

CO5BOLD User Manual

Bernd Freytag

Matthias Steffen
Jorrit Leenaarts

Sven Wedemeyer-Böhm
Werner Schaffenberger

Hans-Günter Ludwig

May 13, 2015

Contents

Contents	11
List of figures	13
List of tables	15
1 Introduction	17
2 Equations	19
2.1 Basic equations	19
2.2 Magnetohydrodynamics (W. Schaffenberger)	20
2.3 A collection of thermodynamic relations (M. Steffen, AIP)	23
2.3.1 Basic thermodynamic equations	23
2.3.2 Definition of often-used thermodynamic coefficients	23
2.3.3 CO5BOLD equation of state	24
2.3.4 Derived thermodynamic coefficients	24
2.3.5 Ideal gas with constant specific heats (polytropic gas)	28
3 CO5BOLD file overview	29
3.1 Fortran directories	29
3.2 Fortran files	30
3.3 Script files	32
3.4 Documentation files	32
4 Compilation & installation	33
4.1 Quickstart: How to compile CO5BOLD	33
4.2 Compilation procedure for CO5BOLD	33
4.3 Configure script	37
4.3.1 Control environment variables	37
4.3.1.1 F90_COLOR	38
4.3.1.2 F90_COMPILER	38
4.3.1.3 F90_PREFLAGS	38
4.3.1.4 F90_POSTFLAGS	38
4.3.1.5 F90_PARALLEL	38
4.3.1.6 F90_DEBUG	38
4.3.1.7 F90_OPTIMIZE	39
4.3.1.8 F90_LHDRAD	39
4.3.1.9 F90_MS RAD	39
4.3.1.10 F90_SHORTRAD	39
4.3.1.11 F90_CHEM	39
4.3.1.12 F90_HION	39
4.3.1.13 F90_DUST	39
4.3.1.14 F90_MHD	40
4.3.1.15 F90_TWEAK	40
4.3.1.16 F90_MACHINE	40

4.3.1.17	F90_BASEPATH	40
4.4	Compiler macros	40
4.4.1	General	41
4.4.1.1	timing_c_factor	41
4.4.1.2	timing_c_range	41
4.4.1.3	timing_r_type	42
4.4.1.4	rhd_box_arrays01	42
4.4.1.5	rhd_box_grav01	42
4.4.1.6	rhd_box_quc01	42
4.4.1.7	rhd_box_bmag01	43
4.4.2	Input/output with UIO	43
4.4.2.1	uio_switch_system_l01	43
4.4.2.2	uio_switch_native_l01	43
4.4.2.3	uio_switch_ieeebe_l01	44
4.4.2.4	uio_switch_ieeele_l01	44
4.4.2.5	uio_switch_ieee_l01	44
4.4.2.6	uio_switch_crayxmp_l01	44
4.4.2.7	uio_switch_open_l01	44
4.4.3	Equation of state	45
4.4.3.1	gasinter_l01	45
4.4.3.2	gasinter_l02	45
4.4.4	Opacity	45
4.4.4.1	opta_switch_l01	45
4.4.5	Hydrodynamics (Roe solver)	45
4.4.5.1	rhd_hyd_gravcorr_p01	45
4.4.5.2	rhd_hyd_entropyfix_p01	46
4.4.5.3	rhd_hyd_upwind_p01	46
4.4.5.4	rhd_roe1d_flux_l01	46
4.4.5.5	rhd_bound_t01	46
4.4.5.6	rhd_roe1d_flux_t01	47
4.4.5.7	rhd_roe1d_step_t01	47
4.4.6	Hydrodynamics (tensor viscosity)	47
4.4.6.1	rhd_vis_density_p01	47
4.4.6.2	rhd_vis_t01	47
4.4.7	Radiation transport	47
4.4.7.1	rhd_r01	47
4.4.7.2	rhd_r02	48
4.4.7.3	rhd_r03	48
4.4.7.4	rhd_rad3d_toray_l01	48
4.4.7.5	rhd_rad3d_fromray_l01	48
4.4.7.6	rhd_rad3d_r02	48
4.4.7.7	rhd_rad3d_solve_t01	49
4.4.7.8	rhd_rad3d_dir_t01	49
4.4.7.9	rhd_rad3d_step_t01	49
4.4.7.10	rhd_shortrad_operator_l01	49
4.4.7.11	rhd_shortrad_operator_l02	50
4.4.7.12	rhd_shortrad_dtauop_l01	50
4.4.7.13	rhd_shortrad_dtauop_l02	50
4.4.7.14	rhd_shortrad_formal_l01	50
4.4.7.15	rhd_shortrad_dir1_l01	50
4.4.7.16	rhd_shortrad_dir_l02	51
4.4.7.17	rhd_shortrad_lambda_l01	51
4.4.7.18	rhd_shortrad_formal_t01	51
4.4.7.19	rhd_shortrad_step_t01	51

4.4.7.20	MSrad_raytas	51
4.4.8	Obsolete macros	52
4.4.8.1	IDF	52
4.4.8.2	rhd_hyd_roe1d_l01	52
4.4.8.3	rhd_roe1d_slope_l01	52
4.5	Optimization, compiler switches	52
4.5.1	OpenMP settings	53
4.5.2	Vectorization	54
4.5.3	Cache usage	54
4.5.4	Inlining	55
4.5.5	Single versus double precision	55
4.6	Specific machines & compilers	55
4.6.1	Cray: SV1	56
4.6.2	Compaq: alpha	56
4.6.3	Hewlett-Packard: V2500	56
4.6.4	Hewlett-Packard: Itanium 2	57
4.6.5	Hitachi SR8000	58
4.6.6	IBM	60
4.6.7	Linux: PGI compiler	61
4.6.8	Linux: Intel compiler	61
4.6.9	Linux: PathScale compiler	64
4.6.10	Linux: GNU g95 compiler	65
4.6.11	Linux: GNU gfortran compiler	65
4.6.12	NEC SX-5, SX-6, SX-8	65
4.6.13	SGI: Origin	66
4.6.14	SGI: Origin 2000/3800 at UKAFF	66
4.6.15	Sun: SunFire	69
5	Programmer's guide	71
5.1	General code organization	71
5.2	Indentation and spaces	71
5.2.1	General layout and indentation recommendations	71
5.2.2	Alignment of assignments and equations	71
5.2.3	Normal code indentation	73
5.2.4	Further recommendations	73
5.3	Naming conventions	74
5.3.1	File names	74
5.3.2	Program names	74
5.3.3	Names of modules, subroutines, and functions	74
5.3.4	Variable names	74
5.4	Comments	75
5.4.1	Header of files	75
5.4.2	Header of modules	75
5.4.3	Header of subroutines and functions	77
5.4.4	Comment lines	78
5.4.5	Short comments after Fortran statements	78
5.5	Compiler switches and directives	79
5.5.1	OpenMP	79
5.5.2	Compiler directives	79
5.5.3	Compiler macros or switches	79
5.6	Unit tests	82
5.6.1	F90_UNIT	82

6	Data file types	83
6.1	File overview	83
6.2	UIO data format	83
6.2.1	Quickstart: Introduction to UIO	83
6.2.2	Example of UIO data file	84
6.2.3	Structure of UIO files	85
6.2.3.1	Data representation: ASCII or binary	85
6.2.3.2	Data file structure	86
6.2.3.3	Tables	87
6.2.3.4	Recommendations for standard file structure	89
6.2.4	Files & directories & paths	89
6.2.5	Fortran90	90
6.2.5.1	Files	90
6.2.5.2	Use of UIO modules in Fortran90	91
6.2.5.3	Compiling and Makefiles	91
6.2.5.4	Sample calls of Fortran UIO routines	92
6.2.6	UNIX scripts	93
6.2.6.1	Installation of UIO UNIX scripts	93
6.2.6.2	Quick examination of files: uiolook	94
6.2.6.3	Transformation of files: uiocat	94
6.2.6.4	Information about conversion types: uioinfo	95
6.2.7	IDL UIO routines	95
6.2.7.1	Initialization of UIO routines under IDL	96
6.2.7.2	Reading data with uio_data.pro	97
6.2.7.3	Reading data with uio_dataset_rd.pro or uio_datasetlist_rd.pro	98
7	Input and control files	101
7.1	Parameter file: rhd.par	101
7.1.1	Quickstart: How to make a proper parameter file	101
7.1.2	Header	102
7.1.2.1	fileform uio	102
7.1.2.2	character file_id	102
7.1.2.3	character description	102
7.1.2.4	character history	103
7.1.3	Fundamental model parameters	103
7.1.3.1	real teff	103
7.1.3.2	character grav_mode	103
7.1.3.3	real grav	103
7.1.3.4	real mass_star	104
7.1.3.5	real r0_grav	104
7.1.3.6	real r1_grav	104
7.1.3.7	real r2_grav	104
7.1.3.8	real r0_core	104
7.1.3.9	character centrifugal_force	105
7.1.3.10	real nu_rotation	105
7.1.3.11	real ar_rotationaxis	105
7.1.4	Boundary conditions (general)	105
7.1.4.1	character side_bound	105
7.1.4.2	character top_bound	106
7.1.4.3	character bottom_bound	106
7.1.4.4	character heat_mode	107
7.1.4.5	character hdcoreheatprofile	107
7.1.4.6	real luminositypervolume	108
7.1.4.7	real s_inflow	108

7.1.4.8	real s_inffradgrad	108
7.1.4.9	real s_inflatgrad	108
7.1.4.10	real c_schange	108
7.1.4.11	real c_pchange	109
7.1.4.12	real c_v3changelinbottom	109
7.1.4.13	real c_v3changesqrbottom	109
7.1.4.14	real c_visbound	109
7.1.4.15	real c_rhochangetop	110
7.1.4.16	real c_tchange	110
7.1.4.17	real c_tsurf	110
7.1.4.18	real c_hptopfactor	110
7.1.4.19	real c_radhtautop	111
7.1.4.20	real r1_rad	111
7.1.4.21	real rho_min	111
7.1.4.22	real c_coredrag	111
7.1.4.23	character hdcoredragprofile	111
7.1.5	Boundary conditions (MHD only)	112
7.1.5.1	character side_bound_mag_x1 and side_bound_mag_x2	112
7.1.5.2	character top_bound_mag	113
7.1.5.3	character bottom_bound_mag	113
7.1.5.4	real b1_inflow	114
7.1.5.5	real c_magthetab	114
7.1.5.6	real c_magphib	114
7.1.6	Equation of state	114
7.1.6.1	character eosfile	114
7.1.6.2	character eospath	115
7.1.7	Opacities	115
7.1.7.1	character opafile	115
7.1.7.2	character opath	116
7.1.8	Hydrodynamics control (HD and MHD)	116
7.1.8.1	character hdscheme	116
7.1.8.2	character hdttimeintegrationscheme	117
7.1.8.3	character hdsplit	117
7.1.8.4	character reconstruction	118
7.1.8.5	real c_gravmu	119
7.1.8.6	integer n_hyditer	120
7.1.8.7	integer n_hydmaxiter	120
7.1.8.8	character hdtmpstructkeepmode	120
7.1.8.9	integer n_hydcellsperchunk	121
7.1.9	Hydrodynamics control (HD only)	121
7.1.9.1	integer n_hydcellsperchunk2	121
7.1.9.2	integer n_hydcellsperchunk3	121
7.1.9.3	integer n_hydrkiter	122
7.1.9.4	real c_hydlowmachcsfactor	122
7.1.9.5	real c_hydlowmachcsbase	123
7.1.9.6	real c_hydsmallfluctfactor	123
7.1.9.7	real c_slopered	123
7.1.9.8	real c_recontshift	124
7.1.9.9	real c_recontsteep	124
7.1.9.10	real c_recwenoweightcenter	125
7.1.9.11	real c_recwenoweightright	125
7.1.9.12	real c_recwenopsifactor	125
7.1.9.13	character hdtransvelomode	126
7.1.9.14	character hdentropywavemode	126

7.1.9.15	character hdenthalpyavgmode	127
7.1.9.16	real c_hydpredfactor	128
7.1.9.17	real c_hydsdiffvelo	128
7.1.9.18	real c_hyvdiffvelo	129
7.1.9.19	real c_hydtdifflin	129
7.1.9.20	real c_hydtdiffmach	130
7.1.10	Hydrodynamics control (MHD only)	130
7.1.10.1	character hdcheckflux	130
7.1.10.2	integer n_orderconstrainedtransport	130
7.1.10.3	integer n_rescellsperchunk	131
7.1.10.4	real c_rescourant	131
7.1.10.5	real c_rescourantmax	131
7.1.10.6	real c_resb	131
7.1.10.7	real c_resbconst	131
7.1.10.8	real c_resepsilon	132
7.1.10.9	real beta_inv	132
7.1.10.10	real va_max	132
7.1.10.11	integer n_magdiffside	132
7.1.10.12	integer n_magdifftop	132
7.1.10.13	integer n_magdiffbottom	133
7.1.11	Tensor-viscosity control	133
7.1.11.1	integer n_visiter	133
7.1.11.2	real c_vissmagorinsky	133
7.1.11.3	real c_visartificial	134
7.1.11.4	real c_visexpansion	134
7.1.11.5	real c_vilinear	134
7.1.11.6	real c_visprturb	134
7.1.11.7	real c_vistensordiag	134
7.1.11.8	real c_vistensoroff	135
7.1.11.9	real c_vistensordiv	135
7.1.11.10	real c_visp2pcoeff	135
7.1.11.11	real c_visp2phypsmagorinsky	135
7.1.11.12	real c_visp2phyppartificial	136
7.1.11.13	real c_visp2phyppexpansion	136
7.1.11.14	real c_visp2pdivrhov	136
7.1.11.15	real c_visp2pincl1	136
7.1.11.16	real c_visp2pincl2	136
7.1.11.17	integer n_viscellsperchunk	137
7.1.12	Dust/molecules/hydrogen ionization: General	137
7.1.12.1	character dustscheme	137
7.1.12.2	character dustreconstruction	138
7.1.12.3	real c_dustOX	138
7.1.12.4	character chem_reacfile	138
7.1.12.5	character chem_reacpath	138
7.1.12.6	real chem_abumetal	138
7.1.12.7	character hion_datapath	139
7.1.12.8	character hion_atomfile	139
7.1.12.9	character hion_abufile	139
7.1.12.10	character hion_edensfile	139
7.1.12.11	character hion_pffile	139
7.1.12.12	real dtime_out_hion	139
7.1.12.13	integer hion_chunks	139
7.1.13	Dust: dustscheme=dust_moment04_c2	139
7.1.13.1	real c_dust01	140

7.1.13.2	real c_dust02	140
7.1.13.3	real c_dust03	140
7.1.13.4	real c_dust04	140
7.1.14	Dust: dustscheme=dust_k3mon_03	140
7.1.14.1	integer n_dustgrainradius	140
7.1.14.2	real ar_dustgrainradius	140
7.1.14.3	real c_dust01	140
7.1.14.4	real c_dust02	141
7.1.14.5	real c_dust03	141
7.1.14.6	real c_dust04	141
7.1.14.7	real c_dust05	141
7.1.14.8	real c_dust06	141
7.1.15	Dust: dustscheme=dust_bins_01	141
7.1.15.1	integer n_dustgrainradius	142
7.1.15.2	real ar_dustgrainradius	142
7.1.15.3	real c_dust01	142
7.1.15.4	real c_dust02	142
7.1.15.5	real c_dust03	142
7.1.15.6	real c_dust04	142
7.1.15.7	real c_dust06	143
7.1.15.8	real c_dust07	143
7.1.15.9	real c_dust08	143
7.1.15.10	real c_dust09	143
7.1.16	Radiation-transport control (general)	143
7.1.16.1	character radscheme	143
7.1.16.2	integer n_radband	144
7.1.16.3	integer n_radminiter	145
7.1.16.4	integer n_raditer	145
7.1.16.5	integer n_radmaxiter	145
7.1.16.6	character radraybase	146
7.1.16.7	character radraystar	146
7.1.16.8	real c_tminlimit	147
7.1.16.9	real c_radimplicitmu	147
7.1.16.10	real c_raditereps	147
7.1.16.11	real c_raditerstep	148
7.1.17	Radiation-transport control (MSrad only)	148
7.1.17.1	integer n_radtheta	148
7.1.17.2	integer n_radphi	148
7.1.17.3	integer n_radsbray	148
7.1.17.4	integer n_radthickpoint	148
7.1.17.5	integer n_radtaurefine	149
7.1.17.6	integer n_radsyslevel	149
7.1.17.7	integer n_radoutput	149
7.1.17.8	real c_radtcool	149
7.1.17.9	real c_raddcool	149
7.1.17.10	real c_radscool	149
7.1.17.11	real c_radtinci	149
7.1.17.12	real c_raddinci	150
7.1.18	Radiation-transport control (LHDrad only)	150
7.1.18.1	real c_radtvisdtau	150
7.1.18.2	real c_radtvis	150
7.1.18.3	real c_radthintimefac	150
7.1.19	Process-time management	150
7.1.19.1	real starttime	151

7.1.19.2	integer starttimestep	151
7.1.19.3	real cputime	151
7.1.19.4	real cputime_remainlimit	151
7.1.19.5	real endtime	151
7.1.19.6	real plustime	152
7.1.19.7	integer endtimestep	152
7.1.19.8	integer plustimestep	152
7.1.20	Time-step control	152
7.1.20.1	real dtime_start	152
7.1.20.2	real dtime_min	152
7.1.20.3	real dtime_max	153
7.1.20.4	real dtime_min_stop	153
7.1.20.5	real dtime_incmax	153
7.1.20.6	real c_courant	153
7.1.20.7	real c_courantmax	153
7.1.20.8	real c_maxeichange	154
7.1.20.9	real c_hydsoundcourant	154
7.1.20.10	real c_hydsoundcourantmax	154
7.1.20.11	real c_hydexpcourant	154
7.1.20.12	real c_hydexpcourantmax	154
7.1.20.13	real c_radcourant	155
7.1.20.14	real c_radcourantmax	155
7.1.20.15	real c_radmaxeichange	155
7.1.20.16	real c_viscourant	155
7.1.20.17	real c_viscourantmax	156
7.1.21	Input/output control	156
7.1.21.1	real dtime_out_full	156
7.1.21.2	real dtime_out_end	156
7.1.21.3	real dtime_out_mean	157
7.1.21.4	integer n_outslicedim_mean	157
7.1.21.5	integer outdim_chu1	157
7.1.21.6	integer outdim_chu2	157
7.1.21.7	integer outdim_chu3	157
7.1.21.8	character infile_start	158
7.1.21.9	integer istep_in_start	158
7.1.21.10	character outfile_end	158
7.1.21.11	character outfile_full	158
7.1.21.12	character outfile_mean	158
7.1.21.13	character outfile_mcyl	158
7.1.21.14	character outfile_chu1	159
7.1.21.15	character outfile_chu2	159
7.1.21.16	character outfile_chu3	159
7.1.21.17	character outform_end	159
7.1.21.18	character outconv_end	159
7.1.21.19	character outform_full	159
7.1.21.20	character outconv_full	160
7.1.21.21	character outform_mean	160
7.1.21.22	character outconv_mean	160
7.1.22	Scale and test parameters	160
7.1.22.1	real time_scalestart	160
7.1.22.2	real time_scaleend	161
7.1.22.3	integer n_test1	161
7.1.22.4	real c_test1	161
7.1.22.5	character strtest1	161

7.1.23	Additional information and obsolete parameters	162
7.1.23.1	real abux	162
7.1.23.2	real abuy	162
7.1.23.3	real qmol	162
7.1.23.4	real gamma	162
7.1.23.5	real c_radkappasmooth	162
7.1.23.6	real c_radtsmooth	163
7.1.23.7	character radpressure	163
7.1.23.8	real c_radtintminfac	163
7.1.23.9	integer dtimestep_out_fine	163
7.1.23.10	character outfile_fine	163
7.1.23.11	character outform_fine	164
7.1.23.12	character outconv_fine	164
7.2	Input model file: rhd.sta	164
7.3	EOS file	164
7.4	Opacity file	164
7.5	Chemistry input	164
7.6	HION input	165
7.7	More control files: rhd.stop, rhd.cont, rhd.dump	166
8	Output and status files	167
8.1	Output model files: rhd.end, rhd.full	167
8.2	Files with additional chunks of data: rhd.chu1, rhd.chu2, rhd.chu3	168
8.3	Files with averaged data: rhd.mean	168
8.4	File with azimuthally averaged data: rhd.mcy1	172
8.5	HION output	174
8.6	Text output: rhd.out	174
8.7	Additional status and output files: rhd.done, rhd.snap	178
9	Running a simulation	179
9.1	Quickstart: How to run CO5BOLD	179
9.2	Using a batch system	180
10	Data analysis with IDL	185
10.1	Preparations	185
10.2	CO5BOLD data in IDL	185
10.2.1	Loading the parameter file	185
10.2.2	Loading CO5BOLD data (.full, .sta, .end, .chu1)	186
10.2.3	Loading the equation of state	186
10.2.4	Loading the opacity table	186
10.2.5	Computation of deduced quantities	186
10.3	IDL data structure	187
10.4	More IDL routines	188
11	Document history	189
12	Glossary	193
13	Trademarks	195
13	Bibliography	198
Index		199

List of figures

4.1	Performance tests on Hitachi SR8000	59
4.2	UKAFF: machine: grand; small model	67
4.3	UKAFF: machine: grand; large model	68
4.4	UKAFF: machine: ukaff; large model	68
9.1	Program scheme	180

List of tables

3.1	List of source directories	29
3.2	List of all high-level modules	30
3.3	List of all low-level modules	31
3.4	List of all tweak modules	31
3.5	List of all unit-test modules	31
3.6	List of Linux script files.	32
3.7	List of documentation files.	32
6.1	CO5BOLD control and data files	84
6.2	UIO conversion types	86
6.3	UIO entry types	87
6.4	UIO header keywords	87
6.5	UIO Fortran90 files	90
6.6	Contents of uio_base_module.f90	90
6.7	Contents of uio_mac_module	90
7.1	Combinations of HD options	116
7.2	Radiation transport parameters	144

Chapter 1

Introduction

CO5BOLD – nickname COBOLD – is the short form of “COnservative COde for the COmputation of COmpressible COnvection in a BOx of L Dimensions with l=2,3”.

It is used to model solar and stellar surface convection (Freytag et al., 2012). For solar-type stars, only a small fraction of the stellar surface layers are included in the computational domain (Wedemeyer et al., 2004). In the case of red supergiants (Freytag et al., 2002; Chiavassa et al., 2011) or AGB-type stars (Freytag & Höfner, 2008), the computational box contains the entire star. The model range has been extended to sub-stellar objects like brown dwarfs (Freytag et al., 2010) and to white dwarfs (Tremblay et al., 2013)

CO5BOLD solves the coupled non-linear equations of compressible hydrodynamics in an external gravity field together with non-local frequency-dependent radiation transport. Operator splitting is applied to solve the equations of hydrodynamics (including gravity), the radiative energy transfer (with a long-characteristics or a short-characteristics ray scheme), and possibly additional 3D (turbulent) diffusion in individual sub steps. The 3D hydrodynamics step is further simplified with directional splitting (usually). The 1D sub steps are performed with a Roe solver (Roe, 1986), accounting for an external gravity field and an arbitrary equation of state from a table.

The radiation transport is computed with either one of three modules:

- **MSrad** module: It uses long characteristics. The lateral boundaries have to be periodic. Top and bottom can be closed or open (“solar module”).
- **LHDrad** module: It uses long characteristics and is restricted to an equidistant grid and open boundaries at all surfaces (old “supergiant module”).
- **SHORTrad** module: It uses short characteristics and is restricted to an equidistant grid and open boundaries at all surfaces (new “supergiant module”).

The code was supplemented with an (optional) MHD version (Schaffenberger et al., 2005) that can treat magnetic fields. There are also modules for the formation and advection of dust available. The current version now contains the treatment of chemical reaction networks, mostly used for the formation of molecules (Wedemeyer-Böhm et al., 2005), and hydrogen ionization (Leenaarts & Wedemeyer-Böhm, 2005), too.

CO5BOLD is written in Fortran90. The parallelization is done with OpenMP directives.

To get a brief overview the “Quickstart Sections” might be helpful:

- “How to compile CO5BOLD” (Sect. 4.1),
- “Introduction to the UIO data format” (Sect. 6.2.1),
- “How to make a proper parameter file” (Sect. 7.1.1),
- “How to run CO5BOLD” (Sect. 9.1).

Chapter 2

Equations

2.1 Basic equations

The hydrodynamics equations are expressed as conservation relations plus source terms for

$$\rho, \rho v_1, \rho v_2, \rho v_3, \rho e_{ik}g, \quad (2.1)$$

the mass density, the three mass fluxes and the total energy density (per volume), respectively. Each quantity q has its corresponding flux $f(q)$ and possibly source term $s(q)$. For convenience,

$$\rho, v_1, v_2, v_3, e_i \quad (2.2)$$

are chosen as independent quantities. The conserved quantities are purely algebraic combinations of these.

The 3D hydrodynamics equations, including source terms due to gravity, are the *mass conservation equation*

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v_1}{\partial x_1} + \frac{\partial \rho v_2}{\partial x_2} + \frac{\partial \rho v_3}{\partial x_3} = 0, \quad (2.3)$$

the *momentum equation*

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho v_1 \\ \rho v_2 \\ \rho v_3 \end{pmatrix} + \frac{\partial}{\partial x_1} \begin{pmatrix} \rho v_1 v_1 + P \\ \rho v_2 v_1 \\ \rho v_3 v_1 \end{pmatrix} + \frac{\partial}{\partial x_2} \begin{pmatrix} \rho v_1 v_2 \\ \rho v_2 v_2 + P \\ \rho v_3 v_2 \end{pmatrix} + \frac{\partial}{\partial x_3} \begin{pmatrix} \rho v_1 v_3 \\ \rho v_2 v_3 \\ \rho v_3 v_3 + P \end{pmatrix} = \begin{pmatrix} \rho g_1 \\ \rho g_2 \\ \rho g_3 \end{pmatrix} \quad (2.4)$$

and the *energy equation* including radiative heating term Q_{rad}

$$\frac{\partial \rho e_{ik}}{\partial t} + \frac{\partial (\rho e_{ik} + P) v_1}{\partial x_1} + \frac{\partial (\rho e_{ik} + P) v_2}{\partial x_2} + \frac{\partial (\rho e_{ik} + P) v_3}{\partial x_3} = \rho (g_1 v_1 + g_2 v_2 + g_3 v_3) + Q_{\text{rad}}. \quad (2.5)$$

The pressure P is computed from density ρ and internal energy e_i via a (tabulated) *equation of state*

$$P = P(\rho, e_i). \quad (2.6)$$

For local models the *gravity* field is simply given by

$$\vec{g} = \begin{pmatrix} 0 \\ 0 \\ -g \end{pmatrix}. \quad (2.7)$$

For global models it is given by

$$\vec{g} = \begin{pmatrix} g_1 \\ g_2 \\ g_3 \end{pmatrix} = - \begin{pmatrix} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_3} \end{pmatrix} \Phi \quad (2.8)$$

with

$$\Phi = - \frac{G M_*}{\left(r_0^4 + r^4 / \sqrt{1 + (r/r_1)^8} \right)^{1/4}}. \quad (2.9)$$

Here, M_* is the mass of the star to be modeled; r_0 and r_1 are free smoothing parameters.

In addition, there are equations for the non-local radiation transport. If grey opacity tables are used, the opacities κ are a simple function of e.g. temperature T and pressure P

$$\kappa = \kappa(T, P) \quad (2.10)$$

and the source function S is given by

$$S = \frac{\sigma}{\pi} T^4 . \quad (2.11)$$

The change in optical depth $\Delta\tau$ along a path with length Δx is than

$$\Delta\tau = \kappa\rho\Delta x . \quad (2.12)$$

The variation of the intensity I with optical depth τ along a ray with orientation (θ, φ) can be described by the simple differential equation

$$\frac{dI}{d\tau} = -I + S . \quad (2.13)$$

The radiative energy flux is given by

$$F_{\text{rad}} = \int_0^{2\pi} \int_0^\pi I \cos\theta \sin\theta \, d\theta \, d\varphi . \quad (2.14)$$

The energy change can than be computed from the flux divergence with

$$\frac{\partial\rho e_i}{\partial t} = Q_{\text{rad}} = - \left(\frac{\partial F_{x1,\text{rad}}}{\partial x1} + \frac{\partial F_{x2,\text{rad}}}{\partial x2} + \frac{\partial F_{x3,\text{rad}}}{\partial x3} \right) . \quad (2.15)$$

2.2 Magnetohydrodynamics (W. Schaffenberger)

The MHD module solves the equations of ideal MHD, given in compact vector form

$$\begin{aligned} \frac{\partial\rho}{\partial t} + \nabla \cdot (\rho\mathbf{v}) &= 0 , \\ \frac{\partial\rho\mathbf{v}}{\partial t} + \nabla \cdot \left(\rho\mathbf{v}\mathbf{v} + \left(P + \frac{\mathbf{B} \cdot \mathbf{B}}{2} \right) \mathbf{I} - \mathbf{B}\mathbf{B} \right) &= \rho\mathbf{g} , \\ \frac{\partial\mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{v}\mathbf{B} - \mathbf{B}\mathbf{v}) &= 0 , \\ \frac{\partial\rho e_{\text{tot}}}{\partial t} + \nabla \cdot \left(\left(\rho e_{\text{tot}} + P + \frac{\mathbf{B} \cdot \mathbf{B}}{2} \right) \mathbf{v} - (\mathbf{v} \cdot \mathbf{B}) \mathbf{B} + \mathbf{F}_{\text{rad}} \right) &= 0 . \end{aligned} \quad (2.16)$$

Here, \mathbf{B} is the magnetic field vector, where the units are such that the magnetic permeability μ is equal to one. \mathbf{I} is the identity matrix and $\mathbf{a} \cdot \mathbf{b} = \sum_k a_k b_k$ the scalar product of the two vectors \mathbf{a} and \mathbf{b} . The dyadic tensor product of two vectors \mathbf{a} and \mathbf{b} is the tensor $\mathbf{a}\mathbf{b} = \mathbf{C}$ with elements $c_{mn} = a_m b_n$ and the n th component of the divergence of the tensor \mathbf{C} is $(\nabla \cdot \mathbf{C})_n = \sum_m \partial c_{mn} / \partial x_m$. The total energy is given by

$$\rho e_{\text{tot}} = \rho e_i + \rho \frac{\mathbf{v} \cdot \mathbf{v}}{2} + \frac{\mathbf{B} \cdot \mathbf{B}}{2} + \rho\Phi , \quad (2.17)$$

where e_i is the internal energy per unit mass. The additional solenoidality constraint,

$$\nabla \cdot \mathbf{B} = 0 , \quad (2.18)$$

must also be fulfilled.

The aim was to create a stable and easy to use module (Schaffenberger et al., 2005). The module has the following features:

- Use of the HLL solver with the Janhunen source terms (Janhunen, 2000).
 - Extension to 2nd order with linear or parabolic reconstruction and a Hancock predictor step or Runge-Kutta-TVD timeintegration scheme.

- The following limiters are available: Minmod, vanLeer, Superbee, Piecewise Parabolic (PP).
- Hybridization of 1st and 2nd order flux to ensure positivity of pressure and density.
- Use of Roe solver.
- Flux interpolated constrained transport step.
- Small violation of strict energy conservation after the constrained transport step to keep the pressure positive \mathcal{E} -term of Balsara & Spicer (1999).
- Electric conductivity and additional energy diffusion.
- Use of thermal energy equation instead of total energy equation possible (for HLL solver only).
- Use of both, thermal energy equation and total energy equation possible (dual energy method, HLL solver only).
- Reduction of Alfvén speed to avoid small time steps (with HLL solver only and in combination with thermal energy equation or dual energy method only).
- Use of multiple MHD-substeps.
- Boundary conditions for the magnetic field can be specified independently from the hydro boundary conditions.
- Diffusive boundary layers possible.
- Dimensional splitting or unsplit scheme possible.

The magnetic field is located at the cell boundaries rather than in the cell centers. Therefore, the format of the magnetic field arrays is slightly different from that of the other hydrodynamic variables.

Staggered grid representation of the magnetic field in 2 dimensions:

```

+---^---+---^---+---^---+---^---+---^---+---^---+
|      |      |      |      |      |      |      |
> * > * > * > * > * > * > * > * >
|      |      |      |      |      |      |
+---^---+---^---+---^---+---^---+---^---+---^---+
|      |      |      |      |      |      |      |
> * > * > * > * > * > * > * > * >
|      |      |      |      |      |      |      |
+---^---+---^---+---^---+---^---+---^---+---^---+
|      |      |      |      |      |      |      |
> * > * > * > * > * > * > * > * >
|      |      |      |      |      |      |      |
+---^---+---^---+---^---+---^---+---^---+---^---+
|      |      |      |      |      |      |      |
> * > * > * > * > * > * > * > * >
|      |      |      |      |      |      |      |
+---^---+---^---+---^---+---^---+---^---+---^---+

```

* hydrodynamic variables
> x1 component of the magnetic field
^ x2 component of the magnetic field

The extension to 3 dimensions should be clear. Variables at the left or the bottom boundary have the same indices as the cell.

For a box with $120 \times 120 \times 120$ cells, the header for the magnetic field arrays in the start model may look like

```
real bb1 d=(1:121,1:120,1:120) f=E13.6 p=4 b=4 &
      n='cell boundary magnetic field 1' u=G*sqrt(4pi)
real bb2 d=(1:120,1:121,1:120) f=E13.6 p=4 b=4 &
      n='cell boundary magnetic field 2' u=G*sqrt(4pi)
real bb3 d=(1:120,1:120,1:121) f=E13.6 p=4 b=4 &
      n='cell boundary magnetic field 3' u=G*sqrt(4pi)
```

For simplicity, the MHD module uses units such that the 4π factors do not appear in the MHD equations.

Therefore one has to multiply the original magnetic fields in gauss with the factor $1/\sqrt{4\pi}$ in order to get the correct magnetic field strength for CO5BOLD!!!

After the computation, one has to multiply the magnetic fields from the CO5BOLD output with the factor $\sqrt{4\pi}$ in order to get the magnetic field strength in gauss!!!

The CO5BOLD analysis tool CAT does this automatically when reading the model data, so that CAT outputs the field strength in gauss.

Positivity of pressure and density:

A special problem of MHD simulations is that pressure or density can become negative in some circumstances. This problem is also present in pure hydrodynamic simulations but gets worse for MHD. The original hydrodynamic version of CO5BOLD tries to fix this problem by reducing the time step. In hydrodynamics, this works in most cases. In MHD, however, reduction of the time step often does not help and other methods are necessary to avoid this problem. Therefore, the MHD module uses a HLL solver instead of a Roe solver, which is used in the hydrodynamic module (Roe, 1986). It was shown numerically by Janhunen (2000), that using a HLL solver together with additional source terms in the induction equation keeps pressure and density positive under all circumstances. Because the constrained transport step, which is performed after the 1D sweeps with the MHD solver, changes the magnetic field, a correction of the internal energy in each cell is necessary to keep the total energy conserved. Because this correction can lead to negative pressure, it is omitted if the internal energy would become too small. Therefore, the total energy is not exactly conserved but this affects only a few cells in the simulation box. (See also Balsara & Spicer (1999) on this topic.)

The methods described above result in a very robust scheme, which guarantees positivity of pressure and density under almost all conditions. However, this does not mean, that these values are accurate! The pressure and temperature distribution may be very inaccurate in regions with strong magnetic fields. This may be relevant, if one includes special chromospheric physics such as dynamic hydrogen ionization and CO formation in the simulation. A possibility to get more accurate pressure and temperature would consist in the use of the entropy equation instead of the energy equation for the computation of the internal energy in regions with strong magnetic field. This was included in the original test version of the MHD module. In the present version, we make use of the equation for the thermal energy itself depending on the ratio of thermal to magnetic pressure, i.e., the plasma β . The limiting β can be specified by the model parameter `beta_inv`. This is the dual energy approach, used in many MHD codes. Its advantage goes at the expense of violation of strict conservation of the total energy.

Due to the Courant condition, the time step in case of MHD can become considerably smaller than in the hydrodynamic case. This happens because the time step is also limited by the Alfvén speed which is large in regions with strong magnetic field and low density (small plasma β).

To avoid an extreme time step reduction, the Alfvén speed can be artificially limited. This is done by reducing the Lorentz force in the momentum equation by a factor f . This factor is calculated with the following formula:

$$f = \frac{v_{A\max}^2}{(v_A^2 + v_{A\max}^2)}, \quad (2.19)$$

where v_A is the original Alfvén speed and $v_{A\max}$ is the desired maximum value of the Alfvén speed. Currently, this feature works only with the HLL-solver. It is advisable to use this feature only in combination

with either the thermal energy equation (`beta_inv` = 0.0) or the dual energy method. In the latter case, `beta_inv` should be chosen small enough so that the region where the Lorentz-force reduction is active is handled by the thermal energy equation. This is obtained with `beta_inv` $\lesssim \gamma v_{A\max}^2 / c_s^2$, where c_s is the speed of sound and γ the adiabatic exponent.

This module has been extensively tested. It should be able to handle many MHD flows of astrophysical interest. Bugs and problems can be reported to `werner.schaffnerberger@gmx.at`.

2.3 A collection of thermodynamic relations (M. Steffen, AIP)

2.3.1 Basic thermodynamic equations

Differential relations:

$$de = Tds + \frac{p}{\rho^2}d\rho \quad (20)$$

where e is the **internal energy** .

$$dh = Tds + \frac{1}{\rho}dp \quad (21)$$

where the **specific enthalpy** , h , is defined as

$$h = e + p/\rho \quad (22)$$

This implies:

$$\left(\frac{\partial e}{\partial s}\right)_\rho = T \quad (23)$$

$$\left(\frac{\partial e}{\partial \rho}\right)_s = \frac{p}{\rho^2} \quad (24)$$

$$\left(\frac{\partial h}{\partial s}\right)_p = T \quad (25)$$

$$\left(\frac{\partial h}{\partial p}\right)_s = \frac{1}{\rho} \quad (26)$$

2.3.2 Definition of often-used thermodynamic coefficients

Definition of specific heats:

$$c_p \equiv \left(\frac{\partial h}{\partial T}\right)_p = T \left(\frac{\partial s}{\partial T}\right)_p = \left(\frac{\partial s}{\partial \ln T}\right)_p \quad (27)$$

$$c_v \equiv \left(\frac{\partial e}{\partial T}\right)_\rho = T \left(\frac{\partial s}{\partial T}\right)_\rho = \left(\frac{\partial s}{\partial \ln T}\right)_\rho \quad (28)$$

Definitions of further thermodynamic coefficients:

$$\chi_T \equiv \left(\frac{\partial \ln p}{\partial \ln T}\right)_\rho \quad (29)$$

$$\chi_\rho \equiv \left(\frac{\partial \ln p}{\partial \ln \rho}\right)_T \equiv (Kp)^{-1} \quad (30)$$

$$\delta \equiv -\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_p \equiv \alpha T = \frac{\chi_T}{\chi_\rho} \quad (31)$$

It can be shown that

$$c_p - c_v = \alpha^2 T / (K\rho) = \frac{p}{\rho T} \delta^2 \chi_\rho = \frac{p}{\rho T} \delta \chi_T = \frac{p}{\rho T} \chi_T^2 / \chi_\rho \quad (32)$$

Definition of adiabatic exponents:

$$\Gamma_1 \equiv \left(\frac{\partial \ln p}{\partial \ln \rho} \right)_s \quad (33)$$

$$\Gamma_3 \equiv \left(\frac{\partial \ln T}{\partial \ln \rho} \right)_s + 1 \quad (34)$$

$$\nabla_{\text{ad}} \equiv \left(\frac{\partial \ln T}{\partial \ln p} \right)_s \equiv \frac{\Gamma_2 - 1}{\Gamma_2} \quad (35)$$

2.3.3 CO5BOLD equation of state

CO5BOLD equation of state input:

$$\rho; e \quad (36)$$

CO5BOLD equation of state output:

$$s; P; T; \left(\frac{\partial p}{\partial e} \right)_\rho; \left(\frac{\partial p}{\partial \rho} \right)_e; \left(\frac{\partial T}{\partial e} \right)_\rho \quad (37)$$

All required thermodynamic coefficients can be expressed in terms of $\left(\frac{\partial p}{\partial e} \right)_\rho$, $\left(\frac{\partial p}{\partial \rho} \right)_e$, $\left(\frac{\partial T}{\partial e} \right)_\rho$:

2.3.4 Derived thermodynamic coefficients

First, the missing derivative $\left(\frac{\partial T}{\partial \rho} \right)_e$ can be found from the relation:

$$\left(\frac{\partial T}{\partial \rho} \right)_e = \frac{T}{\rho^2} \left(\frac{\partial p}{\partial e} \right)_\rho - \frac{p}{\rho^2} \left(\frac{\partial T}{\partial e} \right)_\rho \quad (38)$$

which is obtained from the equality of the mixed derivatives in Eq.(20), written as:

$$ds = \frac{1}{T} de - \frac{p}{T\rho^2} d\rho \quad (39)$$

Then

$$\frac{\partial^2 s}{\partial e \partial \rho} = \frac{\partial}{\partial \rho} \left(\frac{1}{T} \right)_e = \frac{\partial}{\partial e} \left(-\frac{p}{T\rho^2} \right)_\rho \quad (40)$$

First adiabatic exponent:

$$\Gamma_1 \equiv \left(\frac{\partial \ln p}{\partial \ln \rho} \right)_s = \frac{\rho}{p} \left(\frac{\partial p}{\partial \rho} \right)_e + \frac{1}{\rho} \left(\frac{\partial p}{\partial e} \right)_\rho \quad (41)$$

This relation is obtained by combining Eq.(20) with the identity

$$dp = \left(\frac{\partial p}{\partial \rho} \right)_e d\rho + \left(\frac{\partial p}{\partial e} \right)_\rho de \quad (42)$$

The **adiabatic sound speed** is then obtained as

$$c_s \equiv \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s} = \sqrt{\Gamma_1 \frac{p}{\rho}} \quad (43)$$

Third adiabatic exponent:

$$\Gamma_3 \equiv 1 + \left(\frac{\partial \ln T}{\partial \ln \rho}\right)_s = 1 + \frac{1}{\rho} \left(\frac{\partial p}{\partial e}\right)_\rho \quad (44)$$

This relation is obtained by combining Eq.(20) with the identity

$$dT = \left(\frac{\partial T}{\partial \rho}\right)_e d\rho + \left(\frac{\partial T}{\partial e}\right)_\rho de \quad (45)$$

and then using Eq.(38).

Adiabatic temperature gradient:

$$\nabla_{\text{ad}} \equiv \left(\frac{\partial \ln T}{\partial \ln p}\right)_s = \frac{\Gamma_3 - 1}{\Gamma_1} \quad (46)$$

since

$$\left(\frac{\partial \ln T}{\partial \ln p}\right)_s = \left(\frac{\partial \ln T}{\partial \ln \rho}\right)_s \cdot \left(\frac{\partial \ln \rho}{\partial \ln p}\right)_s = \frac{\Gamma_3 - 1}{\Gamma_1}. \quad (47)$$

Adiabatic energy changes:

$$\rho \left(\frac{\partial e}{\partial p}\right)_s = \frac{p}{\rho} \left(\frac{\partial \rho}{\partial p}\right)_s = \left(\frac{\partial \ln \rho}{\partial \ln p}\right)_s = \frac{1}{\Gamma_1} \quad (48)$$

or

$$\left(\frac{\partial \rho e}{\partial p}\right)_s = e \left(\frac{\partial \rho}{\partial p}\right)_s + \rho \left(\frac{\partial e}{\partial p}\right)_s = \frac{1}{\Gamma_1} \left(1 + \frac{\rho e}{p}\right) \quad (49)$$

We define the coefficients c'_v and c'_p through the relation

$$ds = c'_v d \ln p - c'_p d \ln \rho \quad (50)$$

Entropy change at constant density:

$$c'_v = \left(\frac{\partial s}{\partial \ln p}\right)_\rho = \frac{p}{\rho T} \left(\frac{\partial \ln \rho}{\partial \ln T}\right)_s = \frac{p}{\rho T} \frac{1}{\Gamma_3 - 1} \quad (51)$$

This relation is obtained from the equality of the mixed derivatives in Eq.(20) together with Eq.(44).

Entropy change at constant pressure:

$$c'_p = - \left(\frac{\partial s}{\partial \ln \rho}\right)_p = \frac{p}{\rho T} \left(\frac{\partial \ln p}{\partial \ln T}\right)_s = \frac{p}{\rho T} \frac{\Gamma_1}{\Gamma_3 - 1} \quad (52)$$

This relation is obtained from the equality of the mixed derivatives in Eq.(21) together with Eq.(46).

Specific heat at constant density:

$$c_v = c'_v \chi_T = \left(\frac{\partial s}{\partial \ln T} \right)_\rho = \left(\frac{\partial e}{\partial T} \right)_\rho = 1 / \left(\frac{\partial T}{\partial e} \right)_\rho \quad (53)$$

To derive the specific heat at constant pressure, we start from the relation

$$d \ln T = \left(\frac{\partial \ln T}{\partial \ln \rho} \right)_s d \ln \rho + \left(\frac{\partial \ln T}{\partial s} \right)_\rho ds \quad (54)$$

from which we get

$$\left(\frac{\partial s}{\partial \ln \rho} \right)_T = - \left(\frac{\partial \ln T}{\partial \ln \rho} \right)_s / \left(\frac{\partial \ln T}{\partial s} \right)_\rho \quad (55)$$

Using Eqs.(44) and (53), we obtain

$$\left(\frac{\partial s}{\partial \ln \rho} \right)_T = -c_v (\Gamma_3 - 1) \quad (56)$$

Now

$$ds = \left(\frac{\partial s}{\partial \ln p} \right)_\rho d \ln p + \left(\frac{\partial s}{\partial \ln \rho} \right)_p d \ln \rho \quad (57)$$

or

$$ds = \left(\frac{\partial s}{\partial \ln p} \right)_\rho d \ln p + \left(\frac{\partial s}{\partial \ln \rho} \right)_p \left\{ \left(\frac{\partial \ln \rho}{\partial \ln T} \right)_s d \ln T + \left(\frac{\partial \ln \rho}{\partial s} \right)_T ds \right\} \quad (58)$$

hence

$$ds \left\{ 1 - \left(\frac{\partial s}{\partial \ln \rho} \right)_p \left(\frac{\partial \ln \rho}{\partial s} \right)_T \right\} = \left(\frac{\partial s}{\partial \ln p} \right)_\rho d \ln p + \left(\frac{\partial s}{\partial \ln \rho} \right)_p \left(\frac{\partial \ln \rho}{\partial \ln T} \right)_s d \ln T \quad (59)$$

and finally

$$\left(\frac{\partial \ln T}{\partial s} \right)_p = \left\{ 1 - \left(\frac{\partial s}{\partial \ln \rho} \right)_p \left(\frac{\partial \ln \rho}{\partial s} \right)_T \right\} / \left\{ \left(\frac{\partial s}{\partial \ln \rho} \right)_p \left(\frac{\partial \ln \rho}{\partial \ln T} \right)_s \right\} \quad (60)$$

or

$$\left(\frac{\partial \ln T}{\partial s} \right)_p = \left(\frac{\partial \ln T}{\partial \ln \rho} \right)_s \left\{ \left(\frac{\partial \ln \rho}{\partial s} \right)_p - \left(\frac{\partial \ln \rho}{\partial s} \right)_T \right\} \quad (61)$$

Using Eqs.(27), (44), (52), (56), we finally obtain the relation for the **specific heat at constant pressure**:

$$\frac{1}{c_p} = \frac{1}{c_v} - \frac{\rho T}{p} \frac{(\Gamma_3 - 1)^2}{\Gamma_1} = \frac{1}{c_v} - T \left(\frac{\Gamma_3 - 1}{c_s} \right)^2 \quad (62)$$

Alternatively, c_p can be obtained from Eq.(32)

$$c_p = c_v + \frac{p}{\rho T} \delta \chi_T \quad (63)$$

or from

$$c_p = \delta c'_p = \frac{p}{\rho T} \delta \frac{\Gamma_1}{\Gamma_3 - 1} \quad (64)$$

once δ and χ_T are known (see below).

We can now express the thermodynamic coefficients provided by CO5BOLD in terms of c_v , Γ_1 , Γ_3 , and ∇_{ad} :

$$\left(\frac{\partial p}{\partial e}\right)_\rho = \rho(\Gamma_3 - 1) \quad (65)$$

$$\left(\frac{\partial p}{\partial \rho}\right)_e = \frac{p}{\rho}(1 - \Gamma_3 + \Gamma_1) \quad (66)$$

$$\left(\frac{\partial T}{\partial e}\right)_\rho = \frac{1}{c_v} \quad (67)$$

$$\left(\frac{\partial T}{\partial \rho}\right)_e = \frac{T}{\rho}(\Gamma_3 - 1) - \frac{p}{\rho^2} \frac{1}{c_v} \quad (68)$$

$$\left(\frac{\partial e}{\partial \rho}\right)_T = -\left(\frac{\partial T}{\partial \rho}\right)_e / \left(\frac{\partial T}{\partial e}\right)_\rho = \frac{p}{\rho^2} \left\{ 1 - \frac{\rho T}{p} c_v (\Gamma_3 - 1) \right\} \quad (69)$$

$$\left(\frac{\partial e}{\partial \rho}\right)_p = -\left(\frac{\partial p}{\partial \rho}\right)_e / \left(\frac{\partial p}{\partial e}\right)_\rho = \frac{p}{\rho^2} \left\{ 1 - \frac{\Gamma_1}{\Gamma_3 - 1} \right\} = \frac{p}{\rho^2} \frac{\nabla_{\text{ad}} - 1}{\nabla_{\text{ad}}} \quad (70)$$

We consider again Eq.(39), replacing de by

$$de = \left(\frac{\partial e}{\partial T}\right)_\rho dT + \left(\frac{\partial e}{\partial \rho}\right)_T d\rho \quad (71)$$

so

$$ds = \frac{1}{T} \left(\frac{\partial e}{\partial T}\right)_\rho dT + \left\{ \frac{1}{T} \left(\frac{\partial e}{\partial \rho}\right)_T - \frac{p}{T\rho^2} \right\} d\rho \quad (72)$$

The requirement that the mixed derivatives must be equal then yields

$$\frac{\partial}{\partial \rho} \left(\frac{1}{T} \left(\frac{\partial e}{\partial T}\right)_\rho \right)_T = \frac{\partial}{\partial T} \left(\frac{1}{T} \left(\frac{\partial e}{\partial \rho}\right)_T - \frac{p}{T\rho^2} \right)_\rho \quad (73)$$

or

$$0 = -\frac{1}{T^2} \left(\frac{\partial e}{\partial \rho}\right)_T - \frac{1}{\rho^2} \left\{ \frac{1}{T} \left(\frac{\partial p}{\partial T}\right)_\rho - \frac{p}{T^2} \right\} \quad (74)$$

Finally,

$$\left(\frac{\partial e}{\partial \rho}\right)_T = \frac{p}{\rho^2} \left\{ 1 - \left(\frac{\partial \ln p}{\partial \ln T}\right)_\rho \right\} = \frac{p}{\rho^2} (1 - \chi_T) \quad (75)$$

Comparison with Eq.(69) implies

$$\chi_T = \frac{\rho T}{p} c_v (\Gamma_3 - 1) \quad (76)$$

Similarly, replacing de by

$$de = \left(\frac{\partial e}{\partial p}\right)_\rho dp + \left(\frac{\partial e}{\partial \rho}\right)_p d\rho \quad (77)$$

in Eq.(39), we get

$$ds = \frac{1}{T} \left(\frac{\partial e}{\partial p}\right)_\rho dp + \left\{ \frac{1}{T} \left(\frac{\partial e}{\partial \rho}\right)_p - \frac{p}{T\rho^2} \right\} d\rho \quad (78)$$

and the requirement that the mixed derivatives must be equal then yields

$$\frac{\partial}{\partial \rho} \left(\frac{1}{T} \left(\frac{\partial e}{\partial p} \right)_\rho \right)_p = \frac{\partial}{\partial p} \left(\frac{1}{T} \left(\frac{\partial e}{\partial \rho} \right)_p - \frac{p}{T \rho^2} \right)_\rho \quad (79)$$

or

$$\left(\frac{\partial e}{\partial p} \right)_\rho \left(\frac{\partial T}{\partial \rho} \right)_p = \left(\frac{\partial T}{\partial p} \right)_\rho \left\{ \left(\frac{\partial e}{\partial \rho} \right)_p - \frac{p}{\rho^2} \right\} + \frac{T}{\rho^2} \quad (80)$$

or

$$\left(\frac{\partial e}{\partial p} \right)_\rho \left(\frac{\partial \ln T}{\partial \ln \rho} \right)_p = \left(\frac{\partial \ln T}{\partial \ln p} \right)_\rho \left\{ \frac{\rho}{p} \left(\frac{\partial e}{\partial \rho} \right)_p - \frac{1}{\rho} \right\} + \frac{1}{\rho}. \quad (81)$$

Since

$$\left(\frac{\partial \ln T}{\partial \ln \rho} \right)_p / \left(\frac{\partial \ln T}{\partial \ln p} \right)_\rho = - \left(\frac{\partial \ln p}{\partial \ln \rho} \right)_T = -\chi_\rho \quad (82)$$

we finally obtain, using Eqs.(29), (65) and (70),

$$\chi_\rho = \Gamma_1 - \chi_T (\Gamma_3 - 1) \quad (83)$$

and

$$\delta = \chi_T / \{ \Gamma_1 - \chi_T (\Gamma_3 - 1) \} \quad (84)$$

The **isothermal sound speed** is then obtained as

$$c_T \equiv \sqrt{\left(\frac{\partial p}{\partial \rho} \right)_T} = \sqrt{\chi_\rho \frac{p}{\rho}} = \sqrt{\Gamma_1 \frac{p}{\rho} \left\{ 1 - \chi_T \frac{\Gamma_3 - 1}{\Gamma_1} \right\}} = c_s \sqrt{(1 - \chi_T \nabla_{\text{ad}})} \quad (85)$$

2.3.5 Ideal gas with constant specific heats (polytropic gas)

In this case, we obtain much simpler relations:

$$e = c_v T = \frac{p}{\rho} \frac{1}{\gamma - 1} \quad (86)$$

$$h = c_p T = \frac{p}{\rho} \frac{\gamma}{\gamma - 1} \quad (87)$$

$$s = c_v \{ \ln p - \gamma \ln \rho \} + \text{const.} \quad (88)$$

$$\gamma \equiv \frac{c_p}{c_v} = \Gamma_1 = \Gamma_2 = \Gamma_3 = \text{const.} \quad (89)$$

$$c_p - c_v = \frac{p}{\rho T} \equiv \mathcal{R} \quad (90)$$

$$c_v = \mathcal{R} \frac{1}{\gamma - 1} = c'_v \quad (91)$$

$$c_p = \mathcal{R} \frac{\gamma}{\gamma - 1} = c'_p \quad (92)$$

$$\chi_T = \chi_\rho = \delta = 1 \quad (93)$$

$$c_s \equiv \sqrt{\left(\frac{\partial p}{\partial \rho} \right)_s} = \sqrt{\gamma \frac{p}{\rho}} \quad (94)$$

$$c_T \equiv \sqrt{\left(\frac{\partial p}{\partial \rho} \right)_T} = \sqrt{\frac{p}{\rho}} \quad (95)$$

Chapter 3

CO5BOLD file overview

In this section, all the files and modules CO5BOLD contains are listed.

3.1 Fortran directories

The files necessary to compile CO5BOLD are distributed over a few directories in the main directory `for`. The source files are located as shown in Tab. 3.1.

Paths	Abb.	Description
<code>for/cons/f90/</code>	CON	constants and units
<code>for/eos/f90/</code>	EOS	equation of state
<code>for/hd/chem/</code>	CHEM	chemical reaction network
<code>for/hd/dust/</code>	DUST	source terms due to dust or molecules
<code>for/hd/hion/f90/</code>	HION	time-dependent hydrogen ionization
<code>for/hd/mhd/</code>	MHD	MHD
<code>for/hd/rhd/</code>	RHD	RHD: main, HD, Bernd's radiation transport
<code>for/hd/rhdb/</code>	RHDB	basic RHD: I/O, box handling, averaging
<code>for/hd/tweak/</code>	TWEAK	various optional tweak modules
<code>for/hd/unitt/</code>	UT	unit-test subroutines and main program
<code>for/mat/str/</code>	STR	string handling
<code>for/opa/opta/</code>	OPTA	opacities
<code>for/rad/hdrad/</code>	RAD	Matthias' radiation transport
<code>for/time/f90/</code>	TIME	timing
<code>for/uio/f90/</code>	UIO	I/O

Table 3.1: List of source directories with path name, abbreviation, and a short description.

The executables (and Makefiles, object files, module information files) are usually located in subdirectories of the source code directories. These subdirectories typically have the name of the machine, architecture, or operating system the executable is compiled for.

3.2 Fortran files

Tables 3.2 and 3.3 show a list of all source files necessary to compile the complete version of CO5BOLD.

File and path	Abb.	Description
hd/rhd/rhd.F90	RHD	main program
hd/rhd/rhd_hyd_module.F90	RHD	hydrodynamics routines
hd/rhd/rhd_baserad_module.f90	RHD	basic radiative transfer
hd/rhd/rhd_lhtrad_module.F90	RHD	radiative transfer routines
hd/rhd/rhd_shortrad_module.F90	RHD	long characteristics, global models radiative transfer
hd/rhd/rhd_shortrad_dtauop01.f90	RHD	short characteristics, global models short-characteristics tau coupling
hd/rhd/rhd_shortrad_dtauop02.f90	RHD	short-characteristics tau coupling
hd/rhd/rhd_shortrad_operator00.f90	RHD	short-characteristics operator
...		
hd/rhd/rhd_shortrad_operator05.f90	RHD	short-characteristics operator
hd/rhd/rhd_shortrad_operator06.f90	RHD	short-characteristics operator
hd/rhd/rhd_shortrad_bound01.f90	RHD	short-char. boundary condition
hd/rhd/rhd_vis_module.F90	RHD	tensor viscosity
hd/mhd/rhd_mhd_module.F90	MHD	magnetic fields
rad/hdrad/rhd_rad_module.F90	RAD	interface for:
rad/hdrad/MSrad3D.F90	RAD	Matthias' radiation-transport long characteristics, local models
eos/f90/gasinter_routines.F90	EOS	equation of state
opa/opta/cubit_module.f	OPTA	cubic interpolation
opa/opta/opta_par_module.f90	OPTA	parameters for opacity routines
opa/opta/opta_routines.F90	OPTA	opacity reading & interpolation
opa/opta/opta_dust.f90	OPTA	dust opacity
hd/dust/rhd_dust_module.F90	DUST	dust/molecule-formation master
hd/dust/dust_k3mon_module.f	DUST	1- or 2-component dust model
hd/dust/dust_bins_module.f90	DUST	multi-bin dust model
hd/dust/dust_momentc2_module.f	DUST	4-moment C dust model
hd/dust/C2.INC	DUST	dust include file: C ₂ molecule
hd/dust/C2H.INC	DUST	dust include file: C ₂ H molecule
hd/dust/C2H2.INC	DUST	dust include file: C ₂ H ₂ molecule
hd/dust/CHPAR_CT.INC	DUST	dust include file
hd/dust/DINDEX.INC	DUST	dust include file
hd/dust/DKSPLINT.INC	DUST	dust include file
hd/dust/H2.INC	DUST	dust include file: H ₂ molecule
hd/chem/chem_rn_module.F90	CHEM	chemical reaction network
hd/chem/chem_rn_dvode.F90	CHEM	chemical reaction network: solver
hd/hion/f90/hion_main_module.f90	HION	hydrogen ionization
hd/hion/f90/hion_io_module.f90	HION	hydrogen ionization: I/O
hd/hion/f90/hion_def_module.f90	HION	hydrogen ionization: definitions
hd/hion/f90/hion_dvode_module.f90	HION	hydrogen ionization: solver
hd/hion/f90/hion_lineq_module.f90	HION	hydrogen ionization: linear algebra
hd/hion/f90/hion_util_module.f90	HION	hydrogen ionization: utility package
hd/hion/f90/hion_devel_module.f90	HION	hydrogen ionization: developer kit
hd/hion/f90/edens_module.f90	HION	electron densities

Table 3.2: List of all high-level modules: the table shows the file name with part of its path, the shortcut for the directory, and its description.

