Smoothed Particle Hydrodynamics (SPH) numerical methods

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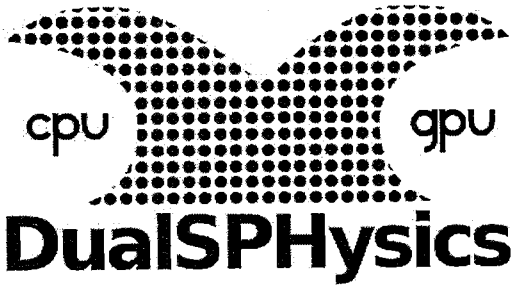


Renato Vacondio

Objectives

Outcomes of the course

- By the end of this course, you will have been **introduced** to the **basics of SPH**. The main objective is that you will be able to understand any basic SPH material completely and be given enough to understand new material that is continually appearing on SPH. We will cover the following elements in this course:

- The basic theoretical foundation of SPH
- How to derive the basic formulation
- Understand the basic building blocks of DualSPHysics

Outline of course

Day 1 – Tuesday 19/02/2019

- Fundamentals of meshless spatial interpolations (SPH, Moving Least Square, Radial Basis Functions) and consistency of SPH interpolation
- SPH discretization of continuity and Euler equations for compressible fluids

Day 2 – Wednesday 20/02/2019

- second-order SPH operators, time integration schemes, boundary conditions
- SPH through Lagrangian, introduction to data structures for SPH numerical schemes

Day 3 – Thursday 21/02/2019

- High Performance Computing applied to Smoothed particle Hydrodynamics
- Latest achievements and Current Challenges
- Practical training for DualSPHysics – exercises in the computer lab

Textbooks

Most of the literature on SPH is contained in research papers, but there are a few books:

- G R Liu: **Mesh Free Methods - Moving Beyond the finite element method**, 712 pages, CRC Press, 2002, ISBN: 0849312388.
- G R Liu & M B Liu: **Smoothed Particle Hydrodynamics: A Meshfree Particle Method**, 472 pages, World Scientific, 2003, ISBN: 981-238-456-1.
- Li, Shaofan, Liu, Wing K: **Meshfree Particle Methods**, 502 pages, Springer, 2004, ISBN: 3-540-22256-1.

- **D VIOLEAU**: **Fluid Mechanics and the SPH Method**, Oxford University Press, 2012.

- In my opinion, all are decent, but the last is the best. Liu & Liu's has a code in the back.
- See http://www.readinglists.manchester.ac.uk/index.html , search for MACE61070

Mesh-based methods 1

- Mesh-based methods:

  Finite-difference method (FDM)
  Finite-element method (FEM)
  Finite-volume method (FVM)

- Mesh-based methods that you use are very mature, both mathematically and algorithmically

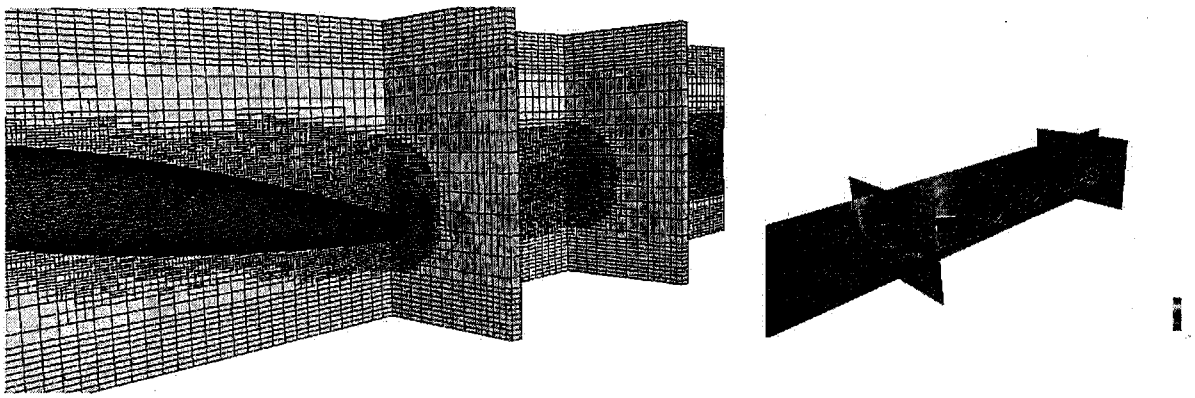
- Mesh-based methods have dominated the field of Computational Fluid Dynamics (CFD)

  … because they are **robust**, **well-developed**, have been applied to many applications where these methods produce a very accurate answer

Mesh-based methods 2

- What are the drawbacks of mesh-based methods?

- **Mesh generation** is a **very expensive** and **very time-consuming & needs great experience/expertise!!**
  industrial example: generate a 3-D mesh for a rotating turbine?
  3-4months just to generate the mesh:



- And only then, can you run the simulations !!

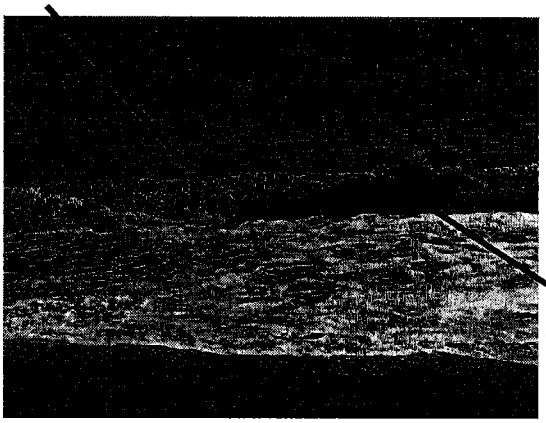
Mesh-based methods 3

- How do they handle cases where the mesh MUST deform? → extra mathematics & unwieldy

  e.g. A cylinder wall that is flexing

- How can a mesh-based method deal with **highly non-linear deformation**?

MultiPhase!!



Splash up

(Photo courtesy of F. Raichlen)

Pelton Runner

Mesh-based methods 4

In summary:

Mesh-based methods are **good** for
(i) confined computational domains
(ii) computations where the boundaries are not moving

Mesh-based methods are **bad** for:
(i) mesh generation – can be very expensive
(ii) highly nonlinear deformation of the fluid body

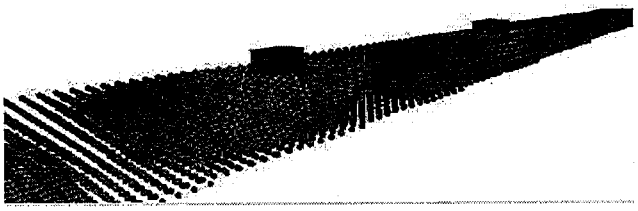
- → So, we need numerical methods where we are not constrained by the restrictions of the numerical mesh.... Hence, **Meshless methods**

Meshless methods (also Meshfree)

- What is a **Meshless** method? No computational grid or mesh

The computational points now take the form of 'particles' or 'points', similar (but different) to the nodal points in the Finite Element Method

Different meshless techniques are presented in **Lagrangian** form



Different meshless techniques are presented in **Lagrangian** form

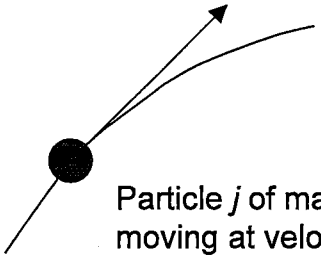
Meshless methods: Basic Idea of SPH

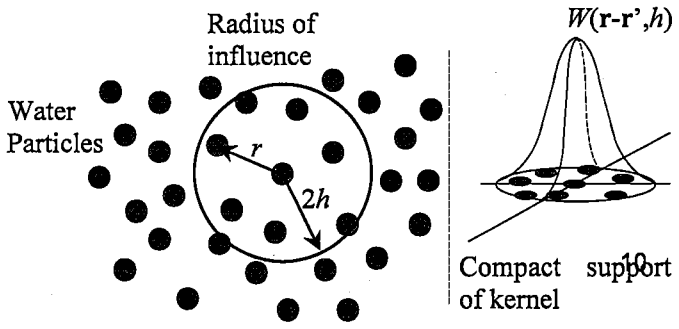
Meshless Our computation points are **particles** that now **move** according to governing dynamics , e.g. Navier-Stokes Equations

Particles move along a trajectory by **integrating** in time their velocity & acceleration

Particles possess **fluid properties** that travel with them, e.g. density, pressure; these can change with time

Local Interpolation (summation) with a **weighting function** (kernel) around each particle to obtain fluid properties





Meshless methods: Terminology

Eulerian description of motion: describes changes as they occur at a fixed point in the fluid

Lagrangian description of motion: describes changes which occur as you follow a fluid particle along its trajectory

The Eulerian derivative is the rate of change at a fixed position
e.g. measuring the flow in a river at a fixed location

$$\text{Eulerian derivative} = \frac{\partial}{\partial t}$$

The Lagrangian derivative is the '**total** rate of change' and is the derivative along a fluid trajectory

$$\text{Lagrangian derivative} = \frac{\mathrm{d}}{\mathrm{d}t}$$

Meshless methods: Terminology

More on the Lagrangian derivative .....

The Lagrangian derivative is also referred to as the
Total, **material** or **substantive** derivative and is also commonly written as

$$\text{Lagrangian derivative} = \frac{\mathrm{d}}{\mathrm{d}t} = \frac{D}{Dt}$$

The Eulerian derivative operator is related to the Total derivative by:

$$\underbrace{\frac{D}{Dt}}_{\text{Lagrange}} = \underbrace{\frac{\partial}{\partial t}}_{\text{Euler}} + \mathbf{u} \cdot \nabla$$

In 3-D cartesian form

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla = \boxed{\frac{\partial}{\partial t} + u\frac{\partial}{\partial x} + v\frac{\partial}{\partial y} + w\frac{\partial}{\partial z}}$$

Meshless methods

Why use **meshless/meshfree** methods?

