UNIVERSITY OF TWENTE.

An Introduction to Smoothed Particle Hydrodynamics

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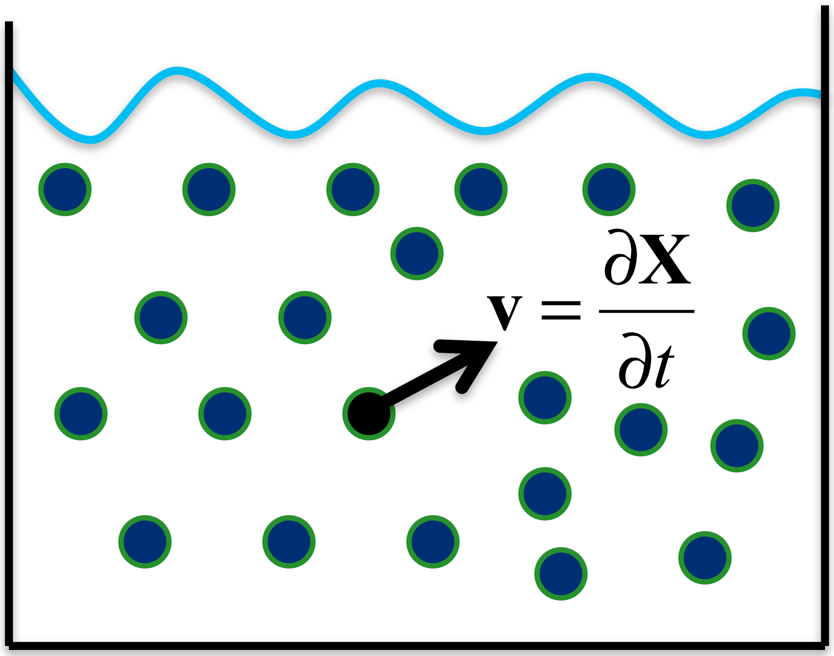
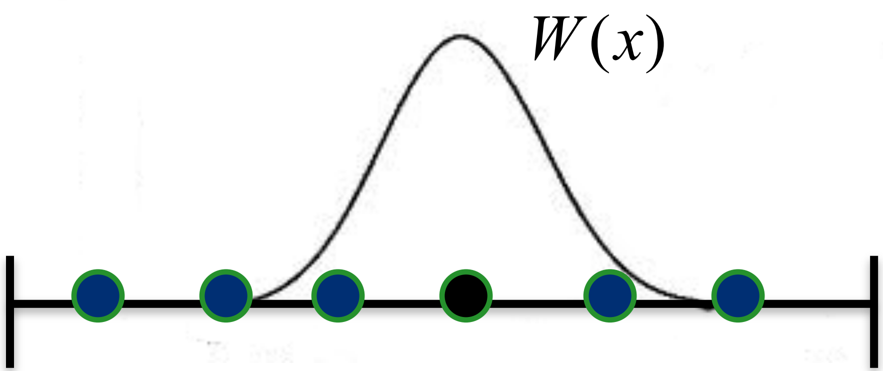
Outline

1. Introduction to SPH
   - Kernel Interpolation
   - First and second derivatives
   - Derivation of main SPH equations

Smoothed Particle Hydrodynamics

- Smoothed Particle Hydrodynamics is a Lagrangian scheme
- The fluid is discretised into particles that move with the fluid velocity





- Fluid variables are interpolated between particles using kernel interpolation.

