Smoothed Particle Hydrodynamics

Or how I learnt to stop worrying and love Lagrangians

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SPH starts here...

What is the density?
Not the SPH density estimate

\[ \rho_a = \frac{\sum_b m_b}{V_a} \]
The SPH density estimate

Kernel-weighted sum:

\[ \rho(\mathbf{r}) = \sum_{j=1}^{N} m_j W(|\mathbf{r} - \mathbf{r}_j|, h) \]

\[ W = \frac{\sigma}{h^3} e^{-r^2/h^2} \]
Resolution follows mass

\[
\frac{dx}{dt} = \mathbf{v}
\]
From density to hydrodynamics

\[ L_{\text{sph}} = \sum_j m_j \left[ \frac{1}{2} v_j^2 - u_j(\rho_j, s_j) \right] \quad \text{Lagrangian} \]

\[ \frac{d}{dt} u = \frac{P}{\rho^2} d\rho \quad \text{1st law of thermodynamics} \]

\[ \nabla \rho_i = \sum_j m_j \nabla W_{ij}(h) \quad \text{density sum} \]

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{v}} \right) - \frac{\partial L}{\partial \mathbf{r}} = 0 \quad \text{Euler-Lagrange equations} \]

\[ \frac{dv_i}{dt} = - \sum_j m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_i W_{ij}(h) \quad \text{equations of motion!} \]
What this gives us: Advantages of SPH

- An exact solution to the continuity equation
- Resolution follows mass
- ZERO dissipation
- Advection done perfectly
- EXACT conservation of mass, momentum, angular momentum, energy and entropy
- A guaranteed minimum energy state
Zero dissipation - Example I.

Propagation of a circularly polarised Alfvén wave
Zero dissipation - example II: Advection of a current loop

1000 crossings (Rosswog & Price 2007)

1000 crossings (Rosswog & Price 2007)

First 25 crossings

2 crossings (Gardiner & Stone 2005)

Fig. 3. Gray-scale images of the magnetic pressure $(B_x^2 + B_y^2)$ at $t = 2$ for an advected field loop ($v_0 = \sqrt{3}$) using the $\delta^*_{\parallel}$ (top left), $\delta^*_{\perp}$ (top right) and $\delta^*_{\parallel}$ (bottom) CT algorithm.

Fig. 8. Magnetic field lines at $t = 0$ (left) and $t = 2$ (right) using the CTU + CT integration algorithm.
Zero dissipation...
From density to hydrodynamics

\[ L_{sph} = \sum_j m_j \left[ \frac{1}{2} v_j^2 - u_j(\rho_j, s_j) \right] \]

Lagrangian

1st law of thermodynamics

\[ du = \frac{P}{\rho^2} d\rho \]

Here we assume that density is differentiable and that the entropy does not change

Density sum

\[ \nabla \rho_i = \sum_j m_j \nabla W_{ij}(h) \]

density sum

Euler-Lagrange equations

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{v}} \right) - \frac{\partial L}{\partial r} = 0 \]

Equations of motion!

\[ \frac{d\mathbf{v}_i}{dt} = - \sum_j m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_i W_{ij}(h) \]
Zero dissipation...

...so we have to add some
Must treat EVERY discontinuity

Viscosity + Conductivity
Must treat discontinuities properly...

Agertz et al. 2007, Price 2008 and too many others

This issue has nothing to do with the instability itself
It is related to the treatment of the contact discontinuity
dissipation terms need to be explicitly added
The key is a good switch

Figure 2. As Fig. 1, but for SPH with standard \((\alpha = 1)\) or Morris & Monaghan (1997) artificial viscosity, as well as our new method (only every fifth particle is plotted). Also shown are the undamped wave (solid) and lower-amplitude sinusoids (dashed). Only with our method the wave propagates undamped, very much like SPH without any viscosity, as in Fig. 1.

6 Lee Cullen & Walter Dehnen

Figure 6. Steepening of a 1D sound wave: velocity and viscosity parameter vs. position for standard SPH, the M&M method, our new scheme, and Godunov particle hydrodynamics of first and second order (GPH, Cha & Whitworth 2003), each using 100 particles per wavelength. The solid curve in the top panel is the solution obtained with a high-resolution grid code.

Switch for artificial viscosity: Cullen & Dehnen (2010)
What this gives us: Advantages of SPH

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- EXACT conservation of mass, momentum, angular momentum, energy and entropy
- A guaranteed minimum energy state
Exact conservation: Advantages

Orbits are orbits... even when they’re not aligned with any symmetry axis.

