# Introduction to Numerical Hydrodynamics and Radiative Transfer

# Part II: Hydrodynamics

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### Susanne Höfner Susanne.Hoefner@physics.uu.se

# Structure & Content

#### **1. Equations of Fluid Dynamics**

- basic concepts, derivation of the equations
- waves and shocks
- some basic mathematical and numerical considerations

#### 2. The Linear Advection Equation

- introduction of the linear advection equation
- discretization: basics concepts and examples
- analysis of schemes

#### 3. Non-linear Advection: Burgers' Equation

- introduction of Burgers' equation
- numerical examples

#### 4. Hydrodynamics: Selected Topics

- the Riemann problem
- numerical methods

Introduction to Numerical Hydrodynamics

# 1. The Equations of Fluid Dynamics

### 1.1 Basic Concepts of Fluid Mechanics

# **Dynamical Theories**

### General characteristics of dynamical theories

- state of the system at a given instant: described by a set of variables
- evolution of the system/variables with time: described by a set of equations giving time derivatives of the variables

#### Levels of dynamical theories for fluids

system	description of state	dynamical equations
<i>N</i> classical particles distribution function continuum model	$(x_1,, x_N, v_1,, v_N)$ f(x, v, t) $\rho(x), T(x), v(x)$	Newton's laws Boltzmann equation hydrodynamic equations

consider a typical fluid ...



... and define a fluid element



#### Definition of fluid element:

A region over which we can define local variables (density, temperature, etc.) The size of this region is assumed to be such that it is

(i) small enough that we can ignore systematic variations across it for any variable q we are interested in:

$$|_{\text{region}} \ll |_{\text{scale}} \sim q / |\nabla q|$$

(ii) large enough to contain sufficient particles to ignore fluctuations due to the finite number of particles (discreteness noise):

$$n |_{region}^3 >> 1$$

In addition, collisional fluids must satisfy:

(iii)  $|_{region} >> mean free path of particles$ 

# Mean Free Path - Examples

### Mean Free Path

- depends on number density and cross section
- elastic scattering cross section of neutral atoms:  $10^{-15}$  cm<sup>2</sup>

### Examples

gas in	density	MFP	size
	[cm <sup>-3</sup> ]	[cm]	[cm]
typical room	10 <sup>19</sup>	$10^{-4}$	$10^{3}$
HI region (ISM)	10	10 <sup>-14</sup>	$10^{19}$

- frequent collisions, small mean free path compared to the characteristic length scales of the system → coherent motion of particles
- definition of fluid element: mean flow velocity (bulk velocity)
- particle velocity = mean flow velocity + random velocity component



random-walk trajectory

coherent motion of particles



coherent motion of particles



coherent motion of particles







• The fluid is described by local macroscopic variables (e.g., density, temperature, bulk velocity)

• The dynamics of the fluid is governed by internal forces (e.g. pressure gradients) and external forces (e.g. gravity)

• The changes of macroscopic properties in a fluid element are described by conservation laws

Introduction to Numerical Hydrodynamics

# 1. The Equations of Fluid Dynamics

### 1.2 Fluid Dynamics: Conservation Laws

#### Mass conservation:



Mass conservation:

*divergence theorem* 

$$\frac{d}{dt} \int_{V} \rho \ dV = -\oint_{A} \rho \, \boldsymbol{u} \cdot \boldsymbol{\hat{n}} \ dA = -\int_{V} \nabla \cdot (\rho \, \boldsymbol{u}) \ dV$$

rate of change of mass in V = mass flux across the surface

rewrite as:

$$\int_{V} \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) \right] dV = 0$$

... but the volume V is completely arbitrary

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$
  
equation of continuity

Momentum conservation:

$$\frac{d}{dt} \int_{V} \rho u_{i} \, dV = -\oint_{A} \rho u_{i} u_{j} \hat{n}_{j} \, dA - \oint_{A} P \delta_{ij} \hat{n}_{j} \, dA + \int_{V} \rho a_{i} \, dV$$
rate of change of momentum in V =
momentum flux across the surface (fluid flow)
- effect of pressure on surface
+ effect of forces

applying divergence theorem (surface to volume integrals):

$$\Rightarrow \frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \rho a_i$$
  
equation of motion

Energy conservation:

$$\frac{d}{dt} \int_{V} \left( \frac{1}{2} \rho u^{2} + \rho e \right) dV = -\oint_{A} \left( \frac{1}{2} \rho u^{2} + \rho e \right) u \cdot \hat{n} \quad dA - \oint_{A} u_{i} P \delta_{ij} \hat{n}_{j} dA + \int_{V} \rho u \cdot a \quad dV$$
  
rate of change of energy in V =  
energy flux across the surface (due to fluid flow)  
- work done by pressure

