Introduction to Numerical Hydrodynamics and Radiative Transfer

Part II: Hydrodynamics

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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

<table>
<thead>
<tr>
<th>system</th>
<th>description of state</th>
<th>dynamical equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N$ classical particles</td>
<td>$(x_1, ..., x_N, v_1, ..., v_N)$</td>
<td>Newton’s laws</td>
</tr>
<tr>
<td>distribution function</td>
<td>$f(x, v, t)$</td>
<td>Boltzmann equation</td>
</tr>
<tr>
<td>continuum model</td>
<td>$\rho(x), T(x), v(x)$</td>
<td>hydrodynamic equations</td>
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</tbody>
</table>
Fluid Dynamics: Basic Concepts

consider a typical fluid ...
Fluid Dynamics: Basic Concepts

... and define a fluid element
Fluid Dynamics: Basic Concepts

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:

\[ l_{\text{region}} \ll l_{\text{scale}} \sim q / |\nabla q| \]

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

\[ n l_{\text{region}}^3 \gg 1 \]

In addition, collisional fluids must satisfy:

(iii) \[ l_{\text{region}} \gg \text{mean free path of particles} \]
Mean Free Path - Examples

Mean Free Path

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

Examples

<table>
<thead>
<tr>
<th>gas in</th>
<th>density [cm$^{-3}$]</th>
<th>MFP [cm]</th>
<th>size [cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>typical room</td>
<td>$10^{19}$</td>
<td>$10^{-4}$</td>
<td>$10^3$</td>
</tr>
<tr>
<td>HI region (ISM)</td>
<td>10</td>
<td>$10^{14}$</td>
<td>$10^{19}$</td>
</tr>
</tbody>
</table>
Fluid Dynamics: Basic Concepts

- 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
Fluid Dynamics: Basic Concepts

cohereit motion of particles
Fluid Dynamics: Basic Concepts

coherent motion of particles
Fluid Dynamics: Basic Concepts

coherent motion of particles
Fluid Dynamics: Basic Concepts

- 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.
1. The Equations of Fluid Dynamics

1.2 Fluid Dynamics: Conservation Laws
Fluid Dynamics: The Conservation Laws

Mass conservation:
Fluid Dynamics: The Conservation Laws

Mass conservation:

\[ \frac{d}{dt} \int_V \rho \ dV = -\oint_A \rho \mathbf{u} \cdot \mathbf{n} \ dA = -\int_V \nabla \cdot (\rho \mathbf{u}) \ dV \]

rate of change of mass in \( V \) = mass flux across the surface

rewrite as:

\[ \int_V \left[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) \right] \ dV \ = \ 0 \]

... but the volume \( V \) is completely arbitrary

\[ \Rightarrow \quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]

equation of continuity
Fluid Dynamics: The Conservation Laws

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
Fluid Dynamics: The Conservation Laws

Energy conservation:

\[
\frac{d}{dt} \int_V \left( \frac{1}{2} \rho u^2 + \rho e \right) dV = -\oint_A \left( \frac{1}{2} \rho u^2 + \rho e \right) u \cdot \hat{n} \ dA - \oint_A u_i P \delta_{ij} \hat{n}_j \ dA + \int_V \rho u \cdot a \ dV
\]

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):

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

ergy equation
Fluid Dynamics: The Conservation Laws

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]

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

\[ \frac{\partial}{\partial t} \left( \frac{1}{2} \rho u^2 + \rho e \right) + \nabla \cdot \left( \frac{1}{2} \rho u^2 + \rho e \right) \mathbf{u} = - \nabla \cdot (P \mathbf{u}) + \rho \mathbf{u} \cdot \mathbf{a} \]

general form of conservation laws:

\[ \frac{\partial}{\partial t} \left( \text{density of quantity} \right) + \nabla \cdot \left( \text{flux of quantity} \right) = \text{sources} - \text{sinks} \]
Fluid Dynamics: The Conservation Laws

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]

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

\[ \frac{\partial}{\partial t}\left(\frac{1}{2} \rho u^2 + \rho e\right) + \nabla \cdot \left(\frac{1}{2} \rho u^2 + \rho e\right) \mathbf{u} = - \nabla \cdot (P \mathbf{u}) + \rho \mathbf{u} \cdot \mathbf{a} \]

... and what about external forces?

