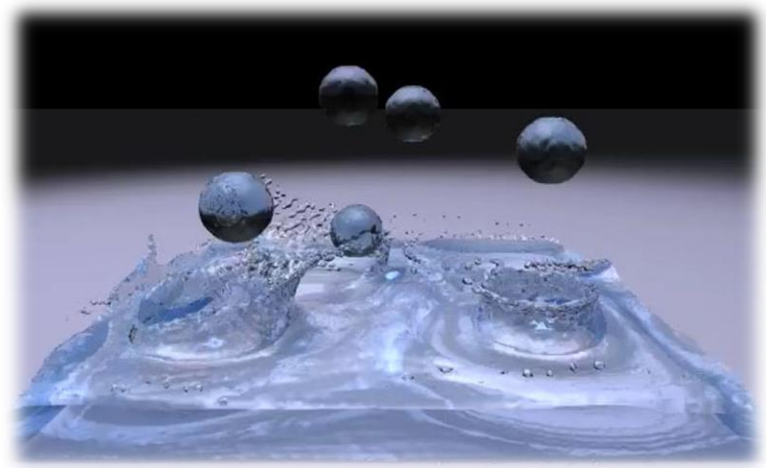

Alternative Numerical Methods in Continuum Mechanics

Smoothed Particle Hydrodynamics

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Mars 2010

Outline

- Introduction
- Basic Concepts and Essential Formulation
- Construction of Smoothing Functions
- SPH for General Dynamic Fluid Flows
- Implementation
- Issues and Limitations
- Conclusion

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Procedure for Numerical Simulations

Physical phenomena — Simplification and extraction of important physics

Mathematical model — Governing equations (PDEs, ODEs, …)

Domain discretization — Mesh/grid, cell, node or particle generation
→ Computational frame

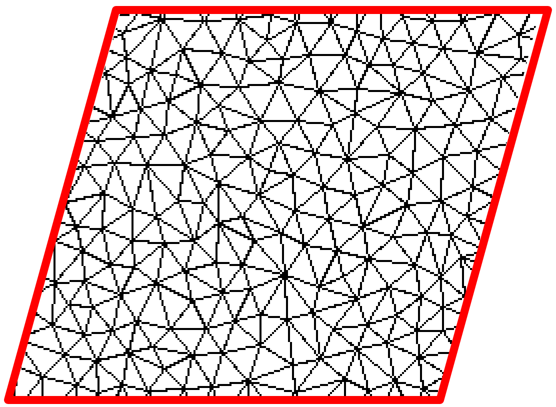
Numerical algorithms — Initial and/or boundary conditions,
Numerical discretization, function approximation
ODE and/or algebraic equation solver

Codind and implementation — Computational accuracy, Speed and storage,
Robustness and user friendlyness

Numerical simulation

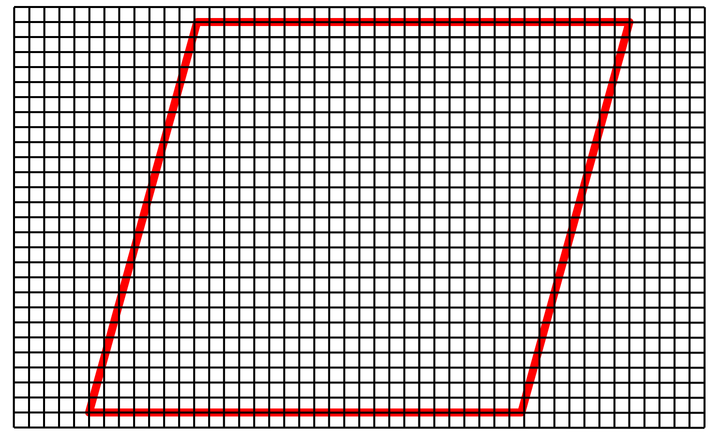
Grid-based Methods

- Lagrangian grid



- Attached on the material
- Does not deal with large deformations (remesh)
- History of all the variables can be easily obtained
- Used by FEM (CSM)

- Eulerian grid



- Fixed in space and with time
- Not easy to treat the irregular or complicated geometries
- Difficult to track moving boundary and interface
- Used by FDM, FVM (CFD)

Meshfree Methods

Key idea:

Provide accurate and stable numerical solutions for governing equations with a set of arbitrarily distributed nodes without using any mesh (~~nodes connectivity~~).

- To cope with problems of grid-based methods, such as free surface, deformable boundary, complex mesh generation, mesh adaptivity and multi-scale resolution.
- Can be coupled with other meshfree methods or conventional numerical ones.
- Used for large deformation and vibration analyses, explosion simulation, …
- 3 types of meshfree methods:
  - Strong form formulation (simple to implement but instable in some cases)
  - Weak form formulation (excellent accuracy but required a background mesh)
  - Particle methods

Meshfree Particle Methods

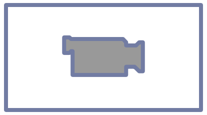
*Employ a set of finite number of discrete **particles** to represent the state of a system and to record its movement.*

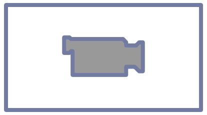
- Particles can be
  - associated with a discrete physical object (stars, atoms, …).
  - generated to represent a part of a continuum domain (fluid particles, …).
- Each particle possesses a set of field variables (mass, position, charge, vorticity, …) for which the evolution is determined by the conservation laws.
- Most MPMs
  - are inherently Lagrangian methods.
  - use explicit methods for the time integration.
- Discretization of complex geometry is simple.
- Refinement of the particles is much easier to perform than the mesh refinement

Smoothed Particle Hydrodynamics

The state of the system is represented by a set of particles, which possess individual material properties and move according to the governing equations.

- Illustrations:





- SPH is not affected by the arbitrariness of the particle distribution.

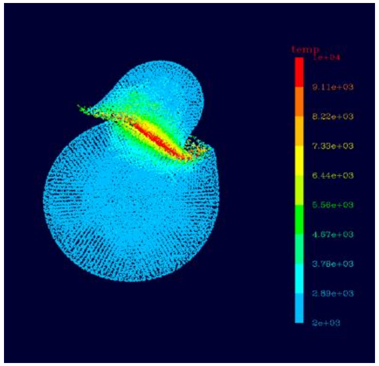
  → *adaptive nature*

- SPH works well even without particle refinement operation.

- In other MPMs, meshfree nodes are only used as interpolation points and do not carry material properties.

Brief History of the SPH Method

- Invention
  - 1977 – Monaghan & Gingold
  - 3D astrophysical problems modeled by classical Newtonian hydrodynamics
- Extension
  - Many areas in astrophysics (discrete formulation)
  - Since 1990s, applied to computational fluid/solid mechanics (discretization of continuum media)
- Applications
  - 1992 – elastic flow
  - 1995 – fracture of brittle solids
  - 1998 – high explosive charge explosion
  - 1999 – flow trough porous media
  - 2000 – metal forming
  - 2002 – atomistic scale simulations



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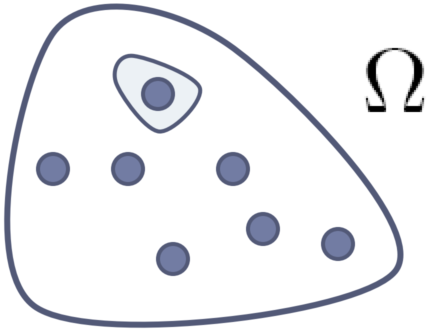
Basic Ideas of SPH

- Domain discretization
  - Set of arbitrarily distributed particles
  - No connectivity is needed



- Numerical discretizations (at each time step)
  1. *Kernel approximation* : field functions approximated by integral representation method (smoothing effect like weak form)

  2. *Particle approximation* : replacing integrations with summations at the neighboring particles in a local domain so-called *support domain* (sparse matrices)

$$\text{PDEs} \xrightarrow{1} \int_\Omega \text{PDEs} \xrightarrow{2} \text{ODEs}$$

Integral Representation of a Function

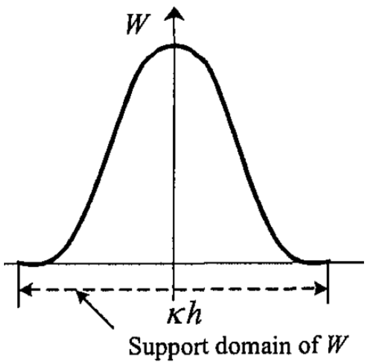
- Starts from

$$f(\mathbf{x}) = \int_\Omega f(\mathbf{x}')\delta(\mathbf{x}-\mathbf{x}')d\mathbf{x}'$$

where f is a continuous function of $\mathbf{x} = (x\ y\ z)^T$ in Ω (*problem domain*) and δ is the Dirac delta function.

- Replacing δ by a *smoothing function* $W(\mathbf{x}-\mathbf{x}', h)$, one gets

$$\boxed{\langle f(\mathbf{x})\rangle \triangleq \int_\Omega f(\mathbf{x}')W(\mathbf{x}-\mathbf{x}', h)d\mathbf{x}'} \quad (1)$$



where W is the so-called *kernel* which usually satisfies :

- even function
- compact condition
- normalization condition
- delta function property when $h \to 0$

second order accuracy (cf. Appendix I)

h = *smoothing length*

Derivative of a Function

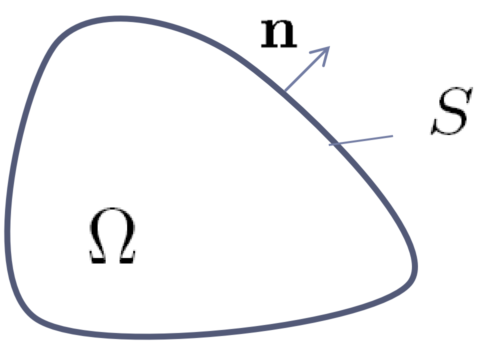
- Substituting $f(\mathbf{x})$ with $\nabla f(\mathbf{x})$ in equation (1), we obtain

$$\langle \nabla f(\mathbf{x}) \rangle = \int_{\Omega} [\nabla f(\mathbf{x}')] W(\mathbf{x}-\mathbf{x}', h) d\mathbf{x}'$$

- Integrating by parts and using the Gauss theorem, one gets

$$< \nabla f(\mathbf{x}) >= \underbrace{\int_{S} f(\mathbf{x}') W(\mathbf{x}-\mathbf{x}', h).\mathbf{n} dS}_{= 0 \text{ if compact support}} - \int_{\Omega} f(\mathbf{x}') \nabla W(\mathbf{x}-\mathbf{x}', h) d\mathbf{x}'$$

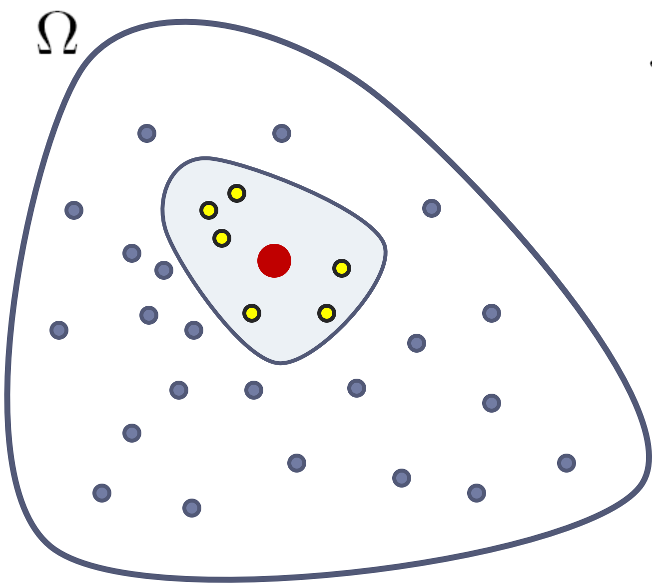
$$\boxed{< \nabla f(\mathbf{x}) >= - \int_{\Omega} f(\mathbf{x}') \nabla W(\mathbf{x}-\mathbf{x}', h) d\mathbf{x}'} \quad (2)$$



- The gradient is determined from the values of f and the derivatives of W rather than from the derivative of f.

Particle approximation (1)

- Aim : Convert continuous integral representation to discretized forms of summation over all the particles in the *support domain.*



$$
\begin{aligned}
f(\mathbf{x}) &= \int_\Omega f(\mathbf{x}')W(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}' \\
&\cong \sum_{j=1}^{N} f(\mathbf{x}_j)W(\mathbf{x}-\mathbf{x}_j,h)\Delta V_j \\
&= \sum_{j=1}^{N} f(\mathbf{x}_j)W(\mathbf{x}-\mathbf{x}_j,h)\frac{1}{\rho_j}(\rho_j \Delta V_j) \\
&= \sum_{j=1}^{N} f(\mathbf{x}_j)W(\mathbf{x}-\mathbf{x}_j,h)\frac{1}{\rho_j}(m_j)
\end{aligned}
$$

Particle of interest (i)

Support domain of i

Neighboring particles of i

$$
\boxed{\langle f(\mathbf{x}_i)\rangle = \sum_{j=1}^{N} \frac{m_j}{\rho_j} f(\mathbf{x}_j)W(\mathbf{x}_i-\mathbf{x}_j,h)}
$$

(**the same for the gradient**)

Other formulations

- Employing these identities

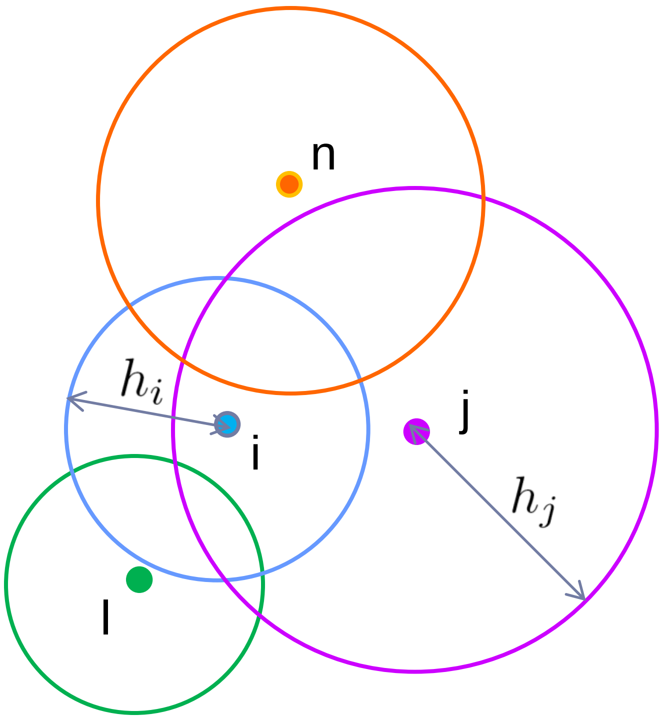
$$\begin{aligned}\nabla f(\mathbf{x}) &= \frac{1}{\rho}\left[\nabla(\rho f(\mathbf{x})) - f(\mathbf{x})\nabla\rho\right]\\ \nabla f(\mathbf{x}) &= \rho\left[\nabla\left(\frac{f(\mathbf{x})}{\rho}\right) + \frac{f(\mathbf{x})}{\rho^2}\nabla\rho\right]\end{aligned}$$

one gets these other equivalent forms

$$\begin{aligned}\nabla f(\mathbf{x}_i) &= \frac{1}{\rho_i}\left[\sum_{j=1}^{N} m_j\left[f(\mathbf{x}_j) - f(\mathbf{x}_i)\right]\nabla_i W_{ij}\right]\\ \nabla f(\mathbf{x}_i) &= \rho_i\left[\sum_{j=1}^{N} m_j\left[\frac{f(\mathbf{x}_j)}{\rho_j^2} + \frac{f(\mathbf{x}_i)}{\rho_i^2}\right]\nabla_i W_{ij}\right]\end{aligned}$$