+ work done by forces

applying divergence theorem (surface to volume integrals):

$$\frac{\partial}{\partial t} \left( \frac{1}{2} \rho u^2 + \rho e \right) + \nabla \cdot \left( \left( \frac{1}{2} \rho u^2 + \rho e \right) u \right) = - \nabla \cdot \left( P u \right) + \rho u \cdot a$$
  
energy equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$
$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \rho a_i$$
$$\frac{\partial}{\partial t} \left( \frac{1}{2} \rho u^2 + \rho e \right) + \nabla \cdot \left( (\frac{1}{2} \rho u^2 + \rho e) \boldsymbol{u} \right) = - \nabla \cdot (P \boldsymbol{u}) + \rho \boldsymbol{u} \cdot \boldsymbol{a}$$

general form of conservation laws:

 $\frac{\partial}{\partial t} (density of quantity) + \nabla \cdot (flux of quantity) = sources - sinks$ 

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \rho a_i$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2}\rho u^2 + \rho e\right) + \nabla \cdot \left(\frac{1}{2}\rho u^2 + \rho e\right) \boldsymbol{u} = -\nabla \cdot (P \boldsymbol{u}) + \rho \boldsymbol{u} \cdot \boldsymbol{a}$$
... and what about external forces ?
$$\boldsymbol{a} = \frac{F}{m}$$

## Fluid Dynamics: External Forces



#### Gravitation:

a = g ... acceleration

where *g* is given by Poisson's equation

$$\nabla \cdot \boldsymbol{g} = -4 \pi G \rho$$

## Fluid Dynamics: External Forces



Radiation pressure:

$$f_{rad} = \rho/c \ \int \kappa_v \mathbf{F}_v \, dv$$

 $f_{_{rad}}$ 

force per volume, • • • added to equation of motion

 $\boldsymbol{u} \cdot \boldsymbol{f}_{rad} \dots$  work done by radiation pressure, added to energy equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$

$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \rho g_i + f_{rad}^i$$

$$\frac{\partial}{\partial t} \left( \frac{1}{2} \rho u^2 + \rho e \right) + \nabla \cdot \left( (\frac{1}{2} \rho u^2 + \rho e) \boldsymbol{u} \right) = -\nabla \cdot (P \boldsymbol{u}) + \rho \boldsymbol{u} \cdot \boldsymbol{g}$$

$$+ \boldsymbol{u} \cdot \boldsymbol{f}_{rad} + \Gamma - \Lambda$$
... including: gravity  
radiation pressure  
heating & cooling by radiation

# Fluid Dynamics: Limit Cases of Energy Transport

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$
$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \rho a_i$$

Barotropic equation of state:

 $P = P(\rho)$ 

 $P \propto \rho T$ Examples: - ideal gas: \* isothermal case  $P \propto \rho$  $P = K \rho^{\gamma}$ \* adiabatic case

Efficient radiative heating and cooling:  $\Gamma - \Lambda = 0 \rightarrow T \rightarrow P(\rho, T)$  $(\rightarrow radiative equilibrium)$ 

Introduction to Numerical Hydrodynamics

# 1. The Equations of Fluid Dynamics

### 1.3 Acoustic Waves and Shock Waves

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$
$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \rho a_i$$
$$\frac{\partial}{\partial t} \left( \frac{1}{2} \rho u^2 + \rho e \right) + \nabla \cdot \left( (\frac{1}{2} \rho u^2 + \rho e) \boldsymbol{u} \right) = - \nabla \cdot (P \boldsymbol{u}) + \rho \boldsymbol{u} \cdot \boldsymbol{a}$$

general form of conservation laws:

 $\frac{\partial}{\partial t} (density of quantity) + \nabla \cdot (flux of quantity) = sources - sinks$ 

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$
$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial P}{\partial x_i} + \rho a_i$$

replacing energy equation:

 $P = K \rho^{\gamma}$ 

1D, no external forces:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) = 0$$
$$\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u u) = - \frac{\partial P}{\partial x}$$

small-amplitude disturbances in gas which initially is at rest with constant pressure and density

$$P = P_0 + P_1(x, t)$$
  

$$\rho = \rho_0 + \rho_1(x, t)$$
  

$$u = u_1(x, t)$$

replacing energy equation:  $P = K \rho^{\gamma}$ 

1D, no external forces:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) = 0$$
$$\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u u) = - \frac{\partial P}{\partial x}$$

small-amplitude disturbances in gas which initially is at rest with constant pressure and density

insert into equations & linearise:

$$P = P_0 + P_1(x, t)$$
  

$$\rho = \rho_0 + \rho_1(x, t)$$
  

$$u = u_1(x, t)$$

$$P_1 = \gamma K \rho_0^{\gamma - 1} \rho_1 = \gamma \frac{P_0}{\rho_0} \rho_1$$

$$\frac{\partial \rho_1}{\partial t} + \rho_0 \frac{\partial u_1}{\partial x} = 0$$
$$\rho_0 \frac{\partial u_1}{\partial t} = - \frac{\partial P_1}{\partial x}$$

small-amplitude disturbances in gas which initially is at rest with constant pressure and density

$$P = P_0 + P_1(x, t)$$
  

$$\rho = \rho_0 + \rho_1(x, t)$$
  

$$u = u_1(x, t)$$

$$P_1 = \gamma K \rho_0^{\gamma - 1} \rho_1 = \gamma \frac{P_0}{\rho_0} \rho_1$$

use sound speed:

