Smoothed Particle Hydrodynamics (SPH)

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Calculating density
SPH density estimator

Weighted summation over nearby particles:

$$\rho(r) = \sum_{b=1}^{N_{\text{neigh}}} m_b W(r - r_b, h)$$

$W$ weight function with dimension of inverse volume. $h$ scale parameter determining fall-off rate of $W$.

Conservation of mass implies $W$ normalisation:

$$\int_{V} W(r' - r_b, h) dV' = 1$$
The smoothing kernel (Weight function)

- Positive weighting, monotonically decreasing with relative distance, smooth derivatives.
- Symmetry with respect to \((r - r')\) i.e., \(W(r' - r, h) \equiv W(|r' - r|, h)\)
- Flat central portion (No strong influence by small change in near neighbour position change)

A natural choice that satisfies all of the properties is the Gaussian:

\[
W(r - r', h) = \frac{\sigma}{h^d} \exp \left[ -\frac{(r-r')^2}{h^2} \right]
\]

\(d\) number of dimensions.
\(\sigma\) normalisation factor.
The smoothing kernel (Weight function)

Problem with Gaussian: Interaction with all particles in the domain necessary, although the contribution of particles quickly becomes negligible with increasing distance.

Better choice: Gaussian shaped kernel, but truncated at some finite distance (a few times the scale length h).

A popular choice is the Schoenberg (1946) B-Spline:

\[ w(q) = \sigma \left\{ \begin{array}{ll}
\frac{1}{4}(2 - q)^3 - (1 - q)^3, & 0 \leq q < 1; \\
\frac{1}{4}(2 - q)^3, & 1 \leq q < 2; \\
0, & q \geq 2,
\end{array} \right. \]

There is a large number of alternative Kernels.
The smoothing length (scale length) $h$

- Specifies the fall-off of the kernel weighting with respect to particle separation.
- The number of neighbours (inside the smoothing kernel) can change without changing $h$ (Higher order B-splines)

To resolve clustered and sparse regions evenly a natural choice is to relate $h$ to the local number density of particles:

$$h(r) \propto n(r)^{-1/d} \quad n(r) = \sum_b W[r - r_b, h(r)].$$

For equal mass particles this is equivalent to making $h$ proportional to density itself. Since in turn density itself is a function of $h$, this leads to the idea of iterative summation to simultaneously obtain density and $h$. This is done for the two equations:

$$\rho(r_a) = \sum_b m_b W(r_a - r_b, h_a) \quad h(r_a) = \eta \left( \frac{m_a}{\rho_a} \right)^{1/d}$$
From density to equations of motion

How to calculate arbitrary quantities $A(\mathbf{r})$ (which could be velocity, energy, etc.) using the density estimate?

First use the identity

$$A(\mathbf{r}) = \int A(\mathbf{r}') \delta(\mathbf{r} - \mathbf{r}') d\mathbf{r}'$$

and approximate using the smoothing kernel instead of the Dirac delta function.

$$A(\mathbf{r}) = \int A(\mathbf{r}') W(\mathbf{r} - \mathbf{r}', h) d\mathbf{r}' + O(h^2)$$

Now discretise onto a finite set of interpolation points.

$$\langle A(\mathbf{r}) \rangle = \int \frac{A(\mathbf{r}')}{\rho(\mathbf{r}')} W(\mathbf{r} - \mathbf{r}', h) \rho(\mathbf{r}') d\mathbf{r}' \approx \sum_{b=1}^{N_{\text{neigh}}} m_b \frac{A_b}{\rho_b} W(\mathbf{r} - \mathbf{r}_b, h)$$
From density to equations of motion

The summation interpolant forms the base of all SPH formalisms. Gradient terms can now be straightforwardly calculated.