Introduction

- Grew out of the astrophysics community in the late seventies
  - Gingold, R. A. & Monaghan, J. J. (1977), 'Smoothed particle hydrodynamic: theory and application to non-spherical stars', *Monthly Notices of the Royal Astronomical Society* **181,** 375–389.
  - Lucy, L. B. (1977), 'A numerical approach to testing the fission hypothesis', *The Astronomical Journal* **82**(12), 1013–1924**.**

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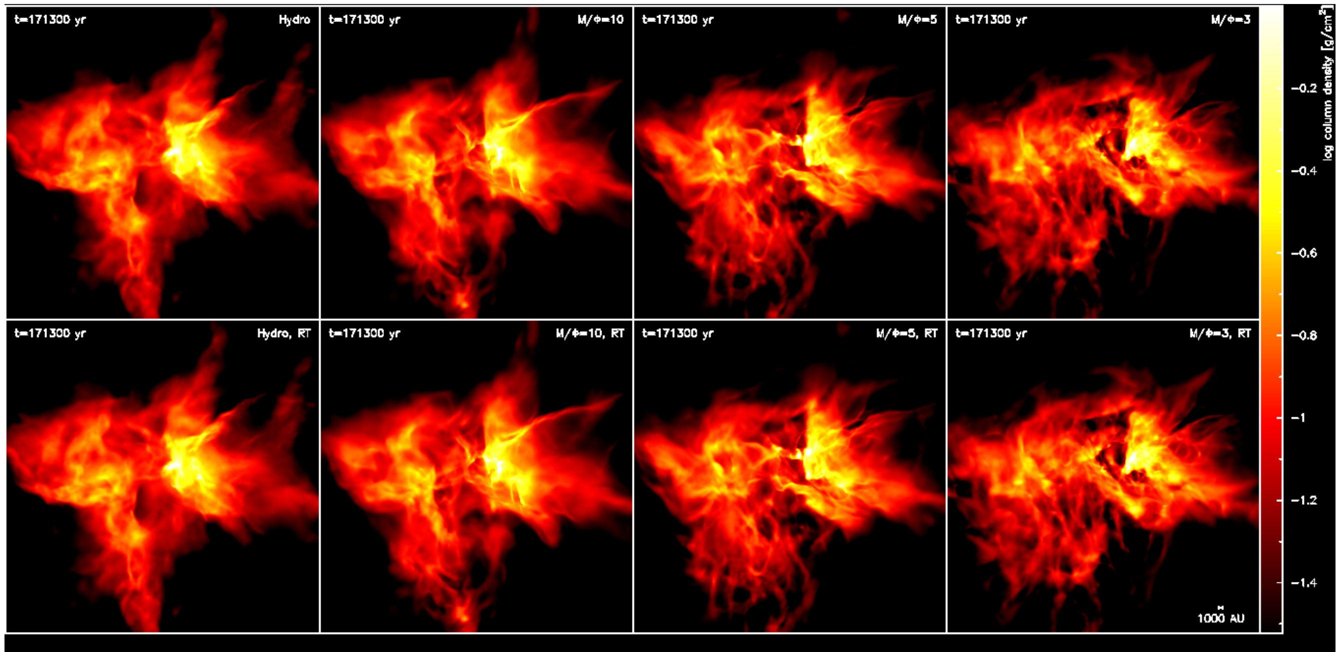
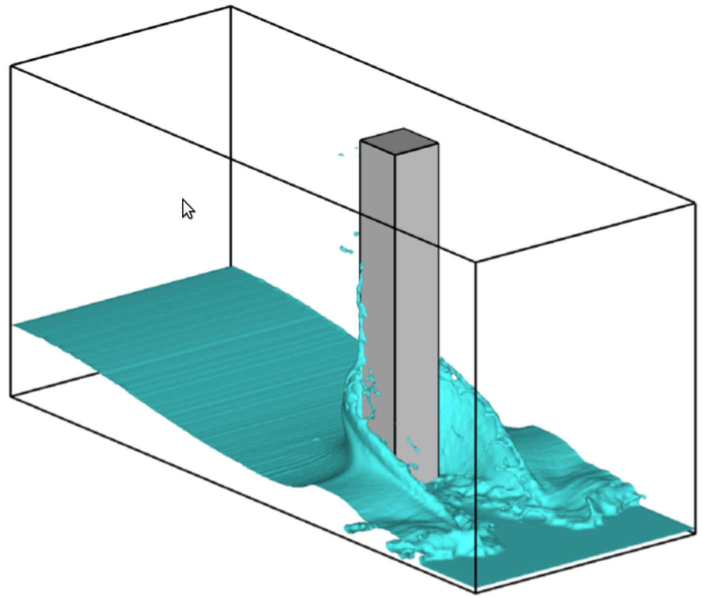


