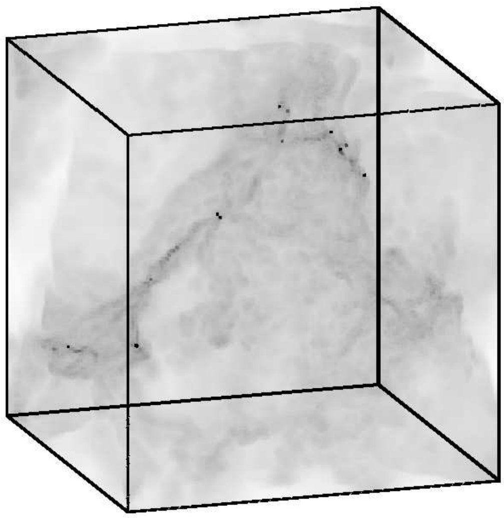
SPH Basics

Introduction into Smoothed Particle Hydrodynamics



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Overview

- Some words about hydrodynamics
- SPH – The Standard Implementation
- Modifications and Extensions
- Some Caveats

Hydrodynamics:

- text books on hydrodynamics
  - Landau & Lifshitz, Volume VI - Hydrodynamics
  - Landau & Lifshitz, Volume X - Kinetic theory
  - Reichl, A modern course in statistical physics, Wiley, New York (1998)
  - Shu, The physics of astrophysics 2, Univ. Sc. Books, Mill Valley (1992)

- derivation
  - gases and fluids are *large* ensembles of interacting particles
  - $\longrightarrow$ state of system is described by location in $6N$ dimensional phase space $f^{(N)}(\vec{q}_1 ... \vec{q}_N, \vec{p}_1 ... \vec{p}_N) d\vec{q}_1 ... d\vec{q}_N d\vec{p}_1 ... d\vec{p}_N$
  - time evolution governed by 'equation of motion' for $6N$-dim probability distribution function $f^{(N)}$
  - $f^{(N)} \rightarrow f^{(n)}$ by integrating over all but n coordinates $\longrightarrow$ BBGKY hierarchy of equations of motion (after Born, Bogoliubov, Green, Kirkwood and Yvon)
  - physical observables are typically associated with 1- or 2-body probability density $f^{(1)}$ or $f^{(2)}$
  - at lowest level of hierarchy: 1-body distribution function describes the probability of finding a particle at time t in the volume element $d\vec{q}$ at $\vec{q}$ with momenta in the range $d\vec{p}$ at $\vec{p}$.
  - **Boltzmann equation** – equation of motion for $f^{(1)}$

$$\begin{aligned}\frac{df}{dt} &\equiv \frac{\partial f}{\partial t} + \dot{\vec{q}} \cdot \vec{\nabla}_{\mathrm{q}} f + \dot{\vec{p}} \cdot \vec{\nabla}_{\mathrm{p}} f \\ &= \frac{\partial f}{\partial t} + \vec{v} \cdot \vec{\nabla}_{\mathrm{q}} f + \vec{F} \cdot \vec{\nabla}_{\mathrm{p}} f = f_{\mathbf{c}}\,.\end{aligned}$$

Hydrodynamics:

- derivation

  - **Boltzmann equation**

$$\frac{df}{dt} \equiv \frac{\partial f}{\partial t} + \dot{\vec{q}} \cdot \vec{\nabla}_{\rm q} f + \dot{\vec{p}} \cdot \vec{\nabla}_{\rm p} f$$
$$= \frac{\partial f}{\partial t} + \vec{v} \cdot \vec{\nabla}_{\rm q} f + \vec{F} \cdot \vec{\nabla}_{\rm p} f = f_{\mathbf{c}} \, .$$

  $\longrightarrow$ first line: transformation from comoving to spatially fixed coordinate system.

  $\longrightarrow$ second line: velocity $\vec{v} = \dot{\vec{q}}$ and force $\vec{F} = \dot{\vec{p}}$

  $\longrightarrow$ all higher order terms are 'hidden' in the collision term $f_{\mathbf{c}}$

  - observable quantities are typically (velocity) moments of the Boltzmann equation, e.g.

  $\longrightarrow$ density:

$$\rho = \int m \, f(\vec{q}, \vec{p}, t) d\vec{p}$$

  $\longrightarrow$ momentum:

$$\rho \vec{v} = \int m\vec{v} \, f(\vec{q}, \vec{p}, t) d\vec{p}$$

  $\longrightarrow$ kinetic energy density:

$$\rho \vec{v}^{\,2} = \int m\vec{v}^{\,2} \, f(\vec{q}, \vec{p}, t) d\vec{p}$$

Hydrodynamics:

