Physical processes by characteristic timescale

<table>
<thead>
<tr>
<th>Timescale</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diffusive timescale</td>
<td>$t_{\text{diff}} \sim \frac{L^2}{D}$</td>
</tr>
<tr>
<td>Sound-crossing timescale</td>
<td>$t_{\text{sound}} \sim \frac{L}{a}$</td>
</tr>
<tr>
<td>Flow timescale</td>
<td>$t_{\text{flow}} \sim \frac{L}{u}$</td>
</tr>
<tr>
<td>Free-fall timescale</td>
<td>$t_{\text{ff}} \sim \frac{1}{\sqrt{\rho G}}$</td>
</tr>
<tr>
<td>Cooling timescale</td>
<td>$t_{\text{cool}} \sim \frac{\rho \varepsilon}{</td>
</tr>
<tr>
<td>Reaction timescale</td>
<td>$t_{\text{react}} \sim \min_i \frac{X_i}{</td>
</tr>
</tbody>
</table>

largest to smallest
Continuity equation source terms

Multiple fluid components

\[
\begin{align*}
\rho_1 + \rho_2 + \rho_3 + \ldots + \rho_{N_f} &= \rho \\
X_1 + X_2 + X_3 + \ldots + X_{N_f} &= 1
\end{align*}
\]

\[
X_i \equiv \frac{\rho_i}{\rho}
\]

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

\[
\frac{\partial X_i}{\partial t} + \mathbf{u} \cdot \nabla X_i = 0
\]

Reactions that convert one fluid component into another

\[
\frac{\partial X_i}{\partial t} + \mathbf{u} \cdot \nabla X_i = \sum_{j=1}^{N_f} X_i X_j R_{ij}
\]

Mass diffusion – usually negligible in astrophysical settings

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \nabla \cdot [D(\rho) \nabla \rho]
\]
Importance of conservation in continuity equations

The sum \( \sum X_i = 1 \) is not always preserved by an update step:

- **Interpolants**: different flattening of the \( X_i \)
- **Source terms**: not always guaranteed to preserve sum

Solutions:

- **Rescaling**
  \[
  X_i \rightarrow \frac{X_i}{\sum_j X_j}
  \]

- **Restricting**
  \[
  X_i \rightarrow \min\left[1, \max\left(0, X_i\right)\right]
  \]

  **Problem**: no error control

- **Solving only** \( N_f - 1 \) **equations**
  \[
  X_{N_f} = 1 - \sum_{j=1}^{N_f-1} X_j
  \]

  **Problem**: error tends to accumulate in the assumed fluid abundance

- **Flatten all abundances** when \( |\sum X_i - 1| > \epsilon \), otherwise none of them

  **Problem**: reduces spatial order, leads to numerical mixing
Momentum equation source terms

Gravitational forces and viscosity

\[
\frac{\partial}{\partial t} \rho \mathbf{u} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) + \nabla P = \rho \mathbf{g} + \nabla \cdot (\mu \mathbf{D}) = \nabla \cdot [\mathbf{G} + \mu \mathbf{D}]
\]

For momentum equation these terms can be written as the divergence of a conserved flux.

Can also have “true” momentum source terms: e.g., AGN jets modelled as pistons.
Energy equation source terms

Energy sources/sinks – gravity, radiation

\[
\frac{\partial \varepsilon}{\partial t} + \mathbf{u} \cdot \nabla \varepsilon + \frac{P}{\rho} \nabla \cdot \mathbf{u} = \frac{\Gamma - \Lambda}{\rho}
\]

\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot [(\rho E + P) \mathbf{u}] = \rho \mathbf{u} \cdot \mathbf{g} + (\Gamma - \Lambda)
\]

Thermal conduction and viscous heating

\[
\frac{\partial \varepsilon}{\partial t} + \mathbf{u} \cdot \nabla \varepsilon + \frac{P}{\rho} \nabla \cdot \mathbf{u} = \nabla \cdot [K \nabla \varepsilon] + \frac{1}{2} \mu \| \mathbf{D} \|^2
\]

\[
D_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \nabla \cdot \mathbf{u}
\]

Equation of state

\[
\varepsilon \equiv \varepsilon (\rho, T, X_1, \ldots, X_{N_f})
\]

for ideal gases: Dalton's law of partial pressures

\[
P = P(\rho_1, T) + P(\rho_2, T) + \ldots + P(\rho_{N_f}, T)
\]
**Unsplit methods**