Introduction

Some advantages:

- Lack of mesh simplifies problems involving complex, moving and deforming geometries (e.g. Solid fracture), free surfaces and multi-phase / interfaces.
- Advection is obtained from the movement of the particles and the time history of fluid particles is easy to obtain (e.g. Mixing visualisation/measurement).
- Strong conservation properties for energy, linear and angular momentum.
- No computational effort

  … if there is no mass.



Marrone S., Colagrossi A., Le Touz´ D., Graziani G. (2009) A fast algorithm for free-surface particles detection in 2D and 3D SPH methods, *Proc. Of 4th SPHERIC Workshop*, 61-68.

GPU-SPHysics
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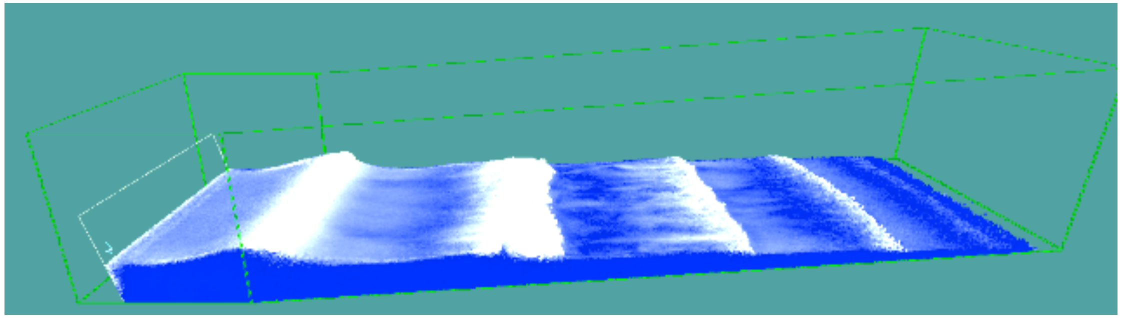
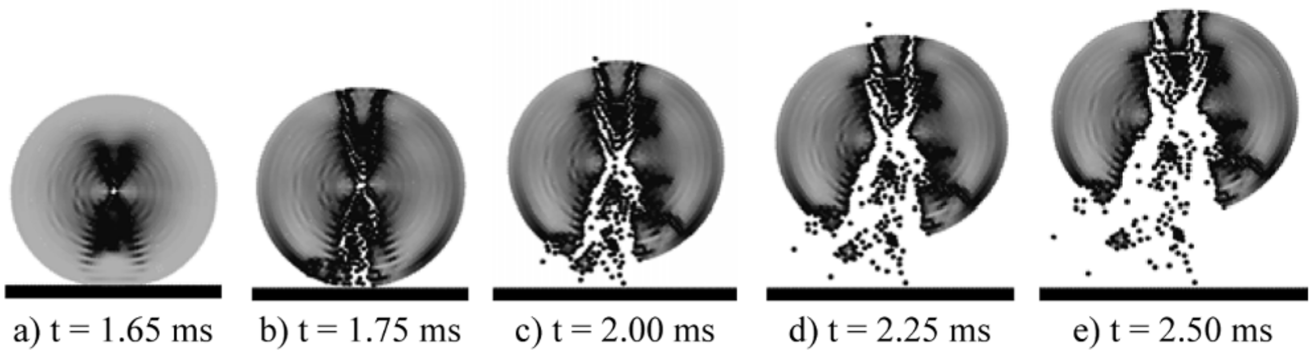