  - Symmetric forms
  - Linear forms : $\langle \alpha f_1 + \beta f_2\rangle = \alpha\langle f_1\rangle + \beta\langle f_2\rangle$
  - Commutative forms : $\langle f_1\rangle\langle f_2\rangle = \langle f_1 f_2\rangle = \langle f_2 f_1\rangle = \langle f_2\rangle\langle f_1\rangle$

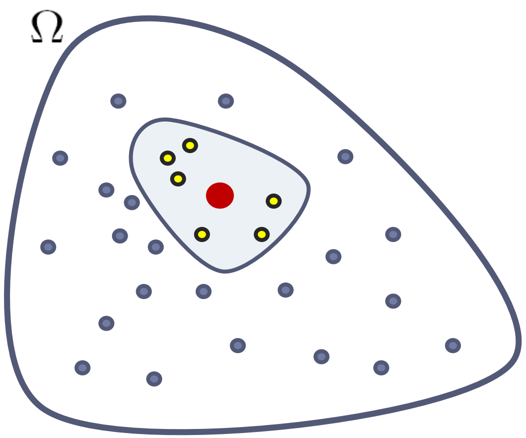
Support and influence domains



- *Support domain* at $\mathbf{x} = (x\ y\ z)^T$ is the domain where the information for all the points inside this domain is used to determine the information at the **point** $\mathbf{x}$.
- *Influence domain* is the domain where a **node** exerts its influences.
- If a node *i* is within the support domain of point $\mathbf{x}$ then node *i* exerts an influence on point $\mathbf{x}$, and then the point $\mathbf{x}$ is within the influence domain of node *i*.
- If $h_i \neq h_j$, $i \in infl(j)$ but $j \notin infl(i)$
  → Nonphysical solution !

Concluding remarks

- SPH method is
  - meshfree
  - particle
  - Lagrangian
  - adaptive



- Domain discretization with moving particles
- Numerical discretization
  - kernel approximation (integration on continuum domain)
  - particle approximation (summation on particles inside the support domain)
- Using of *smoothing function* and *smoothing length*
  - keystones of the SPH method
  - … but have to be determined !

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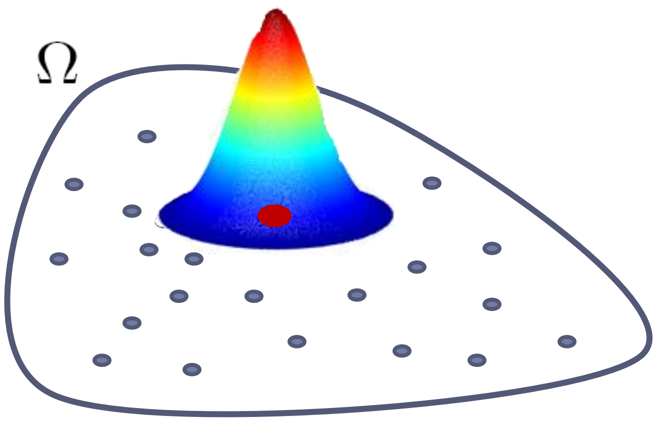
- Construction of Smoothing Functions
- SPH for General Dynamic Fluid Flows
- SPH for Other Fields
- Issues and Limitations
- Conclusion

Introduction

- SPH method employs the integral representation using a *smoothing function*
- *Smoothing functions*
  - Determine the pattern for the function approximation
  - Define the dimension of the support domain
  - Determine the consistency and the accuracy of both the kernel and particle approximations
- Other appellations
  - Smoothing kernel function
  - Smoothing kernel
  - Kernel
- How to construct these functions?



Consistency of the Kernel Approximation (1)

Consistency:

If an approximation can reproduce a polynomial of up to k-th order exactly, the approximation is said to have k-th order or C^k consistency.

- For a constant field function $f(\mathbf{x}) = c$, we should have

$$f(\mathbf{x}) = \int_\Omega c\, W(\mathbf{x}-\mathbf{x}', h)d\mathbf{x}' = c$$

→ $\boxed{\int_\Omega W(\mathbf{x}-\mathbf{x}', h)d\mathbf{x}' = 1}$ (3)

The unity condition is the condition for the kernel approximation to have the 0-th order consistency.

- For a linear function $f(\mathbf{x}) = c_0 + c_1\, \mathbf{x}$, we should have

$$f(\mathbf{x}) = \int_\Omega (c_0 + c_1\, \mathbf{x}')\ W(\mathbf{x}-\mathbf{x}', h)d\mathbf{x}' = c_0 + c_1\, \mathbf{x}$$

→ $\int_\Omega \mathbf{x}'\, W(\mathbf{x}-\mathbf{x}', h)d\mathbf{x}' = \mathbf{x}$ (4)

Consistency of the Kernel Approximation (2)

- Multiplying $\mathbf{x}$ to both side of equation (3), one gets

$$\int_{\Omega} \mathbf{x}\, W(\mathbf{x}-\mathbf{x}', h) d\mathbf{x}' = \mathbf{x} \qquad (5)$$

and subtracting (4) from (5) leads to

$$\boxed{\int_{\Omega} (\mathbf{x}-\mathbf{x}')\, W(\mathbf{x}-\mathbf{x}', h) d\mathbf{x}' = 0} \qquad (6)$$

→ $W(\mathbf{x}-\mathbf{x}', h)$ has to be symmetric.

- Generalization to the *k*-th order

$$\boxed{\int_{\Omega} (\mathbf{x}-\mathbf{x}')^{k}\, W(\mathbf{x}-\mathbf{x}', h) d\mathbf{x}' = 0} \qquad (7)$$

Consistency of the Particle Approximation

- The discrete counterparts of the constant and linear consistency conditions (3) and (6) are

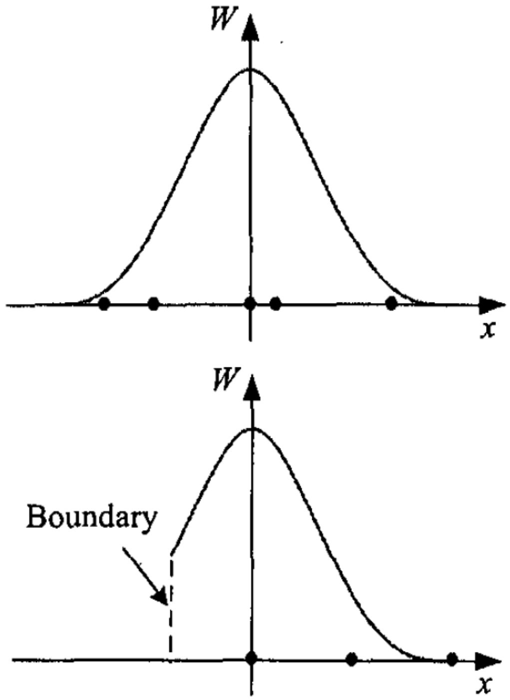
$$\boxed{\sum_{j=1}^{N} W(\mathbf{x}-\mathbf{x}_j,h)\Delta\mathbf{x}_j = 1} \quad \& \quad \boxed{\sum_{j=1}^{N} (\mathbf{x}-\mathbf{x}_j)\,W(\mathbf{x}-\mathbf{x}_j,h)\Delta\mathbf{x}_j = 0}$$

- Other way to establish the consistency conditions:

  → cf. Appendix II and Appendix III

- Consistency of the kernel approximation do not ensure consistency for the discrete form produced after the particle approximation.
  → *Irregular distribution problem*

- The integral and discretized consistency conditions are not always satisfied
  → *Boundary deficiency problem*



Important properties

- The *smoothing function*
  - must be normalized (*unity*),

$$\int_{\Omega} W(\mathbf{x}-\mathbf{x}', h)d\mathbf{x}' = 1$$

  - should be compactly supported (*compact support*),

$$W(\mathbf{x}-\mathbf{x}') = 0 \qquad \text{for} \quad |\mathbf{x}-\mathbf{x}'| > \kappa\, h$$

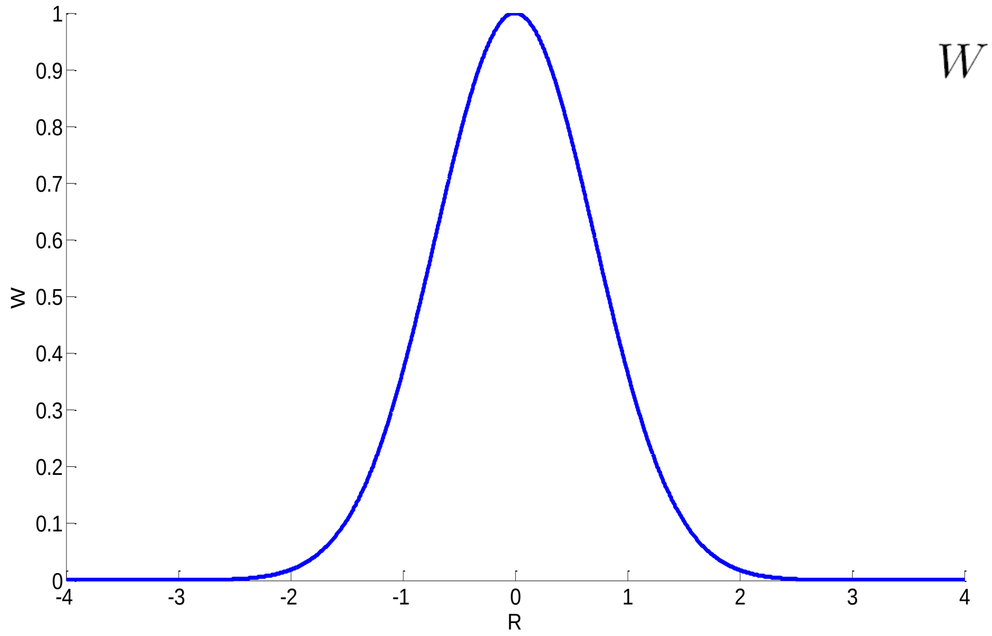
  - must be non negative within the support domain of the particle (*positivity*),
  - should be monotonically decreasing with the distance away from the particle (*decay*),
  - should satisfy the Dirac delta function condition as the *smoothing length* approaches to zero (*delta function property*) ,

$$\lim_{h \to 0} W(\mathbf{x}-\mathbf{x}') = \delta(\mathbf{x}-\mathbf{x}')$$

  - should be an even function (*symmetric property*),
  - should be sufficiently smooth (*smoothness*).

Examples (1)

- Gaussian kernel



$$W(R,h) = \alpha_d \, e^{-R^2}$$

with $R = \dfrac{|\mathbf{x} - \mathbf{x}'|}{h}$

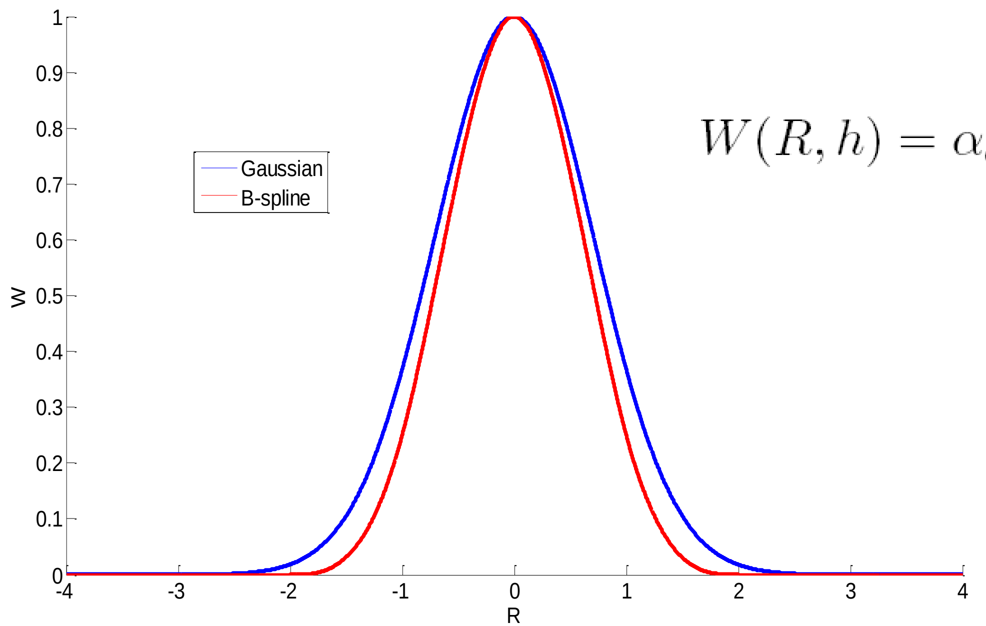
$$\alpha_d = f(d,h)$$

- Sufficiently smooth
- Very stable and accurate
- Not really compact

  → computationally more expensive

Examples (2)

- B-spline or cubic spline function

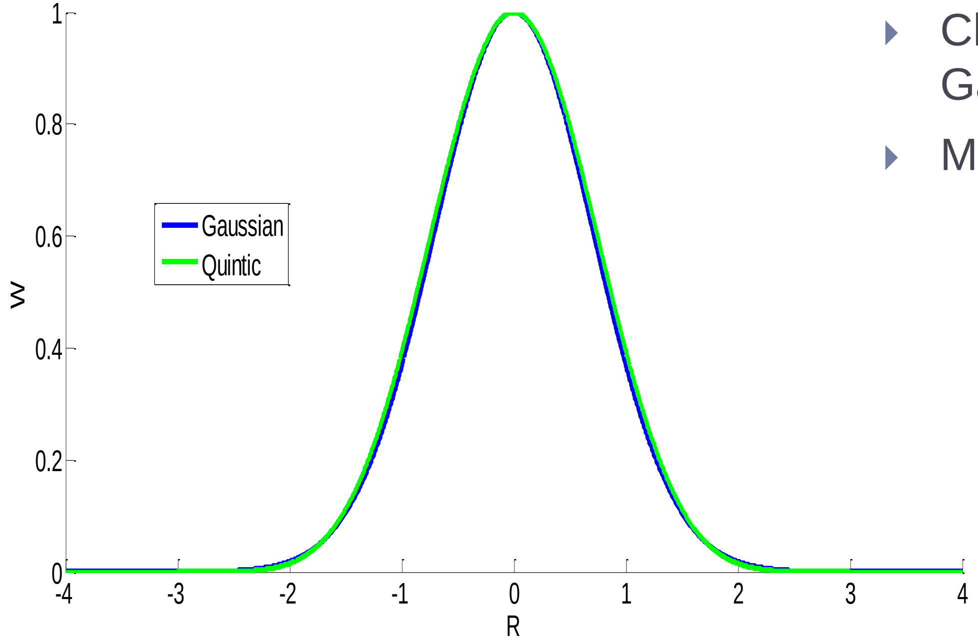


$$W(R,h) = \alpha_d \cdot \begin{cases} \frac{2}{3} - R^2 + \frac{1}{2}R^3 & 0 \le R \le 1 \\ \frac{1}{6}(2-R)^3 & 1 \le R < 2 \\ 0 & R \ge 2 \end{cases}$$

  - Most popular
  - In pieces → more difficult to use
  - Narrower compact support than Gaussian one
  - The 2nd derivative is piecewise linear function

Examples (3)

- Quintic function



- Closely approximating the Gaussian kernel
- More stable than Gaussian kernel

$$W(R,h) = \alpha_d \cdot \begin{cases} (3-R)^5 - 6(2-R)^5 + 15(1-R)^5 & 0 \leq R < 1 \\ (3-R)^5 - 6(2-R)^5 & 1 \leq R < 2 \\ (3-R)^5 & 2 \leq R < 3 \\ 0 & R > 3 \end{cases}$$

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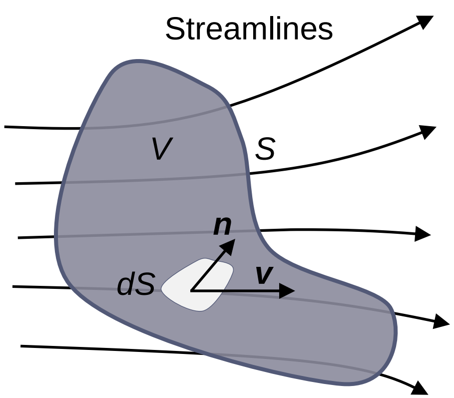
Navier-Stokes equations (1)

- The basic governing equations of fluid dynamics are based on the following 3 fundamental laws of conservation
  - Conservation of mass
  - Conservation of momentum
  - Conservation of energy

- Spatial discretization with SPH formulation



Navier-Stokes PDEs $\xrightarrow{\text{SPH}}$ ODEs $\xrightarrow{\int dt}$ Solution

- SPH method being a Lagrangian method, we should consider the Lagrangian form of these equations.