1. Can handle easily simulations of very large deformations (because the connectivity between nodes is changing and being calculated at run-time)
2. Data structure can be linked more easily to a CAD database since no mesh generation is needed
3. Method is designed to adapt to the changes of the topological structure

Meshless methods

Quick comparison of Lagrangian & Eulerian methods:

	Lagrangian Methods	**Eulerian Methods**
Grid	Attached to moving particles	Fixed in space
Track	Movement of any point on materials	Mass, momentum & energy flux across grid nodes & mesh cell boundary
Time history	Easy to obtain time-history on point attached to materials	Difficult to obtain time-history on point attached to materials
Moving boundaries & interfaces	Easy to track	Difficult to track
Irregular geometry	Easy to model	Difficult to model with accuracy

From Liu & Liu (2003)

Different Meshless methods

Methods	Methods of approximation
Smoothed Particle Hydrodynamics (SPH)	**Integral representation**
Finite point method	Finite difference representation
Diffuse element method	Moving least square (MLS) approximation - Galerkin
Element free Galerkin (EFG) method	MLS approximation - Galerkin
Reproducing Kernel particle method (RKPM)	Integral representation - Galerkin
Free mesh method	Galerkin method
Meshless local Petrov-Galerkin (MLPG) method	MLS approximation Petrov-Galerkin method
Point interpolation method (PIM)	Point interpolation (radial & polynomial basis), Galerkin method, Petrov-Galerkin method
Meshfree weak-strong form (MWS)	MLS, PIM, radial PIM (RPIM), Collocation plus Petrov-Galerkin

Chronological order

(Liu & Liu, 2003)

Applications of SPH

Astrophysics (the origin of SPH – Gingold & Monaghan 1977)

- Stellar Collisions
- Cloud Fragmentations & collisions
- Collapse and Formation of Galaxies

Magneto-Hydrodynamics

- Magnetic Collapse of Gas Clouds
- Development of expansive wave in a magnetic cloud

Solid Mechanics

- Impact problems
- Fracture simulation
- Metal Forming
- Moulding

Fluid Dynamics

- Free-surface flows
- Heat Conduction
- Wave breaking
- Multi-phase flows

Recent Applications of SPH in CFD

Long Waves

Tsunamis, breaking waves at beaches, landslide generated waves

Sediment Transport & Suspension

Solves convection-diffusion equation for suspended sediment concentration under waves

Two-phase SPH

Bubbles, modelling air & water, oil spills (EDF)

Incompressible SPH

Enforces correct pressure at all times throughout the domain

Short Waves

Breaking Waves & Wave Impact Studies on Offshore Structures

Bio-medical applications

hear valves, flexible membranes, etc.

Fundamentals of SPH

- SPH describes a fluid by replacing its continuum properties with locally (smoothed) quantities at discrete Lagrangian locations ⇒ **meshless**
- SPH is based on integral interpolants invented in 1970s for astrophysics (Lucy 1977, Gingold & Monaghan 1977), but turned out to be very useful for many other fields

Fundamentals of SPH

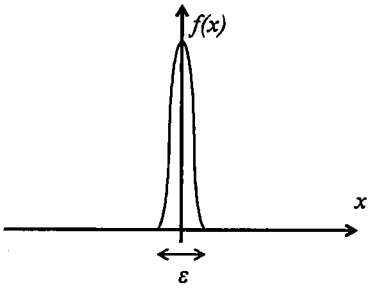
The Delta Function

The interpolation procedure within SPH is based on the (discrete) approximation that the value of a function $A(\mathbf{x})$ at a point $\mathbf{x}$ in space can be expressed as:

$$A(\mathbf{r}) = \int_{\Omega} \delta(\mathbf{r} - \mathbf{r}')\ A(\mathbf{r}')\, \mathrm{d}\,\Omega$$

where $\delta(\mathbf{x})$ is the Dirac delta function defined as

$$\delta_\varepsilon(x) = \lim_{\varepsilon \to 0} \begin{cases} 0 & x < -\varepsilon/2 \\ 1/\varepsilon & -\varepsilon/2 < x < \varepsilon/2 \\ 0 & x > \varepsilon/2 \end{cases}$$



The delta function has the useful properties

$$\int_{-\infty}^{+\infty} \delta(x - x') f(x')\, \mathrm{d}\,x' = f(x) \qquad \int_{-\infty}^{+\infty} \delta(x)\, \mathrm{d}\,x = \int_{-\varepsilon/2}^{\varepsilon/2} \frac{1}{\varepsilon}\, \mathrm{d}\,x = 1$$

Fundamentals of SPH

The SPH Integral Interpolation

In our computations, we cannot use a delta function since it is *infinitesimally narrow* which means that the interpolation region, Ω, would not overlap with other particles/nodal interpolation points. Hence, the interpolation procedure within SPH approximates the delta function with its own weighting function called the **SMOOTHING KERNEL,** W

$$\langle A(\mathbf{r}) \rangle = \int_{\Omega} W(\mathbf{r} - \mathbf{r}', h)\ A(\mathbf{r}')\, \mathrm{d}\,\Omega$$

where $< \cdot >$ is the integral SPH averaged quantity and h is the **SMOOTHING LENGTH** (more later on this). Compare this with the delta function interpolation from before:

$$A(\mathbf{r}) = \int_{\Omega} \delta(\mathbf{r} - \mathbf{r}')\ A(\mathbf{r}')\, \mathrm{d}\,\Omega$$

(Qu: What's the difference?)

Fundamentals of SPH

The SPH Smoothing Kernel

As stated, the interpolation procedure within SPH approximates the delta function with its own weighting function called the **SMOOTHING KERNEL**

$$\langle A(\mathbf{r})\rangle = \int_{\Omega} W(\mathbf{r}-\mathbf{r}', h)\ A(\mathbf{r}')\,\mathrm{d}\,\Omega$$

We can choose the Smoothing kernel – this gives the SPH technique some key advantages as it allows us to use a kernel of sufficiently high order for a particular problem.

The kernel depends on the two quantities:

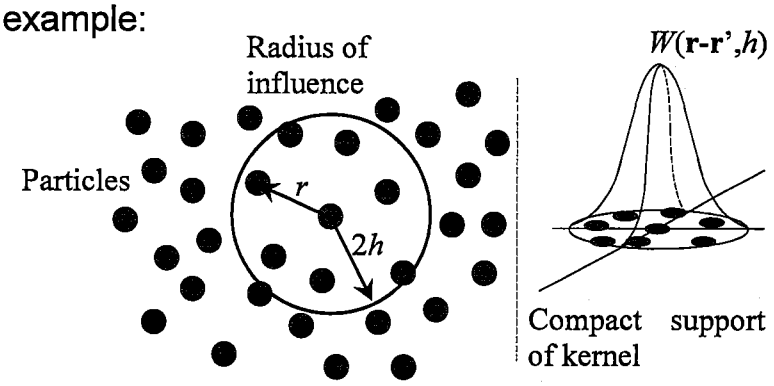
(i) The interpolation distance (distance between particles) = $\mathbf{r} - \mathbf{r}'$

(ii) The smoothing length, (h=characteristic length)

Fundamentals of SPH

The SPH Smoothing Kernel and smoothing length

•Smoothing Kernel example:



The smoothing length h defines the extent of the kernel. In SPH simulations, it is either:

(i) Kept constant at a present value $h = coefficient \times \Delta x$

(ii) Adapted during the simulation according to some criterion (variable smoothing length)

The radius of influence of each kernel is often set to be twice the smoothing length, $2h$

Fundamentals of SPH

The SPH Smoothing Kernel

How do we define a smoothing kernel? The kernel must approximate to the delta function as the smoothing length, tends to zero $h \rightarrow 0$.

$$\langle A(\mathbf{r}) \rangle = \int_{\Omega} W(\mathbf{r} - \mathbf{r}', h)\, A(\mathbf{r}')\, \mathrm{d}\,\Omega$$

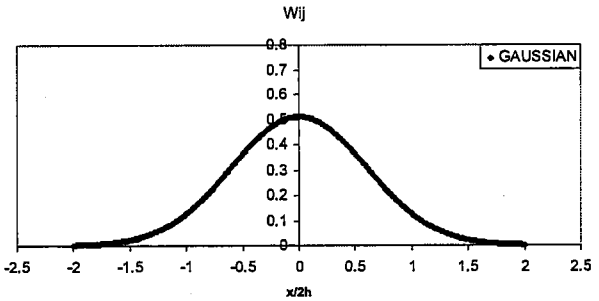
Hence, we can generate a smoothing kernel we want. Some common choices are:

1. Gaussian
2. Cubic Spline (B-spline)
3. Quadratic
4. Higher-order kernels, e.g. 4th & 5th-order

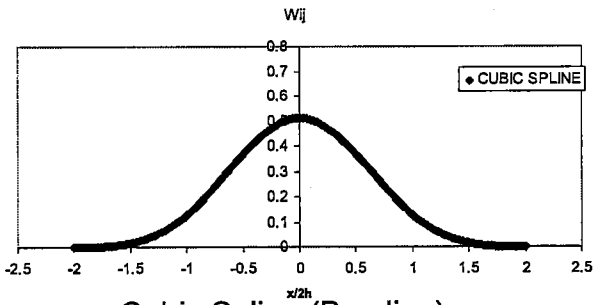
We will now take a look at these in turn.