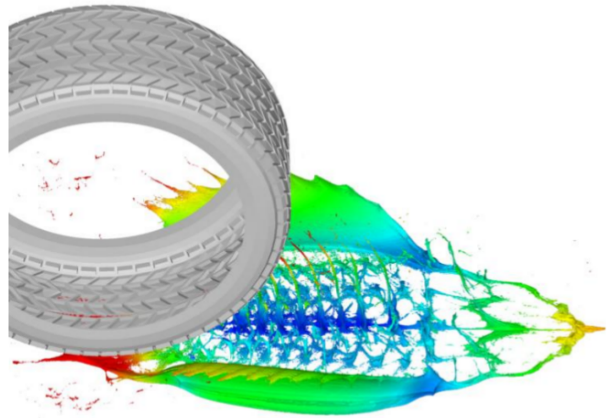
Introduction

Common Application Areas:

- Astrophysics (e.g. Binary star systems, shocks, impact of planetesimals)
- Marine or coastal hydrodynamics (e.g. Breaking waves, sloshing in gas tankers, gravity currents)
- Fluid Structure Interaction
- Industrial flows (e.g. die casting, resin transfer moulding, sag mills)
- Deformation or fracture of brittle or elastic solids



Reddy, B. D., Cleary, P., Das, R. (2008) The Potential for SPH Modelling of Solid Deformation and Fracture, *IUTAM Symposium on Theoretical, Computational and Modelling Aspects of Inelastic Media,* 287-296



Oger G., Leroy C., Jacquin E., Le Touzé D., Alessandrini B (2009) Specific pre/post treatments for 3-D SPH applications through massive HPC simulations, *Proc. Of 4th SPHERIC Workshop*, 52-60.

SPH Basics – Kernel Interpolation

- Smoothed Particle Hydrodynamics is a Lagrangian scheme, whereby the fluid is discretised into particles that move with the fluid velocity
- Navier-Stokes equations are discretised using kernel interpolation between particles.

$$A_I(x) = \int A(x')W(x - x', h)\,dx'$$

Integral Interpolant

$$A_S(x) = \sum_b A_b W(x - x_b, h)\frac{m_b}{\rho_b}$$

Summation Interpolant

$$A_a = \sum_b A_b W(x_a - x_b, h)\frac{m_b}{\rho_b}$$

Calculated on particle *a*

SPH Basics – Kernel Interpolation

- SPH Kernels are Gaussian-like with a compact support
- Cubic Spline kernel commonly used:

$$W(q) = \frac{\beta}{h^d} \begin{cases} 4 - 6q^2 + 3q^3 & \text{for } 0 \le q < 1 \\ (2-q)^3 & \text{for } 1 \le q < 2 \\ 0 & \text{for } q > 2 \end{cases}$$

$$\text{where } q = |r/h|$$

$$\int W(r - r', h)\,dr' = 1$$

therefore β= 1/6, 15/(14π) and 1/(4π) for one, two and three dimensions, respectively

SPH Basics – Kernel Interpolation

- SPH kernels are normally made symmetric
- This ensures symmetric force contributions between particles and conservation of linear and angular momentum

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

$$W_{ab} = W\left(x_a - x_b, 0.5(h_a + h_b)\right)$$

or

$$W_{ab} = 0.5\left(W(x_a - x_b, h_a) + W(x_a - x_b, h_b)\right)$$

Example – interpolate density

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

$$\rho_a = \sum_b m_b \frac{\rho_b}{\rho_b} W_{ab}$$

Let A = ρ

$$= \sum_b m_b W_{ab}$$

Example – interpolate density

$$\rho_a = \sum_b m_b W_{ab}$$

- Physical interpretation:
  SPH particles represent a constant mass of fluid
- Density field is particle mass smoothed according to the kernel
- Particle smoothing length can vary according to density:

$$h_a = \sigma \left(\frac{m_a}{\rho_a} \right)^{1/d}$$

Ideally, iterate the calculations of *h* and *σ* each timestep, until they converge