- derivation
  - in general: the i-th velocity moment $\langle \xi_i \rangle$ (of $\xi_i = m\vec{v}^{\,i}$) is

    $$\langle \xi_i \rangle = \frac{1}{n} \int \xi_i \, f(\vec{q}, \vec{p}, t) d\vec{p}$$

    with the mean particle number density n defined as

    $$n = \int f(\vec{q}, \vec{p}, t) \, d\vec{p}$$

  - the equation of motion for $\langle \xi_i \rangle$ is

    $$\int \xi_i \left\{ \frac{\partial f}{\partial t} + \vec{v} \cdot \vec{\nabla}_{\mathrm{q}} f + \vec{F} \cdot \vec{\nabla}_{\mathrm{p}} f \right\} d\vec{p} = \int \xi_i \, \{ f_{\mathbf{c}} \} \; d\vec{p} \, ,$$

    which after some complicated rearrangement becomes

    $$\boxed{\frac{\partial}{\partial t} n \langle \xi_i \rangle + \vec{\nabla}_{\mathrm{q}} (n \langle \xi_i \vec{v} \rangle) + n\vec{F} \langle \vec{\nabla}_{\mathrm{p}} \xi_i \rangle = \int \xi_i f_{\mathbf{c}} \, d\vec{p}}$$

    (Maxwell-Boltzmann transport equation for $\langle \xi_i \rangle$)

  - if the RHS is zero, then ξ_i is a conserved quantity. This is only the case for first three moments, mass $\xi_0 = m$, momentum $\vec{\xi}_1 = m\vec{v}$, and kinetic energy $\xi_2 = m\vec{v}^{\,2}/2$.
  - MB equations build a hierarically nested set of equations, as $\langle \xi_i \rangle$ depends on $\langle \xi_{i+1} \rangle$ via $\vec{\nabla}_{\mathrm{q}} (n \langle \xi_i \vec{v} \rangle)$ and because the collision term cannot be reduced to depend on ξ_i only.
    $\longrightarrow$ need for a closure equation
    $\longrightarrow$ in hydrodynamics this is typically the equation of state.

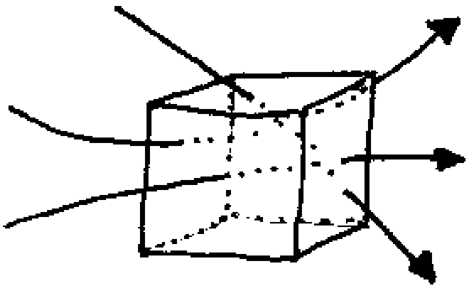
Hydrodynamics:

- assumptions
  - **continuum limit:**
    - $\longrightarrow$ distribution function f must be a 'smoothly' varying function on the scales of interest $\longrightarrow$ local average possible
    - $\longrightarrow$ stated differently: the averaging scale (i.e. scale of interest) must be larger than the mean free path of individual particles
    - $\longrightarrow$ stated differently: microscopic behavior of particles can be neglected
    - $\longrightarrow$ concept of fluid element must be meaningful
  - **only 'short range forces':**
    - $\longrightarrow$ forces between particles are short range or saturate $\longrightarrow$ collective effects can be neglected
    - $\longrightarrow$ stated differently: correlation length of particles in the system is finite (and smaller than the scales of interest)
- limitations
  - shocks (scales of interest become smaller than mean free path)
  - phase transitions (correlation length may become infinite)
  - description of self-gravitating systems
  - description of fully fractal systems

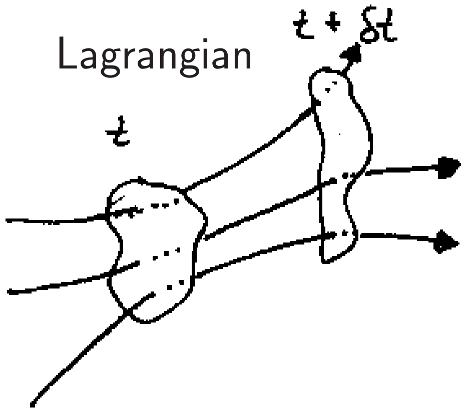
Hydrodynamics:

- the equations of hydrodynamics
  - hydrodynamics $\equiv$ book keeping problem
    One must keep track of the 'change' of a fluid element due to various physical processes acting on it. How do its 'properties' evolve under the influence of compression, heat sources, cooling, etc.?
  - Eulerian vs. Lagrangian point of view

Eulerian



Lagrangian



consider spatially fixed volume element

following motion of fluid element

  - hydrodynamic equations = set of equations for the five conserved quantities $(\rho, \rho\vec{v}, \rho\vec{v}^{\,2}/2)$ plus closure equation (plus transport equations for 'external' forces if present, e.g. gravity, magnetic field, heat sources, etc.)

Hydrodynamics:

- the equations of hydrodynamics
  - equations of hydrodynamics

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \vec{v} \cdot \vec{\nabla}\rho = -\rho\vec{\nabla} \cdot \vec{v} \qquad \text{(continuity equation)}$$

$$\frac{d\vec{v}}{dt} = \frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \vec{\nabla})\vec{v} = -\frac{1}{\rho}\vec{\nabla}p - \vec{\nabla}\phi + \eta\vec{\nabla}^2\vec{v} + \left(\zeta + \frac{\eta}{3}\right)\vec{\nabla}(\vec{\nabla} \cdot \vec{v})$$

$$\text{(Navier-Stokes equation)}$$

$$\frac{d\epsilon}{dt} = \frac{\partial \epsilon}{\partial t} + \vec{v} \cdot \vec{\nabla}\epsilon = T\frac{ds}{dt} - \frac{p}{\rho}\vec{\nabla} \cdot \vec{v} \qquad \text{(energy equation)}$$

$$\vec{\nabla}^2\phi = 4\pi G\rho \qquad \text{(Poisson's equation)}$$

$$p = \mathcal{R}\rho T \qquad \text{(equation of state)}$$

$$\vec{F}_B = -\vec{\nabla}\frac{\vec{B}^2}{8\pi} + \frac{1}{4\pi}(\vec{B} \cdot \vec{\nabla})\vec{B} \qquad \text{(magnetic force)}$$

$$\frac{\partial \vec{B}}{\partial t} = \vec{\nabla} \times (\vec{v} \times \vec{B}) \qquad \text{(Lorentz equation)}$$