Navier-Stokes equations (2)

- Remember your fluid dynamics course:

$$\boxed{\begin{aligned} \frac{D\rho}{Dt} &= -\rho \frac{\partial \mathbf{v}^\beta}{\partial \mathbf{x}^\beta} \\ \frac{D\mathbf{v}^\alpha}{Dt} &= \frac{1}{\rho}\frac{\partial \sigma^{\alpha\beta}}{\partial \mathbf{x}^\beta} \\ \frac{De}{Dt} &= \frac{\sigma^{\alpha\beta}}{\rho}\frac{\partial \mathbf{v}^\alpha}{\partial \mathbf{x}^\beta} \end{aligned}}$$

$$\left\{\begin{aligned} \sigma^{\alpha\beta} &= -p\delta^{\alpha\beta} + \tau^{\alpha\beta} \\ \tau^{\alpha\beta} &= \mu\epsilon^{\alpha\beta} \qquad \text{(for Newtonian fluids)} \\ \epsilon^{\alpha\beta} &= \frac{\partial \mathbf{v}^\beta}{\partial \mathbf{x}^\alpha} + \frac{\partial \mathbf{v}^\alpha}{\partial \mathbf{x}^\beta} - \frac{2}{3}(\nabla \cdot \mathbf{v})\delta^{\alpha\beta} \end{aligned}\right.$$

$$\longrightarrow \quad \boxed{\frac{De}{Dt} = -\frac{p}{\rho}\frac{\partial \mathbf{v}^\beta}{\partial \mathbf{x}^\beta} + \frac{\mu}{2\rho}\epsilon^{\alpha\beta}\epsilon^{\alpha\beta}}$$

  - Having neglected the heat flux and the body forces
  - The total time derivatives are taken in the moving Lagrangian frame
  - Greek superscripts are used to denote the coordinate directions

Particle Approximation of Density (1)

- The density approximation is very important in the SPH method since density determines the particle distribution and the *smoothing length* evolution.

- 2 approaches to evolve density
  - *Summation density* : applies the SPH approx to ρ itself
  - *Continuity density* : approximates ρ according to the continuity equation

- <u>*Summation approach*</u>

$$\rho_i = \sum_{j=1}^{N} \frac{m_j}{\rho_j} \rho_j W_{ij} \longrightarrow \boxed{\rho_i = \sum_{j=1}^{N} m_j W_{ij}} \quad (1)$$

  - The density of a particle can be approximated by the weighted average of density of the neighboring particles.

Particle Approximation of Density (2)

- *Continuity approach*

$$\frac{D\rho_i}{Dt} = -\rho_i \frac{\partial \mathbf{v}_i^\beta}{\partial \mathbf{x}_i^\beta} = -\rho_i \sum_{j=1}^{N} \frac{m_j}{\rho_j} \mathbf{v}_j^\beta \frac{\partial W_{ij}}{\partial \mathbf{x}_j^\beta} \qquad (2)$$

- Since

$$0 = \nabla 1 = \int 1 \cdot \nabla W(\mathbf{x} - \mathbf{x}', h) d\mathbf{x}' = \sum_{j=1}^{N} \frac{m_j}{\rho_j} \frac{\partial W_{ij}}{\partial \mathbf{x}_i^\beta}$$

- Thus

$$0 = \rho_i \mathbf{v}_i^\beta \left(\sum_{j=1}^{N} \frac{m_j}{\rho_j} \frac{\partial W_{ij}}{\partial \mathbf{x}_i^\beta} \right) = \rho_i \sum_{j=1}^{N} \frac{m_j}{\rho_j} \mathbf{v}_i^\beta \frac{\partial W_{ij}}{\partial \mathbf{x}_i^\beta} \qquad (3)$$

- (2) + (3) :

$$\boxed{\frac{D\rho_i}{Dt} = \rho_i \sum_{j=1}^{N} \frac{m_j}{\rho_j} \mathbf{v}_{ij}^\beta \frac{\partial W_{ij}}{\partial \mathbf{x}_i^\beta}} \qquad \mathbf{v}_{ij}^\beta = \mathbf{v}_i^\beta - \mathbf{v}_j^\beta \qquad (4)$$

Particle Approximation of Density (3)

- Other formulations

  - $$\frac{D\rho}{Dt} = -\rho \frac{\partial \mathbf{v}^\beta}{\partial \mathbf{x}^\beta} = -\left(\frac{\partial(\rho \mathbf{v}^\beta)}{\partial \mathbf{x}^\beta} - \mathbf{v}^\beta \frac{\partial \rho}{\partial \mathbf{x}^\beta} \right)$$

$$\boxed{\frac{D\rho_i}{Dt} = \sum_{j=1}^{N} m_j \mathbf{v}_{ij}^\beta \frac{\partial W_{ij}}{\partial \mathbf{x}_i^\beta}} \qquad (5)$$

  - *Modified summation density approach* :

This expression improves the accuracy near both the free boundaries and the material interfaces with a density discontinuity. It is well suited for simulating general fluid flow problem without discontinuities such as shock waves (cf. later CSPM).

$$\boxed{\rho_i = \frac{\sum_{j=1}^{N} m_j W_{ij}}{\sum_{j=1}^{N} \frac{m_j}{\rho_j} W_{ij}}} \qquad (6)$$

Particle Approximation of Density (4)

- *Density summation* (1)
  - The total mass is exactly conserved.
  - Edge effects appear when being applied to particles at the boundary of the fluid domain or near the material interfaces (*boundary particle deficiency*).

    → Normalized SPH (cf. eq (6))
  - More computational efforts
  - More popular
  - Used for simulating general fluid phenomena

- *Continuity density* (4) & (5)
  - Related to the relative velocities between the particles
  - The total mass is not exactly conserved.
  - Faster and can be parallelized
  - Used for simulating events with strong discontinuity (explosion, HVI, …)

Particle Approximation of Momentum (1)

- Momentum equation

$$\frac{D\mathbf{v}_i^{\alpha}}{Dt} = \frac{1}{\rho_i}\frac{\partial \sigma_i^{\alpha\beta}}{\partial \mathbf{x}^{\beta}} = \frac{1}{\rho_i}\sum_{j=1}^{N}\frac{m_j}{\rho_j}\sigma_j^{\alpha\beta}\frac{\partial W_{ij}}{\partial x_i^{\beta}}$$

- Adding

$$0 = \frac{\sigma_i^{\alpha\beta}}{\rho_i}\sum_{j=1}^{N}\frac{m_j}{\rho_j}\frac{\partial W_{ij}}{\partial \mathbf{x}_i^{\beta}} = \sum_{j=1}^{N} m_j \frac{\sigma_i^{\alpha\beta}}{\rho_i\rho_j}\frac{\partial W_{ij}}{\partial \mathbf{x}_i^{\beta}}$$

- One gets the symmetric form :

$$\boxed{\frac{D\mathbf{v}_i^{\alpha}}{Dt} = \sum_{j=1}^{N} m_j \frac{\sigma_i^{\alpha\beta} + \sigma_j^{\alpha\beta}}{\rho_i\rho_j}\frac{\partial W_{ij}}{\partial \mathbf{x}_i^{\beta}}}$$

Particle Approximation of Momentum (2)

- Using

$$\begin{cases} \sigma^{\alpha\beta} = -p\delta^{\alpha\beta} + \tau^{\alpha\beta} \\ \tau^{\alpha\beta} = \mu\epsilon^{\alpha\beta} \quad \text{(for Newtonian fluids)} \\ \epsilon^{\alpha\beta} = \dfrac{\partial \mathbf{v}^\beta}{\partial \mathbf{x}^\alpha} + \dfrac{\partial \mathbf{v}^\alpha}{\partial \mathbf{x}^\beta} - \dfrac{2}{3}(\nabla \cdot \mathbf{v})\delta^{\alpha\beta} \end{cases}$$

- one gets

$$\boxed{\frac{D\mathbf{v}_i^\alpha}{Dt} = -\sum_{j=1}^{N} m_j \frac{p_i + p_j}{\rho_i \rho_j} \frac{\partial W_{ij}}{\partial \mathbf{x}_i^\alpha} + \sum_{j=1}^{N} m_j \frac{\mu_i \epsilon_i^{\alpha\beta} + \mu_j \epsilon_j^{\alpha\beta}}{\rho_i \rho_j} \frac{\partial W_{ij}}{\partial \mathbf{x}_i^\beta}}$$

with $$\boxed{\epsilon_i^{\alpha\beta} = \sum_{j=1}^{N} \frac{m_j}{\rho_j} \mathbf{v}_j^\beta \frac{\partial W_{ij}}{\partial \mathbf{x}_i^\alpha} + \sum_{j=1}^{N} \frac{m_j}{\rho_j} \mathbf{v}_j^\alpha \frac{\partial W_{ij}}{\partial \mathbf{x}_i^\beta} - \left(\frac{2}{3} \sum_{j=1}^{N} \frac{m_j}{\rho_j} \mathbf{v}_j \cdot \nabla_i W_{ij} \right) \delta^{\alpha\beta}}$$

Particle Approximation of Energy

- Energy equation :

$$\frac{De}{Dt} = -\frac{p}{\rho}\frac{\partial \mathbf{v}^\beta}{\partial \mathbf{x}^\beta} + \underbrace{\frac{\mu}{2\rho}\epsilon^{\alpha\beta}\epsilon^{\alpha\beta}}_{\text{known from the previous slide}}$$

- First term

$$-\frac{p}{\rho}\frac{\partial \mathbf{v}^\beta}{\partial \mathbf{x}^\beta} = \frac{p}{\rho^2}\left(-\rho\frac{\partial \mathbf{v}^\beta}{\partial \mathbf{x}^\beta}\right) = \frac{p}{\rho^2}\frac{D\rho}{Dt}$$

which can be approximated by directly using the continuity equation.

- Other formulation

$$\boxed{\frac{De_i}{Dt} = \frac{1}{2}\sum_{j=1}^{N} m_j \frac{p_i + p_j}{\rho_i \rho_j}\mathbf{v}_{ij}^\beta \frac{\partial W_{ij}}{\partial \mathbf{x}_i^\beta} + \frac{\mu_i}{2\rho_i}\epsilon_i^{\alpha\beta}\epsilon_i^{\alpha\beta}}$$

Numerical Aspects

- *Artificial viscosity*
  - Special treatments are required to model shock wave, or else the simulation will develop unphysical oscillations in the numerical results.
  - Application of the conservation laws across a shock wave front requires the simulation of creation of entropy.
  - This energy transformation can be represented as a form of viscous dissipation.
  - This idea leads to the *artificial viscosity* concept, which spread the shock wave and regularize the numerical instabilities.

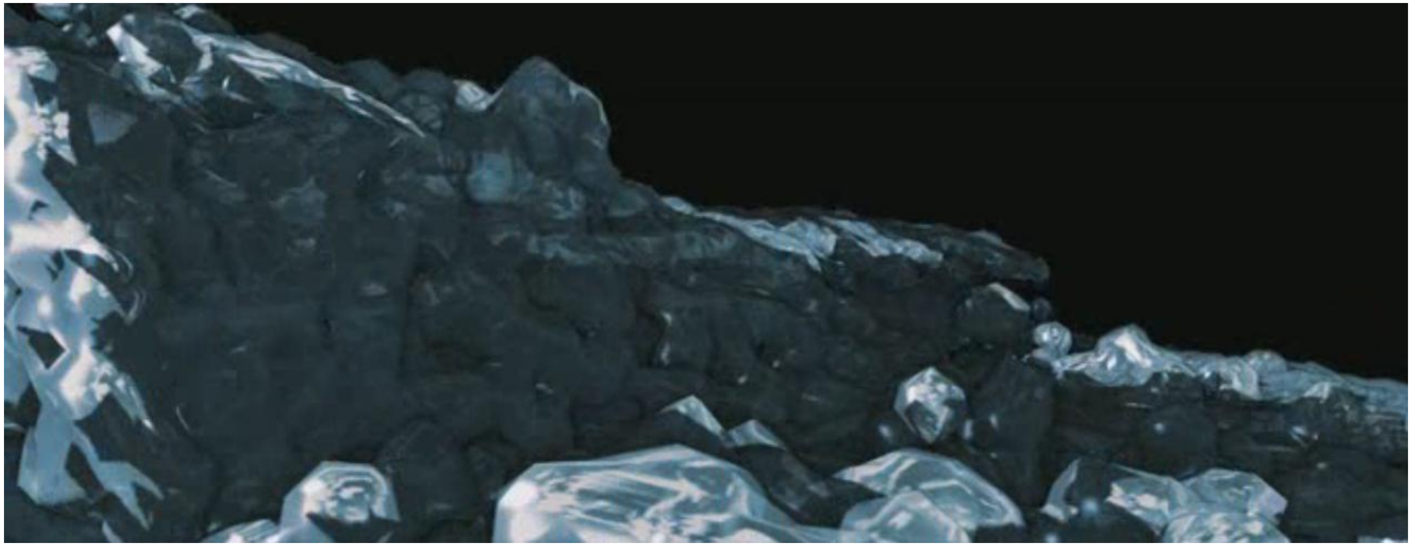
- *Artificial heat*
  - The *artificial viscosity* generates excessive heating under some circumstances.
  - This can be fixed by adding an artificial heat conduction term to the energy equation.