Example – interpolate velocity (simple minded)

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

$$\mathbf{v}_a = \sum_b m_b \frac{\mathbf{v}_b}{\rho_b} W_{ab}$$

Let A = **v**

Example – interpolate velocity (optimized version)

$$\mathbf{v}_a = \frac{1}{\rho_a}(\mathbf{v}\rho)_a$$

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

$$= \frac{1}{\rho_a}\sum_b m_b \frac{\mathbf{v}_b \rho_b}{\rho_b} W_{ab}$$

$$= \frac{1}{\rho_a}\sum_b m_b \mathbf{v}_b W_{ab}$$

Shepard Correction

- Use Shepard correction to make interpolation more accurate near boundaries/free surface:

$$A_s(x) = \frac{1}{\sum_b \frac{m_b}{\rho_b} W_{ab}} \sum_b m_b \frac{A_b}{\rho_b} W_{ab}$$

- Correction denominator is ~1 for kernel summations with full support, but <1 near a free surface or some boundaries

Interpolation of Derivatives

- First approach:

$$\nabla A_a = \sum_b \frac{m_b}{\rho_b} A_b \nabla_a W_{ab}$$

- But, does not vanish when A(x) is constant! Instead use:

$$\nabla A = \frac{1}{\Phi}\left(\nabla(\Phi A) - A\nabla\Phi\right)$$

$$\nabla A_a = \frac{1}{\Phi_a}\sum_b m_b \frac{\Phi_b}{\rho_b}(A_b - A_a)\nabla W_{ab}$$

$$\nabla \cdot \mathbf{a}_a = \frac{1}{\Phi_a}\sum_b m_b \frac{\Phi_b}{\rho_b}(\mathbf{a}_b - \mathbf{a}_a)\cdot\nabla W_{ab}$$

Φ is any continuous field

Interpolation of Derivatives

- For a radially symmetric kernel:

$$\nabla_a W_{ab} = \frac{r_{ab}}{|r_{ab}|}\frac{\partial W}{\partial r}$$

$$= \frac{r_{ab}}{|r_{ab}|}\frac{1}{h}\frac{\partial W}{\partial q}$$

Example – Continuity Equation

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v}$$

- Use SPH derivatives to evaluate divergence of velocity

$$\nabla \cdot \mathbf{a}_a = \frac{1}{\Phi_a} \sum_b m_b \frac{\Phi_b}{\rho_b} (\mathbf{a}_b - \mathbf{a}_a) \cdot \nabla W_{ab}$$

Let a = **v**
Let Φ = ρ

$$\frac{d\rho_a}{dt} = \rho_a \left[\frac{1}{\rho_a} \sum_b m_b \frac{\rho_b}{\rho_b} (\mathbf{v}_a - \mathbf{v}_b) \cdot \nabla W_{ab} \right]$$

$$= \sum_b m_b \mathbf{v}_{ab} \cdot \nabla W_{ab}$$

Example – Internal Energy

- From first law of thermodynamics:

Heat added = 0

u is internal energy per unit mass

$dV=(m/\rho^2)d\rho$

$$Tds = dU - PdV$$

$$0 = du - \frac{P}{\rho^2} d\rho$$

$$\frac{du}{dt} = \frac{P}{\rho^2} \frac{d\rho}{dt}$$

$$\frac{du_a}{dt} = \frac{P_a}{\rho_a^2} \sum_b m_b \mathbf{v}_{ab} \cdot \nabla W_{ab}$$

Example – The Pressure Gradient

- Momentum equation from Euler equations:

$$\frac{Dv}{Dt} = -\frac{1}{\rho}\nabla P$$

$$\nabla A = \frac{1}{\Phi}\left(\nabla(\Phi A) - A\nabla\Phi\right)$$

Let A = P
Let Φ = 1/ρ

$$\frac{1}{\rho}\nabla P = \frac{1}{\rho}\rho\left(\nabla(P/\rho) - P\nabla(1/\rho)\right)$$

$$= \nabla\left(P/\rho\right) - \frac{P}{\rho^2}\nabla\rho$$

Example – The Pressure Gradient

- SPH Momentum equation becomes…

$$\frac{D\mathbf{v}}{Dt} = -\frac{1}{\rho}\nabla P = -\nabla(P/\rho) + \frac{P}{\rho^2}\nabla\rho$$