$\rho =$ density, $\vec{v} =$ velocity, $p =$ pressure, $\phi =$ gravitational potential, ζ and η viscosity coefficients, $\epsilon = \rho\vec{v}^{\,2}/2 =$ kinetic energy density, $T =$ temperature, $s =$ entropy, $\mathcal{R} =$ gas constant, $\vec{B} =$ magnetic field (cgs units)

Hydrodynamics:

- the equations of hydrodynamics
  - mass transport – continuity equation

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \vec{v}\cdot\vec{\nabla}\rho = -\rho\vec{\nabla}\cdot\vec{v}$$

(conservation of mass)

  - transport equation for momentum – Navier Stokes equation

$$\frac{d\vec{v}}{dt} = \frac{\partial \vec{v}}{\partial t} + (\vec{v}\cdot\vec{\nabla})\vec{v} = -\frac{1}{\rho}\vec{\nabla}p - \vec{\nabla}\phi + \eta\vec{\nabla}^2\vec{v} + \left(\zeta + \frac{\eta}{3}\right)\vec{\nabla}(\vec{\nabla}\cdot\vec{v})$$

momentum change due to

$\longrightarrow$ pressure gradients: $(-\rho^{-1}\vec{\nabla}p)$

$\longrightarrow$ (self) gravity: $-\vec{\nabla}\phi$

$\longrightarrow$ viscous forces (internal friction, contains $\mathrm{div}(\partial v_i/\partial x_j)$ terms): $\eta\vec{\nabla}^2\vec{v} + \left(\zeta + \frac{\eta}{3}\right)\vec{\nabla}(\vec{\nabla}\cdot\vec{v})$

(conservation of momentum, general form of momentum transport: $\partial_t(\rho v_i) = -\partial_j \Pi_{ij}$)

  - transport equation for internal energy

$$\frac{d\epsilon}{dt} = \frac{\partial \epsilon}{\partial t} + \vec{v}\cdot\vec{\nabla}\epsilon = T\frac{ds}{dt} - \frac{p}{\rho}\vec{\nabla}\cdot\vec{v}$$

$\longrightarrow$ follows from the thermodynamic relation $d\epsilon = T\,ds - p\,dV = T\,ds + p/\rho^2 d\rho$ which described changes in ϵ due to entropy changed and to volume changes (compression, expansion)

$\longrightarrow$ for adiabatic gas the first term vanishes ($s =$constant)

$\longrightarrow$ heating sources, cooling processes can be incorporated in ds

(conservation of energy)

Hydrodynamics:

- the equations of hydrodynamics
  - closure equation – equation of state
    - $\longrightarrow$ general form of equation of state $p = p(T, \rho, ...)$
    - $\longrightarrow$ ideal gas: $p = \mathcal{R}\rho T$
    - $\longrightarrow$ special case – isothermal gas: $p = c_\mathrm{s}^2 T$ (as $\mathcal{R}T = c_\mathrm{s}^2$)

SPH Basics:

- literature
  - Benz, W., SPH, in 'The Numerical Modeling of Nonlinear Stellar Pulsations' ed. J. R. Buchler, Kluwer (1990)
  - Monaghan, J. J., Particle Methods for Hydrodynamics, Comp. Phys. Reports (1985)
  - Monaghan, J. J., SPH, ARA&A (1992)
- concept of SPH
  - 'invented' independently by Lucy (1977) and Gingold & Monaghan (1977)
  - originally proposed as Monte Carlo approach to calculate the time evolution of gaseous systems
  - more intuitively understood as interpolation scheme:

    The fluid is represented by an ensemble of particles i, each carrying mass m_i, momentum $m_i\vec{v}_i$, and hydrodynamic properties (like pressure p_i, temperature T_i, internal energy ϵ_i, entropy s_i, etc.). The time evolution is governed by the equation of motion plus additional equations to modify the hydrodynamic properties of the particles. Hydrodynamic observables are obtained by a local averaging process.

SPH Basics:

- properties of local averaging processes
  - local averages $\langle f(\vec{r})\rangle$ for any quantity $f(\vec{r})$ can be obtained by convolution with an appropriate smoothing function $W(\vec{r},\vec{h})$:

$$\langle f(\vec{r})\rangle \equiv \int f(\vec{r}\,')W(\vec{r}-\vec{r}\,',\vec{h})\,d^3r'\,.$$

    the function $W(\vec{r},\vec{h})$ is called smoothing kernel
  - the kernel must satisfy the following two conditions:

$$\int W(\vec{r},\vec{h})\,d^3r = 1 \quad \text{and} \quad \langle f(\vec{r})\rangle \longrightarrow f(\vec{r}) \;\; \text{for} \;\; \vec{h}\to 0$$

    the kernel W therefore follows the same definitions as Dirac's delta function $\delta(\vec{r})$: $\lim_{h\to 0} W(\vec{r},h) = \delta(\vec{r})$.
  - most SPH implementations use spherical kernel functions

$$W(\vec{r},\vec{h}) \equiv W(r,h) \quad \text{with} \quad r=|\vec{r}| \;\; \text{and} \;\; h=|\vec{h}|.$$