SPH form of the Navier-Stokes equations

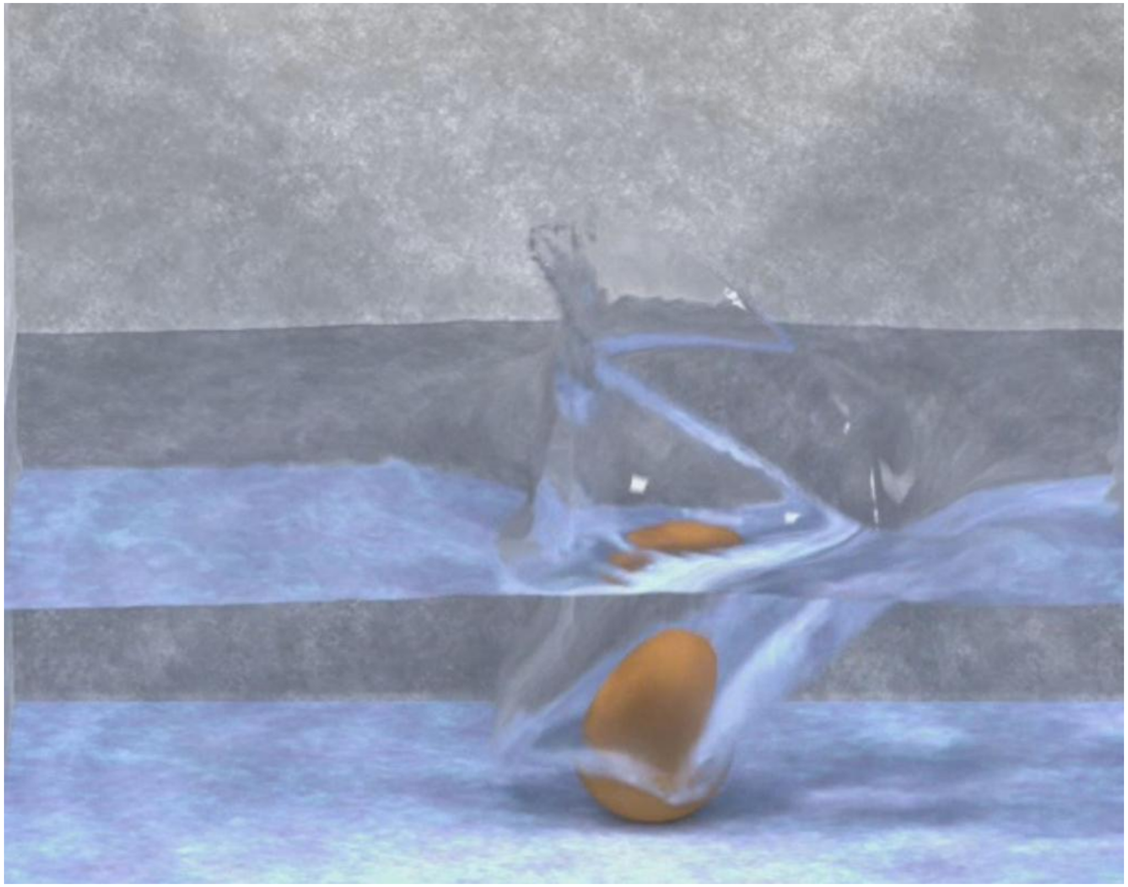
- Taking into account the *artificial viscosity* Π_{ij} and *artificial heat* H_i , one finally gets

$$
\begin{aligned}
\frac{D\rho_i}{Dt} &= \sum_{j=1}^{N} m_j \mathbf{v}_{ij}^{\beta} \frac{\partial W_{ij}}{\partial \mathbf{x}_i^{\beta}} \\
\frac{D\mathbf{v}_i^{\alpha}}{Dt} &= -\sum_{j=1}^{N} m_j \left(\frac{\sigma_i^{\alpha\beta}}{\rho_i^2} + \frac{\sigma_j^{\alpha\beta}}{\rho_j^2} + \Pi_{ij} \right) \frac{\partial W_{ij}}{\partial \mathbf{x}_i^{\beta}} \\
\frac{De_i}{Dt} &= \frac{1}{2} \sum_{j=1}^{N} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} + \Pi_{ij} \right) \mathbf{v}_{ij}^{\beta} \frac{\partial W_{ij}}{\partial \mathbf{x}_i^{\beta}} + \frac{\mu_i}{2\rho_i} \epsilon_i^{\alpha\beta} \epsilon_i^{\alpha\beta} + H_i
\end{aligned}
$$

SPH in Fluid Dynamics : Illustration (1)



SPH in Fluid Dynamics : Illustration (2)



Outline

- Introduction
- Basic Concepts and Essential Formulation
- Construction of Smoothing Functions
- SPH for General Dynamic Fluid Flows
- <u>Implementation</u>
- Issues and Limitations
- Conclusion

Variable Smoothing Length

- The smoothing length has direct influence on the efficiency of the computation and the accuracy of the solution.
  - If h too small : low accuracy
  - If h too large : low accuracy and high computational effort
- First, h depended on the initial average density. Now, an individual smoothing length is assigned each particle according to the local density.
- The smoothing length can vary both in space and time and can be a scalar, a vector or a tensor.
- Many ways to evolve h :

$$h = h_0 \left(\frac{\rho_0}{\rho} \right)^{1/d} \qquad \frac{dh}{dt} = -\frac{1}{d} \frac{h}{\rho} \frac{d\rho}{dt}$$

Symmetrization of Particle Interaction

- Hence previous slides, each particle has its own smoothing length. Therefore, the influencing domain of particle i may cover particle j but not necessarily vice versa (violation of the action-reaction law)

- 2 approaches to preserve the symmetry of particle interaction
  - Symmetric smoothing length

$$h_{ij} = \frac{h_i + h_j}{2} \qquad h_{ij} = \frac{2h_i h_j}{h_i + h_j}$$

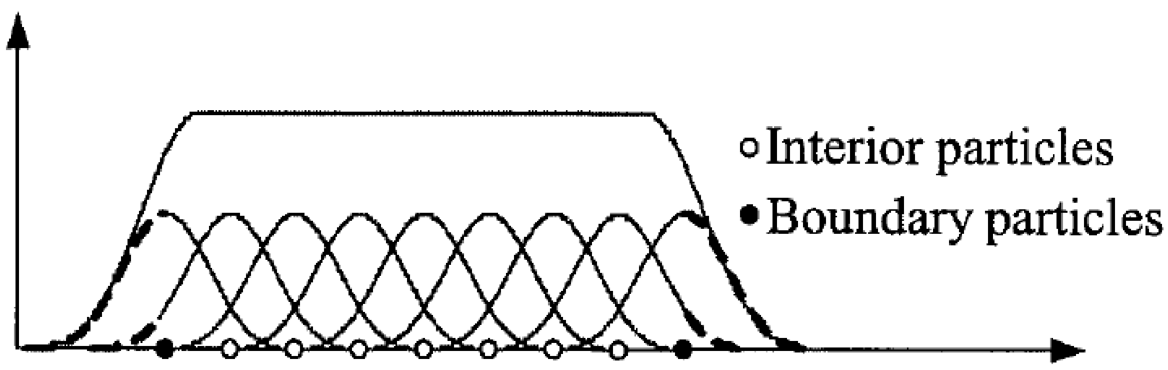
$$h_{ij} = \min(h_i, h_j) \qquad h_{ij} = \max(h_i, h_j)$$

  - Average of smoothing function

$$W_{ij} = \frac{1}{2}\left(W(h_i) + W(h_j)\right)$$

Boundary Treatment (1)

- One of the largest problem of SPH is the particle deficiency near or on the boundary. The truncated integrals (*cf.* slide 21) result in the violation of the consistency conditions.

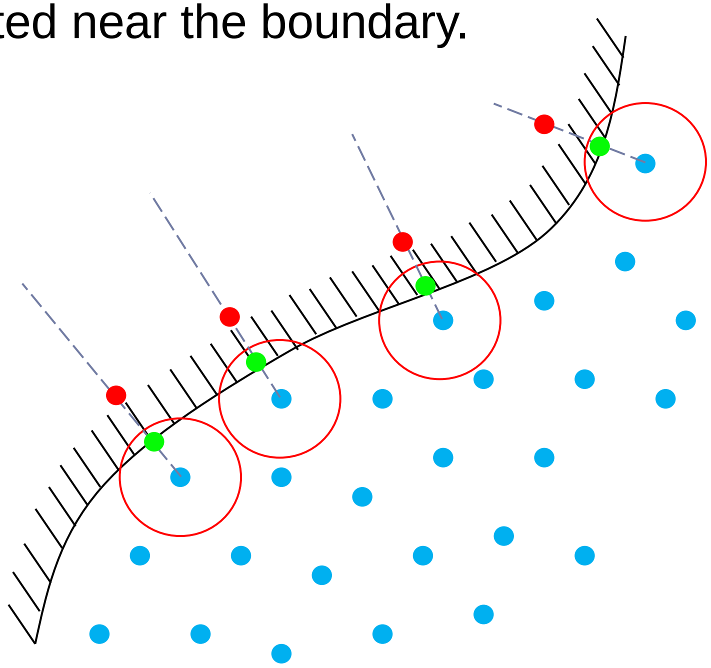


- Lots of treatments have been proposed:
  - Monaghan : ghost particles producing a repulsive force near the boundary
  - Campbell : used the completed definition of the original kernel gradient
  - Libersky & Petschek : used a symmetrical surface boundary condition

Boundary Treatment (2)

- Liu has used 2 types of virtual particles :
  - Type I : to produce a highly repulsive force near the boundary
  - Type II : to recover consistency conditions
- A type II virtual particle is placed symmetrically on the outside of the boundary if the concerned real particle is located near the boundary.

  This added particle has the same density and pressure but opposite velocity.
- To prevent real particles from penetrating outside the boundary, type I virtual particles are placed on the boundary.



Nearest Neighboring Particle Searching (1)

- To perform the particle approximation, one needs to find the particles in the support domain of the concerned particle (NNPS methods).

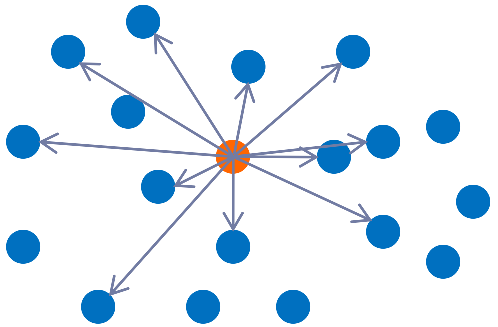
- Unlike a grid-based method (FEM, FVM,…) the neighboring elements can vary with time.

- 4 techniques are commonly used :

1. <u>All-pair search</u>

   This approach calculates the distance r_{ij} from i to each and every particle j .

   - Complexity : $O(N^2)$
   - Computational time too long
   - Used for problems of very small scale

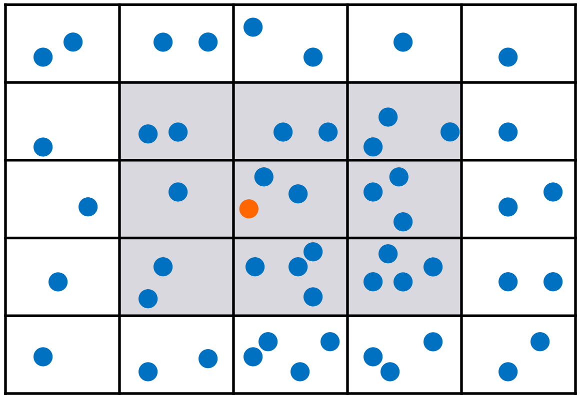


Nearest Neighboring Particle Searching (2)

2. <u>Linked-list algorithm</u>

In this method, a temporary mesh is overlaid on the problem domain. The mesh spacing is selected to match the dimension of the support domain.

Then, the nearest neighboring particles of a particle i can only be in the same grid cell or the adjoining ones.

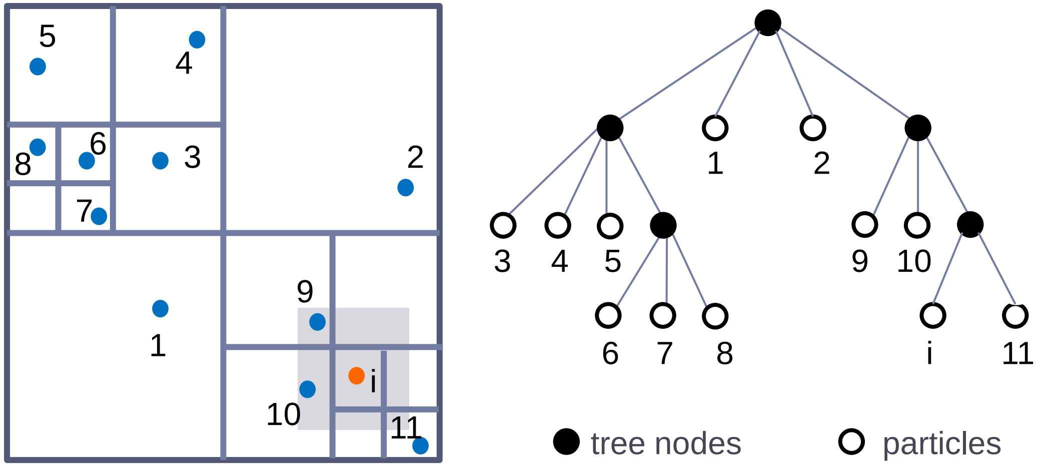


- Complexity : $O(N)$ if the particle density of the cells is sufficiently small.
- Mesh spacing may not be optimal when variable smoothing length is used.

Nearest Neighboring Particle Searching (3)

3. <u>Tree search algorithm</u>

Tree method recursively splits the problem domain into octants that contain particles, until just one left.



For a particle i , a $2h_i$ side cube is used to enclose the particle. The tree search algorithm is performed by checking if the volume of this cube overlaps with the volume represented by the current node.

