EXCOSM computing school

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Git repository for hands-on examples

https://github.com/rainerweinberger/CosmoComputingSchool

1 Modelling gas using computers

1.1 Theoretical foundations

Let $f = f(\mathbf{x}, \mathbf{u}, t)$ be the distribution function of an ensemble of identical particles with no internal degrees of freedom, position $\mathbf{x}$ and velocity $\mathbf{u}$ such that the number of particles is

$$N = \iint f(\mathbf{x}, \mathbf{u}, t)\, d^3x\, d^3u. \tag{1}$$

Assuming the particle number is conserved, we get

$$\frac{d}{dt} f(\mathbf{x}, \mathbf{u}, t) = \frac{\partial f}{\partial t} + \frac{\partial \mathbf{x}}{\partial t} \cdot \nabla f + \frac{\partial \mathbf{u}}{\partial t} \cdot \nabla_u f = \left[\frac{df}{dt}\right]_c, \tag{2}$$

$$\frac{d}{dt} f(\mathbf{x}, \mathbf{u}, t) = \frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f + \mathbf{g} \cdot \nabla_u f = \left[\frac{df}{dt}\right]_c, \tag{3}$$

with $\left[\frac{df}{dt}\right]_c$ denoting changes due to collisions and $\mathbf{g}$ the accelerations due to a potential force, e.g., gravity. Equation 3 is called the Boltzmann equation. It describes the time evolution of the 6 dimensional phase space distribution function.

We speak of a fluid in the limit of frequent collision, if the mean free path, i.e., the mean travelling distance of a particle between collisions is negligible compared to the size of the system in question[1]. This allows us to simplify the Boltzmann equation significantly. First, one can assume the velocity distribution of the particles follows a Maxwell-Boltzmann distribution. Second, one can

[1] This is the opposite limit to a collisionless fluid you would have for dark matter in cosmological structure formation.

take moments of the equation, i.e.

$$\int \left(\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f + \mathbf{g} \nabla_u f \right) d^3u = \int \left[\frac{df}{dt} \right]_c d^3u, \tag{4}$$

$$\int \mathbf{u} \left(\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f + \mathbf{g} \nabla_u f \right) d^3u = \int \mathbf{u} \left[\frac{df}{dt} \right]_c d^3u, \tag{5}$$

$$\int \mathbf{u}^2 \left(\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f + \mathbf{g} \nabla_u f \right) d^3u = \int \mathbf{u}^2 \left[\frac{df}{dt} \right]_c d^3u. \tag{6}$$

Defining the mass density ρ, fluid velocity $\mathbf{v}$ and energy density e as

$$\rho(\mathbf{x}, t) = \int m\, f(\mathbf{x}, \mathbf{v}, t)\, d^3u, \tag{7}$$

$$\mathbf{v}(\mathbf{x}, t) = \frac{1}{\rho} \int \mathbf{u}\, m\, f(\mathbf{x}, \mathbf{u}, t)\, d^3u, \tag{8}$$

$$e(\mathbf{x}, t) = \int \frac{1}{2} u^2\, m\, f(\mathbf{x}, \mathbf{u}, t)\, d^3u, \tag{9}$$

with m being the particle mass, one can drive the equations of ideal hydrodynamics. These describe the time evolution of the 3 dimensional fluid quantities $\rho, \mathbf{v}$ and e. (Note this step is non-trivial, but not shown here for brevity).

1.2 Ideal hydrodynamics

The equation for an ideal fluid with density ρ, velocity $\mathbf{v}$ and energy density e are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \tag{10}$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \left(\rho \mathbf{v} \mathbf{v}^T + \mathbf{I} p \right) = \rho \mathbf{g}, \tag{11}$$

$$\frac{\partial e}{\partial t} + \nabla \cdot \left(\mathbf{v} \left(e + p \right) \right) = \rho \left(\mathbf{v} \cdot \mathbf{g} \right), \tag{12}$$

with

$$e_{th} = e - \frac{1}{2} \rho \mathbf{v}^2,$$
$$p = (\gamma - 1) e_{th}.$$

Note that the thermal energy density is related to the temperature T

$$k_B\, T = (\gamma - 1) \mu m_p\, \frac{e_t h}{\rho},$$

with k_B is the Boltzmann constant, $\gamma = 5/3$ for an ideal fluid (with no internal degrees of freedom), μ is the mean particle weight in units of the proton mass m_p.

1.3 Finite volume approach

The Euler equations have the form

$$\frac{\partial q}{\partial t} + \nabla \cdot \mathbf{F}(q) = 0 \tag{13}$$

with $q = \rho, \rho v, e$.