    (one could also use triaxial kernels, e.g. Martel et al. 1995)
  - as the kernel function W can be seen as approximation to the δ-function for small but finite h we can expand the averaged function $\langle f(\vec{r})\rangle$ into a Taylor series for h to obtain an estimate for $f(\vec{r})$; if W is an even function, the first order term vanishes and the errors are second order in h

$$\langle f(\vec{r})\rangle = f(\vec{r}) + \mathcal{O}(h^2)$$

    this holds for functions f that are smooth and do not exhibit steep gradients over the size of W ($\longrightarrow$ problems in shocks).
    (more specifically the expansion is $\langle f(\vec{r})\rangle = f(\vec{r}) + \kappa h^2\vec{\nabla}^2 f(\vec{r}) + \mathcal{O}(h^3)$)

SPH Basics:

- properties of local averaging processes
  - within its intrinsic accuracy, the smoothing process therefore is a linear function with respect to summation and multiplication:

$$\langle f(\vec{r}) + g(\vec{r})\rangle = \langle f(\vec{r})\rangle + \langle g(\vec{r})\rangle$$
$$\langle f(\vec{r}) \cdot g(\vec{r})\rangle = \langle f(\vec{r})\rangle \cdot \langle g(\vec{r})\rangle$$

(one follows from the linearity of integration with respect to summation, and two is true to $\mathcal{O}(h^2)$)

  - derivatives can be 'drawn into' the averaging process:

$$\frac{d}{dt}\langle f(\vec{r})\rangle = \left\langle \frac{d}{dt} f(\vec{r})\right\rangle$$
$$\vec{\nabla}\langle f(\vec{r})\rangle = \langle \vec{\nabla} f(\vec{r})\rangle$$

Furthermore, the spatial derivative of f can be transformed into a spatial derivative of W (no need for finite differences or grid):

$$\vec{\nabla}\,\langle f(\vec{r})\rangle = \left\langle \vec{\nabla} f(\vec{r})\right\rangle = \int f(\vec{r}\,')\,\vec{\nabla} W(|\vec{r}-\vec{r}\,'|,h)\,d^3r'\;.$$

(shown by integrating by parts and assuming that the surface term vanishes; if the solution space is extended far enough, either the function f itself or the kernel approach zero)

  - basic concept of SPH is a particle representation of the fluid $\longrightarrow$ *integration* transforms into *summation* over discrete set of particles; example density ρ:

$$\langle \rho(\vec{r}_i)\rangle = \sum_j m_j W(|\vec{r}_i - \vec{r}_j|, h)\;.$$

in this picture, the mass of each particle is smeared out over its kernel region; the density at each location is obtained by summing over the contributions of the various particles $\longrightarrow$ *smoothed particle hydrodynamics!*

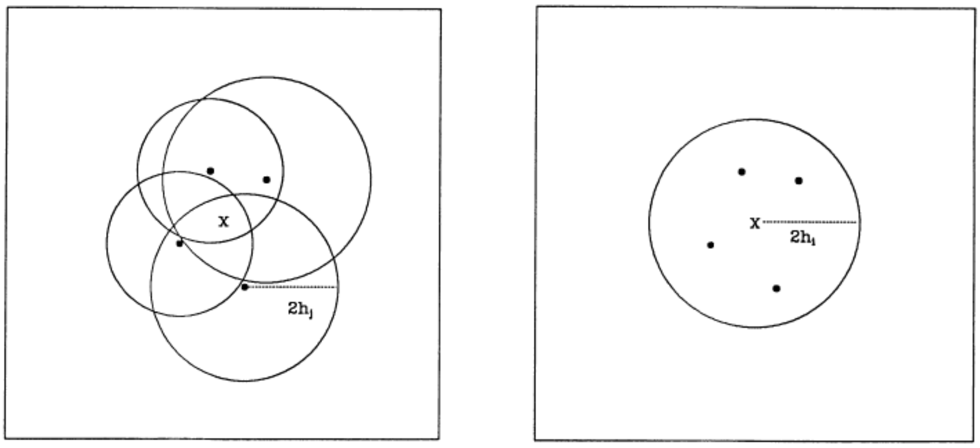
SPH Basics:

- properties of local averaging processes
  - 'scatter' versus 'gather' approach:

$$\langle \rho(\vec{r}_i) \rangle = \sum_j m_j W(|\vec{r}_i - \vec{r}_j|, h) \; .$$

allows for two different interpretations...