Fundamentals of SPH

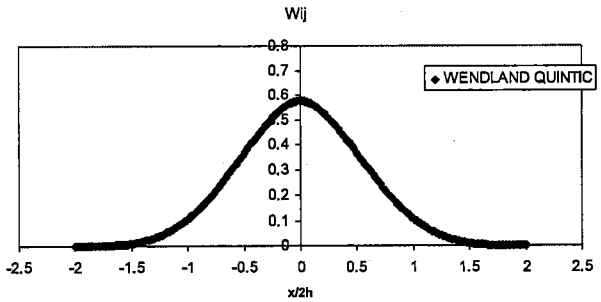
The SPH Smoothing Kernel



Gaussian



Cubic Spline (B-spline)



Higher-order kernels, e.g. 4th & 5th-order

Note symmetry of each kernel, and that the kernels =0 beyond $\pm 2h$

Fundamentals of SPH

Axioms of SPH Integral Interpolation

The interpolation procedure within SPH with the smoothing kernel depends on 3 axioms in order to give accurate results

Partition of unity: $\int_{\Omega} W(\mathbf{r}-\mathbf{r}',h)\ \mathrm{d}\Omega = 1$

Kernel tends to delta fn: $W(\mathbf{r}-\mathbf{r}',h) \to \delta(\mathbf{r}-\mathbf{r}'), \qquad h \to 0$

Kernel is k-times differentiable and derivative is continuous: $W(\mathbf{r}'-\mathbf{r},h) \in C_0^k$

(Qu1: When might these not be satisfied?)
(Qu2: What might happen when these are not satisfied?)

Fundamentals of SPH

The SPH Smoothing Kernel: Gaussian

The Gaussian smoothing kernel is defined as:

$$W(r,h) = \alpha_D \exp(-q^2)$$

$$q = \frac{r-r'}{h}, \text{ or } q = \frac{r_i - r_j}{h}$$

α_D is normalisation factor to ensure the integral of the kernel itself reproduces unity, and is defined as:

1-D: (an exercise for you)
2-D: $1/(\pi h^2)$
3-D: $1/(3\pi/2h^3)$

The advantage of the Gaussian kernel are that it approximates the dirac delta function very well.
There are 2 disadvantages:

(i) It is computationally expensive as it is an infinite series and extends well beyond $2h$
(ii) It has a point of maximum (extremum) in its gradient

We will return to this very important 2nd point again later

Fundamentals of SPH

The SPH Smoothing Kernel: Cubic Spline (3rd-order)

The Cubic Spline smoothing kernel is defined as:

$$W(r,h) = \alpha \begin{cases} 1 - \frac{3}{2}q^2 + \frac{3}{4}q^3 & 0 \le q \le 1 \\ \frac{1}{4}(2-q)^3 & 1 \le q \le 2 \\ 0 & q \ge 2 \end{cases}$$

α_D is normalisation factor to ensure the integral of the kernel itself reproduces unity, and is defined as:

- 1-D: $2/3h$
- 2-D: $10/(7\pi h^2)$
- 3-D: $1/(\pi h^3)$

$$q = \frac{r - r'}{h}, \text{ or } q = \frac{r_i - r_j}{h}$$

Advantage: approximates the Gaussian kernel very closely and is therefore computationally cheap.

Disadvantage: has a point of maximum (extremum) in its gradient

Fundamentals of SPH

The SPH Smoothing Kernel: Example 5th-order (Wendland kernel)

•The Gaussian smoothing kernel is defined as:

$$W(r,h) = \alpha_D \left(1 - \frac{q}{2}\right)^4 (2q+1) \qquad 0 \le q \le 2$$

α_D is normalisation factor to ensure integral of the kernel itself reproduces unity, and is defined as:

- 1-D: $15/8h$
- 2-D: $7/(4\pi h^2)$
- 3-D: $21/(16\pi h^3)$

$$q = \frac{r - r'}{h}, \text{ or } q = \frac{r_i - r_j}{h}$$

Advantages: (i) is high–order & therefore captures higher-order effects
(ii) has improved accuracy

Disadvantage: (i) is high–order & therefore computationally expensive
(ii) has a point of maximum (extremum) in its gradient

Accuracy of SPH interpolation

How accurate is the SPH interpolation (in 1D)?

$$\langle A(r)\rangle = \int_\Omega A(r')\, W_h(r-r')\, \mathrm{d}r'$$

Taylor Serie of $A(r')$:

$$A(r') = A(r) + \frac{\partial A(r)}{\partial r}(r-r') + \frac{1}{2}\frac{\partial^2 A(r)}{\partial r^2}(r-r')^2 + O(r-r')^3$$

Substituting the TS in the SPH interpolation leads to:

$$\langle A(r)\rangle = A(r)\int_\Omega W_h(r-r')\,\mathrm{d}r' + \frac{\partial A(r)}{\partial r}\int_\Omega W_h(r-r')\,(r-r')\mathrm{d}r'$$

$$+\frac{1}{2}\frac{\partial^2 A(r)}{\partial r^2}\int_\Omega W_h(r-r')\,(r-r')^2\mathrm{d}r' + \dots$$

$=1$

$=\phi$

Accuracy of SPH interpolation

Recalling the following properties of the SPH interpolation:

Partition of unity: $\int_\Omega W_h(\mathbf{r}-\mathbf{r}')\ \mathrm{d}\Omega = 1$

Kernel is an even function $W_h(\mathbf{r}) = W_h(-\mathbf{r})$

Which leads to: $\int_\Omega W_h(\mathbf{r}-\mathbf{r}')\cdot(\mathbf{r}-\mathbf{r}')\,\mathrm{d}\Omega = 0$

So we get:

$$\langle A(r)\rangle = A(r)\cdot 1 + \frac{1}{2}\frac{\partial^2 A(r)}{\partial r^2}\int_\Omega W_h(r-r')\,(r-r')^2\mathrm{d}r' + \cdots$$

$= M_{2,W}$

Accuracy of SPH interpolation

Second-order moment: $M_{2,w} = \int_{\Omega} W_h(r - r')\,(r - r')^2 \mathrm{d}\,r'$

$$\langle A(r)\rangle = A(r)\cdot 1 + \frac{1}{2}\frac{\partial^2 A(r)}{\partial r^2} M_{2,w} + \cdots$$

$$q = \frac{r - r'}{h} \Longmapsto W_h(r - r') = \frac{c}{h^d} w(q) \qquad M_{2,w} = ch^2 \int_{\Omega_q} q^2 w(q)\,\mathrm{d}\,q$$

d: dimension number

Non-dimensional

If Kernel function is defined as: $w(q) \geq 0;\ \forall\, q$

$$M_{2,w} \geq 0 \Longrightarrow \langle A(r)\rangle = A(r) + O(h^2)$$

Accuracy of SPH interpolation

$$\langle A(r)\rangle = A(r) + O(h^2)$$

- SPH interpolation is second order in space at continuous level
- We imposed that the kernel function is always positive
- Order of interpolation does not depends on the order of the kernel function (example: 5° order Wendland gives 2° order of accuracy)

Accuracy of SPH interpolation

If the rule $w(q) \geq 0;\ \forall\, q \in \mathbb{R}$ is violated

We can derive a kernel function that guarantes: $M_{2,w} = 0$

And, recalling the SPH approximation for a generic scalar function *A*:

$$\langle A(r) \rangle = A(r) + \cancel{\frac{1}{2}\frac{\partial^2 A(r)}{\partial r^2} M_{2,w}} + \frac{1}{2}\frac{\partial^4 A(r)}{\partial r^4} M_{4,w} + \cdots$$

$$\langle A(r) \rangle = A(r) + A(r) + O(h^4)$$

The same procedure can be applied to $M_{4,w}$ ...

SPH interpolation at continuous level can reach arbitrarily order of accuracy.

SPH Gradients

Now we can tackle gradients

How do we take the gradient of potentially scattered data?

$$\left\langle \frac{\partial A(r)}{\partial r} \right\rangle = ???$$

SPH Gradients

Now we can tackle gradients

Consider the gradient of a integral interpolation. (Like Finite Elements)

The definition of the integral interpolation is

$$\left\langle \frac{\partial A(r)}{\partial r} \right\rangle = \int_\Omega \frac{\partial A(r')}{\partial r'} W_h(r - r')\,\mathrm{d}\,r'$$

But we cannot evaluate this because we don't know $\frac{\partial A(x')}{\partial x'}$

So, We use integration by parts:

$$\left\langle \frac{\partial A(x)}{\partial x} \right\rangle = \int_\Omega \frac{\partial}{\partial r'}[A(r')W_h(r - r')]\,\mathrm{d}\,r' - \int_\Omega A(r')\frac{\partial W_h(r - r')}{\partial r'}\,\mathrm{d}\,r'$$

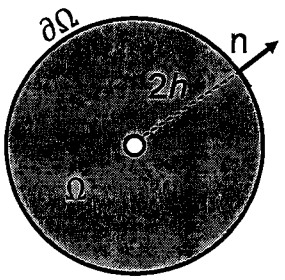
SPH Gradients

In 1D: $\int_\Omega \frac{\partial}{\partial r'}[A(r')W_h(r - r')]\,\mathrm{d}\,r' = 0$

In 2D and 3D: $\int_\Omega \frac{\partial}{\partial r'}[A(\mathbf{r}')W_h(\mathbf{r} - \mathbf{r}')]\,\mathrm{d}\,\mathbf{r}' = \oint_{\partial\Omega} A(\mathbf{r}')W_h(\mathbf{r} - \mathbf{r}')\mathbf{n}(\mathbf{r}')\mathrm{d}s$