Solve the advection, diffusion, and source terms together

e.g., upwind differencing for advection, FTCS for diffusion, and FT for source:

\[
\frac{\partial q}{\partial t} = -\frac{\partial q u}{\partial x} + D \frac{\partial^2 q}{\partial x^2} + \Gamma
\]

\[
q_{i}^{n+1} = q_{i}^{n} - \frac{\Delta t}{\Delta x} \left[ \left( (qu)^{n}_{i+s} - (qu)^{n}_{i+s-1} \right) - \frac{D}{\Delta x} \left( q_{i+1}^{n} - 2q_{i}^{n} + q_{i-1}^{n} \right) - \Gamma_{i}^{n} \right]
\]

where \( s = 1 \) if \( u_{i}^{n} < 0 \), \( s = 0 \) if \( u_{i}^{n} > 0 \)

**Advantage:** avoids errors introduced by operator splitting

**Disadvantage:** difficult to develop Godunov-type methods and multidimensional methods; usually no exact solution to Riemann problem
**Split (fractional-step) methods**

Apply difference operators for each piece of physics in sequence. Consider

\[ D = D_1 + D_2 + D_3 \]

First order (time):

\[ D[q] = D_1 [D_2 [D_3 [q]]] + O(\Delta t) \]

Second order (time) – Strang splitting:

\[ D[q] = D_1^{1/2} [D_2^{1/2} [D_3^{1/2} [D_3^{1/2} [D_2^{1/2} [D_1^{1/2} [q]]]]]] + O(\Delta t^2) \]

With operator splitting we cannot do better than the time accuracy of the splitting method, no matter what the accuracy of the component operators is.

Solve the advection part of our equation with a standard CFD method, with the diffusion terms split off and solved with a parabolic solver, and the source terms split off and solved with an ordinary differential equation solver:

\[
\begin{align*}
\frac{\partial q}{\partial t} &= -\frac{\partial q u}{\partial x} + D \frac{\partial^2 q}{\partial x^2} + \Gamma \\
\frac{\partial q}{\partial t} &= D \frac{\partial^2 q}{\partial x^2} \\
\frac{d q}{d t} &= \Gamma
\end{align*}
\]
Stiffness

Often have very different timescales for flow and source terms.

e.g., thermonuclear runaway in a white dwarf (Type Ia supernova)

nuclear burning timescale \((^{12}\text{C} + ^{12}\text{C})\)

\[ t_{\text{burn}} \sim \frac{\varepsilon}{\dot{\varepsilon}} \sim 4 \times 10^{18} \left( \frac{n}{\text{cm}^{-3}} \right)^{-1} \text{ sec} \sim 10^{-12} \text{ sec} \]

sound-crossing timescale

\[ t_{\text{sound}} \sim \frac{R}{a} \sim \frac{6 \times 10^8 \text{ cm}}{2 \times 10^{-2} c} \sim 1 \text{ sec} \]

If we stick to explicit time-integration schemes, we are forced to integrate on the shortest timescale in order to maintain numerical stability!

Yet doing everything implicitly causes problems when shock waves are involved.

So commonly we:

• Use explicit methods for longest-timescale physics (advection, diffusion)
• Use implicit methods for shortest-timescale physics (reactions, diffusion)
• Set timestep using explicit method and then “sub-cycle” the implicit method
Sub-cycling

Intervals $\Delta t_n$ between $\bullet$ determined by stability needs of explicit scheme

Intervals $\Delta t_{n,m}$ between $\bullet$ determined by accuracy needs of implicit scheme; last interval set to make $t_{n,m_{\text{max}}}$ = $t_{n+1}$

Cannot have $\Delta t_n \gg \max_m \Delta t_{n,m}$ – causes advection and source terms to decouple
Explicit ODE methods

Consider the system of linear ordinary differential equations

\[
\frac{dq}{dt} = -A \cdot q
\]

with \( A \) symmetric and positive definite (all positive eigenvalues).

The number of elements in the vector \( q \) is the number of simultaneous source-term equations we are solving. One such system is solved for every zone in our grid.

*Forward Euler* (explicit) differencing gives

\[
q^{m+1} = (I - A \Delta t) \cdot q^m
\]

For stability, the timestep must satisfy

\[
|1 - \lambda_{\text{max}} \Delta t| < 1 \quad \Rightarrow \quad \Delta t < \frac{2}{\lambda_{\text{max}}}
\]

where \( \lambda_{\text{max}} \) is the maximum eigenvalue of \( A \).
**Runge-Kutta methods**

Explicit ODE integration schemes that achieve higher order than forward Euler by computing derivatives at intermediate points.