1. particle i collects the contributions from all other particles j which smoothing volumes h_j *scatter* onto location $\vec{r}_i$
   $h \rightarrow h_j$, 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
   $h \rightarrow h_i$, i.e. use $W(|\vec{r}_i - \vec{r}_j|, h_i)$ 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

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

SPH Basics:

- the kernel function
  - different functions meet the requirement $\int W(|\vec{r}|, h)\, d^3r = 1$ and $\lim_{h\to 0} \int W(|\vec{r} - \vec{r}'|, h) f(\vec{r}')\, d^3r' = f(\vec{r})$:

    $\longrightarrow$ Gaussian kernel:

    $$W(r, h) = \frac{1}{\pi^{3/2} h^3} \exp\left(-\frac{r^2}{h^2}\right)$$

    · *pro:* mathematically sound

    · *pro:* derivatives exist to all orders and are smooth

    · *contra:* all particles contribute to a location

    $\longrightarrow$ spline functions with compact support

    $\longrightarrow$ the standard kernel: cubic spline
    with $\xi = r/h$ it is defined as

    $$W(r, h) \equiv \frac{1}{\pi h^3} \begin{cases} 1 - \frac{3}{2}\xi^2 + \frac{3}{4}\xi^3, & \text{for } 0 \le \xi \le 1; \\ \frac{1}{4}(2 - \xi)^3, & \text{for } 1 \le \xi \le 2; \\ 0, & \text{otherwise.} \end{cases}$$

    · *pro:* compact support $\longrightarrow$ all interactions are zero for $r > 2h$ $\longrightarrow$ number of particles involved in the average remains small (typically between 30 and 80)

    · *pro:* second derivative is continuous

    · *pro:* dominant error term is second order in h

    $\longrightarrow$ in principle different kernel functions could be used for different equations (but it brings no obvious advantage, except maybe in the case of XSPH)

    $\longrightarrow$ specialized kernels can be constructed for different types of problems

SPH Basics:

- variable smoothing length h
  - spatial resolution of SPH is limited by h, the scale over which forces and physical properties are smeared out
  - to make optimum use of the Lagrangian nature of SPH one has to allow for variations of h: in high-density regions h should be small, in regions of low density h should be large
  - the optimum value of h is such that every particle has ~ 50 neighbors within the smoothing volume
  - caveats:

    $\longrightarrow$ introduction of *additional errors* (the Taylor series now contains contributions from $\vec{\nabla} h$, furthermore time derivatives $\partial h/\partial t$ occur); however, these errors are of second or higher order and thus the same as the one inherent to SPH anyway

    $\longrightarrow$ *modification* of the kernel *gradient*

    $$\vec{\nabla} W(|\vec{r}-\vec{r}\,'|, h) = \vec{\nabla} W(|\vec{r}-\vec{r}\,'|, h)\Big|_h + \frac{\partial}{\partial h} W(|\vec{r}-\vec{r}\,'|, h) \vec{\nabla} h\Big|_{\vec{r}}$$

    the new term is $\propto \vec{\nabla} h$ and becomes important only if the smoothing length varies on scales less than the smoothing lengths itself $\longrightarrow$ it is generally *neglected* (see Nelson & Papaloizou 1994).
  - equation of 'motion' for h can be coupled to the density: from $h = h_0\,(\rho_0/\rho)^3$ it follows from using the continuity equation

    $$\frac{\mathrm{d}h}{\mathrm{d}t} = -\frac{1}{3}\frac{h}{\rho}\frac{\mathrm{d}\rho}{\mathrm{d}t} = \frac{1}{3}\,h\,\vec{\nabla}\cdot\vec{v} \tag{1}$$

    alternative methods exist (see e.g. Steinmetz & Müller 1993)

SPH Basics:

- the fluid equations in SPH
  - there is an infinite number of possible SPH implementations of the hydrodynamic equations!
  - some notation: $h_{ij} = (h_i + h_j)/2$, $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$, $\vec{v}_{ij} = \vec{v}_i - \vec{v}_j$, and $\vec{\nabla}_i$ is the gradient with respect to the coordinates of particle i; all measurements are taken at particle positions (e.g. $\rho_i = \rho(\vec{r}_i)$)
  - *general form of SPH equations:*

$$\boxed{\langle f_i \rangle = \sum_{j=1}^{N_i} \frac{m_j}{\rho_j} f_j W(r_{ij}, h_{ij})}$$

  - *density* — continuity equation (conservation of mass)

$$\boxed{\rho_i = \sum_{j=1}^{N_i} m_j W(r_{ij}, h_{ij})}$$

or $$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = \sum_{j=1}^{N_i} m_j \vec{v}_{ij} \cdot \vec{\nabla}_i W(r_{ij}, h_{ij})$$

(the second implementation is almost never used, see however Monaghan 1991 for an application to water waves)

important

density is needed for *ALL* particles *BEFORE* computing other averaged quantities $\longrightarrow$ at each timestep, SPH computations consist of *TWO* loops, first the *density* is obtained for each particle, and then in a second round, all *other* particle properties are updated.

  - *pressure* is defined via the equation of state (for example for isothermal gas $p_i = c_s^2 \rho_i$)

SPH Basics:

- the fluid equations in SPH
  - *velocity* — Navier Stokes equation (conservation of momentum)

$\longrightarrow$ consider for now *only* pressure contributions: Euler's equation

$$\frac{\mathrm{d}\vec{v}}{\mathrm{d}t} = \frac{\partial \vec{v}}{\partial t} + (\vec{v}\cdot\vec{\nabla})\vec{v} = -\frac{1}{\rho}\vec{\nabla}p = -\vec{\nabla}\left(\frac{p}{\rho}\right) - \frac{p}{\rho^2}\vec{\nabla}\rho \qquad (*)$$

here, the identity $\vec{\nabla}(p\rho^{-1}) = \rho^{-1}\vec{\nabla}p - p\rho^{-2}\vec{\nabla}\rho$ is used

$\longrightarrow$ in the SPH formalism this reads as

$$\frac{d\vec{v}_i}{dt} = -\sum_{j=1}^{N_i} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right)\vec{\nabla}_i W(r_{ij}, h_{ij})$$

where the first term in (*) is neglected because it leads to surface terms in the averaging procedure; it is assumed that either the pressure or the kernel becomes zero at the integration border; if this is not the case *correction terms* need to be added above.
the equation is anti-symmetric in i and j and conserves momentum locally and globally.