Path and file	Abb.	Description
hd/rhdb/rhd_action_module.f90	RHDB	control-parameter passing
hd/rhdb/rhd_box_module.F90	RHDB	box handling
hd/rhdb/rhd_dat_module.F90	RHDB	handling of averages
hd/rhdb/rhd_gl_module.f90	RHDB	global parameters
hd/rhdb/rhd_io_module.F90	RHDB	input/output
hd/rhdb/rhd_mean_module.f90	RHDB	averaging routines
hd/rhdb/rhd_mpi_module.F90	RHDB	MPI routines (under construction)
hd/rhdb/rhd_phys_module.f90	RHDB	physics routines, source terms
hd/rhdb/rhd_prop_module.f90	RHDB	box properties
hd/rhdb/rhd_rec_module.f90	RHDB	reconstruction routines
hd/rhdb/rhd_sub_module.f90	RHDB	additional routines
cons/f90/const_module.f90	CON	physical & mathematical constants
mat/str/str_module.f90	STR	string handling
time/f90/timing_module.F90	TIME	timing routines
uio/f90/uio_base_module.f90	UIO	I/O routines
uio/f90/uio_bulk_module.f90	UIO	I/O routines
uio/f90/uio_filedef_module.f90	UIO	I/O routines
uio/f90/uio_mac_module.F90	UIO	I/O routines, machine-dependend part

Table 3.3: List of all low-level modules: the table shows the file name with part of its path, the shortcut for the directory, and its description.

Path and file	Abb.	Description
hd/tweak/rhd_scale_module.F90	TWEAK	scale parameters
hd/tweak/rhd_tweak_massreduction_module.F90	TWEAK	reduce mass
hd/tweak/rhd_tweak_ppdamp_module.F90	TWEAK	damp plane-parallel modes
hd/tweak/rhd_tweak_ppdamp12_module.F90	TWEAK	damp plane-parallel modes
hd/tweak/rhd_tweak_ppdamp45_module.F90	TWEAK	damp plane-parallel modes
hd/tweak/rhd_tweak_smallrhodamp_module.F90	TWEAK	damp fluctuation at small densities
hd/tweak/rhd_tweak_smallrhodampmassred_module.F90	TWEAK	damp fluctuations and change mass
hd/tweak/rhd_tweak_smallrhodampnurotinc_module.F90	TWEAK	damp fluctuations and change rotation

Table 3.4: List of all tweak and sscale modules: the table shows the file name with part of its path, the shortcut for the directory, and its description.

Path and file	Abb.	Description
hd/unitt/rhdut.F90	UT	unit-test program
hd/unitt/UT_module.F90		unit-test routines
hd/rhd/rhd_baseradUT_module.f90		unit tests of basic radiative transfer
hd/rhdb/rhd_meanUT_module.f90		unit tests of averaging routines
hd/rhdb/rhd_recUT_module.f90		unit tests of reconstruction routines

Table 3.5: List of all unit-test modules (including the unit-test main program): the table shows the file name with part of its path, the shortcut for the directory, and its description.

3.3 Script files

The Linux scripts in Tab. 3.6 perform various tasks like producing the CO5BOLD (or UIO or gas2eos.exe) Makefile, starting or aiding the compilation of the manual from the \LaTeX source, etc.

Path (and files)	Description
bin/collect_for	Collect all CO5BOLD files in a tar file <code>for.tar.gz</code>
bin/ls_for	List all CO5BOLD Fortran files
bin/*	Further utility scripts
doc/manual/extractmpi	Create dummy Fortran file with MPI routine calls
doc/manual/for2tex_co5bold	Transform CO5BOLD source code into \LaTeX
doc/manual/for2tex	Transform Fortran source code into \LaTeX
doc/manual/mk_co5bold	Produce PDF and HTML versions of the manual
eos/f90/conf/configure	Produce the gas2eos.exe Makefile
eos/f90/job/j2/eos_r8tor4.sh	Transform EOS tables from double to single precision
hd/rhd/conf/configure	Produce the CO5BOLD Makefile, see Sect. 4.3
uio/bin/uiocat	Concatenate files in UIO form, see Sect. 6.2.6.3
uio/bin/uioinfo	Print machine-dependent UIO information, see Sect. 6.2.6.4
uio/bin/uiolook	Print entry headers of file in UIO form, see Sect. 6.2.6.2
uio/f90/conf/configure	Produce the UIO Makefile
uio/f90/conf/install	Set some paths to install UIO

Table 3.6: List of Linux script files.

3.4 Documentation files

The files in Tab. 3.7 provide various information. Among them is the general README file and the \LaTeX source of the CO5BOLD manual. PDF and HTML versions of the manual are not included and have to be compiled individually (by executing `mk_co5bold`).

Path (and files)	Description
README	CO5BOLD installation instructions
README_MHD	Short description of MHD parameters
doc/examples/ReadMe	Description of some CO5BOLD parameter files
doc/examples/*.par	Some CO5BOLD sample parameter files
doc/info/*.txt	A mix of info files (release notes, todo list,...)
doc/manual/co5bold.tex	The \LaTeX source of the manual
uio/man/man1/	man pages for UIO scripts, see Sect. 6.2.6

Table 3.7: List of documentation files.

Chapter 4

Compilation & installation

In this section, the installation procedure is outlined and compiler switches necessary to compile CO5BOLD and to optimize its performance are described.

4.1 Quickstart: How to compile CO5BOLD

If you are going to install CO5BOLD on a machine with a “known” (to setup script and generated Makefile) operating system and compiler (see Sections 4.3 and 4.5), then the procedure should be fairly easy. The general compilation procedure is now:

```
tar -zxvf for.tar.gz
cd for/hd/rhd
mkdir -p YOUR_MACHINE
cd YOUR_MACHINE
ln -s ../conf/configure .
./configure
make
```

The compilation process is explained in more detail in Sect. 4.2. The configure script is described in its header and in Sect. 4.3. The directory structure is shown in Tab. 3.1. All Fortran files are listed in Tables 3.2 and 3.3.

4.2 Compilation procedure for CO5BOLD

The installation procedure has changed significantly since the early releases: now, there is a configure script (see Sect. 4.3) that creates the complete (temporary) Makefile, which can be used to compile CO5BOLD and produce the executable `rhd.exe`. The detailed installation procedure is:

1. Choose/create a proper base directory. This could be `$HOME`. Then the master directory will typically be `$HOME/for` – this is the default created by the tar file. However, you might prefer to put the files into `$HOME/CO5BOLD` or `$HOME/CO5BOLD/VersionNumber` instead.
2. Put all source files and the configure script there. This will be done typically by expanding the gzipped tar file `for.tar.gz` e.g. with

```
tar -zxvf for.tar.gz
```

(or by copying all files from an existing installation). On a restricted UNIX you might be forced to use

```
gunzip for.tar.gz
tar -xvf for.tar
```

instead. Unpacking the tar file creates a sub directory `for` in the local directory (and possibly overwrites existing files!). You get sub sub directories as described in Sect. 3.1 and files as listed in Tables 3.2 and 3.3. See the Readme file `'for/README'`.

3. Change with

```
cd for/hd/rhd
```

into the main directory.

4. Look at the existing sub directories, e.g. with

```
ls -og | grep "^d"
```

to see if you find one that fits your machine. The directory

```
for/hd/rhd/conf
```

should not be used. It contains only the configure script. But any other directory will do. If you don't like any of the existing directories – or there are none, create your own e.g. with

```
mkdir YOUR_MACHINE
```

Change into this directory with

```
cd YOUR_MACHINE
```

5. Check if there is a configure script or a link to it with

```
ls -og configure
```

which should give something like

```
lrwxrwxrwx  1  17 2014-01-07 15:15 configure -> ../conf/configure
```

If it is not there, create the link with

```
ln -s ../conf/configure .
```

6. Start the configure script to create the (first version of the) Makefile with

```
./configure
```

A partly colored output can be generated with

```
./configure -c
```

This gives you a screen output like

```
Configuration script for C05BOLD Makefile
=====
```

```
No ./configurerc file found.
Writing template ./configurerc.
```

```
Checking default settings for environment variables:
```

```

No compiler          specified                : F90_COMPILER=
No parallelization  requested, assuming default: F90_PARALLEL= scalar
No debugging        requested, assuming default: F90_DEBUG   = 0
No LHDrad module    requested, assuming default: F90_LHDRAD   = 0
No MSrad module     requested, assuming default: F90_MS RAD    = 0
No SHORTrad module  requested, assuming default: F90_SHORTRAD = 1
No chem. module     requested, assuming default: F90_CHEM    = 0
No hion. module     requested, assuming default: F90_HION    = 0
No dust module      requested, assuming default: F90_DUST    = 0
No MHD module       requested, assuming default: F90_MHD     = 0
No TWEAK module     requested, assuming default: F90_TWEAK   = 0
No explicit machine specified, assuming default: F90_MACHINE = local
No explicit path    specified, assuming default: F90_BASEPATH= /home/bf/for

```

List of control environment variables:

```

F90_COMPILER =
F90_PREFLAGS =
F90_POSTFLAGS=
F90_PARALLEL = scalar
F90_DEBUG    = 0
F90_LHDRAD   = 0
F90_MS RAD   = 0
F90_SHORTRAD = 1
F90_CHEM     = 0
F90_HION     = 0
F90_DUST     = 0
F90_MHD      = 0
F90_TWEAK    = 0
F90_MACHINE  = local
-> MACHINE   = i686
    MACMODEL = Intel Pentium
F90_BASEPATH = /home/bf/for

```

System and compiler info:

```

Linux system with i686 architecture
  PGI compiler
  version=3.3-2

```

Compiler call:

```
pgf90 -byteswapio -fast -Mvect=sse -Mcache_align -Minfo=inline
```

Write compiler name and flags into file compiler_flags.info

New Makefile written.....

A new 'Makefile' is produced. An existing one is appended to 'Makefile_old'. Additionally, the file 'compiler_flags.info' is written which contains the compiler call in Fortran format.

7. Check the output of the configure script and the header of the new Makefile. You get an overview over the existing environment variables that control the configure script (see Sect. 4.3) with

```
env | grep F90_
```

Obs.: at the beginning there might be none.

It is convenient to collect the control environment variables in the configure resource file `.configurerc`. During the first call of `configure` in any directory, a template `.configurerc` file is produced.

8. Look into the header (and if necessary the rest) of the configure script or into Sect. 4.3 or try

```
./configure -h
```

to find out how to change the environment variables to control the script. For instance, if you want to enable debugging options, type:

```
export F90_DEBUG=1
```

Restart the configure script after every change in the control variables! With e.g.

```
export F90_MACHINE=dummy
export F90_PREFLAGS="-Oprettyfast +Qsomethingelse"
./configure
```

it is possible to specify all machine-dependent settings yourself (see Sect. 4.3.1.16 and Sect. 4.3.1.3). This is useful when dealing with a compiler hitherto unknown to the configure script.

9. Start the compilation with

```
make
```

to produce the executable `rhd.exe`. Symbolic links are created that point from the current directory to each source-code file needed to compile CO5BOLD in its requested configuration.

A simple sample installation might look like the following (the sub directory 'for' is put directly into the home directory).

```
# --- Choose the base directory ---
cd $HOME

# --- Put the tar file there ---
# ...

# --- Expand the tar file ---
tar -zxvf for.tar.gz

# --- Go into (default) master directory ---
cd for/hd/rhd/YOUR_MACHINE

# --- Activate OpenMP und MSrad radiation transport ---
export F90_PARALLEL=openmp
export F90_MSRAD=1

# --- Start the configure script to produce the Makefile ---
./configure

# --- Compile using the Makefile ---
make

echo 'Voila!'
```

If you want to compile in a directory in a completely different place (not in a sub directory of `for` as described above), you have to set the environment variable `F90_BASEPATH` (see Sect. 4.3.1.17) to make the paths to the source files known to the configure script. That might look like

```
mkdir SOME_REMOTE_PLACE
cd SOME_REMOTE_PLACE
export F90_BASEPATH=$HOME/for
ln -s $F90_BASEPATH/hd/rhd/conf/configure .
./configure
```

The variable `F90_BASEPATH` also has to be set explicitly if the main directory `for` should have another name. Renaming the sub-directories with the source files is not a good idea – it requires modifications of the configure script itself.

If you install a new CO5BOLD version on top of an older one it might be safer (particularly, if Fortran file names have change), to remove all earlier generated temporary links and files with

```
make removeall
```

so that the entire sequence looks like:

```
./configure
make removeall
make
```

If you want to remove temporary object and info files after a successful compilation, you could use

```
make clean
```

as in:

```
./configure
make
make clean
```

4.3 Configure script

The configure script produces a Makefile.

It is controlled by environment variables (see below). It tries to use reasonable default values if they are not set (properly). In the script the machine type is determined with ‘`uname -m`’. According to the control variables and the machine architecture the compiler name and its compiler flags are composed. These are written into the header of a Makefile which is produced in the end. An existing Makefile is appended to

```
Makefile_old.
```

Additionally, the compilation command is written into the file

```
'compiler_flags.info'
```

in a form ready to be included in a Fortran program.

4.3.1 Control environment variables

The environment variables that control the script are listed in the following. It is convenient to put them into the configure resource file `.configurerc` that is read by the configure script.

4.3.1.1 F90_COLOR

Activate color output of the `configure` script:

- 0: standard black & white output
- 1: color output

4.3.1.2 F90_COMPILER

Fortran compiler, e.g.:

- '': a machine-dependent default is chosen individually for each architecture
- `f90`: general default
- `gfortran`: GNU compiler
- `ifort`: Intel compiler

See Sect. 4.6 for a more complete list and further details.

4.3.1.3 F90_PREFLAGS

Compiler flags to be put at the beginning of the list. Usually, the list of compiler flags produced by the `configure` script should be pretty complete. But you might want to add special switches like `'-Bstatic'` to enforce static linking of libraries.

- '': no extra flags

4.3.1.4 F90_POSTFLAGS

Compiler flags to be put at the end of the list. Usually, the list of compiler flags produced by the `configure` script should be pretty complete. However, you might want to overwrite some settings. This can be done by setting this variable to a none-empty value because typically a compiler should interpret the flags from left to right.

- '': no extra flags

4.3.1.5 F90_PARALLEL

Parallelization scheme:

- `scalar`: no parallelization (default)
- `openmp`: OpenMP (appropriate for CO5BOLD)
- `auto`: auto-parallelization (not implemented for all machines)

4.3.1.6 F90_DEBUG

Debugging level:

- 0: no extra debugging information produced, full optimization is chosen (default)
- 1: standard debugging mode (typically switch `'-g'` instead of `'-fast'`)
- 2: other debugging (or array checking) modes possible if implemented for the requested machine

4.3.1.7 F90_OPTIMIZE

Optimization:

- 0: no explicit optimization (default if F90_DEBUG=1)
- 1: try to find automatically sensible optimization flags. That's the default if F90_DEBUG=0. However, often it is better to specify the optimization flags explicitly
- `-ipo -O3 -xHost` (example): set the optimization flags by hand. This is a better way to specify the optimization than using F90_POSTFLAGS

4.3.1.8 F90_LHDRAD

LHDRad radiation transport:

- 0: do not activate (compile and link) this module (default)
- 1: activate this radiation transport module

4.3.1.9 F90_MS RAD

MSrad radiation transport:

- 0: do not activate (compile and link) this module (default)
- 1: activate this radiation transport module

4.3.1.10 F90_SHORTRAD

SHORTrad radiation transport:

- 0: do not activate (compile and link) this module (default)
- 1: activate this radiation transport module

4.3.1.11 F90_CHEM

CHEM module (chemical reaction networks):

- 0: do not activate (compile and link) this module (default)
- 1: activate this source step module

Setting this variable to 1 will set F90_DUST=1. The compiler is then called with `-Drhd_chem01`.

4.3.1.12 F90_HION

HION module (time-dependent hydrogen ionization):

- 0: do not activate (compile and link) this module (default)
- 1: activate this source step module

Setting this variable to 1 will set F90_DUST=1. The compiler is then called with `-Drhd_hion01`.

4.3.1.13 F90_DUST

DUST module:

- 0: do not activate (compile and link) this module (default)
- 1: activate this source step module

If this variable is set to 1 the compiler is called with `-Drhd_box_quc01=1`, see Sect. 4.4.1.6.

4.3.1.14 F90_MHD

MHD module:

- 0: do not activate (compile and link) this module (default)
- 1: activate this magnetohydrodynamics module (MHD HLL solver)

If CO5BOLD is compiled with the MHD module, your start model should include magnetic fields, otherwise zero magnetic fields are created and used. In the latter case, the magnetic field arrays are not written into the output files.

4.3.1.15 F90_TWEAK

TWEAK module:

- 0: do not activate (compile and link) this module (default)
- 1: activate the TWEAK module `rhd_tweak_module.F90`
- `rhd_tweak_name_module`: activate the TWEAK module with this name

A TWEAK module is a user-provided set of routines performing some simple but non-standard task.

4.3.1.16 F90_MACHINE

Explicit machine specification. This is usually not necessary, use 'local' or '' instead.

- '': local machine
- `sun4u`: Sun
- ...: See the header of the configure script for an up-to-date list
- `local`: local machine (default)
- `dummy`: do not use any machine-dependent flags but use module selections
- `empty`: compiler flags are composed from `F90_PREFLAGS` and `F90_POSTFLAGS` only

4.3.1.17 F90_BASEPATH

Path for the CO5BOLD base directory.

- '': the configure script tries to determine the base-directory name automatically (default). This should work if the local directory is located somewhere below `.../hd/rhd/`
- otherwise: this string is used as base directory name (e.g. `/home/user/for`)

Some examples can be found in Sect. 4.2.

4.4 Compiler macros

Some of the modules of the CO5BOLD code (with suffix “.F90”) employ compiler macros to switch between code versions during compile time. Typically you define at least one of the three switches `rhd_r01`, `rhd_r02`, or `rhd_r03` to choose a radiation transport module. The others have reasonable default values. To find the combination with the optimal performance, you should look into Sect. 4.5

The macros are sorted into different categories:

Some *activate a certain feature* (like a radiation transport module or the dust module). They have to be selected by the user (typically via environment variables and the configure script, see Sect. 4.3) each time the code is compiled for a certain purpose.

Other macros are meant to *improve the performance* by offering the choice between e.g. different loop structures or case distinctions. These macros are set by the configure script to the best knowledge of the author(s). Ideally, they should be checked and modified if necessary each time CO5BOLD is compiled on a new machine. It should be save to modify these settings: the results between runs with different settings should only differ slightly due to round-off errors.

Some macros *select between different numerical approximations*. A change here should be visible in a (more or less drastic) change of the results of a simulation. Usually, the default values should be accepted. Other settings typically only exist to allow the comparison with older versions of CO5BOLD or because there are new developments going on which have not yet managed to become the default.

A couple of macros only activate timing measurements and result in *additional output*. Some of them are not thread-save und should only be activated for runs on one thread (as done by the configure script). It is always save to switch any of them off (by removing or undefining them).

The macros in the category *test* mark parts of code under development. The default values should only be changed with great care (typically by the author of that code segment). The configure script does not touch these settings.

4.4.1 General

4.4.1.1 `timing_c_factor`

(“timing count factor”) in `timing_module.F90`.

Category: account for property of machine.

To produce the timing statistics printed at the end of a simulation run the standard Fortran routine `SYSTEM_CLOCK` is used. The macro `timing_c_factor` specifies by how much the count rate of this routine is reduced when storing its count value. This does not prevent all overflows but can make the output much more useful. Values:

- 1: (default) count rate of `SYSTEM_CLOCK` is used directly.
- otherwise: e.g. 1000, count rate of `SYSTEM_CLOCK` is reduced by this factor.

By a proper choice of this factor the timing measurements of individual routines can be made meaningful: the reduction of the count rate prevents overflows due to the addition of several measurements. An overflow during an individual measurement can not be prevented. Therefore, the count rate for the entire program still tends to produce overflows.

4.4.1.2 `timing_c_range`

(“timing counter range”) in `timing_module.F90`.

Category: account for property of machine.

To produce the timing statistics printed at the end of a simulation run the standard Fortran routine `SYSTEM_CLOCK` is used. The macro `timing_c_range` specifies the number of digits (the “range”) used for the integers storing the counters. The value appears in the code e.g. in `integer(kind=selected_int_kind(timing_c_range)) :: count_total`.

Fortran standard is the use of 4-byte integers. However, that is often not sufficient and can lead to overflows. Many compilers can use longer integers, though. That can be tried by setting the `timing_c_range` not to 9 (the default) but e.g. to 15. If it works, overflows are essentially ruled out. If it does not work, the compilation stops with an error message. Values:

- 9: (default) use standard 4-byte integers for timing counters.
- 15 or otherwise: use this number for the range of Fortran integers

By a proper choice of this number all the timing measurements can be made meaningful, even for long runs on machines with fast counters.

4.4.1.3 `timing_r_type`

(“timing rate type”) in `timing_module.F90`.

Category: account for property of machine.

During a CO5BOLD run, the total execution time is measured and printed after each time step. The type of clock used can be chosen with:

- 1: Use `call system_clock()` (default).
- 2: Use `call Date_and_Time()`.
- 3: Use `t=etime()` (Sun version, used in most cases).
- 4: Use `call etime()` (gfortran version).
- 5: Use `call tremain()` (Cray version).
- 6: Use `call clock()` (Hitachi version).

4.4.1.4 `rhd_box_arrays01`

(“rhd box arrays 01”) in `rhd_box_module.F90`.

Category: performance enhancement.

Switch to choose between the (“classical”) use of pointer arrays within the box structure to store arrays, or the (“new”) version with allocatable arrays, that is potentially faster. Values:

- 0: classical pointer arrays (default).
- 1: new allocatable arrays (probably faster)

4.4.1.5 `rhd_box_grav01`

(“rhd box gravitation 01”) in `rhd_box_module.F90`.

Category: feature activation.

Switch to activate the array for the gravitational potential in the box structure. If the switch is set to 1, a 3D array for the potential is created, copied, removed, ... There is no module to compute the gravitational potential, yet. Therefore the entire thing has no practical value, yet. Values:

- 0: (default) no handling of array.
- 1: array handling activated.

4.4.1.6 `rhd_box_quc01`

(“rhd box quantity centered 01”) in `rhd_box_module.F90` and `rhd.F90`.

Category: feature activation.

CO5BOLD is able to handle a number of further quantities (`quc`: “quantity centered”) in addition to the basic hydrodynamics quantities (ρ , e_i , ...) if this compiler switch is activated. These additional quantities can be e.g. densities of dust distribution moments or densities of molecules. They are required for the treatment of chemical reaction networks and time-dependent hydrogen ionization. For the latter the `quc` arrays contain the number densities of the atomic level populations. For the chemical reaction network, the arrays contain the species number densities in cm^{-3} and with headers following this example: ”Number density of H2”. Values:

- 0: (default) no handling of additional quantities (density arrays).
- 1: handling of additional density arrays is activated.

To actually include dust formation in a simulation, it is necessary to

1. set the switch `-Drhd_box_quc01=1` during compilation (this is done by the configure script if the environment variable `F90_DUST` is set to 1, see the description of the variable in Sect. 4.3.1.13),
2. put arrays specifying the initial conditions of the additional density into the start model (as `real quc001, real quc002, ...`),
3. select a proper model describing dust (or molecule) formation in the parameter file (with character `dustscheme`).

4.4.1.7 rhd_box_bmag01

(“rhd box b magnetic 01”) in `rhd_box_module.F90` and `rhd.F90`.

Category: feature activation.

CO5BOLD can handle magnetic field arrays if this compiler switch is set. Values:

- : (default) no handling of magnetic field arrays.
- : handling of magnetic field arrays is activated.

To actually account for magnetic fields in a simulation, it is necessary to

1. set the switch `-Drhd_box_bmag01=1` during compilation (this is done by the configure script if the environment variable `F90_MHD` is set to 1, see Sect. 4.3),
2. put arrays specifying the initial conditions of the boundary-centered magnetic-field arrays into the start model (as `real bb1, real bb2, real bb3`),
3. select an hydrodynamics scheme that is able to handle magnetic fields in the parameter file (with character `hdscheme`).

4.4.2 Input/output with UIO

4.4.2.1 uio_switch_system_l01

(“uio switch system list 01”) in `uio_mac_module.F90`.

Category: I/O, account for property of machine.

Sometimes, it is useful to have in the header of a UIO file information about the system that wrote the file. How Fortran gets this information depends on the machine. Values:

- 0: Read information from file `uioenvfile.txt`. Don't write or delete the file.
- 1: Call external function `system()` to produce the file `uioenvfile.txt`. Read and delete the file (default).
- 2: Call routine `system()` to produce `uioenvfile.txt`. Read and delete the file.
- 3: Call external routine `HF_SH()` to produce `uioenvfile.txt`. Read and delete it.
- 4: Call external function `uname()` to get system information.
- 5: Call external routine `pxfuname()` to get system information.

4.4.2.2 uio_switch_native_l01

(“uio switch native list 01”) in `uio_mac_module.F90`.

Category: I/O, account for property of machine.

All machines can read and write their native format – only that it might differ from one machine to the other. It is there, if needed, but should be avoided in practise. Values:

- 1: Get information about word lengths from `uio_deform()` (default).
- 0,2: Set word lengths explicitly.

4.4.2.3 `uio_switch_ieeebe_l01`

(“uio switch ieee big endian list 01”) in `uio_mac_module.F90`.

Category: I/O, account for property of machine.

This is the standard for files read of written by CO5BOLD. All machine/compiler combinations should support it – either natively or via some conversion process. Values:

- 0: Don’t include this conversion type (default).
- 1: Get information about word lengths from `uio_deform()`.
- 2: Set word lengths explicitly.

4.4.2.4 `uio_switch_ieeele_l01`

(“uio switch ieee little endian list 01”) in `uio_mac_module.F90`.

Category: I/O, account for property of machine. Values:

- 0: Don’t include this conversion type (default).
- 1: Get information about word lengths from `uio_deform()`.
- 2: Set word lengths explicitly.

4.4.2.5 `uio_switch_ieee_l01`

(“uio switch ieee list 01”) in `uio_mac_module.F90`.

Category: I/O, account for property of machine.

This is a fallback for reading of UIO files, that should be activated for compilation if either of the Endian formats above is allowed. It should not be used for writing. Values:

- 0: Don’t include this conversion type (default).
- 1: Get information about word lengths from `uio_deform()`.
- 2: Set word lengths explicitly (4-byte words).
- 3: Set word lengths explicitly (8-byte words).

4.4.2.6 `uio_switch_crayxmp_l01`

(“uio switch cray x-mp list 01”) in `uio_mac_module.F90`.

Category: I/O, account for property of machine.

This is the native format on old Cray X-MP and Cray TS machines. Values:

- 0: Don’t include this conversion type (default).
- 1: Get information about word lengths from `uio_deform()`.

4.4.2.7 `uio_switch_open_l01`

(“uio switch open list 01”) in `uio_mac_module.F90`.

Category: I/O, account for property of machine.

Many compilers support a transparent conversion between number representations during reading and writing. This is not a Fortran standard, though, and has to be activated in different ways:

- 0: No conversion (default).
- 1: Use the `convert` keyword in the `open()` statement (Intel and gfortran compilers on Linux machines, standard compiler on Dec Alphas).
- 2: Use `asnunit()` Cray X-MP style.
- 3: Use `asnunit()` Cray TS style.

4.4.3 Equation of state

4.4.3.1 `gasinter_l01`

(“gas interpolation l01”) in `gasinter_routines.F90`.

Category: performance enhancement.

This switch determines how temporary arrays are handled and loops are split to improve performance.

Values:

- 0: (old default) Temporary coefficient arrays are actually copied.
- 1: Temporary coefficient arrays just get a pointer link into the big arrays.
- 2: No temporary coefficient arrays.
- 3: Experimental; testing only (avoid!).
- 4: (default) Split inner loop into three to give better vectorization.

4.4.3.2 `gasinter_l02`

(“gas interpolation l02”) in `gasinter_routines.F90`.

Category: performance enhancement.

This switch determines how coefficient arrays are handled to improve performance. Values:

- 0: Coefficients are stored as pointer arrays (old version).
- 1: (default) Coefficients are stored as allocatable arrays.

4.4.4 Opacity

4.4.4.1 `opta_switch_l01`

(“opacity table switch l01”) in `opta_switch_routines.F90`.

Category: performance enhancement.

This switch determines how arrays are handled and loops are split to improve performance. Values:

- 0: 3D-array single-loop scheme (old default)
- 1: 1D-array single-loop scheme
- 2: 3D-array three-loop scheme (default)
- 3: 1D-array three-loop scheme

4.4.5 Hydrodynamics (Roe solver)

4.4.5.1 `rhd_hyd_gravcorr_p01`

(“rhd hydrodynamics gravitation correction parameter 01”) in `rhd_hyd_module.F90`.

Category: selection of approximation.

This parameter controls the way the Roe solver handles the source terms due to gravity. A different choice results in different simulation results and not just in slightly faster (or slower) code. The problem is that the original Roe solver interpretes the pressure gradient in a hydrostatic stratification a fluctuation due to shock waves. In case of strong stratification this can lead to weird effects. With activated correction the Roe solver treats only the deviations from a hydrostatic stratification as due to waves (or shocks). Several correction formulas have been tried. The latest is the recommended default. Values:

- 0: No pressure correction terms in Roe solver.
- 1: Simple correction with rhomean, no new average pressure.

- 2: Simple correction with rhomean, new average pressure.
- 3: Correction with local rho, limited, new average pressure.
- 4: Correction with local rho, new (different formula) average pressure.
- 5: (default) Correction with local rho, new limit, new average pressure.
- 6: Modification of 5 with different geometry factors in case of non-equidistant grid.

4.4.5.2 `rhd_hyd_entropyfix_p01`

(“rhd hydrodynamics entropy fix parameter 01”) in `rhd_hyd_module.F90`.

Category: performance enhancement.

The entropy fix can be done in one of two ways to get optimum performance (with essentially the same results). Values:

- 0: (default) “if...then...else” construction
- 1: use a mask and the signum function

4.4.5.3 `rhd_hyd_upwind_p01`

(“rhd hydrodynamics upwind parameter 01”) in `rhd_hyd_module.F90`.

Category: performance enhancement.

The determination of the upwind direction can be done in one of two ways to get optimum performance (with essentially the same results). Values:

- 0: (default) “if...then...else” construction
- 1: use a mask and the signum function

4.4.5.4 `rhd_roe1d_flux_l01`

(“rhd roe 1 dimension flux loop 01”) in `rhd_hyd_module.F90`.

Category: performance enhancement.

This switch allows to choose between various ways of computing the upwind-centered Roe states. Values:

- 0: Use upwind-index arrays in all Roe-state computations. Do it in one step (old default).
- 1: Use if-then-else-constructs in all Roe-state computations. Do it in one step (default, recommended).
- 2: Use upwind-index arrays in all Roe-state computations. Do it in two steps.
- 3: Use if-then-else-constructs in all Roe-state computations. Do it in two steps.

4.4.5.5 `rhd_bound_t01`

(“rhd bound timing 01”) in `rhd_hyd_module.F90`.

Category: additional output.

Produce timing information for “inner boundary” routine (central potential) or lower and upper boundary routines (constant gravitation). It can be used together with OpenMP. Values:

- `undefined`: (default) no timing information.
- `defined`: call subroutines to measure elapsed time.

4.4.5.6 rhd_roe1d_flux_t01

(“rhd roe 1 dimension flux timing 01”) in `rhd_hyd_module.F90`.

Category: additional output.

Produce timing information for the routine which computes the Roe fluxes. It should not be used in conjunction with OpenMP. Values:

- **undefined:** (default) no timing information
- **defined:** call subroutines to measure elapsed time

4.4.5.7 rhd_roe1d_step_t01

(“rhd roe 1 dimension step timing 01”) in `rhd_hyd_module.F90`.

Category: additional output.

Produce timing information for the routine which performs the Roe step. It should not be used in conjunction with OpenMP. Values:

- **undefined:** (default) no timing information
- **defined:** call subroutines to measure elapsed time

4.4.6 Hydrodynamics (tensor viscosity)

4.4.6.1 rhd_vis_density_p01

(“rhd viscosity density parameter 01”) in `rhd_vis_module.F90`.

Category: selection of approximation.

Choose formula for density average at cell boundary in tensor-viscosity routines. Values:

- 0: $\rho_{\text{mean}} = \min(\rho_{\text{left}}, \rho_{\text{right}})$
- 1: (default) $\rho_{\text{mean}} = 0.5 * (\rho_{\text{left}} + \rho_{\text{right}})$

4.4.6.2 rhd_vis_t01

(“rhd viscosity timing 01”) in `rhd_vis_module.F90`.

Category: additional output.

Produce timing information for 2D/3D tensor-viscosity routines. It should not be used in conjunction with OpenMP. Values:

- **undefined:** (default) no timing information
- **defined:** call subroutines to measure elapsed time

4.4.7 Radiation transport

4.4.7.1 rhd_r01

(“rhd radiation 01”) in `rhd.F90`.

Category: feature activation.

Switch to include LHDrad radiation transport module. It uses long characteristics and is restricted to an equidistant grid and open boundaries at all surfaces (old “supergiant module”). Values:

- **undefined:** (default) LHDrad routines are deactivated.
- 1: LHDrad routines are recognized by the compiler.

4.4.7.2 rhd_r02

(“rhd radiation 02”) in `rhd.F90`.

Category: feature activation.

Switch to include MSrad radiation transport module. It uses long characteristics. The lateral boundaries have to be periodic. Top and bottom can be closed or open (“solar module”). Values:

- **undefined:** (default) MSrad routines are deactivated.
- **1:** MSrad routines are recognized by the compiler.

4.4.7.3 rhd_r03

(“rhd radiation 03”) in `rhd.F90`.

Category: feature activation.

Switch to include SHORTrad radiation transport module. It uses short characteristics and is restricted to an equidistant grid and open boundaries at all surfaces (new “supergiant module”). Values:

- **undefined:** (default) SHORTrad routines are deactivated.
- **1:** SHORTrad routines are recognized by the compiler.

4.4.7.4 rhd_rad3d_toray_l01

(“rhd radiation 3 dimensions to ray loop 01”) in `rhd_lhdrad_module.F90`,

Category: performance enhancement.

There might be a performance gain by splitting the main loop in routine `rhd_rad3d_toray` into three separate loops. Typically, one big loop is to be preferred. Values:

- **undefined:** (default) One big loop
- **defined:** Three smaller loops

4.4.7.5 rhd_rad3d_fromray_l01

(“rhd radiation 3 dimensions from ray loop 01”) in `rhd_lhdrad_module.F90`,

Category: performance enhancement.

There might be a performance gain by splitting a big loop in routine `rhd_rad3d_fromray` into two separate loops. Typically, one big loop is to be preferred. Values:

- **undefined:** (default) One big loop
- **defined:** Two smaller loops

4.4.7.6 rhd_rad3d_r02

(“rhd radiation 3 dimensions radiation 02”) in `rhd_lhdrad_module.F90`,

Category: test.

Module `rhd_lhdrad_module` contains a routine for the handling of periodic boundaries. It is in an experimental state and is deactivated by default. Values:

- **undefined:** (default) Skip routine `rhd_rad3d_dirper` during compilation
- **defined:** Compile routine `rhd_rad3d_dirper`

4.4.7.7 rhd_rad3d_solve_t01

(“rhd radiation 3 dimensions solve timing 01”) in `rhd_lhdrad_module.F90`,

Category: additional output.

Produce timing information for the routines which solves the 1D radiation transport equation along single ray. This routine is called very frequently. The timing measurement might slow it down somewhat. It should not be used in conjunction with OpenMP. Values:

- **undefined:** (default) no timing information
- **defined:** call subroutines to measure elapsed time

4.4.7.8 rhd_rad3d_dir_t01

(“rhd radiation 3 dimensions direction timing 01”) in `rhd_lhdrad_module.F90`,

Category: additional output.

Produce timing information for the routines which solves the radiation transport equation for one direction field. The timing measurement are called very frequently and might slow down the code. It should not be used in conjunction with OpenMP. Values:

- **undefined:** (default) no timing information
- **defined:** call subroutines to measure elapsed time

4.4.7.9 rhd_rad3d_step_t01

(“rhd radiation 3 dimensions step timing 01”) in `rhd_lhdrad_module.F90`,

Category: additional output.

Produce timing information with main 3D radiation transport routine. It can be used together with OpenMP and should cause no noticeable performance loss. Values:

- **undefined:** (default) no timing information
- **defined:** call subroutines to measure elapsed time

4.4.7.10 rhd_shortrad_operator_l01

(“rhd short-characteristics radiation operator loop 01”) in `rhd_shortrad_module.F90`.

Category: performance enhancement, selection of approximation.

Choose type of short characteristics operator. The operators usually come in pairs (1/2, 3/4, 5/6). There is a development from 1/2 over 3/4 to 5/6 towards higher stability. Both members of each pair should do the same operation but use different ways to do a case distinction. The 'even' operator has in some cases the better performance. But the 'odd' operator might be saver to use. Values:

- 0: simple test operator, fast but results are utterly useless!
- 1: case distinction with “if..then..else” construct.
- 2: case distinction with masks (weights 0.0 or 1.0).
- 3: case distinction with “if..then..else” construct, slope reduction of source function.
- 4: case distinction with masks (weights 0.0 or 1.0), slope reduction of source function.
- 5: (default) case distinction with “if..then..else” construct, modified slope reduction of source function.
- 6: (old default) case distinction with masks (weights 0.0 or 1.0), modified slope reduction of source function.
- 8: test version.

4.4.7.11 `rhd_shortrad_operator_l02`

(“rhd short-characteristics radiation operator loop 02”) in `rhd_shortrad_module.F90`.

Category: performance enhancement.

Select the way the short characteristics operator is accessed. Values:

- 0: (old default) The routine with the short characteristics operator is called within a loop and should be inlined.
- 1: (default) The program fragment with the short characteristics operator is included. No inlining necessary.

4.4.7.12 `rhd_shortrad_dtauop_l01`

(“rhd short-characteristics radiation delta tau operator loop 01”) in `rhd_shortrad_module.F90`.

Category: performance enhancement.

Choose type of short characteristics tau coupling operator. Values:

- 1: case distinction with “if..then..else” construct, default if `rhd_shortrad_operator_l01=1,3,5`.
- 2: case distinction with masks (weights 0.0 or 1.0), default if `rhd_shortrad_operator_l01=2,4,6`.

4.4.7.13 `rhd_shortrad_dtauop_l02`

(“rhd short-characteristics radiation delta tau operator loop 02”) in `rhd_shortrad_module.F90`.

Category: performance enhancement.

Select the way the operator for the tau coupling (short characteristics module) is accessed. Values:

- 0: (old default) The routine with the tau coupling operator is called within a loop and should be inlined.
- 1: (default) The program fragment with the tau coupling operator is included. No inlining necessary.

4.4.7.14 `rhd_shortrad_formal_l01`

(“rhd short-characteristics radiation formal loop 01”) in `rhd_shortrad_module.F90`.

Category: performance enhancement.

Select version of loop splitting for $\exp(-d\tau)$ computation. Values:

- 0: (default) `dtauhalf`, `exp_mdtauhalf`, `expl2t_mdtauhalf` are computed in a single loop
- 1: (`dtauhalf`, `exp_mdtauhalf`), (`expl2t_mdtauhalf`) are computed in separate loops. This prevents the SUN1 machine (Sunfire, Solaris, Forte 6.2) from doing some performance degrading optimization

4.4.7.15 `rhd_shortrad_dir1_l01`

(“rhd short-characteristics radiation direction 1 loop 01”) in `rhd_shortrad_module.F90`.

Category: performance enhancement.

Choose routine version for rays in x1 direction. Values:

- 0: (old default) Use routine with permuted indices for rays in x1 direction. In this case the innermost loop index is the third array index. The transposition of arrays is not needed but some machines (e.g. SUN1) do not like this index arrangement.
- 1: (default) Transpose arrays and use routine `rhd_shortrad_dir3` for rays in x1 direction. The extra step for the transposition of some arrays (and the reverse procedure) needs some time. But now the routine with the optimum index ordering can be used.
- 2: Transpose arrays serially and use routine `rhd_shortrad_dir3` for rays in x1 direction. The extra step for the transposition of some arrays (and the reverse procedure) needs some time. But now the routine with the optimum index ordering can be used.

4.4.7.16 rhd_shortrad_dir_l02

(“rhd short-characteristics radiation direction loop 02”) in `rhd_shortrad_module.F90`.

Category: performance enhancement, OpenMP.

Determine position of PARALLEL statement relative to outer loop in `rhd_shortrad_dirX`. Both settings give the same results but might show a different performance on a specific machine. Values:

- 0: (old default) PARALLEL statement inside of outer loop.
- 1: (default) PARALLEL statement outside of outer loop.

4.4.7.17 rhd_shortrad_lambda_l01

(“rhd short-characteristics radiation lambda loop 01”) in `rhd_shortrad_module.F90`.

Category: feature activation.

Handling of extra arrays to allow partially implicit Lambda* iteration. Values:

- 0: (default) Only fully implicit Lambda* iteration allowed (or fully explicit treatment).
- 1: Also partially implicit Lambda* iteration allowed.

4.4.7.18 rhd_shortrad_formal_t01

(“rhd short-characteristics radiation formal timing 01”) in `rhd_shortrad_module.F90`.

Category: additional output.

Produce timing information for routine which gives the formal solution of the radiation transport equation with the help of short characteristics. It can be used together with OpenMP and should cause no noticeable performance loss. Values:

- `undefined`: (default) no timing information
- `defined`: call subroutines to measure elapsed time

4.4.7.19 rhd_shortrad_step_t01

(“rhd short-characteristics radiation step timing 01”) in `rhd_shortrad_module.F90`.

Category: additional output.

Produce timing information for main short characteristics routine. It can be used together with OpenMP and should cause no noticeable performance loss. Values:

- `undefined`: (default) no timing information
- `defined`: call subroutines to measure elapsed time

4.4.7.20 MSrad_raytas

(“Matthias Steffen radiation ray tau s”) in `MSrad3D.F90`.

Category: performance enhancement.

Values:

- 0: (default) Loop with IF..THEN..ELSE
- 1: Loop with ABS,SIGN
- 2: Loop with MIN,MAX

4.4.8 Obsolete macros

4.4.8.1 IDF

(“Integer Delta Flux”) in `rhd_hyd_module.F90`.

Category: performance enhancement.

Number of padding cells for flux-like variables. This number was introduced to check whether the increase of the size of vectors for flux-like quantities (defined at cell boundaries) can improve the performance (especially on a CRAY machine). The gain is marginal (if present at all). The parameter is usually set to zero or left undefined. Values:

- 0: (default) no padding cells
- 1,2,3,...: extra padding cells

This switch is not recognized anymore.

4.4.8.2 `rhd_hyd_roe1d_l01`

(“rhd hydrodynamics roe 1 dimension loop 01”) in `rhd_hyd_module.F90`.

Category: performance enhancement.

The computation of the Roe fluxes can be done by either of two sets of routines to find the set which gives optimum performance (with essentially the same results). Values:

- 0: (default) lots of small routines acting on scalars, inlining needed, cache reuse is optimized
- 1: routines acting on arrays, more temporary arrays necessary, vectorization is easier

This switch is not recognized anymore.

4.4.8.3 `rhd_roe1d_slope_l01`

(“rhd roe 1 dimension slope loop 01”) in `rhd_hyd_module.F90`.

Category: feature activation.

When this compiler switch is set, a new extra stabilization mechanism can be activated: If one of the reconstruction methods `VanLeer`, `Superbee`, or `PP` (see Sect. 7.1.8.4) is activated, the slope can be reduced (by averaging with the results from a `MinMod` reconstruction) by setting `c_slopered` (see Sect. 7.1.9.7) to a positive non-zero value. This can improve the stability without significantly reducing the effective numerical resolution. Switch values:

- 0: (default) no slope reduction.
- 1: slope reduction in case of expansion wave.
- 2: slope reduction in case of strong density contrast.

This switch is not recognized anymore.

4.5 Optimization, compiler switches

In this section some mandatory or useful compiler flags are described. These have different functions:

- Enable necessary macro processing/expansion for the `.F90` files.
- Force proper handling of binary I/O.
- Choose module for radiative transfer.
- Activate module for dust formation and/or magnetic field transport.
- Enable parallelization with OpenMP directives.

- Choose a version of a subroutine or loop which is optimized for a specific architecture.
- Tell the compiler if and what to inline.
- Improve the general performance.

4.5.1 OpenMP settings

The OpenMP specifications and many related links can be found on the OpenMP.org homepage. Overviews can be found in “Shared Memory Programming With OpenMP” (M. D. Jones 2013) and “Intel Parallel Studio XE. Facing the Multicore-Challenge II” (Hans Pabst 2011). A complete online tutorial is “Parallel Computing and OpenMP Tutorial” (Shao-Ching Huang 2013).

To activate OpenMP in the CO5BOLD executable you have to set the corresponding environment variable (see 4.3.1.5) before calling the configure script, like

```
export F90_PARALLEL=openmp
./configure
make
```

This will insert the corresponding compiler switch (e.g. `-openmp`, `-omp`, `-mp`,... confer the following sections) into the compiler calls in the Makefile (see Sect. 4.3).

The calls to the timing routines that would be executed in parallel are removed by (not) setting the appropriate compiler macros (see Sect. 4.4).

In addition, the switch `rhd_shortrad_dir_102` (see Sect. 4.4.7.16) might be set, according to experience about performance enhancements.

The user has to find optimum values for the parameters `n_hydcellsperchunk` (for the Roe and the HLLMHD solver module, see Sect. 7.1.8.9) and `n_viscellsperchunk` (for the tensor-viscosity module, see Sect. 7.1.11.17) to optimize the size of the chunk given to one thread per time. For the Roe solver of the hydrodynamics module, there exist also the optional parameters `n_hydcellsperchunk2` (see Sect. 7.1.9.1) and `n_hydcellsperchunk3` (see Sect. 7.1.9.2).

For several modules the environment variable `OMP_SCHEDULE` can be set (before running CO5BOLD) to control its OpenMP scheduling behavior. Important parallel loops in the SHORTrad module have a `SCHEDULE(RUNTIME)` modifier that allows this external control. The old default is achieved by not defining the variable or by setting

```
export OMP_SCHEDULE="STATIC,1"
```

On some machines (e.g. an older Intel Xeon with Linux and PGI compiler), a dynamic scheduling activated with

```
export OMP_SCHEDULE="DYNAMIC,1"
```

is advantageous. The size of the individual chunks might be set to larger values than 1 (in the examples above). The optimal value has to be found empirically. A good starting point is `number_of_grid_points_in_1D/Number_of_treads`, which gives for a model with 171^3 grid points on a 4-processor machine

```
export OMP_NUM_THREADS=4
export OMP_SCHEDULE="STATIC,43"
```

However, usually the general default

```
export OMP_SCHEDULE="STATIC"
```

is a good choice. The number of threads should equal the number of available processors and has to be set at run-time with the environment variable `OMP_NUM_THREADS`, e.g. with

```
export OMP_NUM_THREADS=16
```

The size of the stack per thread can be set with `OMP_STACKSIZE`, as e.g. in

```
export OMP_STACKSIZE=300M
```

Usually, the default value is too small. On machines with many cores, experiments with `KMP_AFFINITY` might be beneficial for the performance as e.g. in

```
export KMP_AFFINITY=verbose,granularity=core,compact
```

4.5.2 Vectorization

To ensure a good performance on modern CPUs vectorization has to be enabled usually by enabling a sufficiently high optimization level with for instance `-O3`, `-Ofast`, `-fast`, etc, see Sect. 4.6.

The performance can be improved by choosing optimal branches in `CO5BOLD`, i.e., by determining the optimal values for

- `rhd_box_arrays01`: pointer or (better) allocatable arrays in the data structure “box”, see Sect. 4.4.1.4. The classical implementation with pointer arrays works in most (all?) cases and is the default. However, the implementation with allocatable arrays is a bit faster but causes runtime errors with several – current – compilers.
- `gasinter_101`: array treatment in the EOS routines, see Sect. 4.4.3.1.
- `gasinter_102`: pointer or (better) allocatable arrays in the data structure for the EOS tables, see Sect. 4.4.3.2.
- `opta_switch_101`: array treatment in the opacity routines, see Sect. 4.4.4.1.
- `rhd_hyd_entropyfix_p01`: loop with “if..then..else” or masks in `rhd_hyd_module.F90`, see Sect. 4.4.5.2.
- `rhd_hyd_upwind_p01`: loop with “if..then..else” or masks in `rhd_hyd_module.F90`, see Sect. 4.4.5.3.
- `rhd_roe1d_flux_101`: treatment of upwind direction in `rhd_hyd_module.F90`, see Sect. 4.4.5.4.
- `rhd_shortrad_operator_101`: operator version in `rhd_shortrad_module.F90`, see Sect. 4.4.7.10.
- `rhd_shortrad_operator_102`: way of operator inlining in `rhd_shortrad_module.F90`, see Sect. 4.4.7.11.
- `rhd_shortrad_dtauop_101`: operator version in `rhd_shortrad_module.F90`, see Sect. 4.4.7.12.
- `rhd_shortrad_dtauop_102`: way of operator inlining in `rhd_shortrad_module.F90`, see Sect. 4.4.7.13.
- `rhd_shortrad_dir1_101`: direct integration or transpose for nearly vertical rays in `rhd_shortrad_module.F90`, see Sect. 4.4.7.15.
- `MSrad_raytas`: loop type in `MSrad3D.F90`, see Sect. 4.4.7.20.

4.5.3 Cache usage

The user has to find optimum values for the parameters `n_hydcellsperchunk` (for the Roe and the HLLMHD solver module, see Sect. 7.1.8.9) and `n_viscellsperchunk` (for the tensor-viscosity module, see Sect. 7.1.11.17) to optimize the size of the chunk given to one thread per time. For the Roe solver of the hydrodynamics module, there exist also the optional parameters `n_hydcellsperchunk2` (see Sect. 7.1.9.1) and `n_hydcellsperchunk3` (see Sect. 7.1.9.2).

4.5.4 Inlining

Candidate routines for inlining are (i.e. they should be inlined if anyhow possible):

- file `rhd_hyd_module.F90`:
`rhd_hyd_avg, rhd_hyd_upwind, rhd_hyd_pred0, rhd_hyd_predm, rhd_hyd_predp,`
`rhd_hyd_alpha, rhd_hyd_constanteq, rhd_hyd_minmodeq, rhd_hyd_minmod,`
`rhd_hyd_vanleereq, rhd_hyd_vanleer, rhd_hyd_superbeeeq, rhd_hyd_superbee,`
`rhd_hyd_ppeq, rhd_hyd_pp, rhd_hyd_hdflux`
- file `rhd_lhdrad_module.F90`:
`rhd_rad3d_raylhd, rhd_rad3d_solve, rhd_rad3d_solveeq`
- file `rhd_shortrad_module.F90`:
`rhd_shortrad_operator, rhd_shortrad_dtauop.`

On some machines the Makefile generated by the configure script contains such a list explicitly. On others, one has to rely on automatic inlining (see the following sections).

4.5.5 Single versus double precision

Usually, the files containing the hydrodynamics and EOS data use 4 byte to represent a single number and most of the computations within CO5BOLD are performed in single precision – except for certain routines in e.g. MSrad or some dust modules.

To switch to double precision everywhere one has to deal with the binary files and force the transformation of single precision variables to double precision during the compilation. Compiling all CO5BOLD files with such a switch produces problems with the UIO modules: there would be a name conflict between the routines that usually deal with double precision reals and those that are written to deal with single precision reals and are now forced to pretend to be also a double precision version.

Therefore, one should compile the UIO routines and the rest with separate settings, e.g. for the Intel compiler:

```
./configure
make UIO
```

```
export F90_PREFLAGS="-r8 -fpconstant"
```

```
./configure
make
```

Code compiled in this way cannot read anymore single precision binary UIO files. However, there are no problems with the opacity tables (ASCII files) and *formatted* UIO files. To make existing single precision binary UIO files readable one could transform them to the formatted version with `uiocat` (see 6.2.6.3), e.g. like:

```
uiocat -f formatted -o rhd_ascii.sta rhd_binary.sta
```

New start models could be written in double precision binary UIO format directly using the `double_flag` in the IDL routine `rhd_wrboxdata.pro`.

For the EOS table `eos_mm00_15.eos` there exists a double precision binary version.

4.6 Specific machines & compilers

A (slightly outdated) overview about comparable switches of different compilers can be found in the “Compiler and tools tricks” by Arnaud Desitter (2008).

4.6.1 Cray: SV1

On `craSHi` in Kiel (a “CRAY SV1 20-32768 SN9542”, now out of service) CO5BOLD could use all 4 processors per board. The new configure script still includes a branch for this system even if has never been tested on that machine.

In some cases the non-default versions of loops in the CO5BOLD code vectorize better and are preferred over the standard ones:

- `-F`: Enable macro expansion
- `-Otask1`: Parallelization: Enable tasking (in this case OpenMP).
- `-Oinline3`: Optimization: enable (high level) of inlining.
- `-Ovector3 -Oscalar3`: General optimization
- `-Drhd_hyd_roe1d_101=1`: Optimization: Choose non-standard set of routines for Roe solver. See Sect. 4.4.8.2.
- `-Drhd_hyd_entropyfix_p01=1`: Optimization: version with masks (weights). See Sect. 4.4.5.2
- `-Drhd_hyd_upwind_p01=1`: Optimization: version with masks (weights).
- `-Drhd_shortrad_operator_101=2`: Optimization: short characteristics operator with masks (weights).
- `-Drhd_shortrad_dir_102=1`: Optimization: OMP PARALLEL statement outside of outer loop in `rhd_shortrad_dirX`.

4.6.2 Compaq: alpha

The UIO module allows the reading and writing of files in `little_endian` and `big_endian` format. In 4.4.2 the preprocessor switches are listed, that control the modern – single – version `uio_mac_module.F90` of this file.

- `-assume byterecl`: Necessary for the UIO routines: specify that the length of a record is measured in bytes (and not in words).
- `-cpp`: invoke the preprocessor on all source files.
- `-inline speed -V`: Force automatic inlining, optimized for speed.
- `-O4`: General optimization.
- `-Drhd_hyd_roe1d_101=0`: Optimization: Choose standard set of routines for Roe solver. See Sect. 4.4.8.2.
- `-DMSrad_raytas=0`: Optimization: choose default version of loop in SUBROUTINE `raytas` in file `MSrad3D.F90`. See Sect. 4.4.7.20.

4.6.3 Hewlett-Packard: V2500

The 12-processor machine “zeipel” from Hewlett-Packard was a “V2500 PA 2.0” system. There was some success to force the compiler to accept the OpenMP directives in CO5BOLD. Yet, when running on several processors, only some routines (e.g. `rhd_shortrad_dirsimple1`) in CO5BOLD could benefit while others (`rhd_shortrad_dirsimple2`, `rhd_shortrad_dirsimple3`) were significantly slower than on one processor. In addition, the single-processor performance was not very good, partly because the achievable optimization level is not very high.

Some macros, which seemed to be necessary:

- `+U77`: Link proper library to make the machine understand e.g. `call flush(6)`.

- `+cpp=yes`: Switch on the C preprocessor. Note that all Fortran90 files have to end with “.f90”. The “.F90” suffix does not seem to work.
- `+0parallel +0openmp +0noautopar`: Try to enable parallelization with OpenMP directives, disable auto-parallelization.
- `+0noinline`: Disables inlining. This can simplify things. With a proper choice of routine versions inlining is not really necessary anymore.
- `+03 +0limit`: General optimization with limited resource usage during compilation. Some modules should only be compiled with `+02`, others compile even with `+03 +0nolimit`.

The UIO modules and the string handling module should be compiled in debug mode. A proposed compiling sequence is (MSrad does not compile; all other modules are activated):

```
export F90_LHDRAD=1
export F90_MSRAD=0
export F90_SHORTRAD=1
export F90_DUST=1
export F90_MHD=1
export F90_PARALLEL=openmp
```

```
export F90_DEBUG=1
./configure
make UIO STR
```

```
export F90_DEBUG=0
./configure
make
```

4.6.4 Hewlett-Packard: Itanium 2

The 2-processor system “gunnar” from Hewlett-Packard is a dual Itanium 2 machine with two 900MHz ia64 CPU modules, 4GB of RAM and 70GB user disk space.

The single-processor performance of CO5BOLD is very good. On two processor the code runs even faster but just stops after a few time steps. The number of time steps varies even for simulations with the very same start model and parameter file. Therefore, OpenMP should not be activated currently.

The compiler settings are somewhat similar to the settings of the HP V2500 system in Section 4.6.3:

- `+U77`: Link proper library to make the machine understand e.g. `call flush(6)`.
- `+cpp=yes`: Switch on the C preprocessor. Note that all Fortran90 files have to end with “.f90”. The “.F90” suffix does not seem to work.
- `+0fast`: High optimization level. And `+0faster` is even higher.
- `+0openmp +0noautopar`: Try to enable parallelization with OpenMP directives, disable auto-parallelization. The code compiles and runs fast but crashes after a few time steps.

A proposed compiling sequence is (LHDrad, DUST, MHD do not compile):

```
export F90_MSRAD=1
export F90_SHORTRAD=1
./configure
make
```

4.6.5 Hitachi SR8000

Some information about the Hitachi compiler is here.

In 4.4.2 the preprocessor switches are listed, that control the modern – single – version `uio_mac_module.F90`.