Gauss theorem

If we make the following hypothesis:
- Inside the fluid (away from the boundaries)
- Compact kernel support

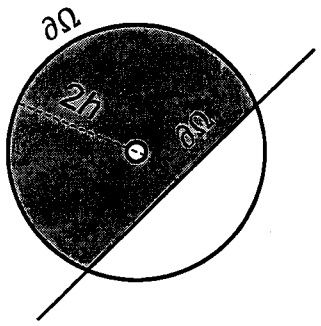


$$\oint_{\partial\Omega} A(\mathbf{r}')W_h(\mathbf{r} - \mathbf{r}')\mathbf{n}(\mathbf{r}')\mathrm{d}s = 0$$

SPH Gradients

Please note that near the boundaries:

$$\oint_{\partial\Omega} A(\mathbf{r}')W_h(\mathbf{r}-\mathbf{r}')\mathbf{n}(\mathbf{r}')\mathrm{d}s \neq 0$$



Going back to the SPH approximation of the derivative of *A*:

$$\left\langle \frac{\partial A(r)}{\partial r} \right\rangle = \int_{\Omega} A(r') \boxed{\frac{\partial W_h(r-r')}{\partial r'}} \mathrm{d}\,r'$$

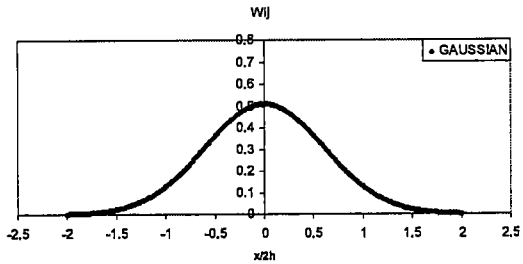
= "transfer the derivative onto the kernel"

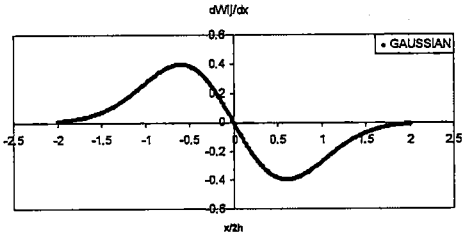
This is **fantastic** since we specify the kernel and therefore know its gradient!

SPH Gradients

We use the fact that the smoothing kernel is symmetric, and if the kernel is symmetric, then its gradient is .... ?

Asymmetric! $W_h(r-r') = W_h(r+r') \Rightarrow \frac{\partial W_h(r-r')}{\partial r'} = -\frac{\partial W_h(r-r')}{\partial r}$



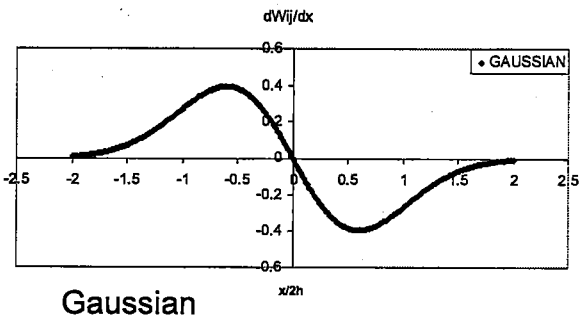


So the integral interpolation of a gradient becomes:

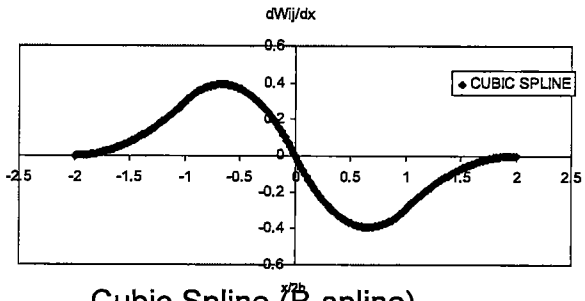
$$\left\langle \frac{\partial A(x)}{\partial x} \right\rangle = \int_{\Omega} A(r') \frac{\partial W_h(r-r')}{\partial r} \mathrm{d}\,r'$$

SPH Gradients

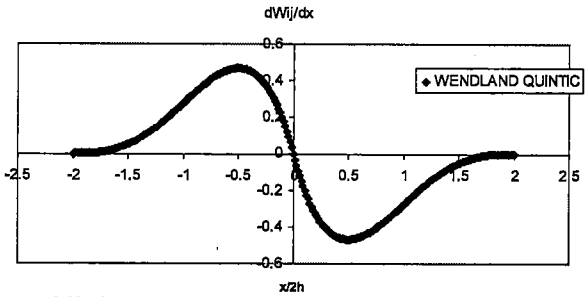
The SPH Smoothing Kernel Gradient



Gaussian



Cubic Spline (B-spline)



Higher-order kernels, e.g. 4th & 5th-order

Note **asymmetry** of each kernel gradient, and they have extremum in the gradient!

SPH Gradients

In 2D/3D this corresponds to:

$$\langle \nabla A(\mathbf{r}) \rangle = \int_{\Omega} A(\mathbf{r}') \nabla W_h(r - r') \, \mathrm{d}\boldsymbol{r}'$$

for the divergence of **A**:

$$\langle \nabla \cdot \mathbf{A}(\mathbf{r}) \rangle = \int_{\Omega} \mathbf{A}(\mathbf{r}') \cdot \nabla W_h(r - r') \, \mathrm{d}\boldsymbol{r}'$$

for the Laplacian of *A*:

$$\langle \nabla^2 A(\mathbf{r}) \rangle = \int_{\Omega} A(\mathbf{r}') \cdot \nabla^2 W_h(r - r') \, \mathrm{d}\boldsymbol{r}'$$

But this is not a very good idea (more on this later)

Accuracy of the SPH gradient

We start from the previous formula: $\left\langle \frac{\partial A}{\partial r} \right\rangle = \int_\Omega A(\mathrm{r}') \frac{\partial W_h(r-r')}{\partial r} \mathrm{d}\, r'$

Sustituting the TS:

$$A(r') = A(r) + \frac{\partial A(r)}{\partial r}(r-r') + \frac{1}{2}\frac{\partial^2 A(r)}{\partial r^2}(r-r')^2 + O(r-r')^3$$

We get this:

$$\left\langle \frac{\partial A}{\partial r} \right\rangle = A(r)\int_\Omega \frac{\partial W_h(r-r')}{\partial r}\mathrm{d}\, r' + \frac{\partial A(r)}{\partial r}\int_\Omega \frac{\partial W_h(r-r')}{\partial r}(r-r')\,\mathrm{d}\, r' + \\ + \frac{1}{2}\frac{\partial^2 A(r)}{\partial r^2}\int_\Omega \frac{\partial W_h(r-r')}{\partial r}(r-r')^2\,\mathrm{d}\, r' + O(h^2)$$

Accuracy of the SPH gradient

So, to get second order convergence, we need the following conditions to be fulfilled:

$$\int_\Omega \frac{\partial W_h(r-r')}{\partial r}\mathrm{d}\, r' = 0$$

$$\int_\Omega \frac{\partial W_h(r-r')}{\partial r}(r-r')\,\mathrm{d}\, r' = 1$$

$$\int_\Omega \frac{\partial W_h(r-r')}{\partial r}(r-r')^2\, d\, r' = 0$$

Those conditions are due to the kernel symmetry

an exercise, for you:

Prove that: $\int_\Omega \frac{\partial W_h(r-r')}{\partial r}(r-r')^3\, d\, r'$ converges as $O(h^2)$

Accuracy of the SPH gradient

Second exercise:

Prove that: $$\int_{\Omega} \frac{\partial W_h(r-r')}{\partial r}(r-r')\,\mathrm{d}r' = 1$$

Is equivalent to partition of unity: $$\int_{\Omega} W_h(\mathbf{r}-\mathbf{r}')\;\mathrm{d}\Omega = 1$$

(Hints: use integration by parts and the Gauss Theorem)

Discrete SPH interpolation

In the numerical SPH method, we must approximate the integral interpolation procedure

$$\langle A(\mathbf{r})\rangle = \int_{\Omega} A(\mathbf{r}')\,W(\mathbf{r}-\mathbf{r}',h)\,\mathrm{d}\mathbf{r}'$$

$$\downarrow$$

$$\langle A(\mathbf{r}_i)\rangle \approx \sum_{j=1}^{N} A(\mathbf{r}_j)\,W(\mathbf{r}_i-\mathbf{r}_j,h)\,V_j$$

$$\langle \nabla A(\mathbf{r})\rangle = \int_{\Omega} A(\mathbf{r}')\,\nabla W(\mathbf{r}-\mathbf{r}',h)\,\mathrm{d}\mathbf{r}'$$

$$\downarrow$$

$$\langle \nabla A(\mathbf{r}_i)\rangle \approx \sum_{j=1}^{N} A(\mathbf{r}_j)\,\nabla W(\mathbf{r}_i-\mathbf{r}_j,h)\,V_j$$

where $\mathrm{d}\mathbf{r}'=\mathrm{d}\Omega$ becomes the volume of each particle

$$V_j = \frac{m_j}{\rho_j} = \frac{\text{mass of particle } j}{\text{density of particle } j}$$

Subscripts i or j denotes particles i or j

Discrete SPH interpolation

How accurate is the discrete SPH interpolation?

Difficult to know, it really depends on the particle distribution.