$\longrightarrow$ if self-gravity is taken into account, the gravitational force needs to be added on the RHS

$$\vec{F}_{\mathrm{G}} = -\vec{\nabla}\phi_i = -G\sum_{j=1}^{N} \frac{m_j}{r_{ij}^2}\frac{r_{ij}}{r_{ij}}$$

note that the sum needs to be taken over *ALL* particles $\longleftarrow$ computationally expensive

SPH Basics:

- the fluid equations in SPH
  - *velocity* — Navier Stokes equation (conservation of momentum)

  $\longrightarrow$ the contribution of viscosity:

  · converts ordered kinetic energy into random kinetic energy (heat)

  · molecular viscosity in most astrophysical problems is small (except maybe in shocks) $\longrightarrow$ SPH normally has NO explicit treatment of physical viscosity.

  · however, artificial viscosity is needed to prevent particle interpenetration.

  · this is achieved by smearing out shocks and by introducing dissipation in regions with strong velocity divergence

  · there are MANY ways to formulate artificial viscosity!!

  $\longrightarrow$ the standard formulation of viscous pressures is

$$p_\alpha = \Pi_\alpha \rho^2 = -\alpha \rho \ell c_s (\vec{\nabla} \cdot \vec{v}) \,,$$

and

$$p_\beta = \Pi_\beta \rho^2 = -\beta \rho \ell^2 (\vec{\nabla} \cdot \vec{v})^2 \,.$$

α and β are free parameters and control the strength of the viscous terms (typical values are $\alpha = 1$ and $\beta = 2$); ℓ is the scale over which shocks are smeared out (typically $\ell \approx 2h$).

  · p_α is a combined *shear* and *bulk* viscosity – it dampens post-shock oscillations

  · p_β is a von Neumann-Richtmyer viscosity – necessary to prevent interpenetration in high Mach number shocks

SPH Basics:

- the fluid equations in SPH
  - *velocity* — Navier Stokes equation (conservation of momentum)

$\longrightarrow$ the SPH implementation of the standard artificial viscosity is

$$\vec{F}_i^{\rm visc} = -\sum_{j=1}^{N_i} m_j \Pi_{ij} \vec{\nabla}_i W(r_{ij}, h_{ij})\,,$$

where the viscosity tensor Π_{ij} is defined by

$$\Pi_{ij} = \begin{cases} (-\alpha c_{ij}\mu_{ij} + \beta\mu_{ij}^2)/\rho_{ij} & \text{for} \quad \vec{v}_{ij}\cdot\vec{r}_{ij} \le 0\,, \\ 0 & \text{for} \quad \vec{v}_{ij}\cdot\vec{r}_{ij} > 0\,, \end{cases}$$

where

$$\mu_{ij} = \frac{h\vec{v}_{ij}\cdot\vec{r}_{ij}}{\vec{r}_{ij}^{\,2} + 0.01h^2}\,.$$

with $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$, $\vec{v}_{ij} = \vec{v}_i - \vec{v}_j$, mean density $\rho_{ij} = (\rho_i + \rho_j)/2$, and mean sound speed $c_{ij} = (c_i + c_j)/2$.

$\longrightarrow$ Advantages of the standard artificial viscosity

- Galilean invariant
- vanishes for rigid body rotation (but not for differential rotation!!!)
- conserved linear and angular momenta

$\longrightarrow$ Disadvantages of the standard formula

- generates entropy in shear flows $\longrightarrow$ Balsara viscosity
- leads to strong dissipation (one simulates 'honey' instead of interstellar gas) $\longrightarrow$ time-dependent viscosity & XSPH
- arbitrariness (no physical motivation) $\longrightarrow$ Flebbe-type viscosities

$\longrightarrow$ many alternative formulations exist

$\longrightarrow$ set together, the momentum equation is

$$\boxed{\frac{d\vec{v}_i}{dt} = -\sum_{j=1}^{N_i} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} + \Pi_{ij}\right)\vec{\nabla}_i W(r_{ij}, h_{ij}) - \nabla\phi_i}$$

SPH Basics:

- the fluid equations in SPH
  - *energy equation* (conservation of momentum)

  $\longrightarrow$ recall the hydrodynamic energy equation:

$$\frac{d\epsilon}{dt} = \frac{\partial \epsilon}{\partial t} + \vec{v} \cdot \vec{\nabla}\epsilon = \frac{ds}{dt} - \frac{p}{\rho}\vec{\nabla} \cdot \vec{v}$$