- `-cont199`: Up to 199 continuation lines can be interpreted (otherwise not more than 39 continuation lines are accepted).
- `-limit`: Limits the amount of time and memory for compilation.
- `-opt=ss`: use highest possible optimization level.
- `-nopredicate`: this option switches off a sub-option activated by `opt=ss`. It is necessary to disable the `-predicate` option because the code crashes otherwise (segmentation violation). The switch must appear *after* setting `-opt=ss`.
- `-pvfunc=2`: References the pseudo-vectorizing mathematical function and applies the temporary array to reference the pseudo-vectorizing mathematical function.
- `-omp -parallel=1`: parallelize based on OpenMP directives only.
- `-procnum=8`: generate code for 8 processors on one node.
- `-orphaned=1`: Checks if the regions sequentially executed contain orphaned directives during runtime when `PROCNUM=8` is specified. If a sequentially executed region contains an orphaned directive, the system outputs a message and terminates the program.
- `-nestcheck=1`: Checks for nesting errors in parallel regions. If a parallel region is nested, the system returns an error and terminates the program. *Without this option, the code aborts with an error message, indicating illegal nesting. Compiler bug?*
- `-pmpar`: Collects the performance monitor information for each parallelization unit.
- `-pmfunc`: Collects the performance monitor information for each procedure.
- `-Drhd_hyd_roe1d_101=1`: Optimization: Choose non-standard set of routines for Roe solver. See Sect. 4.4.8.2.
- `-DMSrad_raytas=0`: Optimization: choose default version of loop in SUBROUTINE `raytas` in file `MSrad3D.F90`. See Sect. 4.4.7.20.
- **Important note:** The UIO routines need in addition the compiler option `-subchk`: Array bound checking. Without this checking option, some UIO routines are not working properly (compiler bug?).

A proposed compiling sequence is (only default modules activated):

```
export F90_PREFLAGS="-subchk"
./configure
make UIO
```

```
export F90_PREFLAGS=
./configure
make
```

Performance tests on hwwsr8k

Some tests have been performed on the machine `hwwsr8k` at HLR Stuttgart in order to determine the optimum chunk sizes which are set by the parameters `n_hydcellsperchunk` and `n_visccellsperchunk`

Performance test on Hitachi SR8000 at HLRS

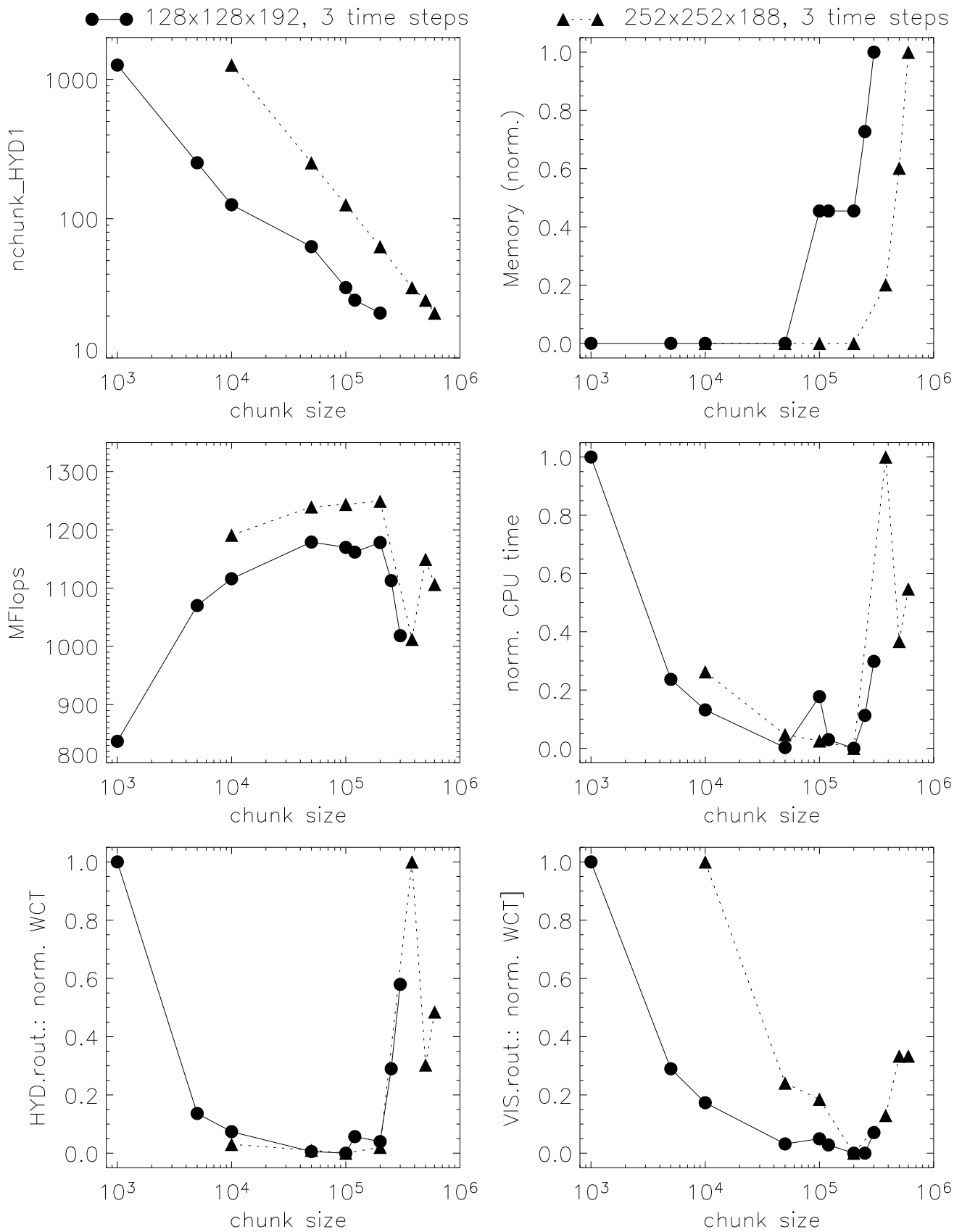


Figure 4.1: Performance tests on Hitachi SR8000 at HLR Stuttgart. For models with $128 \times 128 \times 192$ and $252 \times 252 \times 188$ grid cells different values for the hydrodynamics and viscosity chunk size parameters were used. See text for more details.

(see Sect. 7.1.8.9 and Sect. 7.1.11.17). Two different models have been used, one consisting of 128x128x192 grid cells, the other of 252x252x188, respectively. Grey radiative transfer has been performed with the MSrad module. Different values for the chunk size(s) have been assumed where the hydrodynamics and the viscosity parameter were set equal. In all cases three time steps have been computed. The results are shown in Fig. 4.1. The number of resulting chunks for step HYD1 (the values for HYD2, HYD3, and VIS are very similar), total memory, performance, and the wall clock duration of the hydrodynamics and the viscosity routines are shown as functions of the chunk size parameter(s). Clearly, the number of chunks decreases towards larger chunk sizes whereas the required memory increases – in particular for very large chunk size values. Moreover, performance and CPU time can be optimized by choosing the right parameter values. Interestingly, the optimum chunk size is different for hydrodynamics and viscosity. Based on these tests, a larger value seems to be preferable for the viscosity (`n_viscellsperchunk`). In the case of the smaller model, 50000 seems to be fine for the hydrodynamics whereas the optimum viscosity chunk size is 200000. This difference explains the double-peaked structure of performance and CPU time. Note that the optimum values do not only depend on the architecture used but also on the dimensions of the model. We recommend to test some chunk size values since it might lead to a higher performance.

4.6.6 IBM

Useful links:

IBM compiler documentation: “IBM: XL Fortran”, especially “IBM AIX compiler information center”. Particularly useful hints: “Porting Programs from the Crays to the SP”.

The compiler to be used for OpenMP runs is called with `xlf90_r` which “binds the object files to the thread-safe components” (IBM documentation). For scalar code `xlf90` might be sufficient.

Important switches are:

- `-qsuffix=f=f90 -qsuffix=cpp=F90`: To tell the compiler about the existence of Fortran90 and to enable the preprocessing for files with suffix “F90”.
- `-qextname=flush:etime`: Append underscore to both routine names. In 4.4.2 the preprocessor switches are listed, that control the modern – single – version `uio_mac_module.F90`.
- `-WF, -Drhd_r03`: The compiler does not send switches starting with `-D` to the preprocessor but tries to interpret them itself – unlike all other compilers. Therefore, each switch (e.g. `-Drhd_r03`) has to “escaped” with `-WF`, (as e.g. `-WF, -Drhd_r03`).
- `-q64`: Activate the 64-bit mode. In the default 32-bit mode a very small model (with total memory requirements far below the 2 GByte limit) might run. However, experienced IBM users might experiment instead with the compiler switches `-bmaxstack`, `-bmaxdata`, and `-qsmallstack`, with the UNIX commands `limit` or `ulimit`, or with the settings in the header of the batch script...
- `-O3`: Choose optimization level. Higher levels that involve interprocedural analysis cause the compiler to stop with an error message.
- `-qarch=auto -qtune=auto -qcache=auto`: To allow optimization specific for the local machine (default in the configure script). “Cross compilation” can be activated e.g. with `-qarch=pwr3 -qtune=pwr3` or `-qarch=pwr4 -qtune=pwr4` (by setting an environment variable, e.g. `F90_MACHINE="(pwr3)"` before calling `configure`).
- `-Q -Q+...`: To activate inlining and to specify the list of routines that should be inlined (see Sect. 4.5.4).
- `-qsmp=noauto:omp`: Parallelization: OpenMP directives are activated.

A job script `rhd.job` on the Loadleveler batch system on `io.cines.fr` can be submitted with

```
llsubmit rhd.job
```

The jobs in the queue for user `testuser` can be checked with

```
llq -u testuser
```

A job with ID `n34.56789.0` can be cancelled with

```
llcancel n34.56789.0
```

4.6.7 Linux: PGI compiler

Under Linux the compiler of the Portland Group was first used to compile CO5BOLD. It is called with `pgf90`.

Important switches are:

- `-byteswapio`: With this flag set, binary files in `big_endian` format (the standard for UIO files) are automatically transformed to `little_endian` and vice versa.
- `-fast`: General optimization flag to choose (close to) optimum optimization for local machine.
- `-Mvect=sse`: Optimization: Allow Pentium III vector commands.
- `-Mcache_align`: Optimization: Align some data object on cache-line boundaries.
- `-fastsse`: From compiler version 4.0 on, this option can be used instead of the three previous ones. It contains and supersedes them.
- `-Minline=...`: Optimization: the routines that should be inlined are listed in Sect. 4.5.4.
- `-DMSrad_raytas=2`: Optimization: choose non-default version of loop in SUBROUTINE `raytas` in file `MSrad3D.F90`. See Sect. 4.4.7.20.
- `-Drhd_hyd_roe1d_101=0`: Optimization: choose standard set of routines for Roe solver. See Sect. 4.4.8.2.
- `-Drhd_shortrad_operator_102=1`: Optimization: use the “manually inlined version” of the short characteristics operator.
- `-Drhd_shortrad_dtauop_102=1`: Optimization: use the “manually inlined version” of the optical coupling operator.

4.6.8 Linux: Intel compiler

The compiler is called with `ifort` (`ifc` on older compiler versions).

With Version 7.0 and 7.1 of the Intel compiler (version 15.0 here) CO5BOLD compiled (with tricks, see below). Version 8.0 still caused trouble. With version 9.1 (and up) everything compiles, with some glitches for certain version every now and then.

The native binary format on Intel machines is `little_endian`. With

```
export F_UFMTENDIAN=big
```

(to be set at runtime after compilation before running CO5BOLD) the default can be changed to `big_endian`. In 4.4.2 the preprocessor switches are listed, that control the modern – single – version `uio_mac_module.F90`. Important switches are:

- `-fast`: Optimization: choose a general optimization (close to) optimal for the local machine. It actually activates a number of other optimization flags, that might change with compiler version. This option currently is *not recommended* for CO5BOLD because the too aggressive optimization causes runtime errors (the offending sub flag appears to be `no-prec-div`). Instead, the – working – sub flags are specified individually.

- **-ip:** Optimization:
activate interprocedural optimization within each source file. This enables some inlining.
- **-ipo:** Optimization:
enable interprocedural optimization between files. The compiler makes a first step with a pre-compilation and syntax check for each source file and then finishes the compilation and optimization of *all* source files together in a second – time-consuming – step. It allows some global optimizations and appears to have at least no adverse effects – in all recent compiler versions.
- **-O3:** Optimization:
activate a generally high level of optimization.
- **-xHost:** Optimization for hardware:
optimize for the architecture of the compiling host. This flag is recommended, although there are a few issues: On AMD machines this might work less than perfect, because the features of the processors might now be properly recognized: check it! Compiling with this option on a new machine with a recent set of vector instructions will likely generate code that will not run on older machines. In the – rather uncommon – case that the CO5BOLD executable is distributed a combination of other flags has to be used that ensures that the code runs in an optimal way on a range of machines, see below and see the manual.
- **-tpp6 -xK:** Optimization for hardware (old):
optimize especially for Pentium III (and Athlon, includes SSE vector commands).
- **-tpp7 -xW:** Optimization for hardware (old):
optimize especially for Pentium IV (includes SSE2 vector commands).
- **-xP:** Optimization for hardware (old):
optimize especially for Core 2 Duo and similar architectures.
- **-xSSE4.2:** Optimization for hardware:
Optimize for machines with SSE 4.2 vector instructions.
- **-xAVX:** Optimization for hardware:
Optimize for machines with AVX vector instructions. By now, there are several – more advanced – versions of this.
- **-Drhd_box_arrays01=1:** Optimization:
activate a faster way of handling arrays in structures (see Sect. 4.4.1.4). That works e.g. in version 12.1 of the compiler but not in more recent ones.
- **-DMSrad_raytas=2:** Optimization:
choose non-default version of loop in SUBROUTINE `raytas` in file `MSrad3D.F90`. See Sect. 4.4.7.20.
- **-Drhd_shortrad_dir1_l01=1:** Optimization:
Transpose arrays and use routine `rhd_shortrad_dir3` for rays in x1 direction. See Sect. 4.4.7.15.
- **-openmp:** Parallelization:
activate OpenMP directives. Note that for compiler versions before 9.0 the UIO routines should be compiled without OpenMP support (even if they do not contain any OpenMP directives themselves).
- **-static:** Linking:
prevent linking with shared libraries. This is usually part of **-fast** and does not seem to have any positive effect on the performance.
- **-static-intel:** Linking:
link Intel-provided libraries statically. This option is recommended. This has the nice effect that the executable now can be safely transferred from the compile node – where the Intel libraries are available – to any of the compute nodes – where the Intel libraries should be available, but aren't.

- `-assume byterecl`: I/O:
specify that the length of a record is measured in bytes (and not in words). That is necessary for the UIO routines.
- `-Duiio_switch_system_l01=1 -Duiio_switch_native_l01=1 -Duiio_switch_ieeebe_l01=1 -Duiio_switch_ieeele_l01=1 -Duiio_switch_ieee_l01=1 -Duiio_switch_open_l01=1`: I/O:
activate the appropriate set of UIO switches.
- `-Dtiming_c_range=15 -Dtiming_r_type=7`: General:
configure the timing routines.
- `-r8 -fpconstant`: General:
force compilation in double precision (see 4.5.5). In general, single precision is sufficient. However, e.g. for very cool objects with small-Mach-number flows, the general activation of double-precision arithmetic is necessary.
- `-fpp`: General:
activate the preprocessor.
- `-W0`: General:
suppress warning messages.

On Macintosh machines the typical optimization flags are `-O3 -no-prec-div -fno-alias -ip`. A big problem is the tiny stack size on those machines: large arrays taken from the stack should be avoided. For the SHORTRad module, this can be achieved by setting `-Drhd_arrays_l01=2` during compilation. In addition, relatively small chunk sizes should be specified in `rh.d.par`, see Sect. 7.1.8.9 and Sect. 7.1.11.17.

Using the Intel compiler (before version 9.1) there was a problem with the UIO modules when OpenMP is activated. This was a bit weird because the UIO modules do not contain any OpenMP directives. However, this means that OpenMP can be safely deactivated for these modules. A proposed compiling sequence was:

```
export F90_COMPILER=ifort
export F90_MSRAD=1

export F90_PARALLEL=scalar
./configure
make UIO

export F90_PARALLEL=openmp
./configure
make
```

With more recent compiler version, this is much simpler. A realistic example (with several modules activated, with an explicit choice if optimization flags) might look like:

```
export F90_COMPILER=ifort
export F90_MSRAD=1
export F90_SHORTRAD=1
export F90_MHD=1
export F90_PARALLEL=openmp
export F90_OPTIMIZE="-ipo -O3 -xHost -static-intel -W0 -Drhd_box_arrays01=1"
export F90_POSTFLAGS="-Drhd_hyd_gravcorr_p01=6 -Dtiming_c_range=15 -Dtiming_r_type=7"

./configure -c
make
```

For OpenMP (see Sect. 4.5.1), the number of threads can be set for instance with

```
export OMP_NUM_THREADS=16
```

for a machine with 16 threads (e.g., 2 processors, 4 cores per processor, 2 threads per core). With

```
export OMP_NUM_THREADS='cat /proc/cpuinfo | grep "processor.*:" | wc -l'
```

the number of OpenMP threads is determined from the number of – logical – processors. Experimenting with the scheduling, e.g. by setting

```
export OMP_SCHEDULE=DYNAMIC,1
```

or

```
export OMP_SCHEDULE=GUIDED,2
```

or (most often just)

```
export OMP_SCHEDULE=STATIC
```

might improve the performance (see Sect. 4.5.1). The last two OpenMP variables are recognized by several compilers. However, there are Intel-specific ones.

In some cases it was helpful to set

```
export LD_ASSUME_KERNEL=2.4.19
```

when encountering problems with OpenMP. However, that seems not to be necessary with recent compiler versions. Still, often the stack memory per thread is too small, which can be increased e.g. with

```
export KMP_STACKSIZE=300000000
```

or

```
export OMP_STACKSIZE=300M
```

To optimize the performance, particularly on many-core systems, the thread affinity (see “Intel Thread Affinity Interface”) can be specified at runtime (i.e., after compilation but before running the code) e.g. with

```
export KMP_AFFINITY=verbose,granularity=core,compact
```

4.6.9 Linux: PathScale compiler

Some experiments with the PathScale compiler have been made. It is called with `pathf90`. The result is not entirely satisfying, yet.

Important switches are:

- `-byteswapio`: With this flag set, binary files in `big_endian` format (the standard for UIO files) are automatically transformed to `little_endian` and vice versa.
- `-O3`: General optimization flag. More aggressive optimization can be activated with `-Ofast` or `-Ofast -ipa`.
- `-mp`: Parallelization: OpenMP directives are activated.

4.6.10 Linux: GNU g95 compiler

One of the available GNU Fortran compilers is the g95 compiler with the g95 home page. It is called with `g95`.

Important switches are:

- `-fendian=big`: With this flag set, binary files in `big_endian` format (the standard for UIO files) are automatically transformed to `little_endian` and vice versa.
- `-O3`: General optimization flag.

In 4.4.2 the preprocessor switches are listed, that control the modern – single – version `uio_mac_module.F90`.

OpenMP is not there yet. The binary I/O format (“unformatted”) is incompatible with the one used before in CO5BOLD: no existing binary UIO files can be read.

4.6.11 Linux: GNU gfortran compiler

The Fortran compiler of the GNU project is called with `gfortran`. See this discussion for some recommendations of options. There is a full list of Optimize Options available. Important switches are:

- `-fconvert=big-endian -frecord-marker=4`: With this flag set, binary files in `big_endian` format (the standard for UIO files) are automatically transformed to `little_endian` and vice versa. In addition, the old 32-bit record marker convention is maintained and existing UIO files can be read.
- `-O3`: General optimization flag.
- `-fopenmp`: Activates the OpenMP directives.
- `-fdefault-real-8 -fdefault-double-8`: Useful to force compilation in double precision (see 4.5.5).

In 4.4.2 the preprocessor switches are listed that control the modern – single – version `uio_mac_module.F90` of the UIO module.

The scalar code is slower than code compiled e.g. with the Intel compiler (see Sect. 4.6.8). However, the factor is not prohibitive. For not too demanding runs the `gfortran` compiler can be useful.

4.6.12 NEC SX-5, SX-6, SX-8

First attempts to compile CO5BOLD on neSH at the Rechenzentrum Kiel and on hwwsx5 at HLR Stuttgart:

An environment variable has to be set to `F_RECLUNIT=BYTE` (before execution of a program) to enable UIO to compute proper record lengths. The cross compiler (on sunsrv or crossi) is called with `sxf90`. Thus, the environment variable `F90_COMPILER=sx90` has to be set before running the configure script.

No optimized version of CO5BOLD has been achieved yet.

Some maybe useful switches are

- `sx5`: generate instructions for SX-5. Use `sx6` or `sx8` when appropriate.
- `C vopt`: normal optimization in vector mode
- `-Wf'-M noflunf -M noinv -M noinexact -M setall'`: suppress some exceptions
- `-P openmp`: parallelization with OpenMP
- `-Ep`: call cpp preprocessor
- `-pi exp=...`: inlining of a list of routines (see Sect. 4.5.4)

- `-dw -float0` (no special environment variable): use internally and in files the 4 Byte `big_endian` format

For the SX-5 the compiler flags in the configure script are

```
F90FLAGS="-C hopt -sx5 -dw -float0
-Wf'-L nostdout -L fmtlist -L inclist -L mrgmsg -L transform -M noflunf
-M noinv -M noinexact -M setall'
-pi exp=rhd_shortrad_operator exp=rhd_shortrad_dtauop $F90MODULES
$F90TIME -DMSrad_raytas=1"
```

For the SX-8 the configure scripts gives the output

```
sxf90 -EP -P openmp -Chopt -sx8 -Wl'-Z 8G -m' -dw -float0
-Wf'-L nostdout -L fmtlist map summary transform -L inclist
-L mrgmsg -M noflunf -M noinv -M noinexact -M setall'
-Drhd_r03 -Drhd_shortrad_step_t01 -Drhd_shortrad_formal_t01 -DMSrad_raytas=1
-Drhd_hyd_entropyfix_p01=1 -Drhd_hyd_upwind_p01=1 -Drhd_hyd_roe1d_l01=1 -Dgasinter_l01=2
```

4.6.13 SGI: Origin

CO5BOLD has been compiled and tested on up to 8 processors on the SGI 2000 machine at TAC in Copenhagen and the SGI 3800 machine at the NSC in Linköping. The code was used on the UKAFF machines (see Sect. 4.6.14) and the computers at CINES.

See e.g. the excellent SGI Fortran90 manual (or here). Information about the CINES machines can be found under CINES.

Important switches are:

- `-macro_expand`: Enable macro expansion
- `-mp`: Enable parallelization with OpenMP directives
- `-INLINE:aggressive=0N -INLINE:list -INLINE:preempt=0N`: General keywords for inlining
- `-INLINE:must=...`: Optimization: routines that should be inlined (see Sect. 4.5.4).
- `-Ofast -OPT:0limit=0`: General optimization. On older compiler versions `-03` was the achievable optimum.
- `-IPA:plimit=5500`: Even more optimization. This option requires lots of memory (> 1 GByte). To get it it might be necessary to ask for more than one processor for the compilation (especially on the CINES machines).
- `-CG:longbranch_limit=60000`: This switch limits needed compiler resources. It is suggested by the compiler (on the CINES machines) itself.
- `-Drhd_roe1d_step_101=1`: Slight performance improvement

4.6.14 SGI: Origin 2000/3800 at UKAFF

CO5BOLD has been also compiled and tested on up to 22 processors on the machines of the UK Astrophysical Fluids Facility (UKAFF) in Leicester, England. UKAFF operates two machines: an SGI Origin 3800 with 128 processors (named “ukaff”), and an older SGI Origin 2000 with 22 processors (named “grand”) which is mainly used for development and test purposes. Both machines are binary compatible. At the time of testing (April 2003) the SGI MIPSpro Compilers (Version 7.4) was installed.

Most of the compiler switches given in the previous section were used, except for the following modifications which either gave empirically a better performance or were recommended by the UKAFF *Hints for users*:

- `-Ofast`: Replaces `-O3`, gave better performance
- `-LN0:cs1=32k:ls1=32:cs2=8M:ls2=128`: Explicit cache architecture added

The option `-Ofast` is now the default selected by the configure script for all SGIs with IP35 architecture. The cache architecture settings are activated for the UKAFF machines only.

A glitch in the system libraries made it necessary to add a work-around to the source code (file `rhdf.F90`). A “bus error” occurred whenever the system routine “flush” was trying to flush an empty file buffer. The temporary work-around was simply to add a write statement before every call of “flush”. This made the log-file look less nice but did the job. Now, the few “flush” statements that are not necessarily preceded by a write statement are removed.

The main goal was to investigate the scaling of the performance of CO5BOLD with the number of processors. This was done only for the MSrad module, considering local surface convection models. Two model sizes were tested: a small one with 125x125x81 grid points employing non-grey radiative transfer (4 frequency bands), and a large one with 315x315x81 grid points employing grey radiative transfer. Rather short runs of 10 (small model) and 3 (large model) time steps were performed. Even for the large model the memory demand was ca. 800Mb, which is very modest considering that every sub-node of the machine — consisting of 4 processors — has 2Gb of memory.

The results are summarized in the following three figures. The black lines give the scaling of the total time, the green lines the scaling of the time needed by the hydrodynamics routines, and the red lines the scaling of the radiative transfer routines. The scaling is presented as the increase of processing time per processors as the problem is distributed among more and more processors. The times are normalized to the time that is used in a scalar, i.e. single processor setup. Ideally, one would like a constant behavior which stays close to one.

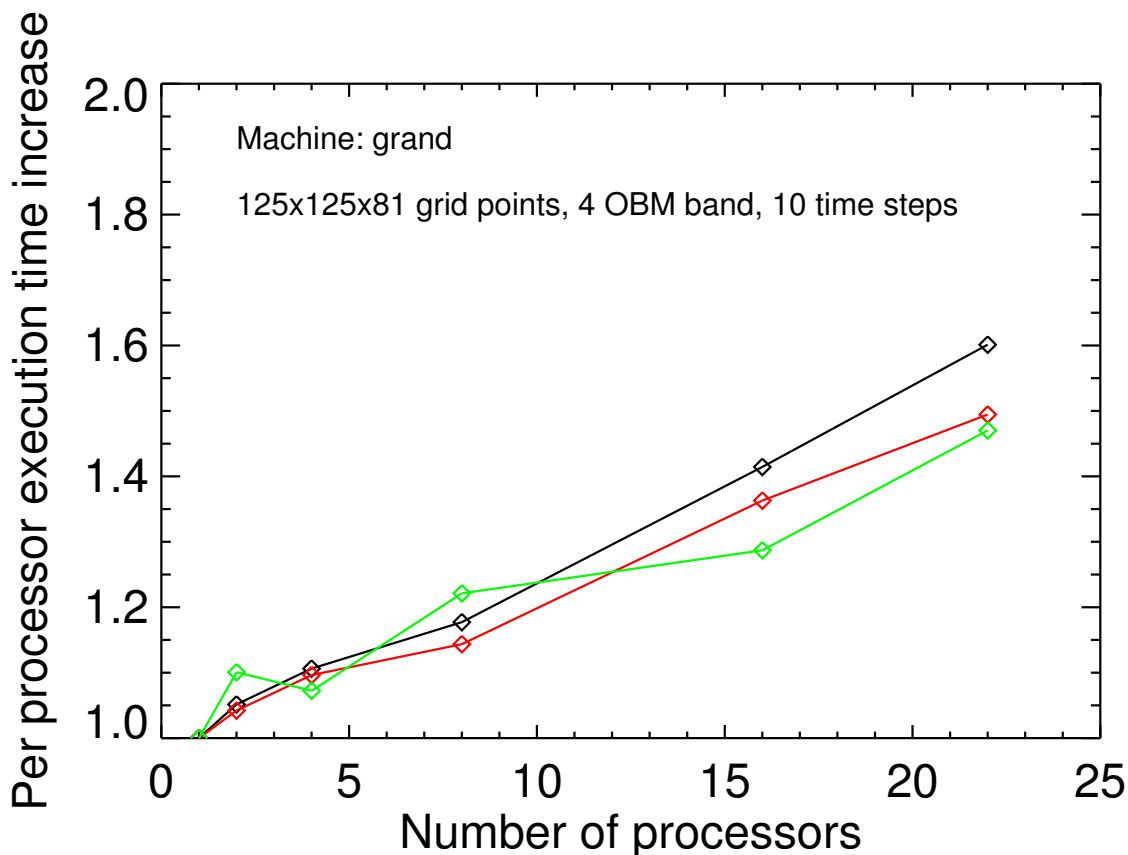


Figure 4.2: UKAFF: machine: grand; small model

The perhaps most interesting result is that the speedup on “ukaff” is about 11 for the large model on 16 processors. Perhaps not ideal, but within the range of practical interest. In general, the hydrodynamics

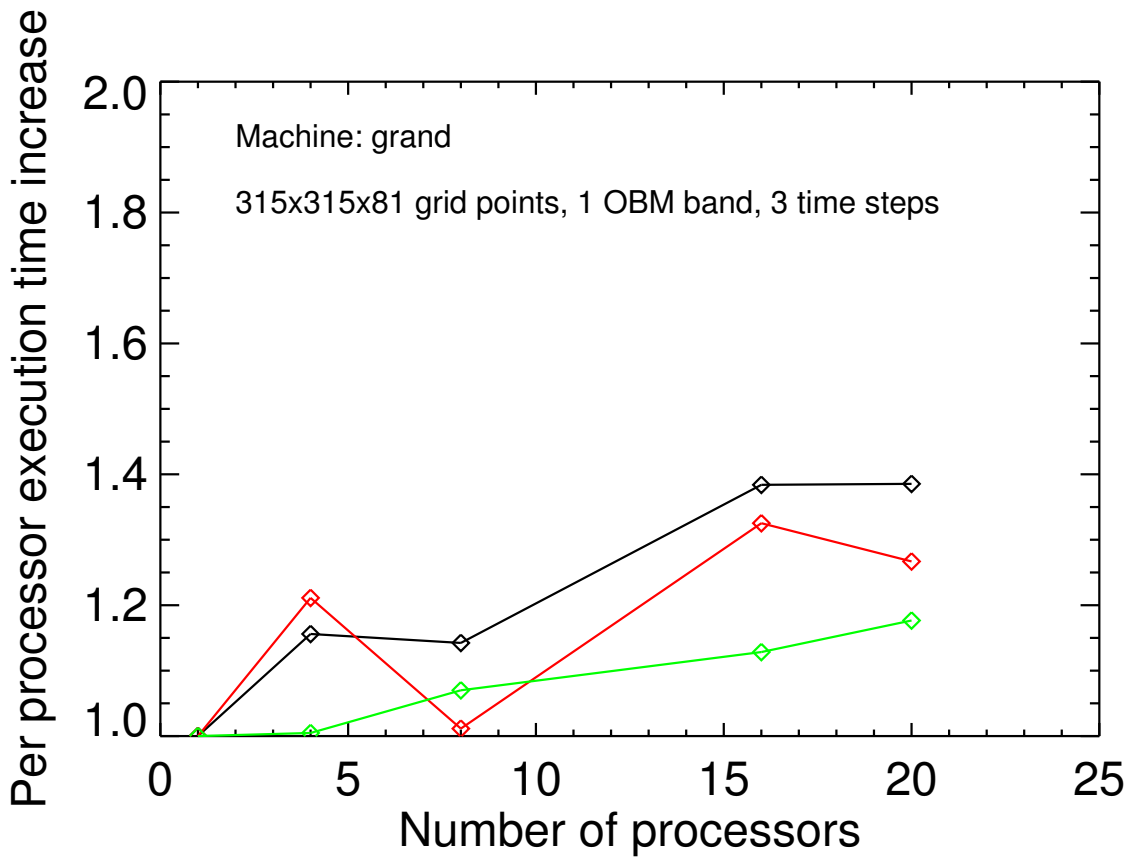


Figure 4.3: UKAFF: machine: grand; large model

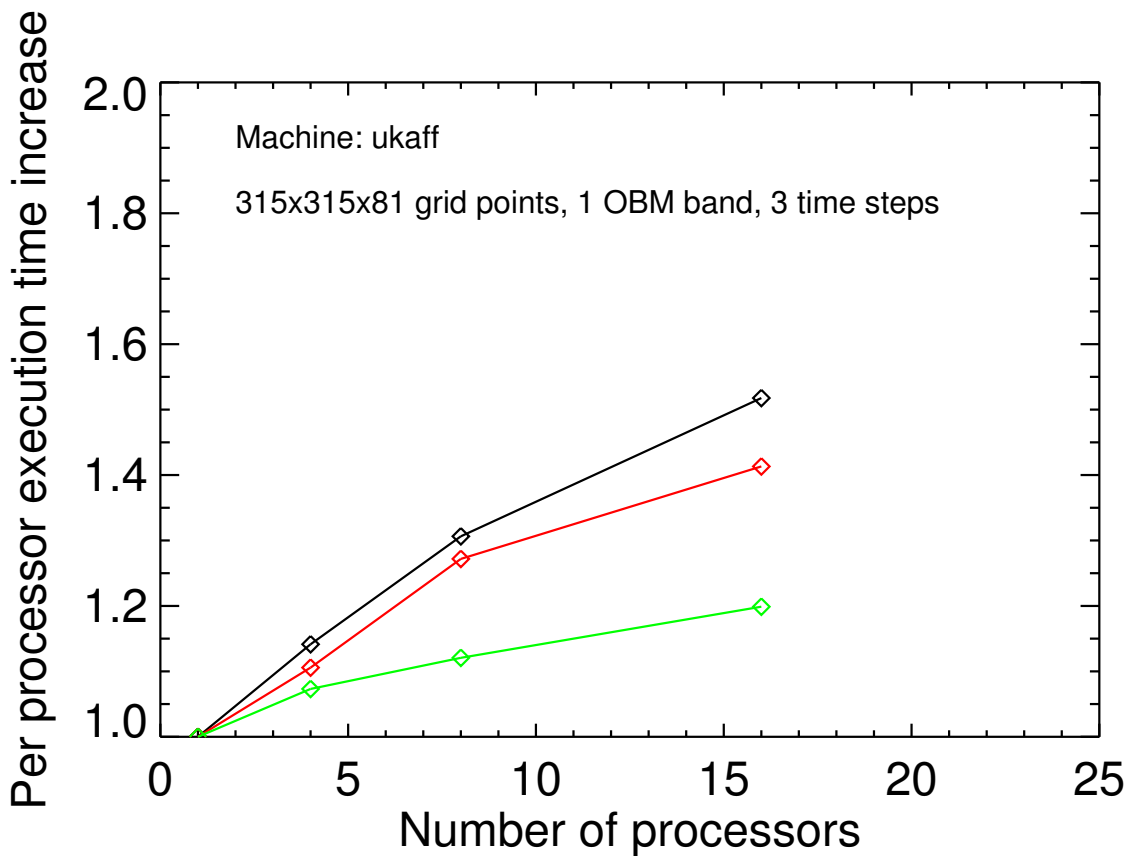


Figure 4.4: UKAFF: machine: ukaff; large model

routines scale more favorably than the radiation routines. This is perhaps simply related to the fact that in explicit hydrodynamics communication is restricted to neighboring grid cells.

For those wondering: the black curves do not lie between the red and green curve since more components than just radiation and hydrodynamics add up to the total time. Furthermore, the normalization of the execution times given by CO5BOLD is not exact.

4.6.15 Sun: SunFire

CO5BOLD has been used on the SunFire machines “fire1”, “fire2”, and “fire3” in Uppsala with compiler version “Sun WorkShop 6 update 2 Fortran 95 6.2 2001/05/15” and later. An older version was not able to compile CO5BOLD properly.

Important switches are:

- `-openmp`: Enable OpenMP.
- `-fast -xvector=yes/no`: General optimization. On the Sun the `-fast` option switches on more or less all optimization features of the compiler. That works reasonable well. However, during the compilation of `gasinter_routines.f90` (and only there) the switch `-xvector=no` is required! This is done automatically in the Makefile.
- `-inline=...`: Optimization: routines that should be inlined: see Sect. 4.5.4.
- `-DMSrad_raytas=2`: Optimization: choose non-default version of loop in SUBROUTINE `raytas` in file `MSrad3D.F90`. See Sect. 4.4.7.20.
- `-Drhd_shortrad_formal_l01=1`: Optimization: split loop for $\exp(-dt\tau)$ computation into two loops. See Sect. 4.4.7.14.
- `-Drhd_shortrad_dir1_l01=1`: Optimization: Transpose arrays and use routine `rhd_shortrad_dir3` for rays in x1 direction. See Sect. 4.4.7.15.
- `-Drhd_hyd_entropyfix_p01=1`: Optimization: version with masks (weights). See Sect. 4.4.5.2.
- `-xarch=native64`: Produces 64-bit code optimized for local machine.

Chapter 5

Programmer's guide

5.1 General code organization

The directory structure is shown in Tab. 3.1. In the master directory `for` (for “Fortran”), there are a number of sub directories for groups of files. Most of the files are located somewhere below `for/hd`. Exceptions are files with modules that might be used outside CO5OLD, like the UIO, EOS, or OPTA routines. A master group (as e.g., `for/hd` or `for/uio`) can have a number of sub-group directories (as e.g., `for/hd/rhd` and `for/hd/mhd` or just one (as e.g., `for/uio/f90`), that contain the actual Fortran files.

Although a few ancient subroutines still use the FORTRAN fixed format, for newer code parts, the Fortran free format is strongly recommended.

Subroutines, functions, type definitions, global data, etc. should be collected in modules. Typically, there is one module per file – with some exceptions.

Standard Fortran statements and commands (`if`, `then`, `subroutine`,...) is written in lower case. Preprocessor directives (e.g., `#ifdef`) are written in lower case. OpenMP declarations and compiler directives are written in upper case. Names of variables, subroutines, and modules can use CamelCase (and underscores).

Implicit type declarations should be avoided, although there is still the tendency to start integer variables with `i`, `m`, or `n`. Instead, all type declarations should be preceded by

```
implicit none
```

which enforces an explicit type declaration of all variables.

All quantities are measured in cgs units.

5.2 Indentation and spaces

5.2.1 General layout and indentation recommendations

Lines should be limited to a maximum of 101 characters, if anyhow possible. That ensures that an editor window with this width does not wrap or cut lines. The version of the CO5BOLD manual that includes the source code cannot display much more than 100 characters in a line.

The code should be carefully indented. Each indentation level shifts the text by 2 spaces to the right. Tabs should not be used. Special care should be taken for the indentation and alignment of stencil operations of assignments and equations (see below). To have sufficient “screen estate” left for these, the recommended indentation amount per level (2 spaces) is rather small. For the same reason, module and subroutine headers should not be indented, even if logically a contained subroutine is a level below the corresponding module.

5.2.2 Alignment of assignments and equations

Indentation and alignment of stencil operations are important, as in

```
! --- Save original values into local copies ---  
rho=model%rho
```

```
ei =model%ei
v1 =model%v1
```

OR

```
eip_ll=ei(i1-2,i2,i3) + P(i1-2,i2,i3)/rho(i1-2,i2,i3)
eip_l =ei(i1-1,i2,i3) + P(i1-1,i2,i3)/rho(i1-1,i2,i3)
eip_r =ei(i1 ,i2,i3) + P(i1 ,i2,i3)/rho(i1 ,i2,i3)
eip_rr=ei(i1+1,i2,i3) + P(i1+1,i2,i3)/rho(i1+1,i2,i3)
```

OR

```
! --- Fill buffer zones of temperature array ---
T(m1-1 , m2 :n2 , m3 :n3 )=T(m1 , m2 :n2 , m3 :n3 )
T( n1+1, m2 :n2 , m3 :n3 )=T( n1 , m2 :n2 , m3 :n3 )
T(m1-1:n1+1, m2-1 , m3 :n3 )=T(m1-1:n1+1, m2 , m3 :n3 )
T(m1-1:n1+1, n2+1, m3 :n3 )=T(m1-1:n1+1, n2 , m3 :n3 )
T(m1-1:n1+1, m2-1:n2+1, m3-1 )=T(m1-1:n1+1, m2-1:n2+1, m3 )
T(m1-1:n1+1, m2-1:n2+1, n3+1)=T(m1-1:n1+1, m2-1:n2+1, n3 )
```

In this case, blanks around the “=” sign might be appropriate. Other examples are

```
lambda_til_mi(i1,i2,i3)=(1.0-mask_up_mi) * (v1(i1-1,i2,i3)-cs(i1-1,i2,i3)) + &
mask_up_mi * (v1(i1 ,i2,i3)-cs(i1 ,i2,i3))
```

OR

```
! --- Delete all global boxes ---
if (rhd_box_Exist(modelVis)) call rhd_box_Delete(modelVis)
if (rhd_box_Exist(modelB )) call rhd_box_Delete(modelB )
if (rhd_box_Exist(modelA )) call rhd_box_Delete(modelA )
```

Properly aligned assignments facilitate the understanding and debugging enormously.

In more complex assignments, corresponding brackets should be carefully positioned. However, different styles and conventions can be used, as e.g.,

```
model%v1(i1,i2,i3)=model%v1(i1,i2,i3) - &
( dtimeoverrhodx1 * (flux_rhov11(i1+1, i2 , i3 ) - &
flux_rhov11(i1 , i2 , i3 )) + &
dtimeoverrhodx3 * (flux_rhov13(i1 , i2 , i3+1) - &
flux_rhov13(i1 , i2 , i3 )) )
```

OR

```
model%v1(i1,i2,i3)=model%v1(i1,i2,i3) - &
( dtimeoverrhodx1 * (flux_rhov11(i1+1, i2 , i3 ) - &
flux_rhov11(i1 , i2 , i3 )) + &
dtimeoverrhodx3 * (flux_rhov13(i1 , i2 , i3+1) - &
flux_rhov13(i1 , i2 , i3 )) &
)
```

OR

```
model%v1(i1,i2,i3)=model%v1(i1,i2,i3) - &
( dtimeoverrhodx1 * (flux_rhov11(i1+1, i2 , i3 ) - &
flux_rhov11(i1 , i2 , i3 )) &
) + &
dtimeoverrhodx3 * (flux_rhov13(i1 , i2 , i3+1) - &
flux_rhov13(i1 , i2 , i3 )) &
) &
)
```

Sometimes, the “fluffy” (third) form can greatly increase the readability. Sometimes (probably in the example above), it might just be overdoing it.

5.2.3 Normal code indentation

Usual if..then..else constructs and do loops should be indented with 2 blanks per level as for instance in

```
do i3=m3,n3
  do i2=m2,n2
    do i1=m1,n1
      rho(i1,i2,i3)=model%rho(i1,i2,i3)
    end do ! i1
  end do ! i2
end do ! i3
```

OR

```
if (Copyrho_flag) then
  ! --- Copy original rho array into array with buffer zones ---
  rho(m1:n1,i2,i3)=model%rho(m1:n1,i2,i3)
  !
  ! --- Copy original quc array into array with buffer zones ---
  do iquc=1,nquc
    quc(m1:n1,i2,i3,iquc)=model%quc(m1:n1,i2,i3,iquc)
  end do ! iquc
endif ! (Copyrho_flag)
```

OR

```
if (time_flag > 0) then
  boxout%itime =box%itime
  boxout%time =box%time
  boxout%time_db=box%time_db
endif (time_flag > 0)
```

OR

```
! --- Set default value ---
if (present(grid_flag)) then
  grid_flag0=grid_flag
else
  grid_flag0=1
endif
```

5.2.4 Further recommendations

To save space for the alignments of assignments, headers of files, modules, subroutines, or programs should not be indented.

Usually, there should be no blanks around the “=” in an assignment. However, in some cases they can be inserted to improve readability. Likewise, a blank after a comma in parameter lists is inserted in some but not all cases.

In if..then..else constructs, the new comparison operators are preferred over the old ones, i.e. “==” instead of “.eq.”. A single space is used before and after the comparison operator. The general outline should be

```
if (Copyrho_flag) then
if (time_flag > 0) then
if (ierr /= 0) then
if (model%n1 == model%m1) then
```

The use of possibly redundant brackets is encouraged as in

```
if ((par%OutFile_full /= '') .or. (par%OutFile_mean /= '')) then
if ((par%A%hdScheme == hdScheme_RoeWave ) .or. &
  (par%A%hdScheme == hdScheme_RoeState ) .or. &
  (par%A%hdScheme == hdScheme_RoeMagKin) ) then
if ((ierr > 0) .and. (ierr < 100)) then
```

There is no space between subroutine or function name and following open bracket.

5.3 Naming conventions

5.3.1 File names

(Most of) the file names of the CO5BOLD tar ball are shown in Tables 3.2 and 3.3. Available tweak and scaling files are listed in Tab. 3.4. The – few – corresponding unit-test files are listed in Tab. 3.5.

Program-file names are short, without hyphen (`rhdf90`, `rhdfmpi.F90`, `rhdfut.F90`). However, to avoid name-space pollution, very short names for subroutines, functions, modules and their corresponding files are strongly discouraged. Instead, one level of grouping as, e.g., subroutine `timing_start` and subroutine `timing_stop` in `timing_module`, or two levels as, e.g., subroutine `rhdf_hyd_Step` in `rhdf_hyd_module`, are recommended. In these cases, the files are named as the modules they contain, i.e., `timing_module.F90` and `rhdf_hyd_module.F90`, respectively.

As Fortran free format is preferred, the normal file suffix is `.f90` (or `.F90` for files that have to be processed with a preprocessor during the compiling step), even if language elements beyond Fortran90 are used.

5.3.2 Program names

Program names are short, without hyphen (`rhdf`, `rhdfmpi`, `rhdfUT`). Programs should reside in files with the same name (plus suffix).

5.3.3 Names of modules, subroutines, and functions

Module names should end in `_module`. They should have at least one and at most two underscores indicating the module group name and subgroup name like `group_module` or `group_subgroup_module`.

Contained routines are then named `group_DoThis` or `group_subgroup_DoThat` or `group_subgroup_SomeOperation`. Routine names should contain at least one, at most three underscores. Thus, the name should indicate the module the routine belongs to. Short names like `Init` or `Output` should not be used to avoid name-space pollution and be called `group_Init` or `group_subgroup_Output`, instead. Ideally, all routines should have a globally uniq name even if that not strictly necessary because modules are never used together or some subroutines are kept private in the modules. The use of CamelCase for the subroutine name is encouraged.

If unit-test routines for a `group_module` or `group_subgroup_module` are collected in a separate module this should be called `groupUT_module` or `group_subgroupUT_module`, respectively.

5.3.4 Variable names

As variable names are “more local” than subroutine or module names and the naming conventions vary even more, depending on author and date.

Mathematical conventions should be used as guide lines (e.g., `gamma` for γ or `Gamma1` for Γ_1). Camel-Case and/or underscores can be used to make variable names easier to read.

Variable names in often used structures (e.g., the `box` structure) should be used as guide for further names (see, e.g., Sect. 8.1 and Sect. 8.3). The individual components of vector quantities (axes, velocities, magnetic-field components) don't get individual letters but indices 1, 2, 3 for the respective spatial dimension. So far, these stand for the x , y , and z direction. But these names should be avoided, leaving the possibility of – for instance – spherical coordinates open. Names of basic quantities are, e.g., `rho`, `v1`, `ei` for density ρ , velocity v_1 in x_1 direction, and internal energy e_i per mass unit. The centering of variables can be indicated by `c` for cell-centered quantities and `b` for boundary-centered quantities (as in `xc1` or `xb1`). As cell centering is the default the `c` is often omitted (as in `rho` or `ei`).

Names of quantities that are simple combinations of existing quantities are often constructed as combinations, as, e.g., `rhov1` for the momentum `rho*v1`, instead of inventing an entirely unrelated name (as, e.g., `m1`). The name of an energy tells about its components, e.g., `eikg = ei + ek + eg` (sum of internal, kinetic, and potential energy per mass unit). Likewise, `rhoeikg = rhoei + rhoek + rhoeg` (sum of internal, kinetic, and potential energy per volume). The convention of combining names obviously has limits for more complex functions (as, e.g., fluxes). Due to the lack of a sufficient number of letters in the alphabet loop indices don't all get their individual letters, either. Instead, they look like `i1`, `i2`,

`i3`, `iquc`, `inu`, `idir`, `itime`. The lower grid index is `m`, the upper is `n`. So, cell-centered quantities (in the absence of ghost cells) go from `m` to `n`, whereas boundary-centered quantities go from `m` to `n+1`.

5.4 Comments

5.4.1 Header of files

The header of a file should contain a short summary of its contents, as for example:

```
!*****
!  
! ##### # # ##### # # # # #####  
! # # # # # # # # # # # # #  
! # # ##### # # ##### # # #  
! ##### # # # # # # # # # # #  
! # # # # # # # # # # # # #  
! # # # # # ##### ##### # # # ##### _module  
!  
! Radiation-Hydrodynamics Code: hydrodynamics module  
!  
!*****  
! Fortran90  
! 2015-04-04  
!*****  
! With contributions from:  
! Bernd Freytag: Kiel, Copenhagen, Uppsala, Montpellier, Lyon, Naples  
! Werner Schaffenberger: Exeter  
! Sven Wedemeyer-Boehm: Freiburg  
!*****  
! MODULES:  
! rhd_hyd_module: Hydrodynamics routines  
!  
!*****
```

Dates should be written in the form `YYYY-MM-DD`. The date in the header should be updated each time a file is edited. The banner at the top can be generated, e.g., with the ASCII Generator (Font=banner, Width=100). Usually, a file contains one module with more detailed information in its respective header.

5.4.2 Header of modules

The header of a module could look like:

```
!-----*****-----  
module rhd_hyd_module  
!-----  
! NAME:  
! rhd_hyd_module ('rhd_hydrodynamics_module')  
!  
! PURPOSE:  
! Provide hydrodynamics routines for rhd.  
!  
! CATEGORY:  
! Hydrodynamics  
!  
! CALLING SEQUENCE:  
! use rhd_hyd_module  
!  
! TYPES:  
! None  
!  
! VARIABLES:  
! None  
!  
! ROUTINES: (all contained routines; public ones are marked with '>>')
```

```

! > rhd_hyd_SwitchInfo:    Print information about used compiler switches
!   rhd_bound_3DTransmit: Adjust density values in top cells for the open boundary condition
!   rhd_bound_3DInOutFlow: Adjust values in bottom cells to fulfill the open boundary condition
! > rhd_bound_3DCenter:    Modify energy in central cells to keep entropy constant
! > rhd_bound_3DHeatBottom: Modify energy in bottom cells to keep entropy constant.
!   rhd_bound_1DTransmit: Adjust values in top or bottom cells for transmitting boundary condition
!   rhd_hyd_Roe1DOutput:   Extract some averaged quantities
!   rhd_hyd_sDiff:         Compute 1D energy flux down an entropy step with state reconstruction
!   rhd_hyd_FluxState:     Compute 1D flux from state vector for single quantity
!   rhd_hyd_Pred:         Compute reduced pressure as gravity correction for Roe solver.
!   rhd_hyd_RoeWavealpha12: Compute 1D Roe sound-wave fluxes
!   rhd_hyd_RoeWavealpha36: Compute 1D Roe entropy-wave and ionization-energy fluxes
!   rhd_hyd_RoeWavealpha45: Compute 1D Roe transversal-momentum fluxes
!   rhd_hyd_Fluxrhoei:     Compute 1D internal energy flux from the fluxes of individual waves
!   rhd_hyd_RoeWave1Dflux: Compute 1D Roe fluxes with wave reconstructions
!   rhd_hyd_RoeState1Dflux: Compute 1D Roe fluxes with state reconstructions
!   rhd_hyd_Dust:         Advect passive tracers
!   rhd_hyd_mhd:         Advect magnetic fields
!   rhd_hyd_Roe1DStep:     Perform 1D hydrodynamics step in x1 direction with Roe scheme
!   rhd_hyd_Roe1DMincedStep: Perform 1D hydro step in x1 direction, call Roe solver repeatedly
!   rhd_hyd_SingleStep:    Perform entire (single) 2D or 3D hydrodynamics step, employ Roe scheme
! > rhd_hyd_Step:         Perform entire 3D hydro step, possibly composed of multiple time-steps
!
! CALLING TREE:
!   rhd_hyd_SwitchInfo
!   |
!   rhd_bound_3DCenter
!   | * eosinter
!   |
!   rhd_bound_3DHeatBottom
!   | * eosinter
!   |
!   rhd_hyd_Step
!   * rhd_hyd_SingleStep
!     + rhd_hyd_CoriolisOMP
!     + rhd_bound_3DTransmit
!     | * eosinter
!     + rhd_bound_3DInOutFlow
!     | * eosinter_all
!     + rhd_hyd_Roe1DMincedStep
!     | * rhd_hyd_Roe1DStep
!     | ...
!     + rhd_hyd_Roe1DStep
!     * rhd_bound_1DGhost
!     * rhd_grav
!     * rhd_bound_1DTransmit
!     * + eosinter_PdPTdT
!     * rhd_bound_1DGhost
!     * eosinter_all
!     * eosinter_PdPTdT
!     * eosinter_PdP
!     * rhd_hyd_RoeState1Dflux
!     | + rhd_hyd_RecVecEq
!     | + rhd_hyd_RecVec
!     * rhd_hyd_RoeWave1Dflux
!     | + rhd_hyd_Pred
!     | + rhd_hyd_RoeWavealpha12
!     |   * rhd_hyd_Fluxalpha
!     |   * rhd_hyd_FluxalphaEq
!     | + rhd_hyd_RoeWavealpha36
!     |   * rhd_hyd_Fluxalpha
!     |   * rhd_hyd_FluxalphaEq
!     |   * rhd_hyd_FluxState
!     |     . rhd_hyd_RecVecEq
!     |     . rhd_hyd_RecVec
!     |   * rhd_hyd_sDiff
!     |     . rhd_hyd_RecVecEq

```

```

!           |      . rhd_hyd_RecVec
!           | + rhd_hyd_RoeWavealpha45
!           | * rhd_hyd_FluxState
!           |      . rhd_hyd_RecVecEq
!           |      . rhd_hyd_RecVec
!           | + rhd_hyd_Fluxrhoei
!           | * rhd_hyd_Roe1Doutput
!           | + rhd_mean_weight
!           | + rhd_mean_x23mean
!           | + rhd_mean_x23weight
!           | + rhd_mean_rindex
!           | + rhd_mean_rcmean
!           | + rhd_mean_VecProj
!           | + rhd_mean_rbmean
!           | * rhd_hyd_Dust
!           | + rhd_hyd_FluxState
!           | * rhd_hyd_RecVecEq
!           | * rhd_hyd_RecVec
!           | + rhd_hyd_Rossow78tfall
!           | + rhd_hyd_RecVecEq
!           | + rhd_hyd_RecVec
!           | + rhd_mean_weight
!           | + rhd_mean_x23mean
!           | * rhd_hyd_mhd
!           | + rhd_hyd_Fluxalpha
!
! MODIFICATION HISTORY:
!   1997-06-19 (B.F. Kiel) First version
!   1999-05-11 (B.F. Copenhagen) Routine bound3d_inoutflow added
!   ...
!   2014-08-17 (B.F.) Use global boxes for working copies
!   2014-12-02 (B.F.) Remove "rhd_roe1d_step_l01=0" option
!-----

```

The description of modules, routines, and functions should start at column 27, unless the name is too long.

5.4.3 Header of subroutines and functions

```

!-----*****-----
subroutine rhd_bound_3DTransmit(model, action, dtime)
!-----
! NAME:
!   rhd_bound_3DTransmit ('rhd_boundary_conditions_3_Dimensions_Transmit')
!
! PURPOSE:
!   Adjust density values in top cells to contribute to the open upper boundary condition.
!
! CATEGORY:
!   Hydrodynamics
!
! CALLING SEQUENCE:
!   call rhd_bound_3DTransmit(model, action, dtime)
!
! INPUT:
!   action:      ('action') derived type with collection of control parameters
!   dtime:       ('delta_time') real, time step to be used
!
! INPUT/OUTPUT:
!   model:       ('model') derived type, model data: rho, ei, v, x, time, ...
!
! OUTPUT:
!
! LOCAL VARIABLES:
!
! ROUTINES:

```

```

!   eosinter:           Solve EOS by bicubic interpolation: rho, e -> P, dPdrho, dPde, T, dTde, s
!   MPI_AllReduce:     Perform a reduction and send result to all processes
!   MPI_Comm_Split:    Split a communicator
!
! MODULES:
!   rhd_gl_module:     Global type definitions and parameters for RHD
!   rhd_action_module: Routines to handle the control structure 'action'
!   rhd_box_module:    Box-handling routines
!   rhd_prop_module:   Properties of quantities in 'box' structure
!   gasinter_module:   Routines for interpolating GAS or EOS quantities
!   MPI:               Standard MPI routines and definitions
!
! SIDE EFFECTS:
!
! RESTRICTIONS:
!   Works only for upper (bound_r3) boundary, not for all 6 sides.
!
! PROCEDURE:
!
! EXAMPLE:
!   call rhd_bound_3DTransmit(model, action, 0.5)
!
! MODIFICATION HISTORY:
!   2010-04-05 (B.F.) First Version
!   2010-04-28 (B.F.) bound_transmitting3
!   2012-11-08 (B.F.) Minor modifications
!   2012-11-09 (B.F.) New parameters in call, MPI version
!   2012-11-12 (B.F.) MPI parameters put into prop structure
!-----

```

The description of modules and routines should start at column 27, unless the name is too long. With the script `listroutines` these entries can be generated (almost) automatically.

The description of a variable should start at column 18, unless the name is too long. It should start with a long variable name (`delta_time` for `dtime`) that explains the short name, followed by a short comment about the purpose of the variable.

5.4.4 Comment lines

A subroutine, function, or program should not contain completely empty lines but should start such a line with a – properly indented – exclamation mark.

Comments should be indented as the surrounding Fortran code.

Comments should typically be formulated as an order and start with a verb.