Convert to SPH derivatives

$$\frac{d\mathbf{v}_a}{dt} = -\sum_b \frac{m_b}{\rho_b}\left(\frac{P_b}{\rho_b}\right)\nabla_a W_{ab} + \frac{P_a}{\rho_a^2}\sum_b \frac{m_b}{\rho_b}(\rho_b)\nabla_a W_{ab}$$

$$= -\sum_b m_b\left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2}\right)\nabla_a W_{ab}$$

Artificial Viscosity

- Artificial viscosity originally developed to stabilise shocks and prevent the build-up of acoustic energy due to integration errors.

$$\frac{d\mathbf{v}_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} + \Pi_{ab} \right) \nabla_a W_{ab}$$

- Modern SPH viscosity terms approximate the viscous term in the Navier-Stokes equations

Artificial Viscosity – some examples

$$\Pi_{ab} = -\frac{\alpha \bar{h}_{ab} \bar{c}_{ab}}{\bar{\rho}_{ab}} \left(\frac{v_{ab} \cdot \mathbf{r}_{ab}}{r_{ab}^2 + \varepsilon \bar{h}_{ab}^2} \right)$$

Monaghan and Gingold (1983)

$$\Pi_{ab} = -\frac{16 \mu_a \mu_b}{\rho_a \rho_b (\mu_a + \mu_b)} \left(\frac{v_{ab} \cdot \mathbf{r}_{ab}}{r_{ab}^2 + \varepsilon \bar{h}_{ab}^2} \right)$$

Cleary (1998)

- Conserve linear and angular momentum.
- But derivation is rather ad-hoc….

Second Derivatives in SPH

- Better approach:
  construct a second derivative in SPH to approximate
  $$\mu \nabla^2 \mathbf{v}$$
- Could try:
  $$\left(\frac{d^2 v}{dx^2} \right) = \sum_b m_b v_b \frac{d^2 W_{ab}}{dx_a^2}$$
- But:
  - Sensitive to particle disorder
  - Sign of this expression can change with particle separation due to second derivative of the kernel.

Second Derivatives in SPH

- More stable and accurate -> start with an integral approximation (Cleary and Monaghan 1999, heat conduction)

$$\nabla \cdot \kappa \nabla T + O(h^2) = \int \big(\kappa(r) + \kappa(r')\big)\big(T(r) - T(r')\big) \frac{1}{|r - r'|} \nabla W(|r - r'|) dr'$$

$$= \sum_b \frac{m_b}{\rho_b} \left(\kappa_a + \kappa_b\right)\left(T_a - T_b\right) \frac{1}{r_{ab}} \frac{\partial W_{ab}}{\partial r_a}$$

- (Morris 1997) applied this to the viscosity term

$$(\nabla \cdot \mu \nabla)\mathbf{v} = \sum_b \frac{m_b}{\rho_b} \left(\mu_a + \mu_b\right)\left(\mathbf{v}_a - \mathbf{v}_b\right) \frac{1}{r_{ab}} \frac{\partial W_{ab}}{\partial r_a}$$