\[\mathbf{A}(\mathbf{r}) \approx \sum_b m_b \frac{\mathbf{A}_b}{\rho_b} W(\mathbf{r} - \mathbf{r}_b, h)\]

\[\nabla \cdot \mathbf{A}(\mathbf{r}) \approx \sum_b m_b \frac{\mathbf{A}_b}{\rho_b} \cdot \nabla W(\mathbf{r} - \mathbf{r}_b, h)\]

\[\nabla \times \mathbf{A}(\mathbf{r}) \approx -\sum_b m_b \frac{\mathbf{A}_b}{\rho_b} \times \nabla W(\mathbf{r} - \mathbf{r}_b, h)\]

\[\nabla^j A^i(\mathbf{r}) \approx \sum_b m_b \frac{A^i_b}{\rho_b} \nabla^j W(\mathbf{r} - \mathbf{r}_b, h)\]

In case of a non-constant smoothing length also the derivative of the smoothing length has to be taken into account.
From density to equations of motion
(Example: continuity equation)

Start with the base expression for $\rho$:

$$\rho_a = \sum_b m_b W(r_a - r_b, h_a)$$

Time derivative:

$$\frac{d\rho_a}{dt} = \sum_b m_b (v_a - v_b) \cdot \nabla_a W_{ab}(h).$$

Rewrite:

$$\frac{d\rho_a}{dt} = v_a \cdot \sum_b \frac{m_b}{\rho_b} \rho_b \nabla_a W_{ab} - \sum_b \frac{m_b}{\rho_b} (\rho_b v_b) \cdot \nabla_a W_{ab}$$

Which is an approximate expression for (derivatives from the last slide):

$$\approx v_a \cdot \nabla \rho - \nabla \cdot (\rho v) \approx -\rho_a (\nabla \cdot v)_a$$
Non constant smoothing length

In the case of a non-constant smoothing length, also the derivative of the smoothing length needs to be taken into account.

Using the time derivative of the density again:

$$\frac{d\rho_a}{dt} = \sum_b m_b (v_a - v_b) \cdot \nabla_a W_{ab}(h).$$

Changes to:

$$\frac{d\rho_a}{dt} = \frac{1}{\Omega_a} \sum_b m_b (v_a - v_b) \cdot \nabla_a W_{ab}(h_a)$$

With the correction term $\Omega_a$:

$$\Omega_a \equiv \left[ 1 - \frac{\partial h_a}{\partial \rho_a} \sum_b m_b \frac{\partial W_{ab}(h_a)}{\partial h_a} \right]$$
Generalised first derivate operators

The gradient operators can be generalised using the expressions

\[ \nabla A = \frac{1}{\phi} [\nabla (\phi A) - A \nabla \phi] \approx \sum_b \frac{m_b}{\rho_b} \frac{\phi_b}{\phi_a} (A_b - A_a) \nabla_a W_{ab} \]

and

\[ \nabla A = \phi \left[ \frac{A}{\phi^2} \nabla \phi + \nabla \left( \frac{A}{\phi} \right) \right] \approx \sum_b \frac{m_b}{\rho_b} \left( \frac{\phi_b}{\phi_a} A_a + \frac{\phi_a}{\phi_b} A_b \right) \nabla_a W_{ab} \]

where \( \phi \) is any arbitrary, differentiable scalar quantity defined on the particles.

Various alternative SPH formulations are based on different choices for \( \phi \).

Two examples using the expression for acceleration:

(Hernquist, Katz, 1989) \( \frac{dv}{dt} = - \sum_b m_b \left( 2 \frac{\sqrt{P_a P_b}}{\rho_a \rho_b} \right) \nabla_a W_{ab} \)

(Morris, 1996) \( \frac{dv}{dt} = \sum_b m_b \left( \frac{P_a - P_b}{\rho_a \rho_b} \right) \nabla_a W_{ab} \)
Choice of the derivative

