Numerical hydrodynamics

The fluid equations (for a *perfect*, *ideal* fluid) are the most common type of PDEs to be solved in astrophysics, even more common than the Poisson equation as there are many problems in which gravity can be treated as a fixed external force (eg interstellar medium, accretion disks, turbulent flows in interstellar clouds). Most often are coupled with Poisson, as in the study of galaxy or star formation.

Two approaches: *eulerian* and *lagrangian.*

In *eulerian approach*, one seeks the solution of the flow (velocity, density, pressure/temperature) from a static reference frame (**v=0**) from which the flow is observed

In *lagrangian approach*, one seeks the solution of the flow in a reference frame co-moving with the flow (**v=v(x,** t**)**)

The first approach lends itself naturally to the adoption of grid-based codes, in which a fixed mesh introduces the static reference frame (eg def **x=0, v=0** at the center of the mesh)

The second approach lends itself naturally to particle-based codes, in which some "macroparticle" tracers of the fluid model the trajectories of fluid elements analogously to the case of star clusters or dark matter lumps in collisionless systems. Recall fluid equations are moments of the Boltzmann equation, perfectly consistent with the idea of using "macroparticles" to sample the various quantities, while actual atoms and molecules obey the underlying Boltzmann equation
In this one can start with the fluid at rest (all particles have zero velocity) or not, and the coordinate system will be chosen appropriately at t=0 but there is no mesh forcing it.

In the remainder we will *neglect viscous forces* until further notice as this is often a good enough approximation.

Recap inviscid fluid equations (Euler)

In eulerian form the full set of PDEs, including those for the internal energy e, are:

$$\frac{\partial \rho}{\partial t} + \mathbf{u} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{u} = 0$$

mass cons.

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{\nabla p}{\rho} = 0$$

momentum cons. (with no. applied ext. force)

$$\frac{\partial e}{\partial t} + \mathbf{u} \cdot \nabla e + \frac{p}{\rho} \nabla \cdot \mathbf{u} = 0$$

energy cons.

Note the total energy, the sum of internal energy per unit mass e plus the kinetic energy per unit mass, $v^2/2$, is conserved (can be shown) but the internal energy would be conserved only in an *incompressible flow* for which the divergence of the velocity is zero (last term in third equation = 0).
In astrophysics we normally consider *compressible flows.*

To have a *closed* system of PDEs one needs an extra equation that describes the relation between pressure, density and internal energy - the equation of state. For an ideal gas:

$$P = (\gamma - 1)\rho u,$$

with the adiabatic index $\gamma = c_p/c_v$ =5/3 for monoatomic gas (eg hydrogen)

To obtain the lagrangian formulation one uses the convective derivative to express that fluid flow properties as observed by an observer moving with the flow:

$$\mathrm{d}/\mathrm{d}t = \partial/\partial t + \mathbf{v} \cdot \nabla$$

The equations in lagrangian from (note change of notation, now **v** is the velocity while *u* is the internal energy) are:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \nabla \cdot \mathbf{v} = 0,$$

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} + \frac{\nabla P}{\rho} = 0,$$

$$\frac{\mathrm{d}u}{\mathrm{d}t} + \frac{P}{\rho} \nabla \cdot \mathbf{v} = 0,$$

The two formulations are equivalent. In general the solution of the Euler equations does not depend on the reference frame. If we rotate or translate the frame the same solution still holds given fixed initial conditions (i.e. **v**, ρ, P at each coordinare **x** at t=0 in the eulerian form).

This leads to the important notion of *galilean invariance*. This means that the geometry of a numerical infrastructure used to solve these PDEs (eg a mesh should not affect the solution of

Smoothed particle hydrodynamics (SPH)

It is a particle-based method for the solution of the lagrangian form of the fluid equations based on interpolation technique:

- That is, particles are used as interpolation points to obtain the values of the hydrodynamical variables at the location of a particle.

- The values of the hydro variables are obtained using convolution integrals in order to obtain a smooth estimate

- The convolution kernel is chosen based on a trade-off between interpolating on a volume large enough to have a as smooth as possible function reconstruction (eg smooth-out Poisson noise due to discretization) and have enough resolution locally to identify features in the flow (eg resolves sudden density/pressure changes)

- the method is formally and naturally conserving mass, momentum and angular momentum, as well as gas internal energy in absence of shocks. With shocks *artificial viscosity* needs to be introduced and energy conservation is lost.