  $\longrightarrow$ for *adiabatic* systems ($c = \mathrm{const}$) the SPH form follows as

$$\frac{d\epsilon_i}{dt} = \frac{p_i}{\rho_i^2} \sum_{j=1}^{N_i} m_j \, \vec{v}_{ij} \cdot \vec{\nabla}_i W(r_{ij}, h_{ij}) \; ,$$

(note that the alternative form

$$\frac{d\epsilon_i}{dt} = \frac{1}{2} \sum_{j=1}^{N_i} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) \vec{v}_{ij} \cdot \vec{\nabla}_i W(r_{ij}, h_{ij})$$

can lead to unphysical solutions, like negative internal energy)

  $\longrightarrow$ *dissipation* due to (artificial) viscosity leads to a term

$$\frac{d\epsilon_i}{dt} = \frac{1}{2} \sum_{j=1}^{N_i} m_j \Pi_{ij} \, \vec{v}_{ij} \cdot \vec{\nabla}_i W(r_{ij}.h_{ij})$$

  $\longrightarrow$ the presence of *heating* sources or *cooling* processes can be incorporated into a function Γ_i.

  $\longrightarrow$ altogether:

$$\boxed{\frac{d\epsilon_i}{dt} = \frac{p_i}{\rho_i^2} \sum_{j=1}^{N_i} m_j \, \vec{v}_{ij} \cdot \vec{\nabla}_i W_{ij} \; + \; \frac{1}{2} \sum_{j=1}^{N_i} m_j \Pi_{ij} \, \vec{v}_{ij} \cdot \vec{\nabla}_i W_{ij} \; + \; \Gamma_i}$$

SPH Basics:

- the fluid equations in SPH
  - *entropy equation*
    - $\longrightarrow$ alternatively to the energy equation one can integrate an equation for the 'entropy'
    - $\longrightarrow$ the *entropic function* $A(s)$ is defined by

$$p = A(s)\rho^{\gamma} \ .$$

the internal energy follows as

$$\epsilon = \frac{A(s)}{\gamma - 1}\rho^{\gamma-1} \qquad (*)$$

- $\longrightarrow$ the time evolution of $A(s)$ depends on the emissivity per unit volume Γ (heat sources and sinks) and on the viscosity; one possible SPH implementation is

$$\frac{\mathrm{d}A_i}{\mathrm{d}t} = -\frac{\gamma - 1}{\rho_i}\Gamma_i + \frac{1}{2}\frac{\gamma - 1}{\rho_i^{\gamma-1}}\sum_{j=1}^{N_i} m_j \Pi_{ij} \vec{v}_{ij} \cdot \vec{\nabla}_i W(r_{ij}, h_{ij}) \ .$$

- $\longrightarrow$ the time evolution of ϵ_i is then derived from this equation via (*), the temperature T_i of particle i is directly proportional to ϵ_i.

SPH Basics:

- time integration
  - time integration is done similar to N-body methods
  - there are two main schemes: *leap-frog* and *predictor-corrector methods*
  - *variable timesteps*
    - $\longrightarrow$ efficient use of CPU power in strongly inhomogeneous systems
    - $\longrightarrow$ typically, the lengths of timestep bins differ by factor 2
    - $\longrightarrow$ criteria for chosing the timestep
      - *Courant-Friedrichs-Lewy* plus *viscosity* criterion

$$\delta t_{\mathrm{cv}} = \frac{0.3\,h}{c_{\mathrm{s}} + h|\vec{\nabla}\cdot\vec{v}| + 1.2(\alpha c_{\mathrm{s}} + \beta h|\vec{\nabla}\cdot\vec{v}\,|)}\;.$$

      - *force* criterion

$$\delta t_{\mathrm{f}} = 0.3\sqrt{\frac{h}{|\vec{F}\,|}}\;,$$

      - *global error tolerance* criteria are possible in Runge-Kutta schemes

- boundary conditions
  - closed (or periodic) boundaries can be handled by introducing 'ghost' particles
  - open boundaries are difficult, because of large pressure gradients (e.g. water surface on air)

Modifications of SPH:

o

- alternative ways to force anti-symmetry
  - instead of using one kernel and take a mean value for h, average of the kernel contributions of each particle:

    $$W\left(|\vec{r}_i - \vec{r}_j|, \frac{h_i + h_j}{2}\right) \longrightarrow \frac{1}{2}\left\{W(|\vec{r}_i - \vec{r}_j|, h_i) + W(|\vec{r}_i - \vec{r}_j|, h_j)\right\}$$

  - instead of the artithmetic mean for the quantity p/ρ^2 use the geometric one:

    $$\frac{1}{2}\left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right) \quad \longrightarrow \quad \frac{\sqrt{p_i p_j}}{\rho_i \rho_j}$$

- XSPH (Monaghan 1989)
  - in the standard formulation the particle is advanced by integrating

    $$\frac{d\vec{r}_i}{dt} = \vec{v}_i$$

  - it may be more physical (and in the spirit of SPH) when moving the particle with the smoothed flow velocity

    $$\frac{d\vec{r}_i}{dt} = \hat{\vec{v}}_i \quad \text{with} \quad \hat{\vec{v}}_i = \vec{v}_i + \eta \sum_{j=1}^{N_i} \frac{m_j}{\rho_{ij}} (\vec{v}_i - \vec{v}_j) W(|\vec{r}_i - \vec{r}_j|, h_{ij})$$

    where $\eta \approx 0.5$.
  - this allows for a strongly reduced artificial viscosity term $\longrightarrow$ reach higher Reynolds numbers when modeling interstellar turbulence
  - XSPH also allows for the introduction of the *Cassama-Holm subgrid model of turbulence* (Monaghan 2002 – astro-ph/0204118)