Nixon, King & Price (2012)
Exact conservation: Disadvantages

In grid codes, "screwing it up" => CRASH

In SPH, "screwing it up" => NOISE

What this gives us:
Advantages of SPH

- An exact solution to the continuity equation
- Resolution follows mass
- ZERO dissipation
- Advection done perfectly
- EXACT conservation of mass, momentum, angular momentum, energy and entropy
- A guaranteed minimum energy state
The minimum energy state

The “grid” in SPH...
SPH gradients 101

\[
A_a = \sum_b \frac{m_b}{\rho_b} A_b W_{ab}
\]

\[
\nabla A_a = \sum_b \frac{m_b}{\rho_b} A_b \nabla W_{ab}
\]

BAD

\[
\nabla A_a = \sum_b \frac{m_b}{\rho_b} (A_b - A_a) \nabla W_{ab}
\]

Exact constant

\[
\chi_{\mu\nu} \nabla^\mu A_a = \sum_b m_b (A_b - A_a) \nabla W_{ab}
\]

\[
\chi_{\mu\nu} = \sum_b m_b (x^\mu - x'^\mu) \nabla^\nu W_{ab}
\]

Exact linear

\[
\frac{\nabla A_a}{\rho_a} = - \sum_b m_b \left( \frac{A_a}{\rho_a^2} + \frac{A_b}{\rho_b^2} \right) \nabla W_{ab}
\]

Huh?
What happens to a random particle arrangement?

$\frac{dv_i}{dt} = -\sum_j m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_i W_{ij}$

SPH particles know how to stay regular
Why better gradients are a bad idea

Abel 2010, Price 2012

\[
\frac{d\mathbf{v}_i}{dt} = \sum_j m_j \left( \frac{P_i - P_j}{\rho_j^2} \right) \nabla_i W_{ij}
\]

Improving the gradient operator leads to WORSE results

Corollary: Better to use a worse but conservative gradient operator
Corollary: Need positive pressures

\[ S_{ij} = \left( P + \frac{B^2}{2\mu_0} \right) \delta_{ij} - \frac{B_i B_j}{\mu_0} \]

This is known as the tensile instability in SPH: occurs when net stress is negative.
Smoothed Particle Magnetohydrodynamics

\[ L_{sph} = \sum_b m_b \left[ \frac{1}{2} u_b^2 - u_b(\rho_b, \sigma_b) - \frac{1}{2\mu_0} \frac{B_b^2}{\rho_b} \right] \]

\[ \int \delta L dt = 0 \]

\[ \delta \rho_b = \sum c m_c (\delta r_b - \delta r_c) \cdot \nabla_b W_{bc}, \]

\[ \delta \left( \frac{B_b}{\rho_b} \right) = -\sum c m_c (\delta r_b - \delta r_c) \frac{B_b}{\rho_b^2} \cdot \nabla_b W_{bc} \]

\[ \frac{dv^i_a}{dt} = -\sum_b m_b \left[ \left( \frac{S^{ij}}{\rho^2} \right)_a + \left( \frac{S^{ij}}{\rho^2} \right)_b \right] \nabla^j_a W_{ab}, \]

\[ S_{ij} = \left( P + \frac{B^2}{2\mu_0} \right) \delta_{ij} - \frac{B_i B_j}{\mu_0} \]
Compromise approach gives stability

Subtract $-\mathbf{B}(\nabla \cdot \mathbf{B})$ from MHD force:

Stable but nonconservative

Børve, Omang & Trulsen (2001)
2D shock tube

- intrinsic “remeshing” of particles
Why you cannot use “more neighbours”: The pairing instability

\[ \text{STOP} \]

Pairing occurs for > 65 neighbours for the cubic spline in 3D
2D shock tube: M6 quintic

- Use smoother M6 quintic kernel - truncated at 3h instead of 2h (NOT the same as “more neighbours” with the cubic spline)

- Resolution length given by different kernels scales with standard deviation of the kernel (Dehnen & Aly 2012, Leroy & Violeau 2013)
Pairing + Wendland kernels

Dehnen & Aly (2012)

- pairing depends on Fourier transform of the kernel
- Wendland Kernels: Fourier transform positive definite, hence no pairing, but are always biased
- B-splines: Fourier transform changes sign, pairing occurs at large neighbour number, but errors much smaller than Wendland for same number of neighbours
How to stop worrying and love Lagrangians
From density to hydrodynamics

\[ L_{sph} = \sum_j m_j \left[ \frac{1}{2} v_j^2 - u_j(\rho_j, s_j) \right] \]

1st law of thermodynamics

\[ du = \frac{P}{\rho^2} d\rho + \sum_j m_j \nabla W_{ij}(h) \]

\[ \nabla \rho_i = \sum_j m_j \nabla W_{ij}(h) \]

Euler-Lagrange equations of motion

\[ \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{v}} \right) - \frac{\partial L}{\partial v} = 0 \]

\[ \frac{d\mathbf{v}_i}{dt} = - \sum_j m_j \left( \frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} \right) \nabla_i W_{ij}(h) \]

\[ \left( \frac{d\mathbf{v}}{dt} = - \frac{\nabla P}{\rho} \right) \]
Example I: Variable h


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

\[ h_a = \eta \left( \frac{m_a}{\rho_a} \right)^{1/n_{\text{dim}}} \]

\[ \frac{d\mathbf{v}_a}{dt} = -\sum_b m_b \left[ \frac{P_a}{\Omega_a \rho_a^2} \nabla_a W_{ab}(h_a) + \frac{P_b}{\Omega_b \rho_b^2} \nabla_a W_{ab}(h_b) \right] \]

\[ \Omega_a = \left[ 1 - \frac{dh_a}{d\rho_a} \sum_c m_c \frac{\partial W_{ab}(h_a)}{\partial h_a} \right] \]