- the method is naturally galilean invariant because it is mesh-free. It is also naturally adaptive because the smoothing kernel, which defines the region of interpolation, adapts to the flow - i.e. it shrinks as the density increases

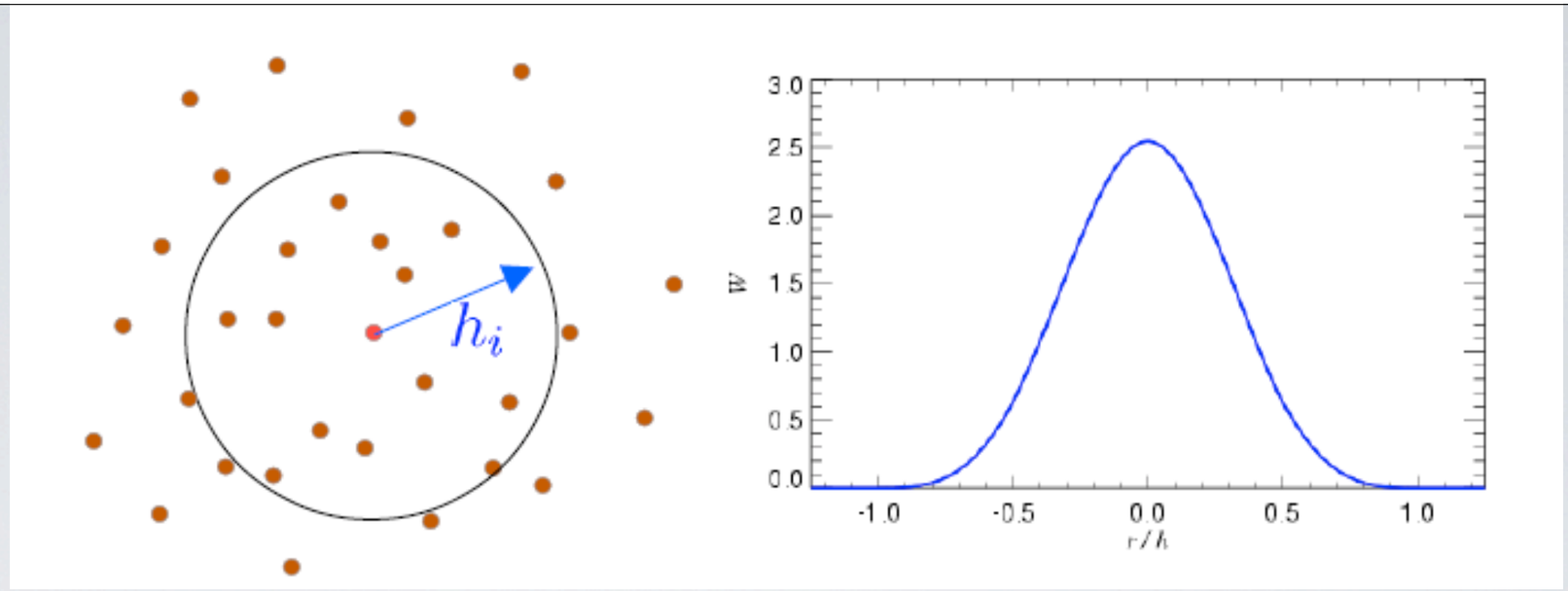
In SPH for any fluid field F(**r**) one writes the corresponding smoothed interpolated version using a finite set of particles as

$$F_s(\mathbf{r}) = \int F(\mathbf{r}')\,W(\mathbf{r}-\mathbf{r}',h)\,\mathrm{d}\mathbf{r}'.$$

with the spherical kernel **W**(**r,** h) = **W**(2**r**/h), "h" smoothing length

A standard kernel choice is the cubic spline with finite support

$$w_{3\mathrm{D}}(q) = \frac{8}{\pi}\begin{cases} 1-6q^2+6q^3, & 0 \le q \le \frac{1}{2}, \\ 2(1-q)^3, & \frac{1}{2} < q \le 1, \\ 0, & q > 1, \end{cases}$$



The smoothing length *h* defines the characteristic size of the interpolation kernel. By choosing a finite support kernel rather than eg a gaussian one defines finite volume that has short tails, which means the interpolation is inherently local. This enables high resolution in principle by weighing only on the region quite close to a particle + makes the calculation fast as only a few interpolation points are needed to get values at particle positions A typical choice is to fixed the *number of neighbors* to define *h* at any given tim, where this is number of particles used in the interpolation. This makes the estimate of any field F(**r**) automatically adapitve

Assume we have a field $F(\mathbf{r})$ is sampled with a finite set of particles (i.e. known at a finite set of points) $F_i = F(\mathbf{r}_i)$ then integrals have to be replaced by sums. Each particle is given a mass m_i and thus associated density $\rho i = m_i/V_i$, so that we can write:

$$F_s(\mathbf{r}) \simeq \sum_j \frac{m_j}{\rho_j} F_j W(\mathbf{r} - \mathbf{r}_j, h).$$