 $\Rightarrow$  homogeneous wave equation:

$$\frac{\partial^2 \rho_1}{\partial t^2} - a_0^2 \frac{\partial^2 \rho_1}{\partial x^2} = 0$$

general solution:

 $\rho_1 = f(x - a_0 t) + g(x + a_0 t)$ 

waves propagating with sound speed  $a_{o}$ 



In the absence of dissipation and spatial inhomogeneities (or dispersion), the waveform of a disturbance governed by a linear wave equation maintains its size and shape forever, apart from propagation at a constant wave speed.

# Waves: Steepening of Acoustic Waves



An acoustic wave of finite amplitude, even if it starts with a perfect sinusoidal shape and propagates in an undisturbed medium of exactly uniform properties, would inevitably steepen in its waveform.

### Waves: Steepening of Acoustic Waves



The tendency for nonlinearities to steepen the wave profile, which would produce multiple values for fluid properties such as gas density and velocity, must be eventually offset by the onset of strong viscous forces. The balance of the viscous forces and the steepening tendency mediates a shock, which is approximated in ideal fluid flow as a discontinuous jump of gas properties across the front.

 $\boldsymbol{x}$ 

### Waves: Structure of Shock Waves



Across a viscous shock, the pressure and density increase and the velocity decreases as the gas flows from the upstream state to the downstream state. The transition is made in a characteristic distance  $\Delta x$  that equals a few mean free paths  $\ell$  for the elastic scattering of the gas particles.

### Waves: Structure of Shock Waves



On macroscopic scales, shock transitions may be approximated as single discontinuous jumps.

1D,

no external forces 
$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) = 0$$
$$\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u u) = -\frac{\partial P}{\partial x}$$
$$\frac{\partial}{\partial t} \left( \frac{1}{2} \rho u^2 + \rho e \right) + \frac{\partial}{\partial x} \left( (\frac{1}{2} \rho u^2 + \rho e) u \right) = -\frac{\partial}{\partial x} (P u)$$

1D, no external forces, stationary flow:

$$\frac{\partial}{\partial x}(\rho u) = 0$$
$$\frac{\partial}{\partial x}(\rho u u) = -\frac{\partial P}{\partial x}$$
$$\frac{\partial}{\partial x}\left((\frac{1}{2}\rho u^{2}+\rho e)u\right) = -\frac{\partial}{\partial x}(P u)$$

1D, no external forces, stationary flow:  $\frac{\partial}{\partial x}(\rho uu) = 0$  $\frac{\partial}{\partial x}(\rho uu) + \frac{\partial P}{\partial x} = 0$  $\frac{\partial}{\partial x}\left((\frac{1}{2}\rho u^{2} + \rho e)u\right) + \frac{\partial}{\partial x}(P u) = 0$ 

1D, no external forces, stationary flow:

$$\frac{\partial}{\partial x}(\rho u) = 0$$
$$\frac{\partial}{\partial x}(\rho u u + P) = 0$$
$$\frac{\partial}{\partial x}\left(\left(\frac{1}{2}u^2 + e + \frac{P}{\rho}\right)\rho u\right) = 0$$

jump conditions:  
specific enthalpy  

$$h \equiv e + \frac{P}{\rho} = \frac{\gamma}{\gamma - 1} \frac{P}{\rho}$$

$$\rho_2 u_2^2 = \rho_1 u_1$$

$$\rho_2 u_2^2 + P_2 = \rho_1 u_1^2 + P_1$$

$$\frac{1}{2} u_2^2 + h_2 = \frac{1}{2} u_1^2 + h_1$$

### Adiabatic Shocks: Jump Conditions

From these relations one can obtain expressions for the ratios of upstream to downstream quantities in terms of the upstream Mach number  $M_1 \equiv u_1/a_s$ , where  $a_s^2 \equiv \gamma P/\rho$ . The quantity  $M_1$  is known as the Mach number of the shock. For a perfect gas we find:

$$\frac{\rho_2}{\rho_1} = \frac{(\gamma+1)M_1^2}{(\gamma+1) + (\gamma-1)(M_1^2 - 1)} = \frac{u_1}{u_2}$$
(75)

$$\frac{P_2}{P_1} = \frac{(\gamma+1) + 2\gamma(M_1^2 - 1)}{(\gamma+1)} \tag{76}$$

$$\frac{T_2}{T_1} = \frac{[(\gamma+1)+2\gamma(M_1^2-1)][(\gamma+1)+(\gamma-1)(M_1^2-1)]}{(\gamma+1)^2M_1^2}$$
(77)