Combine with adaptive step size control for robust integration to modest accuracy ($\approx 10^{-4}$) – either by halving $\Delta t$ or by combining different orders to get error estimate ("embedding")

Second-order Runge-Kutta (midpoint method):

$$k_1 = \Delta t f(t_m, q^m)$$
$$k_2 = \Delta t f(t_m + \frac{1}{2} \Delta t, q^m + \frac{1}{2} k_1)$$
$$q^{m+1} = q^m + k_2 + O(\Delta t^3)$$

Fourth-order Runge-Kutta method:

$$k_1 = \Delta t f(t_m, q^m)$$
$$k_2 = \Delta t f(t_m + \frac{1}{2} \Delta t, q^m + \frac{1}{2} k_1)$$
$$k_3 = \Delta t f(t_m + \frac{1}{2} \Delta t, q^m + \frac{1}{2} k_2)$$
$$k_4 = \Delta t f(t_m + \Delta t, q^m + k_3)$$
$$q^{m+1} = q^m + \frac{1}{6} k_1 + \frac{1}{3} k_2 + \frac{1}{3} k_3 + \frac{1}{6} k_4 + O(\Delta t^5)$$
Bulirsch-Stoer method

Can also use midpoint method on successively smaller intervals $\Delta t$ and use *Richardson extrapolation* to estimate solution at $\Delta t \to 0$.

Advantage: much more efficient than Runge-Kutta for large systems & high accuracy
Disadvantage: not as robust for nonsmooth or singular source terms
Implicit and semi-implicit ODE methods

*Backward Euler* (implicit) differencing gives

\[
q^{m+1} = q^m - A q^{m+1} \Delta t
\]

\[
q^{m+1} = (I + A \Delta t)^{-1} \cdot q^m
\]

which is unconditionally stable, since

\[
(1 + \lambda \Delta t)^{-1} < 1
\]

for all eigenvalues \(\lambda\) and timesteps \(\Delta t\).

For nonlinear systems of equations

\[
\frac{d}{dt} \frac{dq}{dt} = f(q) \quad \rightarrow \quad q^{m+1} = q^m + f(q^{m+1}) \Delta t
\]

we use Newton's method:

\[
q^{m+1} = q^m + \Delta t \left[ I - \Delta t \left. \frac{\partial f}{\partial q} \right|_m \right]^{-1} \cdot f(q_m)
\]

\(\partial f/\partial q\) is the Jacobian matrix. This type of method is called *semi-implicit*. 
Rosenbrock methods

Semi-implicit generalization of Runge-Kutta methods.

Look for a solution of the form

\[ q^{m+1} = q^m + \sum_{i=1}^{s} c_i k_i \]

where

\[ \left( I - \gamma \Delta t \frac{\partial f}{\partial q} \bigg|_m \right) \cdot k_i = \Delta t f \left( q^m + \sum_{j=1}^{i-1} \alpha_{ij} k_j \right) + \Delta t \frac{\partial f}{\partial q} \bigg|_m \cdot \sum_{j=1}^{i-1} \gamma_{ij} k_j \]

s is the order of the method.

By combining third- and fourth-order methods, can obtain an estimate of truncation error to use for adaptive step size control.

Method is not guaranteed to be stable (semi-implicit), but fairly robust nevertheless, even for nonsmooth right-hand sides (e.g., from tabular interpolation).

For large vectors \( q \) (> 10 elements) and high accuracy (< \( 10^{-5} \)), methods based on Richardson extrapolation are more efficient.
Intermission
Reaction networks – example: diffuse gas + radiation

Partially or fully ionized diffuse gas experiences several types of “reaction:”

- Photoionization: \( X + \gamma \rightarrow X^+ + e \)
- Recombination: \( X^+ + e \rightarrow X + \gamma \)
- Photon absorption: \( X + \gamma \rightarrow X^* \)
- Photon emission: \( X^* \rightarrow X + \gamma \)
- Stimulated emission: \( X^* + \gamma \rightarrow X + 2\gamma \)
- Collisional excitation: \( X + e \rightarrow X^* + e \)
- Collisional ionization: \( X + e \rightarrow X^+ + 2e + \gamma \)
- Charge exchange: \( X + p \rightarrow X^+ + H \)
- Dielectronic recombination: \( X^+ + e \rightarrow X^* \)
- Bremsstrahlung: \( X + e \rightarrow X + e + \gamma \)
- ...