The paradox of SPH is that choosing a less accurate derivate estimator can actually be a good decision. Using the accurate derivate estimator of Morris for a constant density box of particles (randomly distributed, which is a bad choice) the particle-particle force is:

\[-m_a m_b \left( \frac{P_a - P_b}{\rho_a \rho_b} \right) F_{ab}(\hat{r}_a - \hat{r}_b).\]

Here, the force vanishes when the pressure is constant regardless of the particle distribution. Using a less accurate estimate:

\[-m_a m_b \left( \frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} \right) F_{ab}(\hat{r}_a - \hat{r}_b).\]

there will be a net (repulsive) force between the particles until a certain arrangement of particles is reached (locally isotropic and regular).
Alternative derivation of the SPH formalism

Price derives the equations of motion for SPH from first principles using only the Lagrangian $L = T - V$ inserted into the Euler-Lagrange equations:

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \mathbf{v}_a} \right) - \frac{\partial L}{\partial \mathbf{r}_a} = 0$$

From this the whole SPH equations of motion can also be derived. The full equations of motion are (including the treatment of magnetic fields):

$$\frac{d \mathbf{v}_i}{dt} = \sum_b m_b \left[ \frac{S_{ij} a}{\Omega_a \rho_a^2} \nabla_j W_{ab}(h_a) + \frac{S_{ij} b}{\Omega_b \rho_b^2} \nabla_j W_{ab}(h_b) \right]$$

with $S^{ij} \equiv - \left( P + \frac{1}{2 \mu_0} B^2 \right) \delta^{ij} + \frac{1}{\mu_0} B^i B^j$

Induction equation for the evolution of the magnetic field:

$$\frac{d \mathbf{B}_i}{dt} = \frac{1}{\Omega \rho_i} \cdot \left[ \sum_{j=1}^{N} m_j \left[ \boldsymbol{B}_i (\mathbf{v}_{ij} \cdot \nabla_i W_i) - \mathbf{v}_{ij} (\boldsymbol{B}_i \cdot \nabla_i W_i) \right] \right]$$
Higher order derivatives

With some work one can introduce higher order derivatives to calculate quantities such as $\langle \nabla^2 A \rangle$ or $\langle \nabla (\nabla \cdot A) \rangle$

Those higher order derivatives can be used to discretise additional physics (depending on higher order derivatives) like viscosity or thermal conductivity. Taking viscosity as an example, the 'standard' formulation of artificial viscosity is given by:

$$
\left( \frac{dv}{dt} \right)_{\text{diss}} = - \sum_b m_b \frac{-\alpha \bar{c}_{s,ab} \mu_{ab} + \beta \mu_{ab}^2}{\bar{\rho}_{ab}} \hat{r}_{ab} \hat{F}_{ab}
$$

where

$$
\mu_{ab} = \frac{h v_{ab} \cdot \hat{r}_{ab}}{r_{ab} + \epsilon h_{ab}^2}
$$

Barred quantities correspond to an average

$c_s$ is the sound speed

$\alpha$ and $\beta$ are dimensionless parameters ($\alpha = 1$, $\beta = 2$ normally)

$\epsilon \approx 0.01$ is a small parameter to prevent divergences.
Example for particle rearrangement and (artificial) viscosity
Treatment of discontinuities using artificial viscosity and artificial conductivity

\[
\left( \frac{du}{dt} \right)_\text{diss} = - \sum_b \frac{m_b}{\rho_{ab}} \left[ \frac{1}{2} \alpha_{\text{sig}} (v_{ab} \cdot \hat{r}_{ab})^2 + \alpha_u \nu_{\text{sig}} (u_a - u_b) \right] \bar{F}_{ab}
\]
SPH

**Advantage**

- No geometry constraints
- Auto resolution
- Perfect advection
- Energy conservation
- Easy NBody coupling

**Disadvantage**

- Shocks broadened
- Mixing
- Conduction by hand
- Derivative estimator
- Visualisation
SPH Codes

Gadget       Seren
Phantom       VINE
NDSPMHD       GCSPH
SPHNG         SPARTACUS