\[ \mathbf{a} = \frac{\mathbf{F}}{m} \]
Fluid Dynamics: External Forces

Gravitation:

\[ a = g \quad \text{... acceleration} \]

where \( g \) is given by Poisson's equation

\[ \nabla \cdot g = -4 \pi G \rho \]
Fluid Dynamics: External Forces

Radiation pressure:

\[ f_{\text{rad}} = \rho / c \int \kappa_v F_v \, dv \]

\[ f_{\text{rad}} \] ... force per volume, added to equation of motion

\[ u \cdot f_{\text{rad}} \] ... work done by radiation pressure, added to energy equation
Fluid Dynamics: The Conservation Laws

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0
\]

\[
\frac{\partial}{\partial t} (\rho \mathbf{u}_i) + \frac{\partial}{\partial x_j} (\rho \mathbf{u}_i \mathbf{u}_j) = - \frac{\partial P}{\partial x_i} + \rho \mathbf{g}_i + f_{rad}^i
\]

\[
\frac{\partial}{\partial t} \left( \frac{1}{2} \rho \mathbf{u}^2 + \rho e \right) + \nabla \cdot \left( \left( \frac{1}{2} \rho \mathbf{u}^2 + \rho e \right) \mathbf{u} \right) = - \nabla \cdot (P \mathbf{u}) + \rho \mathbf{u} \cdot \mathbf{g} + \mathbf{u} \cdot f_{rad} + \Gamma - \Lambda
\]

... including:  
gravity  
radiation pressure  
heating & cooling by radiation
Fluid Dynamics: Limit Cases of Energy Transport

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

Barotropic equation of state:

\[
P = P(\rho)
\]

Examples:  - ideal gas:

\[
P \propto \rho T
\]

* isothermal case

\[
P \propto \rho
\]

* adiabatic case

\[
P = K \rho^\gamma
\]

Efficient radiative heating and cooling:

\[\Gamma - \Lambda = 0 \rightarrow T \rightarrow P(\rho, T)\]

(\rightarrow \text{radiative equilibrium})
Introduction to Numerical Hydrodynamics

1. The Equations of Fluid Dynamics

1.3 Acoustic Waves and Shock Waves
Fluid Dynamics: The Conservation Laws

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]

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

\[ \frac{\partial}{\partial t} \left( \frac{1}{2} \rho u^2 + \rho e \right) + \nabla \cdot \left( \frac{1}{2} \rho u^2 + \rho e \right) \mathbf{u} = - \nabla \cdot (P \mathbf{u}) + \rho \mathbf{u} \cdot \mathbf{a} \]

general form of conservation laws:

\[ \frac{\partial}{\partial t} \, \left( \text{density of quantity} \right) + \nabla \cdot \left( \text{flux of quantity} \right) = \text{sources} - \text{sinks} \]
Waves: Small-Amplitude Sound Waves

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) &= 0 \\
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j) &= - \frac{\partial P}{\partial x_i} + \rho a_i
\end{align*}
\]

replacing energy equation:

\[
P = K \rho^y
\]

1D, no external forces:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) &= 0 \\
\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho uu) &= - \frac{\partial P}{\partial x}
\end{align*}
\]
Waves: Small-Amplitude Sound Waves

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

replacing energy equation:

1D, no external forces:
Waves: Small-Amplitude Sound Waves

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

insert into equations & linearise:

\[ P = P_0 + P_1(x, t) \]
\[ \rho = \rho_0 + \rho_1(x, t) \]
\[ u = u_1(x, t) \]

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

\[ \frac{\partial \rho_1}{\partial t} + \rho_0 \frac{\partial u_1}{\partial x} = 0 \]
\[ \rho_0 \frac{\partial u_1}{\partial t} = - \frac{\partial P_1}{\partial x} \]
Waves: Small-Amplitude Sound Waves

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:

\[ \frac{\partial \rho_1}{\partial t} + \rho_0 \frac{\partial u_1}{\partial x} = 0 \]
\[ \rho_0 \frac{\partial u_1}{\partial t} + a_0^2 \frac{\partial \rho_1}{\partial x} = 0 \]
\[ \gamma \frac{P_0}{\rho_0} = a_0^2 \]
Waves: Small-Amplitude Sound Waves

⇒ 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 \(a_0\)

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.
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

\[ P_2 \quad \rho_2 \quad u_2 \quad \rho_1 \quad P_1 \]

\[ \text{shock "jump" if } \ell \ll L \]

On macroscopic scales, shock transitions may be approximated as single discontinuous jumps.
Waves: Shocks and Conservation Laws