Again, we treat different elements and ionization states as different fluids:

\( H^0, H^+, H^-, He^0, He^+, He^{++}, \ldots \)

Overall charge neutrality gives free electron number density: \( n_e = \sum_i Z_i n_i \)

In optically thin limit all radiation escapes; in optically thick limit it is absorbed; in other regimes we need to keep track of radiation field and do radiation transfer
Thermal and ionization equilibrium

If we have *local thermodynamic equilibrium* conditions (necessary for a fluid approach!), the Boltzmann relation gives relative abundances of excited states:

\[ n_i = \frac{n}{U_i} g_i e^{-E_i/kT} \]

- \( n_i \) = number density of atomic/ionic species in \( i \)th excited state
- \( n \) = total number density of species
- \( U_i \) = partition function for \( i \)th state
- \( g_i \) = statistical weight for \( i \)th state
- \( E_i \) = energy of \( i \)th state relative to ground state

If we have *ionization equilibrium* conditions, we can use Saha equation to determine ionic abundances rather than following them separately:

\[ \frac{n_{i+1} n_e}{n_i} = \frac{2 U_{i+1}}{U_i} \left( \frac{2 \pi m_e kT}{\hbar^2} \right)^{3/2} e^{-\chi_i/kT} \]

- \( n_i \) = number density of ions in ionization state \( i \)
- \( n_e \) = free electron number density
- \( U_i \) = partition function for ionization state \( i \)
- \( \chi_i \) = ionization energy of for ionization state \( i \)

Then we just track the atomic abundances and use the Saha equation whenever we need an ionic abundance.
Collisional ionization equilibrium

A common situation in the intergalactic medium is collisional ionization equilibrium, in which atoms are collisionally ionized and radiatively recombine. If the gas is optically thin, this causes a net loss of energy from the gas.

Treat this situation using:

• One continuity equation for each element (or a single metallicity for all of them)

• Ionization fraction is a known function of temperature and abundances – use to determine $n_e$ (needed for emissivity and equation of state)

$$n_{X,i} = n_{X,i}(T, n_H, n_{H+}, n_{He}, n_{He+}, n_{He++}, ... )$$

$$P = \left( n_e + \sum_{X,i} n_{X,i} \right) kT$$

• Radiative cooling via a local energy sink term – cooling rate is a known function of density, temperature, and abundances:

$$\rho \frac{d\varepsilon}{dt} = -\Lambda(T, n_H, ...)$$
Radiative cooling rate for collisionally ionized gas

Primordial abundances (from Black 1981)
Photoionization equilibrium

Another common situation: a source of ultraviolet photons ionizes nearby gas; medium is optically thick to recombination photons (“Strömgren sphere”)

In the interior of the nebula the ionization state is set by the equilibrium between:

- Photoionization by photons from central source and from locally produced recombination photons
- Collisional ionization by local free electrons
- Recombination

The size of the nebula increases with time unless collisional processes produce radiation that can escape.

Inside cloud treat using:

- Ionic abundances from photoionization equilibrium given known external photon source: varying optical depth to known source, local recombination radiation produces local re-ionization (“on-the-spot” approximation)
- Net heating source term for energy equation includes collisional cooling effects
- Near the edge of the cloud finite optical depth to local recombination photons must be taken into account
Photoionization equilibrium – 2

Case 1: no external radiation field, optically thin, collisional cooling only – $T$ decreases with time

Case 2: known external radiation field, net photoionization energy input exceeds collisional cooling rate – $T$ increases with time

Case 3: known external radiation field, collisional cooling rate exceeds net photoionization energy input – $T$ decreases with time

Case 4: known external radiation field, net photoionization energy input balances collisional cooling – thermal equilibrium
Cooling curves including photoionization

Representative curves for uniform external $J_\nu = 10^{-22} (\nu L / \nu) \text{ erg s}^{-1} \text{ cm}^{-2} \text{ sr}^{-1} \text{ Hz}^{-1}$ (N. Katz)

- At lower density, almost complete ionization – so gas transparent to recombination photons, allowing them to act as a coolant
- At higher density, recombination photons are locally absorbed – cooling occurs by collisionally excited line emission and bremsstrahlung

\[ n_H = 2.89 \times 10^{-6} \text{ cm}^{-3} \quad n_H = 2.89 \times 10^{-3} \text{ cm}^{-3} \]