Notice that  $P_2 \ge P_1$ ,  $\rho_2 \ge \rho_1$ , and  $T_2 \ge T_1$  if  $M_1 \ge 1$  (supersonic upstream) with equality if  $M_1 = 1$  (no shock at all). In the limit of a very strong shock,  $M_1 \to \infty$ , the density jump is bounded by a finite value  $(\gamma + 1)/(\gamma - 1)$ , which equals 4 if  $\gamma = 5/3$ . In the same limit, the pressure and temperature jumps have no bound. In any case the deceleration of a gas from supersonic to subsonic speeds in a shock results in compression and heating.



jump conditions: specific enthalpy  $h \equiv e + \frac{P}{\rho} = \frac{\gamma}{\gamma - 1} \frac{P}{\rho}$   $\rho_2 u_2^2 = \rho_1 u_1$   $\rho_2 u_2^2 + P_2 = \rho_1 u_1^2 + P_1$  $\frac{1}{2} u_2^2 + h_2 = \frac{1}{2} u_1^2 + h_1$ 



jump conditions:

$$\rho_2 u_2 = \rho_1 u_1$$

$$\rho_2 u_2^2 + P_2 = \rho_1 u_1^2 + P_1$$

$$T_2 = T_1$$

### Strong Shocks: Jump Conditions

#### adiabatic

isothermal

 $\frac{\rho_2}{\rho_1} = \frac{u_1}{u_2} \rightarrow \frac{\gamma+1}{\gamma-1} \qquad \qquad \frac{\rho_2}{\rho_1} = \frac{u_1}{u_2} \rightarrow M_1^2$ 

for Mach number  $M_1 \rightarrow \infty$ 

density jump is limited

density jump is unlimited

Radiative cooling increases the compression ratio!

Introduction to Numerical Hydrodynamics

# 1. The Equations of Fluid Dynamics

### 1.4 Basic Mathematical and Numerical Considerations

# Equations of Fluid Dynamics: Euler Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$
$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial P}{\partial x_i}$$
$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho u^2 + \rho e\right) + \nabla \cdot \left((\frac{1}{2} \rho u^2 + \rho e) \boldsymbol{u}\right) = -\nabla \cdot (P \boldsymbol{u})$$

based on simplifying assumptions:

- no external forces (e.g. gravity, radiation pressure)
- no heating or cooling by radiation or heat conduction
- no viscosity (friction at microscopic level, shear)

# Equations of Fluid Dynamics: Euler Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$
$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j + P \delta_{ij}) = 0$$
$$\frac{\partial}{\partial t} \left( \frac{1}{2} \rho u^2 + \rho e \right) + \nabla \cdot \left( (\frac{1}{2} \rho u^2 + \rho e + P) \boldsymbol{u} \right) = 0$$

based on simplifying assumptions:

- no external forces (e.g. gravity, radiation pressure)
- no heating or cooling by radiation or heat conduction
- no viscosity (friction at microscopic level, shear)

## Equations of Fluid Dynamics: Euler Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0$$
$$\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j + P \delta_{ij}) = 0$$
$$\frac{\partial}{\partial t} \left( \frac{1}{2} \rho u^2 + \rho e \right) + \nabla \cdot \left( (\frac{1}{2} \rho u^2 + \rho e + P) \boldsymbol{u} \right) = 0$$

... can be re-written in the following form:

$$\frac{\partial}{\partial t} \mathbf{q} + \mathbf{f}(\mathbf{q}) = 0 \quad \text{where} \quad \mathbf{q} = \left( \rho, \rho u_i, \frac{1}{2} \rho u^2 + \rho e \right)$$

# Euler Equations ... A Recipe for a Solution?

The equations describe the time-evolution of q

$$\frac{\partial}{\partial t} \mathbf{q} = -\mathbf{f}(\mathbf{q}) \quad \text{where} \quad \mathbf{q} = \left( \rho, \rho u_i, \frac{1}{2} \rho u^2 + \rho e \right)$$

- So: 1. define a spatial grid
  - 2. specify initial conditions for q at t=0 for all grid period and suitable boundary conditions
  - 3. compute  $u_i$ , e and P
  - 4. compute right-hand side (spatial derivatives)
  - 5. take a small step in time and get a small change in q
  - 6. update *q*
  - 7. restart at 3.

But: there are many ways how this can go wrong, as we will see ...