Comments should start with a space-separated triple-hyphen block as in

```
! --- Show a typical comment ---
```

5.4.5 Short comments after Fortran statements

The final statement of a counting do loop should have the loop index as comment as in:

```

do i3=m3,n3
  do i2=m2,n2
    do i1=m1,n1
      rho(i1,i2,i3)=model%rho(i1,i2,i3)
    end do ! i1
  end do ! i2
end do ! i3

```

Long `if..then..else` constructs can have the branching condition (or an abbreviated version) as comment after the `endif` statement as in the (very short) example:

```

if (Copyrho_flag) then
  rho(m1:n1,i2,i3)=model%rho(m1:n1,i2,i3)
endif ! (Copyrho_flag)

```

5.5 Compiler switches and directives

5.5.1 OpenMP

CO5BOLD is parallelized with OpenMP directives. They should be capitalized and indented with the surrounding code, as in:

```
!$OMP PARALLEL DEFAULT(SHARED), PRIVATE(i1, i2, i3)
!
! --- Set bulk HD quantities to zero ---
!$OMP DO SCHEDULE(RUNTIME)
do i3=m3-nghost3,n3+nghost3
  do i2=m2-nghost2,n2+nghost2
    !DIR$ IVDEP
    do i1=m1-nghost1,n1+nghost1
      box%rho(i1,i2,i3)=0.0
      box%ei( i1,i2,i3)=0.0
      box%v1( i1,i2,i3)=0.0
      box%v2( i1,i2,i3)=0.0
      box%v3( i1,i2,i3)=0.0
    end do ! i1
  end do ! i2
end do ! i3
!$OMP END DO
!
!$OMP END PARALLEL
```

5.5.2 Compiler directives

Some directives are inserted into the code to improve performance. They are only understood by the Intel compiler, though. In the following example, unrolling is enforced (or highly recommended) by the directive:

```
do i3=m3,n3
  do i2=m2,n2
    do i1=m1,n1+1
      !DIR$ UNROLL
      do j=-1,1
        alpha_til_1(i1,j,i2,i3)=alpha0_til_1(i1,i_up_mi(i1,i2,i3)-i1+j,i2,i3)
      end do ! j
    end do ! i1
    !
    do i1=m1,n1+1
      !DIR$ UNROLL
      do j=-1,1
        alpha_til_2(i1,j,i2,i3)=alpha0_til_2(i1,i_up_pl(i1,i2,i3)-i1+j,i2,i3)
      end do ! j
    end do ! i1
  end do ! i2
end do ! i3
```

5.5.3 Compiler macros or switches

Compiler switches are used to (des)activate modules or compile alternative branches to improve performance. The default values are set in the header section of each file as, e.g., in:

```
!# /* --- Default values for some preprocessor macros ----- */
!#
!# /* --- Number of additional quantities --- */
# ifndef rhd_box_quc01
#   define rhd_box_quc01 0
# endif
!#
```

```

!# /* --- Gravity correction: 0:'off0', 1:'default0', 2,3,4,5,6,11:'defaultn' --- */
# ifndef rhd_hyd_gravcorr_p01
#   define rhd_hyd_gravcorr_p01 5
# endif
!#
!# /* --- Method of entropy-fix calculation: 0, 1, 2 --- */
# ifndef rhd_hyd_entropyfix_p01
#   define rhd_hyd_entropyfix_p01 0
# endif
!#
!# /* --- Method of upwind calculation: 0 or 1 --- */
# ifndef rhd_hyd_upwind_p01
#   define rhd_hyd_upwind_p01 0
# endif
!#
!# /* --- Loop type for alpha value (amplitude) calculation: 0 (default), 1, 2, 3 --- */
# ifndef rhd_roeid_flux_l01
#   define rhd_roeid_flux_l01 1
# endif
!#
!# /* --- MPI activation --- */
# ifndef rhd_mpi_l01
#   define rhd_mpi_l01 0
# endif
!#
!# /* ----- */

```

To document which switches were used to compile the code each module that uses compiler switches should contain a `_SwitchInfo` routine, that is called by the main program. It can look like:

```

!-----*****-----
subroutine rhd_hyd_SwitchInfo(ncp)
!-----
! NAME:
!   rhd_hyd_SwitchInfo ('rhd_hydrodynamics_Switch_Information')
!
! PURPOSE:
!   Print information about used compiler switches.
!
! CATEGORY:
!   Hydrodynamics
!
! CALLING SEQUENCE:
!   call rhd_hyd_SwitchInfo(ncp)
!
! INPUT:
!   ncp:           ('number_channel_print') integer with output channel number (usually 6)
!
! OUTPUT:
!   None
!
! LOCAL VARIABLES:
!
! ROUTINES:
!   None
!
! MODULES:
!   None
!
! SIDE EFFECTS:
!   Write to requested output channel.
!
! RESTRICTIONS:
!   If another compiler switch is used anywhere in the module it has to be explicitly
!   included in this routine.
!
! PROCEDURE:

```



```

!   Just print the value of all compiler switches used for the module.
!
! EXAMPLE:
!   call rhd_hyd_SwitchInfo(6)
!
! MODIFICATION HISTORY:
!   2002-08-12 (B.F.) Written
!-----
implicit none
!
! --- I/O parameters ---
integer,          intent(in)  :: ncp
!
! --- Local variables ---
character(len=*), parameter    :: defstr='  defined', undefstr='undefined'
!-----
!
write(ncp,'(A)')      'Compiler switches: rhd_hyd_module .....'
!
write(ncp,'(A,I6)') ' rhd' // '_hyd_gravcorr_p01:      ', rhd_hyd_gravcorr_p01
write(ncp,'(A,I6)') ' rhd' // '_hyd_entropyfix_p01:    ', rhd_hyd_entropyfix_p01
write(ncp,'(A,I6)') ' rhd' // '_hyd_upwind_p01:       ', rhd_hyd_upwind_p01
write(ncp,'(A,I6)') ' rhd' // '_roe1d_flux_l01:       ', rhd_roe1d_flux_l01
write(ncp,'(A,I6)') ' rhd' // '_mpi_l01:              ', rhd_mpi_l01
!
!#
# ifdef rhd_bound_t01
!#
write(ncp,'(A,A)') ' rhd' // '_bound_t01:              ', defstr
!#
# else
!#
write(ncp,'(A,A)') ' rhd' // '_bound_t01:              ', undefstr
!#
# endif
!#
!
!#
# ifdef rhd_roe1d_flux_t01
!#
write(ncp,'(A,A)') ' rhd' // '_roe1d_flux_t01:        ', defstr
!#
# else
!#
write(ncp,'(A,A)') ' rhd' // '_roe1d_flux_t01:        ', undefstr
!#
# endif
!#
!
!#
# ifdef rhd_roe1d_step_t01
!#
write(ncp,'(A,A)') ' rhd' // '_roe1d_step_t01:         ', defstr
!#
# else
!#
write(ncp,'(A,A)') ' rhd' // '_roe1d_step_t01:         ', undefstr
!#
# endif
!#
!
end subroutine rhd_hyd_SwitchInfo

```

5.6 Unit tests

For a number of subroutines in a few modules, there exist automated unit tests. The master unit-test routine `hd/unitt/UT_module.F90` and the corresponding main program `hd/unitt/rhdut.F90` reside in `for/hd/unitt/`.

The Makefile is produced with the usual `configure` script (see Sect.4.3). The usual environment variables e.g. for optimization are still valid. However, the unit testing is controlled with the variable `F90_UNIT` and the new make target is `UT` or `rhdut.exe`. A complete installation, compilation, and run of the unit tests could look like:

```
tar -zxvf for.tar.gz
cd for/hd/rhd
mkdir -p UNIT_TESTS_ON_YOUR_MACHINE
cd UNIT_TESTS_ON_YOUR_MACHINE
ln -s ../conf/configure .
export F90_UNIT=1
./configure
make UT
echo -e "$(/rhdut.exe)"
```

The trickery with `echo` causes colored output – that is activated by default – to be properly displayed.

So far, the coverage of the unit tests is microscopic, i.e., a successful unit-test run does not tell much about the correctness of the entire code. While the coverage will hopefully increase with time, there is no intention to try to cover higher-level modules or the entire code. Such tests are and will be made with normal test runs of the entire code – hopefully better automated in the future.

5.6.1 F90_UNIT

Specify, which unit-test modules should be activated:

- 0: Don't activate any unit-test modules. This is the default for normal code compilation and does not make much sense for actual unit testing.
- 1: Activate all unit-unit test modules.
- `rhd_baseradUT_module`: Activate this module.
- `rhd_meanUT_module`: Activate this module.
- `rhd_recUT_module`: Activate this module.
- `rhd_baseradUT_module rhd_meanUT_module`: Activate these two modules (this is an example; any combination is possible).

Chapter 6

Data file types

6.1 File overview

Table 6.1 shows a list of all files necessary to run CO5BOLD. Figure 9.1 gives similar information but is not quite up to date. Executing the Makefile produces an executable `rh.d.exe`. Its name can of course be changed afterwards. The names of the control files `rh.d.par`, `rh.d.stop`, `rh.d.cont`, and `rh.d.dump` and of the status file `rh.d.done` cannot be changed (without modification of the source code). The names of EOS, opacity, and CO5BOLD data files can be chosen freely in the parameter file `rh.d.par`. Table 6.1 only contains dummy names.

6.2 UIO data format

6.2.1 Quickstart: Introduction to UIO

The UIO (“Universal Input Output”) routines are a set of routines in Fortran90 and IDL to manage I/O of scalars, arrays and a certain table type. Files can be formatted or unformatted. The formatted (ASCII text) data representation is machine-independent and appropriate for human reading (for short files).

The binary representation uses the Fortran “unformatted” read and write routines, provides much faster I/O, gives smaller files, and the IEEE format is a quasi-standard among many platforms/compiler. On all machines the native binary representation can be chosen. On some platforms additional conversion types are offered (IEEE on most machines, CRAY format an CRAYs).

The Fortran standard does not guarantee that unformatted (i.e. also UIO) files are readable on all machines. But it is always possible to produce (formatted) UIO files on a machine which are readable on all others. And with some fiddling with compile options or the call of machine-specific subroutines provided by the compiler vendor it was up to now always possible to enable the access to binary UIO files (of one common format: IEEE `big_endian`) on all machines and compilers tested: Compaq alpha, Cray, Hitachi, HP V2500, HP Itanium2, IBM, Intel/AMD (with Linux OS and PGI, Intel, or Pathscale compiler), NEC SX-5, SGI, and Sun. Problems might arise with the transition to records larger than 2 GByte which require an extension of the current standard. The GNU Fortran compilers (particularly g95) might introduce a 64-bit system that does not allow to read older 32-bit files (even small ones).

Each file entry is a header-data-unit. The header contains information to identify the entry and to specify the format and size of the following data block. This block usually consists of a scalar or an array. In some cases it is empty (e.g. for labels) or it contains more complex information (for tables).

The first version of UIO routines was written in FORTRAN77. It still exists. However, further development was done with the Fortran90 versions. Therefore, the use of the FORTRAN77 routines is not recommended anymore. The current Fortran version of the UIO routines is a set of Fortran90 modules.

To allow a communication between Fortran and IDL programs, an IDL version of the UIO routines has been written. The correspondence between Fortran and IDL routines is rather close. But in detail, there are differences. Currently, IDL Version 6.0 is used. Amazingly, the UIO routines also used to work under *PV-WAVE* (Version 6.01, sun4 solaris sparc).

File	Sect.	I/O	Type	Description
rhd.exe	4.2	-	executable	main program
rhd.par	7.1	I	ctrl/data: UIO	central control file
rhd.par2	7.1.22.1	I	ctrl/data: UIO	additional control file
rhd.stop	7.7	I	ctrl: empty	file to force controlled stop of simulation
rhd.cont	7.7	I	ctrl: empty	file to force continuation after stop
rhd.dump	7.7	I	ctrl: empty	file to request output of current model
data.eos	7.1.6	I	data: UIO	tabulated equation of state
data.opta	7.1.7	I	data	tabulated opacities
rhd.sta	8.1	I	data: UIO	start model (e.g. end file of last run)
rhd.done	8.7	O	status: text	exit status: written if run was successful
rhd.end	8.1	O	data: UIO	end model
rhd.full	8.1	O	data: UIO	sequence of (2D or 3D) snapshots, large
rhd.mean	8.3	O	data: UIO	horizontal and spherical means, intensity
rhd.mcycl	8.3	O	data: UIO	azimuthal means (of global models)
rhd.chu1	8.2	O	data: UIO	small chunk of full dataset, written often
rhd.chu2	8.2	O	data: UIO	small chunk of full dataset, written often
rhd.chu3	8.2	O	data: UIO	small chunk of full dataset, written often
rhd.snap	8.7	O	data: UIO	model snapshot if requested
rhd.out	8.6	O	data: text	human readable text output
data.dat	7.5	I	data: text	chemical reaction data
data.atom	7.6	I	data: text	HION data file (model atom)
edens.dat	7.6	I	data: UIO	HION data file (electron density table)
abundance.input	7.6	I	data: text	HION data file (abundances)
pf_kurucz.dat	7.6	I	data: UIO	HION data file (partition functions)
HION.time.H.*.out	8.5	O	data: UIO	HION: additional output
HION.step.H.*.out	8.5	O	data: UIO	HION: additional output

Table 6.1: List of all control and data files of CO5BOLD with the file name, where e.g., “rhd” and “data” are in most cases only placeholders for the real model or data table name, a reference to a section with a more detailed description of the file, a column indicating whether the file is used for input or output, the type of the file distinguishing between executable, control, data, and status files, and a (slightly) more detailed description.

So far, there exist three UNIX shell scripts (calling Fortran routines) useful to quickly examine data sets or to change the format or conversion type of files. The installation of these scripts with a “configure-make-make install” sequence is described in Sect. 6.2.6.1.

Without these scripts an UIO file in ASCII format can be examined with any text editor or with more. To get an overview about the contents of a binary file the command

```
strings -30 uio_example_file.dat
```

can be useful.

6.2.2 Example of UIO data file

To give a first impression about the data structure, here follows a simple test file, which contains the header, a label, a couple of scalars, an array, and a short table:

```
fileform uio form=formatted convert=native version=0.1.1997.11.29 &
date='29.11.1997 21:23:39.835' system=IRIX machine=atlas osrelease=6.3 &
osversion=12161207 hardware=IP32 language=Fortran90 program=uiotst
```

```
label testdata n='sample test data field' date='29.11.1997 21:23:39.835'
```

```

integer ia f=I3 b=4 n='This is the answer'
  42
complex ca f='''('',E13.6,'',''',E13.6,'')''' b=8 n='This is a complex answer'
( 0.400000E+01, 0.200000E+01)
real da f=E23.15 b=8 n='precise answer'
  0.4200000000000000E+02
real answer f=F4.0 b=4 n=answer u=1
  42.

real real2d d=(100:103,200:204) f=E13.6 p=4 b=4
  0.100000E+01 0.200000E+01 0.300000E+01 0.400000E+01
  0.500000E+01 0.600000E+01 0.700000E+01 0.800000E+01
  0.900000E+01 0.100000E+02 0.110000E+02 0.120000E+02
  0.130000E+02 0.140000E+02 0.150000E+02 0.160000E+02
  0.170000E+02 0.180000E+02 0.190000E+02 0.200000E+02

table f77table d=(1:5,1:7) f=1X b=1 n='test table to test the table routines'
integer   int1  f=I5    b=4  n='Integer: 1. column'
real      real1 f=F5.1  b=4  n='Real: 2. column'
character char1 f=A16   b=16 n='Char: 3. column'
real      real2 f=E13.6 b=4  n='Real: 4. column'
integer   int2  f=I5    b=4  n='Integer: 5. column'
  int1 real1          char1          real2  int2
    1   2.0 a          0.100000E+02    1
    2   4.0 ab         0.200000E+02    2
    3   6.0 abc        0.300000E+02    3
    4   8.0 abcd       0.400000E+02    4
    5  10.0 abcde      0.500000E+02    5
    6  12.0 abcdef     0.600000E+02    6
    7  14.0 abcdefg    0.700000E+02    7

```

6.2.3 Structure of UIO files

6.2.3.1 Data representation: ASCII or binary

While opening a file for writing, the file format (“formatted” or “unformatted”) and the conversion type (“native”, e.g. “ieee_4”, ...) have to be specified.

The *formatted* ASCII data representation allows I/O independent of platform or compiler. It is useful for parameter files which can be read and edited by hand, for the direct inspection of data, the transfer between very different systems, or for the import of data which exist e.g. in a table format. From the specified conversion type only the default output format for numbers (e.g. “E13.6” for 4 byte reals) is determined.

The *unformatted* binary I/O is much faster and gives usually more compact files with higher accuracy (ideally exact) in the numerical data representation. But – in principle – the file format is machine dependent. Fortunately, the IEEE format turns out to become a quasi-standard among a variety of machines. Most workstations work internally with this format. Some CRAYS which have a different internal data representation allow the hidden transformation between the internal and IEEE format during the I/O process. The UIO routines support this feature of CRAY FORTRAN compilers by means of a module (`uio_mac_module`), individually designed for (two types of) CRAY machines using certain CRAY specific system calls (CRAY FFIO assign logic). Nevertheless, there is also a machine independent version of this module, written completely in standard Fortran90 but providing less features than the machine-dependent versions.

Besides the format, the conversion type (see table 6.2) has to be specified. The “native” conversion type is the internal binary-data representation, which is also standard for unformatted Fortran output. If this representation happens to be conformal with the IEEE standard the conversion type “ieee_4” should be used. It gives the same data format, but in the header of the file the term “convert=ieee_4” instead of “convert=native” describes the data format precisely – in a way also understandable by other machines. On CRAY machines the native format is equal to the conversion type “crayxmp_8”, but also

the conversion types “`ieee_4`”, and “`ieee_8`” can be chosen. The last two conversion types correspond to the CRAY internal types “`ieee_32`” and “`ieee_64`”, respectively.

On a machine with an internal data representation not within the list in the existing `uio_mac_module.F90` file, one could use the “native” conversion type only. But it is better to invent an appropriate name for the new data format and to build a proper machine-dependent branch with its own compiler switch. However, it was possible in all cases so far to activate some internal conversion process, which allowed the handling of UIO files in the standard Big-Endian-IEEE format.

conversion type	I	R	D	description
<code>native</code>	?	?	?	internal data format on all machines (sometimes useful but not recommended)
<code>ieee_4</code>	4	4	8	standard IEEE <code>big_endian</code> format (recommended)
<code>ieeele_4</code>	4	4	8	IEEE <code>little_endian</code> format
<code>ieee_8</code>	8	8	16	double precision IEEE <code>big_endian</code> format (on some machines possible)
<code>crayxmp_8</code>	8	8	16	CRAY internal data format
<code>idl</code>	4	4	8	IDL format (but IDL also supports <code>ieee_4</code>)
<code>xdr</code>	4	4	8	format possible with IDL
<code>ieee_4_limit</code>	4	8	8	standard IEEE format → <code>ieee_4</code>
<code>ieee</code>	?	?	?	IEEE format, unknown length (not recommended)

Table 6.2: UIO conversion types with length of integers, single precision reals, and double precision reals in bytes, and an explanation.

Some attention has to be paid if weird compiler switches (as e.g. `-r16 -i2`) are used to modify the accuracy and standard memory size of variables.

If an existing file is opened for reading, the file format and conversion type are determined automatically from the file if the conversion type of the data in the file is among the conversion types supported by the compiler. If the file has a conversion type “native” but is created on a machine with different internal data representation, the file header might be readable, but an error will probably occur during the reading of a real variable.

6.2.3.2 Data file structure

The UIO routines only handle sequential files. Each file consists of a list of entries. The first entry describes the file format, conversion type, and the machine who is responsible for it. The following entries contain data (scalars and 1D ... 4D arrays of type integer, real (single & double precision), complex (single precision), character; tables with columns of type integer, real (single precision), or character), or structuring information (labels).

Each entry consists of the header and the (possibly empty) data block.

Each header is a list of at most 20 terms separated by blanks or linefeeds. The first term is the entry type (e.g. `real`, see table 6.3), followed by an identifier. This identifier should follow the standard rules for variables (lowercase letters, numbers, underscore; starting with letter). It is a name as e.g. `rho`, `v_1`. The rest of the terms come in the form “keyword=value”. See Tab. 6.4 for some pre-defined keywords.

A header line has a maximum length of 80 characters. A continuation line is indicated by `&` at the end of the line. A header consists of 20 lines at maximum. It can be preceded by empty lines (except for the file header entry). Example:

```
real time f=F9.2 b=4 n='Time' u=s c0='Simulation time in seconds' &
  c1='Time count starts at 0.0'
  12.34
```

The entry header is followed by the entry data block. This block is empty for labels and the fileform entry but non-empty otherwise.

entry type	entry contents
fileform	file description (first entry)
integer	scalars, 1D ... 4D arrays
real	scalars, 1D ... 4D arrays, single & double precision
complex	scalars, 1D ... 4D arrays, single precision
character	scalars, 1D ... 4D arrays
table	table with integer, real, character columns
label	label entry for file structuring

Table 6.3: UIO entry types

keyword	description	example	descriptor	info.	necessary
b	byte number	4	format		yes
d	dimension	(0:9)	format		yes (arrays)
ds	dimension shift	(1:1)		yes	
f	Fortran format	E13.6	format		yes
p	values per line	4	format		yes (arrays)
t	transformation	log10	format		
n	name	density		yes	
u	unit	g/cm ³		yes	
date	date	1.1.98		yes	
c0...9	comment	Dichte		yes	
form	file format	formatted	file		yes (file header)
convert	conversion	ieee_4	file		yes (file header)
version	version	0.1.1997.11.29		yes	
system	system	IRIX		yes	
machine	machine name	atlas		yes	
osrelease	OS release	6.3		yes	
osversion	OS version	12161207		yes	
hardware	machine hardware	IP32		yes	
language	program. language	Fortran90		yes	
program	program	uiotst		yes	
xyz...	user defined	source		yes	

Table 6.4: Standard UIO entry header keywords: The keyword is given with a short description and an example. The fourth, fifth, and sixth column indicate if the keyword is a mandatory descriptor (in the file header or for the format of an entry) or if it gives only additional information and is optional and therefore not necessary to specify.

In an *unformatted* file each header line is an individual record containing a string with exactly 80 characters. The following data block (scalar or array) is one single record.

In a *formatted* file each header line is a string of at most 80 characters delimited by a LINEFEED of whatever the operating system decided to be appropriate as EOL character (sequence). The following data block is written as sequence of lines. The number of items per line is specified by the “p=?” keyword in the header.

6.2.3.3 Tables

For a table the entry header is followed by a list of headers for the individual table columns, a single table header line consisting of (abbreviations of) the table entry identifiers and the table itself (see the example in section 6.2.2). The dimension keyword gives the number of columns and rows in the form “d=(1:columns,1:rows)”.

The Holweger-Müller-Atmosphere is chosen as the following “real world” example for a file with a

table in UIO format:

```

fileform uiio form=formatted convert=ieee_4 version=0.0.1996.10.29 &
  date='20-Feb-1997 18:40:45' system=SunOS machine=saturn osrelease=4.1.3 &
  osversion=3 hardware=sun4m language='IDL 4.0' program='by hand'

character description d=(0:3) f=A80 p=1 b=80 d='13-Nov-1996 18:29:48'
Holweger-Mueller-Atmosphere,
Hartmut Holweger & Edith Mueller (1974) Solar Physics 39, 19-30, table II,
empirical solar temperature stratification to fit solar spectral lines and
limb darkening

character history d=(0:3) f=A80 p=1 b=80 d='13-Nov-1996 18:29:52'
Holweger-Mueller-Atmosphere, from 1974
uiio-form:          13-Nov-1996 18:29:52
conversion type added: 20-Feb-1997 18:21:01
xi -> vmicro:      20-Feb-1997 18:23:43

real teff f=F6.1 b=4 n='effective temperature' u=K texa='T_eff'
5780.0

table atmosphere d=(1:7,1:29) f=X b=1 n=Holweger-Mueller-Atmosphere &
  c0='Hartmut Holweger & Edith Mueller (1974) Solar Physics 39, 19-30, table II' &
  c1=Teff(Sun)=5780K
real tauross f=E9.2 b=4 n='optical depth (Rosseland)' u=1
real tau5000 f=F7.3 b=4 n='optical depth (lambda5000)' u=1 t=log10
real t      f=F7.0 b=4 n=temperature u=K
real pgas   f=F6.3 b=4 n='gas pressure' u=dyn/cm^2
real pel    f=F6.3 b=4 n='electron pressure' u=dyn/cm^2
real vmicro f=F4.2 b=4 n=microturbulence u=km/s
real q      f=F8.5 b=4 n='Hopf function' u=1 c0='q=((T(tau)/Teff)^4)/0.75)-tau'
  tauross tau5000      t      pgas      pel vmic      q
2.00E-07 -6.539  3900.  0.769 -3.140 0.00  0.27637
2.50E-07 -6.279  3920.  1.171 -2.752 0.00  0.28208
5.00E-07 -5.868  3970.  1.598 -2.342 0.00  0.29675
1.00E-06 -5.588  4030.  1.842 -2.105 0.00  0.31510
2.00E-06 -5.334  4080.  2.042 -1.910 0.00  0.33103
5.00E-06 -5.001  4160.  2.279 -1.674 0.00  0.35776
1.00E-05 -4.747  4210.  2.450 -1.508 0.00  0.37527
2.00E-05 -4.486  4270.  2.618 -1.341 0.00  0.39712
5.00E-05 -4.131  4340.  2.835 -1.128 0.00  0.42377
1.00E-04 -3.856  4400.  2.999 -0.967 0.50  0.44765
2.00E-04 -3.577  4460.  3.162 -0.804 0.50  0.47248
5.00E-04 -3.200  4530.  3.377 -0.596 0.50  0.50256
1.00E-03 -2.912  4590.  3.541 -0.437 0.50  0.52925
2.00E-03 -2.621  4640.  3.704 -0.279 0.50  0.55173
5.00E-03 -2.233  4720.  3.919 -0.070 0.50  0.58792
1.00E-02 -1.939  4800.  4.083  0.094 0.50  0.62415
2.00E-02 -1.645  4900.  4.245  0.266 0.65  0.66867
5.00E-02 -1.256  5080.  4.460  0.504 0.85  0.74558
1.00E-01 -0.961  5260.  4.622  0.705 1.00  0.81447
2.50E-01 -0.571  5560.  4.830  1.002 1.25  0.89163
4.00E-01 -0.371  5850.  4.926  1.251 1.40  0.99911
7.00E-01 -0.133  6260.  5.022  1.613 1.50  1.13453
1.00E+00  0.019  6570.  5.070  1.879 1.60  1.22581
1.50E+00  0.191  6880.  5.114  2.140 1.70  1.17659
2.00E+00  0.312  7160.  5.140  2.363 1.80  1.13964
4.00E+00  0.597  7920.  5.191  2.889 1.80  0.70033
6.00E+00  0.761  8250.  5.213  3.092 1.80 -0.46595
8.00E+00  0.877  8420.  5.229  3.196 1.80 -1.99552
1.00E+01  0.967  8500.  5.242  3.245 1.80 -3.76404

```


6.2.3.4 Recommendations for standard file structure

The very first entry in an UIO file is always the fileform `uio` entry, containing information about the file format and conversion type. Afterwards, entries can follow in any order. But it is perhaps a good idea to start the file with three special entries (`file_id`, `description`, `history`) as in

```
fileform uio form=formatted convert=ieee_4 ...

character file_id f=A80 b=80 n='File identification'
uio-demofile

character description d=(1:2) f=A80 p=1 b=80 n='File description'
This is a file to demonstrate the recommended start entries for all
UIO files.

character history d=(1:1) f=A80 p=1 b=80 n='File history'
UIO demo file: 22-Dec-1997 14:15:15
```

A recommended format for sets of multi-dimensional arrays (e.g. hydrodynamics: x-axis, y-axis, z-axis, density, velocities, energy, ...) is shown in Sect. 8.1.

6.2.4 Files & directories & paths

All UIO-routines are located in sub-directories of a common directory `uio`. The subdirectories and their contents are

```
uio/bin/      : shell scripts: uiolook (Sect.6.2.6.2), uiocat (Sect.6.2.6.3), uioinfo (Sect.6.2.6.4)
uio/f90/      : Fortran90 source code, see Tab.6.5
uio/man/man1/ : manual pages for shell scripts: uiolook, uiocat, uioinfo
idl/bflib/uio/: IDL routines (Sect.6.2.7)
```

To use the UNIX scripts and the Makefile you could set a global system variable **UIOPATH** pointing to this directory. The path to the shell scripts and to the man pages could be added to your shell path variables e.g. in one of the login scripts:

C-shell (`.cshrc`):

```
# --- uio ---
setenv UIOPATH "$HOME/uio"
setenv PATH "$PATH:$UIOPATH/bin"
setenv MANPATH "$MANPATH:$UIOPATH/man"
# --- *** ---
```

Korn-shell (`.kshrc`) or bash (`.bashrc`):

```
# --- uio ---
UIOPATH=$HOME/uio
export UIOPATH
PATH=$PATH:$UIOPATH/bin
export PATH
MANPATH=$MANPATH:$UIOPATH/man
export MANPATH
# --- *** ---
```

However, with the UIO `configure` script and `make`, `make install` there is a different method available that adds the path declarations automatically, see Sect. 6.2.6.1.

File	Contents
<code>uio_base_module.f90</code>	Collection of basic modules
<code>uio_mac_module.F90</code>	Machine-dependent routines for all machines
<code>uio_bulk_module.f90</code>	Main part of UIO routines
<code>uio_filedef_module.f90</code>	Standard file descriptors and labels
<code>uio_table_module.f90</code>	Table manipulation routines
<code>uio_var_module.f90</code>	Definition and handling of UIO flexible variable
<code>uio_varfile_module.f90</code>	Definition and handling of file structure of UIO flexible variables
<code>uiocop.f90</code>	Program to copy and transform UIO files
<code>uiolok.f90</code>	Program to look into UIO files
<code>uioinf.f90</code>	Program to give information about conversion types
<code>uiotst.f90</code>	Program to produce test UIO file

Table 6.5: UIO Fortran90 files

Module	Contents
<code>uio_cst_module</code>	Channel status information
<code>uio_cvl_module</code>	Convert type list of current machine
<code>uio_inf_module</code>	Information about environment
<code>uio_nam_module</code>	Definition of names
<code>uio_siz_module</code>	String length, table size
<code>uio_base_module</code>	Basic set of UIO-routines: string processing, header handling, I/O channel management

Table 6.6: Contents of `uio_base_module.f90`

6.2.5 Fortran90

6.2.5.1 Files

The Fortran UIO package is a collection of Fortran90 modules and programs described in Table 6.5. The file `uio_base_module.f90` contains the basic set of modules (see Table 6.6).

In older version of CO5BOLD, the files `uio_mac*_module.f90` (Tab. 6.5) contained machine-dependent routines collected in the module `uio_mac_module` (see Tab. 6.7).

Routine	Purpose
<code>uio_getenv</code>	Get information about environment
<code>uio_mkcvls</code>	Make list with possible conversion types
<code>uio_uopen</code>	Open file with special handling for conversion type
<code>uio_uclose</code>	Close file with special handling for conversion type

Table 6.7: Contents of `uio_mac_module`

In the current version of CO5BOLD, there is only one file `uio_mac_module.F90` – with a capital F90 – that can be changed during the compilation by preprocessor switches, see 4.4.2.

The main set of routines is contained in `uio_bulk_module.f90` in the module `uio_bulk_module`. The three files `uio_base_module.f90`, `uio_mac_module.F90`, and `uio_bulk_module.f90` comprise the standard set of UIO routines. Additionally, there exists a file `uio_table_module.f90` with the single module `uio_table_module` which permits the I/O and manipulation of a certain table format (see the example in section 6.2.2).

The latest extension comes within the modules `uio_var_module.f90` and `uio_varfile_module.f90`. The module `uio_var_module.f90` contains a type definition for a variable (“uio flexible variable”) of gen-

eral type (i.e. it may be a scalar integer value or a 1D character array or a 3D real array. . .) together with some routines for the basic handling of the variables (I/O in UIO format, construction and modification of variables. . .). The module `uio_varfile_module.f90` contains a type definition for a file built of UIO flexible variables together with routines for the handling of these files.

6.2.5.2 Use of UIO modules in Fortran90

To make the UIO routines available in a Fortran program the appropriate modules have to be specified in a `USE` statement.

At maximum five modules play a role: The `uio_bulk_module` contains the main part of the UIO routines (and also uses the relevant sub-modules). Instead of `uio_bulk_module` the module `uio_table_module` is used if the UIO table routines are needed. The modules `uio_siz_module` and `uio_nam_module` contain specifications about the size of some arrays and the length of strings, and the names of types and keywords, respectively. The module `uio_filedef_module` contains some definitions in addition to the basic UIO standard as e.g. the label names which delimit a data set (`label dataset` and `label enddataset`).

A typical case for the use of UIO modules is

```
use uio_bulk_module
use uio_siz_module
use uio_nam_module
```

6.2.5.3 Compiling and Makefiles

For a certain platform, it was necessary to change the name of the module file with the machine-dependent routines (`uio_mac*_module.f90`) in a Makefile for the UIO routines. For this purpose the environment variable `UIOMAC` had to be set to the name of the appropriate routine (see Sect. 3.1).

In the current version of CO5BOLD, there is only one file `uio_mac_module.F90` – with a capital F90 – that can be changed during the compilation by preprocessor switches, see 4.4.2.

For CO5BOLD or the UIO Unix scripts, the respective configure script takes care of either of these steps. Many compilers generate module information files with suffixes like `.M`, `.mod`, or `.kmo`. To clean up information files with other suffixes, they have to be included in the cleaning step. Calling examples:

```
make
make UIO
make UIO "F90FLAGS=-g"
make clean
make cleanall
make remove
make removeall
```

A section of a typical Makefile using the UIO routines may be

```
...
# --- Compiler options ---
F90C=f90
F90FLAGS=
# --- Libraries ---
UIOMAC=uio_mac_module
...
# --- Dependencies of exe-files on object files and libraries ---
test.exe: test.o
    $(F90C) $(F90FLAGS) -o $@
    $(UIOPATH)/f90/uio_base_module.o $(UIOPATH)/f90/$(UIOMAC).o
    $(UIOPATH)/f90/uio_bulk_module.o
```

```

test.o: $(UIOPATH)/f90/UIO test.f90
        $(F90C) -c $(F90FLAGS)          -M$(UIOPATH)/f90          test.f90
...
# --- Dependencies on used modules ---
$(UIOPATH)/f90/UIO:
        cd $UIOPATH/f90 ; make UIO "F90FLAGS=$(F90FLAGS)"

```

6.2.5.4 Sample calls of Fortran UIO routines

Examples for routines with UIO input/output in CO5BOLD are `tabinter_rdcoeff`, `tabinter_wrcoeff`, `rhd_box_RdData`, `rhd_box_WrData`, `rhd_datx_Write`, and `rhd_par_RdData`. The needed modules have to be declared by a `use` statement like:

```
use uio_bulk_module
```

In the initial phase of the program the UIO routine package has to be initialized by exactly one call of the `uio_init` routine with the name of the program as optional parameter:

```
call uio_init(progname='uiotst')
```

The internal list of logical I/O unit numbers may be changed with calls of `uio_chunit` and `uio_chconv`. A file can be opened for writing with

```

file='test.txt'
form='formatted' ! or: 'unformatted'
conv='ieee_4'    ! or: 'native', 'crayxmp_8',...
call uio_openwr(ncout, file, form=form,conv=conv)

```

Header and data block are written together with one command as e.g. in:

```

call uio_wr(ncout, time, 'time', name='time', unit='s' )
call uio_wr(ncout, rho(1:10), 'rho', name='density', unit='g/cm^3')

```

There are two different routines to close a file after reading or writing. A file opened for writing is closed by:

```
call uio_closwr(ncout)
```

To open a file for reading, only the file name has to be specified. File form and conversion type are determined automatically:

```

file='test.txt'
call uio_openrd(ncin, file)

```

In contrast to the writing of an entry by one routine call the reading is performed in two separate sub-steps for the header and the data part. After the reading of the header e.g. with

```

use uio_siz_module
use uio_nam_module
...
integer                :: ntt
character*(let)        :: termt(2,nttmx)
...
call uio_rdhd(ncin, termt,ntt)

```

the identifier, type, and dimension (if any) of the entry is contained in the character array `termt` with `ntt` entries and special actions may be taken: The data part may be skipped with

```
uio_skipda(ncin, termt,ntt)
```

or it can be read with:

```
call uio_rd(ncin, termt,ntt, time, ident)
```

If the entry is an array it may be necessary to allocate memory:

```
call uio_exkeyw(termt,ntt, dimna,dimstr)
call uio_st2dim(dimstr, ilow, iup, ndim=ndim)
allocate(rho(ilow(1):iup(1)))
call uio_rd(ncin, termt,ntt, rho, ident, ilb=ilow(1:1))
```

Alternatively, it is possible to search in the file for a special entry or to search in a specially generated entry list with:

```
call uio_srhdc(ncin, termt,ntt, type='real',ident='rho',outstr=outstr,ierr=ierr)
```

Additionally, the `uio_var_module` makes it possible to read any entry into an UIO flexible variable, and the `uio_varfile_module` allows the reading of a complete file into a special file structure of UIO flexible variables.

To close a file after reading use

```
uio_closrd(ncin)
```

There are several examples of programs with UIO routines like `uio_var_test.f90`, `uio_varfile_test.f90`, `uiotst.f90`, (`uio_demo.f90`) and – of course – `CO5BOLD`.

6.2.6 UNIX scripts

So far, there exist three UNIX shell scripts useful to quickly examine data sets (`uiolook`), to change the format or conversion type of files (`uiocat`), or to print some information about the conversion types possible on the local machine (`uioinfo`).

6.2.6.1 Installation of UIO UNIX scripts

The installation procedure for the UIO scripts has been updated to make use of its own configure script. Therefore, the procedure should now look like

```
tar -zxvf for.tar.gz
cd for/uio/f90/YOUR_MACHINE
./configure
make
make install
```

or

```
tar -zxvf for.tar.gz
cd for/uio/f90
mkdir YOUR_MACHINE
cd YOUR_MACHINE
ln -s ../conf/configure .
./configure
make
make install
```

Some of the environment variables that control the `CO5BOLD` configure script are also recognized (see the header of the UIO configure script). The command

```
make install
```

generates a directory `/${HOME}/local` and sub-directories. An init script is put into `/${HOME}/bin`. And the resource files `.cshrc` and `.bashrc` are modified to call it. Therefore, this installation step is *potentially dangerous*, because its effect is not restricted to the local directory!

6.2.6.2 Quick examination of files: uiolook

The shell script uiolook calls the Fortran program uiolok.f90. The man page:

```
UIOLOOK(1V)          Misc. Reference Manual Pages          UIOLOOK(1V)

NAME
    uiolook - print entry headers of file in uio form

SYNOPSIS
    uiolook [ -h ] [ -p ] [ filename ... ]

AVAILABILITY

DESCRIPTION
    The routine uiolook reads each filename (file in uio form)
    in sequence and displays the headers of the entries in
    pretty form.

OPTIONS
    -h    Print usage of uiolook.

    -p    Entry header keywords in (long) pretty form

SunOS 5.5.1          Last change: 27 November 1996          1
```

6.2.6.3 Transformation of files: uiocat

The shell script uiocat calls the Fortran program uiocat.f90. The man page:

```
UIOCAT(1V)          Misc. Reference Manual Pages          UIOCAT(1V)

NAME
    uiocat - concatenate file(s) in uio form

SYNOPSIS
    uiocat [ -c conversion ] [ -f format ] [ -h ] [ -l copylist
    ] [ -o outputfilename ] [ filename ... ]

DESCRIPTION
    The routine uiocat reads each filename (file in uio form) in
    sequence and displays its contents formatted on standard
    output or writes it into a file. In the latter case the
    format change from 'formatted' to 'unformatted' or vice
    versa is possible.

OPTIONS
    -c    Conversion type: 'native', 'ieee_4', ... (machine
    dependent), its specification is only relevant, if an
    output file is specified with the -o option and output
    format='unformatted'.

    -f    Output format: 'formatted' or 'unformatted'. Its
    specification is only relevant, if an output file is
    specified with the -o option.

    -h    Help: print usage of uiocat.

    -l    List of entries to be copied. E.g.
    uiocat ... -l"real rho"
    uiocat ... -l"real rho,integer i"
```

```
uiocat ... -l"label *,real rho,integer i"
uiocat ... -l"label *,real rho,* i"
```

Here, copylist is a list, separated by ",". Each item consists of exactly two items, separated by a blank. No additional blanks are allowed. Use copylist with "" as above.

- o Output file name. If omitted, standard output is used and "-c" and "-f" are meaningless.

SunOS 5.5.1 Last change: 12 January 1998 1

6.2.6.4 Information about conversion types: uioinfo

The shell script uioinfo calls the Fortran program uioinf.f90. The man page:

uioinfo(1V) Misc. Reference Manual Pages uioinfo(1V)

NAME

uioinfo - print machine-dependent information

SYNOPSIS

uioinfo

DESCRIPTION

The routine uioinfo prints information about its environment and a list of possible conversion types.

OPTIONS

SunOS 5.5.1 Last change: 12 January 1998 1

6.2.7 IDL UIO routines

The UIO package for IDL comes as a list of routines with names quite similar to the Fortran90 version. Instead of using global variables as in Fortran90 there are now common blocks in Include-files.

```
*****
; Routines, functions : uio_*.pro:
;
; (!: most important, +: user-routine, -: comfortable, .:useful)
; . adkey1: Add one keyword to term table, keyword-value=' ', no link character
; . adkey2: Add one keyword to term table with keyword-value
; . adkey3: Add one keyword to term table with keyword-value or default
; . chconv: Actualize list of conversion types for all channels
; + chpos: Give current file position or jump to specified position
; . chunit: Initialize, store and actualize a list of free and occupied unit
;          numbers
; + closrd: Close file after reading
; + closwr: Close file after writing
; - cpenr: Copy entry from one file to another
; + d: Read data from uio-file(s) in quasi direct-access mode
; + data: Handle uio-file(s) in quasi direct access mode
; ! dataset_rd: Read uio file and put data into anonymous structure
; ! datasetlist_rd: Read data from list of files and put it into an. structure
; deform: Determine the default output format for numbers
; dim2st: Compose dimension string
; . exkeyw: Extract value of keyword from table
; ex1trm: Extract one term from the input line
; exmtrm: Transform a list of items into its components
```

```

; . filcon:      Determine file contents: list of all entries with its positions
;  getenv:      Get information about environment
; ! init:       Initialization procedure for input/output routines
;  me1trm:     Merge the input term: 'keyword', 'value' -> 'keyword=value'
;  memtrm:     Merge a list of terms (keywords and their values) into a line table
;  mkcvls:     Make list with possible conversion types
; . nc2nt:     From column number or entry name find table entry number
; + openrd:    Open file for reading, read header
; + openwr:    Open file for writing, write header
; - pptrmt:    Print term table in pretty form
;  qmaadd:     Transform a string into a string with quotation marks if necessary
;  qmadel:     Parse string "inline" and remove quotation marks if necessary
; + rd:        Reading scalar and array data of all types
; . rdfifo:    Read file header
; + rdhdex:    Read header of variable and extract keywords
;  rdhead:     Read header
; + rdlabl:    Read label
; + rdtab:     Read table of integer, real, and/or character data from file
; + skipda:    Skip data block
; - slhdex:    Search header of variables given by list and extract keywords
; . st2dim:    Parse dimension string
; ! struct_rd: Read uio file and put data into anonymous structure
; . tab0:      Create empty table structure
; + tabc:      Change and modify table contents: rearrange lines.
; + tabm:      Merge two tables in different ways
; + tabr:      Read 1d array from 2d table array (all types)
; + tabw:      Write 1d array into table (all types)
;  ucloze:    Close file with special handling for conversion type
;  uopen:     Open file with special handling for conversion type
;  vnanrm:    Transform a string to give a correct name of a variable
;  wf2rf:     Produce from write format string corresponding read format string
; + wr:       Writing scalar and array data of all types
; . wrfifo:   Write file header
;  wrhdme:    Write header of variable, input: term table.
;  wrhead:    Write header of variable, input: line table.
; + wrlabl:   Write label
; + wrtab:    Write table of integer, real, and/or character data to file
;*****
; Include-Files uio_*.pro:
;  filedefinc:
;  uiocstinc:  channel status information (common uio_chainf)
;  uiocvlinc:  convert type list of current machine (common uio_cvlist)
;  uionaminc:  names of types, keywords, identifiers; default formats
;              (common uio_defnam)
;  uiosizinc:  length of strings, size of tables (trmtab, lintab)
;  uiotabinc:  empty table structure (common uio_taborg)
;*****

```

Most of the routines are low-level ones and do not have to be worried about because they rarely will be used directly.

For accessing data in UIO format within IDL the initialization routine `uio_init` (see Sect. 6.2.7.1) and the high-level reading routines (`uio_struct_rd.pro`, `uio_dataset_rd.pro`, and `uio_datasetlist_rd.pro`, see Sect. 6.2.7.3) might suffice.

6.2.7.1 Initialization of UIO routines under IDL

The directory containing the IDL UIO routines should be added to the IDL variable `!PATH`. This could be done by a program segment in the startup procedure, like:

```

; --- Try to determine language ---
if (n_elements(!X.TICKV) eq 150) then langua='WAVE' else langua='IDL'

```



```

;
; --- Add user IDL directory to search path ---
if (langua eq 'IDL') then begin &$
  addpath=expand_path('+$UIOPATH/idl') &$
endif else begin &$
  addpath='/home/supas024/uio/idl' + ':' + '/home/supas024/wave' &$
endif
if strtrim(addpath,2) ne '' then !path=addpath+':'+!path
delvar, addpath

```

Alternatively, one might want to set the IDL path variable accordingly like

```
export IDL_PATH="+$UIOPATH/idl"
```

for example in the `.bashrc` file. Or one just copies or links the UIO IDL routines to a location in the standard IDL search path.

It is reasonable to include the UIO initialization in the startup procedure as e.g.:

```

; --- Initialize uio-routines ---
uio_init, progrm='by hand'

```

IDL can handle the conversion types `native`, `ieee_4`, `ieeele_4`, `ieee`, `idl`, `xdr` (compare Tab. 6.2 in Sect 6.2.3.1). Here, `ieee_4` is the default and should be used as a standard.

Attention: The IDL type “long” corresponds to the standard Fortran type “integer”. The IDL types “byte” and “integer” are not known in standard Fortran and are therefore transformed to the IDL type “long” before writing (in the IDL routine `uio_wr`).

Be aware of: The parsing and interpretation of the entry headers can only be done by scalar operations which are comparatively slow in IDL.

6.2.7.2 Reading data with `uio_data.pro`

The IDL routine `uio_data` and the IDL function `uio_d` were the first set of “high-level” routines to read UIO data in IDL. They were useful for the easy reading of not too complex data files. By now, they are replaced by the routines `uio_struct_rd` and `uio_dataset_rd` (see see next Section and Sect 10).

The old routines allow the opening,

```

uio_data, mode='open', filename='model.dat'
uio_data, mode='open', filename='model*.txt'
uio_data, mode='open', filename='model.dat', family='mod1'
uio_data, mode='open', filename='model*.txt', family='mod2'

```

examination,

```

uio_data, mode='content'
uio_data, mode='files'

```

reading,

```

uio_data, mode='read', value=rho, 'rho'
uio_data, value=temp, 'temp'
uio_data, value=p, 'p', filename='model.dat'
uio_data, value=p, 'p', family='mod1'
plot_oi, uio_d('p'), uio_d('t')

```

and closing,

```

uio_data, mode='close', filename='model.dat'
uio_data, mode='close', filename='model*.txt'
uio_data, mode='close', family='mod2'
uio_data, mode='allclose'

```

of UIO files.

6.2.7.3 Reading data with `uio_dataset_rd.pro` or `uio_datasetlist_rd.pro`

For a detailed description of how to handle UIO files in IDL see Sect 10.

With the new IDL routines `uio_struct_rd.pro`, `uio_dataset_rd.pro`, and `uio_datasetlist_rd.pro` files are not read entry by entry anymore but in larger blocks (or “data sets”).

With `uio_struct_rd` all entries in a file are read and put into an IDL structure variable. This is appropriate for the CO5BOLD parameter file or for the UIO table file in Sect. 6.2.3.3, e.g.

```
par=uio_struct_rd('st35gm04n05_03.par')
atm=uio_struct_rd('holmu.atm')
```

When groups of entries in an UIO file are properly marked with `label dataset` and `label enddataset` delimiters (confer the example in Sect. 8.1) each group can be accessed with `uio_dataset_rd`. The first block can be read with

```
ful=uio_dataset_rd('st35gm04n05_03.full')
```

or

```
ful=uio_dataset_rd('st35gm04n05_03.full', ndataset=0)
```

Dataset number `i+1` (counting starts at zero) can be read with

```
ful=uio_dataset_rd('st35gm04n05_03.full', ndataset=i)
```

If a dataset with that number does not exist, an empty structure is returned. In this case, when called with additional keywords like

```
ful=uio_dataset_rd('st35gm04n05_03.full', ndataset=i, outstr=outstr, ierr=ierr)
```

an error message is returned in `outstr` and `ierr` is set to a value larger than 0.

To read all entries in a list of files in sequence the routine `uio_datasetlist_rd.pro` is convenient, as in the short example

```
ierr=0
delvar, listdata
;
; --- Loop over all datasets ---
while (ierr eq 0) do begin &$
; --- Read the next dataset ---
ful=uio_datasetlist_rd('testmodel_0?.full', listdata=listdata, ierr=ierr) &$
if (ierr eq 0) then begin &$
print, '--- ', ful.z.time, format='(A,E15.8)' &$
;
; --- Now do the data handling (demo) ---
print, 'Mean density: ', avg(ful.z.rho) &$
endif &$
endwhile
```

or in the more detailed example

```
model='st33gm06n03' & modelident='_??' & parmodelident='_01'
modeldisk=getenv('HOME') + '/dat/rhd/d' + model + '/'
;
modelfile=modeldisk + model + modelident + '.full'
parfile =modeldisk + model + parmodelident + '.par'
;
; --- Read parameter file ---
par=uio_struct_rd(parfile)
```

```

;
; --- Open first dataset to get some information about array sizes ---
delvar, listdata
ful=uiio_datasetlist_rd(modelfile, listdata=listdata, ierr=ierr)
uiio_closrd, listdata.channel
delvar, listdata
;
nxc1=n_elements(ful.z.xc1)
nxc2=n_elements(ful.z.xc2)
nxc3=n_elements(ful.z.xc3)
;
n_timestep=1000 ; --- Some huge value to get everything. Reduce for tests! ---
ierr=0
i=0
;
; --- Loop over all datasets ---
while ((ierr eq 0) and (i lt n_timestep)) do begin &$
; --- Read the next dataset ---
ful=uiio_datasetlist_rd(modelfile, listdata=listdata, ierr=ierr) &$
if (ierr eq 0) then begin &$
print, '--- ', i, ful.z.itime, ful.z.time, format='(A,I4,I6,E15.8)' &$
;
; --- Now do the data handling (demo) ---
print, 'Mean density: ', avg(ful.z.rho) &$
;
i=i+1 &$
endif &$
endwhile

```

All necessary counter information is stored in the structure `listdata`.

Note, that you can specify an entire group of files with e.g. `modelident='_*`, `modelident='_??'`, `modelident='_3?'`, or `modelident='_[29,3[0-2]]'`.

Chapter 7

Input and control files

7.1 Parameter file: `rhd.par`

The parameter file `rhd.par` also has the UIO format. But it will be usually Fortran “formatted” (ASCII).

It contains a list of parameter entries, which are collected in groups to make it easier to find an entry. Otherwise, the order is arbitrary (except for the very first `fileform uio` entry). If there are more than one entry with the same name, the first occurrence will be used by CO5BOLD. But the doubling of entries is strongly discouraged because it will almost certainly lead to confusion at some time. In addition, the IDL routine to read the parameter file will fail with an error message.

Additional entries can be added if the names differ from the standard ones described below. These entries will be ignored by CO5BOLD but read by the IDL input routine. They can be used to provide comments, additional information about the model, or control parameters for further processing.

7.1.1 Quickstart: How to make a proper parameter file

You will never write a new parameter file from scratch. Typically, you take an old file (e.g. the one controlling the simulation which produced the model which is used to start the new run) and edit it:

1. Take the parameter file corresponding to the model you want the new simulation to start with. Most of the parameters should be already OK.
2. Write a brief description of the purpose of the planned simulation into the `character description` array (Sect. 7.1.2.3). You might add a remark about the parent file of the parameter file under construction and the current date into the `character history` (Sect. 7.1.2.4) array in the header (see Sect. 7.1.2).
3. Check/modify the name of start model and output files: `infile_start` (Sect. 7.1.21.8), `outfile_end` (Sect. 7.1.21.10), `outfile_full` (Sect. 7.1.21.11), `outfile_mean` (Sect. 7.1.21.12), etc. On a system with batch queue this has not to be done in the parameter file itself but in the external command file (see Sect. 7.1.21).
4. Check/modify the fundamental parameters including boundary condition specifiers (see Sections 7.1.3 and 7.1.4, respectively)
 - effective temperature: `heat_mode` (Sect. 7.1.4.4), `s_InFlow` (Sect. 7.1.4.7), `Teff` (Sect. 7.1.3.1), `LuminosityPerVolume` (Sect. 7.1.4.6), ...
 - gravity: `grav_mode` (Sect. 7.1.3.2), `grav` (Sect. 7.1.3.3), `mass_star` (Sect. 7.1.3.4), ...
 - abundances: `eosfile` (Sect. 7.1.6.1), `opafile` (Sect. 7.1.7.1). Check the paths `eospath` (Sect. 7.1.6.2) and `opapath` (Sect. 7.1.7.2)!
 - boundary conditions:
5. If the gravity of the new model – and therefore the characteristic length and time scales – significantly deviate from the values of the old one, some values have to be scaled accordingly:

- the time specifications controlling the output frequency: `dttime_out_full`, `dttime_out_mean`, ...
- the total length of the simulation if specified as stellar time: `endtime`, `plustime`,
- absolute boundaries for the time step: `dttime_min`, `dttime_min_stop`, `dttime_max`, `dttime_start`
- some radii for global models,
- some scale length for some boundary conditions,

Look for parameters with units `u=s` or `u=cm` (see Sections 7.1.20 and 7.1.21).

6. The rest of the parameters controls additional details. Most of the constants are specified in dimensionless form and keep their value in a class of related simulations. The previously used values will probably be reasonable for the new simulation, too. However, if typical Mach numbers or ratios of radiative to advective time scales change significantly, also the values of the dimensionless parameters should be checked.

Of course, a complete control of CO5BOLD is only possible after studying of the meaning of the parameters in detail (e.g. by reading the following pages) AND – unfortunately – an accompanying look into the source codetself.

7.1.2 Header

The header of the parameter file contains information about the file format and contents. The `description` array can be used to specify the goal of the simulation, special model characteristics, or important parameter changes compared to a previous or standard model. The `history` array may contain the predecessor of the parameter file to simplify a tracing of parameter changes.

7.1.2.1 fileform uio

The header of the parameter file, e.g.

```
fileform uio form=formatted convert=ieee_4 date='2002-01-01' &
  program='by hand'
```

can be abbreviated to

```
fileform uio form=formatted convert=ieee_4
```

which indicates that the file is in UIO form and Fortran “formatted” (ASCII). The specification of the conversion type (“`convert=ieee_4`”) is more relevant for unformatted files. These terms should not be changed. But it can be of interest to append e.g. the date of the last modification (e.g. “`date='2002-12-24'`”).

7.1.2.2 character file_id

The file identification string

```
character file_id f=A80 b=80 n='File identification'
rhd-parameter
```

indicates the intended use of the file as parameter file for the RHD code CO5BOLD. Do not edit!

7.1.2.3 character description

The header of the file can (should) contain a short description of the simulation, as in e.g.

```
character description d=(1:4) f=A80 p=1 b=80 n='File description'
Parameter file for RHD code:
Full size 3D Betelgeuse model: 5 M_Sun, 650 R_Sun
Start with st35gm04n03_09.end (127^3 -> 171^3)
Run with SHORTrad
```

This entry is optional (it can be omitted completely) but it is recommended to put at least some relevant keywords into this array. If you change the number of lines (between 1 and 20) you have to adjust the size specification (“`d=(1:4)`” in the example above).

7.1.2.4 character history

The file history has a similar purpose as the previous entry. It can be used to keep information about the “parent” parameter file, as in

```
character history d=(1:2) f=A80 p=1 b=80 n='File history'
Taken from st35gm04n03_09.par
Last Modification:      2002-01-01
```

Its use is optional.

7.1.3 Fundamental model parameters

7.1.3.1 real teff

The effective temperature is one of the basic model parameters and is specified e.g. with

```
real teff f=F13.3 b=4 n='Effective Temperature' u=K
3500.0
```

(for a relatively cool star). Note that this parameter specifies the average output flux only for local models with closed radiative lower boundary and that in many cases the actual effective temperature can only be determined a posteriori. For other lower (or inner boundary conditions) the entropy of the instreaming material `s_inflow` (see below) is more important than `teff` itself. See Sect. 7.1.4.4 for different heating modes controlled with `heat_mode`.

7.1.3.2 character grav_mode

Gravity is another characteristic of a stellar atmosphere. The type (or geometry) of the external gravity field has to be specified e.g. with

```
character grav_mode f=A80 b=80 n='Type of gravity field' &
c0='constant/central'
central
```

Three values are possible so far:

- **central**: For the global “star-in-a-box” case, a central potential is assumed with origin at $x=0$. The stellar mass `mass_star` (Sect. 7.1.3.4) as well as some characteristic radii (`r0_grav`, `r1_grav`, `r2_grav`, `r1_core`) have to be specified.
- **constant**: In the standard local “box-in-a-star” case, the constant gravity specified with `grav` (Sect. 7.1.3.3) is directed downward in x_3 direction.
- **localboxtide**: This activates a simple model for the action of a tidal wave on convection in a local box model. It adds to the case of **constant** gravity a potential $\hat{\Phi}_{\text{ex}}$ which is harmonic in space and time according to

$$\Phi_{\text{ex}} = \hat{\Phi}_{\text{ex}} \cos(k_{\text{h}}x_1 + \omega t). \quad (7.1)$$

It is intended to mimic a travelling tidal wave. Since the setup is considered experimental the parameters are set by the `C_test` parameters according:

$$\begin{aligned} \hat{\Phi}_{\text{ex}} &= \text{C_test1} \text{ (amplitude of potential variations)} \\ k_{\text{h}} &= \text{C_test2} \text{ (horizontal wavenumber)} \\ \omega &= \text{C_test3} \text{ (frequency)} \end{aligned}$$

Boundary conditions: in order to be compatible with periodic lateral boundaries k_{h} should be an integer multiple of 2π times the inverse lateral box size.

7.1.3.3 real grav

In the case of a constant gravity the amount of the acceleration has to be specified with

```
real grav f=E15.8 b=4 n='Gravity' u=cm/s^2
27500.0
```

Setting this value to zero switches off gravity.

7.1.3.4 real mass_star

In the case of a central the mass (in cgs units) of the star has to be specified with

```
real mass_star f=E15.8 b=4 n='Stellar Mass'      u=g
  9.94500e+33
```

7.1.3.5 real r0_grav

To avoid the central singularity in a $1/r$ potential it is smoothed in the center to give a central potential of $1/r0_grav$, specified with

```
real r0_grav   f=E15.8 b=4 n='Inner Smoothing Radius'  u=cm
  9.45833e+12
```

This parameter should always be non-zero for a central potential of a global model. For local models, this parameter specifies the depth of the lower heating and damping region, see Sect. 7.1.4.4.

7.1.3.6 real r1_grav

The density in an atmosphere in hydrostatic equilibrium can decline to very low values. To artificially enlarge the pressure (and density) scale height in the outer layers of the star (the corners of the box) the gravity can be reduced by defining the potential at infinity to be $1/r1_grav$, specified with

```
real r1_grav   f=E15.8 b=4 n='Outer Smoothing Radius'  u=cm &
  c0='0.0: Not used'
  11.35000e+13
```

Setting this parameter to zero gives the usual $1/r$ behavior of the potential in the outer layers but also chooses another smoothing formula in the central part (where $r0_grav$ is relevant). But a value somewhat larger than the remotest corner of the box effectively cancels this artificial smoothing in the outer layers.

7.1.3.7 real r2_grav

Using $r2_grav$ instead of $r1_grav$ means that a potential function more appropriate for a polytropic stellar interior model is used. It can be set, e.g. with

```
real r2_grav   f=E15.8 b=4 n='Outer Smoothing Radius'  u=cm &
  c0='0.0: Not used'
  11.35000e+13
```

Setting this parameter to zero means the potential parameterized with $r1_grav$ is used. This parameter is similar to $r1_grav$, i.e., it enlarges the pressure scale height in the outer layers but does not change the smoothing formula in the center. This parameter is only effective if $r1_grav$ is set to zero.