For Cartesian grid (Quinlan et al. 2006):

$$\frac{\partial A(r)}{\partial r} - \left\langle \frac{\partial A(r)}{\partial r} \right\rangle = h^2 \frac{\partial^3 A(r)}{\partial r^3} \int_{\Omega_q} q^2 w(q) \mathrm{d}\, q + C \left(\frac{\Delta x}{h}\right)^{\beta+2}$$

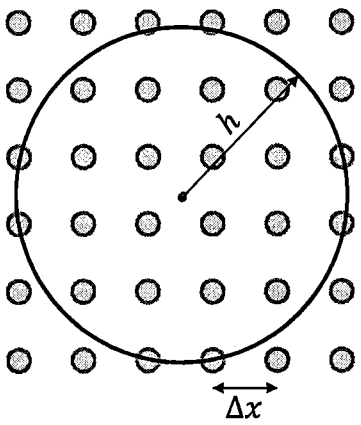
Where:
C is a constant
Δx is the particle spacing (Cartesian grid size)
β smoothness of the kernel at the boundaries

Discrete SPH interpolation

SPH discrete interpolation accuracy can be analyzed for:

$h \to 0$; $\frac{\Delta x}{h} = const$ which corresponds to reducing the smoothing error

$h = const$; $\frac{\Delta x}{h} \to 0$ which corresponds to reducing the discretization error



$\frac{\Delta x}{h}$ controls the number of neighbours and so the efficiency of the SPH interpolation

Discrete SPH interpolation

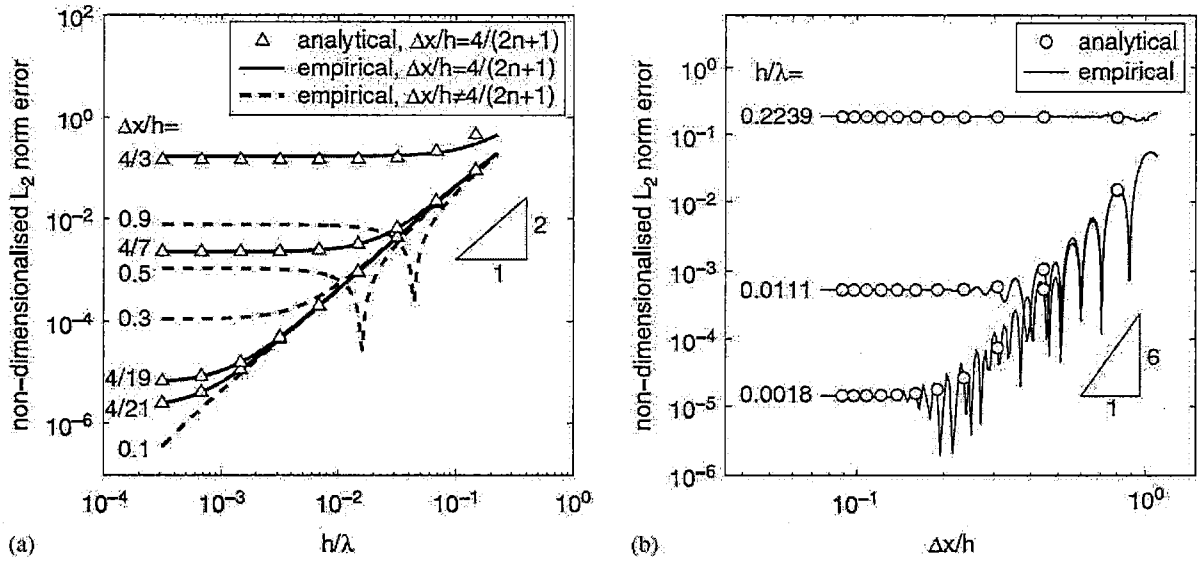


Figure 2. Analytically and empirically calculated L_2 norm of error in SPH estimates of the first derivative of $A(x) = A_0 \sin(2\pi x/\lambda)$: (a) as a function of smoothing length for various values of particle spacing; and (b) as a function of particle spacing for various smoothing lengths.

(Quinlan et al. 2006)

Discrete SPH interpolation

σ being the standard deviation of the perturbation

λ the wavelength

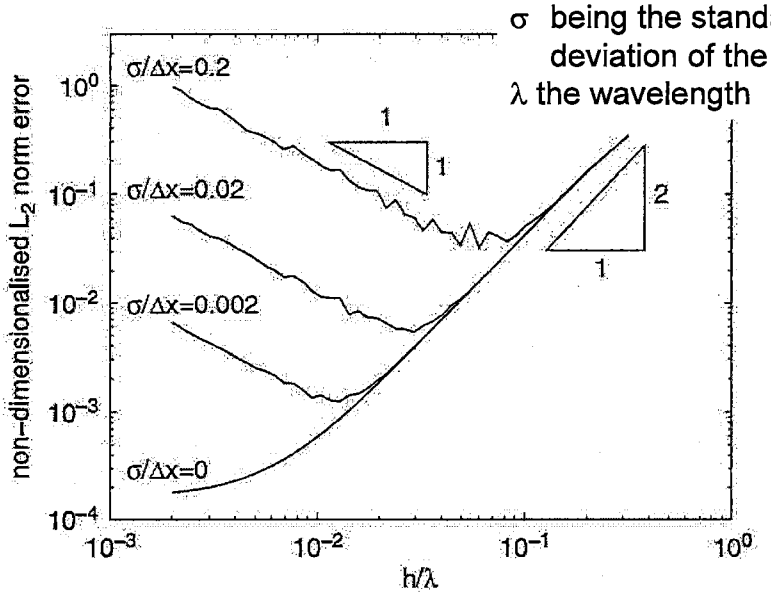


Figure 4. Observed L_2 norm error in SPH estimates of the first derivative of $A(x) = A_0 \sin(2\pi x/\lambda)$ as a function of smoothing length, for various particle spacing perturbations, computed with $\Delta x/h = 0.364$.

(Quinlan et al. 2006)

Discrete SPH interpolation

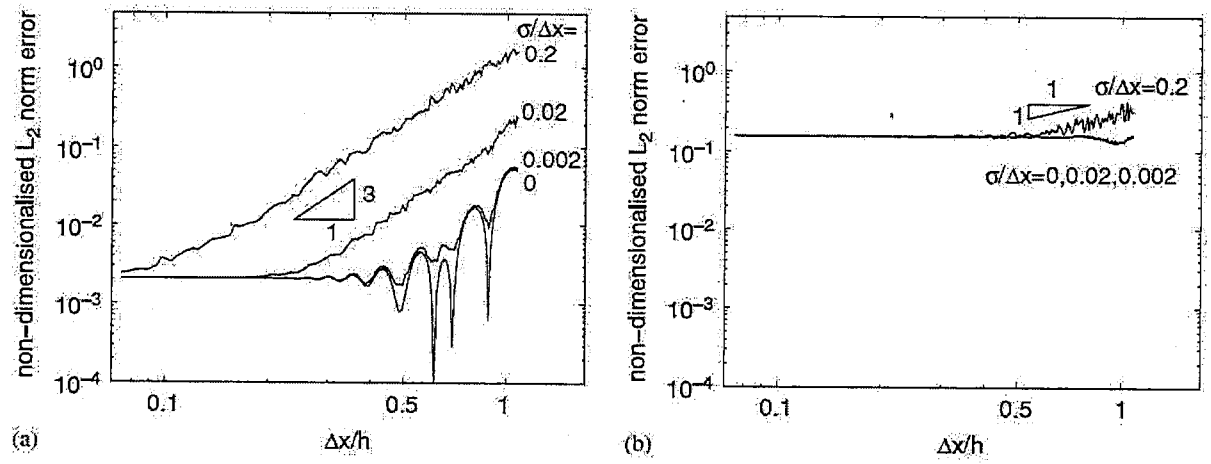


Figure 5. Observed L_2 norm error in SPH estimates of the first derivative of $A(x) = A_0 \sin(2\pi x/\lambda)$ as a function of particle spacing for various particle spacing perturbations with: (a) $h/\lambda = 0.022$; and (b) $h/\lambda = 0.2$.

(Quinlan et al. 2006)

Accuracy of SPH discrete interpolation

When we go from:

Continuous $\int_\Omega A(\mathbf{r}')\, W(\mathbf{r}-\mathbf{r}', h)\, \mathrm{d}\,\mathbf{r}'$ to

discrete $\sum_{j=1}^{N} A(\mathbf{r}_j)\, W(\mathbf{r}-\mathbf{r}_j, h)\, V_j$

We loose second order of accuracy **and the SPH interpolation might not converge to the exact solution**, if particles are disordered.

Interpolation might even diverge! (bigger error for higher resolution)

How do we fix this?

One option is introducing Kernel Correction to enforce consistency.