Modifications of SPH:

- alternative formulations of viscosity
  - Balsara viscosity:
    - $\longrightarrow$ standard viscosity generates entropy in shear flows (Balsara 1989)
    - $\longrightarrow$ add a correction term $\propto \vec{\nabla} \times \vec{v}$
    - $\longrightarrow$ new viscosity:

$$\Pi_{ij} = \begin{cases} (-\alpha c_{ij}\mu_{ij} + \beta\mu_{ij}^2)/\rho_{ij} & \text{for} \quad \vec{v}_{ij} \cdot \vec{r}_{ij} \leq 0\,, \\ 0 & \text{for} \quad \vec{v}_{ij} \cdot \vec{r}_{ij} > 0\,, \end{cases}$$

where now

$$\mu_{ij} = \frac{h\vec{v}_{ij} \cdot \vec{r}_{ij}}{\vec{r}_{ij}^{\,2} + 0.01h^2} \frac{f_i + f_j}{2}$$

with

$$f_i = \frac{|\vec{\nabla} \cdot \vec{v}|_i}{|\vec{\nabla} \cdot \vec{v}|_i + |\vec{\nabla} \times \vec{v}|_i + 0.0001c_i/h}$$

    - $\longrightarrow$ this representation vanishes in pure shear flows, but is identical to the standard version in purely compressional flows

  - for more physically motivated viscosity see
    - $\longrightarrow$ Flebbe et al., ApJ, 431, 754 (1994)
    - $\longrightarrow$ Watkins et al., ApJS, 119, 177 (1996)
    - $\longrightarrow$ etc

Modifications of SPH:

- alternative formulations of viscosity
  - switch to reduce viscosity (Morris & Monaghan 1997)

    $\longrightarrow$ artificial viscosity is a strongly *undesired quantity*, as it leads to dissipation that is much higher than in astrophysical gases

    $\longrightarrow$ for realistic models one wants as little artificial viscosity as possible (e.g. important for turbulence simulations — we model 'honey' instead of interstellar gas)

    $\longrightarrow$ in priciple, artificial viscosity is only needed in regions of strong compression (shocks)

    $\longrightarrow$ introduce a switch which leads to high Π_{ij} when $\vec{\nabla} \cdot \vec{v}$ becomes strongly negative and then let Π_{ij} 'decay' to zero afterwards

    $\longrightarrow$ implementation:

    · each particle i carries its own value α_i (and β_i, e.g. with $\beta_i = 2\alpha_i$)

    · time evolution

$$\alpha_i = \alpha_{\mathrm{min}} + A \exp(-t/\tau)$$

with decay time $\tau \approx 10h/c_{\mathrm{s}}$.

Modifications of SPH:

- fully conservative formulation using Lagrange multipliers
  - Springel & Hernquist (2002, astro-ph/0111016)
  - Monaghan (2002, astro-ph/0204118)

  ◦ the Lagrangian for compressible flows which are generated by the thermal energy $\epsilon(\rho, s)$ acts as effective potential is

  $$\mathcal{L} = \int \rho \left\{ \frac{1}{2} v^2 - u(\rho, s) \right\} d^3 r.$$

  equations of motion follow with $s = \mathrm{const}$ from

  $$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \vec{v}} - \frac{\partial \mathcal{L}}{\partial \vec{r}} = 0$$

  ◦ after some SPH arithmetics, one can derive the following acceleration equation for particle i

  $$\frac{d\vec{v}_i}{dt} = - \sum_{j=1}^{N_i} m_j \left\{ \frac{1}{f_i} \frac{p_i}{\rho_i^2} \vec{\nabla}_i W(r_{ij}, h_i) + \frac{1}{f_j} \frac{p_j}{\rho_j^2} \vec{\nabla}_i W(r_{ij}, h_j) \right\}$$

  where

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

  ◦ the Lagrange multiplier used here is the constraint that h_i is adjusted such that each smoothing volume contains a fixed amount of mass

  ◦ under this contraint, the formulation conserves energy, entropy, linear and angular momentum ($\vec{\nabla} h$ terms are taken into account implicitely)

Properties of SPH:

- *no clear mathematical convergence study* $\longrightarrow$ reliability of method needs to rely on comparison with analytic solutions and on empirical tests (e.g. comparing results obtained with different particle numbers)
- SPH is more *dissipative* than most grid-based methods
- SPH is *Lagrangian*, it can resolve large density contrasts whereever needed (regions of interest need not to be defined in advance)
- SPH provides *good* resolution in *high-density* regions, however, only *poorly* resolves *low-density* regions
- SPH generally performes poorly when handling shocks (but see GPH)
- SPH is a particle scheme $\longrightarrow$ good for describing the *transition* from gaseous to stellar-dynamical systems (i.e. good for describing the formation of stellar clusters)
- SPH *cannot* (yet) handle *magnetic field* satisfactory (problems with stability and with $\vec{\nabla} \cdot \vec{B} = 0$ requirement)
- SPH can be combined with the special purpose hardware GRAPE