7.1.3.8 real r0_core

To insert energy in a sphere different with a radius other than $r0_grav$ (the default), the heating radius $r0_core$ can be specified separately, e.g. with

```
real r0_core   f=E15.8 b=4 n='Core Radius'      u=cm
  9.45833e+12
```

If this parameter is not specified or set to zero $r0_grav$ is used as the radius of the core.

7.1.3.9 character centrifugal_force

Usually, a centrifugal force is applied if `nu_rotation` $\neq 0$. To switch it off even for a non-zero rotation rate, the parameter `centrifugal_force` can be used, e.g. by setting

```
character centrifugal_force f=A80 b=80 n='Switch on/off the centrifugal force' &
  c0='on: default, off: no centrifugal force, even for non-zero nu_rotation'
off
```

Two alternative values are possible so far:

- **on:** This is the default and can be set even for non-rotating objects.
- **off:** This skips the application of the centrifugal force in case of a non-zero rotation rate. In this case, only the Coriolis force is applied.

By default, the centrifugal force is activated if the rotation rate `nu_rotation` is non-zero, but only for global models as the centrifugal force for local models would in effect only modify the value of the gravity constant.

7.1.3.10 real nu_rotation

To transform onto a rotating coordinate-system a rotation rate can be specified with e.g.

```
real nu_rotation f=E15.8 b=4 n='Rotation frequency' u=1/s
0.01
```

The potential is modified by adding terms due to a centrifugal force unless `centrifugal_force` is set to `off`. In addition, a Coriolis force is applied during the hydrodynamics step.

7.1.3.11 real ar_rotationaxis

The rotation axis can be specified with

```
real ar_rotationaxis f=E10.4 b=4 p=1 d=(1:3) n='Rotation axis' u=1
1.0
0.0
0.0
```

The default value is $(0.0, 0.0, 1.0)$ and should be used for rotating global models. A different axis only makes sense for local models.

7.1.4 Boundary conditions (general)

The boundary conditions at the six sides of the computational box cannot be specified independently. For the naming convention of the boundaries a gravitational acceleration in $-x_3$ direction is assumed. Accordingly, there is a bottom and a top boundary, and four side boundaries.

All boundary conditions of the hydrodynamic case are available in the MHD module.

7.1.4.1 character side_bound

The boundary condition at all four sides is given by e.g.

```
character side_bound f=A80 b=80 n='side boundary conditions' &
  c0='closed, transmitting, periodic'
transmitting
```

Possible values are:

- **reflective:** closed wall, no gravity, no radiation. The velocity vector is mirrored at the boundary.
- **constant:** open boundary with constant extrapolation of all values, no gravity, no radiation.
- **closed, closedtop:** closed wall, can handle gravity, open for outward radiation.

- **periodic**: periodic boundaries for hydrodynamics, radiation.
- **transmitting**: transmitting boundary for hydro and outward radiation.

Any of these values can be specified. But in fact, not all of them are recognized by all modules. Therefore some parameters are for test purposes (e.g. shock calculations) only. In simulations of a solar-like star with the MSrad radiation transport module the side boundaries *have* to be **periodic**. In simulations of a red supergiant all boundaries (including the sides) will typically be **transmitting**. As an alternative, closed boundaries can be chosen in this case.

7.1.4.2 character top_bound

The boundary condition at the top of the model is given by for instance

```
character top_bound    f=A80 b=80 n='top boundary conditions'
transmitting
```

Possible values are:

- **reflective**: closed wall, no gravity, no radiation. The velocity vector is mirrored at the boundary.
- **constant**: open boundary with constant extrapolation of all values, no gravity, no radiation
- **closed, closedtop**: closed wall, can handle gravity, open for outward radiation.
- **periodic**: periodic boundaries for hydrodynamics.
- **transmitting**: transmitting boundary for hydro and outward radiation: exponential decrease of density (standard open boundary condition).
- **transmitting2**: transmitting boundary for hydro and outward radiation: exponential decrease of density and extra velocity treatment.
- **transmitting3**: transmitting boundary for hydro and outward radiation: constant density extrapolation.

In almost every simulation of stellar convection a **transmitting** top boundary will be selected, the **closed** one is an alternative. The **periodic** condition is only recognized by the hydrodynamics routines and not by any radiation transport routine.

7.1.4.3 character bottom_bound

The boundary condition at the bottom of the model is given for instance by

```
character bottom_bound f=A80 b=80 n='bottom boundary conditions' &
c0=closedbottom
transmitting
```

Possible values are:

- **reflective**: closed wall, no gravity, no radiation. The velocity vector is mirrored at the boundary.
- **constant**: open boundary with constant extrapolation of all values, no gravity, no radiation.
- **closed, closedtop**: closed wall, can handle gravity, open for outward radiation.
- **closedbottom**: closed wall, handles gravity, radiation in diffusion approximation.
- **closedbottom2**: closed wall, handles gravity, radiation in diffusion approximation. In this version, the extrapolation of quantities should be smoother than for **closedbottom**.
- **periodic**: periodic boundaries for hydrodynamics.

- **transmitting**: transmitting boundary for hydro and outward radiation. The parameters `real c_tchange`, `real c_tsurf`, and `real c_hptopfactor` have to be specified.
- **inoutflow**: "classical" open lower boundary for deep convection, gravity and radiation possible. The parameters `real s_inflow`, `real c_schange`, and `real c_pchange` have to be specified.
- **inoutflow2**: variant of the open lower boundary condition. The parameters `real s_inflow`, `real c_schange`, and `real c_pchange` have to be specified. In this version, the extrapolation of quantities should be smoother than for `inoutflow`.

In simulations of a solar-like star with the MSrad radiation transport module the bottom boundary is typically of type "inoutflow". A supergiant simulation will have a `transmitting` lower boundary.

7.1.4.4 character heat_mode

The mode in which energy is supplied can be adjusted with this parameter. The classical choice is to leave it empty, in which case the mode is chosen from `s_inflow` (see Sect. 7.1.4.7) and `luminositypervolume` (see Sect. 7.1.4.6). Example:

```
character heat_mode f=A80 b=80 n='Heating mode' &
c0='-/'bottom_entropy1/bottom_energy1' &
c1='core_entropy1/core_energientropy1/core_energy1/core_energy2'
bottom_entropy1
```

Possible values, so far:

- : (empty). The classical value. For local models the energy comes through the lower boundary, either by radiation (for a closed bottom boundary `closedbottom`) or by convection + radiation (for an open bottom boundary `inoutflow`).
- `bottom_entropy1`: The entropy in the bottom layers (defined as being less than `r0_grav` above the bottom of the model) is adjusted towards `s_inflow` on a rate given by `c_schange`.
- `bottom_energy1`: Energy in the bottom layers (defined as being less than `r0_grav` above the bottom of the model) is added according to `teff`.
- `core_entropy1`: The entropy in the core is adjusted towards `s_inflow` on a rate given by `c_schange`.
- `core_energientropy1`: The entropy in the core is adjusted towards the mean core entropy (i.e., smoothed) on a rate given by `c_schange`. However, the total energy input is added according to `luminositypervolume`. This avoids a local pile up of energy in case of a strong core drag force (Sect. 7.1.4.22) or just slow flows.
- `core_energy1`: Energy in the core is added according to `luminositypervolume`.
- `core_energy2`: Energy in the core is added according to `luminositypervolume` with a Gaussian distribution of the energy source.

7.1.4.5 character hcoreheatprofile

This parameter allows to choose between various radial profiles for the core heating. It may be called by

```
character hcoreheatprofile f=A80 b=80 n='Core heat profile'
Constant
```

Possible values are:

- `Constant`, `Constantdei`: Apply the same change of e_i in all core volume elements, (old) default. This gives a larger change of ρe_i than `Constantdrhoei` in the central part of the core where the density is higher.
- `Constantdrhoei`: Apply the same change of ρe_i in all core volume elements.

7.1.4.6 real luminositypervolume

The luminosity of a “star-in-a-box” or a local model with the appropriate `heat_mode` can be set with this parameter. To avoid numbers that do not fit into a 4 Byte real the luminosity per volume has to be specified as e.g. in

```
real luminositypervolume f=E15.8 b=4 n='Luminosity per core volume' &
  u='erg/cm^3/s'
4.5E-02
```

The reference volume is $4/3 \pi r_{\text{grav}}^3$ or $4/3 \pi r_{\text{core}}^3$. If this parameter is set to a value of 0.0 or below the entropy of the material within the core (defined by as all cells within radius `r0_grav`) is adjusted instead.

7.1.4.7 real s_inflow

The entropy of the material streaming through an open boundary of type “inoutflow” into the model can be specified e.g. with

```
real s_inflow f=E15.8 b=4 n='Entropy of core material' &
  u=erg/K/g
3.25E+09
```

In the case of a `central` potential, the entropy in a sphere with radius `r0_grav` is adjusted towards this entropy value. In both geometries (supergiant as well as solar) this value is very important as it finally (but indirectly) determines the luminosity and effective temperature of the star. A value of 0.0 (default) or below disables this energy input.

7.1.4.8 real s_inflradgrad

In the case of a `central` potential, one can decrease the entropy in the very center of the core to generate some extra braking buoyancy, e.g. with

```
real s_inflradgrad f=E15.8 b=4 n='Radial gradient of core entropy' &
  u=erg/K/g
1.0E+06
```

While the value of the core entropy `s_inflow` is typically of the order of 1.0E+09, this parameter is typically of the order of 1.0E+06. A value of 0.0 (default) causes a zero gradient.

7.1.4.9 real s_inflatgrad

In the case of a `central` potential, one can enforce a meridional flow (the x_3 axis is the z axis) by enforcing a lateral entropy gradient in the core, e.g. with

```
real s_inflatgrad f=E15.8 b=4 n='Lateral gradient of core entropy' &
  u=erg/K/g
1.0E+06
```

This might come useful in the case of rotating models. While the value of the core entropy `s_inflow` is typically of the order of 1.0E+09, this parameter is typically of the order of 1.0E+06. A value of 0.0 (default) causes a zero gradient.

7.1.4.10 real c_schange

The entropy `s_inflow` of the material in the bottom layer (solar case, `inoutflow` boundary condition) or the central region of the (global) model is not just set to the specified but adjusted towards it. The adjustment rate can be controlled with e.g.

```
real c_schange f=E15.8 b=4 &
  n='Rate of entropy change for open lower boundary' u=1
0.3
```

Guide values are

- 1.0: fast adjustment
- 0.3: typical value
- 0.1: slow adjustment
- <=0.0: not allowed

7.1.4.11 real c_pchange

The `inoutflow` boundary condition not only controls entropy and velocity but also the pressure in the bottom layers: It is locally adjusted towards the global average to damp out possible instabilities. The adjustment rate can be specified e.g., with

```
real c_pchange f=E15.8 b=4 &
  n='Rate of pressure change for open lower boundary' u=1
1.0
```

7.1.4.12 real c_v3changelinbottom

For the open lower boundary condition (`inoutflow` and `inoutflow2`), a damping of the vertical velocity at the open boundary can be specified, e.g., with

```
real c_v3changelinbottom f=E15.8 b=4 &
  n='Linear velocity reduction rate at bottom' u=1
0.0025
```

The open lower boundary condition tends to produce a slight reduction of the horizontal velocities at the very bottom. As the HD solver does not apply any extra viscosity at the bottom layers (the MHD solver has this option), there is a tendency to produce a slight predominance of vertical velocities in the regions where matter enters the computational box through the lower boundary. By introducing a little bit of damping of the vertical velocity component, this tendency can be significantly reduced. Guide values are

- 0.0: off: no linear damping
- 0.002: small reasonable value
- 0.005: large, possible useful value

7.1.4.13 real c_v3changesqrbottom

For the open lower boundary condition (`inoutflow` and `inoutflow2`), an additional damping of the vertical velocity at the open boundary can be specified, e.g., with

```
real c_v3changesqrbottom f=E15.8 b=4 &
  n='Quadratic velocity reduction rate at bottom' u=1
0.002
```

This damping is stronger for velocities that exceed the rms value of the velocities averaged over the entire bottom layers.

7.1.4.14 real c_visbound

An additional drag force can be added locally in inflow cells in the outer layer when the `transmitting` boundary condition is chosen. The value can be set e.g. with

```
real c_visbound f=E15.8 b=4 &
  n='Boundary drag viscosity parameter' u=1
0.001
```

This extra drag force is usually not necessary and should be switched off (with `c_visbound=0.0`).

7.1.4.15 real c_rhochangetop

The `transmitting` upper boundary condition can smooth density fluctuations with this parameter. It is locally adjusted towards the global average to damp out possible instabilities. It appears to be useful for the HLLMHD solver. For simulations without magnetic fields, there is no need to set this parameter, so far. The adjustment rate can be specified e.g. with

```
real c_rhochangetop f=E15.8 b=4 &
  n='Rate of density change for open upper boundary' u=1
  1.0
```

Obs.: So far, this parameter only switches the density damping on or off. All positive values have the same effect as a value of 1.0.

7.1.4.16 real c_tchange

In the case of a `transmitting` upper or outer boundary the temperature of the material streaming into the model is adjusted with a rate given e.g. by

```
real c_tchange f=E15.8 b=4 &
  n='Rate of temperature change for open upper boundary' u=1
  0.3
```

7.1.4.17 real c_tsurf

In the case of a `transmitting` upper or outer boundary the temperature of the material streaming into the model is adjusted towards a temperature $t_{\text{eff}} \cdot c_{\text{tsurf}}$. This temperature can be specified as fraction of the effective temperature e.g. with

```
real c_tsurf f=E15.8 b=4 n='Temperature factor for open upper boundary' u=1
  0.62
```

The value depends on where the outer boundary is located relative to the photosphere: If the boundary lies at a point where the solar photospheric minimum temperature is located, it can be fairly small. If the boundary is far away from the photosphere of a red supergiant, the value can be even smaller. On the other hand, if the boundary lies somewhere within the solar chromosphere even values above 1.0 might be reasonable.

7.1.4.18 real c_hptopfactor

In the case of a `transmitting` upper or outer boundary the density stratification outside the model has to be extrapolated properly. Assumptions about this density affects the amount of mass flowing into the model. For the extrapolation it is assumed that the density scale H_ρ scales with the pressure scale height H_p as $H_\rho = H_p / c_{\text{hptopfactor}}$.

```
real c_hptopfactor f=E15.8 b=4 &
  n='Correction factor for surface pressure scale height' u=1
  0.8
```

Possible values are

- $C < 0.0$: No effect (actually, a value of 1.0 is chosen).
- $0.0 \leq C < 1.0$: The density scale height is enlarged to account for possible effects of turbulent pressure on the scale height: The density decays less rapidly with height than in an (isothermal) hydrostatic stratification.
- $C = 1.0$: Density scale height is pressure scale height.
- $C \geq 1.0$: Density scale height is smaller than pressure scale height. Not really useful.

7.1.4.19 real c_radhtautop

Boundary conditions open for (essentially) emergent radiation need the specification of the scale height of the optical depth to allow for small amounts of irradiation. The parameter can be set e.g. with

```
real c_radhtautop f=E15.8 b=4 n='Scale height of optical depth at top' u='1'
60.0E+05
```

Possible values are

- $C > 0.0$: Older version: $\tau_0(x1, x2) = C * \kappa(x1, x2)$ (both MSrad and SHORTRAD).
- $C \leq 0.0$: New version: $\tau_0(x1, x2) = \text{abs}(C) * H_p(x1, x2) * \kappa(x1, x2)$. In this case, a value of `C_radHtautop=-1.0` might be a good choice (MSrad only).

7.1.4.20 real r1_rad

For a “star-in-a-box” and particularly when only “simple” ray directions are allowed in the radiation transport step the temperature in the outer corners of the box tends to become very small. To artificially increase the effect of radiative heating the parameter `r1_rad` can specify a radius beyond which only positive contributions of the radiative energy transport to the energy budget are taken into account. This ruins the conservativity of the code in these layers and should be applied only in very remote corners which are then considered only as sort of extended boundary region but not as part of the “real” model. The parameter can be specified e.g. with

```
real r1_rad f=E15.8 b=4 n='Outer radiation transport radius' u=cm &
c0='0.0: Not used'
8.00000e+13
```

A value of 0.0 (default) or below deactivates this feature.

7.1.4.21 real rho_min

During long periods of matter infall the density at an open outer boundary can become very low. To limit the decrease of the density a lower limit in the extrapolated ghost cells can be set e.g. with

```
real rho_min f=E15.8 b=4 n='Minimum boundary density' u=g/cm^3
1.0E-25
```

The density within the model will typically not fall much below this value. A value of 0.0 (default) or below deactivates this feature.

7.1.4.22 real c_coredrag

To damp the flow in the core of models with central potential a drag force restricted to the inner part of the model ($r < r0_grav$) can be applied. It is controlled e.g. with

```
real c_coredrag f=E15.8 b=4 n='Core drag force parameter' u=1
1.0
```

A value of 0.0 (default) or below deactivates this feature.

7.1.4.23 character hcoredragprofile

This parameter allows to choose between various radial profiles for the core drag force used to damp motions in the core of global models. It may be called by

```
character hcoredragprofile f=A80 b=80 n='Core drag profile'
Linear
```

Possible values are:

- **Constant**: Use a local drag force that depends on core radius `r0_grav`, local sound speed, and `real c_coredrag` (default). The overlaid radial profile is a constant.

- **Linear**: Use a local drag force that employs as overlay a linear decay from center to `r0_grav`.
- **Cosine**: Use a local drag force that employs as overlay a cosine function from center to `r0_grav`.
- **CosSqr**: Use a local drag force that employs as overlay a (\cosine^2) function from center to `r0_grav`.
- **Constant-Radial**: Use the same radial profile as **Constant** but apply the drag force to the radial velocity component only.
- **Linear-Radial**: Use the same radial profile as **Linear** but apply the drag force to the radial velocity component only.
- **Cosine-Radial**: Use the same radial profile as **Cosine** but apply the drag force to the radial velocity component only.
- **CosSqr-Radial**: Use the same radial profile as **CosSqr** but apply the drag force to the radial velocity component only.
- **Constant-Meridional**: Use the same radial profile as **Constant** but apply the drag force to the meridional velocity components only (x_3 is the z axis).
- **Linear-Meridional**: Use the same radial profile as **Linear** but apply the drag force to the meridional velocity components only.
- **Cosine-Meridional**: Use the same radial profile as **Cosine** but apply the drag force to the meridional velocity components only.
- **CosSqr-Meridional**: Use the same radial profile as **CosSqr** but apply the drag force to the meridional velocity components only.

7.1.5 Boundary conditions (MHD only)

The following parameters are specific to MHD simulations. For MHD calculations they must be set additional to the hydrodynamic boundary parameters.

7.1.5.1 `character side_bound_mag_x1` and `side_bound_mag_x2`

The boundary condition at the sides perpendicular to the x_1 direction and perpendicular to the x_2 direction, respectively. They are given by e.g.

```
character side_bound_mag_x1  f=A80 b=80 n='side boundary conditions magnetic x1'
fixed
character side_bound_mag_x2  f=A80 b=80 n='side boundary conditions magnetic x2'
periodic
```

Possible values are:

- **constant**: constant extrapolation of all magnetic field components into the ghost cells.
- **periodic**: periodic continuation of all magnetic field components into the ghost cells.
- **fixed**: the component normal to the boundary is kept fixed at its initial value. Constant extrapolation applies for the transversal components.
- **vertical**: constant extrapolation for the vertical component. The transversal cell-centered field is mirrored, with the opposite sign. That should result in transversal components of the boundary-centered field being zero at the boundary.
- **vertical2**: constant extrapolation for the vertical component. The transversal cell-centered field is set to zero.

- **reflective**: The magnetic field is mirrored at the boundary. This boundary condition is unphysical, because the magnetic field is an axial vector and because it violates the divergence free property of the magnetic field. Therefore, this boundary condition should be used with caution.

The **fixed** conditions are realized by setting the electric field at those cell edges that coincide with the physical boundary zero. This is done in the constrained transport module.

7.1.5.2 character top_bound_mag

The boundary condition at the top of the model is given by for instance

```
character top_bound_mag f=A80 b=80 n='bottom boundary conditions magnetic'
vertical
```

Possible values are:

- **constant**: constant extrapolation of all magnetic field components into the ghost cells.
- **periodic**: periodic continuation of all magnetic field components into the ghost cells.
- **fixed**: the component normal to the boundary is kept fixed at its initial value. Constant extrapolation applies for the transversal components.
- **vertical**: constant extrapolation for the vertical component. The transversal cell-centered field is mirrored, with the opposite sign. That should result in transversal components of the boundary-centered field being zero at the boundary.
- **vertical2**: constant extrapolation for the vertical component. The transversal cell-centered field is set to zero.
- **oblique**: magnetic fields with a given inclination at the boundary. The inclination is specified through parameters `C_magthetaB` and `C_magphiB`.

7.1.5.3 character bottom_bound_mag

The boundary condition at the bottom of the model is given by for instance

```
character bottom_bound_mag f=A80 b=80 n='bottom boundary conditions magnetic'
inoutflow
```

Possible values are:

- **constant**: constant extrapolation of all magnetic field components into the ghost cells.
- **periodic**: periodic continuation of all magnetic field components into the ghost cells.
- **fixed**: the component normal to the boundary is kept fixed at its initial value. Constant extrapolation applies for the transversal components.
- **vertical**: constant extrapolation for the vertical component. The transversal cell-centered field is mirrored, with the opposite sign. That should result in transversal components of the boundary-centered field being zero at the boundary.
- **vertical2**: constant extrapolation for the vertical component. The transversal cell-centered field is set to zero.
- **oblique**: magnetic fields with a given inclination at the boundary. The inclination is specified through parameters `C_magthetaB` and `C_magphiB`.
- **inoutflow**: magnetic field can be advected into the computational domain by ascending material flow. Its strength can be specified with the parameter `b1_inflow`. The boundary condition for the hydrodynamic variables must be set to `inoutflow` too, otherwise this boundary condition is the same like constant.

In the case of `inoutflow` the magnetic field, which is advected into the computational domain has a unique component which is in the `x1` direction and it is only present where a velocity in the positive `x3` direction exists. In all other places, the magnetic field components are constantly extrapolated into the ghost cells.

7.1.5.4 real `b1_inflow`

This parameter controls the strength of the inflowing horizontal magnetic field at the lower boundary in connection with `bottom_bound_mag=inoutflow`. The default value is 0.0. Example:

```
real b1_inflow f=E15.8 b=4 &
    n='Strength of inflowing horizontal magnetic field'          u=G
10.0
```

The unit of this parameter is gauss (no factor $\sqrt{4\pi}$!).

7.1.5.5 real `c_magthetab`

This parameter specifies the angle between the magnetic field vector and the `x3`-axis (in radians) in the case of oblique boundary conditions. The default value is 0.0. Example:

```
real c_magthetab f=E15.8 b=4 &
    n='angle magnetic field w.r. to the vertical direction' &
    u=rad c0='used in combination with oblique conditions'
0.523598775598299
```

7.1.5.6 real `c_magphib`

This parameter specifies the angle between the horizontal component of the magnetic field vector and the `x1`-axis (in radians) in the case of oblique boundary conditions. The default value is 0.0. Example:

```
real c_magphib f=E15.8 b=4 n='angle magnetic field w.r. to the x-axis' &
    u=rad c0='used in combination with oblique conditions'
0.0
```

7.1.6 Equation of state

7.1.6.1 character `eosfile`

The equation of state file together with the opacity file implicitly determine the chemical composition. The EOS file can be specified for instance with

```
character eosfile f=A80 b=80 n='EOS file name' &
    c0=eos_gamma140.eos/eos_mm20_1.eos/eos_mm00_13.eos
eos_mm00_15.eos
```

There exists an increasing number of files, e.g.:

- `eos_mm00_13.eos`: Standard EOS file for solar composition with extra large density range (towards low densities). There exist two other files for the same composition but smaller density range (`eos_mm00.eos`, `eos_mm00_1.eos`)
- `eos_XXXX_14.eos`: Several EOS tables for various compositions.
- `eos_mm00_15.eos`: EOS file for solar composition, with temperature range extended to very low values by keeping μ fixed below 500 K. The number of points for the density sampling has been reduced. The number of points for the energy sampling has been increased.
- `eos_mm20_1.eos`: Standard EOS file for metal-poor star ($[M/H]=-2.0$) with extended range in internal energy and density (towards lower values). The older file (`eos_mm20.eos`) did not reach far enough.

- `eos_gamma140.eos`: EOS table for simple gas with constant $\Gamma=1.4$. In this case all quantities could be faster computed than by interpolation in a table. Nevertheless, for compatibility reasons (to be able to use the existing EOS Fortran routines), the table is provided.
- `eos_gamma166.eos`: EOS table for simple gas with constant $\Gamma=5/3$.
- `cpheos_mm00.eos`: Copenhagen EOS for (their) solar composition.

7.1.6.2 character eospath

The equation of state file does not have to be in the working directory. Instead, its path can be specified e.g. with

```
character eospath f=A80 b=80 n='path of EOS file' &
  c0=/astro/b/bf/for/eos/dat
/home/bf/for/eos/dat
```

7.1.7 Opacities

7.1.7.1 character opafile

The opacity file can be specified with e.g.

```
character opafile f=A80 b=80 n='opacity file name' &
  c0=g2va.opta/big_grey.opta &
  c1='empty -> no radiation transport'
phoenix_opal_grey.opta
```

So far, there exist already a couple of files, for example:

- `davmf.opta`:
- `f5v.opta`:
- `g2va.opta`:
- `g2v_lowhe.opta`:
- `g2v_m20.opta`:
- `g2v.opta`:
- `hmin_p00.opta`:
- `opal_lowhe.opta`:
- `opal_m05.opta`:
- `opal_m10.opta`:
- `opal_m20.opta`:
- `phoenix_dust_grey.opta`:
- `phoenix_dust_ob4.opta`:
- `phoenix_opal_grey.opta`:
- `ross_m05.opta`:
- `ross_m10.opta`:
- `ross_m20.opta`:

- sunur1.opta:
- sunur2.opta:
- t5000g44mm20.opta:
- t5000g47mm20.opta:
- t6300g40mm20.opta:
- t6500g44mm20.opta:
- zzceti1g.opta:
- zzceti1.opta:

7.1.7.2 character opapath

The opacity file does not have to be in the working directory. Instead, its path can be specified e.g. with

```
character opapath f=A80 b=80 n='path of opacity file' &
c0=/astro/b/bf/for/opa/dat
/home/bf/for/opa/dat
```

7.1.8 Hydrodynamics control (HD and MHD)

Many parameters in the control file that are valid for the HD module also apply for the MHD module. A few parameters have somewhat different options for both modules (`hdtimeintegrationscheme`: Sect. 7.1.8.2, `hdsplit`: Sect. 7.1.8.3, `character reconstruction`: Sect. 7.1.8.4). Several parameters have meanings only for the HD (see Sect. 7.1.9) or the MHD module (see Sect. 7.1.10) and are ignored in the other one.

hdScheme	hdTimeIntegrationScheme	hdSplit	C_{CourMax}	$C_{\text{SndCourMax}}$	comment
Roe	Single	123	1		old default
Roe	Single	unsplit	$1/D$		don't use
Roe	Single	CTU	1	$1/2$ for $D=3$	recommended default
Roe	RungeKutta2	unsplit	$1/D$		small Mach-number flow
Roe	RungeKutta3	unsplit	$1/D$		
HLLMHD	Hancock	123	≈ 1		recommended default
HLLMHD	Hancock	unsplit	≈ 1		
HLLMHD	RungeKutta2	unsplit	$\approx 1/D$		
HLLMHD	RungeKutta3	unsplit	$\approx 1/D$		

Table 7.1: List of reasonable combinations of options for HD and MHD solver. The columns are the type of the (M)HD scheme, see Sect. 7.1.8.1, the time-integration scheme, see Sect. 7.1.8.2, the (directional) splitting method, see Sect. 7.1.8.3, the maximum Courant number (where D is the dimension of the computational box), see Sect. 7.1.20.6, the maximum sound-Courant number (where D is the dimension of the computational box) only specified for the case where it is actually a new constraint in addition to the normal Courant condition, see Sect. 7.1.20.9, and a comment.

7.1.8.1 character hdscheme

With this parameter, the type of the hydrodynamics scheme can be specified as in

```
character hdscheme f=A80 b=80 n='Hydrodynamics scheme' &
c0='Roe (approximate Riemann solver of Roe type)' &
c1='RoeMagKin (Roe solver + kinetic magnetic field transport)' &
c2='RoeMHD/HLLMHD (MHD solver)' &
```

```
c3='None (skip hydrodynamics step entirely)'
Roe
```

Possible values are

- **None:** The hydrodynamics step is skipped entirely (for test purposes). Note that in this case some initializations necessary for the generation of the mean file are omitted, too.
- **Roe:** (default) The standard approximate Riemann solver of Roe-type is activated. This value will be chosen for pure HD simulations without magnetic fields.
- **RoeMagKin:** The standard Roe solver is extended to transport passively a magnetic field. This is a test implementation to check if the general magnetic-field handling works. For proper MHD simulations use HLLMHD instead. This option is currently deactivated.
- **RoeMHD:** Use the MHD Roe solver. This option is currently deactivated.
- **HLLMHD:** Use the MHD HLL solver (the recommend value for MHD simulations).

7.1.8.2 character hdttimeintegrationscheme

With this parameter, the type of the time-integration scheme can be specified as in

```
character hdttimeintegrationscheme f=A80 b=80 n='Time-integration scheme' &
c0='Single/Hancock/Euler1/RungeKutta2/RungeKutta3'
Single
```

Possible values are

- **Single:** (default for HD Roe) Compute all updates in one single step. Terms higher order in time are provided by the Roe solver depending on the order of the reconstruction scheme.
- **Hancock:** (default for MHD HLLE) Terms of second order in time are approximated by a Hancock predictor step.
- **Euler1:** (only for MHD) A single Euler step is used, which is only first order in time.
- **RungeKutta2:** A two-step (predictor-corrector) Runge-Kutta step is used.
- **RungeKutta3:** A three-step Runge-Kutta step is used.

For possible combinations see Tab. 7.1.

7.1.8.3 character hdsplit

With this parameter, the type of the hydrodynamics operator (directional) splitting scheme can be specified as in

```
character hdsplit f=A80 b=80 n='Hydrodynamics directional splitting scheme' &
c0='123: directional splitting (default)' &
c1='unsplit: unsplit (direct) operator' &
c2='CTU: Colellas Corner Transport Upwind scheme (Colella, 1990)'
123
```

Possible values are

- **123:** (default) The standard directional splitting is activated, where the 1D operators for the individual directions are applied in the given order. So far, only the order 123 is possible.
- **unsplit:** The standard solver is applied. However, the changes from the individual steps are computed from (and applied to) the same model configuration. The result is an unsplit scheme.

- **CTU**: Use Colella’s ”Corner Transport Upwind” scheme (’CTU’, see Colella, 1990). It first computes and stores the changes from hydrodynamics in x_1 , x_2 , and x_3 direction. Then (half of) the contributions from the steps in x_1 and x_2 direction are used as sort of a predictor step for the full (’corrector’) step in x_3 direction (and accordingly for the two other directions). At the end, the three corrector-step contributions are added. That means, that two hydrodynamics steps have to be performed in each direction with some overhead for copying and adding the contributions. Still, together with e.g., `reconstruction=FRweno`, there is a significant improvement for convection at small Mach numbers compared to 123, `vanLeer`.

This parameter is recognized by `hdscheme=Roe` and `hdscheme=HLLMHD`, although `hdscheme=HLLMHD` does not know `hdsplit=CTU`.

7.1.8.4 character reconstruction

This parameter determines the order and “aggressiveness” of the reconstruction scheme with e.g.

```
character reconstruction f=A80 b=80 n='Reconstruction method' &
  c0=Constant c1=Minmod/VanLeer/Superbee c2=PP/PPmimo &
  c3=FRmimo,FRmono(2),FRweno(2),FRcont
FRweno2
```

Possible values are

- **Constant**: The run of the partial waves inside the cells is assumed to be constant. A highly dissipative first order scheme results. This values will usually only be used for test (or comparison) purposes.
- **Minmod**: Chooses the smallest slope which still results in a second-order scheme. It is the most diffusive (and most stable) one in this class.
- **VanLeer**: (default) The first-order reconstruction method. It was recommended and used in various simulations but is now replaced by a second-order reconstruction.
- **Superbee**: The “most aggressive” first-order reconstruction method. It results in the steepest shocks, which works well in some test cases but tends to turn smooth gradients into steps and might be too difficult for the radiation transport module to handle.
- **PPmimo**: MinMod reconstruction based on boundary values from PP.
- **PP**: Chooses the piecewise parabolic reconstruction of the PPM scheme (“Piecewise Parabolic Method”, see Colella & Woodward, 1984). Results in 3rd order accuracy for the advection.
- **FRmimo**: MinMod reconstruction based on boundary values from FRmono.
- **FRmono**: 2nd-order monotonic reconstruction derived from PP, WENO, and MinMod: “Frankenstein’s Method”.
- **FRmono2**: 2nd-order monotonic reconstruction derived from PP, WENO, and MinMod. It is identical to FRmono if `c_slopered=0.0` (the usually adopted default choice, see Section. 7.1.9.7). However, for `c_slopered>$>0.0`, it uses **Constant** reconstruction as fallback, instead of Minmod as FRmono does. This is the recommended fallback version for red-supergiant models.
- **FRweno**: 2nd-order non-monotonic version of FR. This (or **FRweno2**) is now the recommended value.
- **FRweno2**: 2nd-order non-monotonic version of FR. It is identical to FRweno if `c_slopered=0.0` (the usually adopted default choice, see Section. 7.1.9.7). However, for `c_slopered>$>0.0`, it uses **Constant** reconstruction as fallback, instead of Minmod as FRweno does. This is the recommended version for red-supergiant models.
- **FRcont**: 2nd-order continuous version of FR, unstable except for low Mach numbers.

- **HBweno**: Common WENO scheme based on three parabolas in a stencil, with an additional “handbrake” to fall back to a more stable (monotonic) scheme if the smoothness of all parabolas is bad. This scheme is (depending on the parameters) even less diffusive than **FRweno**. It is not strictly monotonic, neither.
- **VAweno**: Common (“vanilla”) WENO scheme based on three parabolas in a stencil. This scheme achieves very high resolution if the lack of monotonicity and general diffusivity can be accepted. It is identical to **HBweno**, but without the “handbrake” and therefore even a bit faster.

Usually, the **VanLeer** reconstruction has been a good choice. If a more stable (and diffusive) scheme was needed, **Minmod** could have been used. However, now the variants of the more recent 2nd-order “Frankenstein’s Method” are better choices, if the additional computational cost is acceptable. Even if it is not strictly monotonic, the **FRweno2** scheme seems to be a good general default for pure-HD models computed with the Roe solver. The **PP** reconstruction gives the highest accuracy. However, there is the possibility that it produces somewhat “noisy” models with small wiggles e.g. in the velocity for extreme cases – solar models look fine with **PP**. The newest options are **HBweno** and **VAweno**, which are closer to standard WENO schemes.

The options **Constant**, **SuperBee**, and **FRcont** are just for testing purposes: they have either too much, sometimes the wrong sign of, or too little diffusion, respectively.

The order of decreasing diffusivity and increasing accuracy is roughly (schemes on a line are similar; schemes in brackets are for testing only):

(**Constant**)

MinMod

FRmimo, **PPmimo**, **vanLeer**

FRmono

FRweno, **HBweno**, (**Superbee**)

PP, **VAweno**

(**FRcont**).

However, there are differences how the increase in accuracy is achieved: **vanLeer** uses (potentially dangerous) anti-diffusion (in contrast to **MinMod**) but needs only a 3-point stencil, whereas **PPmimo** and **FRmimo** don’t have anti-diffusion but need a (more expensive) 5-point stencil. **FRweno** achieves actually a 2nd-order-accurate reconstruction also near extrema for reasonably resolved structures (e.g., sufficiently long wavelengths of sine waves). I.e., it gives up strict monotonicity, whereas **PP** is strictly monotonic and achieves low dissipation from avoiding jumps at cell boundaries wherever possible. However, it chops off (flattens) extrema like all TVD schemes and it shows Gibbs wiggles near a jump that is not surrounded by constant plateaus but lies in a slope. The 2nd-order scheme **FRmono** is designed to suppress these wiggles, too. The highest-resolution schemes are **PP** (implemented in the MHD module, too) and **VAweno** (HD module only).

7.1.8.5 real c_gravmu

The time centering of the density that is used for the computation of the gravitational acceleration can be selected e.g. with

```
real c_gravmu f=E15.8 b=4 n='Gravity time centering' u=1 &
  c0='-1.0: use defaults depending on time-integration scheme' &
  c1='0.0: density at old time step; 0.5: centered; 1.0: new time step'
0.5
```

A value of 0.0 is the default for Runge-Kutta-type time integration. The others use 0.5. However, a larger value (the maximum is 1.0) leads to damping of oscillations in a stratified atmosphere. This is due to the fact that in a “normally stratified” atmosphere – where the density increases with depth – the density in any given grid cell usually increases with time during an *upward* motion (of course, the divergence of the flow field plays a role, too). Using the density for the computation of the *downward*-directed gravitational acceleration at a slightly later time increases this value leading to a stronger deceleration of the upward motion. This works analogously for downward motions. The parameter is recognized by the HD and the MHD module.

7.1.8.6 integer `n_hyditer`

After each complete hydrodynamic time step the recommendation for the next time step will be chosen so that `n_hyditer` iterations will (probably) be needed. The parameter can be set e.g. with

```
integer n_hyditer f=I4 b=4 &
      n='Number of hydrodynamics iterations' c0=10
8
```

For a simulation of a solar-type star it will typically be set to 1. E.g. for brown dwarfs with shorter hydrodynamical time scales values around 10 may be considered. Note, that the hydrodynamics iteration works somewhat differently than the radiation transport iteration: in the latter case the size of the actual time step can be determined after computing the fluxes, whereas the hydrodynamics step is (possibly) of at least second order in time and the time step has to be known in advance.

In the case of the MHD module, this can reduce the computation time significantly because the MHD time step is often much smaller than the other timestep limits. However, this parameter does not determine the number of substeps directly. Instead, the number of substeps is determined by the requested timestep and the timestep of each MHD substep which is determined by the standard Courant condition. So, the number of MHD substeps varies during the simulation. So, the exact value of this parameter has no direct influence on the number of substeps. If this parameter is set to zero, this feature is turned off. (See also parameter `va_max` for speeding up MHD simulations.)

7.1.8.7 integer `n_hydmaxiter`

The absolute maximum number of hydro iterations can be specified e.g. with

```
integer n_hydmaxiter f=I4 b=4 &
      n='Maximum number of hydro iterations' c0=14
0
```

If more iterations are needed the computation for the current time step is stopped and resumed with a smaller one. Usually, `n_hydmaxiter` will either be set to a value somewhat larger than the recommended number of iterations (`n_hyditer`) or to 0 which disables the check for too many iterations completely. This can be safely allowed in many cases. To disable the iteration of the hydrodynamics sub-step set `n_hyditer=0`.

In case of the MHD module, this parameter sets the maximum number of MHD-substeps. If this parameter is set to zero, the number of MHD substeps is not limited.

7.1.8.8 character `hdtmpstructkeepmode`

With this parameter, one can control if some temporary large 3D-array structures are kept during the run of the program or are only allocated when needed (and deleted immediately afterwards). The structures are used in the HYD, the MHD, and the VIS module. The parameter can be set e.g. with:

```
character hdtmpstructkeepmode f=A80 b=80 &
      n='Retaining mode for large temporary structures' &
      c0='Keep(new,default)/Delete(old)'
Keep
```

The choices are

- **Keep:** Keep the large temporary structures until the end of the program. This requires somewhat more memory (which during normal CO5BOLD runs is of no concern) but can improve the performance slightly, because particularly the deallocation of large arrays costs time (*new*, *default*).
- **Delete:** Delete the large temporary structures immediately after they have been used. This mode can be chosen if memory is a problem (*old*).

7.1.8.9 integer n_hydcellsperchunk

In every directional sub-step neighboring 1D columns are independent from each other. They can be grouped and computed in chunks of arbitrary size. The approximate number of grid cells per chunk can be specified e.g. with

```
integer n_hydcellsperchunk f=I9 b=4 &
  n='Number of cells per hydro chunk' &
  c0='0 => one 2D slice at a time' &
  c1='1 => minimum chunk size (inefficient)' &
  c2='1200: reasonable value' &
  c3='1000000000: maximum chunk size (inefficient and memory intensive)'
1600
```

The exact number is determined at run time to get (approximately) equal sizes of the individual chunks. The choice of this parameter does not affect the result of the computation but the memory usage and performance: smaller (and more) chunks may result in an optimum cache usage and need the smallest amount of memory, but result in additional overhead due to frequent subroutine calls. Bigger (and less) chunks are to be preferred for vector machines and processors with large caches. Very rough guide values may be

- 1200: Intel Xeon processor
- 2500: Intel Pentium III or Core 2 Duo processor
- 20000: RISC processor
- 100000: Vector machine

Note: For simulations with activated OpenMP on a parallel machine the chunk size has to be made small enough to allow at least as many chunks as processors (or threads) available. This is particularly important for models with a small number of grid points (e.g. 2D models). An example is given for the Hitachi SR8000 in Sect. 4.6.5.

7.1.9 Hydrodynamics control (HD only)

7.1.9.1 integer n_hydcellsperchunk2

Only for the HD solver and `hdsplit=CTU`, the chunk size in *i2* direction can be specified independently. The default is to used `integer n_hydcellsperchunk`. The approximate number of grid cells per chunk can be specified e.g. with

```
integer n_hydcellsperchunk2 f=I9 b=4 &
  n='Number of cells per hydro chunk 2' &
  c0='around 2400 or 1; 0: (default) use n_hydcellsperchunk'
1
```

The exact number is determined at run time to get (approximately) equal sizes of the individual chunks. The choice of this parameter does not affect the result of the computation but the memory usage and performance, similar to `integer n_hydcellsperchunk`. However, as accesses to chunks in *i2* direction span many memory pages, the access time is longer than for properly aligned chunks in *i1* direction and somewhat larger (twice...) values might be optimal. Alternatively, a value of `n_hydcellsperchunk2=1` causes a two-stage access where first an entire 2D slice is transposed and copied to achieve proper alignment and then the normal chunk size (specified with `integer n_hydcellsperchunk`) is used in a consecutive step.

7.1.9.2 integer n_hydcellsperchunk3

Only for the HD solver, the chunk size in *i3* direction can be specified independently. The default is to used `integer n_hydcellsperchunk`. The approximate number of grid cells per chunk can be specified e.g. with

```
integer n_hydcellsperchunk3 f=I9 b=4 &
  n='Number of cells per hydro chunk 3' &
  c0='around 2400 or 1; 0: (default) use n_hydcellsperchunk'
1
```

The exact number is determined at run time to get (approximately) equal sizes of the individual chunks. The choice of this parameter does not affect the result of the computation but the memory usage and performance, similar to `integer n_hydcellsperchunk`. However, as accesses to chunks in *i2* direction span many memory pages, the access time is longer than for properly aligned chunks in *i1* direction and somewhat larger (twice...) values might be optimal. Alternatively, a value of `n_hydcellsperchunk3=1` causes a two-stage access where first an entire 2D slice is transposed and copied to achieve proper alignment and then the normal chunk size (specified with `integer n_hydcellsperchunk`) is used in a consecutive step.

7.1.9.3 integer n_hydrkiter

In the case of `hdscheme = Roe` and `hdttimeintegrationscheme = RungeKutta2` (and only there), the default number of Runge-Kutta sub steps can be increased relative to the default value 2 to improve the performance in the case of a large ratio of radiative to hydrodynamical time scales. The parameter can be set e.g. with

```
integer n_hydrkiter f=I9 b=4 &
  n='Number of Runge-Kutta sub steps' &
  c0='2: default; 3: some acceleration'
3
```

Reasonable values are

- 2: (default) The standard predictor-corrector 2nd-order Runge-Kutta step number.
Cost: 2; advance 1; $C_{\text{hydSoundCourantMax}}=1/3$ = 0.333
- 3: Typical recommended value.
Cost: 3; advance 2; $C_{\text{hydSoundCourantMax}}=1/3*(3/2)^{(1/3)}=0.381$
- 5: Rather large, still sensible value.
Cost: 5; advance 4; $C_{\text{hydSoundCourantMax}}=1/3*(5/4)^{(1/3)}=0.358$

7.1.9.4 real c_hydlowmachcsfactor

For very low Mach numbers the over-sensitive sound-wave detection of the Roe solver (for 2D and 3D cases) can be suppressed by choosing a non-zero value for `real c_hydlowmachcsfactor`. This is in fact a tiny modification of the Roe solver but changes its behavior significantly and requires (for $C_{\text{hydLowMachcsFactor}} > 0.0$) `hdsplit=unsplit` and `hdttimeintegrationscheme=RungeKutta2` or `hdttimeintegrationscheme=RungeKutta3`. The value can be set e.g. with

```
real c_hydlowmachcsfactor f=E15.8 b=4 &
  n='Low-Mach-Number sound-speed reduction parameter' &
  c0='<=0.0: off (old settings, recommended default)' &
  c1='1.0: small value; 2.0: reasonable value; 5.0: large value'
2.0
```

Typical choices are

- 0.0: The extra reduction factor is not applied. This is the standard Roe scheme. It is still the recommended default, exceptd for very-low-Mach-number flows.
- 1.0: Smallest meaningful value to switch on the reduction.
- 2.0: Reasonable value
- 5.0: Rather large value

The default is not to use this reduction and leave the parameter at 0.0. However, the improvement for low-Mach-number flows is significant. This parameter is not recognized by the MHD module.

7.1.9.5 real c_hydlowmachcsbase

For very low Mach numbers the over-sensitive sound-wave detection of the Roe solver (for 2D and 3D cases) can be suppressed by choosing a non-zero value for `real c_hydlowmachcsfactor`. With `real c_hydlowmachcsbase`, a minimum value can be chosen as, e.g., in

```
real c_hydlowmachcsbase f=E15.8 b=4 &
  n='Low-Mach-Number sound-speed reduction base value' &
  c0='<=0.0: off (old settings); 0.001-0.02: reasonable values'
0.001
```

Typical choices are

- 0.0: The extra reduction factor is not applied. This is the standard Roe scheme. It is still the recommended default, exceptd for very-low-Mach-number flows.
- <1.0E-06: Dangerously small values
- 1.0E-06: Default
- 0.001 to 0.02: Reasonable values
- 1.0: Switch off the low-Mach-number sound-speed reduction

7.1.9.6 real c_hydsmallfluctfactor

In various equations in the Roe solver, an estimate of the relative size of fluctuations is made. With `real c_hydsmallfluctfactor`, a scaling factor can be chosen to fine tune the regime of the small-fluctuation treatment, as, e.g., in

```
real c_hydsmallfluctfactor f=E15.8 b=4 &
  n='Small/large-fluctuation estimate parameter' &
  c0='<1.0: smaller relative fluctuations ; 1.0: default; >1.0: larger fluctuations'
1.0
```

Typical choices are

- <1.0: Extend the small-fluctuation treatment towards larger fluctuations. This can can result in a nicer entropy profile but might be unstable.
- 1.0: Default
- 0.5, 1.0, 2.0, 5.0: Reasonable values
- >1.0: Extend the large-fluctuation treatment towards smaller fluctuations. This improves stability but leads to artefacts in the entropy stratification under near-adiabatic conditions.

7.1.9.7 real c_slopered

A new extra stabilization mechanism can be activated that reduces the slope and flattens the reconstruction function in case of a strong density contrast ($\rho_{\text{oneside}}/\rho_{\text{otherside}} > 2$ between neighboring cells). This value can be set e.g. with

```
real c_slopered f=E15.8 b=4 &
  n='Slope reduction parameter in case of strong density contrast' u=1 &
  c0='0.00: off (default), 0.02: reasonable value, 0.10: large value'
0.02
```

Typical choices are

- 0.0: Slope reduction switched off. Original reconstruction is used.
- 0.02: Moderate slope reduction in case of large density jumps.
- 0.10: More pronounced slope reduction in case of strong density contrast.

The default is not to use this trick and leave the parameter at 0.0. However, if numerical problems occur close to strong density jumps one can try to cure them by setting it e.g., to 0.02 or so. One could even think off other criteria (e.g., low temperatures, very high Mach numbers,...) to activate this slope reduction. That could be implemented if it would deem beneficial. This parameter is not recognized by the MHD module.

7.1.9.8 real c_recontshift

The second-order reconstruction schemes except `FRcont` have the option to make the reconstruction even more continuous in the case of very low Mach numbers, controlled with `C_RecContShift` and `C_RecContSteep`. The value can be set e.g. with

```
real c_recontshift f=E15.8 b=4 &
  n='Enhanced reconstruction continuation parameter 1 for shifting' &
  c0='0.0: off; 1.0: reasonable value'
0.2
```

Typical choices are

- 0.0: No attempt is made to make the reconstruction more continuous. The original reconstruction is used.
- 0.1: Make the transition to a smoother reconstruction at lower Mach numbers.
- 1.0: Reasonable value.
- 10.0: Make the transition to a smoother reconstruction at higher Mach numbers.

While the resulting scheme works for solar simulations, the parameters are really of benefit only in the case of brown dwarfs or exoplanets or the deep layers of M dwarfs. This parameter is not recognized by the MHD module.

7.1.9.9 real c_recontsteep

The second-order reconstruction schemes except `FRcont` have the option to make the reconstruction even more continuous in the case of very low Mach numbers, controlled with `C_RecContShift` and `C_RecContSteep`. The value can be set e.g. with

```
real c_recontsteep f=E15.8 b=4 &
  n='Enhanced reconstruction continuation parameter 2 for steepening' &
  c0='0.0: off; 0.1: reasonable value'
0.5
```

Typical choices are

- 0.0: No attempt is made to make the reconstruction more continuous. The original reconstruction is used.
- 0.01: Make the transition to a smoother reconstruction steeper (at even lower Mach numbers)
- 0.1: Reasonable value.
- 1.0: Make the transition to a smoother reconstruction smoother

While the resulting scheme works for solar simulations, the parameters are really of benefit only in the case of brown dwarfs or exoplanets or the deep layers of M dwarfs. This parameter is not recognized by the MHD module.

7.1.9.10 real c_recwenweightcenter

The WENO-style reconstruction schemes **VAweno** and **HBweno** (but not the “Frankenstein” versions like **FRweno**) allow to set the basic weights for the stencil of each of the three polynomials. This possibility is given mainly for development purposes. Users will likely not change the default values.

The specifiers “central” and “right” refer to the central and right stencil for finding the value at the right side of a cell. The “central” stencil includes the left and right neighbor cells. The “right” stencil is shifted on point to the right. The “left” stencil is shifted on point to the left, furthest away from the (right) cell boundary under consideration. The value for the central stencil can be set e.g. with

```
real c_recwenweightcenter f=E15.8 b=4 &
  n='Weight of central polynomial' &
  c0='Reasonable values: 0.5..0.8; recommended: 0.6'
0.6
```

Typical choices are

- 0.3333333: Give the central polynomial 1/3 of the total weight. Together with `c_recwenweightright=0.5` (Sect. 7.1.9.11), this attributes equal weights to all three stencils.
- 0.5: Low, but reasonable value.
- 0.6: Recommended value. Found by a number of empirical tests to be a good choice together with `c_recwenweightright=0.6666666` (Sect. 7.1.9.11).
- 1.0: Give all weight to the central polynomial. This essentially kills the central idea of the WENO scheme and only makes sense for test purposes.

7.1.9.11 real c_recwenweightright

The WENO-style reconstruction schemes **VAweno** and **HBweno** (but not the “Frankenstein” versions like **FRweno**) allow to set the basic weights for the stencil of each of the three polynomials. The value for the “right” stencil can be set e.g. with

```
real c_recwenweightright f=E15.8 b=4 &
  n='Weight of right polynomial' &
  c0='Reasonable values: 0.5..0.8; recommended: 0.6666666'
0.6666666
```

Typical choices are

- 0.0: Give all weight (that does not go to the central polynomial) to the left polynomial. For test purposes.
- 0.5: Give left and right polynomial equal weight.
- 0.6666666: Recommended value. Found by a number of empirical tests to be a good choice together with `c_recwenweightcenter=0.6` (Sect. 7.1.9.10).
- 1.0: Give all weight (that does not go to the central polynomial) to the right polynomial. For test purposes.

7.1.9.12 real c_recwenopsifactor

This parameter represents a factor to the “Pairwise Smoothness Indicator” controlling the “handbrake” that further stabilizes **HBweno** compared to the standard “Vanilla” WENO scheme **VAweno**. The value of the parameter can be set e.g. with

```
real c_recwenopsifactor f=E15.8 b=4 &
  n='Smoothing factor in case of bad pairwise smoothness match' &
  c0='Reasonable values: 0.0..30.0; works only with HBweno'
10.0
```

Typical choices are

- 0.0: No additional smoothing. This reduces HBweno to the (faster) VAweno. For test purposes only.
- 1.0: Weak smoothing
- 4.0: Reasonable value.
- 16.0: Strong smoothing.

Those values might have to be increased if `c_recontshift` (Sect. 7.1.9.8) is used. Typically, `c_recwenopsifactor` \rightarrow `c_recwenopsifactor/c_recontshift`.

7.1.9.13 character hdtransvelomode

This parameter controls the treatment of advection of transverse velocities. It can be set e.g. with:

```
character hdtransvelomode f=A80 b=80 &
  n='Mode for transverse velocity advection' &
  c0='Normal(default)/CA1/CA2/CA3/CA4(recommended)'
CA4
```

The choices are

- `Normal`, ' ': Compute flux of transversal momentum with standard Roe treatment (old, *default*)
- `CA1`: Compute flux of transversal momentum with consistent advection, version 1. Use mass flux and upwind density to determine flow speed. Actually recompute transversal velocities.
- `CA2`: Compute flux of transversal momentum with consistent advection, version 2. Use mass flux and Roe-mean density ($\tilde{\rho}$) to determine flow speed. Actually recompute transversal velocities.
- `CA3`: Compute flux of transversal momentum with consistent advection, version 3. Use mass flux and upwind density to determine flow speed. Compute transversal momentum fluxes from mass flux and diffusive momentum flux.
- `CA4`: Compute flux of transversal momentum with consistent advection, version 4. Use mass flux and Roe-mean density ($\tilde{\rho}$) to determine flow speed. Compute transversal momentum fluxes from mass flux and diffusive momentum flux (*recommended*).

For instance for a 2D Sedov blast wave problem, the new modes give less artifacts close to the axes than the old mode `Normal`. The four new advection types are made of to choices for the way to compute the effective flow speed across a cell boundary (different density values can be used) and two ways to compose the final transversal momentum fluxes. Version `CA4` is recommended. This parameter is not recognized by the MHD module.

7.1.9.14 character hdentropywavemode

This parameter controls the computation of the Roe correction flux for the entropy wave. It can be set e.g. with:

```
character hdentropywavemode f=A80 b=80 &
  n='Mode for entropy wave type' &
  c0='Normal/Entropy1/Entropy2/Entropy3M/Entropy3Ms/Entropy3gMps(recommended)'
Entropy3gMps
```

The choices are

- `Normal`, ' ': Compute entropy-wave flux with standard Roe treatment from pressure and density, (old, *default*).
- `Entropy1`: Compute entropy-wave flux from entropy. This only works well for small Mach numbers.

- **Entropy2**: Compute entropy-wave flux from entropy and pressure.
- **Entropy3M**: Compute entropy-wave flux from entropy, pressure, and density. In fact, an cases **Normal** and **Entropy1** are interpolated according to the Mach number.
- **Entropy3Ms**: Compute entropy-wave flux from entropy, pressure, and density. In fact, an cases **Normal** and **Entropy1** are interpolated according to the Mach number and entropy fluctuations.
- **Entropy3gMps**: Compute entropy-wave flux from entropy, pressure, and density. In fact, an cases **Normal** and **Entropy1** are interpolated according to the Mach number and fluctuations in pressure (directly and after subtracting the hydrostatic pressure correction) and entropy. This case is *recommended*.

The **Normal** computation with the standard Roe procedure is optimized for shocks and works also for small fluctuations in density and pressure. However, in the case of a nearly adiabatic stratification, the density and pressure fluctuations between adjacent depth points induce some spurious fluxes. These are avoided by reconstructing the entropy directly (**Entropy1**). However, that does not work well for shocks. Therefore, an interpolation between the standard reconstruction based on pressure and density and another one based on entropy is *recommended* (**Entropy3gMps**). This parameter is not recognized by the MHD module.

7.1.9.15 character henthalpyavgmode

This parameter controls the type of averaging used to get from the cell-centered enthalpy (flux) the boundary-centered enthalpy (flux). To this flux, the Roe corrections are added. It can be set e.g. with:

```
character henthalpyavgmode f=A80 b=80 &
  n='Mode for enthalpy averaging' &
  c0='Normal(old default)/CA1/CA1g/CA1gMps(recommended)/CA1M/CA1Ms/CA1p/CA1s' &
  c1='CA2/CA2g/CA2M/CA2p/CA2s/CA3/CA4'
CA1gMps
```

The choices are

- **Normal**, ' ': Use the standard Roe-averaging of the enthalpy + kinetic-energy fluxes, (old, *default*).
- **CA1**: Average the enthalpy and multiply with the average mass flux. Average the kinetic energy fluxes as in the standard Roe case.
- **CA1g**: Use the consistent-advection centering for the average enthalpy flux as in **CA1** for small fluctuations. Switch smoothly to the **Normal** Roe averaging for large non-hydrostatic pressure fluctuations.
- **CA1gMps**: Use the consistent-advection centering for the average enthalpy flux as in **CA1** for small Mach numbers. Switch smoothly to the **Normal** Roe averaging for large Mach numbers or large fluctuations in pressure (directly and after subtracting the hydrostatic pressure correction) and entropy. This case is *recommended*.
- **CA1M**: Use the consistent-advection centering for the average enthalpy flux as in **CA1** for small Mach numbers. Switch smoothly to the **Normal** Roe averaging for large Mach numbers.
- **CA1Ms**: Use the consistent-advection centering for the average enthalpy flux as in **CA1** for small Mach numbers. Switch smoothly to the **Normal** Roe averaging for large Mach numbers or large entropy fluctuations.
- **CA1p**: Use the consistent-advection centering for the average enthalpy flux as in **CA1** for small pressure fluctuations. Switch smoothly to the **Normal** Roe averaging for large pressure fluctuations.
- **CA1s**: Use the consistent-advection centering for the average enthalpy flux as in **CA1** for small entropy fluctuations. Switch smoothly to the **Normal** Roe averaging for large entropy fluctuations.