Accuracy of SPH discrete interpolation

Starting from the SPH interpolation of a scalar function

$$\langle A(r_a)\rangle = \sum_{b=1}^{N} A(r_b)\, W_h(r_a - r_b)\, V_j$$

And substituting the Taylor Serie of $A(r_b)$:

$$A(r_b) = A(r_a) + \frac{\partial A(r_a)}{\partial r_a}(r_b - r_a) + \frac{1}{2}\frac{\partial^2 A(r_a)}{\partial r_a^2}(r_b - r_a)^2 + O(r_b - r_a)^3$$

Leads to:

$$\langle A(r_a)\rangle = A(r_a)\sum_{b=1}^{N} W_h(r_a - r_b)\, V_j + \frac{\partial A(r_a)}{\partial r_a}\sum_{b=1}^{N} W_h(r_a - r_b)\cdot(r_b - r_a)\, V_j +$$

$$\frac{1}{2}\frac{\partial^2 A(r_a)}{\partial r_a^2}\sum_{b=1}^{N} W_h(r_a - r_b)\cdot(r_b - r_a)^2\, V_j$$

Accuracy of SPH discrete interpolation

If the following conditions hold $\forall\, a \in D$

For the scalar function *A*:

$$\begin{cases} \sum_{b=1}^{N} W_h(r_a - r_b)\, V_j = 1 \\ \sum_{b=1}^{N} W_h(r_a - r_b)\cdot(r_b - r_a)\, V_j = 0 \end{cases}$$

For the gradient of scalar function *A*:

$$\begin{cases} \sum_{b=1}^{N} \partial W_h(r_a - r_b)\, V_j = 0 \\ \sum_{b=1}^{N} \partial W_h(r_a - r_b)\cdot(r_b - r_a)\, V_j = 1 \end{cases}$$

The SPH interpolation is 1° order consistent, which means that:

1 – linear functions can be exactly reproduced by the SPH interpolation

2 – it converges with order $O(h^2)$

Accuracy of SPH discrete interpolation

How do we enforce consistency?

Different proposals are available in literature for the kernel function and/or the derivatives:

- Bonet and Lok 1999,
- Chen et al.1999,
- G.A. Dilts 1999,
- Liu & Liu 2006 = BEST but EXPENSIVE → 2 loops : 1/ correction kernel (first (L_a)) 2/ gradient (then)

Key idea: derive a corrected kernel $\widehat{W}_h$ (or kernel gradient $\nabla\widehat{W}_h$) for each particle *a* which fulfils the consistency conditions.

Kernel corrections

Bonet and Lok (1999)

$\wedge$ = corrected kernel

$$\underbrace{\langle \nabla A(\mathbf{r}_a) \rangle}_{\text{= gradient}} \approx \sum_{b=1}^{N} A(\mathbf{r}_b) \nabla\widehat{W}(\mathbf{r}_a - \mathbf{r}_b, h) V_b$$

Where the corrected kernel is defined as: (= normal "kernel")

$$\nabla\widehat{W}(\mathbf{r}_a - \mathbf{r}_b, h) = \mathbf{L}_a \nabla W(\mathbf{r}_a - \mathbf{r}_b, h)$$

in 1D: $\begin{cases} \sum_b \partial \hat{W}_R (r_a - r_b) \cdot V_b = \phi \\ \sum_b \partial \hat{W}_R (r_a - r_b) \cdot (r_a - r_b) = \end{cases}$

And matrix $\mathbf{L}_a$ is obtained enforcing that, for each particle (a)

in 3D: $$\left\{ \sum_{b=1}^{N} (\vec{\mathbf{r}}_b - \vec{\mathbf{r}}_a) \otimes \nabla\widehat{W}(\vec{\mathbf{r}}_a - \vec{\mathbf{r}}_b, h) V_b = \sum_{b=1}^{N} (\vec{\mathbf{r}}_b - \vec{\mathbf{r}}_a) \otimes \nabla W(\vec{\mathbf{r}}_a - \vec{\mathbf{r}}_b, h) V_b \mathbf{L}_a = \mathbf{I} = \text{Identity Matrix} = \begin{bmatrix} 1 & \phi \\ \phi & 1 \end{bmatrix} \right.$$

Which means that the matrix can be calculated as follows:

$$\mathbf{L}_a = \left[\sum_{b=1}^{N} (\vec{\mathbf{r}}_b - \vec{\mathbf{r}}_a) \otimes \nabla W(\vec{\mathbf{r}}_a - \vec{\mathbf{r}}_b, h) V_b \right]^{-1}$$

= "Consistency (or) Correction of Kernel or Gradient?"

{ 3x3 in 3D
  2x2 in 2D $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

Kernel corrections

Liu & Liu (2006)

Multidimensional Tayor series of A (first order only):

$$A(\mathbf{r}_b) = A(\mathbf{r}_a) + \nabla A(\mathbf{r}_a) \cdot (\mathbf{r}_b - \mathbf{r}_a) + O(\mathbf{r}_b - \mathbf{r}_a)^2$$

Can be rewritten using Einstein notation as:

$$A(\mathbf{r}_b) = A(\mathbf{r}_a) + \frac{\partial A(\mathbf{r}_a)}{\partial r_a^\alpha} \cdot (r_b^\alpha - r_a^\alpha) \text{ where } \alpha \text{ is a dimension index}$$

If we multiply the previous equation by the kernel function W_{ab} and sum over b we obtain:

$$\sum_{b=1}^{N} A(\mathbf{r}_b) W_{ab} V_b = A(\mathbf{r}_a) \sum_{b=1}^{N} W_{ab} V_b + \frac{\partial A(\mathbf{r}_a)}{\partial r_a^\alpha} \cdot \sum_{b=1}^{N} r_{ba}^\alpha W_{ab} V_b$$

Kernel corrections

Similarly, we can multiply the same equation by the kernel derivative $\partial^\beta W(\mathbf{r}_{ab})$ and sum over b:

$$\sum_{b=1}^{N} A(\mathbf{r}_b) \partial^\beta W(\mathbf{r}_{ab}) V_b = A(\mathbf{r}_a) \sum_{b=1}^{N} \partial^\beta W(\mathbf{r}_{ab}) V_b + \frac{\partial A(\mathbf{r}_a)}{\partial r_a^\alpha} \cdot \sum_{b=1}^{N} (r_{ba}^\alpha) \partial^\beta W(\mathbf{r}_{ab}) V_b$$

$\partial^\beta W(\mathbf{r}_{ab})$: is the kernel derivative accordingly to β direction

this is a scalar equation, which in 3D can be repeated for $\beta = x, y, z$

In total we have written 4 equations

Unknowns:

$$\mathbf{x} = \begin{bmatrix} A(\mathbf{r}_b) \\ \frac{\partial A(\mathbf{r}_a)}{\partial r_a^x} \\ \frac{\partial A(\mathbf{r}_a)}{\partial r_a^y} \\ \frac{\partial A(\mathbf{r}_a)}{\partial r_a^z} \end{bmatrix} \qquad \mathbf{b} = \begin{bmatrix} \sum_{b=1}^{N} A(\mathbf{r}_b) W_{ab} V_b \\ \sum_{b=1}^{N} A(\mathbf{r}_b) \partial^x W(\mathbf{r}_{ab}) V_b \\ \sum_{b=1}^{N} A(\mathbf{r}_b) \partial^y W(\mathbf{r}_{ab}) V_b \\ \sum_{b=1}^{N} A(\mathbf{r}_b) \partial^z W(\mathbf{r}_{ab}) V_b \end{bmatrix}$$

Kernel corrections

$$\mathbf{A} = \begin{bmatrix} \sum_b W_{ab}V_b & \sum_b r_{ba}^x W_{ab}V_b & \sum_b r_{ba}^y W_{ab}V_b & \sum_b r_{ba}^z W_{ab}V_b \\ \sum_b \partial^x W(\mathbf{r}_{ab})V_b & \sum_b r_{ba}^x \partial^x W(\mathbf{r}_{ab})V_b & \sum_b r_{ba}^y \partial^x W(\mathbf{r}_{ab})V_b & \sum_b r_{ba}^z \partial^x W(\mathbf{r}_{ab})V_b \\ \sum_b \partial^y W(\mathbf{r}_{ab})V_b & \sum_b r_{ba}^x \partial^y W(\mathbf{r}_{ab})V_b & \sum_b r_{ba}^y \partial^y W(\mathbf{r}_{ab})V_b & \sum_b r_{ba}^x \partial^y W(\mathbf{r}_{ab})V_b \\ \sum_b \partial^z W(\mathbf{r}_{ab})V_b & \sum_b r_{ba}^x \partial^z W(\mathbf{r}_{ab})V_b & \sum_b r_{ba}^y \partial^z W(\mathbf{r}_{ab})V_b & \sum_b r_{ba}^z \partial^z W(\mathbf{r}_{ab})V_b \end{bmatrix}$$

By solving the following linear system: $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$

The corrected SPH approximation for $A(\mathbf{r}_a)$ and $\frac{\partial A(\mathbf{r}_a)}{\partial r_a^\alpha}$ are obtained

They ensure 1st order consistency (2nd order accuracy) both for the function *A* and its derivatives both inside the domain and close to the boundaries.

Kernel corrections

Despite this seems very promising, kernel corrections are not very popular for several reasons:

- They are computationally expensive and SPH is already quite expensive in itself
- They destroy conservation properties of SPH method (see later)
- The matrix which has to be inverted becomes ill-conditioned when particles are very disordered making imposssible to apply the correction where/when it is really needed.

Navier – Stokes equations

So do we have enough to try discretising the governing equations?

Let's have a go!

The governing equations we want to solve are the Navier-Stokes equations expressed in **Lagrangian form**:

- density

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho \nabla \cdot \mathbf{v}$$

- Velocity

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\frac{1}{\rho}\nabla p + v_o \nabla^2 \mathbf{v} + \mathbf{F}$$

ρ is density, $\mathbf{v}$ is velocity vector, t is time, p is pressure, v_o is viscosity and $\mathbf{F}$ are body forces

Deriving SPH Equations: A quick note

One of the **really nice features of SPH** is that the equations for fluids can be derived 3 different ways and all give the same result!

1. Considering a weighted interpolation of the governing equations
2. Using a Least-Action Principle (Calculus of Variations)
3. Using an error minimisation approach with Moving Least Squares (MLS)

Here, we will only consider the first option as initially that is the easiest …

The Basics of SPH

Deriving the basic equations ....