Then can be rewritten integrating over a volume V to

$$\frac{\partial}{\partial t} \int\limits_V q \, dV + \int\limits_V \nabla \cdot \mathbf{F}(q) \, dV = 0, \tag{14}$$

$$\frac{\partial}{\partial t} Q + \oint\limits_{\partial V} \mathbf{F}(q) \cdot d\mathbf{S} = 0, \tag{15}$$

where we defined $Q = \int\limits_V q \, dV$, denoting mass, momentum and total energy. Discretizing the time derivative (here in a forward Euler fashion with timestep δt), as well as the surface integral in terms of a discrete number of surfaces, we get

$$Q_{n+1} = Q_n + \sum_i \mathbf{F}(q_i) \cdot \mathbf{A}_i \, \delta t, \tag{16}$$

where the sum over index i denotes a sum over all interfaces to neighbouring cells. The key question is then how to obtain the flux across cell interfaces. One common way to get fluxes is to treat the interface as a Riemann problem.

A Riemann problem is defined as a problem with initial state

$$q(\mathbf{x}, t = 0) = \begin{cases} q_L & \text{for} \quad x \leq 0 \\ q_R & \text{for} \quad x > 0 \end{cases} \tag{17}$$

while the details of theory of the solution of the Riemann problem is somewhat involved (the textbook by Toro is an excellent reference for this), algorithms that compute the solutions, and, most importantly the fluxes $\mathbf{F}(q_l, q_r)$ either exact iteratively or approximately exist and are used in finite volume solvers.

The time-integration is done in timesteps δt, with a single timestep consisting of the following steps

1. reconstruct q from Q
2. evolve: calculate the fluxes given q and the amount of material flowing over interfaces
3. average: add the changes due to interface fluxes to state Q in every cell

1.4 Smoothed particle hydrodynamics

A different approach to modelling fluids is though the use of particles that serve as interpolation points for the fluid field. The basic idea of smoothed particle hydrodynamics (SPH) is to then find equations of motion for these particles that represent the Euler equations in a Lagrangian fashion. This means that SPH discretizes the equations of hydrodynamics in mass, which is a quite desirable aspect making it particularly attractive for structure formation simulations, where SPH particles move analogous (but not identical!) to the collisionless particles of the n-body solver. For any field F, one can define a smoothed version F_s though convolution with a kernel

$$F_s(\mathbf{x}) = \int F(\mathbf{x}')W(\mathbf{x} - \mathbf{x}'d\mathbf{x}' \tag{18}$$

e.g.

$$\rho_s(\mathbf{x}) = \sum_j m_j W(|\mathbf{x} - \mathbf{x}_j|, h) \tag{19}$$

with one possibility of a kernel being a cubic spline interpolation of a Gaussian

$$W(r,h) = \frac{8}{\pi}\begin{cases} 1 - 6\left(\frac{r}{2\,h}\right)^2 + 6\left(\frac{r}{2\,h}\right) & \text{for} \quad 0 \le r \le h \\ 2\,\left(1 - \frac{r}{2h}\right)^3 & \text{for} \quad h < r \le 2h \\ 0 & \text{else} \end{cases} \tag{20}$$

One can show that the quation of motion for SPH particles are

$$\frac{d\mathbf{v}_i}{dt} = -\sum_{j=1}^{N} m_j \left[f_i \frac{P_i}{\rho_i^2}\nabla_i W_{ij}(h_i) + f_j \frac{P_j}{\rho_j^2}\nabla_i W_{ij}(h_j) \right] \tag{21}$$

with

$$f_i = \left[1 + \frac{h_i}{3\rho_i}\frac{\partial \rho_i}{\partial h_i}\right]^{-1} \tag{22}$$

Conveniently, we do not have to explicitly solve for mass conservation as this is already taken care of by the movement of the simulation particles. The energy equation is, up to this stage, is also not needed since the entropy will stay constant. This, however, is not true at shocks, which require the introduction of an artificial viscosity to allow for entropy generation. This can be added as an additional term in the equation of motion as

$$\left.\frac{d\mathbf{v}_i}{dt}\right|_{\text{visc}} = -\sum_{j=1}^{N} m_j \Pi_{ij} \nabla_i \frac{W_{ij}(h_i) + W_{ij}(h_j)}{2}, \tag{23}$$

and increase the entropy accordingly. Note that sometimes, $W_{ij}((h_i + h_j)/2)$ is used instead of the average over the weighting kernels.

One possible choice for the artivicial viscosity Π_{ij} is

$$\Pi_{ij} = \begin{cases} (-\alpha c_{ij}\mu_{ij} + \beta\mu_{ij}^2)/\rho_i j & \text{if} \quad \mathbf{v}_{ij} \cdot \mathbf{r}_{ij} < 0, \\ 0 & \text{otherwise.} \end{cases} \tag{24}$$

Here,

$$\mu_{ij} = \frac{h_{ij}\mathbf{v}_{ij} \cdot \mathbf{r}_{ij}}{|\mathbf{r}_{ij}|^2 + \epsilon h_{ij}^2} \tag{25}$$

and h_{ij} and ρ_{ij} are means of the corresponding quantities of the two particles i and j.