- **CA2**: Average the enthalpy plus kinetic energy and multiply with the average mass flux.
- **CA2g**: Use the consistent-advection centering for the average enthalpy plus kinetic energy flux as in **CA2** for small fluctuations. Switch smoothly to the **Normal** Roe averaging for large non-hydrostatic pressure fluctuations.
- **CA2M**: Use the consistent-advection centering for the average enthalpy plus kinetic energy flux as in **CA2** for Mach numbers. Switch smoothly to the **Normal** Roe averaging for large Mach numbers.
- **CA2p**: Use the consistent-advection centering for the average enthalpy plus kinetic energy flux as in **CA2** for small pressure fluctuations. Switch smoothly to the **Normal** Roe averaging for large pressure fluctuations.
- **CA2s**: Use the consistent-advection centering for the average enthalpy plus kinetic energy flux as in **CA2** for small entropy fluctuations. Switch smoothly to the **Normal** Roe averaging for large entropy fluctuations.
- **CA3**: Take the Roe tilde average enthalpy plus kinetic energy and multiply with the computed mass flux. This is a more experimental version and not generally recommended.
- **CA4**: Averaging the enthalpy and multiply with the computed mass flux. This is a more experimental version and not generally recommended.

Here, 'CA1' and 'CA2' behave in a similar way, whereas 'CA3' and 'CA4' are essentially just for tests. I prefer the **CA1** variant for the time being. However, both **CA1** and **CA2** work only well for small fluctuations and Mach numbers. Therefore, one of the modified schemes should be used. Again, they are rather similar even if the implemented criteria are rather different. While most of the versions work for "ordinary" main-sequence models, the comparably poorly resolved red-supergiant models (with large entropy step and Mach numbers) require a combination of the criteria above. Therefore, **CA1gMps** is recommended (for all type of models in general). This parameter is not recognized by the MHD module.

7.1.9.16 real c_hydpredfactor

The "hydrostatic pressure correction" terms in the two acoustic waves are always present. However, for the entropy wave and the "ionization wave" it is not quite clear if the terms should be there (the classical default) or if they should be set to zero. The value of a factor in front of these terms can be set e.g. with

```
real c_hydpredfactor f=E15.8 b=4 &
  n='hydrostatic pressure reduction in waves 3 and 6' u=1 &
  c0='0.0: Deactivation of pressure reduction terms' &
  c1='1.0: Activation of pressure reduction terms (default)'
0.0
```

Possible choices are

- 0.0: Deactivation of pressure reduction terms in waves 3 and "6" in Roe solver
- 1.0: Activation of pressure reduction terms in waves 3 and "6" in Roe solver (default)

This parameter is only recognized for **hdEntropyWaveMode='Normal'** which is not recommended, anymore. This parameter is not recognized by the MHD module.

7.1.9.17 real c_hydsdiffvelo

With this parameter an extra energy diffusion down an entropy step (after reconstructing the entropy) can be activated. For the diffusion velocity all three velocity components are used, i.e., there is a diffusion even transversal to the flow speed. This makes the diffusion more isotropic and lets numerical solutions to the Sedov-blast-wave problem look smoother. The value can be set e.g. with


```
real c_hydsdiffvelo f=E15.8 b=4 &
      n='Parameter for energy diffusion down an entropy step' u=1 &
      c0='typically 1.0'
1.0
```

Possible choices are for example

- 0.0: No extra energy diffusion down an entropy gradient (default).
- 0.2: Small value
- 1.0: Reasonable value
- 3.0: Large value

It acts on the entropy but only on the fraction of the jump that is still there after the reconstruction – unlike `C_hydTdiffLin` and `C_hydTdiffMach` that act on local temperature minima (see below). This parameter is not recognized by the MHD module.

7.1.9.18 real c_hydvdiffvelo

With this parameter an extra diffusion of the transversal velocities (after reconstructing them) can be activated. For the diffusion velocity all three velocity components are used, i.e., there is a diffusion even transversal to the flow speed. This makes the diffusion more isotropic and lets numerical solutions to the Sedov-blast-wave problem look smoother. The value can be set e.g. with

```
real c_hydvdiffvelo f=E15.8 b=4 &
      n='Parameter for transversal momentum diffusion down a velocity step' u=1 &
      c0='typically 1.0'
1.0
```

Possible choices are for example

- 0.0: No extra energy diffusion down an entropy gradient (default).
- 0.2: Small value
- 0.5: Reasonable value
- 1.0: Reasonable value
- 3.0: Large value

The type of dissipation that can be added with this option is similar to that provided by the tensor viscosity (Sect. 7.1.11). Therefore, I recommend to use only small values (0.5 to 1.0) to reduce the directional dependence of the dissipation applied by the Roe solver and to use an explicite tensor viscosity (Sect. 7.1.11) in case of emergencies. This parameter is not recognized by the MHD module (but in fact, the HLLC solver applies a somewhat similar – but stronger – dissipation by construction).

7.1.9.19 real c_hydtdiffin

The Roe-solver correction does not have any dissipation for standing waves and very little for slowly moving ones – unlike the MHD-HLLC solver that always has quite some minimum dissipation (depending on the reconstruction, though). The small amount of dissipation is a positive feature when it comes e.g., to convection with smaller Mach numbers in the deeper layers of a solar model, or (the absence) of vertical net mass fluxes in a hydrostatic atmosphere. However, it can be a drawback, e.g., in the case of a transsonic rarefaction wave, where an entropy fix is applied (since the beginning, see Leveque “Numerical Methods for Conservation Laws”), or in the (rather quiet) center of a Sedov blast wave where a cross-like structure with comparably low temperature is visible. This artefact can be removed by applying the standard tensor viscosity including the energy dissipation down an entropy gradient (controlled with `C_visPrturb`) or by the new, rather simple option to the Roe solver to apply additional energy dissipation down a temperature gradient but *only* in cells adjacent to a local temperature minimum (in 1D). It works nicely for the Sedov blast wave and does not have any visible adverse impact in any other cases, so far.

I don't expect it to do any harm for convection simulations and recommend to activate it per default. Cautious people might not like it and see how well it works without, though. Still, unlike the tensor viscosity with turbulent Prandtl number there is no viscous flux down the subphotospheric temperature or entropy gradient (unless there is a local minimum at the bottom). The linear diffusion can be set e.g. with

```
real c_hytdiffLin f=E15.8 b=4 &
    n='Parameter 1 for energy diffusion near local temperature minimum' u=1 &
    c0='typically 0.2, if activated; usually 0.0'
0.0
```

It just acts on the temperature gradient (in the neighborhood of a local minimum), whereas `C_hydTdiffMach` (see below) has an additional factor, that takes velocity gradients into account, which prevent this type of diffusion from acting in deeper convective layers. I recommend as a default `C_hydTdiffLin=0.0` and non-zero values only in case of an emergency and `C_hydTdiffMach=1.0` or `2.0` as a default. These parameters are not recognized by the MHD module.

7.1.9.20 real c_hytdiffmach

Analogously to `c_hytdiffLin`, an additional energy dissipation down a temperature gradient but *only* in cells adjacent to a local temperature minimum (in 1D) can be applied, that has a scaling factor derived from the Mach number. This Mach-number-dependent diffusion can be set e.g. with

```
real c_hytdiffmach f=E15.8 b=4 &
    n='Parameter 1 for energy diffusion near local temperature minimum' u=1 &
    c0='typically 0.2, if activated; usually 0.0'
1.0
```

I recommend as a default `C_hydTdiffLin=0.0` and non-zero values only in case of an emergency and `C_hydTdiffMach=1.0` or `2.0` as a default. These parameters are not recognized by the MHD module.

7.1.10 Hydrodynamics control (MHD only)

The following parameters apply only to the MHD module (see also Sect. 2.2 for details).

7.1.10.1 character hdcheckflux

With this parameter the CheckFlux routine of the HLLMHD solver can be (des)activated, as e.g. in

```
character hdcheckflux f=A80 b=80 n='Switch to activate checking of MHD fluxes' &
    c0='on/off'
off
```

This parameter is only recognized by the HLLMHD scheme. Leaving it on might be safer but is definitely (slightly) slower.

7.1.10.2 integer n_orderconstrainedtransport

Order of reconstruction of the electric field in the constrained-transport step. The parameter can be set e.g. with

```
integer n_orderconstrainedtransport f=I4 b=4 &
    n='Number of hydrodynamics iterations' &
    c0='order of reconstruction of electric field in constrained-transport step' &
    c1='1: Simple arithmetic average (default), 2: Quadratic interpolation'
2
```

Possible values:

- 1: Simple arithmetic average of fluxes (default).
- 2: Quadratic interpolation of fluxes to the cell edges

This parameter is only recognized by the `hdscheme=HLLMHD`.

7.1.10.3 integer n_rescellsperchunk

The approximate number of grid cells per chunk in the 3D resistivity scheme can be specified e.g. with

```
integer n_rescellsperchunk f=I9 b=4 &
  n='Number of cells per chunk in resistivity routine' &
  c0='0 => one 2D slice at a time' &
  c1='1 => minimum chunk size (inefficient)' &
  c2='10000: typical value'
20000
```

The exact number is determined at run time to get (approximately) equal sizes of the individual chunks. The choice of this parameter does not affect the result of the computation but the memory usage and performance: Smaller (and more) chunks may result in an optimum cache usage and need the smallest amount of memory, but result in additional overhead due to frequent subroutine calls. Bigger (and less) chunks are to be preferred for vector machines and processors with large caches.

7.1.10.4 real c_rescourant

The tensor resistivity routines have their own time-step restriction. The recommended typical time step can be set e.g. with

```
real c_rescourant f=E15.8 b=4 n='resistivity Courant factor' u=1 &
  c0='range: 0.0 < C_resCourant, typically: 0.5'
0.5
```

7.1.10.5 real c_rescourantmax

The absolute upper limit for the resistivity time scale can be set with

```
real c_rescourantmax f=E15.8 b=4 n='maximum resistivity Courant factor' u=1 &
  c0='range: C_resCourant <= C_resCourantmax, typically 1.0'
0.95
```

Its value should be slightly above `c_rescourant`.

7.1.10.6 real c_resb

This parameter specifies the electric resistivity. Values between 0.0 and 1.0 may be reasonable. Higher values are possible but drastically reduce the time step. The default value is 0.0. Example:

```
real c_resb f=E15.8 b=4 &
  n='Parameter for numerical resistivity' u=1
0.0
```

The artificial electric resistivity of Stone & Pringle (2001) is used. It is given by $\eta_B = c_resB \cdot |j| \cdot (\Delta x)^2 / \sqrt{\rho}$, where η_B is the magnetic diffusivity, j the current density, Δx a mean width of the grid cell, and ρ is the density. Values ≤ 0 deactivate this feature.

7.1.10.7 real c_resbconst

This parameter specifies a constant magnetic diffusivity η_m . The default value is 0.0. Example:

```
real c_resbconstant f=E15.8 b=4 &
  n='Parameter for constant magnetic diffusivity' u=cm^2/s
0.1
```

A reasonable value can be found by choosing a reasonable value for the magnetic Reynolds number $Re_{mag} = (\ell_0 v_0) / \eta_m$. Values ≤ 0 deactivate this feature.

7.1.10.8 real c_resepsilon

This parameter controls an additional numerical energy diffusion. Typical values are between 0.0 and 1.0. The default value is 0.0. Example:

```
real c_resepsilon f=E15.8 b=4 &
    n='Parameter for additional energy diffusion'          u=1
0.5
```

The diffusion coefficient of the additional energy diffusion is given by $\eta_E = c_repsilon \cdot |j| \cdot (\Delta x)^2 / \sqrt{\rho}$, analog to the magnetic diffusivity `c_resB`. Values ≤ 0 deactivate this feature.

7.1.10.9 real beta_inv

This parameter is used for the dual energy method. It determines which cells are updated with the thermal energy equation. Example:

```
real beta_inv f=E15.8 b=4 &
    n='1/beta dual energy parameter'                      u=1
-1.0
```

The criterion is as follows:

if $\beta < 1/\text{beta_inv}$ the equation for the thermal energy is used.

if $\beta > 1/\text{beta_inv}$ the equation for the total energy is used.

β is the plasma β , i.e., the ratio of the gas pressure to the magnetic pressure. If `beta_inv` is set to zero, the thermal energy equation is used for all cells. A reasonable value may be 100.0. To deactivate this feature, set `beta_inv` to a negative value. If not specified, this parameter is set to -1.0. This parameter works only with `hdscheme=HLLMHD`. When `va_max > 0` then a reasonable value is given by $\text{beta_inv} \lesssim v_{A\max}^2 / c_s^2$, where c_s is the speed of sound in the region where $\beta < 1/\text{beta_inv}$.

7.1.10.10 real va_max

This parameter limits the Alfvén speed to `va_max` by an arbitrary reduction of the Lorentz force. Example:

```
real va_max f=E15.8 b=4 &
    n='maximum Alfvén speed' u=cm/s &
-1.0
```

This parameter is only recognized in conjunction with `hdscheme=HLLMHD`. `va_max=5.0E+06` might be a reasonable value for some specific applications to the solar photosphere. If not specified this parameter is set -1.0. Values ≤ 0 deactivate this feature. See also Eq. (2.19).

7.1.10.11 integer n_magdiffside

Increases the diffusivity of the scheme near the side boundaries within a thickness of the diffusion layer of `N_magDiffSide` computational cells. Example:

```
integer n_magdiffside f=I9 b=4 &
    n='Number of cells of diffusive side boundary layer' &
    c0='0 => deactivates this feature' &
    c1='10: reasonable value'
0
```

7.1.10.12 integer n_magdifftop

Increases the diffusivity of the scheme near the top boundary within a thickness of the diffusion layer of `N_magDiffTop` computational cells. Example:

```
integer n_magdifftop f=I9 b=4 &
    n='Number of cells of diffusive top boundary layer' &
    c0='0 => deactivates this feature' &
    c1='10: reasonable value'
0
```

7.1.10.13 integer n_magdiffbottom

Increases the diffusivity of the scheme near the bottom boundary within a thickness of the diffusion layer of N_magDiffBottom computational cells. Example:

```
integer n_magdiffbottom f=I9 b=4 &
  n='Number of cells of diffusive bottom boundary layer' &
  c0='0 => deactivates this feature' &
  c1='10: reasonable value'
0
```

7.1.11 Tensor-viscosity control

In most test problems it is not necessary to activate the 2D/3D tensor viscosity anymore. Even when strong slow shock fronts are aligned with the grid the Roe solver does not run into problems anymore, even without any additional 2D or 3D viscosity. However, even if the Roe solver can handle sharp shocks by its own, the radiation transport algorithm might cause trouble because of the enormous opacity variations across a shock front. Here the tensor viscosity might become useful. In fact, there are two separate tensor-viscosity routines by now:

The classical one is controlled by `c_visSmagorinsky`, `c_visArtificial`, etc. Its use was recommended for the old version of the Roe solver. Nowadays, it is only kept for compatibility reasons.

The new “point-to-point” tensor viscosity is controlled by `c_visP2Pcoeff`, etc. (see Sect. 7.1.11.10 below). It has better stability properties than the old version. However, due to the improved stability of the Roe solver itself the use of this new tensor viscosity formulation is actually less often necessary than the old one.

7.1.11.1 integer n_visiter

While this parameter is named analogously to `n_hyditer`, it controls a somewhat different behavior of the viscosity step. While positive values of `n_visiter` have no meaning, so far, a negative value specifies the number of hydrodynamics substeps per viscosity step (or rather: how often the viscosity step is called during the hydrodynamics iteration). The parameter can be set e.g. with

```
integer n_visiter f=I4 b=4 n='Number of tensor-viscosity iterations' &
  c0='<0: Number of hydro substeps per viscosity substep' &
  c1=' 0: One tensor-viscosity substep per global time step (old, default)' &
  c2='>0: Not implemented, yet'
-1
```

Possible values are:

- 0: Do exactly one viscosity step per global time step, independent of the number of hydrodynamics sub steps. This is the classical behavior (and default).
- -1: Do one viscosity step per hydrodynamics sub step (and vice versa).
- <0: Do $-n_visiter$ hydrodynamics sub steps between viscosity sub steps.
- >0: Not implemented yet. Gives the same result as 0.

For models with long radiative relaxation time scales, a large value of `n_hyditer` can lead to a significant speed up. Choosing a small negative value for `n_visiter` means that the tensor-viscosity sub step is called sufficiently often. Note, there is not parameter `n_vismaxiter`. So far, this parameter is only recognized by the HYD module.

7.1.11.2 real c_vissmagorinsky

A turbulent viscosity of Smagorinsky type can be activated e.g. with

```
real c_vissmagorinsky f=E15.8 b=4 &
  n='Turbulent eddy viscosity parameter (Smagorinsky type)'      u=1
0.5
```

In many cases values around 0.5 are sufficient to stabilize the code. Larger values are only necessary for some nasty under-resolved supergiant models. Setting `c_vissmagorinsky = c_visartificial = c_visexpansion = c_vislinear = c_visp2pcoeff = 0.0` skips the classical tensor-viscosity step entirely.

7.1.11.3 real c_visartificial

A standard artificial viscosity can be activated e.g. with

```
real c_visartificial f=E15.8 b=4 &
      n='Artificial viscosity tensor parameter'          u=1
0.5
```

In many cases values around 0.5 are sufficient to stabilize the code. Larger values are only necessary for some nasty under-resolved supergiant models.

7.1.11.4 real c_visexpansion

An additional viscosity can be activated e.g. with

```
real c_visexpansion f=E15.8 b=4 &
      n='Expansion viscosity tensor parameter'          u=1
1.2
```

While the standard artificial viscosity acts on compressed regions, this viscosity acts in expansion areas. Ususally, it is not activated (`c_visexpansion = 0.0`). However, it might be useful in cases were strong localized expansions cause problems.

7.1.11.5 real c_vislinear

Another viscosity can be activated e.g. with

```
real c_vislinear f=E15.8 b=4 &
      n='Linear viscosity tensor parameter'            u=1
1.2
```

In the formulae for the standard (artificial, compression, Smagorinsky) viscosity velocity gradients appear. That means that in regions with smooth small-amplitude flows these types of viscosity essentially vanish. Here, the linear viscosity comes in. It uses $\sqrt{R_{\text{gas}}T}$ as approximation for the sound speed that is used in the formula for the kinematic viscosity. Ususally, it is not activated (`c_vislinear = 0.0`). It might be useful to damp small-amplitude almost linear waves.

7.1.11.6 real c_visprturb

The Prandtl number for turbulent mixing can be specified e.g. with

```
real c_visprturb f=E15.8 b=4 &
      n='Turbulent Prandtl number'                    u=1
8.0
```

Values between 1.0 and 10.0 appear reasonable. Note that larger values lead to smaller amounts of turbulent mixing! A value of 0.0 switches off the turbulent mixing terms (but not the entire tensor viscosity).

7.1.11.7 real c_vistensorddiag

The factor in the stress tensor in front of of the diagonal terms can be set with

```
real c_vistensorddiag f=E15.8 b=4 &
      n='Diagonal factor for viscous stress tensor'    u=1 &
      c0='typically 1.0'
1.0
```

This is not really parameter one would try to adjust. The total amount of viscosity should be controlled with parameters like `real c_vissmagorinsky` and `real c_visartificial`. But the parameter can be used to tentatively switch off the diagonal terms completely or to change its importance compared to the other terms.

7.1.11.8 `real c_vistensoroff`

The factor in the stress tensor in front of of the off-diagonal terms can be set with e.g.

```
real c_vistensoroff f=E15.8 b=4 &
  n='Off-diagonal factor for viscous stress tensor'          u=1 &
  c0='typically 0.5'
0.5
```

This is not really parameter one would try to adjust. The total amount of viscosity should be controlled with parameters like `real c_vissmagorinsky` and `real c_visartificial`. But the parameter can be used to tentatively switch off the off-diagonal terms completely or to change its importance compared to the other terms.

7.1.11.9 `real c_vistensordiv`

The factor in the stress tensor in front of of the divergence terms (also on the diagonal) can be set with e.g.

```
real c_vistensordiv f=E15.8 b=4 &
  n='Divergence factor for viscous stress tensor'          u=1 &
  c0='typically -1./3.'
0.0
```

This is not really parameter one would try to adjust. The total amount of viscosity should be controlled with parameters like `real c_vissmagorinsky` and `real c_visartificial`. But the parameter can be used to switch off the divergence terms completely or to change its importance compared to the other terms. These divergence terms can be used to reduce the effect of the tensor viscosity in the case of isotropic compression. But this reduction (`c_vistensordiv = -0.333333` in 3D, `c_vistensordiv = -0.5` in 2D) is usually switched off.

In addition to the standard tensor viscosity described above, there is a "point-to-point" viscosity. It relies on a completely different discretization. It should conserve angular momentum exactly and guarantee positivity of dissipated energy (for sufficiently small time steps). The "point-to-point" viscosity can be used in addition to the standard one – or without.

7.1.11.10 `real c_visp2pcoeff`

The strength of the viscosity can be controlled with e.g.

```
real c_visp2pcoeff f=E15.8 b=4 &
  n='Point to point viscosity coefficient'                  u=1
0.20
```

This parameter is somewhat analogous to `real c_visartificial`, see 7.1.11.3. But it acts on compression, expansion, and shear flows. A value of 0.0 switches it off.

7.1.11.11 `real c_visp2phypsmagorinsky`

This parameter can be set with e.g.

```
real c_visp2phypsmagorinsky f=E15.8 b=4 &
  n='Smagorinsky parameter for point-to-point viscosity'  u=1
0.3
```

This parameter is equivalent to `real c_vissmagorinsky` (see 7.1.11.2) with the classical implementation of the viscosity tensor. A value of 0.0 switches it off. Values of 0.3 or 0.5 are reasonable. Although the underlying formula (and theory) is more complex, the effects are rather similar to that of `real c_visp2pcoeff`. If additional smoothing is required, either of these parameters (or both) can be set to non-zero values.

7.1.11.12 real c_visp2phypartificial

This parameter can be set with e.g.

```
real c_visp2phypartificial f=E15.8 b=4 &
    n='Artificial point-to-point tensor-viscosity parameter'    u=1
0.0
```

This parameter is equivalent to `real c_visartificial` (see 7.1.11.3) with the classical implementation of the viscosity tensor. A value of 0.0 switches it off. Values of 0.3 to 1.0 are reasonable. The viscosity controlled with this parameter is meant to act mostly on shocks.

7.1.11.13 real c_visp2phypexpansion

This parameter can be set with e.g.

```
real c_visp2phypexpansion f=E15.8 b=4 &
    n='Parameter for point-to-point expansion tensor viscosity'    u=1
0.0
```

This parameter is equivalent to `real c_visexpansion` (see 7.1.11.4) with the classical implementation of the viscosity tensor. A value of 0.0 switches it off. The viscosity controlled with this parameter is meant to limit or smooth strong expansion events where density, pressure, temperature, and/or entropy can drop significantly. This parameter is not frequently set to non-zero values.

7.1.11.14 real c_visp2pdivrhov

This parameter can be set with e.g.

```
real c_visp2pdivrhov f=E15.8 b=4 &
    n='Point-to-point mass-flux-divergence viscosity coefficient' u=1
0.0
```

A value of 0.0 switches it off. Values of 0.5 or even 2.0 are reasonable. The viscosity controlled with this parameter acts only on compressible flow configurations, i.e., in near-incompressible low-Mach-number flows it should have hardly any effect. Still, it can be used in exactly such a case to dampen spurious sound waves for example at the very top of the computational box.

7.1.11.15 real c_visp2pincl1

The interaction with the edge neighbor cells with indices $(\pm 1 \pm 1 + 0)$ can be specified with e.g.

```
real c_visp2pincl1 f=E15.8 b=4 &
    n='Point to point viscosity inclined cell factor 1'          u=1
1.0
```

Common values are 1.0 (interaction is considered) and 0.0 (no interaction with these cells). The usual value is 1.0.

7.1.11.16 real c_visp2pincl2

The interaction with the corner neighbor cells with indices $(\pm 1 \pm 1 \pm 1)$ can be specified with e.g.

```
real c_visp2pincl2 f=E15.8 b=4 &
    n='Point to point viscosity inclined cell factor 2'          u=1
0.0
```

Common values are 1.0 (interaction is considered) and 0.0 (no interaction with these cells). The usual value is 0.0 to save some computation time.

7.1.11.17 integer n_viscellsperchunk

The number of cells per box (or “chunk”) treated by the tensor-viscosity scheme at one call (and by one thread) can be set e.g. for an Intel Macintosh with

```
integer n_viscellsperchunk f=I9 b=4 &
  n='Number of cells per viscosity chunk' &
  c0='0 => old chopping' &
  c1='50000: reasonable value'
100000
```

It can be adjusted to improve cache efficiency and to modify the work load distribution onto the threads (in case of parallel runs with OpenMP). Due to the special handling of boundary cells the overhead per call increases significantly for small chunks. Typically, larger chunk sizes (compared the the hydrodynamics chunk sizes set with `integer n_hydcellsperchunk`, see Sect. 7.1.8.9) are adequate. On the other hand they should not be too large to limit the usage of temporary memory and to allow parallelization (the distribution of chunks to threads): For simulations with activated OpenMP on a parallel machine the chunk size has to be made small enough to allow at least as many chunks as processors available. This is particularly important for models with a small number of grid points (e.g. 2D models). An example is given for the Hitachi SR8000 in Sect. 4.6.5.

7.1.12 Dust/molecules/hydrogen ionization: General

CO5BOLD can handle a number of additional density arrays. They can be used to describe e.g. the mass density of dust distribution moments or number densities of molecules. These species are properly advected with the gas density. There is also already a small number of dust/molecule formation models available. These models have to be improved in the future and the influence on the radiation field (opacities, radiation pressure on dust) has to be taken into account.

7.1.12.1 character dustscheme

A scheme for dust or molecule formation and transport can be selected e.g. with

```
character dustscheme f=A80 b=80 n='Dust model' &
  c0='none (default), nosource, dust_simple_01, co_component01_01' &
  c1='dust_k3mon_01, dust_k3mon_02'
dust_k3mon_01
```

The following values are currently possible:

- `none`, `None`: No handling of any dust/molecule density at all.
- `nosource`: Skip source term step for dust/molecules entirely, but do the transport.
- `dust_simple_01`: Simple and unrealistic 'dust' formation model (only for testing of the numerics).
- `co_component01_01`: Simple CO formation (from Matthias Steffen) with one component only but realistic time scales.
- `dust_k3mon_01`: Simple C-rich dust formation (routines from Susanne Höfner) with one component only but realistic time scales.
- `dust_k3mon_02`: Simple C-rich dust formation (routines from Susanne Höfner) with two components for dust density and free carbon density.
- `dust_k3mon_03`: Simple forsterite dust formation (based on routines from Susanne Höfner) with two components for dust density and free "forsterite monomer" density.
- `dust_bins_01`: Multi-size-bin forsterite dust formation (based on Rossow's equations, see Rossow, 1978) with one bin for the monomers and several bins for the different grain sizes.
- `dust_moment04_c2`: C-rich dust chemistry, 4 moments (routines from Susanne Höfner).

- `chemreacnet`: chemical reaction networks (routines from Sven Wedemeyer-Böhm and Inga Kamp).
- `hiontd`: time-dependent hydrogen ionization (routines from Jorrit Leenaarts and Sven Wedemeyer-Böhm).

7.1.12.2 character dustreconstruction

While usually (i.e., when this parameter is not set) the reconstruction scheme for the additional density fields is the same as for the normal hydrodynamics quantities (see 7.1.8.4), it can make sense to choose a strictly monotonic scheme for these additional fields. This scheme can be more (e.g. PP) or less (e.g. PPMimo) aggressive. It can be chosen e.g. with

```
character dustreconstruction f=A80 b=80 n='Reconstruction method for qucs' &
  c0=Constant c1=Minmod/VanLeer/Superbee c2=PP/PPmimo &
  c3=FRmimo,FRmono
FRmono
```

Useful combinations are

- `reconstruction=vanLeer, dustreconstruction=Superbee.`
- `reconstruction=FRweno, dustreconstruction=FRmono.`
- `reconstruction=FRweno, dustreconstruction=PP.`
- `reconstruction=HBweno, dustreconstruction=PP.`
- `reconstruction=HBweno, dustreconstruction=PPmimo.`

7.1.12.3 real c_dust0X

There are ten parameters (`real c_dust01` to `c_dust10`) to control each dust formation scheme in detail. A parameter can be given as in

```
real c_dust01 f=E15.8 b=4 n='Dust parameter 1'
0.0
```

The meaning (and unit) can vary from scheme to scheme. The default value is 0.0 in each case.

Important: The parameter `real c_dust01` must be set to 1.0 in order to activate advection of particle densities for the CHEM (`chemreacnet`) and the HION (`hiontd`) module. The default value is 0.0, i.e. advection is switched off.

7.1.12.4 character chem_reacfile

The name of the input file containing the chemical reaction network.

```
character chem_reacfile f=A80 b=80 n='file name of reaction table'
chem.dat
```

7.1.12.5 character chem_reacpath

The path of the input file containing the chemical reaction network.

```
character chem_reacpath f=A80 b=80 n='path of reaction table'
/data/sven/cobold/dat/chem/
```

7.1.12.6 real chem_abumetal

Abundance of the representative metal ('M', if present) relative to hydrogen ($\epsilon_M = [M]/[H]$). A value of $1.0E-04$ means there are 10^4 hydrogen atoms for every metal atom. The metal number density for each grid cell is then derived via $n_H = \epsilon_M \rho / m_H$ (assuming a pure hydrogen gas). This parameter is ignored when a `quc` array for the metal is found in the input model.

```
real chem_abumetal f=E15.8 b=4 n='Chemical abundance of repres. metal'
1.0E-04
```

7.1.12.7 character hion_datapath

The path of all input files for HION.

```
character hion_datapath f=A80 b=80 n='HION data path'
/data/sven/cobold/dat/hion/
```

7.1.12.8 character hion_atomfile

The file name of the model atom for HION.

```
character hion_atomfile f=A80 b=80 n='HION atom file name'
H_6.atom
```

7.1.12.9 character hion_abufile

The name of the HION input file containing the chemical abundances.

```
character hion_abufile f=A80 b=80 n='HION abundance file name'
abundance.input
```

7.1.12.10 character hion_edensfile

The name of the HION input file containing the electron density table.

```
character hion_edensfile f=A80 b=80 n='HION electron density file name'
edens.dat
```

7.1.12.11 character hion_pffile

The name of the HION input file containing the partition functions.

```
character hion_pffile f=A80 b=80 n='HION partition function file name'
pf_kurucz.dat
```

7.1.12.12 real dtime_out_hion

Time increment for additional HION output. Positive values specify the time increment in seconds, negative values the increment in computational time steps. Setting the parameter to zero, suppresses the output.

```
real dtime_out_hion f=E15.8 b=4 n='Output file time step (HION)'
-10.0
```

7.1.12.13 integer hion_chunks

Number of chunks to use for HION in order to limit the required memory. Do not make it bigger than the number of points in the x2 direction.

```
integer hion_chunks f=I9 b=4 n='Number of HION chunks'
1
```

7.1.13 Dust: dustscheme=dust_moment04_c2

In this section the parameters for dustscheme=dust_moment04_c2 (4-bin (4 moments) dust scheme for carbon-rich dust) are described:

7.1.13.1 real c_dust01

The carbon to oxygen ratio is specified with e.g.

```
real c_dust01 f=E15.8 b=4 n='C to O ratio'           u=1
1.4
```

Larger values mean more dust. Values below 1 make no sense for the current dust model.

7.1.13.2 real c_dust02

The oxygen abundance is specified with e.g.

```
real c_dust02 f=E15.8 b=4 n='Oxygen abundance'       u=1
6.606934E-04
```

7.1.13.3 real c_dust03

The cutoff for the integration of the degree of condensation is specified with e.g.

```
real c_dust03 f=E15.8 b=4 n='cutoff for integration of degree of condensation' &
                                                    u=1
1.0E-05
```

7.1.13.4 real c_dust04

The relative dust opacity factor is specified with e.g.

```
real c_dust04 f=E15.8 b=4 n='Relative dust opacity factor' u=1
1.0
```

7.1.14 Dust: dustscheme=dust_k3mon_03

In this section the parameters for dustscheme=dust_k3mon_03 (simple 2-bin dust scheme for forsterite dust) are described:

7.1.14.1 integer n_dustgrainradius

The number of dust grain radius bins (including one for the monomers) is specified with

```
integer n_dustgrainradius f=I8 b=4 n='Number of dust grain radius bins' &
c1='Includes: bin for monomers'
2
```

The default value is 1 (to avoid an empty array). The value should be the same as the upper dimension in real ar_dustgrainradius. For the current dust scheme, there should always be exactly two bins.

7.1.14.2 real ar_dustgrainradius

The radii of the dust grains are specified with e.g.

```
real ar_dustgrainradius f=E10.4 b=4 p=1 d=(1:2) n='Dust grain radii' u=cm
0.0
1.0E-04
```

The default value is 0.0.

7.1.14.3 real c_dust01

The density of the grain material is specified with e.g.

```
real c_dust01 f=E15.8 b=4 n='Density of grain material' u=g/cm^3
3.3E+00
```

7.1.14.4 real c_dust02

The atomic weight of the "dust monomer" is specified with e.g.

```
real c_dust02 f=E15.8 b=4 n='Atomic weight of dust monomer' u=u
140.71
```

The value 140.71 should be appropriate for forsterite (Mg_2SiO_4). The unit is the atomic mass unit. The default value is 0.0.

7.1.14.5 real c_dust03

The number fraction of the rarest component is specified with e.g.

```
real c_dust03 f=E15.8 b=4 n='Number fraction of rarest component' u=1 &
c0='For Mg2SiO4, Mg is the rarest, its fraction is 3.1187E-05' &
c1='Mg2SiO4 contains 2 Mg -> * 1/2 -> 1.55935e-05'
1.55935e-05
```

For Mg_2SiO_4 the rarest component is (usually) Mg_2 . So, half the magnesium abundance is required as value. The default value is 0.0.

7.1.14.6 real c_dust04

The lower dust limit fraction is specified with e.g.

```
real c_dust04 f=E15.8 b=4 n='Lower dust limit fraction' u=1
1.0E-10
```

It is used in the calculation of the settling velocity where a division by the total density of monomers and dust is required. To prevent this denominator to become zero a term $c_{\text{dust04}} \rho$ is added. The default value is 0.0.

7.1.14.7 real c_dust05

The minimum number of monomers during condensation is specified with e.g.

```
real c_dust05 f=E15.8 b=4 n='Minimum number of monomers during condensation' u=1
10.0
```

For very small grains (just one or very few monomers) the condensation rates can be very small in this dust model: nucleation that would form already small clumps of monomers is not considered. Therefore, to speed things up a minimum number of monomers can be given that is considered for the condensation rate. With 1.0 or smaller values the enhancement is switched off. The default value is 0.0.

7.1.14.8 real c_dust06

The sticking coefficient for the condensation rate is specified with e.g.

```
real c_dust06 f=E15.8 b=4 n='Sticking coefficient' u=1 &
c0='For C-rich dust: 0.37; can be between 0 and 1'
1.0
```

The default value is 0.0.

7.1.15 Dust: dustscheme=dust_bins_01

In this section the parameters for `dustscheme=dust_bins_01` (multi-size-bin dust scheme for forsterite dust) are described:

7.1.15.1 integer n_dustgrainradius

The number of dust grain radius bins (including one for the monomers) is specified with

```
integer n_dustgrainradius f=I8 b=4 n='Number of dust grain radius bins' &
  c1='Includes: bin for monomers'
8
```

The default value is 1 (to avoid an empty array). The value should be the same as the upper dimension in `real ar_dustgrainradius`.

7.1.15.2 real ar_dustgrainradius

The radii of the dust grains are specified with e.g.

```
real ar_dustgrainradius f=E15.8 b=4 p=1 d=(1:8) n='Dust grain radii' u='cm'
0.0
0.00390625E-04
0.0156250E-04
0.06250E-04
0.25000E-04
1.00000E-04
4.00000E-04
16.0000E-04
```

The default value is 0.0.

7.1.15.3 real c_dust01

The density of the grain material is specified with e.g.

```
real c_dust01 f=E15.8 b=4 n='Density of grain material' u=g/cm^3
3.3E+00
```

7.1.15.4 real c_dust02

The atomic weight of the "dust monomer" is specified with e.g.

```
real c_dust02 f=E15.8 b=4 n='Atomic weight of dust monomer' u=u
140.71
```

The value 140.71 should be appropriate for forsterite (Mg_2SiO_4). The unit is the atomic mass unit. The default value is 0.0.

7.1.15.5 real c_dust03

The number fraction of the rarest component is specified with e.g.

```
real c_dust03 f=E15.8 b=4 n='Number fraction of rarest component' u=1 &
  c0='For Mg2Si04, Mg is the rarest, its fraction is 3.1187E-05' &
  c1='Mg2Si04 contains 2 Mg -> * 1/2 -> 1.55935e-05'
1.55935e-05
```

For Mg_2SiO_4 the rarest component is (usually) Mg_2 . So, half the magnesium abundance is required as value. The default value is 0.0.

7.1.15.6 real c_dust04

The lower dust limit fraction is specified with e.g.

```
real c_dust04 f=E15.8 b=4 n='Lower dust limit fraction' u=1
1.0E-10
```

If the density in a bin relative to the gas density falls below this value, the bin is completely emptied and the material is added to the bin with the largest dust or monomer density. Typical values are $1.0\text{E}-09$ or so. The default value is 0.0.

7.1.15.7 real c_dust06

The sticking coefficient for the condensation rate is specified with e.g.

```
real c_dust06 f=E15.8 b=4 n='Sticking coefficient' u=1 &
  c0='For C-rich dust: 0.37; can be between 0 and 1'
1.0
```

Typical values are between 0.0 (deactivating this process) and 1.0. The default value is 0.0. The standard choice is 1.0.

7.1.15.8 real c_dust07

The sticking coefficient for the coagulation rate is specified with e.g.

```
real c_dust07 f=E15.8 b=4 n='Sticking coefficient for coagulation' u=1 &
  c0='Typically between 0 and 1'
1.0
```

Typical values are between 0.0 (deactivating this process) and 1.0. The default value is 0.0.

7.1.15.9 real c_dust08

The sticking coefficient for the coalescence rate is specified with e.g.

```
real c_dust08 f=E15.8 b=4 n='Sticking coefficient for coalescence' u=1 &
  c0='Typically between 0 and 1'
1.0
```

Typical values are between 0.0 (deactivating this process) and 1.0. The default value is 0.0.

7.1.15.10 real c_dust09

The sticking coefficient for the nucleation rate is specified with e.g.

```
real c_dust09 f=E15.8 b=4 n='Sticking coefficient for nucleation' u=1 &
  c0='Typically between 0 and 1'
1.0
```

Typical values are between 0.0 (deactivating this process) and 1.0. The default value is 0.0. The standard choice is 1.0.

7.1.16 Radiation-transport control (general)

In this part of the parameter file the radiation transport module has to be selected. Depending on this selection a couple of additional parameters have to be specified. Table 7.2 gives a list of the parameters and the modules they apply to. The standard routines are now in the MSrad module for local models and the SHORTrad module for global “star-in-a-box” models. The LHDrad module is not maintained very much anymore.

7.1.16.1 character radscheme

So far, there exist three different radiation transport modules. The active one can be selected e.g. with

```
character radscheme f=A80 b=80 n='Radiation transport scheme' &
  c0='LHDrad/MSrad/SHORTrad' &
  c1='None (skip radiation transport step entirely)'
SHORTrad
```

Possible values are

- None: Skip radiation transport entirely.

Parameter	Section	LHDrad	MSrad	SHORTrad
radscheme	7.1.16.1	*	*	*
opafile	7.1.7.1	*	*	*
opapath	7.1.7.2	*	*	*
n_radband	7.1.16.2		*	*
n_radminiter	7.1.16.3	*	*	*
n_raditer	7.1.16.4	*	*	*
n_radmaxiter	7.1.16.5	*	*	*
radraybase	7.1.16.6	*	*	*
radraystar	7.1.16.7	*		*
c_tminlimit	7.1.16.8		*	*
c_radimplicitmu	7.1.16.9	*		*
c_raditereps	7.1.16.10	*		*
c_raditerstep	7.1.16.11	*		*
n_radtheta	7.1.17.1		*	
n_radphi	7.1.17.2		*	
n_radsbray	7.1.17.3		*	
n_radthickpoint	7.1.17.4	*	*	
n_radtaurefine	7.1.17.5	*	*	
n_radrsyslevel	7.1.17.6		*	
n_radoutput	7.1.17.7		*	
c_radtcool	7.1.17.8		*	
c_raddcool	7.1.17.9		*	
c_radscool	7.1.17.10		*	
c_radtinci	7.1.17.11		*	
c_raddinci	7.1.17.12		*	
c_radtvisdtau	7.1.18.1	*		
c_radtvis	7.1.18.2	*		
c_radhtaup	7.1.4.19		*	*
c_radcourant	7.1.20.13	*	*	*
c_radcourantmax	7.1.20.14	*	*	*
c_radmaxeichange	7.1.20.15	*	*	*

Table 7.2: List of radiation transport control parameters and the modules they are relevant for.

- **LHDrad:** (old “supergiant module”) It uses long characteristics and is restricted to an equidistant grid and open boundaries at all surfaces. Note that the switch `-Drhd_r01=1` has to be set during compilation (see Sect. 4.4.7.1), usually by setting `export F90_LHDRAD=1` before calling the configure script (see Sect. 4.3.1.8).
- **MSrad:** (“solar module”, local models, “box-in-a-star” models) It uses long characteristics. The lateral boundaries have to be periodic. Top and bottom can be closed or open. Note that the switch `-Drhd_r02=1` has to be set during compilation (see Sect. 4.4.7.2), usually by setting `export F90_MS RAD=1` before calling the configure script (see Sect. 4.3.1.9).
- **SHORTrad:** (new “supergiant module”, global models, “star-in-a-box” models) It uses short characteristics and is restricted to an equidistant grid and open boundaries at all surfaces. Note that the switch `-Drhd_r03=1` has to be set during compilation (see Sect. 4.4.7.3), usually by setting `export F90_SHORTRAD=1` before calling the configure script (see Sect. 4.3.1.10).

7.1.16.2 integer n_radband

It can be specified whether the grey opacity table or the binned frequency-dependent part of the opacity table is used during the computation. The grey part contains only one bin. The other (possibly non-grey) contains one or more bins depending on the table chosen. The parameter is specified with e.g.


```
integer n_radband f=I4 b=4 n='Number of frequency bins' &
  c0='1: grey opacities' &
  c1='2: non-grey opacities (if available from table)' &
  c2='3: two bands: 1.grey, 2.CO (density via XCO)' &
  c3='4: two bands: 1.grey, 2.CO (density from chemistry)'
1
```

Allowed values are

- 1: Use the grey part of the table
- 2: Use the other (possibly non-grey, frequency-dependent) part of the table
- 3: Use a continuum band plus an infrared band with CO opacity, calculated with CO equilibrium density
- 4: Use a continuum band plus an infrared band with CO opacity, calculated with CO density resulting from time-dependent chemistry

7.1.16.3 integer n_radminiter

Usually the stability considerations dictate a radiative time step smaller than the hydrodynamics or tensor-viscosity time step. To remedy this situation it is possible to allow several radiation transport steps per global time step. Hitherto, all three radiation transport modules support this iteration. The minimum number of iterations (radiative sub-steps) can be specified e.g. with

```
integer n_radminiter f=I4 b=4 &
  n='Minimum number of radiation transport iterations' c0=8
1
```

If less iterations are needed the time step limit for the next step is increased. This value will in almost any case (for explicit radiation transport) be set to 1. In the implicit case it is set to a higher value (typically 5).

7.1.16.4 integer n_raditer

After each complete radiative time step the recommendation for the next time step will be chosen so that `n_raditer` iterations will (probably) be needed. The parameter can be set e.g. with

```
integer n_raditer f=I4 b=4 &
  n='Number of radiation transport iterations' c0=10
8
```

For a simulation of a solar-type star (with comparatively long radiative time scales) it will typically be set to 1. For stars with shorter radiative time scales values around 10 may be considered. All three radiation transport modules understand this parameter.

7.1.16.5 integer n_radmaxiter

The absolute maximum number of iterations can be specified e.g. with

```
integer n_radmaxiter f=I4 b=4 &
  n='Maximum number of rad. transport iterations' c0=30
0
```

If more iterations are needed the computation for the current time step is stopped and resumed with a smaller one (which means that the hydrodynamics and the tensor-viscosity step have to be done again). Usually, `n_radmaxiter` will either be set to a value somewhat larger than the recommended number of iterations (`n_raditer`) or to 0 which disables the check for too many iterations completely. This can be safely allowed in many cases and has the advantage that there is no need to save the initial model before calling the radiation transport module, which saves some memory. To disable the iteration of the radiation transport sub-step set `n_radminiter=n_raditer=n_radmaxiter=1`. All three radiation transport modules understand this parameter.

7.1.16.6 character radraybase

Using the modules LHDrad or SHORTrad, the orientation of the base axis system can be selected e.g. with

```
character radraybase f=A80 b=80 n='Base axis system' &
  c0='SHORTrad: unity/random/randomcube/randomgroup/alternate' &
  c1='MSrad: lobatto/dblgaus'
random
```

Allowed values for radscheme=SHORTrad are:

- **unity**: (default) During all time steps and radiative sub-steps the direction of the rays stays the same.
- **random**: At each time step (and radiative sub-step) a new base axis system is chosen at random
- **randomcube**: The distribution of the random angles is tuned to optimize the isotropy of the time-averaged radiation field. Use together with **radraystar=cube**.
- **randomgroup**: At each new time step a new base axis system is chosen at random. It is kept for all radiative sub-steps.
- **alternate**: Alternate between unity and random orientation matrix.
- **drift01**: Slow drift, algorithm 1.
- **drift02**: Slow drift, algorithm 2.

Because typically only a relatively small number of rays is chosen per time step (with **radraystar**) it is advisable to vary the directions of the rays (by choosing **radraybase=random** or **randomgroup**) to cover the entire sphere at least over a longer time.

Allowed values for radscheme=MSrad are:

- **lobatto**:
- **dblgaus**:

7.1.16.7 character radraystar

Using the modules LHDrad or SHORTrad, the list of ray directions (i.e. the number of rays and their coordinates) relative to the base axis system can be specified with e.g.

```
character radraystar f=A80 b=80 n='List of relative ray directions' &
  c0='x1(1)/x2(1)/x3(1)/oktaeder(3)/tetraeder(4)/cube(4)' &
  c1='ikosaeder(6)/dodekaeder(10)'
oktaeder
```

Examples for allowed values are

- **x1**: (N=1) one single ray along x1 axis (not enough to specify fluxes in all directions)
- **x2**: (N=1) one single ray along x2 axis (not enough to specify fluxes in all directions)
- **x3**: (N=1) one single ray along x3 axis (not enough to specify fluxes in all directions)
- **oktaeder**: (N=3, default) octahedron
- **tetraeder**: (N=4) tetrahedron
- **cube**: (N=4)
- **ikosaeder**: (N=6) icosahedron
- **dodekaeder**: (N=10) dodecahedron

- `list-01`, `list-01(3)`: Choose ray systems from a list (oktahedrons, tetrahedrons). If character `radraybase` is set to `unity` the rays will only be aligned to the axes or diagonals and thus avoid the time-consuming interpolation step of the short-characteristics method.

Several other choices are possible, which are meant for test purposes only. Choosing one of the five Platonic solids (Oops! “German-Greek” names only, so far) means that the 3 to 10 rays are equally distributed over the solid angle (from the center to each *corner* of the respective solid). Check the complete list of options in subroutine `rh_d_rad3d_RaySystem`.

7.1.16.8 real `c_tminlimit`

A minimum temperature can be set, that is enforced by the radiation transport modules `MSrad3D` and `SHORTrad` by adding energy to the too cool cells, e.g. with

```
real c_tminlimit f=E15.8 b=4 &
  n='Enforced minimum temperature for radiation transport step' u=K &
  c0='<=0.0: off (default); 500.0: reasonable value'
400.0
```

7.1.16.9 real `c_radimplicitmu`

So far, only the `LHDrad` and the `SHORTrad` module support implicit radiation transport. It can be activated with the parameter

```
real c_radimplicitmu f=E15.8 b=4 &
  n='Implicitness parameter for radiation transport' u=1 &
  c0='0.0: explicit / 0.5: time centered / 1.0: fully implicit'
0.0
```

Allowed values are

- 0.0: Fully explicit radiation transport (possible with all modules)
- $0.0 < C < 1.0$: Partly implicit radiation transport
- 0.5: Radiation transport time-centered
- 1.0: Fully implicit radiation transport

Values outside this range do not have much meaning. The implicit transport does not work efficiently yet: It does not yield significantly larger time steps than possible with a sequence of purely explicit sub time steps. Additionally, it turns out that the hydrodynamics runs into trouble if a too large time step (still well within the Courant condition) is requested.

7.1.16.10 real `c_raditereps`

With activated implicit radiation transport (`LHDrad` and `SHORTrad` modules only) the requested convergence accuracy of the iteration can be set e.g. with

```
real c_raditereps f=E15.8 b=4 &
  n='Relative accuracy for radiation iteration' u=1 &
  c0='Typical value: 1.0E-03'
2.0E-03
```

7.1.16.11 real c_raditerstep

With activated implicit radiation transport (LHDrad and SHORTrad modules only) the step size of the iteration can be restricted with e.g.

```
real c_raditerstep f=E15.8 b=4 &
    n='Step size of radiation iteration'           u=1 &
    c0='Typical values: 0.7,0.81'
1.0
```

Allowed values are

- 0.0 < 1.0: Restricted step size
- 1.0: No restriction, standard step size
- > 1.0: Extra large steps

This value has to be chosen carefully to get optimal performance. Is the step size too small the convergence is safe but too slow. A too large step size inhibits convergence and leads to a decrease in the time step, which results in a bad performance, too.

7.1.17 Radiation-transport control (MSrad only)

7.1.17.1 integer n_radtheta

Using the MSrad module the ray directions have to be specified in a different way: The number of ray sets in theta direction can be chosen with e.g.

```
integer n_radtheta f=I4 b=4 &
    n='NTHETA: Number of ray sets in theta direction' c0=2
2
```

7.1.17.2 integer n_radphi

Using the MSrad module the number of ray sets in phi direction can be set e.g. with

```
integer n_radphi f=I4 b=4 &
    n='NPHI: Number of ray sets in phi direction' c0=2
2
```

7.1.17.3 integer n_radsubray

Using the MSrad module the number of rays per cell (with the same direction) can be specified e.g. with

```
integer n_radsubray f=I4 b=4 n='KPHI: Number of rays per cell' c0=2
2
```

7.1.17.4 integer n_radthickpoint

With the MSrad module the lower part of the model can be computed in diffusion approximation. The number of points in diffusion approximation can be set with e.g.

```
integer n_radthickpoint f=I4 b=4 &
    n='Number of grid points with optically thick (diff.) approximation' &
    c0='0: no diffusion approximation'
0
```

The value should be chosen so that for all points in that region $\Delta\tau > 1$ is valid. Setting this value to 0 means that the diffusion approximation is not used in any part of the model.

7.1.17.5 integer n_radtaurefine

With the LHDrad and the MSrad module, the number of points on the rays can be finer than the number of points in the basic numerical grid. The refinement can be set e.g. with

```
integer n_radtaurefine f=I4 b=4 &
  n='Refinement factor'
0
```

7.1.17.6 integer n_radrsyslevel

This parameter specifies the "zero" point of the ray system, default: 0 (MSrad only). The parameter is specified with e.g.

```
integer n_radrsyslevel f=I4 b=4 n='Zero index of ray system' &
  c0='0: (default)' &
0
```

7.1.17.7 integer n_radoutput

This parameter controls additional output into the file 'rhd.grad', default: 0 (MSrad only). The parameter is specified with e.g.

```
integer n_radoutput f=I4 b=4 n='Output level of MSrad' &
  c0='0: (default)' &
1
```

7.1.17.8 real c_radtcool

Parameter for surface cooling option ($N_{\text{radband}} \leq 0$) of MSrad. It can be activated with the parameter

```
real c_radtcool f=E15.8 b=4 &
  n='Surface cooling'          u=1 &
  c0='0.0: default'
0.0
```

7.1.17.9 real c_raddcool

Parameter for surface cooling option ($N_{\text{radband}} \leq 0$) of MSrad. It can be activated with the parameter

```
real c_raddcool f=E15.8 b=4 &
  n='Surface cooling'          u=1 &
  c0='0.0: default'
0.0
```

7.1.17.10 real c_radscool

Parameter for surface cooling option ($N_{\text{radband}} \leq 0$) of MSrad. It can be activated with the parameter

```
real c_radscool f=E15.8 b=4 &
  n='Surface cooling'          u=1 &
  c0='0.0: default'
0.0
```

7.1.17.11 real c_radtinci

Temperature of black body that emits incident radiation, default: 0.0, (MSrad only). It can be used e.g. with

```
real c_radtinci f=E15.8 b=4 &
  n='Temperature of black body that sends incident radiation' u=K &
  c0='0.0: default'
0.0
```

7.1.17.12 real c_raddinci

Dilution factor $(R_*/d)^2$ of black body that emits incident radiation, default: 0.0, (MSrad only). It can be used e.g. with

```
real c_raddinci f=E15.8 b=4 &
  n='Dilution factor of black body that sends incident radiation' u=1 &
  c0='0.0: default'
0.0
```

7.1.18 Radiation-transport control (LHDrad only)**7.1.18.1 real c_radvisdtau**

Using the LHDrad module the limit in delta optical depth ($\rho \cdot \kappa \cdot dx$) below which the “radiative temperature viscosity” (=temperature smoothing) is to be applied can be set with e.g.

```
real c_radvisdtau f=E15.8 b=4 &
  n='Optical depth limit for temperature viscosity' u=1
0.1
```

The introduction of this “temperature diffusion” is a somewhat desperate and inelegant attempt to improve the behavior of the Greens function (hot cells should be cooled, cool cells should be heated). This diffusion is necessary for not well resolved models. It is switched off with `c_radvisdtau` ≤ 0.0 .

7.1.18.2 real c_radtvis

Using the LHDrad module the amount of the “radiative temperature viscosity” (=temperature smoothing) can be specified e.g. with

```
real c_radtvis f=E15.8 b=4 n='Temperature viscosity' u=1
1.6
```

For well resolved models it should be switched off (with `c_radtvis` ≤ 0.0).

7.1.18.3 real c_radthintimefac

In the LHDrad module only the radiative time step restriction due to energy changes can be relaxed further in the optically thin by specifying e.g.

```
real c_radthintimefac f=E15.8 b=4 &
  n='time scale reduction in optically thin' u=1 &
  c0='range: 0.1 - 1.0, typically: 0.5'
0.60
```

A value ≤ 0.0 or `real c_radvisdtau` ≤ 0.0 switches off this relaxation.

7.1.19 Process-time management

In this group several parameters can be set which control the start of the time counting during a simulation and the total length of a job. If either one of the halt conditions below is met, CO5BOLD finishes the current step, writes a final model (plus some final information to other files), and stops execution.

For example on a CRAY one typically wants to use most of the CPU time given for an individual batch job. In this case one can set e.g. `real cputime_remainlimit=2000.0` and the values for the other halt conditions to `-1.0` or `-1`.

7.1.19.1 real starttime

The start time of a simulation is usually taken from the start model file. But sometimes is simulation is to be started with the final model of a previous run but should start at time=0.0. This can be achieved by setting the start time with

```
real starttime f=E15.8 b=4 n='Start time'          u=s
0.0
```

Allowed values are

- ≥ 0.0 : Set the initial time of the simulation to this value and override value from start model.
- < 0.0 : (default) Take the initial time from start model.

7.1.19.2 integer starttimestep

The start time step count of a simulation is usually taken from the start model file. But sometimes is simulation is to be started with the final model of a previous run but should start at time step=0. This can be achieved by setting the start time step count with

```
integer starttimestep f=I11 b=4 n='Start time step number'  u=1
0
```

Allowed values are

- ≥ 0 : Set the initial time step of the simulation to this value and override value from start model.
- < 0 : (default) Take the initial time step count from start model.

7.1.19.3 real cputime

Because of the long simulation time usually CO5BOLD will run in some sort of batch mode which might impose limits on the execution time per run. On a CRAY the CPU time that is left can be accessed with a special subroutine (in call `tremain` in `timing_module.F90`). On other machines it is possible to specify the allowed total time for the job e.g. with

```
real cputime f=E15.8 b=4 n='CPU time'          u=s
1000000.0
```

During the run of CO5BOLD the leftover CPU time is computed by subtracting the used CPU time (which is given by `e_time=etime(tarray)` in `timing_module.F90`) from the specified total CPU time for the job.

7.1.19.4 real cputime_remainlimit

Because CO5BOLD needs some time to finish the last time step it should start exiting well before all CPU time is used up. This amount of buffer CPU time can be specified e.g. with

```
real cputime_remainlimit f=E15.8 b=4 n='maximum remaining CPU time'  u=s
2000.0
```

Its value depends on the size of the model and the speed of the machine (more precisely the maximum CPU time per time step).

7.1.19.5 real endtime

If the simulation should run up to a certain (stellar) time, its values can be specified e.g. with

```
real endtime f=E15.8 b=4 n='total simulation time limit'          u=s
10000.0
```

A value < 0.0 deactivates this halt condition: it is not checked at all. If this parameter is set to a non-negative value a follow-up simulation should not use the same parameter file: it would stop immediately.

7.1.19.6 real plustime

If the initial model should be advanced by a certain (stellar) time span, this value can be set e.g. with

```
real plustime f=E15.8 b=4 n='simulation advance time'      u=s
5.0E+07
```

A value < 0.0 cancels this halt condition: it is not checked at all. This condition assures (if it is the only one) that all individual simulation runs cover (approximately) the same stellar time.

7.1.19.7 integer endtimestep

If the simulation should run up to a certain time step, its values can be specified e.g. with

```
integer endtimestep f=I11 b=4 n='total simulation time step number'    u=1
1234
```

This might be useful to advance the simulation up to a point shortly before a previous simulation crashed. A value < 0 cancels this halt condition: it is not checked at all.

7.1.19.8 integer plustimestep

If the initial model should be advanced by a certain number of time steps their number can be set e.g. with

```
integer plustimestep f=I11 b=4 n='simulation advance time step number' u=1
2000
```

A value < 0 deactivates this halt condition: it is not checked at all.

7.1.20 Time-step control

In this group parameters to control the time step restrictions can be set.

They are important because decide about performance and stability of CO5BOLD. They should be tested and adjusted for a simulation of a new type of object. But all the dimensionless parameters can stay unchanged for a group of similar simulations. Only the parameters with an explicit time dimension should be checked in all cases (they scale with characteristic timescales and depend particularly on gravity).

7.1.20.1 real dtime_start

The initial time step recommendation of a simulation is usually taken from the start model file. It can be overwritten e.g. with

```
real dtime_start f=E15.8 b=4 n='Start time step'          u=s
1.0E+03
```

A value ≤ 0.0 means that the original value from the start model is used.

7.1.20.2 real dtime_min

In some rare cases it might be useful to specify explicitly the minimum time step with e.g.

```
real dtime_min f=E15.8 b=4 n='Minimum time step'        u=s &
  c0='dtime_min=0.0 => no restriction'
1.0
```

This value is used even if restrictions from the Courant condition try to enforce a smaller value. A fixed time step can be prescribed by setting `dtime_min = dtime_max` to some positive value. A value `dtime_min ≤ 0.0` means that this time step restriction is completely ignored, which is the case that should usually be chosen.