(i) The Conservation of Mass (Continuity)

SPH Continuity Equation

The continuity equation we wish to solve is:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho\nabla\cdot\mathbf{v}$$

Therefore we need to find an SPH approximation for $\rho\nabla\cdot\mathbf{v}$ one possible option is:

$$\rho_a\langle\nabla\cdot\mathbf{v}\rangle_a = \rho_a\sum_{b=1}^{N}\mathbf{v}_b\cdot\nabla W_{ab}\left(\frac{m_b}{\rho_b}\right) \qquad \left(V_b = \frac{m_b}{\rho_b}\right)$$

But this is not a good choice, because $\langle\rho\nabla\cdot\mathbf{v}\rangle_a \neq 0$ for $\mathbf{v}$=const

SPH Continuity Equation

A better option is to re-write: $\rho\nabla\cdot\vec{\mathbf{v}} = \nabla\cdot(\rho\vec{\mathbf{v}}) - \vec{\mathbf{v}}\cdot\nabla\rho$

And then use SPH approximation on the two terms on the RHS:

$$\langle\rho_a\nabla\cdot\mathbf{v}\rangle_a = \sum_{b=1}^{N}\mathbf{v}_b\cdot\nabla W_{ab}m_b - \mathbf{v}_a\cdot\sum_{b=1}^{N}\nabla W_{ab}m_b$$

Which can be re-written as:

$$\langle\rho_a\nabla\cdot\mathbf{v}\rangle_a = -\sum_{b=1}^{N}\mathbf{v}_{ab}\cdot\nabla W_{ab}m_b$$

$\mathbf{v}_{ab} = \mathbf{v}_a - \mathbf{v}_b$ → if velocity=0 the $\mathbf{v}_b = 0$ = good choice

So the continuity equation becomes:

$$\frac{d\rho}{dt} = -\rho\,\nabla\cdot\mathbf{v} \longrightarrow \boxed{\frac{\mathrm{d}\rho}{\mathrm{d}t} = \sum_{b=1}^{N}\mathbf{v}_{ab}\cdot\nabla W_{ab}m_b}$$

SPH is simple because advection term is already inside $\frac{d\rho}{dt}$ (no extra computation) (N. Stokes)

IN = m, W, v
OUT = density

$\neq \rho_a \sum_b \mathbf{v}_b\cdot\nabla W_{ab}\frac{m_b}{\rho_b}$

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The Basics of SPH

Deriving the basic equations ....

(ii) The Conservation of Momentum

SPH MOMENTUM EQUATION

Eq. momentum = be more conservative than more accurate

Eq continuity = mass is conserved anyway in SPH so we can be less accurate

For the momentum equation, we want an SPH discrete version of:

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\frac{1}{\rho}\nabla p$$

$\left(+ v_0 \nabla^2 v + F\right)$? ($F$: gravity)

$\rho(\nabla P) = \nabla(\rho P) - P(\nabla$

We could use the previous result and write

$$\rho_a \nabla P_a = \sum_b m_b (P_a - P_b) \cdot \nabla_a W_{ab}$$ ← not a good choice

But this would not give an **equal and opposite reaction** between each set of particles and hence **conserve linear and angular momenta.**

To do this we make use of the following identity:

$$= \frac{\nabla P}{\rho} - \frac{P}{\rho^2}\nabla\rho + \frac{P}{\rho^2}\nabla\rho$$

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

SPH MOMENTUM EQUATION

So, we make use of the following identity:

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

$$\left\langle \nabla\left(\frac{\rho}{\rho}\right)\right\rangle = \sum_b \left(\frac{\rho_b}{\rho_b}\right)\cdot\nabla W_{ab}\cdot V_b$$

And then use SPH approximation on the two terms on the RHS:

$$\left\langle \nabla\rho\right\rangle = \sum_b \rho_b \nabla W_{ab} V_b$$

$$\left\langle \frac{\nabla P}{\rho}\right\rangle_a = \sum_{b=1}^{N}\left(\frac{P_b}{\rho_b}\right)\nabla W_{ab} V_b \oplus \left(\frac{P_a}{\rho_a^2}\right)\sum_{b=1}^{N}\rho_b \nabla W_{ab} V_b$$

Which, remembering that $V_b = m_b/\rho_b$ can be re-written as:

$$V_b = \frac{m_b}{\rho_b}$$

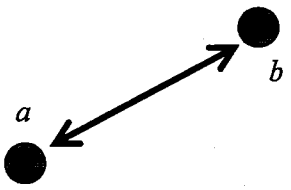
$\frac{dv}{dt}$ — gradient of pressure

$$\left\langle \frac{\nabla P}{\rho}\right\rangle_a = \sum_{b=1}^{N}\left(\frac{P_b}{\rho_b^2} + \frac{P_a}{\rho_a^2}\right)\nabla W_{ab} m_b$$ ✓

IN = $\rho_a, \rho_b, P_a, P_b, m_b, \nabla W_{ab}$

SPH MOMENTUM EQUATION

Why does this form conserve momentum?



$$\left\langle \frac{\nabla P}{\rho} \right\rangle_a = \sum_{b=1}^{N} \left(\frac{P_b}{\rho_b^2} + \frac{P_a}{\rho_a^2} \right) \nabla W_{ab} m_b$$

Consider the force interaction between 2 particles ***a*** and ***b*** and the contributions for each particle (note we multiply the contribution for each particle by its own mass to get the total force on the particle):

Force on particle ***a:*** $m_a \left(\frac{P_b}{\rho_b^2} + \frac{P_a}{\rho_a^2} \right) \nabla W_{ab} m_b$

Force on particle ***b:*** $m_b \left(\frac{P_a}{\rho_a^2} + \frac{P_b}{\rho_b^2} \right) \nabla W_{ba} m_a$

equal to $-F_a$

$= -\nabla W_{ab}$

$\Rightarrow \sum F = F_a + F_b = F_a - F_a = 0$ ↦ conservation of momentum ✓

Since $\nabla W_{ab} = -\nabla W_{ba}$ we hence know that the separate contributions are equal and opposite. This would not be the case for:

$$\left\langle \frac{\nabla P}{\rho} \right\rangle_a = \frac{1}{\rho_a} \sum_b (P_a - P_b) \cdot \nabla_a W_{ab} V_b$$ (Check for yourself)

SPH THERMAL ENERGY EQUATION DERIVATION

We can perform similar operations to obtain an equation for the rate of change of **thermal energy per unit mass**, e

$$\frac{\mathrm{d}e}{\mathrm{d}t} = -\left(\frac{P}{\rho} \right) \nabla \cdot \mathbf{v}$$

which in SPH form (following the same steps used for the momentum) can be derived as:

$$\left\langle \frac{\nabla P}{\rho} \right\rangle_a = \frac{1}{2} \sum_b m_j \left(\frac{p_b}{\rho_b^2} + \frac{p_a}{\rho_a^2} \right) \mathbf{v}_{ab} \cdot \nabla W_{ab}$$

This equation is very similar to the momentum equation so it is very easy to compute.

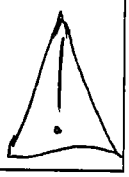
The Basic SPH Equations

$$\begin{cases} \dfrac{\mathrm{d}\rho}{\mathrm{d}t} = \displaystyle\sum_b m_b(\mathbf{v}_a - \mathbf{v}_b)\cdot\nabla W_{ab} & \text{Conservation of Mass} \\ \dfrac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\displaystyle\sum_b m_b\left(\frac{p_b}{\rho_b^2}+\frac{p_a}{\rho_b^2}\right)\nabla W_{ab} & \text{Conservation of Momentum} \\ \dfrac{\mathrm{d}e}{\mathrm{d}t} = \dfrac{1}{2}\displaystyle\sum_b m_b\left(\frac{p_b}{\rho_b^2}+\frac{p_a}{\rho_a^2}\right)\mathbf{v}_{ab}\cdot\nabla W_{ab} & \text{Conservation of Energy} \end{cases}$$

These are the basic (or classical) SPH equations used to solve many problems in the fields mentioned earlier (astrophysics, coastal hydrodynamics, gas dynamics, etc.)

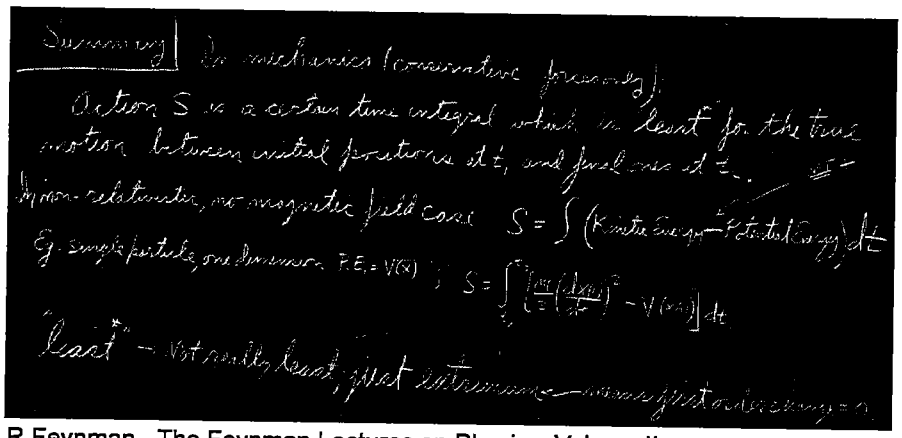
We need one more equation: $\dfrac{\mathrm{d}m_i}{\mathrm{d}t} = 0$ ✓

So, the mass of each equation does not change (in general)



SPH derived from

the Least Action Principle



R Feynman - The Feynman Lectures on Physics, Volume II

SPH from LAP

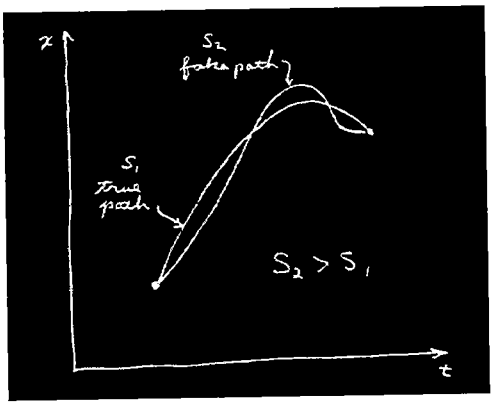
Least Action Principle

Assumption: we derive the motion of a group of particles with mass m_i without boundaries

Action $= S = \int_{t_1}^{t_2} L(\mathbf{v}, \mathbf{r})\, dt$

$L(\mathbf{v}, \mathbf{r})$ is the Lagrangian.