- Complexity : $O(N \log N)$
- Very efficient and robust especially for particles for variable smoothing lengths
- Can not deal with anisotropy

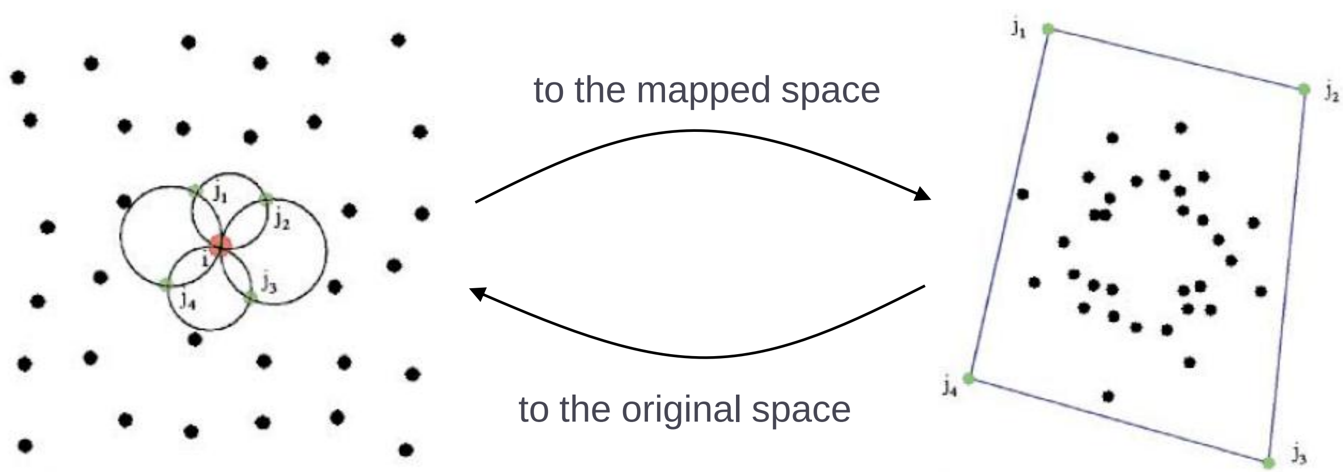
Nearest Neighboring Particle Searching (4)

4. <u>Fast-running convex hull algorithm</u>

- An *inverse square mapping* is used to find a minimal set of neighbors which make up a shell surrounding the particle in question. This mapping is given by

$$\mathbf{x}'_j = \frac{\mathbf{x}_j - \mathbf{x}_i}{|\mathbf{x}_j - \mathbf{x}_i|^2}$$

- This transformation simplifies the search and makes the algorithm faster.

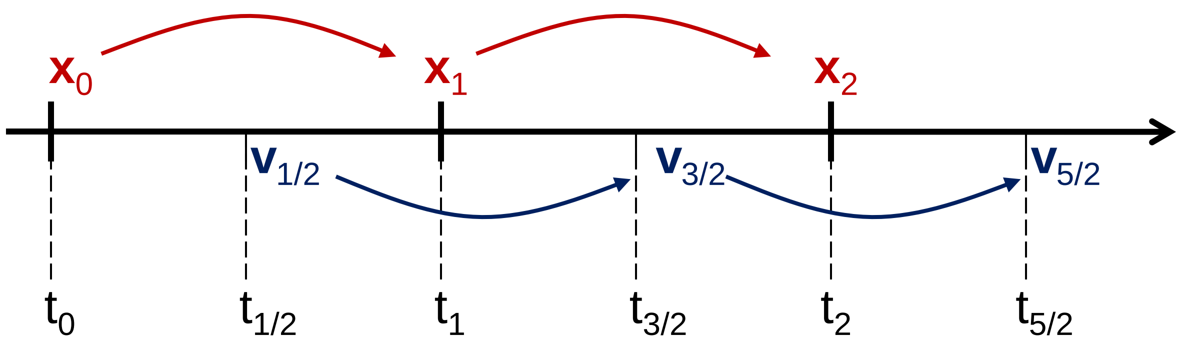


Time integration (1)

- The discrete SPH equations can be integrated with standard methods such as Runge Kutta, predictor-corrector and the second order accurate Leap-Frog schemes.

- Characteristics of the Leap-Frog algorithm
  - Low memory storage required in the computation
  - Efficiency for one force evaluation per step
  - If the smoothing lengths become very small, the time step can become very small to be prohibitive → Runge-Kutta with adaptive time-step is therefore advised.

- Principle



Time integration (2)

- The explicit time integration schemes are subject to the CFL (Courant-Friedrichs-Levy) condition for stability.

- This condition states that the maximum speed of numerical propagation must exceed the maximum speed of physical propagation, which requires the time step to be proportional to the smallest spatial particle resolution.

- In SPH applications, this is represented as

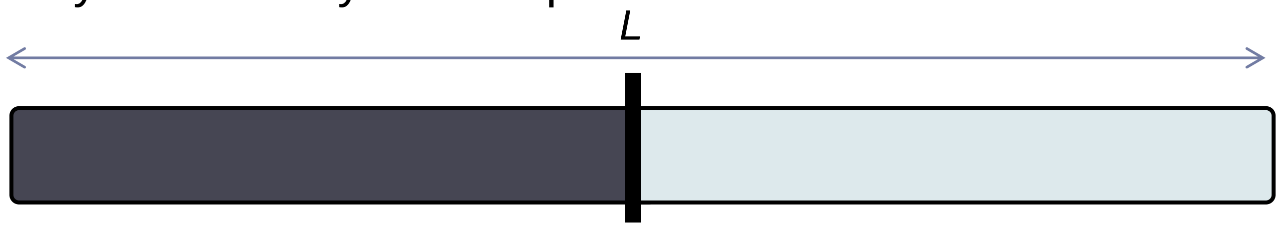
$$\Delta t = \min_i \left(\frac{h_i}{c_i} \right)$$

where c_i is the sound celerity at particle i.

Example – Shock tube problem (1)

- A good numerical benchmark that was investigated by many researchers when studying the SPH method. Exact solution is available.

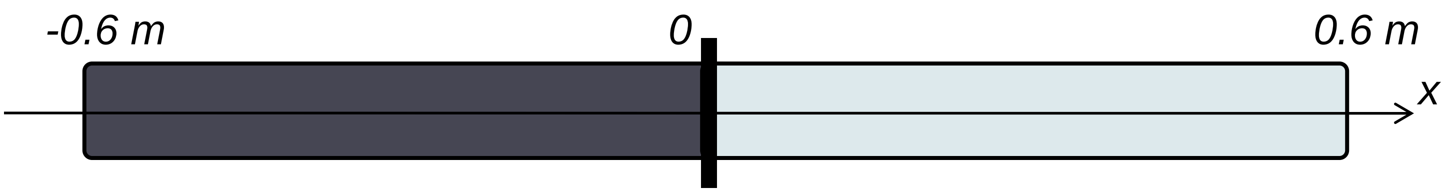
- The shock tube is a long straight tube filled with gas, which is separated by a membrane into two parts of different pressures and densities but are individually in thermodynamic equilibrium.



- When the membrane is taken away the following are produced
  - a *shock wave* - moves into the region with lower density,
  - a *rarefaction wave* - moves into the region with high density
  - a *contact discontinuity* – forms in center and travels into the low-density region, behind the shock

Example – Shock tube problem (2)

- Initial conditions



$$\begin{aligned} \rho &= 1\ kg/m^3 \\ \mathbf{v} &= 0\ m/s \\ e &= 2.5\ J/kg \\ p &= 1\ N/m^2 \\ \Delta x &= 0.001875\ m \\ m &= 0.001875\ kg \end{aligned} \qquad \begin{aligned} \rho &= 0.25\ kg/m^3 \\ \mathbf{v} &= 0\ m/s \\ e &= 1.795\ J/kg \\ p &= 0.1795\ N/m^2 \\ \Delta x &= 0.0075\ m \\ m &= 0.001875\ kg \end{aligned}$$

- The time step is set as 0.001*s* and the simulation is ran for 200 time steps.
- The equation of state for the ideal gas is used (with $\gamma = 1.4$)
- The cubic spline form is used for the smoothing function
- 400 particles of the same mass are used (320 on the left, 80 on the right)

Example – Shock tube problem (3)

- The equations are the Euler equations for evolving density, momentum and energy

$$
\begin{aligned}
\frac{D\rho_i}{Dt} &= \sum_{j=1}^{N} m_j (\mathbf{v}_i - \mathbf{v}_j) \cdot \nabla_i W_{ij} \\
\frac{Dv_i}{Dt} &= -\sum_{j=1}^{N} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} + \Pi_{ij} \right) \nabla_i W_{ij} \\
\frac{De_i}{Dt} &= \frac{1}{2} \sum_{j=1}^{N} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} + \Pi_{ij} \right) (\mathbf{v}_i - \mathbf{v}_j) \nabla_i W_{ij} \\
\frac{D\mathbf{x}_i}{Dt} &= \mathbf{v}_i
\end{aligned}
$$

- Note that the summation density approach can also be used

$$
\rho_i = \sum_{j=1}^{N} m_j W_{ij}
$$

Example – Shock tube problem (4)

- In resolving the shock, the Monaghan type artificial viscosity (Monaghan, 1992) is used, which also solves to prevent unphysical penetration:

$$\Pi_{ij} = \begin{cases} \dfrac{\phi_{ij}^2 - \bar{c_{ij}}\phi_{ij}}{\bar{\rho_{ij}}}, & \mathbf{v}_{ij} \cdot \mathbf{x}_{ij} < 0 \\ 0, & \mathbf{v}_{ij} \cdot \mathbf{x}_{ij} \leq 0 \end{cases}$$

with

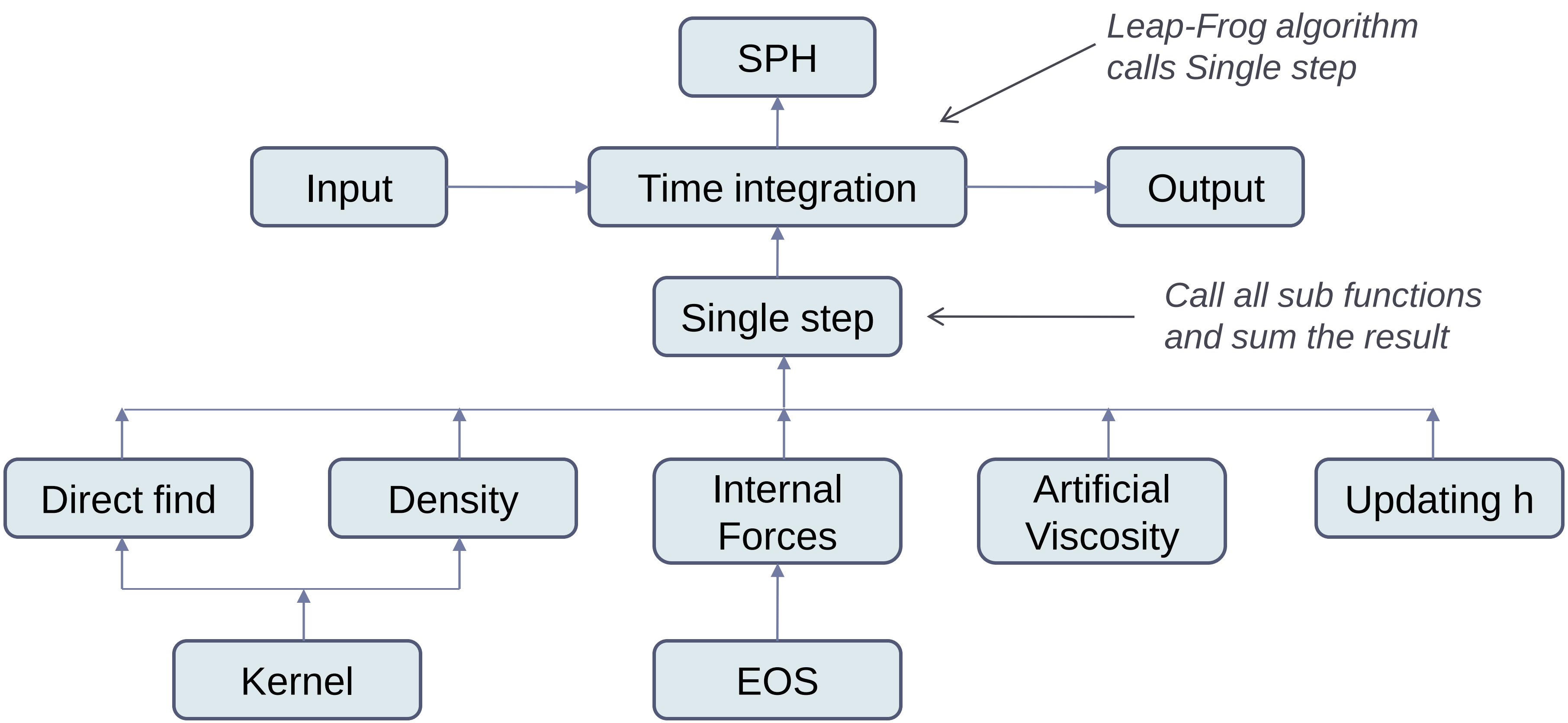
$$\begin{aligned} \phi_{ij} &= \frac{h_{ij}\mathbf{v}_{ij} \cdot \mathbf{x}_{ij}}{|\mathbf{x}_{ij}|^2 + 0.01 h_{ij}^2} \\ \bar{c_{ij}} &= \frac{1}{2}(c_i + c_j) \\ \bar{\rho_{ij}} &= \frac{1}{2}(\rho_i + \rho_j) \\ h_{ij} &= \frac{1}{2}(h_i + h_j) \end{aligned}$$

and

$$\begin{aligned} \mathbf{v}_{ij} &= \mathbf{v}_i - \mathbf{v}_j \\ \mathbf{x}_{ij} &= \mathbf{x}_i - \mathbf{x}_j \end{aligned}$$

Example – Shock tube problem (5)

- Code structure

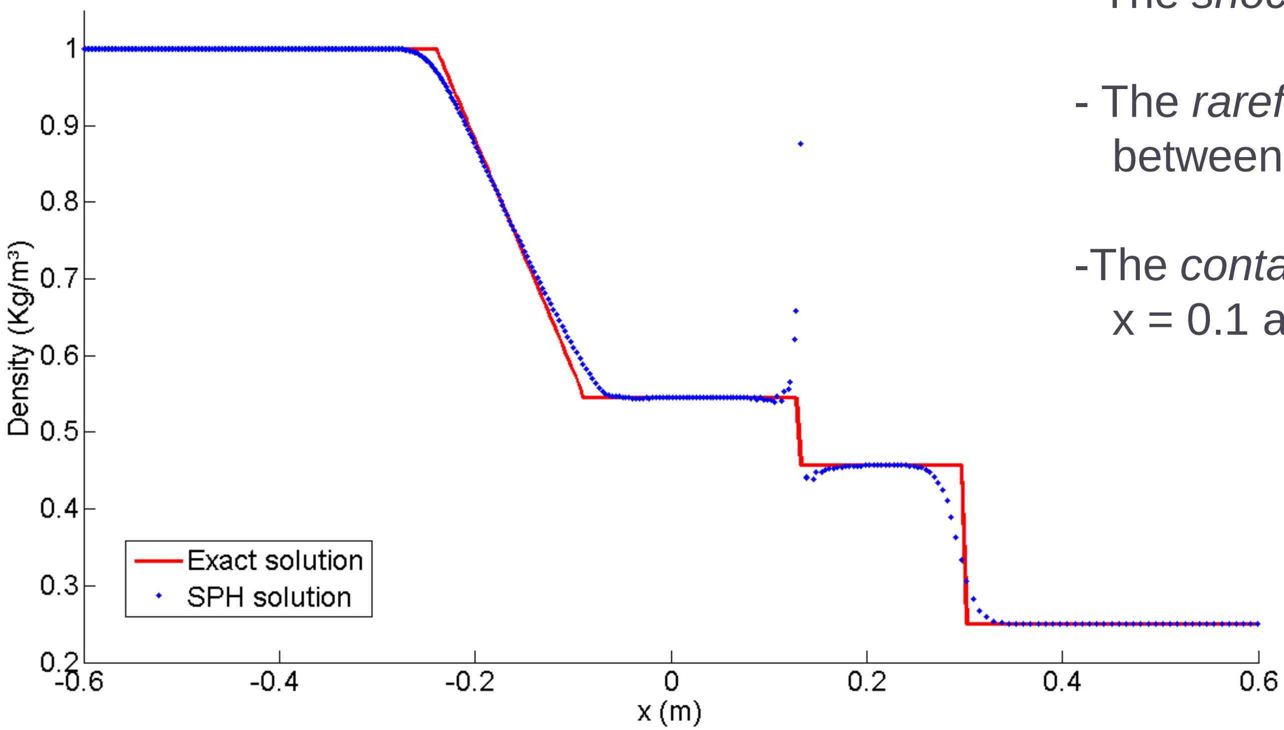


Example – Shock tube problem (6)