Note that particles will be in general distributed in a regular fashion since they will represent physical quantities such as density or pressure profiles (radial profiles $\rho(\mathbf{r})$ or $P(\mathbf{r})$) of physical systems. This helps with the accuracy of the method. For example in 1D if one lies down particle with equal spacing d then one can show
that for $h=d$ the SPH smoothed interpolations of fluid field functions $F(\mathbf{r})$ are second-order accurate.
For not-so-regular particle distributions $h >= d$ and there is no formal error analysis possible in SPH as there is in grid-based approaches (think eg of natural truncation error in finite differencing of Poisson equation)

Note that with the above definition the field functions (**a**) are defined everywhere and not just at the interpolation points (= at particle positions) because the kernel is defined everywhere and (**b**) are differentiable because the kernel is differentiable (although with higher interpolation error).

If F(***r***) = ρ(***r***) we can write the "SPH density" in the form:

$$\rho_s(\mathbf{r}) \simeq \sum_j m_j W(\mathbf{r}-\mathbf{r}_j, h).$$

As mentioned before the smoothing length can be made adaptive in space and time, *h=h(**r**, t)*, for example by fixing the number of neighbors, so that one "adjusts" the density estimate based on the evolution of the flow.

Two basic approaches to introduce adaptive kernels:
"scatter", in which $W(\mathbf{r}, h) = W(\mathbf{r}-\mathbf{r}_j, h(\mathbf{r}))$
"gather", in which $W(\mathbf{r}, h) = W(\mathbf{r}-\mathbf{r}_j, h(\mathbf{r}_j))$

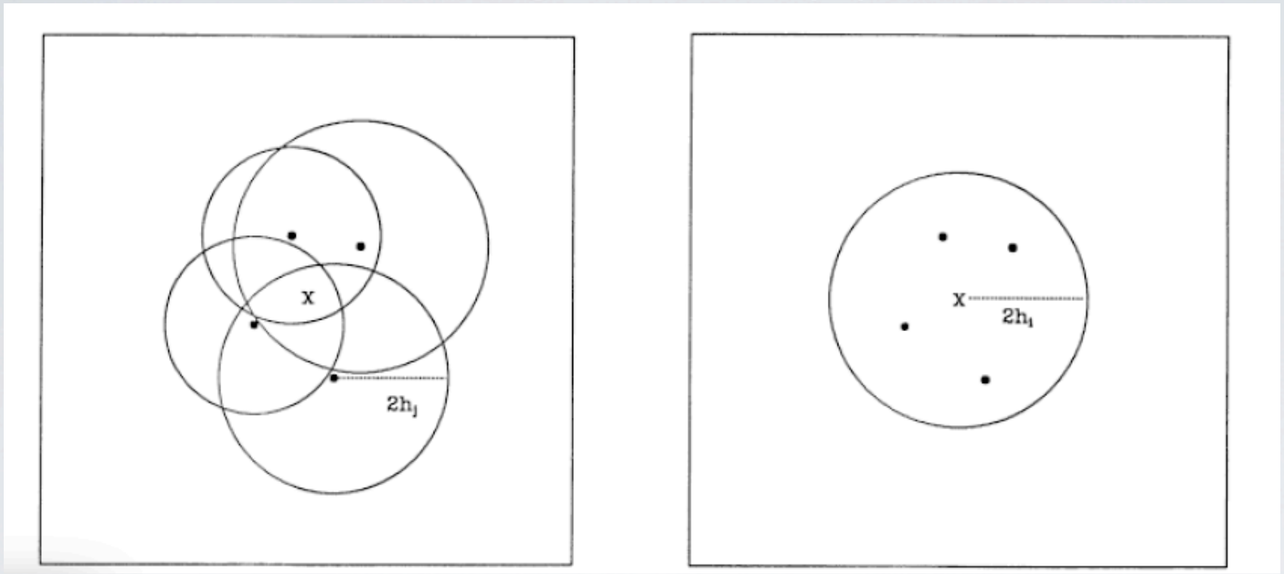
The second approach, "gather", is computationally easier and faster as one uses only the smoothing lengths of the particle *i* to estimate the density at the interpolation point corresponding to it:

$$\rho_i = \sum_{j=1}^{N} m_j W(\mathbf{r}_i - \mathbf{r}_j, h_i).$$

Thanks to the fact that we are using a kernel with finite support the expression above really means that we are summing only over the *N* particles contained within a distance $r = 2h$ because beyond that $W=0$.