7.1.20.3 real dttime_max

It is possible to explicitly specify the maximum time step too, e.g. with

```
real dttime_max f=E15.8 b=4 n='Maximum time step'           u=s &
  c0='dttime_max=0.0 => no restriction'
1.0E+05
```

A fixed time step can be prescribed by setting `dttime_min = dttime_max` to some positive value. A value `dttime_max ≤ 0.0` means that this time step restriction is completely ignored, which is the case that should usually be chosen.

7.1.20.4 real dttime_min_stop

Sometimes a simulation can run into a pathological state where the time step decreases rapidly without recovering. To prevent a simulation in such a case from running forever (or until some other process time restriction applies) without actually advancing significantly in time, it is possible to specify an absolute minimum time step, e.g. with

```
real dttime_min_stop f=E15.8 b=4 n='Minimum time step'       u=s &
  c0='dttime_min_stop=0.0 => no restriction' &
  c1='dttime < dttime_min_stop => program stop'
1.0
```

If the actual time step falls below this value, the simulation finishes gracefully. This values has to specified as absolute time and has to be chosen carefully for each individual model (or each group of models). This time step restriction can be switched off by setting `real dttime_min_stop=0.0`. But in general, one should keep it activated and try to find a proper positive value.

7.1.20.5 real dttime_incmx

Sometimes a time step restriction can lead to a sudden drastic drop in the time step. To prevent unwanted oscillations in the size of the time step its increase can be restricted e.g. with

```
real dttime_incmx f=E15.8 b=4 n='Maximum time step increment factor' u=1 &
  c0='dttime_max<1.0 => no restriction' c1='typically 1.1'
1.2
```

This value specifies the maximum factor by which the time step can be increased from step to step (even if the new Courant condition etc. would allow more). A value `value < 0.0` deactivates this restriction.

7.1.20.6 real c_courant

A typical Courant factor for each 1D hydrodynamics step can be specified with e.g.

```
real c_courant f=E15.8 b=4 n='HD Courant factor'             u=1 &
  c0='range: 0.0 < C_Courant <= 1.0, typically: 0.5'
0.5
```

From the minimum cell crossing time of a partial wave and this factor a recommendation for the *next* time step is computed. A value of 1.0 is the very upper limit that guarantees stability for some simple linear 1D test problems. Recommended upper limits for fully non-linear simulations can be found in Tab. 7.1.

7.1.20.7 real c_courantmax

A typical maximum Courant factor for each 1D hydrodynamics step can be specified with e.g.

```
real c_courantmax f=E15.8 b=4 n='maximum HD Courant factor' u=1 &
  c0='range: C_Courant < C_Courantmax <= 1.0, typically: 0.9'
0.8
```

From the minimum cell crossing time of a partial wave and this factor an upper limit for the *current* time step is computed. If this limit is exceeded the computation is interrupted and resumed with a smaller time step (based on `c_courant`). Usually this parameter should be restricted by `c_courant < c_courantmax ≤ 1.0`. A value of 1.0 is the very upper limit that guarantees stability for some simple linear 1D test problems. Recommended upper limits for fully non-linear simulations can be found in Tab. 7.1.

7.1.20.8 real c_maxeichange

The relative change in internal during a single 1D hydrodynamics step can be used to restrict the time step by specifying

```
real c_maxeichange f=E15.8 b=4 n='maximum hydro energy change'      u=1 &
  c0='range: 0.1 - 1.0, typically 0.5, off:0.0'
  0.5
```

The default is 0.9. Nevertheless, since the Roe solver is constructed to handle shocks and rapid changes in density and energy, this check is usually not needed. It can be switched off by setting `c_maxeichange=0.0`.

7.1.20.9 real c_hydsoundcourant

In addition to the normal Courant factor `c_courant` that gives a time-step restriction based on $c + \text{abs}(v_1)$, another factor can be specified that is based only on the sound speed c , e.g. with

```
real c_hydsoundcourant f=E15.8 b=4 n='HD sound-speed Courant factor'  u=1 &
  c0='range: 0.0 < c_hydsoundcourant <= 0.5, typically: 0.45'
  0.48
```

The check for this condition should be activated (by giving `c_hydsoundcourant` a positive value > 0) for 3D simulations with `hdsplit=CTU`, see Sect. 7.1.8.3 and Table 7.1. In this case, a value slightly smaller than 0.5 is a reasonable choice.

7.1.20.10 real c_hydsoundcourantmax

In addition to the normal maximum Courant factor `c_courantmax` that gives a time-step restriction based on $c + \text{abs}(v_1)$, another factor can be specified that is based only on the sound speed c , e.g. with

```
real c_hydsoundcourantmax f=E15.8 b=4 &
  n='maximum HD sound-speed Courant factor' u=1 &
  c0='range: c_hydsoundcourant < c_hydsoundcourantmax <= 0.5, typically: 0.5'
  0.5
```

The pair `c_hydsoundcourant/c_hydsoundcourantmax` works together in a the same way as described above for `c_courant/c_courantmax`.

7.1.20.11 real c_hydexpcourant

In addition to the usual Courant condition one could restrict the maximum expansion between two adjacent grid cells with e.g.

```
real c_hydexpcourant f=E15.8 b=4 n='HD expansion Courant factor'      u=1 &
  c0='range: 0.0 < C_hydExpCourant < C_hydExpCourantmax, typically: 0.3'
  0.2
```

7.1.20.12 real c_hydexpcourantmax

This parameter can be set e.g. with

```
real c_hydexpcourantmax f=E15.8 b=4 n='HD max. expansion Courant factor' u=1 &
  c0='range: 0.0 < C_hydExpCourant < C_hydExpCourantmax, typically: 0.5'
  0.3
```

The pair `c_hydexpcourant/c_hydexpcourantmax` works analogously to the pair `c_courant/c_courantmax`.

7.1.20.13 real c_radcourant

The radiation transport routines are subject to time step restrictions, too. And in typical scenarios, its the radiative timescale are the shortest one and poses the tightest restriction. Contrary to the hydrodynamics routines the timescale relevant for the stability of the radiation transport scheme can only be estimated using the characteristic timescale of a small sinusoidal temperature disturbance with a wavelength of the grid size in a homogeneous background and grey radiative energy exchange. The “radiative Courant” factor can be set e.g. with

```
real c_radcourant f=E15.8 b=4 n='RAD Courant factor'           u=1 &
  c0='range: 0.0 < C_radCourant, typically: 1.0'
  2.5
```

If the estimate of the timescale would be correct a value of 2.0 would cause the temperature fluctuation on the shortest scale to flip its sign, setting the absolute stability limit. A value of 1.0 would lead to a damping of these fluctuations within one time step. But in practice, even higher values (for example 2.5) show a reasonable behavior. This might be due to the effect that the shortest radiative timescale only occurs at single points (or in 2D layers) but that already the immediate neighbors have longer timescales and can damp the “most sensitive points”. Based on `real c_radcourant` the recommended typical radiative time step is computed.

7.1.20.14 real c_radcourantmax

With this parameter the maximum allowed radiative time step is prescribed as e.g. in

```
real c_radcourantmax f=E15.8 b=4 n='maximum RAD Courant factor' u=1 &
  c0='range: C_radCourant <= C_radCourantmax, typically: 2.0'
  3.0
```

This value will typically be somewhat larger than `real c_radcourant`.

7.1.20.15 real c_radmaxeichange

The relative energy change per radiative sub step can be restricted e.g. with

```
real c_radmaxeichange f=E15.8 b=4 n='maximum radiative energy change' &
  u=1 c0='range: 0.01 - 1.0'
  0.25
```

The default is 0.5. Values between 0.1 and 0.5 seem reasonable. A value ≤ 0.0 deactivates this time step check. However, the check of the radiative energy change should usually be performed. A way to maximize the radiative time step (and therefore the performance of the entire code) can be to first set `real c_radmaxeichange` to a proper value (say 0.25). Then, `real c_radcourant` (and `real c_radcourantmax`) are adjusted (by trial and error) in a way that the radiative time step is almost always restricted by the “Courant” condition and only sometimes in extreme cases by the maximum energy change restriction. The computed output intensity should be checked for the size of its fluctuations due to a possibly too large value of `c_radmaxeichange`.

7.1.20.16 real c_viscourant

The tensor-viscosity routines have their own time step restriction. The recommended typical viscous time step can be set e.g. with

```
real c_viscourant f=E15.8 b=4 n='viscous Courant factor'       u=1 &
  c0='range: 0.0 < C_visCourant, typically: 0.5-1.0, better 0.25'
  0.5
```

As the corresponding viscous timescale is typically longer than the radiative one (and even the Courant timescale from the Roe hydrodynamics routines) this factor is often irrelevant. The absolute upper stability limit is located at `c_viscourant=2.0`. Values around 0.5 to 1.0 are more typical. In some extreme cases in simulations of the solar chromosphere it has turned out that an even lower value (0.2) is necessary to prevent some spikes in the neighborhood of strong colliding shocks.

7.1.20.17 real c_viscourantmax

The absolute upper limit for the viscous time scale can be set with

```
real c_viscourantmax f=E15.8 b=4 n='maximum viscous Courant factor' u=1 &
  c0='range: C_visCourant <= C_visCourantmax, typically smaller than 2.0'
  1.0
```

Its value should be slightly above `c_viscourant` and below 2.0.

7.1.21 Input/output control

With this group of parameters the start model and the type and amount of output can be specified. Parameters with the suffix “_start” describe the initial model, these with suffix “_end” the corresponding final model. Additional data can be written into the file described by the parameters with suffix “_full” (full 2D/3D model dumps, huge, see Sect. 8.1) or into the file described by the parameters with suffix “_mean” (additional information, see Sect. 8.3).

7.1.21.1 real dtime_out_full

The interval between datasets in the `full` file can be set e.g. with

```
real dtime_out_full f=E15.8 b=4 n='Output time step' u=s &
  c0='dtime_out_full < 0.0 => no output' &
  c1='dtime_out_full = 0.0 => output every time step'
  2.0E+06
```

Allowed values are

- `< 0.0`: No output to this file
- `= 0.0`: Output at every time step. Attention: This can produce HUGE files in no time.
- `> 0.0`: Output to `full` file approximately every `dtime_out_full` seconds.

Some examples: The “classical” value for this output for simulations of solar granulation is 20 sec. To save memory this can be increased to 30 sec. But in this case chromospheric shocks are very badly resolved. To cover them properly, a sampling rate of 10 sec or below is needed. On the other hand, if no good time resolution is needed a sampling rate of a few minutes might be sufficient.

7.1.21.2 real dtime_out_end

The interval between outputs into the `end` file can be set e.g. with

```
real dtime_out_end f=E15.8 b=4 n='Output time step' u=s &
  c0='dtime_out_end < 0.0 => output only at very end' &
  c1='dtime_out_end = 0.0 => output every time step' &
  c2='dtime_out_end > 0.0 => output every dtime_out_end seconds (and at end)'
  1.0E+04
```

Allowed values are

- `< 0.0`: Output only at very end of run (classical behavior).
- `= 0.0`: Output at every time step. Attention: This can produce lots of I/O operations and can take a long time. However, it will not produce a large file. Instead, the `end` file is written over and over again.
- `> 0.0`: Output to `end` file approximately every `dtime_out_end` seconds (and at the very end of the simulation).

The standard value is `-1.0`, not enabling any additional output into this file. A value a reasonable factor smaller than `real dtime_out_full` seems appropriate.

7.1.21.3 real dtime_out_mean

The interval between datasets in the `mean` file can be set e.g. with

```
real dtime_out_mean f=E15.8 b=4 n='Output time step'          u=s &
  c0='dtime_out_mean<0.0 => no output'
  0.5E+06
```

Allowed values are

- < 0.0: No output to this file
- = 0.0: Output at every time step.
- > 0.0: Output to `mean` file approximately every `dtime_out_mean` seconds.

Because the size of one `mean` dataset is much smaller than one `full` dataset, it is possible to request a higher sampling rate without using too much disk space.

7.1.21.4 integer n_outslicedim_mean

The index of the optional slice in the `mean` output file can be specified with e.g.

```
integer n_outslicedim_mean f=I4 b=4 n='index of slice in mean output file' u=1 &
  c0='0: no output of slice' &
  c1='1, 2, 3: output of slice with plane perpendicular to this direction'
  2
```

With a value of 0 the output is suppressed. A value of 1, 2, 3 indicates the direction of the normal to the output plane: for instance, in a local 3D "box-in-a-star" model with gravity along direction 3 a value of 3 gives a horizontal plane in the middle of the model (useful only in special cases) whereas a value of 2 (or 1) gives a vertical slice with a horizontal and the vertical axis – useful for movies of 2D slices. The grid index of the slice cannot be specified.

7.1.21.5 integer outdim_chu1

The dimension of an additional output chunk (1) written into a separate file can be specified with this parameter (a 2×3 integer array). The output of a horizontal slice at the 20th layer from the bottom can be requested with:

```
integer outdim_chu1 d=(1:2,1:3) f=I5 b=4 p=6 n='Chunk 1 dimension'    u=1 &
  c0='0: start from first, 9999: end with last'
  0 9999    0 9999    20 20
```

The index ranges go from 1 to the number of elements in that dimension. Specifying a lower first or a larger last dimension (as in the example), means that all elements will be taken. The output sampling rate is the same as for `mean` files. Attention: a high sampling frequency of large chunks can produce large files very quickly.

7.1.21.6 integer outdim_chu2

The dimension of another output chunk 2 written into a separate file can be specified with this parameter, analogously to `integer outdim_chu1` as e.g., in

```
integer outdim_chu2 d=(1:2,1:3) f=I5 b=4 p=6 n='Chunk 2 dimension'    u=1 &
  c0='0: start from first, 9999: end with last'
  0 9999 100 100    0 9999
```

7.1.21.7 integer outdim_chu3

The dimension of another output chunk 2 written into a separate file can be specified with this parameter, analogously to `integer outdim_chu1` as e.g., in

```
integer outdim_chu3 d=(1:2,1:3) f=I5 b=4 p=6 n='Chunk 3 dimension'    u=1 &
  c0='0: start from first, 9999: end with last'
  100 100    0 9999    0 9999
```

7.1.21.8 character infile_start

The filename of the initial model is specified e.g. with

```
character infile_start f=A80 b=80 n='File name of start model'
rhd.sta
```

Default is `rhd.sta` (for a parameter file used within a batch system). Typical filenames are `st35gm04n01_01.sta` or `gt57g44n20dz.end`.

7.1.21.9 integer istep_in_start

The index number of the dataset in the start model file to be used can be specified, e.g. with

```
integer istep_in_start f=I4 b=4 n='Number of dataset to read as start model' &
    u=1 c0='1: first dataset (default), 2: second dataset, ...'
1
```

7.1.21.10 character outfile_end

The file name for the final model can be specified with e.g.

```
character outfile_end f=A80 b=80 n='Output file name'
rhd.end
```

The default is `rhd.end`. Leaving it empty means that no final model is written. This of course inhibits follow-up simulations but can be useful to save time and disk space for some tests.

7.1.21.11 character outfile_full

The name of the file for the output of additional full models at regular intervals (see Sect. 8.1) can be given with e.g.

```
character outfile_full f=A80 b=80 n='Output file name'
rhd.full
```

Leaving it empty means that no file of this type is written.

7.1.21.12 character outfile_mean

The name of the file for the output of additional information (average stratification (1D), mean fluxes (1D), surface intensities(2D)) at regular intervals (see Sect. 8.3) can be specified with e.g.

```
character outfile_mean f=A80 b=80 n='Output file name'
rhd.mean
```

Leaving it empty means that no file of this type is written.

7.1.21.13 character outfile_mcyl

The name of the file for the output of azimuthal averages (2D arrays for 3D models) at regular intervals (see Sect. 8.3) can be specified with e.g.

```
character outfile_mcyl f=A80 b=80 n='Output file name'
rhd.mcyl
```

Leaving it empty means that no file of this type is written. Only in the case of global models such data is computed. It is particularly useful for rotating models.

7.1.21.14 character outfile_chu1

The name of the file for the output of an additional data chunk at regular intervals (the same as for mean file) can be specified with e.g.

```
character outfile_chu1 f=A80 b=80 n='Output file name for chunks'
rhd.chu1
```

The UIO format is the same as specified for mean files. Leaving the name empty means that no file of this type is written.

7.1.21.15 character outfile_chu2

The name of the file for the output of an additional data chunk 2 can be specified with this parameter analogously to `character outfile_chu1`.

7.1.21.16 character outfile_chu3

The name of the file for the output of an additional data chunk 3 can be specified with this parameter analogously to `character outfile_chu1`.

7.1.21.17 character outform_end

The format (see Sect. 6.2.3.1) of the final model files can be chosen e.g. with

```
character outform_end f=A80 b=80 n='Output file format' &
  c0='formatted/unformatted'
unformatted
```

Allowed values are

- **unformatted:** (default) fast compact (possibly machine-dependent) output: strongly recommended
- **formatted:** slow (machine-independent) output, big files

7.1.21.18 character outconv_end

The conversion type (see Sect. 6.2.3.1) of the final model files can be specified e.g. with

```
character outconv_end f=A80 b=80 n='Output file conversion' &
  c0='ieee_4/ieee_8/crayxmp_8/native'
ieee_4
```

The allowed values depend on the machine. Leaving this field empty means that the default is chosen that is build into the local UIO module. If the type `ieee_4` is supported (which is always the case, so far) it should be chosen.

7.1.21.19 character outform_full

The format (see Sect. 6.2.3.1) of the full model files can be chosen e.g. with

```
character outform_full f=A80 b=80 n='Output file format' &
  c0='formatted/unformatted'
unformatted
```

Allowed values are

- **unformatted:** (default) fast compact (possibly machine-dependent) output: strongly recommended
- **formatted:** slow (machine-independent) output, big files

7.1.21.20 character outconv_full

The conversion type (see Sect. 6.2.3.1) of the full model files can be specified e.g. with

```
character outconv_full f=A80 b=80 n='Output file conversion' &
  c0='ieee_4/ieee_8/crayxmp_8/native'
ieee_4
```

The allowed values depend on the machine. Leaving this field empty means that the default is chosen that is build into the local UIO module. If the type `ieee_4` is supported (which is always the case, so far) it should be chosen.

7.1.21.21 character outform_mean

The format (see Sect. 6.2.3.1) of the additional data files can be chosen e.g. with

```
character outform_mean f=A80 b=80 n='Output file format' &
  c0='formatted/unformatted'
unformatted
```

Allowed values are

- `unformatted`: (default) fast compact (possibly machine-dependent) output: strongly recommended
- `formatted`: slow (machine-independent) output, big files

7.1.21.22 character outconv_mean

The conversion type (see Sect. 6.2.3.1) of the additional data files can be specified e.g. with

```
character outconv_mean f=A80 b=80 n='Output file conversion' &
  c0='ieee_4/ieee_8/crayxmp_8/native'
ieee_4
```

The allowed values depend on the machine. Leaving this field empty means that the default is chosen that is build into the local UIO module. If the type `ieee_4` is supported (which is always the case, so far) it should be chosen.

7.1.22 Scale and test parameters

7.1.22.1 real time_scalestart

Usually, parameters are read from `rh.d.par` and are kept constant during a run. A consecutive run could be started with a different set though, e.g., to increase the luminosity of a model. However, in many cases, such an abrupt change causes the generation of spurious (often plane-parallel or radial) waves. And it takes time and effort – by temporarily increasing some viscosity – to damp them. This is particularly annoying when the transient waves reduce the time step of the simulations for some period.

The transition between two parameter sets can be smoothed by interpolating between them. The onset of the transition interval is given by `time_scalestart`, while the end of the interval is given by `time_scaleend` (see Sect. 7.1.22.2). The first set of parameters is given by the usual `rh.d.par` file, while the second set is given by an additional `rh.d.par2` file (see Tab. 6.1). Normally, the scaling is inactive. To activate it, the `rh.d_scale_module` has to be compiled by activating any tweak module, i.e., e.g. by setting `F90_TWEAK=1` (see Sect. 4.3.1.15) before calling the `configure` script (see Sect. 4.3). The file `rh.d.par2` has to exist in the current directory, i.e., at the same place where the `rh.d.par` file resides, and it has to have some entries with values differing from those in `rh.d.par`. Note, though, that so far only a few parameters are treated by the `rh.d_scale_module`. In addition, `0.0<time_ScaleStart<time` and `time_ScaleStart<=time_ScaleEnd` have to be fulfilled. Choosing `0.0<time_ScaleStart=time_ScaleEnd` should work but results in an abrupt change of parameters – not recommended.

For later runs (starting with `time_ScaleEnd<time`) the file `rh.d.par` should be replaced by the previous `rh.d.par2` and both scaling-time parameters should be set to negative values to properly indicate that the scaling is now finished (otherwise, the data in `rh.d.par` don't represent the values actually used for the simulation). The start time of the scaling interval can be set e.g. by


```
real time_scalestart f=E15.8 b=4 n='Start time of scaling interval'      u=s
100.0
```

Allowed values are

- < 0.0 : Don't scale (default).
- ≥ 0.0 : Perform the scaling if all the other conditions are met.

7.1.22.2 real time_scaleend

Together with `time_scalestart` (see a detailed description in Sect. 7.1.22.1), this parameter specifies the scaling interval. The end time of the scaling interval can be set e.g. by

```
real time_scaleend f=E15.8 b=4 n='End time of scaling interval'        u=s
200.0
```

Allowed values are

- < 0.0 : Don't scale (default).
- ≥ 0.0 : Perform the scaling if all the other conditions are met.

With the given example values `time_ScaleStart=100.0` and `time_ScaleEnd=200.0`, values from `rh.d.par` would be used for $100.0 \leq \text{time}$, values from `rh.d.par2` would be used for $\text{time} \geq 200.0$, and values in between (according to the interpolation in `rh.d_scale_module`) for $100.0 < \text{time} < 200.0$.

7.1.22.3 integer n_test1

The integer parameters `n_test1` to `n_test5` are general-purpose parameters to facilitate the testing of new features. They can be used anywhere in the code – but only for a limited time. In any release version of the code, all references to these parameters should be replaced by proper parameters with a dedicated purpose and a descriptive name. In contrast to these recommendation, the parameters are used (more or less permanently) in the various tweak modules. The parameter can be set e.g. by

```
integer n_test1 f=I11 b=4 n='1st integer test parameter'
1.0
```

7.1.22.4 real c_test1

The real parameters `c_test1` to `c_test5` are general-purpose parameters to facilitate the testing of new features. They can be used anywhere in the code – but only for a limited time, see above. The parameter can be set e.g. by

```
real c_test1 f=E15.8 b=4 n='1st real test parameter'
1.0
```

7.1.22.5 character strtest1

The string parameters `strtest1` to `strtest5` are general-purpose parameters to facilitate the testing of new features. They can be used anywhere in the code – but only for a limited time, see above. The parameter can be set e.g. by

```
character strtest1 f=A80 b=80 n='1st character test parameter'
model
```

7.1.23 Additional information and obsolete parameters

7.1.23.1 real abux

This optional information parameter can be specified with

```
real abux f=E15.8 b=4 n='hydrogen abundance (number fraction)' u=1 &
      c0='standard solar mixture'
0.90851003E+00
```

It has no practical consequences because the actually used chemical composition is determined by the files for equation of state and opacity.

7.1.23.2 real abuy

This optional information parameter can be specified with

```
real abuy f=E15.8 b=4 n='helium abundance (number fraction)' u=1 &
      c0='standard solar mixture'
0.90850003E-01
```

It has no practical consequences because the actually used chemical composition is determined by the files for equation of state and opacity.

7.1.23.3 real qmol

This optional information parameter can be specified with

```
real qmol f=E15.8 b=4 n='mean molecular weight' u=u &
      c0='standard solar mixture'
0.13018000E+01
```

It has no practical consequences because the actually used chemical composition is determined by the files for equation of state and opacity.

7.1.23.4 real gamma

This optional information parameter can be specified with

```
real gamma f=E15.8 b=4 n='Adiabatic coefficient' u=1 &
      c0='0.0/1.666666666666666/1.4'
0.0
```

It has no practical consequences because the actually used chemical composition is determined by the files for equation of state and opacity.

7.1.23.5 real c_radkappasmooth

In the LHDrad module the opacity along each ray can be smoothed. The amount of smoothing can be set e.g. with

```
real c_radkappasmooth f=E15.8 b=4 n='Opacity smoothing parameter' u=1 &
      c0='0.0: no smoothing, 0.25: light smoothing, 0.666: strong smoothing'
0.0
```

The smoothing can perhaps reduce the noise in the intensity images somewhat but has no general beneficial effect and should usually not be used.

7.1.23.6 real c_radtsmooth

In the LHDrad module the 3D temperature array can be smoothed. The amount of smoothing can be set e.g. with

```
real c_radtsmooth f=E15.8 b=4 n='Temperature smoothing parameter' u=1 &
    c0='0.0: no smoothing, 0.5: reasonable smoothing, 1.0: max. smoothing'
0.0
```

The smoothing can sometimes reduce the noise in the intensity images but causes/amplifies some anomalies of the radiative Greens function: Some cool cell just above the sharp sub-photospheric temperature drop are not heated but cool further down. Negative temperature spikes may result. This smoothing should not be used anymore.

7.1.23.7 character radpressure

In the LHDrad module there exists a simple prescription for the radiative pressure (reasonable in the optically thin) which can be activated with

```
character radpressure f=A80 b=80 n='Radiation pressure mode' &
    c0='on/off'
on
```

Allowed values are

- on: Radiation pressure on.
- off: Radiation pressure off.

The scheme is pretty slow and wrong in the optically thick. Do not use! However, the SHORTrad version is much more advance and can be used, even if it might require some more testing.

7.1.23.8 real c_radtintminfac

In the LHDrad module: The fraction the interpolated temperature (at a point on the ray) may exceed the minimum temperature at its four neighbors on the HD grid can be set e.g. with

```
real c_radtintminfac f=E15.8 b=4 &
    n='Temperature interpolation parameter' u=1 &
    c0='<1.0: only bilinear, 1.1: reasonable weighting between min. und bil.'
0.0
```

The introduction of this parameter was an attempt to reduce the negative (cooling) effect of a single hot cell on its cool neighbors. It should be switched off e.g. by setting it to 0.0.

7.1.23.9 integer dtimestep_out_fine

This parameter can be specified but there is no corresponding output file in CO5BOLD yet.

```
integer dtimestep_out_fine f=I4 b=4 n='Output time step number' u=1 &
    c0='dtimestep_out_fine<0 => no output'
-1
```

7.1.23.10 character outfile_fine

The name of the file for the output of additional information at regular (small) intervals can be specified with e.g.

```
character outfile_fine f=A80 b=80 n='Output file name'
rhd.fine
```

Leaving it empty means that no file of this type is written. Specifying it means the same (up to now).

7.1.23.11 character outform_fine

The format (see Sect. 6.2.3.1) of the files with frequent output can be chosen e.g. with

```
character outform_fine f=A80 b=80 n='Output file format' &
  c0='formatted/unformatted'
unformatted
```

Allowed values are

- **unformatted**: (default) fast compact (possibly machine-dependent) output: strongly recommended
- **formatted**: slow (machine-independent) output, big files

This parameter can be specified but there is no corresponding output file in CO5BOLD yet.

7.1.23.12 character outconv_fine

The conversion type (see Sect. 6.2.3.1) of the files with frequent output can be specified e.g. with

```
character outconv_fine f=A80 b=80 n='Output file conversion' &
  c0='ieee_4/ieee_8/crayxmp_8/native'
ieee_4
```

The allowed values depend on the machine. Leaving this field empty means that the default is chosen that is build into the local UIO module. If the type `ieee_4` is supported (which is always the case, so far) it should be chosen. This parameter can be specified but there is no corresponding output file in CO5BOLD yet.

7.2 Input model file: rhd.sta

A start file has the same structure as an end file (or a full file containing only one snapshot), see Sect. 8.1.

7.3 EOS file

The equations of state is provided via a table in UIO format, see Sect. 7.1.6.

7.4 Opacity file

The opacity data is provided via an ASCII table, see Sect. 7.1.7.

7.5 Chemistry input

The number densities of the chemical species must be provided as cell-centred quantities `quc` in cm^{-3} (see Sect. 4.4.1.6). The array (UIO) headers must be named following this example: "Number density of H2".

The chemistry input file contains all data for the reaction network. It is a text file with a strict format following the *UMIST 99 ratefile* standard:

```
FORMAT(I4,5(A8,1X),2(1X,A4),1X,1PE8.2,3X,0PF5.2,2X,0PF8.1,A16)
```

It consists of 12 columns with the following meaning:

col.	meaning	format
1	reaction ID	I4
2-4	reactants (max. 3 symbols with 8 characters)	3(A8,1X)
5-8	products (max. 4 symbols, first two with 8 characters, last 2 with 4 characters)	2(A8,1X),2(1X,A4) 2(A8,1X),2(1X,A4)
9	reaction coefficient α	1PE8.2
10	reaction coefficient β	0PF5.2
11	reaction coefficient γ	0PF8.1
12	reference	A16

The symbols are usually the chemical symbols of the involved species, e.g. C for carbon. The present species are recognised automatically. Molecules consisting of more than one atom of the same chemical element, e.g. H₂, are also possible (H2). A special case is the representative metal M which is a catalytic element only, i.e. it must appear as reactant *and* product. The special symbol PHOTON represents a photon as reaction product. Currently no photon can be used as reactant ionising or exciting another species.

The reaction coefficients are needed to calculate the chemical rates at runtime. The basic rate is then given by

$$k = \alpha T_{300}^{\beta} e^{-\gamma/T} , \quad (7.2)$$

where $T_{300} = T/300$ K with T the gas temperature. For catalytic reactions which involve a representative metal also the number density n_M of the metal enters:

$$k = n_M \alpha T_{300}^{\beta} e^{-\gamma/T} . \quad (7.3)$$

An input file could look like this:

```

5001 H      H      H2     H2     H2           9.00E-33  -0.6      0.0  -  AK
5002 H      H      H      H2     H            4.43e-28  -4.0      0.0  DBDDG72
4069 H2     H2     H2     H      H           1.00e-08   0.00    84100.0L 28034
4071 H2     OH     O      H2     H           6.00e-09   0.00    50900.0L 16964
   66 C      OH     O      CH           2.25e-11   0.50    14800.0L 4934
   67 C      OH     CO     H           1.81e-11   0.50     0.0  -  W80
3707 C      O      CO     PHOTON      1.58e-17   0.34    1297.4C  BDD90
7001 C      O      H      CO     H           2.14e-29  -3.08   -2114.0D DBDDG76
4076 CO     M      O      C      M           2.79e-03  -3.52   128700.0D CBDDG76

```

Refer to Wedemeyer-Böhm et al. (2005) for more details.

7.6 HION input

Several input files are required for the time-dependent treatment of hydrogen ionization. Currently, they need to be stored in the same input directory as specified with the parameter `hion_datapath`. There are four input files:

- model atom: The following formatting rules apply. Currently we only provide a hydrogen atom file `H_6-2.atom`. The module might be extended for other species in a future version.
- electron density look-up table (`edens.dat`) as function of total number density of hydrogen in cm^{-3} or m^{-3} , gas temperature in K, and ionization degree of hydrogen.
- chemical abundances (`abundance.input`)
- partition functions (`pf_kurucz.dat`)

The first two files are always needed, whereas the files containing chemical abundances and partition functions are required the initial LTE electron densities for very first time step of a model sequence (and for creating electron density tables). Once the first time step has been calculated the last two input files are obsolete. We plan to implement another initial guess for the LTE densities so that only the model atom and the electron density look-up table are necessary.

Refer to Leenaarts & Wedemeyer-Böhm (2005) for more details.

7.7 More control files: `rhds.stop`, `rhds.cont`, `rhds.dump`

Before each time step CO5BOLD checks in the working directory whether the file `rhds.stop` exists. If it has been generated (e.g. with `touch rhds.stop`), the code exits gracefully, i.e. it produces a proper final model, which can be used to restart the code. This method of stopping a simulation is to be preferred over a simple `kill` or `qdel` command because it allows to analyze the state of the model just at the end of the simulation and a smooth restart.

Before the restart the `rhds.stop` file has to be deleted! The simulation can be continued by just initiating a new run. If the file `rhds.cont` exists at the beginning of a simulation, the code tries to resume an interrupted computation: The initial model will not be taken from the start model file (`infile_start`) but from the final model (`outfile_end`). The data for the full and the mean file is not written into new files but will be appended to the existing ones.

In this way a simulation can be interrupted and continued in a fairly safe way. It is possible to analyze the final model and to change values in the parameter file. Keep in mind that after a restart with `rhds.cont` the specifications about the length of the job (e.g. the number of time steps) will be counted from the restart point and not from the beginning of the original simulation.

To interrupt a job with `rhds.stop` can be very handy. The continuation with `rhds.cont` and the old parameter file is not to be preferred over an ordinary restart with a new parameter file.

At the beginning of every time step CO5BOLD checks in the working directory whether the file `rhds.dump` exists. If it has been generated (e.g. with `touch rhds.dump`) and the file `rhds.snap` does *not* exist, the current model is written into `rhds.snap`. It has the same file properties (format and conversion) as the regular `rhds.end` file. The run of the simulation itself is not modified. This feature might be useful for debugging purposes.

Chapter 8

Output and status files

8.1 Output model files: rhd.end, rhd.full

If the UIO scripts (Sect.6.2.6) are properly installed, you can view the contents (more precisely the headers of the data entries) of an UIO file with `uiolook filename`, e.g.

```
uiolook st35gm04n05_03.end
```

gives the output (slightly edited)

```
fileform uio form=unformatted convert=ieee_4 version=0.1.2000.11.26 &
  date='02.01.2002 16:17:26.036' system=craSHi machine=craSHi osrelease=10.0.0.6 &
  osversion=UoK.4 hardware='CRAY SV1' language=Fortran90 program=RHD
```

```
character file_id f=A8 b=8 n='File identification'
character description d=(1:1) f=A24 p=1 b=24 n='File description'
character history d=(1:20) f=A80 p=1 b=80 n='File history'
character version f=A80 b=80 n='Program version'
```

```
label dataset n='RHD model' date='02.01.2002 16:17:26.043'
  character dataset_id f=A10 b=10 n='Type of box hierarchy'
  real modeltime f=E13.6 b=4 n=time u=s
  real modeltime_db f=E23.15 b=8 n=time u=s
  integer modelitime f=I11 b=4 n='time step number' u=1
  real dtime f=E13.6 b=4 n='time step' u=s
  real time_out_full_last f=E13.6 b=4 n='Time of last output of full model' u=s
  real time_out_mean_last f=E13.6 b=4 n='Time of last output of averaged data' &
  u=s
```

```
label box date='02.01.2002 16:17:26.049'
  character box_id f=A80 b=80 n='Block identification'
  integer dimension d=(1:2,1:3) f=I7 p=6 b=4
  real time f=E13.6 b=4 n=time u=s
  real time_db f=E23.15 b=8 n=time u=s
  integer itime f=I11 b=4 n='time step number' u=1
  real xc1 d=(-63:63,-63:-63,-63:-63) f=E13.6 p=4 b=4 &
  n='x1 coordinates of cell centers' u=cm ds=(0:0,0:1,0:1)
  real xc2 d=(-63:-63,-63:63,-63:-63) f=E13.6 p=4 b=4 &
  n='x2 coordinates of cell centers' u=cm ds=(0:1,0:0,0:1)
  real xc3 d=(-63:-63,-63:-63,-63:63) f=E13.6 p=4 b=4 &
  n='x3 coordinates of cell centers' u=cm ds=(0:1,0:1,0:0)
  real xb1 d=(-63:64,-63:-63,-63:-63) f=E13.6 p=4 b=4 &
  n='x1 coordinates of cell boundaries' u=cm ds=(0:1,0:1,0:1)
  real xb2 d=(-63:-63,-63:64,-63:-63) f=E13.6 p=4 b=4 &
  n='x2 coordinates of cell boundaries' u=cm ds=(0:1,0:1,0:1)
  real xb3 d=(-63:-63,-63:-63,-63:64) f=E13.6 p=4 b=4 &
  n='x3 coordinates of cell boundaries' u=cm ds=(0:1,0:1,0:1)
  real rho d=(-63:63,-63:63,-63:63) f=E13.6 p=4 b=4 n=Density u=g/cm^3
```

```

real ei d=(-63:63,-63:63,-63:63) f=E13.6 p=4 b=4 n='Internal energy' u=erg/g
real v1 d=(-63:63,-63:63,-63:63) f=E13.6 p=4 b=4 n='Velocity 1' u=cm/s
real v2 d=(-63:63,-63:63,-63:63) f=E13.6 p=4 b=4 n='Velocity 2' u=cm/s
real v3 d=(-63:63,-63:63,-63:63) f=E13.6 p=4 b=4 n='Velocity 3' u=cm/s
label endbox
label enddataset date='02.01.2002 16:17:43.322'

```

The UIO format is described in some detail in Sect. 6.2. Each entry has a type (e.g. “label”, “real”, “character”), an identifier (e.g. “box”, “time”, “description”), and additional information about array size (e.g. “d=(-63:63,-63:63,-63:63)”), data format (e.g. “f=E13.6 p=4 b=4”), and properties of the quantity (e.g. “n=Density u=g/cm³”).

Each start (“rhd.sta”) or final (“rhd.end”) model file has a structure as shown above. The (“rhd.full”) file usually contains a sequence of these data sets, which of course can also be used as start model of a simulation.

The axes *xc1*, *xc2*, and *xc3* describe the positions of the cell centers. The axes *xb1*, *xb2*, and *xb3* contain the positions of the cell boundaries: they have one element more than the corresponding cell centered quantity.

Cell boundaries should be centered in the middle between cell centers for the best representation of radiative fluxes with MSrad3D.

8.2 Files with additional chunks of data: rhd.chu1, rhd.chu2, rhd.chu3

If specified, the files “rhd.chu1”, “rhd.chu2”, and “rhd.chu3” contain (parts of) full data sets, written with the same sampling rate as mean files (see below). The dimensions of the output blocks have to be specified in detail with *outdim_chu1*, etc., as described in Sect. 7.1.21.5.

8.3 Files with averaged data: rhd.mean

A “rhd.mean” file contains derived data in addition to the complete data sets in “rhd.full” files: horizontal – and for global models spherically – averaged fluxes and other averaged quantities (all 1D vectors) and surface intensities (2D arrays). It has more entries than a full model file. However, they are much smaller. Therefore, one can afford a higher output sampling rate. The format is usually UIO “unformatted” (binary). A mean file usually consists of several datasets. The overall structure is

```

fileform uio form=unformatted convert=ieee_4

character file_id f=A8 b=8 n='File identification'
character description d=(1:1) f=A14 p=2 b=14 n='File description'
character history d=(1:20) f=A80 p=1 b=80 n='File history'
character version f=A80 b=80 n='Program version'

label dataset n='RHD model'
...
label enddataset

label dataset n='RHD model'
...
label enddataset

.
.
.

```

Each dataset has the following structure (for a supergiant simulation):

```

label dataset n='RHD model' date='25.05.2001 09:41:29.405'
...

```



```

label box date='25.05.2001 09:41:29.408'
character box_id f=A80 b=80 n='Block identification'
rad
...
label endbox

label box date='25.05.2001 09:41:29.983'
character box_id f=A2 b=2 n='Block identification'
z1
...
label endbox

label box date='25.05.2001 09:41:30.078'
character box_id f=A2 b=2 n='Block identification'
z2
...
label endbox

label box date='25.05.2001 09:41:30.170'
character box_id f=A2 b=2 n='Block identification'
z3
...
label endbox

label box date='25.05.2001 09:41:30.260'
character box_id f=A1 b=1 n='Block identification'
r
...
label endbox

label box date='25.05.2001 09:41:30.359'
character box_id f=A80 b=80 n='Block identification'
z
...
label endbox
label enddataset date='25.05.2001 09:41:30.489'

```

There are six sub-blocks delimited with `box` and `endbox` labels. They contain surface intensity and flux arrays (`rad`), averages in the 23-plane (`z1`), the 13-plane (`z2`), the 12-plane (`z3`), and over spherical shells (`r`), and a 2D slice through the model (`z`).

An individual box inside a dataset entry in a mean file can have e.g. the following contents describing horizontal averages in a plane-parallel model. With

```
uiolook chro2D03co08_01.mean | less
```

you get this (and more):

```

label box date='06.11.2002 17:58:05.533'
  character box_id f=A2 b=2 n='Block identification'
  integer dimension d=(1:2,1:3) f=I7 p=6 b=4
  real time f=E13.6 b=4                                n=time &
                                                       u=s
  real time_db f=E23.15 b=8                            n=time &
                                                       u=s
  integer itime f=I10 b=4                              n='time step number' &
                                                       u=1
  real xc1 d=(1:1,1:1,1:1) f=E13.6 p=4 b=4            n='x1 coordinates of cell centers' &
                                                       u=cm &
      ds=(0:0,0:1,0:1)
  real xc2 d=(1:1,1:1,1:1) f=E13.6 p=4 b=4            n='x2 coordinates of cell centers' &

```



```

                                u=G
real ei_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 n='Internal energy' &
                                u=erg/g
real rhoei_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                n='Internal energy' &
                                u=erg/cm^3
real rhoek_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                n='Kinetic energy' &
                                u=erg/cm^3
real rhoeg_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                n='Gravitational energy' &
                                u=erg/cm^3
real t_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 n=Temperature &
                                u=K
real t_xmean4 d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 n=Temperature &
                                u=K
real t_xmeankapparho d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                n=Temperature &
                                u=K
real p_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 n=Pressure &
                                u=dyn/cm^2
real s_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 n=Entropy &
                                u=erg/K/g
real rhos_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                n=Entropy &
                                u=erg/K/cm^3
real gamma1_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                n='1st Adiabatic Coefficient' &
                                u=1
real gamma3_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                n='3rd Adiabatic Coefficient' &
                                u=1
real delta_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                n='Expansion coefficient' &
                                u=1
real kapparho_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                n='Absorption Coefficient' &
                                u=1/cm
real quc001_xmean d=(1:1,1:1,1:120) f=E13.6 p=4 b=4 &
                                n='Number density of CO' &
                                u=1/cm^3
rreal rhovb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                n='Mass flux' &
                                u=g/cm^ &
                                ds=(0:0,0:0,0:1)
real frhov13b_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                n='Momentum x1 flux x3 direction' &
                                u=erg/cm^3 &
                                ds=(0:0,0:0,0:1)
real frhov23b_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                n='Momentum x2 flux x3 direction' &
                                u=erg/cm^3 &
                                ds=(0:0,0:0,0:1)
real frhov33b_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                n='Momentum x3 flux x3 direction' &
                                u=erg/cm^3 &
                                ds=(0:0,0:0,0:1)
real feipb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                n='Enthalpy Flux' &
                                u=erg/cm^2/s &
                                ds=(0:0,0:0,0:1)

```

```

real fekb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                n='Kinetic Energy Flux' &
                                u=erg/cm^2/s &
                                ds=(0:0,0:0,0:1)
real fegb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                n='Gravitational Energy Flux' &
                                u=erg/cm^2/s &
                                ds=(0:0,0:0,0:1)
real fepb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                n='Pressure Energy Flux' &
                                u=erg/cm^2/s &
                                ds=(0:0,0:0,0:1)
real fevb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                n='Viscous Energy Flux' &
                                u=erg/cm^2/s &
                                ds=(0:0,0:0,0:1)
real ferb_xmean d=(1:1,1:1,1:121) f=E13.6 p=4 b=4 &
                                n='Radiative Energy Flux' &
                                u=erg/cm^2/s &
                                ds=(0:0,0:0,0:1)
label endbox

```

The list above was slightly edited (by inserting blanks) to improve readability. In the meantime, several additional entries have been included.

The identifier of an entry together with the name (`n='...'`) and the unit (`u='...'`) should give a first hint about the meaning of the quantity. The suffix `'_xmean'` indicates a simple average. The suffix `'_xmean2'` indicates the root-mean-square average (note: the simple average is not subtracted).

Some entries (e.g. `ferb_xmean`) have a hidden `b` in their name, have one element more (e.g. 121 instead of 120) than most of the others, and are characterized by the `ds` keyword (see Table 6.4). These quantities are located at the cell boundaries in contrast to the usual cell-centered quantities. Clearly, there are also two sets of axes (e.g. `xc3` and `xb3`) corresponding to the cell- or boundary-centered quantities.

Note: The total energy flux can be written as sum

```
feb_total = feipkgvrb = feipb+fekb+fegb+fevb+ferb .
```

The flux `fepb` is already part of `feipb`.

8.4 File with azimuthally averaged data: `rhd.mcyl`

For global models an additional “`rhd.mcyl`” file can be written. It contains azimuthal averages that are particularly useful for global models rotating around the x_3 axis. The format is usually UIO “unformatted” (binary). An individual dataset in “`rhd.mcyl`” so far consists only of one box. With

```
uiolook st36g45n22_005.mcyl | head -105
```

you get (some indentation and blank lines added):

```

fileform uio form=unformatted convert=ieee_4 version=0.1.2013.08.24 &
date='22.09.2013 23:39:54.402' system=Linux machine=c8220node84.ens-lyon.fr &
osrelease=3.2.0-3-amd64 osversion='#1 SMP Mon Jul 23 02:45:17 UTC 2012' &
hardware=x86_64 language=Fortran90 program=RHD
character file_id f=A8 b=8 n='File identification'
character description d=(1:1) f=A14 p=2 b=14 n='File description'
character history d=(1:20) f=A80 p=1 b=80 n='File history'
character version f=A80 b=80 n='Program version'

label dataset n='RHD model' date='22.09.2013 23:40:08.596'
character dataset_id f=A10 b=10 n='Type of box hierarchy'
real modeltime f=E13.6 b=4 n=time u=s
real modeltime_db f=E23.15 b=8 n=time u=s

```

```

integer modelitime f=I10 b=4 n='time step number' u=1

label box date='22.09.2013 23:40:08.599'
character box_id f=A1 b=1 n='Block identification'
integer dimension d=(1:2,1:3) f=I7 p=6 b=4
real time f=E13.6 b=4 n=time u=s
real time_db f=E23.15 b=8 n=time u=s
integer itime f=I10 b=4 n='time step number' u=1
real xc1 d=(1:128,1:1,1:1) f=E13.6 p=4 b=4 &
  n='x1 coordinates of cell centers (radius)' u=cm ds=(0:0,0:1,0:1)
real xc1_volume d=(1:128,1:1,1:1) f=E13.6 p=4 b=4 &
  n='Radius coordinates of cell centers (volume preserving)' u=cm &
  ds=(0:0,0:1,0:1)
real xc2 d=(1:1,1:1,1:1) f=E13.6 p=4 b=4 n='phi coordinates of cell centers' &
  u=1 ds=(0:1,0:0,0:1)
real xc3 d=(1:1,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='x3 coordinates of cell centers (height)' u=cm ds=(0:1,0:1,0:0)
real xb1 d=(1:129,1:1,1:1) f=E13.6 p=4 b=4 &
  n='x1 coordinates of cell boundaries (radius)' u=cm ds=(0:1,0:1,0:1)
real xb1_volume d=(1:129,1:1,1:1) f=E13.6 p=4 b=4 &
  n='Radius coordinates of cell boundaries (volume preserving)' u=cm &
  ds=(0:1,0:1,0:1)
real xb2 d=(1:2,1:1,1:1) f=E13.6 p=4 b=4 &
  n='phi coordinates of cell boundaries' u=1 ds=(0:1,0:1,0:1)
real xb3 d=(1:1,1:1,-127:128) f=E13.6 p=4 b=4 &
  n='x3 coordinates of cell boundaries (height)' u=cm ds=(0:1,0:1,0:1)
real relvol_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Relative Volume' &
  u=1
real rho_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n=Density u=g/cm^3
real ei_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Internal energy' &
  u=erg/g
real rhoei_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Internal energy' &
  u=erg/cm^3
real t_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n=Temperature u=K
real p_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n=Pressure u=dyn/cm^2
real gamma1_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='1st Adiabatic coefficient' u=1
real gamma3_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='3rd Adiabatic coefficient' u=1
real delta_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Expansion coefficient' u=1
real s_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n=Entropy u=erg/K/g
real s_xmean2 d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n=Entropy u=erg/K/g
real rhos_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n=Entropy u=erg/K/cm^3
real v1_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Velocity radial' &
  u=cm/s
real v2_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Velocity azimuthal' &
  u=cm/s
real v3_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Velocity vertical' &
  u=cm/s
real v1_xmean2 d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Velocity radial' &
  u=cm/s
real v2_xmean2 d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Velocity azimuthal' &
  u=cm/s
real v3_xmean2 d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Velocity vertical' &
  u=cm/s
real rhov1_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Mass flux radial' &
  u=g/cm^2/s
real rhov2_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Mass flux azimuthal' u=g/cm^2/s
real rhov3_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Mass flux vertical' &

```

```

u=g/cm^2/s
real rhov1v1_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Momentum flux 11 radial' u=g/cm/s^2
real rhov2v2_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Momentum flux 22 azimuthal' u=g/cm/s^2
real rhov3v3_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Momentum flux 33 vertical' u=g/cm/s^2
real rhov1v2_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Momentum flux 12' &
  u=g/cm/s^2
real rhov1v3_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Momentum flux 13' &
  u=g/cm/s^2
real rhov2v3_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 n='Momentum flux 23' &
  u=g/cm/s^2
real fepc1_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Pressure energy flux radial' u=erg/cm^2/s
real fepc3_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Pressure energy flux vertical' u=erg/cm^2/s
real feipc1_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Enthalpy flux radial' u=erg/cm^2/s
real feipc3_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Enthalpy flux vertical' u=erg/cm^2/s
real fekc1_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Kinetic energy flux radial' u=erg/cm^2/s
real fekc3_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Kinetic energy flux vertical' u=erg/cm^2/s
real ferc1_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Radiative energy flux radial' u=erg/cm^2/s
real ferc2_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Radiative energy flux azimuthal' u=erg/cm^2/s
real ferc3_xmean d=(1:128,1:1,-127:127) f=E13.6 p=4 b=4 &
  n='Radiative energy flux vertical' u=erg/cm^2/s
label endbox
label enddataset date='22.09.2013 23:40:08.608'

```

8.5 HION output

The HION module can produce two types of output. The first is the standard output of the `quc` arrays in the `.full` and `.end` files, holding the level populations. This is all that is needed to restart a computation. The second (optional) output is a HION specific output system that generates files in UIO format after a prescribed number of simulation timesteps or alternatively after a prescribed time interval (see parameter `dtime_out_hion`). Output after a fixed number of timesteps is mainly useful for debugging. The files are named `HION.aaaa.bb.cccc.out` with `aaaa` either `'step'` or `'time'`, indicating output after a fixed number of timesteps or a fixed amount of solar time, `bb` the atom identifier and `cccc` the number of the output file, e.g. `HION.step.H.0001.out`. The HION files can be read with the IDL `uio_dataset_rd` (`'filename'`) function. The resulting data structure contains mass density, gas temperature, electron density of the atmosphere, as well as the axes in the `atmos` substructure. The `atom` substructure contains the time-dependent populations `ntd`, the LTE populations `nstar`, the total population `ntot`, a number of atomic parameters and `l_ntr` and `c_ntr`, arrays of the z-index per column where the radiation temperature in a transition starts to deviate from the gas temperature.

Refer to Leenaarts & Wedemeyer-Böhm (2005) for more details.

8.6 Text output: `rhd.out`

During execution – especially during the initialization phase – CO5BOLD writes lots of information to standard output, which is usually directed into `rhd.out`. the output contains:

After the header, there is a block “Compiler call”, e.g.

```
pgf90 -byteswapio -fast -Mvect=sse -Mcache_align -Minfo=inline -Minline=rhd_hyd_a
vg,rhd_hyd_upwind,rhd_hyd_pred0,rhd_hyd_predm,rhd_hyd_predp,rhd_hyd_alpha,rhd_h
yd_constanteq,rhd_hyd_minmodeq,rhd_hyd_minmod,rhd_hyd_vanleereq,rhd_hyd_vanleer
,rhd_hyd_superbeeeq,rhd_hyd_superbee,rhd_hyd_ppeq,rhd_hyd_pp,rhd_hyd_hdflux,rhd
_hyd_entropyfix -Minline=rhd_rad3d_raylhd,rhd_rad3d_solve,rhd_rad3d_solveeq,rhd
_shorthead_operator,rhd_shorthead_dtauop -Drhd_hyd_roe1d_l01=0 -Drhd_r02 -Drhd_r0
3 -DMSrad_raytas1 -Drhd_hyd_entropyfix_p01=1 -Drhd_roe1d_step_t01 -Drhd_roe1d_f
lux_t01 -Drhd_vis_t01 -Drhd_bound_t01 -Drhd_shorthead_step_t01 -Drhd_shorthead_fo
rmal_t01 -Drhd_shorthead_lambda_t01
```

These lines were produced by the configure script (see Sect. 4.3) and written into the file

```
compiler_flags.info
```

which is accessed from `rhd.F90` via `include` during compilation. Various modules now have a routine “`XXX_SwitchInfo`” that prints the values of the compiler switches used during the compilation of that particular module. The output can look e.g. like

```
Compiler switches: rhd_hyd_module .....
rhd_hyd_gravcorr_p01:          5
rhd_hyd_entropyfix_p01:       1
rhd_hyd_upwind_p01:           0
rhd_hyd_roe1d_l01:            0
rhd_roe1d_step_l01:           0
rhd_roe1d_slope_l01:          0
rhd_roe1d_flux_l01:           undefined
rhd_bound_t01:                 defined
rhd_roe1d_flux_t01:            defined
rhd_roe1d_step_t01:           defined
```

See Sect. 4.4 for more information about the meaning of the values. The reading of the parameter file starts with

```
ACTION: Read parameter file <<<<<<<<
```

After a parameter is read, its value is printed (see Sect. 7.1). The line

```
ACTION: Load EOS data <<<<<<<<
```

indicates the start of the reading of the equation of state data. It is followed by some information about the EOS table in use. Similarly, the line

```
ACTION: Load opacity tables <<<<<<<<
```

indicates the start of the reading of the opacity data. The information that follows is taken directly from the header of the opacity table. Currently, the last file to be read is the start model, which is announced by

```
ACTION: Read start model <<<<<<<<
```

and followed by some information about the start model, e.g. the number of grid points and a new section showing the quantities actually read, e.g.

```
Properties of start model:
time          "time"                      [s]
xc1           "x1 coordinates of cell centers" [cm]
xc2           "x2 coordinates of cell centers" [cm]
xc3           "x3 coordinates of cell centers" [cm]
xb1           "x1 coordinates of cell boundaries" [cm]
xb2           "x2 coordinates of cell boundaries" [cm]
xb3           "x3 coordinates of cell boundaries" [cm]
```

```

rho          "Density"                [g/cm^3]
ei           "Internal energy"        [erg/g]
v1           "Velocity 1"             [cm/s]
v2           "Velocity 2"             [cm/s]
v3           "Velocity 3"             [cm/s]
quc001       "Number density of CO"   [1/cm^3]   advect(1)
bb1          "Magnetic field 1"       [G]
bb2          "Magnetic field 2"       [G]
bb3          "Magnetic field 3"       [G]

```

It might follow

```
ACTION: Initialize MS radiation transport routines <<<<<<<
```

And finally

```
ACTION: Open output files <<<<<<<
```

which indicates that for instance the `rhd.full` file (see Sect 8.1)) and the `rhd.mean` file (see Sect 8.3)) have been opened and now contain a header.

The end of the initialization phase and the beginning of the proper simulation is marked by e.g.

```

===== Start Computation =====
=== Time step number: itime=   47050  time=  2.5821813E+08  t_job=  8.510000E+00 ===

```

The output for a typical simulation time step can look like (for a supergiant model with SHORTrad radiation transport)

```

--- Time step number: itime=   49048  time=  2.6822680E+08  t_job=  1.272180E+06 ---
dtime= 5.3047E+03 HD= 1.4838E+04 RAD= 5.3047E+03 VIS= 1.0723E+05
Luminosity per core volume: 4.49999049E-02
HYD 1: N_cellsperchunk, n_chunks:   10000  1410
HYD 2: N_cellsperchunk, n_chunks:   10000  1410
HYD 3: N_cellsperchunk, n_chunks:   10000  1410
VIS3D: N_cellsperchunk, n_chunks:   10000  1360

=== Start of rhd_shorttrad_step ===
n_subdtime:   1
minmax(T)      1.111651E+03 1.630733E+05
Main ( 1/ 3) ray direction 2:  0.000000  1.000000  0.000000  -----
Main ( 2/ 3) ray direction 3:  0.707105  0.000000  0.707109  -----
Main ( 3/ 3) ray direction 3: -0.707105  0.000000  0.707109  -----
Time step ratio: dtime/dtime_rad:  1.750409E+01
dtime_:rad,drhoei,limit_this,all:  6.667E+02 2.510E+03 6.276E+02 0.000E+00
n_subdtime:   2
minmax(T)      1.116348E+03 1.630658E+05
Main ( 1/ 3) ray direction 1:  1.000000  0.000000  0.000000  -----
Main ( 2/ 3) ray direction 3:  0.000000  0.707105  0.707109  -----
Main ( 3/ 3) ray direction 3:  0.000000 -0.707105  0.707109  -----
Time step ratio: dtime/dtime_rad:  1.836970E+01
dtime_:rad,drhoei,limit_this,all:  6.353E+02 3.188E+03 7.971E+02 6.276E+02
...
n_subdtime:   8
minmax(T)      1.118540E+03 1.630164E+05
Main ( 1/ 3) ray direction 2: -0.707105  0.707109  0.000000  -----
Main ( 2/ 3) ray direction 2:  0.707105  0.707109  0.000000  -----
Main ( 3/ 3) ray direction 3:  0.000000  0.000000  1.000000  -----
Time step ratio: dtime/dtime_rad:  1.791384E+01
dtime_:rad,drhoei,limit_this,all:  6.515E+02 3.894E+03 8.884E+02 4.814E+03
=== End of rhd_shorttrad_step ===

```


A simulation ends with e.g.

```
=== Time step number: itime= 49050 time= 2.6823742E+08 t_job= 1.273407E+06 ===
===== End Computation =====
```

A proper exit is indicated by

```
-----
Exit information: Requested number of time steps done
Exit status:      0
-----
```

In this case a file `rhd.done` (see Sect. 8.7) is produced. A messages like

```
*****
Severe error: SHORTRAD: Time step below absolute limit
Error index:      100
Interrupt computation
*****
```

marks an exit with an error and without `rhd.done` file. A message about the final model like

```
ACTION: Write final model <<<<<<<
Model file 'rhd.end' opened on channel 12
=====
```

is followed by some timing information like e.g.

```
Timing statistics (rate x factor= 1000000 x 10000)
=====
```

Process	Samples	Total time [sec]	Mean time [sec]
RHD code	1	410.830017	410.830017
uio output routines	27	37.469997	1.387778
HYD: bound_3DCenter	2000	3.540000	0.001770
Hydrodynamics routines	2000	48944.660156	24.472330
HYD: 1	2000	16350.610352	8.175305
HYD: 2	2000	16052.459961	8.026230
HYD: 3	2000	16520.798828	8.260400
Viscosity routines 3D	2000	25446.400391	12.723200
VIS: make_box(modelvis)	2000	0.010000	0.000005
VIS: copy_box(modelvis)	2000	1750.960083	0.875480
VIS: delete_box(modelvis)	2000	0.000000	0.000000
Radiation transport routines	2000	243729.000000	121.864502
SHC: step	2020	244064.515625	120.824020
SHC: step: dtime: init: EOS	16024	49312.738281	3.077430
SHC: step: dtime: explicit	16024	174542.343750	10.892558
SHC: formal	16024	170085.437500	10.614418
SHC: formal: init	16024	35591.378906	2.221129
SHC: formal: dirloop	16024	133010.687500	8.300717
SHC: formal: exp	28014	9014.280273	0.321778
SHC: formal: exp: expl2t	28014	3950.409912	0.141016
SHC: formal: dir3	36083	63222.242188	1.752134
SHC: time: dir3	36083	19676.009766	0.545299
SHC: formal: limitei	16024	1306.419922	0.081529
SHC: step: dtime: final	16024	12730.129883	0.794441
SHC: formal: dir2	11959	22205.000000	1.856761
SHC: time: dir2	11959	5731.149902	0.479233
SHC: formal: dir1	4044	10674.429688	2.639572
SHC: time: dir1	4044	1893.760010	0.468289
SHC: step: dtime: final(output)	181	8620.870117	47.629116
Radiation trans.: output only	20	335.929993	16.796499

In this example the value for the overall time (“rhd code 410.830017 sec”) is not useful because of an overflow in the counter. However, it is evident that the radiation transport consumes most of the time (243729.000000 sec), followed by the hydrodynamics routines (48944.660156 sec) and the tensor-viscosity routines (25446.400391 sec). Some of these values are split further.