- Results
  - The shock wave moves into the low-density region (from left to right)
  - The rarefaction wave (reduction in density) moves into the high-density region (from right to left)
  - The contact discontinuity forms in center and travels into the low-density region, behind the shock
  - The contact discontinuity can not be treated with traditional SPH because this formulation suppose the field function to be continuous *a priori*.
  - To perform more accurate simulation, we need another formulation : DSPM

Example – Shock tube problem (7)

- Results – Density profiles in the shock tube at *t = 0.20 s*



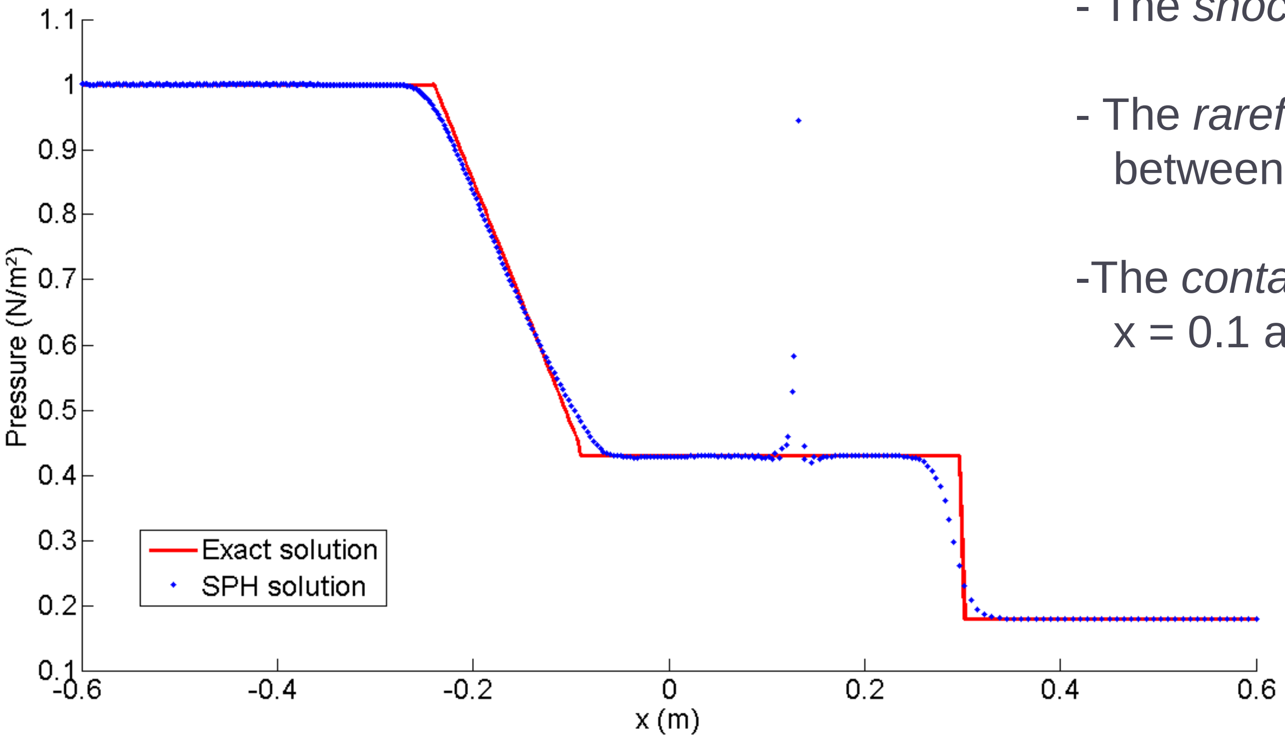
- The *shock* is observed around x = 0.3

- The *rarefaction wave* is located between x = -0.3 and x = 0

-The *contact discontinuity* is between x = 0.1 and x = 0.2.

Example – Shock tube problem (8)

- Results – Pressure profiles in the shock tube at *t = 0.20 s*



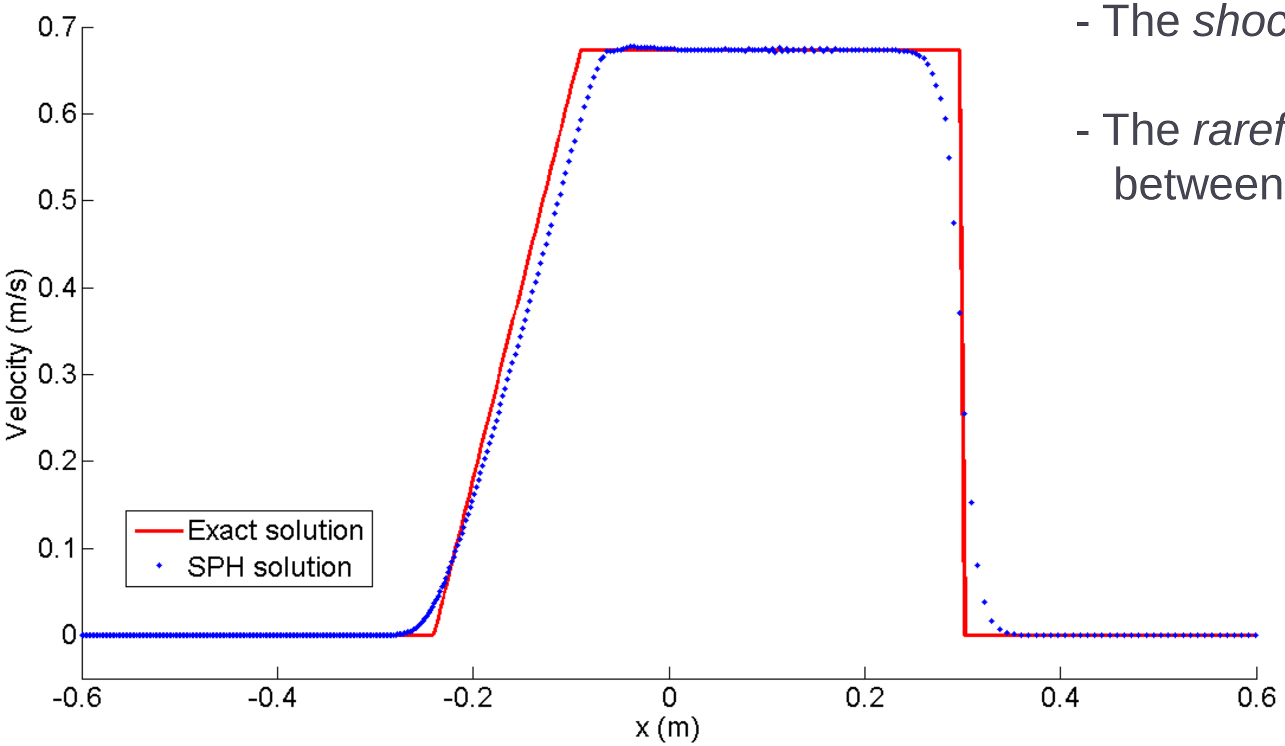
- The *shock* is observed around x = 0.3

- The *rarefaction wave* is located between x = -0.3 and x = 0

-The *contact discontinuity* is between x = 0.1 and x = 0.2.

Example – Shock tube problem (9)

- Results – Velocity profiles in the shock tube at *t = 0.20 s*

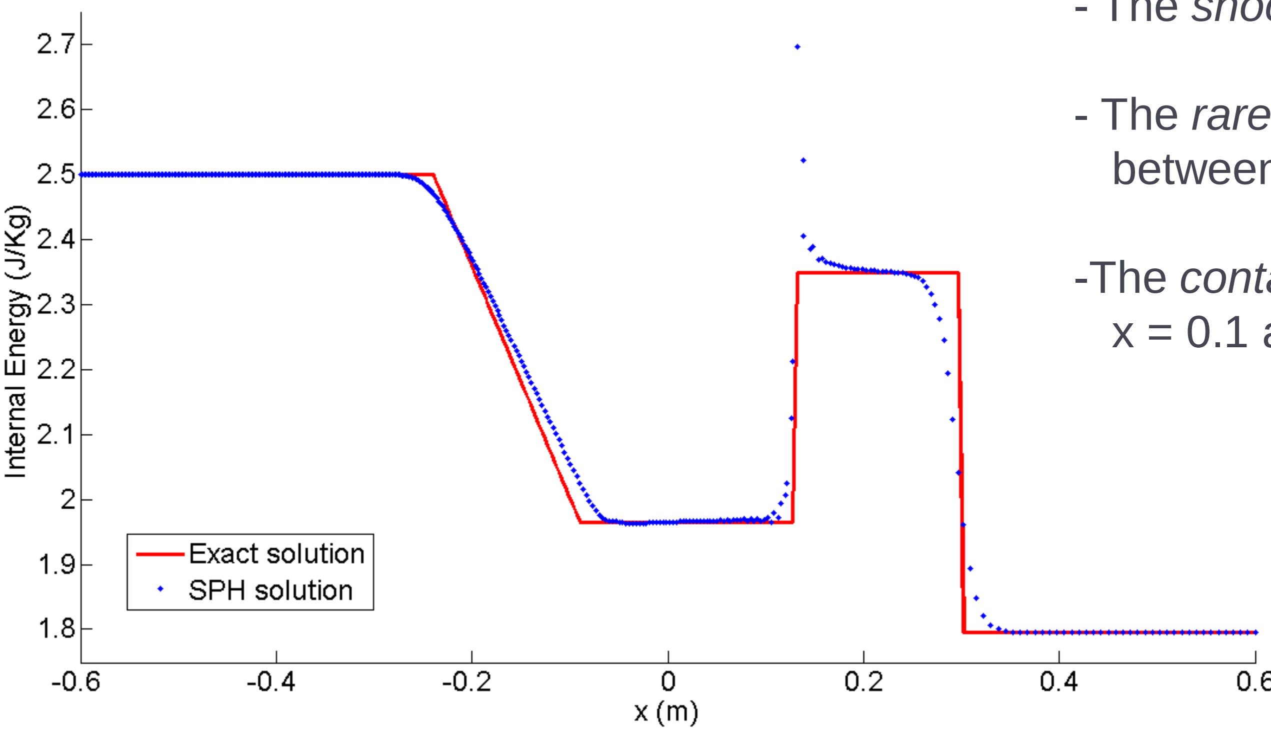


- The *shock* is observed around x = 0.3

- The *rarefaction wave* is located between x = -0.3 and x = 0

Example – Shock tube problem (10)

- Results – Internal energy profiles in the shock tube at *t = 0.20 s*



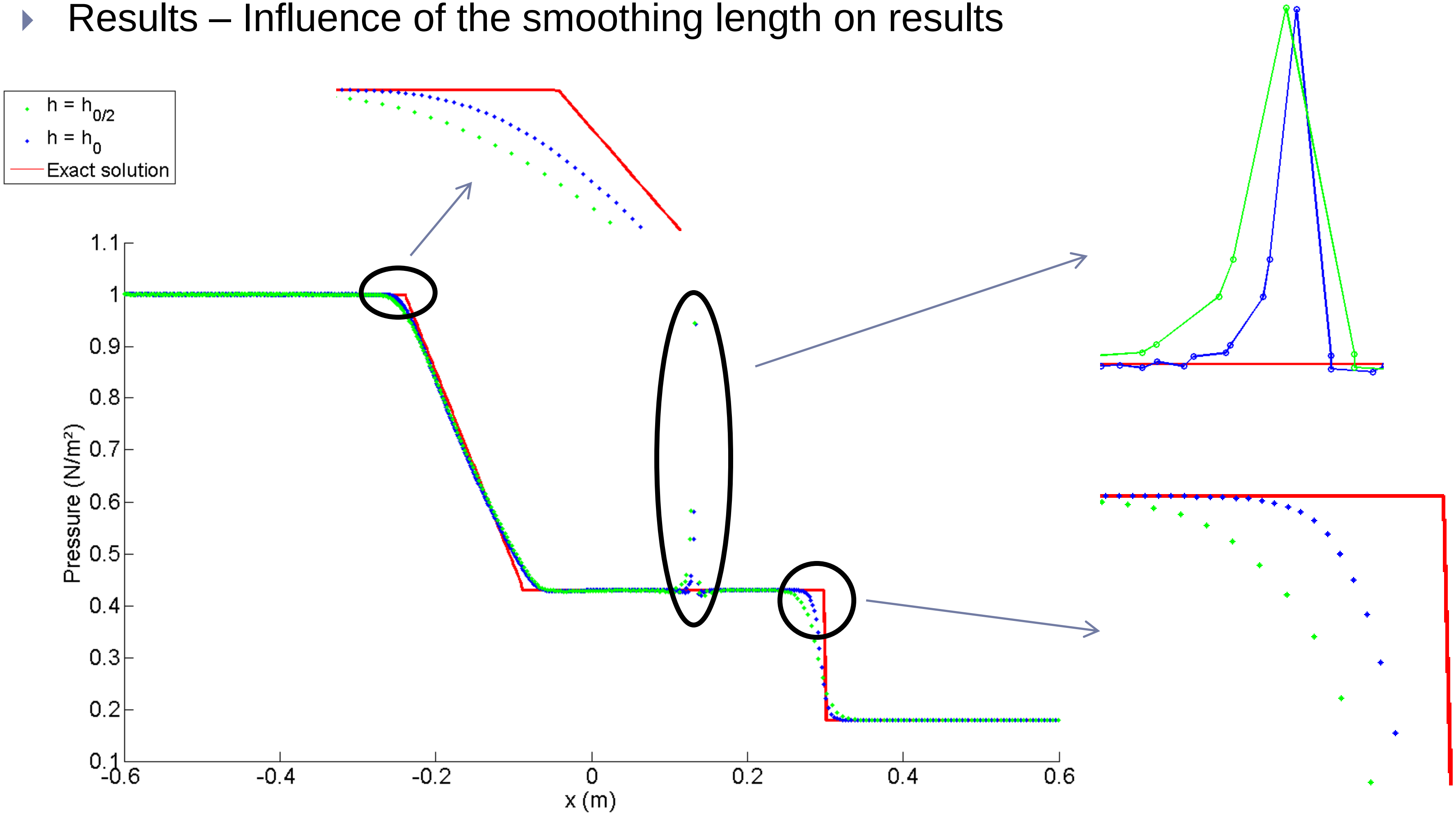
- The *shock* is observed around x = 0.3

- The *rarefaction wave* is located between x = -0.3 and x = 0

-The *contact discontinuity* is between x = 0.1 and x = 0.2.