$L(\mathbf{v}, \mathbf{r}) = K - \pi$
K: kinetic energy
π: potential energy



The Least action principle states that the motion from t_1 to t_2 occurs along the trajectory for which S is minimum

$\Rightarrow \delta S = \int_{t_1}^{t_2} \delta L(\mathbf{v}, \mathbf{r})\, dt$

find the minimum of S

SPH from LAP

For a group of particles, L is:

$$L(\mathbf{v}, \mathbf{r}) = \sum_b m_b \left[\frac{1}{2} v_b^2 - u_b(\rho_b, s_b)\right]$$

K.E^n Pot^l E^n

u_b: thermal energy per unit of mass, function of density and entropy: ρ_b, s_b
v_b : particle velocity magnitude

The equation of motion for particle a can be thus obtained from:

$\frac{dL}{?} = 0$

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

Recalling that $L(\mathbf{v}, \mathbf{r}) = K - \pi$

$$\frac{\partial L}{\partial \mathbf{v}_a} = m_a \mathbf{v}_a$$

$$\frac{\partial L}{\partial \mathbf{r}_a} = -\sum_b m_b \frac{\partial u_b}{\partial \rho_b} \frac{\partial \rho_b}{\partial \mathbf{r}_a}$$

Assuming entropy s=constant, i.e.: no dissipation

no Σ because no dep^t with other particles

Σ because dep^t on all other particles

SPH from LAP

$$\pi_{int} = \sum_a V_a^0 u(J_a)$$

V_a^0: volume of particle *i* at initial time

$u(J_a)$: internal energy per unit of volume

compression rate $J_a := \frac{\rho_a^0}{\rho_a}$

pressure $p := \frac{du}{dJ}$

D_v = directional derivative

the directional derivative along a given vector **v** at a given point **x**: the rate of change of the function, moving through **x** with a velocity specified by **v**

$$D_v \pi_{int} = \sum_a V_a^0 D_v u(J_a)$$

SPH from LAP

$$D_v \pi_{int} = \sum_a V_a^0 D_v u(J_a) = \sum_a V_a^0 \frac{\partial u_a}{\partial J_a} D_v J_a = \sum_a V_a^0 p_a \frac{\partial J_a}{\partial \rho_a} D_v \rho_a$$

$$D_v \pi_{int} = -\sum_a m_a \frac{p_a}{\rho_a^2} D_v \rho_a$$

$D_v \rho_a$ =??? This term comes from the SPH density interpolation:

$$\langle \rho_a \rangle = \sum_b m_b W(\mathbf{r}_a - \mathbf{r}_b, h_a)$$

(Note that here we are assuming a different smoothing length for all particles)

SPH from LAP

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

SPH Kernel can be re-written as:

$$W(\mathbf{r}_b - \mathbf{r}_c, h_b) = \frac{1}{h^d} f(\boldsymbol{q}) \qquad \boldsymbol{q} := \frac{\mathbf{r}_b - \mathbf{r}_c}{h_b}$$

$d :=$ number of dimension

$$D_v\rho_a = \sum_b m_b \left[\frac{\partial W(\mathbf{r}_{ab}, h_a)}{\partial \mathbf{r}_{ab}} D_v \mathbf{r}_{ab} + \frac{\partial W(\mathbf{r}_{ab}, h_a)}{\partial h_a} D_v h_a \right]$$

smoothing length is % to the volume of the particle: $V = \frac{m}{\rho}$ if V↑ then ρ↓

Assuming that: $h_a = \eta \left(\frac{1}{\rho_a}\right)^{1/d} \Rightarrow D_v h_a = \frac{\partial h_a}{\partial \rho_a} D_v \rho_a = -\frac{h_b}{d\rho_a} D_v \rho_a$

$$D_v\rho_a = \sum_b m_b \left[\frac{\partial W(\mathbf{r}_{ab}, h_a)}{\partial \mathbf{r}_{ab}} D_v \mathbf{r}_{ab} + \frac{\partial W(\mathbf{r}_{ab}, h_a)}{\partial h_a} \frac{\partial h_a}{\partial \rho_a} D_v \rho_a \right]$$

$$D_v\rho_a = \frac{1}{\Omega_a} \sum_b m_b \left[\frac{\partial W(\mathbf{r}_{ab}, h_a)}{\partial \mathbf{r}_{ab}} D_v \mathbf{r}_{ab} \right]$$

With: $\Omega_a = 1 - \frac{\partial h_a}{\partial \rho_a} \sum_b m_b \frac{\partial W(\mathbf{r}_{ab}, h_a)}{\partial h_a}$ ← this is just a definition (?)

$= 1 - \sum_b m_b \cdot \frac{\partial W_{ab}}{\partial h_a} \cdot \frac{\partial h_a}{\partial \rho_a}$

SPH from LAP

Now we can substitute $D_v\rho_a$ in the $D_v\pi_{int}$ and we find:

$$D_v\pi_{int} = -\sum_a m_a \frac{p_a}{\rho_a^2} \frac{1}{\Omega_*} \frac{1}{\Omega_*} \sum_b m_b \left[\frac{\partial W(\mathbf{r}_{ab}, h_a)}{\partial \mathbf{r}_{ab}} D_v \mathbf{r}_{ab} \right]$$

Remembering that: $D_v \mathbf{r}_{ab} = \frac{r_a - r_b}{r_{ab}} \cdot (\delta \mathbf{v}_a - \delta \mathbf{v}_b)$

Energy can be expressed as:

$$D_v\pi_{int} = -\sum_a m_a \frac{p_a}{\rho_a^2} \frac{1}{\Omega_a} \sum_b m_b \nabla W_{ab} \cdot (\delta \mathbf{v}_a - \delta \mathbf{v}_b)$$

Re-arranging the summations:

$$D_v\pi_{int} = -\sum_a m_a \left[\sum_b m_b \left(\frac{p_b}{\Omega_b \rho_b^2} \nabla W_{ba} - \frac{p_a}{\Omega_a \rho_a^2} \nabla W_{ab} \right) \right] \delta \mathbf{v}_a$$

SPH from LAP

for h=const we have $\nabla W_{ab} = -\nabla W_{ba}$ and $\Omega_b = 1$

$$D_v \pi_{int} = -\sum_a m_a \left[\sum_b m_b \left(\frac{p_b}{\rho_b^2} + \frac{p_a}{\rho_a^2} \right) \nabla W_{ab} \right] \delta \mathbf{v}_a$$

Recalling that the internal energy dir. Derivative can be expressed also in terms of internal forces $\mathbf{T}_a$ as:

$$D_v \pi_{int} = \sum_a m_a \left(\frac{d\mathbf{v}_a}{dt} \right) \cdot \delta \mathbf{v}_a$$

It is clear that we obtained the same equation as before:

$$\boxed{\frac{d\mathbf{v}_a}{dt} = -\sum_b m_b \left(\frac{p_b}{\rho_b^2} + \frac{p_a}{\rho_a^2} \right) \nabla W_{ab}}$$ MOMENTUM EQ (V)

SPH from LAP

Using Lagrange equation we have obtained the momentum formulation of SPH starting from the density approximation:

$$\langle \rho_a \rangle = \rho_a \cdot \sum_b W(r_a - r_b, h_a) \cdot V_b$$

$$\langle \rho_a \rangle = \sum_b m_b W(\mathbf{r}_a - \mathbf{r}_b, h_a)$$ ← in LAP, we only assume this (p74) ☺

If we differentiate in time we obtain:

$$\frac{\mathrm{d}\rho_a}{\mathrm{d}t} = \rho_a \sum_{b=1}^{N} \mathbf{v}_{ab} \cdot \nabla W_{ab} V_b$$ CONTINUITY EQ (IV)

$m_b = \rho_b \cdot V_b$ ($\rho = \frac{m}{V}$)

$V_b = \left(\frac{m_b}{\rho_b}\right)$

And repeating the same variational procedure we obtain the following formulation for the momentum equation:

$$\frac{d\mathbf{v}_a}{dt} = -\sum_b m_b \left(\frac{p_b + p_a}{\rho_a \rho_b} \right) \nabla W_{ab}$$

Key Components for simulations using SPH

Linking the Equations Together, Closure Submodel 1: Equation of State

SPH Closure Submodels

We will now examine how to close the equations for (i) Gases and (ii) Water using an equation of state.

(i) **For Gases**, the basic equation of state is

$$p = \rho(\gamma - 1)e$$

EoS : $P = f(\rho)$

ρ = density, γ = polytropic index (γ = 1.4 for air), e is the thermal energy.

So, for this system we must solve

(i) continuity equation
(ii) momentum equation
(iii) thermal energy equation