1D, no external forces

\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0 \]

\[ \frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}(\rho uu) = -\frac{\partial P}{\partial x} \]

\[ \frac{\partial}{\partial t}\left(\frac{1}{2}\rho u^2 + \rho e\right) + \frac{\partial}{\partial x}\left(\frac{1}{2}\rho u^2 + \rho e\right)u = -\frac{\partial}{\partial x}(Pu) \]
Waves: Shocks and Conservation Laws

1D, no external forces, stationary flow:

\[
\frac{\partial}{\partial x} (\rho u) = 0
\]

\[
\frac{\partial}{\partial x} (\rho uu) = - \frac{\partial P}{\partial x}
\]

\[
\frac{\partial}{\partial x} \left( \left( \frac{1}{2} \rho u^2 + \rho e \right) u \right) = - \frac{\partial}{\partial x} (Pu)
\]
Waves: Shocks and Conservation Laws

1D, no external forces, stationary flow:

\[ \frac{\partial}{\partial x} (\rho u) = 0 \]
\[ \frac{\partial}{\partial x} (\rho uu) + \frac{\partial P}{\partial x} = 0 \]
\[ \frac{\partial}{\partial x} \left( \left( \frac{1}{2} \rho u^2 + \rho e \right) u \right) + \frac{\partial}{\partial x} (Pu) = 0 \]
Waves: Shocks and Conservation Laws

1D, no external forces, stationary flow:

\[
\frac{\partial}{\partial x}(\rho u) = 0
\]

\[
\frac{\partial}{\partial x}(\rho uu + P) = 0
\]

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

Jump conditions:

\[
\rho_2 u_2 = \rho_1 u_1
\]

\[
\rho_2 u_2^2 + P_2 = \rho_1 u_1^2 + P_1
\]

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

specific enthalpy

\[
h \equiv e + \frac{P}{\rho} = \frac{\gamma}{\gamma-1} \frac{P}{\rho}
\]
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:

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

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

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

Notice that $P_2 \geq P_1$, $\rho_2 \geq \rho_1$, and $T_2 \geq T_1$ if $M_1 \geq 1$ (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.
Waves: Shocks and Conservation Laws

1D, no external forces, stationary flow:

\[
\frac{\partial}{\partial x} (\rho u) = 0
\]

\[
\frac{\partial}{\partial x} (\rho uu + P) = 0
\]

energy conserving (no radiation)

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

jump conditions:

specific enthalpy

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

\[
\rho_2 u_2 = \rho_1 u_1
\]

\[
\rho_2 u_2^2 + P_2 = \rho_1 u_1^2 + P_1
\]

\[
\frac{1}{2} u_2^2 + h_2 = \frac{1}{2} u_1^2 + h_1
\]
Waves: Shocks and Conservation Laws

1D, no external forces, stationary flow:

\[
\frac{\partial}{\partial x}(\rho u) = 0
\]

\[
\frac{\partial}{\partial x}(\rho uu + P) = 0
\]

isothermal (efficient radiative cooling)

\[
\frac{\partial}{\partial x}(T) = 0
\]

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

\[
\frac{\rho_2}{\rho_1} = \frac{u_1}{u_2} \rightarrow \frac{\gamma+1}{\gamma-1}
\]

isothermal

\[
\frac{\rho_2}{\rho_1} = \frac{u_1}{u_2} \rightarrow M_1^2
\]

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

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \]

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

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

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

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]

\[ \frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j + P \delta_{ij}) = 0 \]

\[ \frac{\partial}{\partial t}\left(\frac{1}{2} \rho u^2 + \rho e\right) + \nabla \cdot \left(\left(\frac{1}{2} \rho u^2 + \rho e + P\right) \mathbf{u}\right) = 0 \]

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

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \]

\[ \frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} (\rho u_i u_j + P \delta_{ij}) = 0 \]

\[ \frac{\partial}{\partial t} \left( \frac{1}{2} \rho u^2 + \rho e \right) + \nabla \cdot \left( \left( \frac{1}{2} \rho u^2 + \rho e + P \right) \mathbf{u} \right) = 0 \]

... 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 $q$

$$\frac{\partial}{\partial t} q = -f(q)$$

where

$$q = \left( \rho, \ \rho u, \ \frac{1}{2} \rho u^2 + \rho e \right)$$

So:

1. define a spatial grid
2. specify initial conditions for $q$ at $t=0$ for all grid points
   and suitable boundary conditions
3. compute $u$, $e$ 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 ...