Example – Shock tube problem (10)

- Results – Influence of the smoothing length on results



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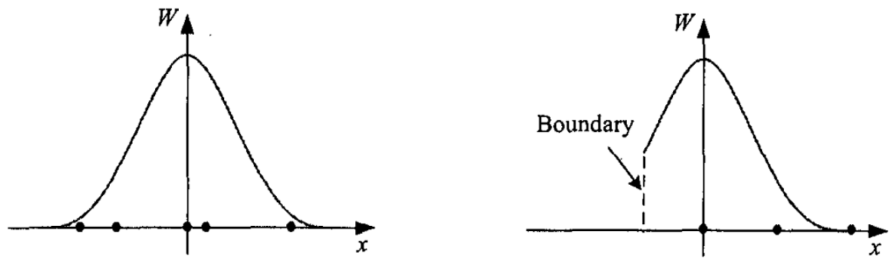
Inconsistencies (1)

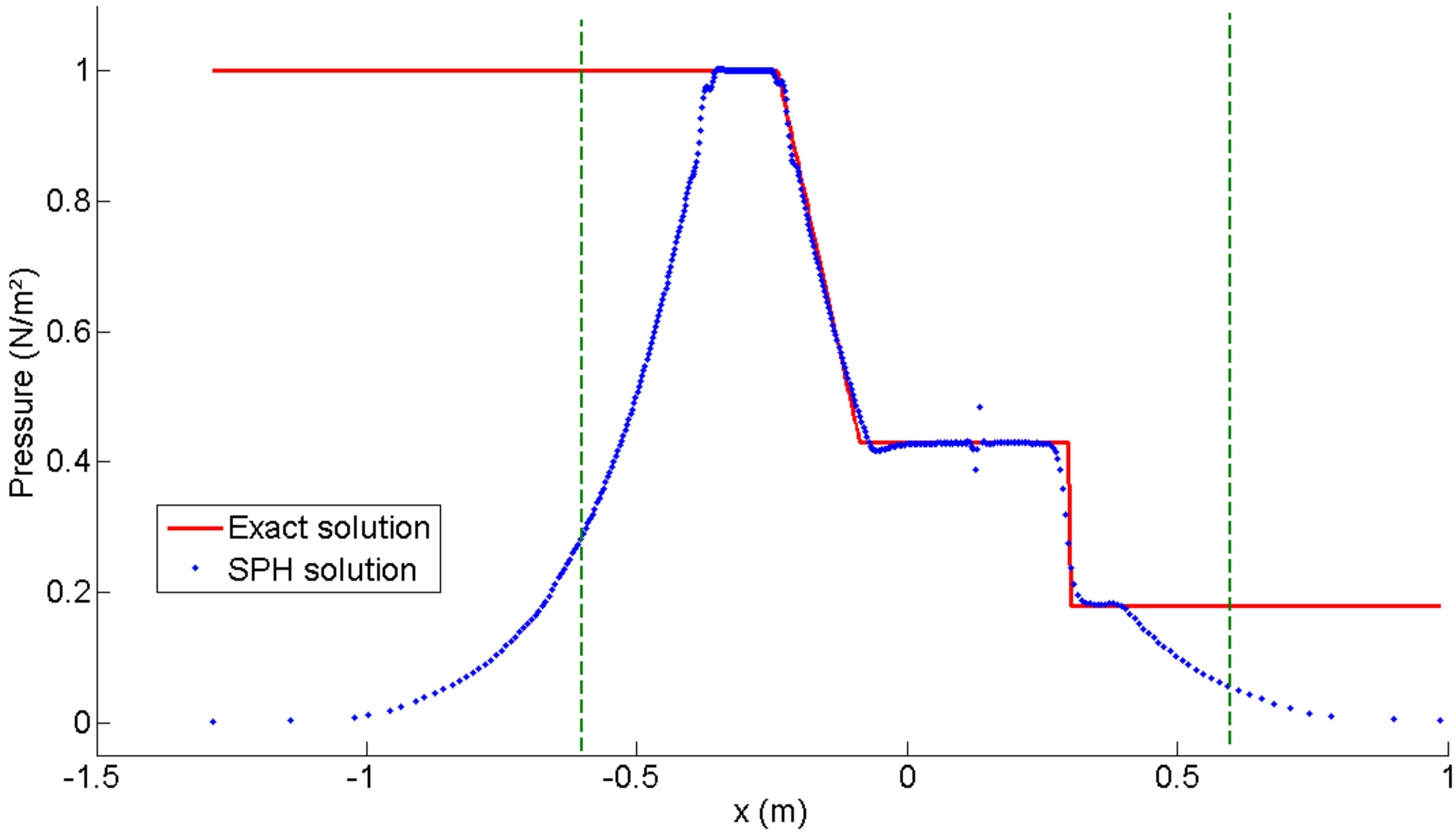
- Remember that, in both cases, the consistency conditions need to be restored :



- There are different ways to do it :
  - Construct the W to ensure *a priori* the discretized consistency to *k*-th order
    - Liu method (Liu, 2003) and RKPM (Liu and Chen, 1995)
  - Enforce 0th order consistency of the derivatives of the field functions in order to achieve the 1st order consistency of the field functions.
    - NSPH (Randles & Libersky, 1996), Symmetrization (Monaghan, 1988), MLSPH (Dilts, 1999), Johnson-Beissel correction (1996) and Krongauz-Belytschko correction (1997)
  - Normalize the kernel and particle approximations inside the problem domain and around the boundary area
    - CSPM (Chen et al, 1999; 2000)

Inconsistencies (2) - Illustration

- Pressure profiles in the shock tube at $t = 0.20$ *s*, <u>without boundary treatment</u>



Inconsistencies (3) – Liu method

- Let's consider the following polynomial representation of W :

$$W(\mathbf{x}-\mathbf{x}_j, h) = \sum_{I=0}^{k} b_I(\mathbf{x}, k) \left(\frac{\mathbf{x}-\mathbf{x}_j}{h}\right)^I$$

- The discrete forms of the consistency conditions (*cf.* slide 21) become:

$$\begin{cases} \displaystyle\sum_{j=1}^{N} \left[\sum_{I=0}^{k} b_I(\mathbf{x}, k) \left(\frac{\mathbf{x}-\mathbf{x}_j}{h}\right)^I\right] \Delta\mathbf{x}_j = 1 \\ \displaystyle\sum_{j=1}^{N} (\mathbf{x}-\mathbf{x}_j) \left[\sum_{I=0}^{k} b_I(\mathbf{x}, k) \left(\frac{\mathbf{x}-\mathbf{x}_j}{h}\right)^I\right] \Delta\mathbf{x}_j = 0 \\ \vdots \\ \displaystyle\sum_{j=1}^{N} (\mathbf{x}-\mathbf{x}_j)^k \left[\sum_{I=0}^{k} b_I(\mathbf{x}, k) \left(\frac{\mathbf{x}-\mathbf{x}_j}{h}\right)^I\right] \Delta\mathbf{x}_j = 0 \end{cases}$$

Inconsistencies (4) – Liu method

- Letting

$$m_k(\mathbf{x}, h) = \sum_{j=1}^{N} \left(\frac{\mathbf{x} - \mathbf{x}_j}{h} \right)^k \Delta_j$$

We can determine the b_l by solving the following system

$$\begin{pmatrix} m_0 & m_1 & \dots & m_k \\ m_1 & m_2 & \dots & m_{1+k} \\ \vdots & \vdots & \ddots & \vdots \\ m_k & m_{k+1} & \dots & m_{k+k} \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_k \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

- After solving the system, W can be calculated.

- But this restoring process leads to some problems:
  - Requires additional CPU time to solve the equations for all the particles at each time step.
  - $\mathbf{M}$ must be non-singular, which means that the particles distribution is not arbitrary anymore.
  - W can lose its fundamental properties (non negativity, symmetry, …).

Inconsistencies (5) - CSPM

- Based on the Taylor expansion, the *Corrective Smoothed Particle Method* provides an approach to normalize the kernel and particle approximations. Therefore it restores the consistencies.
  - Taylor expansion for $f(\mathbf{x})$: $f(\mathbf{x}) = f(\mathbf{x}_i) + (\mathbf{x} - \mathbf{x}_i)\left.\dfrac{\partial f}{\partial \mathbf{x}}\right|_i + O((\mathbf{x} - \mathbf{x}_i)^2)$
  - Multiplying both sides by W and integrating over the problem domain :

$$\int_\Omega f(\mathbf{x}) W_i(\mathbf{x}) d\mathbf{x} = f(\mathbf{x}_i) \int_\Omega W_i(\mathbf{x}) d\mathbf{x} + \left.\frac{\partial f}{\partial \mathbf{x}}\right|_i \int_\Omega (\mathbf{x} - \mathbf{x}_i) W_i(\mathbf{x}) d\mathbf{x} + \dots$$

  - Neglecting the terms involving derivatives, one gets the corrective kernel approximation for f at $\mathbf{x}_i$:

$$\boxed{f(\mathbf{x}_i) = \frac{\int_\Omega f(\mathbf{x}) W_i(\mathbf{x}) d\mathbf{x}}{\int_\Omega W_i(\mathbf{x}) d\mathbf{x}}} \longrightarrow \boxed{f(\mathbf{x}_i) = \frac{\sum_{j=1}^{N} \left(\frac{m_j}{\rho_j}\right) f(\mathbf{x}_j) W_{ij}}{\sum_{j=1}^{N} \left(\frac{m_j}{\rho_j}\right) W_{ij}}}$$

Inconsistencies (6) - CSPM

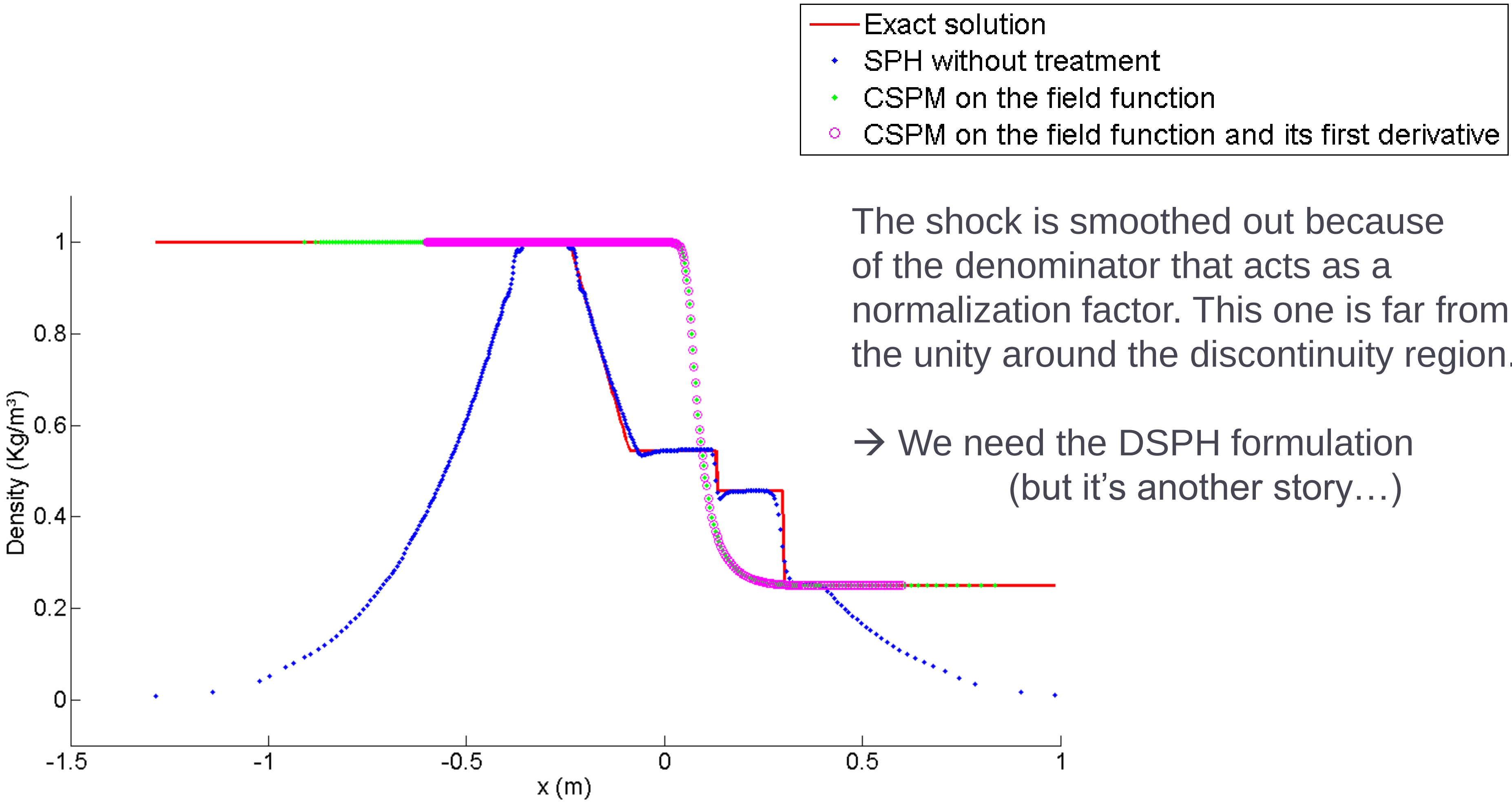
- Similarly, the corrective kernel approximation for the first derivative of f at $\mathbf{x}_i$ is derived as:

$$\left.\frac{\partial f}{\partial \mathbf{x}}\right|_i = \frac{\int_\Omega (f(\mathbf{x}) - f(\mathbf{x}_i))\frac{\partial W_i(\mathbf{x})}{\partial \mathbf{x}} d\mathbf{x}}{\int_\Omega (\mathbf{x} - \mathbf{x}_i)\frac{\partial W_i(\mathbf{x})}{\partial \mathbf{x}} d\mathbf{x}} \longrightarrow \left.\frac{\partial f}{\partial \mathbf{x}}\right|_i = \frac{\sum_{j=1}^{N}\left(\frac{m_j}{\rho_j}\right)(f(\mathbf{x}_j) - f(\mathbf{x}_i))\nabla_i W_{ij}}{\sum_{j=1}^{N}\left(\frac{m_j}{\rho_j}\right)(\mathbf{x}_j - \mathbf{x}_i)\nabla_i W_{ij}}$$

- The numerators are actually the traditional SPH approximations. The denominators are the representations of the normalization property of the *smoothing function*.
- CSPM provides an approach to solve the boundary deficiency problem and reduce the so-called *tensile instability* (*cf.* later).
- Note that in case of discontinuous phenomena, CSPM must be extended to the so-called *DSPH formulation* (Liu et al, 2003).

Inconsistencies (7) – CSPM Illustration

- Illustration of the CSPM results



The shock is smoothed out because of the denominator that acts as a normalization factor. This one is far from the unity around the discontinuity region.