Note: Does **not** conserve angular momentum

Summary

- Navier Stokes Equations for a Newtonian fluid:

$$\rho \frac{D\mathbf{v}}{Dt} = -\nabla P + \mu \nabla^2 \mathbf{v}$$

$$\frac{D\rho}{Dt} = -\rho \nabla \cdot \mathbf{v}$$

- Calculate SPH derivatives using kernel interpolation:

$$\frac{d\mathbf{v}_a}{dt} = -\sum_b m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} + \Pi_{ab} \right) \nabla_a W_{ab}$$

$$\frac{d\rho_a}{dt} = \sum_b m_b \mathbf{v}_{ab} \cdot \nabla W_{ab}$$

$$\rho_a = \sum_b m_b W_{ab}$$

- Use integral approximation for the second derivative to find the viscous term:

$$\frac{1}{\rho} \mu \nabla^2 \mathbf{v} = \sum_b \frac{m_b}{\rho_a \rho_b} (\mu_a + \mu_b)(\mathbf{v}_a - \mathbf{v}_b) \frac{1}{r_{ab}} \frac{\partial W_{ab}}{\partial r_a}$$

Example SPH algorithm

- Let’s use velocity Verlet integration…..
- For each timestep:

$$r^{1/2} = r^0 + \frac{\Delta t}{2} v^0,$$

$$v^1 = v^0 + \Delta t \frac{dv}{dt}(r^{1/2}),$$

$$r^1 = r^{1/2} + \frac{\Delta t}{2} v^1$$

Example SPH algorithm

- Need to update density and *h* field each time-step.
  Here we use the summation form of the density equation.
- For each timestep:

$$r^{1/2} = r^0 + \frac{\Delta t}{2} v^0,$$

$$h^{1/2} = F_1(\rho^0) = \sigma\left(m / \rho\right)^{1/d}$$

$$\rho^{1/2} = F_2(r^{1/2}, h^{1/2}) = \sum_b m_b W_{ab}$$

$$v^1 = v^0 + \Delta t \frac{dv}{dt}(r^{1/2}, \rho^{1/2}, h^{1/2}),$$

$$r^1 = r^{1/2} + \frac{\Delta t}{2} v^1$$

Example SPH algorithm

- Also need an (EOS) Equation Of State….
- For each timestep:

$$r^{1/2} = r^0 + \frac{\Delta t}{2} v^0,$$

$$h^{1/2} = F_1(\rho^0) = \sigma\left(m / \rho\right)^{1/d},$$

$$\rho^{1/2} = F_2(r^{1/2}, h^{1/2}) = \sum_b m_b W_{ab},$$

$$P^{1/2} = F_3(\rho^{1/2}),$$

$$v^1 = v^0 + \Delta t \frac{dv}{dt}(r^{1/2}, P^{1/2}, \rho^{1/2}, h^{1/2}),$$

$$r^1 = r^{1/2} + \frac{\Delta t}{2} v^1$$

Example SPH algorithm

- Finally add viscosity….
- For each timestep:

$$r^{1/2} = r^{0} + \frac{\Delta t}{2} v^{0},$$

$$v^{1/2} = v^{0} + \frac{\Delta t}{2} \frac{dv}{dt} (r^{-1/2}, P^{-1/2}, \rho^{-1/2}, h^{-1/2}, v^{-1/2}),$$

$$h^{1/2} = F_1(\rho^{0}) = \sigma\left(m / \rho\right)^{1/d},$$

$$\rho^{1/2} = F_2(r^{1/2}, h^{1/2}) = \sum_b m_b W_{ab},$$

$$P^{1/2} = F_3(\rho^{1/2}),$$

$$v^{1} = v^{0} + \Delta t \frac{dv}{dt} (r^{1/2}, P^{1/2}, \rho^{1/2}, h^{1/2}, v^{1/2}),$$

$$r^{1} = r^{1/2} + \frac{\Delta t}{2} v^{1}$$

Time step conditions

- Time step calculated on a Courant–Friedrichs–Lewy (CFL) condition:

$$\Delta t << \frac{h_a}{v_{sig}}$$

$$v_{sig} = \frac{1}{2}(c_a + c_b - 2v_{ab} \cdot \hat{\mathbf{r}}_{ab})$$

- V_{sig} is a signal velocity equal to the speed of information exchange between particles