- nonlinear equation for h, rho
- requires iterative solution
- can solve to arbitrary precision
Example II: Hyperbolic divergence cleaning


\[
\left( \frac{d\mathbf{B}}{dt} \right)_{\text{clean}} = -\nabla \psi
\]

\[
\frac{d\psi}{dt} = -c^2(\nabla \cdot \mathbf{B}) - \frac{\psi}{\tau}
\]

these combine to give diffusive wave equation
for propagation of divergence errors:
Divergence cleaning (not from Lagrangian)

5.3. Static cleaning test: free boundaries

A further variant of the divergence advection test we consider replaces the periodic boundaries by a free boundary, since many applications of SPMHD involve free boundaries (e.g. the merger of two neutron stars\cite{36}, or studies of galaxy interactions\cite{15,16}).

5.3.1. Setup

The setup is identical to the divergence advection problem (Section 5.1) with \( r_0 = \frac{1}{\sqrt{8}} \), except that the domain is a circular area of fluid with \( q = 1 \) for \( r \leq 1 \) and \( q = 0 \) (no particles) for \( r > 1 \), set up using a total of 1976 particles placed on a cubic lattice. The divergence perturbation is introduced at the centre of the circle, and the velocity field is set to zero. Rather than impose an external confining potential, we solve only Eqs. (16) and (17) without the full MHD equations, as in Section 5.2.

5.3.2. Results

Fig. 6 shows the results of purely hyperbolic cleaning (\( r = 0 \)) for this case. As in Fig. 4, the top row shows the unconstrained and non-conservative difference/difference formulation, while the bottom row shows results using the conservative difference/symmetric combination. Similar results are also found in this case, with divergence errors piling up at the free boundary in the non-conservative formulation leading to numerical instability, but our constrained formulation remaining stable.

5.4. 2D Blast wave in a magnetised medium

We now turn to tests that are more representative of the dynamics encountered in typical astrophysical simulations, beginning with a blast wave expanding in a magnetised medium. In this case the initial magnetic field is divergence-free, meaning that the only divergence errors are those created by numerical errors during the course of a simulation – rather than the artificial errors we have induced in the previous tests. Based on the results from the previous tests, in this and subsequent tests we apply cleaning only using constrained, energy-conserving formulations – that is, with conjugate operators for \( r/C_1 \) and \( r/w \). We use this problem to examine the effectiveness of the divergence cleaning in the presence of strong shocks, as well as to investigate whether cleaning should be performed using the difference or symmetric \( r/C_1 \) operator. As with the divergence advection test, a key goal is to find optimal values for the damping parameter \( r \).

5.4.1. Setup

The implementation of the blast wave follows that of Londrillo and Del Zanna\cite{18}. The domain is a unit square with periodic boundaries, set up with 512\( \times \)590 particles on a hexagonal lattice with \( q = 1 \). The fluid is at rest with magnetic field \( B_x = 10 \). The pressure of the fluid is set to \( P = 1 \), with \( c = 1.4 \), except a region in the centre of radius \( 0.125 \) has its pressure increased by a factor of 100 by increasing its thermal energy. An adiabatic equation of state is used.
Example II: Divergence cleaning


\[ L_{sph} = \sum_b m_b \left[ \frac{1}{2} v_b^2 - u_b(\rho_b, s_b) - \frac{1}{2\mu_0} \frac{B_b^2}{\rho_b} - \frac{\psi_b^2}{2\mu_0\rho_b c_b^2} \right] \]

\[ \int \delta L dt = 0 \]

\[ \left( \frac{dB}{dt} \right)_{\text{clean}} = -\rho_a \sum_b m_b \left[ \frac{\psi_a}{\rho_a^2 \Omega_a} \nabla_a W_{ab}(h_a) + \frac{\psi_b}{\rho_b^2 \Omega_b} \nabla_a W_{ab}(h_b) \right] \]

\[ \frac{d\psi_a}{dt} = -\frac{c_a^2}{\Omega_a \rho_a} \sum_b m_b (B_b - B_a) \cdot \nabla_a W_{ab}(h_a) - \frac{\psi_a}{\tau_a} \]
Magnetic jets from young stars
Tricco & Price 2012, Price, Tricco & Bate 2012

this explodes without divergence cleaning!
Lagrangian approach gives a powerful way of both deriving and understanding SPH formulations.

Both advantages and disadvantages of SPH can be understood in this context.
Advantages:
- Resolution follows mass
- Zero dissipation until explicitly added
- Exact and simultaneous conservation of all physical quantities is possible
- Intrinsic remeshing procedure
- Does not crash

Disadvantages:
- Resolution follows mass
- Dissipation terms must be explicitly added to treat discontinuities
- Exact conservation means linear errors are worse
- Need to be careful with effects from particle remeshing
- Does not crash