8.7 Additional status and output files: `rhd.done`, `rhd.snap`

At the beginning of every time step CO5BOLD checks in the working directory whether the file `rhd.dump` exists. If it has been generated (e.g. with `touch rhd.dump`) and the file `rhd.snap` does *not* exist, the current model is written into `rhd.snap`. It has the same file properties (format and conversion) as the regular `rhd.end` file. The run of the simulation itself is not modified. This feature might be useful for debugging purposes.

If a run was successful i.e. it was completed because one of the regular termination conditions was fulfilled (e.g. the requested number of time steps was performed) the exit status file `rhd.done` is produced. Currently, it contains the date and time of its generation. The existence of this file can be checked within a script to determine if the simulation was successful (and should be continued). Note: the existence of an `rhd.end` file only indicates that CO5BOLD managed to exit gracefully – due to an error or in a regular way.

Chapter 9

Running a simulation

9.1 Quickstart: How to run CO5BOLD

The generation of a start file and the modification of the parameter file is a somewhat complex process. In short, the following steps have to be performed.

1. Produce an executable `rhds.exe` (see Sect. 4.1) and put it into your working directory.
2. Make sure the environment variable `LD_LIBRARY_PATH` is – still – set correctly, so that all necessary libraries are included (which usually just means: don't change it after a successful compilation).
3. Choose a start model (e.g. the final model of an earlier simulation or a model produced with an IDL routine).
4. Create the parameter file `rhds.par`: typically, you will start with an existing file and edit it just a bit. You should check that the paths names of EOS and opacity files are set correctly (watch the username!). For details about the parameter file see Sect. 7.1.1.
5. Prepare the runtime environment. That might involve – depending on operating system, compiler, and machine – commands like
`ulimit -s unlimited` (to increase the overall stacksize)
`export OMP_STACKSIZE=300M` (to increase the stacksize per thread for an OpenMP run)
`export OMP_NUM_THREADS=8` (to prepare an OpenMP run on 8 cores)
6. Start the simulation with
`nice nohup rhds.exe > rhds.out &`
7. You can see how the simulation proceeds with
`tail -f rhds.out`
8. The other data files usually are in a binary format. You can check them e.g. with – if installed, see Sect. 6.2.6.2 –
`uiolook rhds.mean`
They are usually read and analyzed with IDL routines (see Sect. 6.2.7.3) or processed by a spectrum-synthesis code.

For machines with batch queue there is a script, which can handle an entire sequence of simulations (see Sect. 9.2).

9.2 Using a batch system

For longer simulations it is inconvenient to restart the individual jobs by hand. This task is done by a script originally from Hans-Günter Ludwig. Its basic function is sketched in Fig. 9.1.

CO5BOLD - function diagram

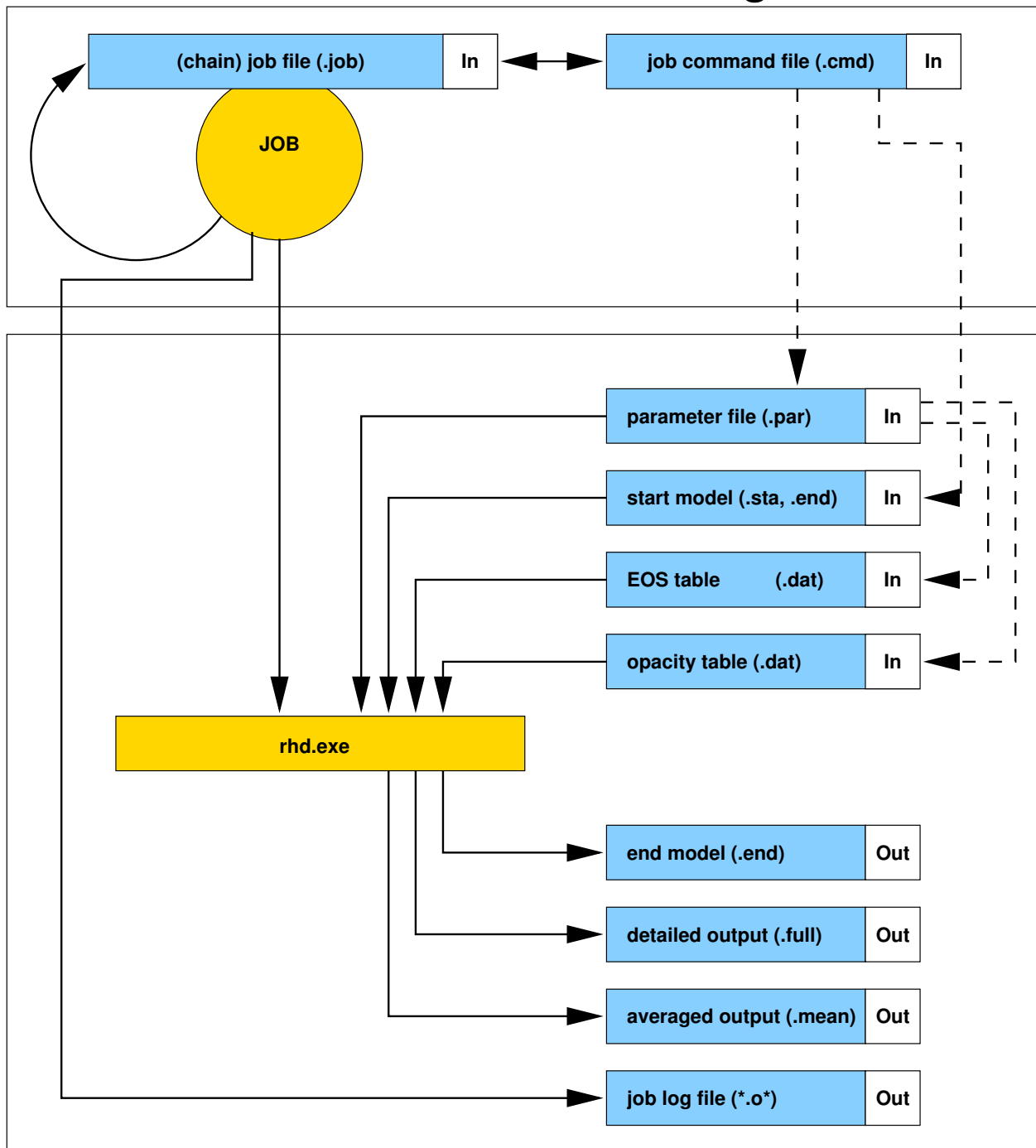


Figure 9.1: Program scheme

Here comes an example of the script (`rhdl.job`) for a system without dedicated batch system. The submission of a job is done via `nohup rhdl.job &`:

```
#!/bin/sh
# --- PBS -N rhdl
# --- PBS -l walltime=72:00:00
# --- PBS -l nodes=1:ppn=4
#
# --- Job file for the execution of CO5BOLD ---
```

```

# --- Source: rhd1.job, original from HGL ---
# --- Last modification: 2014-06-23 ---
#
BASEDIR=/users/bf/dat/job/j1
STADIR=${BASEDIR}/sta      # Start directory: contains *.par, rhd1.cmd, rhd1.job
WRKDIR=${BASEDIR}/wrk      # Work directory
BAKDIR=${BASEDIR}/bak      # Backup and output directory
RHDEXE=${STADIR}/rhd.exe   # RHD program to be executed
#
ulimit -s unlimited
#
export OMP_NUM_THREADS=4
export OMP_STACKSIZE=300M
#
# --- Jump into work directory ---
cd ${WRKDIR}
#
# --- Loop: execute RHD code (possibly) several times in one job -----
for IRUN in 1 2
do
  echo
  echo 'CO5BOLD Run #' $IRUN
  date
  #
  # --- Clear up work directory ---
  rm *
  #
  #####
  #
  # --- Get old command file, select actual command line ---
  # --- and read variables from command line ---
  #
  cp -p $STADIR/rhd1.cmd rhd1.cmd
  #
  awk \
  '
    /#/    { print; next}
    /\*/   { print; next}
    /\+/   { print; next}
    DONE!="T" { print >"cmdline"; printf "%-77s*\n", $0; DONE="T"; next}
    { print} ' rhd1.cmd | cat > dummy_nrhd.cmd
  #
  read INFILE OUTFILE PARFILE ACT < cmdline
  mv dummy_nrhd.cmd ${OUTFILE}_nrhd.cmd
  echo ${INFILE}
  echo ${OUTFILE}
  echo ${PARFILE}
  echo ${ACT}
  #
  #####
  #
  if [ "${ACT}" != dum ]
  then
    #####
    #
    # --- RHD execution ---
    #
    # --- Copy parameter file ---
    cp -p ${STADIR}/${PARFILE} rhd.par
    #
    # --- Copy start file ---
    if test -s ${BAKDIR}/${INFILE}
    then
      cp -p ${BAKDIR}/${INFILE} rhd.sta
    else
      cp -p ${STADIR}/${INFILE} rhd.sta
      cp -p rhd.sta ${BAKDIR}/${INFILE}
    fi
  fi
done

```

```

# --- Copy executable ---
cp -p ${RHDEXE} rhd.exe
#
# --- Execute RHD ---
./rhd.exe > rhd.out
RHD_EXIT=$?
#
if [ "$RHD_EXIT" != 0 ] || [ ! -s rhd.done ]
then
# --- Exit status not zero, ---
# --- error may have occurred during execution of rhd.exe ---
if [ "$RHD_EXIT" != 0 ]
then
echo 'Non-zero exit status ' $RHD_EXIT ' occurred during execution of RHD!'
else
echo 'No rhd.done file found: assume error during execution of RHD!'
fi
echo 'Execution of job chain terminated!'
# --- Modify nrhd.cmd, set termination character "+" ---
awk \
'
    /#/    { print; next}
    /\*/   { print; next}
    /\+/   { print; next}
    DONE!="T" { printf "%-77s+\n", $0; DONE="T"; next}
              { print} ' rhd1.cmd | cat > nrhd.cmd
# --- Terminate chain by simulating ${ACT} = eoc ... ---
ACT=eoc
else
# --- Modify command file: add '*' in appropriate column to indicate ---
# --- proper execution ---
awk \
'
    /#/    { print; next}
    /\*/   { print; next}
    /\+/   { print; next}
    DONE!="T" { print >"cmdline"; printf "%-77s*\n", $0; DONE="T"; next}
              { print} ' rhd1.cmd | cat > nrhd.cmd

fi
#
ls -l
#
# --- Move data into backup directory and modify permissions ---
gzip rhd.out
mv rhd.out.gz ${BAKDIR}/${OUTFILE}.out.gz
cp -p rhd.par ${BAKDIR}/${OUTFILE}.par
mv rhd.end    ${BAKDIR}/${OUTFILE}.end
mv rhd.fine   ${BAKDIR}/${OUTFILE}.fine
mv rhd.full   ${BAKDIR}/${OUTFILE}.full
mv rhd.mcy1   ${BAKDIR}/${OUTFILE}.mcy1
mv rhd.mean   ${BAKDIR}/${OUTFILE}.mean
mv rhd.chu1   ${BAKDIR}/${OUTFILE}.chu1
mv rhd.chu2   ${BAKDIR}/${OUTFILE}.chu2
mv rhd.chu3   ${BAKDIR}/${OUTFILE}.chu3
chmod go+r    ${BAKDIR}/${PARFILE} ${BAKDIR}/${OUTFILE}.*
chmod go-w    ${BAKDIR}/${PARFILE} ${BAKDIR}/${OUTFILE}.*
#
#####
fi
#
#
#####
#
# --- Dispose modified command file for next job ---
cp -p nrhd.cmd $STADIR/rhd1.cmd
#
# --- Exit loop if end of chain reached ---
if test ${ACT} = eoc
then

```

```
    break
fi
#
# --- End of loop -----
done
#
# --- Submit next job if not end of chain reached---
if test ${ACT} != eoc
then
    cd $STADIR
    echo "Resubmit job"
# /usr/local/bin/qsub rhd1.job
# qsub rhd1.job
# nice nohup rhd1.job &
    nohup rhd1.job &
else
    echo "End of job chain"
fi
#
#####
```


Chapter 10

Data analysis with IDL

In this section some basic commands for handling CO5BOLD data in IDL are described. See also Sect. 6.2.7

10.1 Preparations

Make the UIO IDL routines visible to IDL – somehow. There are several ways to do that. Three are described below:

We recommend to create an initialization file (e.g. named `start.pro`) which should be called after starting IDL (e.g. `@start`). This is necessary to define relevant paths of IDL subroutines and to provide the UIO package. Thus, the file should contain the following:

```
; --- Add user IDL directory to search path ---
addpath=expand_path('+$UIOPATH/idl')
addpath=addpath + ':' + expand_path('$HOME/HYDRO/IDL/rhdpro')
if strtrim(addpath,2) ne '' then !path=addpath+'!'+!path
delvar, addpath
; --- Initialize uio-routines ---
uio_init, program='by hand'
```

Note: Before using IDL the environment variables for the CO5BOLD paths should have been set. Use `setarcdeppaths.sh` (or `.ksh`, `.csh`) for this purpose. Important is `UIOPATH` which specifies where to find the IDL routines for the UIO handling in the script above.

Alternatively, one might set the IDL path variable accordingly like

```
export IDL_PATH="+$UIOPATH/idl"
```

for example in the `.bashrc` file before starting IDL.

Or, you just make a symbolic link from the UIO IDL routines at their original location to a sub-directory of the main IDL directory, which should be in the IDL path anyway.

The initial (single) call of `uio_init` is necessary in any case.

10.2 CO5BOLD data in IDL

Important to know is that all operations can be performed in the command line of IDL. This allows an interactive processing of CO5BOLD data. Moreover, there are already prepared IDL scripts for this purpose but most of them are rather complex and still have to be edited (e.g. changing file names – Huuhh!). For the beginning it is more clear to use single commands. We give a short overview of some essential commands.

10.2.1 Loading the parameter file

```
IDL> parfile='mymodel.par'
IDL> par=uio_struct_rd(parfile)
```

All control parameters are provided in the structure `PAR`.

10.2.2 Loading CO5BOLD data (.full, .sta, .end, .chu1)

```
IDL> modelfile='/home/user/mymodel.full' & n=0
IDL> ful=uiio_dataset_rd(modelfile,n=n)
```

First the name and full path (if not in the actual directory) of the model file and the wanted time step should be defined. Here, time step means the consecutive number of the model snapshot in the file. Declaring a time step number greater than the number of snapshots contained in the file will cause an error.

Otherwise all data of the particular time step `n` will be provided in the structure `FUL`. Loading more than one timestep from the same file could be achieved as follows:

```
IDL> uiio_openrd, nc, modelfile, outstr, ierr
IDL> for i=0,ntime-1 do begin &$
IDL>   ful=uiio_dataset_rd(modelfile, channel=nc,ierr=ierr, outstr=err_msg) &$
IDL> endfor &$
IDL> uiio_closrd, nc
```

Again, this operation would cause an error if the wanted time step is not contained in the file. Via checking the error flag `ierr` of the routine `uiio_dataset_rd` such errors can be avoided. This way it is unnecessary to know exactly of how many time steps the model file consists.

```
IDL> uiio_openrd, nc, modelfile, outstr, ierr
IDL> i=0
IDL> repeat begin &$
IDL>   ful=uiio_dataset_rd(modelfile, channel=nc, ierr=ierr) &$
IDL>   if (ierr eq 0) then begin &$
IDL>     ;--- Do the data processing here ---
IDL>     i=i+1 &$
IDL>   endif else begin &$
IDL>     print,'IDL> Reached EOF.' &$
IDL>   endelse &$
IDL> endrep until (ierr ne 0) or (EOF(nc))
IDL> uiio_closrd, nc
```

To read a number of entries from a list of files in sequence the routine `uiio_datasetlist_rd.pro` (see Sect. 6.2.7.3) is appropriate.

10.2.3 Loading the equation of state

```
IDL> eosfile='../eos/dat/' + par.eosfile
IDL> tabinter_rdcoeff, eosfile, eos
```

The table for the equation of state is provided in the structure `EOS`.

NOTE: Always check file name and path!

10.2.4 Loading the opacity table

```
IDL> opafile='../opa/dat/' + par.opafile
IDL> dfopta, opafile
```

The opacity table will be stored as common block `OPTA_COMMON`. **NOTE: Always check file name and path!**

10.2.5 Computation of deduced quantities

After having read the model data `FUL` and the tables for the equation of state (`EOS`) and opacity (`OPTA_COMMON`) (see Sects. 10.2.3, 10.2.4), more quantities can be calculated:

```
IDL> eosbox, ful, eos=eos, /opa, ierror=ierror
```

This operation adds the tags `EOS` and `OPA` to the data structure `FUL`, which contain more quantities like e.g. the temperature (see Sect. 10.3).

Based on the thermodynamic quantities now present in the `FUL` structure, further quantities can be computed with `combox.pro`, as for instance in

```
IDL> cs=combox('cs',ful)
```

10.3 IDL data structure

The data structure `FUL` contains the following variables and substructures. Use `help,/str,ful`, to get this information. See also the short description of the contents of a model file in Sect. 8.1 and particularly the man page of the script `uiolook` in Sect. 6.2.6.2 which gives you even more detailed information directly from the file:

```
** Structure <8287a0c>, 9 tags, length=78404128, refs=1:
TYPE          STRING      'uio'
HEAD          STRUCT      -> <Anonymous> Array[1]
DATASET_ID    STRING      'single_box'
MODELTIME     FLOAT        10050.1
MODELITIME    LONG         64088
DTIME         FLOAT        0.176381
TIME_OUT_FULL_LAST FLOAT    10050.1
TIME_OUT_MEAN_LAST FLOAT    10040.0
Z             STRUCT      -> <Anonymous> Array[1]
```

If the command in Sect. 10.2.5 has been performed, the following substructures are present:

```
EOS          STRUCT      -> <Anonymous> Array[1]
OPA          STRUCT      -> <Anonymous> Array[1]
```

The substructure `FUL.Z` contains the original data arrays from the model file like the spatial axes, density `rho`, internal energy `ei`, and the three spatial components of the velocity (`v1`, `v2`, `v3`):

```
** Structure <8274184>, 16 tags, length=78403900, refs=2:
TYPE          STRING      'uio'
BOX_ID        STRING      'z'
DIMENSION     LONG         Array[2, 3]
TIME          FLOAT        10050.1
ITIME         LONG         64088
XC1           FLOAT        Array[140, 1 , 1 ]
XC2           FLOAT        Array[1 , 140, 1 ]
XC3           FLOAT        Array[1 , 1 , 200]
XB1           FLOAT        Array[141, 1 , 1 ]
XB2           FLOAT        Array[1 , 141, 1 ]
XB3           FLOAT        Array[1 , 1 , 201]
RHO           FLOAT        Array[140, 140, 200]
EI            FLOAT        Array[140, 140, 200]
V1            FLOAT        Array[140, 140, 200]
V2            FLOAT        Array[140, 140, 200]
V3            FLOAT        Array[140, 140, 200]
```

The spatial axes are: `XC1`, `XC2`, `XC3`, `XB1`, `XB2`, `XB3`:

The indices stand for 1:*x*, 2:*y*, 3:*z* (or *h*) `C` for the grid cell centre, `B` for the boundaries. Most of the quantities are defined for the cell centres. In case of doubt, this can be found out by checking the array dimensions: the number of cell boundaries is one larger than the number of cell centers.

The substructure `FUL.Z` can contain additional arrays in case of dust formation, chemical reaction networks, or time-dependent hydrogen ionization:

```

QUC001      FLOAT      Array[140, 140, 200]
QUC002      FLOAT      Array[140, 140, 200]
QUC003      FLOAT      Array[140, 140, 200]
QUC004      FLOAT      Array[140, 140, 200]

```

The meaning of the quantities depends on the used source-term module. The magnetic field components are also stored in this substructure:

```

BB1         FLOAT      Array[141, 140, 200]
BB2         FLOAT      Array[140, 141, 200]
BB3         FLOAT      Array[140, 140, 201]

```

The magnetic field is defined on the cell boundaries in the direction of the spatial components, e.g. BB1 in direction 1, and in the cell-centres for the other directions. The resulting array dimensions differ from the cell-centred quantities like, e.g., rho. The array values must be multiplied with a factor $\sqrt{4\pi}$ in order to obtain the field strength in Gauss.

The substructure FUL.EOS (which is present only after a call of, e.g., eosbox.pro) contains important quantities like the temperature T, gas pressure P, entropy S:

```

** Structure <826a03c>, 6 tags, length=109760000, refs=2:
P           FLOAT      Array[140, 140, 200]
DPDRHO     FLOAT      Array[140, 140, 200]
DPDEI      FLOAT      Array[140, 140, 200]
T          FLOAT      Array[140, 140, 200]
DTDEI      FLOAT      Array[140, 140, 200]
S          FLOAT      Array[140, 140, 200]

```

The substructure FUL.OPA only contains the opacity KAPPA:

```

** Structure <826a5b4>, 1 tags, length=15680000, refs=2:
KAPPA      FLOAT      Array[140, 140, 200]

```

10.4 More IDL routines

In the directory `idl/bflib/` a lot of useful routines can be found which can be used for further processing and visualisation of CO5BOLD data. For the visualisation of 2-D models or 2-D data slices in general we recommend `plotfield.pro`. With `combox.pro` further quantities can be calculated.

Furthermore, we currently develop a widget-based analysis tool called **CO5BOLD AT** (abbrev.: CAT) which will help to work with CO5BOLD data without having to write and edit own IDL code. The routines are stored (if available) in the directory `IDL/COBOLDAT` and have to be started with `@cat`.

Chapter 11

Document history

- 2001-12-30: First version of the manual
- 2002-02-16: First version of the manual on the web
- ... lots of extensions and changes in between...
- 2004-02-23: SGI Origin compiler settings section modified (for CINES machines) 4.6.13, 4.6.14
- 2004-02-23: short example for `uio_datasetlist_rd.pro` usage: 6.2.7.3
- 2004-03-02: Intel compiler settings section modified (`LD_ASSUME_KERNEL=2.4.19`): 4.6.8
- 2004-03-02: SGI Origin compiler settings section modified: 4.6.13
- 2004-03-03: IBM compiler settings section added: 4.6.6
- 2004-03-04: Document history started (pretty late...)
- 2004-03-04: Dedicated OpenMP section: 4.5.1
- 2004-03-04: Dedicated inlining section: 4.5.4
- 2004-03-04: Parameter for core drag force: 7.1.4.22
- 2004-03-04: New EOS table for solar composition: 7.1.6.1
- 2004-03-04: Trademarks: 13
- 2004-03-04: List of new dust files (the table was split into two): 3.2
- 2004-03-04: Installation of UIO UNIX scripts with configure: 6.2.6.1
- 2004-05-03: Thermodynamic relations: 2.3
- 2004-05-14: Point-to-point "tensor" viscosity: 7.1.11.9
- 2004-07-26: New gravitational potential mimicking a travelling tidal wave: 7.1.3.2
- 2004-08-18: New control files `rhd.dump` and `rhd.snap` to request a snapshot of current model: 8.7
- 2005-03-08: New control parameter `dtime_out_end`: 7.1.21.2
- 2006-07-28: Preparation for major code release (beta version) with the new modules CHEM (7.5), and HION(7.6), including new parameters (7.1.12.1) and switches for the configure script (4.3)
- 2006-08-14: MHD section: 2.2, MHD parameters: 7.1.10, 7.1.5
- 2007-02-12: Hydro section with new modii and parameters: heat mode: 7.1.4.4, rotating coordinate system: 7.1.3.10, possible hydrodynamics iteration: 7.1.8.6, new pressure correction scheme: 4.4.5.1 unsplit hydrodynamics operator possible: 7.1.8.3.

- 2007-10-22: Double precision time as additional scalar in model file: 8.1
- 2007-12-18: Rather stable version and parameter-rearrangements for dust model
dustscheme=dust_k3mon_03: 7.1.14
and dustscheme=dust_bins_01: 7.1.15.
- 2008-03-13: Expansion Courant number `C_hydExpCourant`, `C_hydExpCourantmax`: 7.1.20.11
- 2008-03-17: "Hydrostatic pressure correction" in waves 3 and "6" switch-on-and-offable with
`C_hydPredfactor`: 7.1.9.16
- 2008-04-27: Expansion viscosity `C_visExpansion`: 7.1.11.4
- 2008-07-03: Linear viscosity `C_visLinear`: 7.1.11.5
- 2008-08-13: Parameters `N_radrsyslevel`, `N_radoutput`, `C_radTcool`, `C_radDcool`, `C_radscool` in
MSrad: 7.1.17.6, parameters `C_radTinci` and `C_radDinci` to control incident radiation in MSrad:
7.1.17.11
- 2008-08-14: Compiling double precision code: 4.5.5
- 2008-08-19: Some parameters (possibly) valid for MHD module: 7.1.10.6
- 2008-08-28: Rather old parameters for additional I/O control: integer `n_outslicedim_mean`:
7.1.21.4, integer `istep_in_start`: 7.1.21.9
- 2009-01-12: README_MHD: 2.2
- 2010-03-17: Performance enhancement for EOS: `gasinter_102`: 4.4.3.2
- 2010-03-19: Performance enhancement during box handling: `rhd_box_arrays01`: 4.4.1.4
- 2010-04-09: Transmitting upper boundary condition: `c_rhochangetop`: 7.1.4.15
Better counters for timing statistis: `timing_c_range`: 4.4.1.2
- 2010-04-11: Merging of previous introductory text to Sect. 2.2 by BF with README_MHD by WS.
Update of various text passages. Shift of parameter description to Sect. 7.1: 2.2
Removal of remarks relating to the magnetic field in descriptions of parameters `side_bound`,
`top_bound`, and `bottom_bound`: 7.1.5
Description of boundary parameters for the magnetic field: `side_bound_mag_x1`,
`side_bound_mag_x2`, `top_bound_mag`, `bottom_bound_mag`, `b1_inflow`, `C_magthetaB`, and
`C_magphiB`: 7.1.5
Updates for reconstruction:PP, `c_slopered`, `n_hyditer`, `n_hydmaxiter`: 7.1.10
Updates and introduction of parameters for the MHD-module: `c_resb`, `c_resbconst`,
`c_repsilon`, `beta_inv`, `va_max`, `N_magDiffSide`, `N_magDiffTop`, and `n_magbiffbottom`:
7.1.5
F90_MHD: comment about zero magnetic fields: 4.3
Removal of "(first version)" for MHD entry in table of high-level modules: 3.2
References: Balsara & Spicer (1999), Janhunen (2000), Stone & Pringle (2001): 13
- 2010-04-14: Some parameters in MHD module were renamed: `B_theta`, `B_phi`, `N_side`, `N_top`,
`N_bottom` → `C_magthetaB`, `C_magphiB`, `N_magDiffSide`, `N_magDiffTop`, `N_magDiffBottom`
- 2010-04-29: The files `rhd_mac*_module.f90` were removed. The single routine from it was put into
`timing_module.F90`.
- 2010-05-06: Compiler switch `timing_r_type` explained: 4.4.1.3.
Input/output (UIO) compiler switches explained: 4.4.2, accompanied by some changes concerning
the files `uio_mac*_module.[fF]90`.

- 2010-06-14: Output of additional chunks described in 7.1.21.5 and 7.1.21.14
New versions of bottom boundary conditions, better suited for HLLMHD solver: 7.1.4.3
The HLLMHD solver can do different time-integration schemes: 7.1.8.2
In the HLLMHD step the CheckFlux step can be (des)activated: 7.1.10.1
MHD module allows unsplit update: 7.1.8.3.
- 2011-02-10: New parameters for MHD module: 7.1.10.2
- 2011-03-28: New option 'vertical2' for magnetic boundary conditions: 7.1.5.1
- 2011-07-04: MHD equations: 2.2
New parameters `r0_core`, `centrifugal_force`: 7.1.3.8
Heating modes for core heating: 7.1.4.4
- 2011-12-09: New parameter `r2_grav`: 7.1.3.7
New option for old parameter `c_radhtautop`: 7.1.4.19
- 2012-01-10: A few new references including links: 13
Removal of old `uio_mac_modules`, mention of `rhd_rec_module.f90`: 3.3
New reconstruction methods: `PPmimo`, `FRmimo`, `FRmono`, `FRweno`, `FRcont`: 7.1.8.4
New parameters:
`r2_grav`, `r0_core`: 7.1.3.7
`ar_RotationAxis`, `centrifugal_force`: 7.1.3.9
`hdTransVeloMode`: 7.1.9.13
- 2012-01-11: Parameter `real C_visDrag` is obsolete.
Compiler switches `rhd_roe1d_slope_101`, `IDF`, `rhd_hyd_roe1d_101` are obsolete: 4.4.8.3
Updates for `c_slopered`: 7.1.9.7
New options for parameters:
`hdsplit=CTU`: 7.1.8.3
for HD Roe solver: `hdtimeintegrationscheme=Single,RungeKutta2,RungeKutta3` 7.1.8.2
New parameters:
`C_hydTdiffLin`, `C_hydTdiffMach`: 7.1.9.19
`C_RecContShift`, `C_RecContSteep`: 7.1.9.8
`dustReconstruction`: 7.1.12.2
- 2012-01-12: New parameters:
`C_hydSoundCourant`, `C_hydSoundCourantmax`: 7.1.20.9
`C_v3ChangeLinBottom`, `C_v3ChangeSqrBottom`: 7.1.4.12
- 2012-02-16: New parameter: `C_TminLimit`: 7.1.16.8
- 2012-04-06: Added some lines in the Intel compiler section: 4.6.8
- 2012-09-04: New options for `hdTransVeloMode`: 7.1.9.13
New parameters:
`C_hydLowMachcsFactor`: 7.1.9.4
`hdEntropyWaveMode`: 7.1.9.14
`hdEnthalpyAvgMode`: 7.1.9.15
`C_hydsDiffVelo`, `C_hydvDiffVelo`: 7.1.9.17
`C_visP2PhypSmagorinsky`, `C_visP2PhypArtificial`, `C_visP2PhypExpansion`, `C_visP2Pdivrhov`: 7.1.11.11
- 2012-11-07: New options for:
`hdEntropyWaveMode`: 7.1.9.14
`hdEnthalpyAvgMode`: 7.1.9.15
character reconstruction: 7.1.8.4

- 2013-09-11: New parameters:
 outdim_chu2, outdim_chu3: 7.1.21.6
 outfile_chu2, outfile_chu3: 7.1.21.15
 character outfile_mcy1: 7.1.21.13, 8.4
 character hdcoredragprofile: 7.1.4.23
 New compiler options:
 better vectorization of EOS routines, gasinter_101: 4.4.3.1
 better vectorization of opacity routines, opta_switch_101: 4.4.4.1
 better vectorization of Roe-upwind-state computations, rhd_roe1d_flux_101: 4.4.5.4
 Old compiler option removed, rhd_roe1d_slope_101: 4.4.8.3
- 2013-09-18: Optionally, parts of the source code included in the manual. Revised script to produce the manual.
- 2013-09-21: Some long itemize lists transformed into sequences of paragraphs. Cleanup of reference list.
- 2013-09-22: Changed documentclass: article to book (sections become chapters...)
- 2013-09-23: Reorganization and renaming of sections.
- 2013-09-24: Source-code files sorted into groups.
- 2013-09-27: New short subsections about vectorization: 4.5.2 and cache usage: 4.5.3.
- 2014-02-24: Change of default values of some compiler switches.
- 2014-06-20: New option randomcube for parameter radraybase: 7.1.16.6
 parameter C_radHtauTop also in handled in SHORTrad: 7.1.4.19
 new option core_energyentropy1 for parameter heat_mode: 7.1.4.4
 new parameter hdCoreHeatProfile: 7.1.4.5
 new ...-Radial and ...-Meridional options for hdCoreDragProfile: 7.1.4.23
 new parameters s_InFlRadGrad and s_InFlLatGrad: 7.1.4.8
 color output of configure script: 6, 4.3.1.1.
- 2014-07-18: New parameter C_gravmu: 7.1.8.5
- 2014-09-03: New reconstruction methods: HBweno, VAweno: 7.1.8.4
- 2015-04-20: First draft of Programmer's guide: 5
- 2015-04-21: New parameters:
 C_hydLowMachcsBase: 7.1.9.5
 C_hydSmallFluctFactor: 7.1.9.6
 N_hydRKIter: 7.1.9.3
- 2015-05-06: New parameters:
 C_hydCellsPerChunk2 and C_hydCellsPerChunk3: 7.1.9.1
 hdTmpStructKeepMode: 7.1.8.8
 N_visIter: 7.1.11.1
 Removed parameters:
 C_ReconstructionTimeFactor, C_visNeu1, C_visNeu2, C_visDrag
- 2015-05-07: New parameters:
 time_ScaleStart and time_ScaleEnd: 7.1.22.1
 C_recWenoWeightCenter, C_recWenoWeightRight, and C_recWenoPsiFactor: 7.1.9.10
- 2015-05-09: Updated Intel-compiler section: 4.6.8
 New option F90_OPTIMIZE for configure script: 4.3.1.7

Chapter 12

Glossary

- **CAT**: 'CO5BOLD Analysis Tool'
- **CO5BOLD** or **COBOLD** is the short form of "COnservative COde for the COmputation of COmpressible COnvection in a BOx of L Dimensions with l=2,3".
- **EOS**: "Equation Of State"
- **HION**: "Hydrogen IONization"
- **MPI**: "Message Passing Interface"
- **MHD**: "Magneto-HydroDynamics"
- **OpenMP**: "Open Multi-Processing"
- **OpenMPI**: "Open Message Passing Interface"
- **RHD**: "Radiation HydroDynamics"
- **UIO**: the "Universal Input Output" format. It is used in CO5BOLD for parameter, model, mean, and EOS files.

Chapter 13

Trademarks

- AMD is a trademark of Advanced Micro Devices, Inc.
- Compaq is a US trademark of Compaq and/or Hewlett-Packard Company.
- Cray is a trademark of Cray Research.
- HP is a US trademark of Hewlett-Packard Company.
- IBM is a US trademark of International Business Machines.
- IDL is a registered trademark of Research Systems, Inc.
- Intel, Itanium, and Pentium are US trademarks of Intel Corporation.
- Linux is a trademark of Linus Torvalds.
- NEC is a registered trademark of Nippon Electric Company.
- PGI is a trademark of The Portland Group Compiler Technology.
- SGI is a trademark of Silicon Graphics.
- Solaris, Sun, SunOS, and SunFire are US trademarks of Sun Microsystems, Inc.
- Sparc is a US trademark of SPARC International, Inc.
- UNIX is a registered trademark of The Open Group.
- All other product names mentioned in this manual are trademarks or registered trademarks of their respective owners.

Bibliography

- Allard, F., Homeier, D., & Freytag, B. 2011, “Model Atmospheres From Very Low Mass Stars to Brown Dwarfs”, *16th Cambridge Workshop on Cool Stars, Stellar Systems, and the Sun*, eds. Johns-Krull, C., Browning, M. K., West, A. A., ASPCS 448, 91 (link to ADS)
- Balsara, D. S. & Spicer, D. S. 1999, “A Staggered Mesh Algorithm Using High Order Godunov Fluxes to Ensure Solenoidal Magnetic Fields in Magnetohydrodynamic Simulations”, *J.Comput.Phys.* 149, 270-292 (link to ADS)
- Beeck, B., Collet, R., Steffen, M., Asplund, M., Cameron, R. H., Freytag, B., Hayek, W., Ludwig, H.-G., & Schüssler, M. 2012, “Simulations of the solar near-surface layers with the CO5BOLD, MURaM, and Stagger codes”, *A&A* 539, 121 (link to ADS)
- Caffau, E. and Ludwig, H.-G. and Steffen, M. and Freytag, B. and Bonifacio, P. 2011, “Solar Chemical Abundances Determined with a CO5BOLD 3D Model Atmosphere”, *Solar Physics* 268, 255-269 (link to ADS)
- Chiavassa, A., Freytag, B., Masseron, T., & Plez, B. 2011, “Radiative hydrodynamics simulations of red supergiant stars. IV. Gray versus non-gray opacities”, *A&A* 535, 22 (link to ADS)
- Chiavassa, A. and Freytag, B. and Plez, B. 2013, “3D hydrodynamical simulations to interpret observations of stellar surfaces of red supergiant stars”, *EAS Publications Series*, eds. Kervella, P., Le Bertre, T., & Perrin, G., vol. 60, 145-153 (link to ADS)
- Colella, P. 1990, “Multidimensional Upwind Methods for Hyperbolic Conservation Laws”, *J.Comp.Phys.*, 87, 171-200 (link to publisher)
- Colella, P. & Woodward, P. R. 1984, “The Piecewise Parabolic Method (PPM) for Gas-Dynamical Simulations”, *J.Comput.Phys.* 54, 174-201 (link to ADS)
- Freytag, B., Steffen, M., & Dorch, B. 2002, “Spots on the surface of Betelgeuse – Results from new 3D stellar convection models”, *Astron.Nachr.* 323, 213 (link to ADS)
- Freytag, B. & Höfner, S. 2008, “Three-dimensional simulations of the atmosphere of an AGB star”, *A&A* 483, 571-583 (link to ADS)
- Freytag, B., Allard, F., Ludwig, H.-G., Homeier, D., Steffen, M. 2010, “The role of convection, overshoot, and gravity waves for the transport of dust in M dwarf and brown dwarf atmospheres”, *A&A* 513, 19 (link to ADS)
- Freytag, B., Steffen, M., Ludwig, H.-G., Wedemeyer-Böhm, S., Schaffenberger, W., Steiner, O. 2012, “Simulations of stellar convection with CO5BOLD”, *J.Comput.Phys. (Special Issue: Computational Plasma Physics, ed. Barry Koren)* 231, 919-959 (link to ADS, link to publisher)
- Freytag, B. and Chiavassa, A. 2013, “Global radiation-hydrodynamics simulations of red supergiant stars”, *EAS Publications Series*, eds. Kervella, P., Le Bertre, T., & Perrin, G., vol. 60, 137-144 (link to ADS)
- Freytag, B. 2013, “Advances in the hydrodynamics solver of CO5BOLD”, *MemSAIS* 24, 26 (link to ADS)

- Janhunen, P. 2000, “A positive conservative method for magnetohydrodynamics based on HLL and Roe methods”, *J. Comput. Phys.* 160, 649-661 ([link to publisher](#))
- Leenaarts, J. & Wedemeyer-Böhm, S. 2005, “DOT tomography of the solar atmosphere. III. Observations and simulations of reversed granulation”, *A&A* 431, 687-692 ([link to ADS](#))
- Ludwig, H.-G., Caffau, E., Steffen, M., Freytag, B., Bonifacio, P., & Kučinskas, A. 2009, “The CIFIST 3D model atmosphere grid.”, *MemSAIS* 80, 711 ([link to ADS](#))
- Roe, P.L. 1986, “Characteristic-Based Schemes for the Euler Equations”, *Ann.Rev.Fluid.Mech.* 18, 337-365 ([link to publisher](#))
- Rossow, W. B. 1978, “Cloud microphysics – Analysis of the clouds of Earth, Venus, Mars, and Jupiter”, *Icarus* 36, 1-50 ([link to ADS](#), [link to publisher](#))
- Schaffenberger, W., Wedemeyer-Böhm, S., Steiner, O., & Freytag, B. 2005, “Magnetohydrodynamic Simulation from the Convection Zone to the Chromosphere”, in *ESA SP-596: Chromospheric and Coronal Magnetic Fields*, ed. D. E. Innes, A. Lagg, & S. A. Solanki, p. 65.1 ([link to ADS](#))
- Stone, J.M. & Pringle, J.E. 2001, “Magnetohydrodynamical non-radiative accretion flows in two dimensions”, *Mon.Not.R.Astron.Soc.* 322, 461-472 ([link to ADS](#))
- Tremblay, P.-E., Ludwig, H.-G., Freytag, B., Steffen, M., & Caffau, E. 2013, “Granulation properties of giants, dwarfs, and white dwarfs from the CIFIST 3D model atmosphere grid”, *A&A* 557, 7 ([link to ADS](#))
- Wedemeyer, S., Freytag, B., Steffen, M., Ludwig, H.-G., & Holweger, H. 2004, “Numerical simulation of the three-dimensional structure and dynamics of the non-magnetic solar chromosphere”, *A&A* 414, 1121-1137 ([link to ADS](#))
- Wedemeyer-Böhm, S., Kamp, I., Bruls, J., & Freytag, B. 2005, “Carbon monoxide in the solar atmosphere. I. Numerical method and two-dimensional models”, *A&A* 438, 1043-1057 ([link to ADS](#))

Index

- alpha, 56
- AMD, 195
- axis
 - xb1, 168
 - xb2, 168
 - xb3, 168
 - xc1, 168
 - xc2, 168
 - xc3, 168
- batch queue, 180
- big_endian, 56, 61, 64–66, 83, 86
- boundary conditions, 105, 112
- cache usage, 54
- centrifugal force, 105
- chem.dat, 164
- chemical composition, 114
- chemical reaction network, 17, 42, 137, 164, 187
- CINES, 66
- CO5BOLD, 17, 29–32, 193
- Compaq, 195
- compilation, 33–69
- compiler
 - alpha, 44, 56
 - Cray, 56
 - g95, 65
 - gfortran, 65
 - Hewlett-Packard, 56, 57
 - Hitachi SR8000, 58
 - IBM, 60
 - Intel, 61
 - NEC
 - SX-5, 65
 - SX-6, 65
 - SX-8, 65
 - PathScale, 64
 - PGI, 61
 - SGI, 66
 - UKAFF, 66
 - Sun, 69
- compiler macro, 40–52
 - category, 40
 - gasinter_101, 45
 - gasinter_102, 45
 - IDF, 52
 - MSrad_raytas, 51
 - opta_switch_101, 45
 - rhd_shorthead_lambda_101, 51
 - rhd_bound_t01, 46
 - rhd_box_arrays01, 42
 - rhd_box_bmag01, 43
 - rhd_box_grav01, 42
 - rhd_box_quc01, 42
 - rhd_hyd_entropyfix_p01, 46
 - rhd_hyd_gravcorr_p01, 45
 - rhd_hyd_roe1d_101, 52
 - rhd_hyd_upwind_p01, 46
 - rhd_r01, 47
 - rhd_r02, 48
 - rhd_r03, 48
 - rhd_rad3d_dir_t01, 49
 - rhd_rad3d_fromray_101, 48
 - rhd_rad3d_r02, 48
 - rhd_rad3d_solve_t01, 49
 - rhd_rad3d_step_t01, 49
 - rhd_rad3d_toray_101, 48
 - rhd_roe1d_flux_101, 46
 - rhd_roe1d_flux_t01, 47
 - rhd_roe1d_slope_101, 52
 - rhd_roe1d_step_t01, 47
 - rhd_shorthead_dir1_101, 50
 - rhd_shorthead_dir_102, 51
 - rhd_shorthead_dtauop_101, 50
 - rhd_shorthead_dtauop_102, 50
 - rhd_shorthead_formal_101, 50
 - rhd_shorthead_formal_t01, 51
 - rhd_shorthead_operator_101, 49
 - rhd_shorthead_operator_102, 50
 - rhd_shorthead_step_t01, 51
 - rhd_vis_density_p01, 47
 - rhd_vis_t01, 47
 - timing_c_factor, 41
 - timing_c_range, 41
 - timing_r_type, 42
 - uio_switch_crayxmp_101, 44
 - uio_switch_ieeebe_101, 44

- uio_switch_ieee_l01, 44
- uio_switch_ieeele_l01, 44
- uio_switch_native_l01, 43
- uio_switch_open_l01, 44
- uio_switch_system_l01, 43
- configure script, 37–40, 175
 - control variables, 37
 - F90_BASEPATH, 37, 40
 - F90_CHEM, 39
 - F90_COLOR, 38
 - F90_COMPILER, 38
 - F90_DEBUG, 38
 - F90_DUST, 39
 - F90_HION, 39
 - F90_LHDRAD, 39
 - F90_MACHINE, 40
 - F90_MHD, 40
 - F90_MSRAD, 39
 - F90_OPTIMIZE, 39
 - F90_PARALLEL, 38
 - F90_POSTFLAGS, 38
 - F90_PREFLAGS, 38
 - F90_SHORTRAD, 39
 - F90_TWEAK, 40
 - F90_UNIT, 82
- .configurerc file, 36, 37
- Coriolis force, 105
- craSHi, 56
- Cray, 56, 150, 151, 195
- CTU, 118
- data format
 - UIO, 83
- directional splitting, 17, 117
- double precision, 55, 63, 65
- dust, 17, 42, 137
- entropy fix, 46
- environment variable, 40, 53
- EOS, 24, 114
- equation of state, 24, 114
- files, 83, 101, 167
 - configure script, 37–40
 - resource file, 36, 37
 - .configurerc, 36, 37
 - data files, table of, 84
 - documentation, 32
 - documentation files, table of, 32
 - Fortran, 30
 - Fortran files, table of, 30, 31
 - HION, 84
 - IDL
 - UIO, 95
 - input
 - chem.dat, 164
 - EOS, 114
 - opacities, 115
 - rhd.cont, 166
 - rhd.dump, 166
 - rhd.par, 101–164
 - rhd.sta, 164
 - rhd.stop, 166
 - LaTeX
 - CO5BOLD manual, 32
 - Makefile, 33, 34, 37
 - output
 - rhd.chu1, 168
 - rhd.chu2, 168
 - rhd.chu3, 168
 - rhd.done, 178
 - rhd.end, 167
 - rhd.full, 167
 - rhd.mcyl, 172
 - rhd.mean, 168
 - rhd.out, 174
 - rhd.snap, 178
 - rhd.exe, 33, 36
 - script, 32
 - configure, 37–40
 - job file, 180
 - uiocat, 94
 - uioinfo, 95
 - uiolook, 94
 - script files, table of, 32
- fluxes, 168
- formatted, 85
- Fortran, 17, 83
- g95, 65
- gfortran, 65
- HD, 19, 116, 121
- Hewlett-Packard, 56, 57, 195
- HION
 - input, 165
 - output, 174
- Hitachi, 58
- HP, 195
- hydrodynamics, 17, 19, 116, 121
- hydrogen ionization, 17, 42, 137, 187
- IBM, 60, 195
- IDL, 83, 185, 195
 - CAT, 22, 188
 - combox.pro, 187
 - eosbox.pro, 186
 - UIO routines, 95
 - uio_data.pro, 97
 - uio_datasetlist_rd.pro, 98

- uio_dataset_rd.pro, 98
- uio_init.pro, 96
- uio_struct_rd.pro, 98
- inlining, 53, 55
 - alpha, 56
 - Cray VX1, 56
 - IBM, 60
 - Intel compiler on Linux, 62
 - PGI compiler on Linux, 61
 - SGI, 66
 - Sun, 69
- input
 - chemical reaction network, 164
 - HION, 165
- Intel, 61, 195
- Itanium, 57
- KMP_AFFINITY, 54
- LHDrad, 17, 143, 144
- Linux, 61, 64, 65, 195
- little_endian, 56, 61, 64, 65, 86
- Loadleveler, 60
- Macintosh, 63, 137
- magnetic fields, 17, 43, 188
- magnetohydrodynamics, 20
- make, 36
 - clean, 37
 - removeall, 37
- Makefile, 33, 34
 - configure script, 37
 - UIO, 91
- MHD, 20, 116, 130
- molecules, 17, 42, 137, 187
- MSrad, 17, 48, 56, 58, 61, 62, 69, 111, 143, 144
 - cell centering, 168
- NEC, 195
 - SX-5, 65
 - SX-6, 65
 - SX-8, 65
- OMP_NUM_THREADS, 53
- OMP_SCHEDULE, 53
- OMP_STACKSIZE, 54
- opacities, 115
- OpenMP, 17, 52, 53
 - activation in configure script, 38, 53
 - chunk size, 121, 137
 - KMP_AFFINITY, 54, 64
 - KMP_STACKSIZE, 64
 - LD_ASSUME_KERNEL, 64
 - OMP_NUM_THREADS, 53, 63
 - OMP_SCHEDULE, 53, 64
 - OMP_STACKSIZE, 54, 64
 - on Cray VX1, 56
 - on Hitachi, 58
 - on HP, 57
 - on Linux gfortran, 65
 - on Linux Intel, 62
 - on Linux Pathscale, 64
 - on NEC, 65
 - on SGI, 66
 - on Sun, 69
 - thread affinity, 64
- operator splitting, 17, 117
- output
 - chunk data sets, 168
 - full data sets, 167
 - HION, 174
 - mcyl data, 172
 - mean data, 168
- PathScale, 64
- PGI, 195
- precision
 - double, 55, 63, 65
 - single, 55
- quc, 39, 42, 164
- radiation transport, 17, 143, 148, 150
- README, 34
- rhd.cont, 166
- rhd.dump, 166
- rhd.exe, 33, 36
- rhd.out, 174
- rhd.par, 83, 101–164
 - boundary conditions, 105, 112
 - character bottom_bound, 106
 - character bottom_bound_mag, 113
 - character centrifugal_force, 105
 - character chem_reacfile, 138
 - character chem_reacpath, 138
 - character description, 102
 - character dustreconstruction, 138
 - character dustscheme, 137
 - dust_bins_01, 141
 - dust_k3mon_03, 140
 - dust_moment04_c2, 139
 - character eosfile, 114
 - character eospath, 115
 - character file_id, 102
 - character grav_mode, 103
 - character hdcheckflux, 130
 - character hdcoredragprofil, 111
 - character hdcoreheatprofil, 107
 - character hdenthalpyavgmode, 127
 - character hdentropywavemode, 126
 - character hdscheme, 116
 - character hdsplit, 117

- character hdttimeintegrationscheme, 117
- character hdtmpstructkeepmode, 120
- character hdtransvelomode, 126
- character heat_mode, 107
- character hion_abufile, 139
- character hion_atomfile, 139
- character hion_datapath, 139, 165
- character hion_edensfile, 139
- character hion_pffile, 139
- character history, 103
- character infile_start, 158
- character opafile, 115
- character opapath, 116
- character outconv_end, 159
- character outconv_fine, 164
- character outconv_full, 160
- character outconv_mean, 160
- character outfile_chu1, 159
- character outfile_chu2, 159
- character outfile_chu3, 159
- character outfile_end, 158
- character outfile_fine, 163
- character outfile_full, 158
- character outfile_mcyl, 158
- character outfile_mean, 158
- character outform_end, 159
- character outform_fine, 164
- character outform_full, 159
- character outform_mean, 160
- character radpressure, 163
- character radraybase, 146
- character radraystar, 146
- character radscheme, 143
- character reconstruction, 118
- character side_bound, 105
- character side_bound_mag_x1, 112
- character side_bound_mag_x2, 112
- character top_bound, 106
- character top_bound_mag, 113
- chemical reaction network, 137
- dust, 137
- effective temperature, 103, 108
- equation of state, 114
- fileform uio, 102
- gravity, 103
- header, 102
- hydrodynamics, 116, 121
- hydrogen ionization, 137
- input/output, 156
- integer dtimestep_out_fine, 163
- integer endtimestep, 152
- integer hion_chunks, 139
- integer istep_in_start, 158
- integer n_outslicedim_mean, 157
- integer n_dustgrainradius, 140, 142
- integer n_hydcellsperchunk, 60, 121
- integer n_hydcellsperchunk2, 121
- integer n_hydcellsperchunk3, 121
- integer n_hyditer, 120
- integer n_hydmaxiter, 120
- integer n_hydrkiter, 122
- integer n_magdiffbottom, 133
- integer n_magdiffside, 132
- integer n_magdifftop, 132
- integer n_orderconstrainedtransport, 130
- integer n_radband, 144
- integer n_raditer, 145
- integer n_radmaxiter, 145
- integer n_radminiter, 145
- integer n_radoutput, 149
- integer n_radphi, 148
- integer n_radrsyslevel, 149
- integer n_radsubray, 148
- integer n_radtaurefine, 149
- integer n_radtheta, 148
- integer n_radthickpoint, 148
- integer n_rescellsperchunk, 131
- integer n_viscellsperchunk, 137
- integer n_visitor, 133
- integer outdim_chu1, 157
- integer outdim_chu2, 157
- integer outdim_chu3, 157
- integer plustimestep, 152
- integer starttimestep, 151
- luminosity, 108
- MHD, 116, 130
- molecules, 137
- opacities, 115
- process management, 150
- radiation transport, 143, 148, 150
- reading in IDL, 98
- real abux, 162
- real abuy, 162
- real ar_dustgrainradius, 140, 142
- real ar_RotationAxis, 105
- real b1_inflow, 114
- real beta_inv, 132
- real c_magthetab, 114
- real c_radkappasmooth, 162
- real c_visp2pdivrhov, 136
- real c_visp2phypartificial, 136
- real c_visp2phypexpansion, 136
- real c_visp2phypsmagorinsky, 135
- real c_coredrag, 111
- real c_courant, 153
- real c_courantmax, 153

real c_dust01, 140, 142
 real c_dust02, 140–142
 real c_dust03, 140–142
 real c_dust04, 140–142
 real c_dust05, 141
 real c_dust06, 141, 143
 real c_dust07, 143
 real c_dust08, 143
 real c_dust09, 143
 real c_dust0X, 138
 real c_gravmu, 119
 real chem_abumetal, 138
 real c_hptopfactor, 110
 real c_hydexpcourant, 154
 real c_hydexpcourantmax, 154
 real c_hydlowmachcsbase, 123
 real c_hydlowmachcsfactor, 122
 real c_hydpredfactor, 128
 real c_hydsdiffvelo, 128
 real c_hydsmlfluctfactor, 123
 real c_hydsoundcourant, 154
 real c_hydsoundcourantmax, 154
 real c_hydtddiffin, 129
 real c_hydtddiffmach, 130
 real c_hydvdiffvelo, 129
 real c_magphib, 114
 real c_maxeichange, 154
 real c_pchange, 109
 real cputime, 151
 real cputime_remainlimit, 151
 real c_radcourant, 155
 real c_radcourantmax, 155
 real c_raddcool, 149
 real c_raddinci, 150
 real c_radhtautop, 111
 real c_radimplicitmu, 147
 real c_raditereps, 147
 real c_raditerstep, 148
 real c_radmaxeichange, 155
 real c_radscool, 149
 real c_radtcool, 149
 real c_radthintimefac, 150
 real c_radtinci, 149
 real c_radtintminfac, 163
 real c_radtsmooth, 163
 real c_radtvis, 150
 real c_radtvisdtau, 150
 real c_recontshift, 124
 real c_recontsteep, 124
 real c_recwenopsifactor, 125
 real c_recwenoweightcenter, 125
 real c_recwenoweightright, 125
 real c_resB, 131
 real c_resBconst, 131
 real c_rescourant, 131
 real c_rescourantmax, 131
 real c_resepsilon, 132
 real c_rhochangetop, 110
 real c_schange, 108
 real c_slopered, 123
 real c_tchange, 110
 real c_test1, 161
 real c_tminlimit, 147
 real c_tsurf, 110
 real c_v3changelinbottom, 109
 real c_v3changesqrbottom, 109
 real c_visartificial, 134
 real c_visbound, 109
 real c_viscourant, 155
 real c_viscourantmax, 156
 real c_visexpansion, 134
 real c_vislinear, 134
 real c_visp2pcoeff, 135
 real c_visp2pincl1, 136
 real c_visp2pincl2, 136
 real c_visp2prturb, 134
 real c_vissmagorinsky, 133
 real c_vistensordiag, 134
 real c_vistensordiv, 135
 real c_vistensoroff, 135
 real dtime_out_hion, 139, 174
 real dtime_incmax, 153
 real dtime_max, 153
 real dtime_min, 152
 real dtime_min_stop, 153
 real dtime_out_end, 156
 real dtime_out_full, 156
 real dtime_out_mean, 157
 real dtime_start, 152
 real endtime, 151
 real gamma, 162
 real grav, 103
 real luminositypervolume, 108
 real mass_star, 104
 real n_test1, 161
 real nu_rotation, 105
 real plustime, 152
 real qmol, 162
 real r0_core, 104
 real r0_grav, 104
 real r1_grav, 104
 real r1_rad, 111
 real r2_grav, 104
 real rho_min, 111
 real s_infllatgrad, 108
 real s_inflow, 108
 real s_inflradgrad, 108
 real starttime, 151

- real `strtest1`, 161
- real `teff`, 103
- real `time_scaleend`, 161
- real `time_scalestart`, 160
- real `va_max`, 132
- tensor viscosity, 133
- time step, 152
- `rhd.snap`, 178
- `rhd.stop`, 166
- Roe solver, 56, 58, 61
- rotation, 105, 158
 - axis, 105
 - centrifugal force, 105
 - Coriolis force, 105
- SGI, 66, 195
- SHORTrad, 17, 61, 111, 143, 144
- single precision, 55
- Sparc, 195
- Sun, 69, 195
- tensor viscosity, 133
- tests
 - unit, 74, 82
- thermodynamic relations, 23
 - adiabatic gradient, 24, 25
 - enthalpy, 23
 - entropy, 25
 - internal energy, 23, 25
 - polytropic gas, 28
 - sound speed, 25, 28
 - specific heats, 23, 25, 26
- time step, 145
- timing statistics, 41, 177
- total energy flux, 172
- UIO, 83–99
 - conversion type, 85
 - example, 84, 86, 87
 - format, 85
 - Fortran, 90
 - IDL, 95
 - Makefile, 91
 - record length unit, 56, 63
 - `uiocat`, 55, 94
 - `uio_datasetlist_rd.pro`, 98
 - `uio_dataset_rd.pro`, 98
 - `uioinfo`, 95
 - `uio_init.pro`, 96
 - `uiolook`, 94
 - `uio_mac_module`, 90
 - `uio_struct_rd.pro`, 98
 - UNIX scripts, 93
- UKAFF, 66
- unformatted, 85
- unit tests, 74, 82
- UNIX, 195
- vectorization, 54
- viscosity
 - point-to-point, 133, 135
 - tensor, 47, 133
- `xb1`, 168
- `xb2`, 168
- `xb3`, 168
- `xc1`, 168
- `xc2`, 168
- `xc3`, 168