Time step conditions

- Viscous timescale

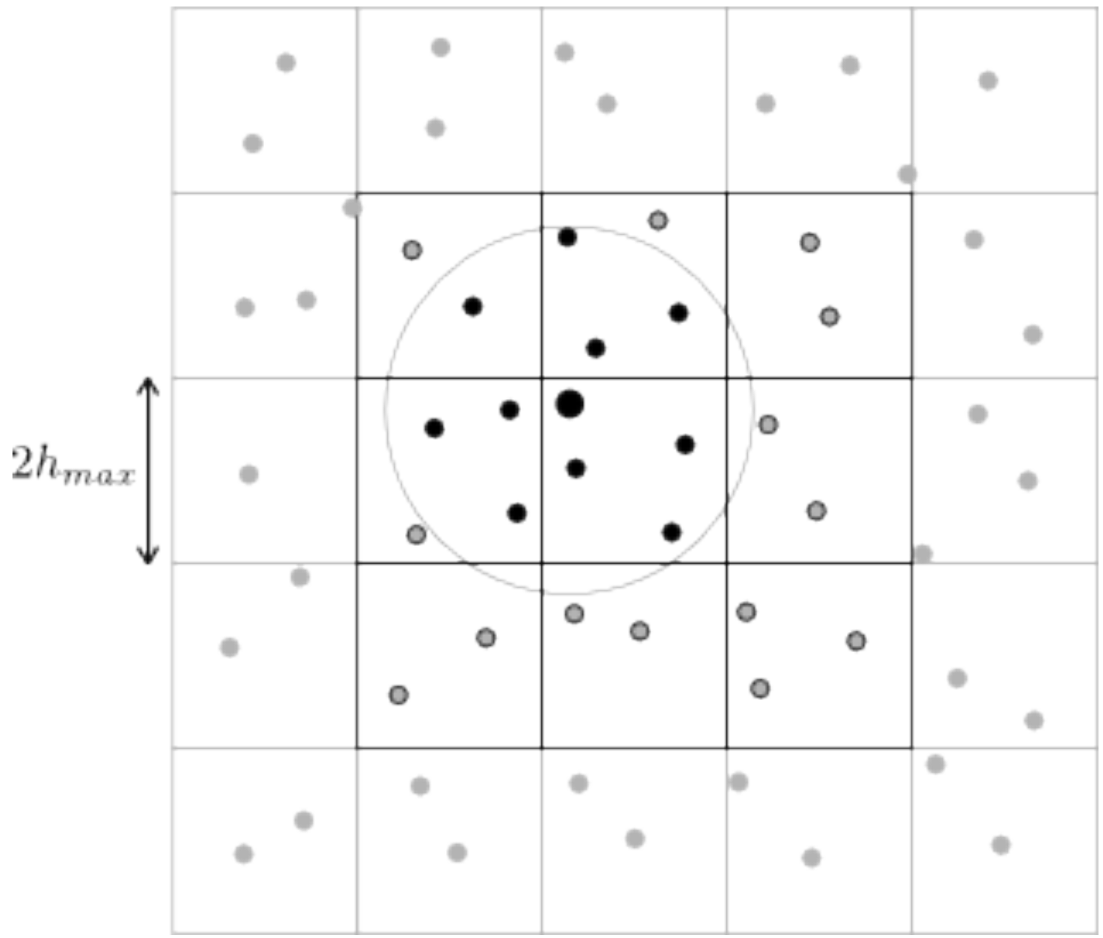
$$\Delta t << \frac{h_a^2}{\nu}$$

- Acceleration timescale

$$\Delta t << \sqrt{\frac{h_a}{dv_a / dt}}$$

Finding Neighbours – Linked Cells (like for MD)

1. Domain divided into "bins" of side length $2h_{max}$
2. Particles placed in bins
3. Each particle's neighbours can be found in its own bin and neighbouring bins
4. Search these bins, keeping particles within 2h.



The End

- Exercise SPH: 1D Sod Shock using SPH….