→ We need the DSPH formulation (but it's another story…)

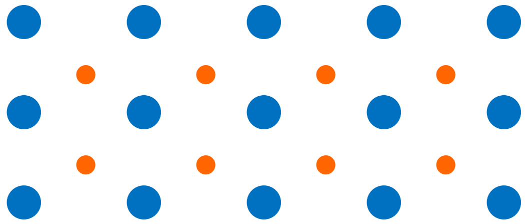
Tensile instability (1)

- Despite its growing popularity, SPH method applied to material mechanics suffers from the so-called *tensile instability.* This refers to the numerical pathology that in a region with tensile stress state, a small perturbation on the positions of particles will result in particle clumping and oscillatory motion.
- Illustration :
- It can be shown that $\partial\sigma^{\alpha\alpha}/\partial x \propto -\sigma^{\alpha\alpha}W_{\alpha\alpha}$, so in case of tensile stress state ($\sigma^{\alpha\alpha} > 0$):
  - If $W_{\alpha\alpha} < 0 \rightarrow \partial\sigma^{\alpha\alpha}/\partial x > 0 \Rightarrow$ Stable
  - If $W_{\alpha\alpha} > 0 \rightarrow \partial\sigma^{\alpha\alpha}/\partial x < 0 \Rightarrow$ Unstable
- Condition for the instability is :

$$\boxed{W_{\alpha\alpha}\sigma^{\alpha\alpha} > 0}$$

Tensile instability (2)

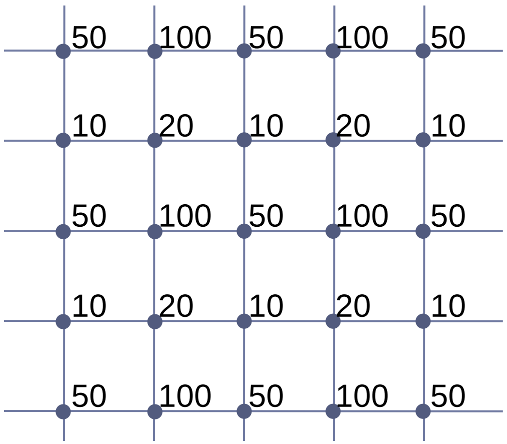
- Several remedies have been proposed to improve or avoid such *tensile instability* :
  - Morris (1996) : special smoothing functions
  - Chen (1999) : CSPM
  - Monaghan (2000) : artificial force
  - Beissel and Belytschko (1996) : additional stabilization terms (as in the Element Free Galerkin Method)
  - Dyka (1997) : additional stress points

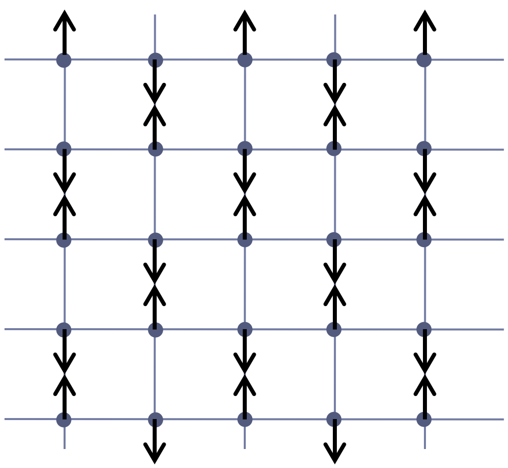


- Note that *tensile instability* remains one of the most critical problems of the SPH method.

Zero-energy Mode (1)

- FDM suffer from a spurious zero-energy mode for which the derivative at certain grid point is 0 when evaluated by the function values at the regular grid points on the both sides.





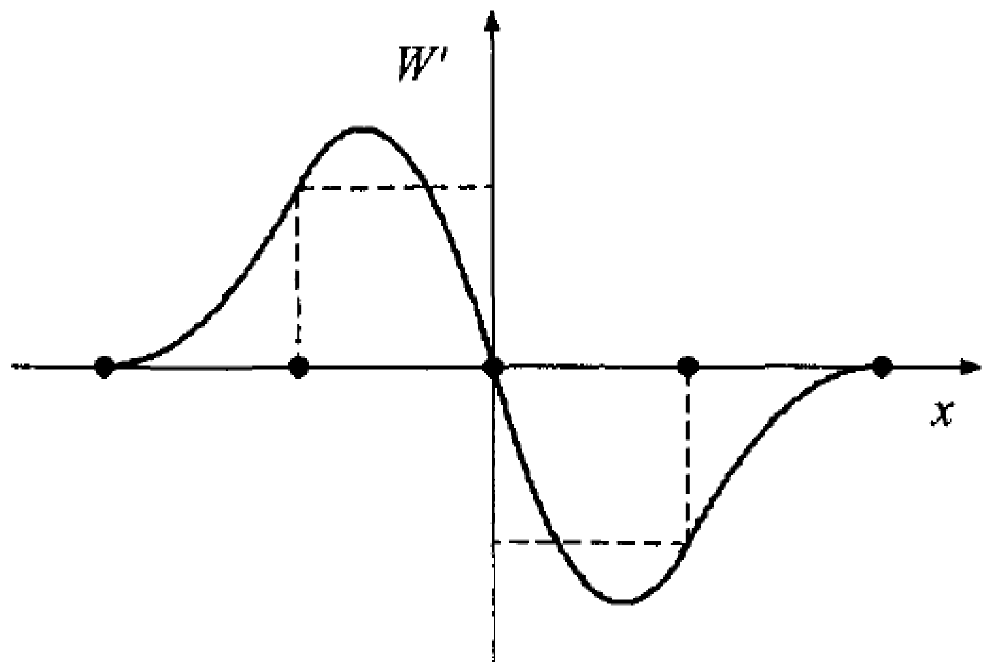
- In FEM, the zero-energy mode happens if quadrilateral elements are employed with reduced integration (Hourglass phenomenon).

Zero-energy Mode (2)

- The same problem also occurs in the SPH method when evaluating the derivatives.

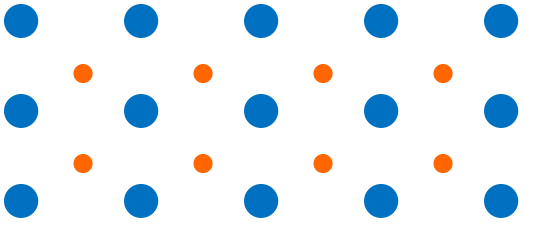
A 1D example with regular particle distribution :

The derivative of W at the particle evaluated is 0, what can be explained by the symmetric property of W.

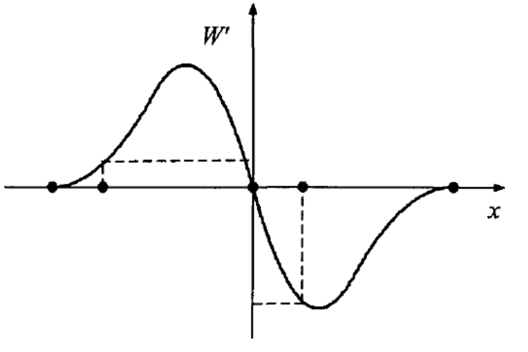


Zero-energy Mode (3)

- The zero-energy mode problem can be solved by using 2 types of particles :
  - velocity points
  - stress points



- However, the zero-energy mode in SPH is not as serious since the particle distribution is usually irregular. In this case, summed contributions from these particles generally will not lead to zero derivatives.



Outline

- Introduction
- Basic Concepts and Essential Formulation
- Construction of Smoothing Functions
- SPH for General Dynamic Fluid Flows
- Implementation
- Issues and Limitations
- <u>Conclusion</u>

Conclusion

- SPH method is a meshfree particle, Lagrangian and adaptive method
- Domain discretization with moving particles
- Numerical discretization
  - Kernel approximation (integration on continuum domain)
  - Particle approximation (summation on particles inside the support domain)
- Effective technique for solving fluid dynamic problems, and many more.
- A lot of numerical treatments have to be performed
  - Inconsistencies of the field functions and their derivatives
  - Boundary treatment
  - Neighbor searching
  - Smoothing length and smoothing function
- Can successfully simulate complex problems at reasonable accuracy and computational effort.

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Appendix I
Second order accuracy of the kernel approximation

Proof of the second order accuracy of the kernel approximation

- From (1)

$$\langle f(\mathbf{x})\rangle \triangleq \int_\Omega f(\mathbf{x}')W(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}'$$

- If $f(\mathbf{x})$ is differentiable, the Taylor series expansion of $f(\mathbf{x}')$ around $\mathbf{x}$ gives

$$f(\mathbf{x}') = f(\mathbf{x}) + f'(\mathbf{x})(\mathbf{x}-\mathbf{x}') + r((\mathbf{x}-\mathbf{x}')^2)$$

- The kernel being an even function with respect to $\mathbf{x}$, we should have

$$\begin{aligned} < f(\mathbf{x}) > &= \int_\Omega [f(\mathbf{x}) + f'(\mathbf{x})(\mathbf{x}' - \mathbf{x}) + r((\mathbf{x}'-\mathbf{x})^2)]W(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}' \\ &= f(\mathbf{x}) \underbrace{\int_\Omega W(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}'}_{=1} + f'(\mathbf{x}) \underbrace{\int_\Omega (\mathbf{x}'-\mathbf{x})W(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}'}_{=0} + r(h^2) \\ &= f(\mathbf{x}) + r(h^2) \end{aligned}$$

Appendix II
Approximation of a Field Function (1)

- Integral representation : $f(\mathbf{x}) = \int_\Omega f(\mathbf{x}')W(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}'$

- If $f(\mathbf{x})$ is sufficiently smooth, applying the Taylor series expansion of $f(\mathbf{x}')$ in the vicinity of $\mathbf{x}$ yields

$$\begin{aligned} f(\mathbf{x}') &= f(\mathbf{x}) + f'(\mathbf{x})(\mathbf{x}'-\mathbf{x}) + \frac{1}{2}f"(\mathbf{x})(\mathbf{x}'-\mathbf{x})^2 + \dots \\ &= \sum_{k=0}^{n} \frac{(-1)^k h^k f^{(k)}(\mathbf{x})}{k!}\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right)^k + r_n\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right) \end{aligned}$$

- Substituting this equation in the integral representation leads to

$$\begin{aligned} f(\mathbf{x}) &= \int_\Omega \sum_{k=0}^{n} \frac{(-1)^k h^k f^{(k)}(\mathbf{x})}{k!}\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right)^k W(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}' + r_n\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right) \\ &= \sum_{k=0}^{n} f^{(k)}(\mathbf{x}) \underbrace{\frac{(-1)^k h^k}{k!}\int_\Omega \left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right)^k W(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}'}_{=A_k} + r_n\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right) \qquad \text{(II.1)} \\ &= \sum_{k=0}^{n} A_k f^{(k)}(\mathbf{x}) + r_n\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right) \end{aligned}$$

Appendix II
Approximation of a Field Function (2)

- Comparing the LHS with the RHS of equation (II.1), in order for $f(\mathbf{x})$ to be approximated to *n*-th order, the coefficients A_k must be equal to the counterparts for $f^{(k)}(\mathbf{x})$ in the LHS of equation (II.1). We obtain in terms of the moments

$$\begin{cases} M_0 &= \int_\Omega W(\mathbf{x}-\mathbf{x}', h)d\mathbf{x}' = 1 \\ M_1 &= \int_\Omega (\mathbf{x}-\mathbf{x}')W(\mathbf{x}-\mathbf{x}', h)d\mathbf{x}' = 0 \\ M_2 &= \int_\Omega (\mathbf{x}-\mathbf{x}')^2 W(\mathbf{x}-\mathbf{x}', h)d\mathbf{x}' = 0 \\ &\vdots \\ M_n &= \int_\Omega (\mathbf{x}-\mathbf{x}')^n W(\mathbf{x}-\mathbf{x}', h)d\mathbf{x}' = 0 \end{cases}$$

- Note that the first equation is the unity condition, and the second equation represents the symmetric property expressed previously. Satisfaction of these two conditions ensures the first order consistency for the SPH kernel approximation for a function.

Appendix III
Approximation of the Derivative of a Field Function

- The approximation of the first derivative can be obtained by replacing the function $f(\mathbf{x})$ in the integral representation with its derivative $f'(\mathbf{x})$, *i.e.*

$$f'(\mathbf{x}) = \int_{\Omega} f'(\mathbf{x}')W(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}'$$

- Integrating by parts, this equation can be rewritten as,

$$f'(\mathbf{x}) = \int_{S} f(\mathbf{x}')W(\mathbf{x}-\mathbf{x}',h)\cdot\vec{\mathbf{n}}dS - \int_{\Omega} f(\mathbf{x}')W'(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}' \qquad \text{(III.1)}$$

- If $f(\mathbf{x})$ is sufficiently smooth, applying the Taylor series expansion of $f(\mathbf{x}')$ in the vicinity of $\mathbf{x}$ yields

$$\begin{aligned} f(\mathbf{x}') &= f(\mathbf{x}) + f'(\mathbf{x})(\mathbf{x}'-\mathbf{x}) + \frac{1}{2}f''(\mathbf{x})(\mathbf{x}'-\mathbf{x})^2 + \ldots \\ &= \sum_{k=0}^{n} \frac{(-1)^k h^k f^{(k)}(\mathbf{x})}{k!}\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right)^k + r_n\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right) \qquad \text{(III.2)} \end{aligned}$$

Appendix III
Approximation of the Derivative of a Field Function

- Substituting (III.2) into the second integral of the RHS of equation (III.1) yields

$$
\begin{aligned}
f'(\mathbf{x}) &= \int_S f(\mathbf{x}')W(\mathbf{x}-\mathbf{x}',h)\cdot\vec{\mathbf{n}}dS - \int_\Omega \left[\left(\sum_{k=0}^{n} \frac{(-1)^k h^k f^{(k)}(\mathbf{x})}{k!}\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right)^k + r_n\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right)\right) W'(\mathbf{x}-\mathbf{x}',h)\right] d\mathbf{x}' \\
&= \int_S f(\mathbf{x}')W(\mathbf{x}-\mathbf{x}',h)\cdot\vec{\mathbf{n}}dS - \left[\sum_{k=0}^{n} \frac{(-1)^k h^k f^{(k)}(\mathbf{x})}{k!}\int_\Omega \left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right)^k W'(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}' + r_n\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right)\right] \\
&= \int_S f(\mathbf{x}')W(\mathbf{x}-\mathbf{x}',h)\cdot\vec{\mathbf{n}}dS + \sum_{k=0}^{n} A'_k f^{(k)}(\mathbf{x}) + r_n\left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right)
\end{aligned}
$$

with

$$
A'_k = \frac{(-1)^{k+1}h^k}{k!}\int_\Omega \left(\frac{\mathbf{x}-\mathbf{x}'}{h}\right)^k W'(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}'
$$

Appendix III
Approximation of the Derivative of a Field Function

- It is clear that, if the following equations are satisfied, $f'(\mathbf{x})$ can be approximated to *n*-th order,

$$\left\{\begin{array}{lcl} M'_0 & = & \int_\Omega W'(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}' = 0 \\ M'_1 & = & \int_\Omega (\mathbf{x}-\mathbf{x}')W'(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}' = 1 \\ M'_2 & = & \int_\Omega (\mathbf{x}-\mathbf{x}')^2 W'(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}' = 0 \\ & \vdots & \\ M'_n & = & \int_\Omega (\mathbf{x}-\mathbf{x}')^n W'(\mathbf{x}-\mathbf{x}',h)d\mathbf{x}' = 0 \end{array}\right. \quad \text{and} \quad W(\mathbf{x}-\mathbf{x}',h)|_S = 0$$

which requires the smoothing function to vanish on the surface of the support domain. This is, in fact, the compact support condition given below.