This way we have that the SPH density estimate has a cost of order $N \times O(N_{neigh})$, where N_{neigh} is the (fixed) number of neighbors that defines the kernel, and is $<< N$ in standard applications. This means of corse that in high density regions the smoothing lengths will be smaller, but the cost of the interpolation will be the same as in low density regions. Note that with a gaussian kernel, which does not have finite support, the cost woul have been $\sim O(N^2)$

Scatter vs. gather approach



1. particle i collects the contributions from all other particles j which smoothing volumes h_j *scatter* onto location $\vec{r}_i$
   $h \to h_j$, i.e. use $W(|\vec{r}_i - \vec{r}_j|, h_j)$ in the summation
2. particle i *gathers* the contributions from all particles which centers fall within the smoothing volume of i
   $h \to h_i$, i.e. use $W(|\vec{r}_i - \vec{r}_i|, h_i)$ in the summation

if all particles have the same smoothing length $h = h_i = h_j$ both approaches are equivalent; otherwise different j contribute to the sum $\longrightarrow$ violation of Newton's 3. law!!
therefore, enforce force anti-symmetry by using the (arithmetic) average of the smoothing lengths for all particle pairs

$$h \longrightarrow h_{ij} = \frac{h_i + h_j}{2} \; .$$

Note that the same mathematical formulation used for the density can be used for all fluid fields and also for differential operators that are needed to solve the Euler equation:

$$(\nabla \cdot \mathbf{v})_i = \sum_j \frac{m_j}{\rho_j} \mathbf{v}_j \cdot \nabla_i W(\mathbf{r}_i - \mathbf{r}_j, h).$$

This is the SPH divergence operator which is obtained by writing the "SPH smoothed" velocity field and taking its derivative. The derivative is applied only to the kernel ultimately because vj is not a function rather it is a scalar value so gives zero under differentiation.

An alternative estimate can be obtained by exploiting the identity

$$\rho \nabla \cdot \mathbf{v} = \nabla(\rho \mathbf{v}) - \mathbf{v} \cdot \nabla \rho,$$

which yields then the more accurate pairwise estimate

$$(\nabla \cdot \mathbf{v})_i = \frac{1}{\rho_i} \sum_j m_j (\mathbf{v}_j - \mathbf{v}_i) \cdot \nabla_i W(\mathbf{r}_i - \mathbf{r}_j, h).$$

(gives zero divergence if particles have equal velocity)

Example of natural adapitvity of SPH formulation: collapsing uniform density sphere

- Initial conditions: particles initially equally spaced everywhere.

- Step 1: turn-on gravity of sphere (eg with treecode).
Now particles get closer to each other due to gravitational forces, so sphere no uniform anymore as
density increases everywhere. Collapse begins.

- Step 2: if number of neighbors fixed all particles have smaller kernels, so they "adjust" the resolution scale (i.e. h) to follow the new higher density.

- Step 3: if adiabatic the fluid would increase its temperature as pressure increases via equation of state

- Step 4: if pressure gradient overcomes gravity sphere expands again, so now the kernels become larger once again

SPH fluid equations from lagrangian

We know want to formulate the inviscid fluid equations, namely the Euler equations, using SPH smoothed interpolations for all the fluid fields and differential operators. In lagrangian form the equations are:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho\,\nabla\cdot\mathbf{v} = 0,$$

mass cons.

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} + \frac{\nabla P}{\rho} = 0,$$

momentum cons. (no ext. forces)

$$\frac{\mathrm{d}u}{\mathrm{d}t} + \frac{P}{\rho}\nabla\cdot\mathbf{v} = 0,$$

internal energy cons.

where $\mathrm{d}/\mathrm{d}t = \partial/\partial t + \mathbf{v}\cdot\nabla$ is the so-called convective or lagrangian derivative (recall how we proceeded for the Vlasov eq.)

One could proceed heuristically, as in the original approach of Monaghan and Gingold, and just recast the equations in SPH form by replacing all individual fields and operators with their SPH versions.

A more elegant approach stars from a lagrangian, from which the Euler equations can be obtained:

$$L = \int \rho \left(\frac{\mathbf{v}^2}{2} - u \right) \mathrm{d}V.$$

where u is the internal energy of the gas

The next step is to discretize the lagrangian and then formulate the corresponding Euler-Lagrange equations. These will then yield the equations of motions for the fluid.

Assuming equal mass particles with mass m_i the discretized lagrangian takes the form

$$L_{\mathrm{SPH}} = \sum_i \left(\frac{1}{2} m_i \mathbf{v}_i^2 |- m_i u_i \right)$$

Note that it does not depend on time and is invariant under translation and rotations (no explicit dependence on spatial coordintes) which expresses energy, momentum and angular momentume conservation