Stability, accuracy and time-integration issues in SPH schemes

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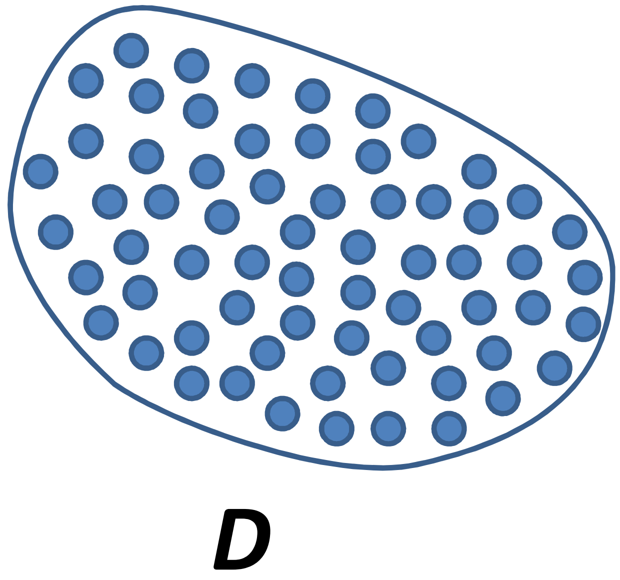
Plan of the Talk

- The standard SPH: general structure
- Weakly-compressibility assumption: issues in pressure evaluation
- Diffusive variants of SPH: main features and limits
- The δ-SPH scheme: a consistent diffusive variant
- Current developments: the δLES-SPH and the δplus-SPH

General features of the SPH

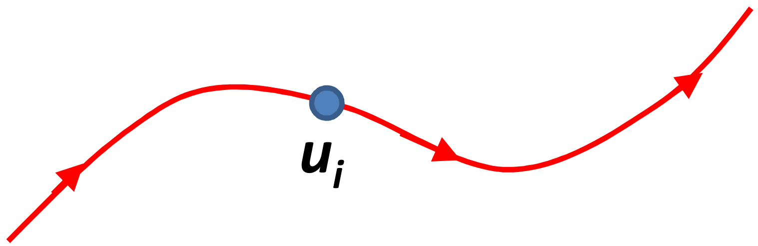
The SPH is a ***particle*** method

The fluid domain (***D*** hereinafter) is discretized into a finite number of particles that represent elementary volumes of fluid



No topological connections
=> the SPH is a ***Meshless*** method

Particles transport the values of the physical quantities (e.g. pressure and velocity), moving with the fluid velocity
=> the SPH is a ***Lagrangian*** method



General features of the SPH

Why smoothing?

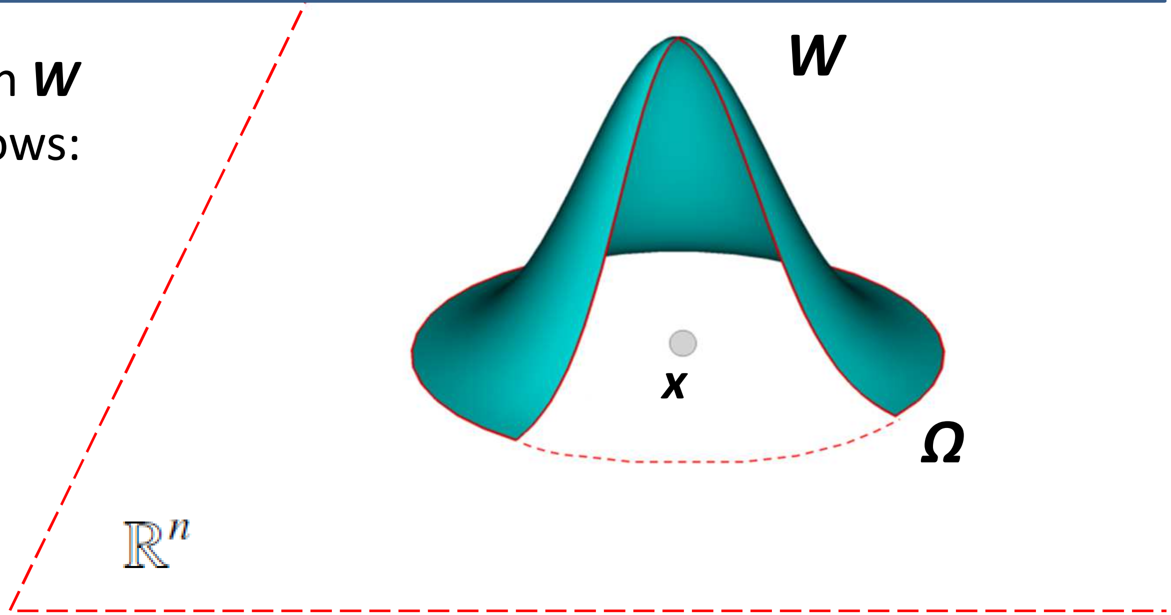
- the Lagrangian nature of the SPH induces **non-uniform spatial distributions** of particles during the flow evolution
- the absence of topological connections between particles (meshless method) makes the **evaluation of _standard_ differential operators very complex**

The smoothing procedure allows us to model the interactions between neighbour particles in a simple and consistent way and to approximate the usual differential operators in a reliable manner

Smoothing

Let us consider a weight function ***W*** (kernel function) defined as follows:

- radial and positive
- with a compact support ***Ω*** (i.e. it is null outside ***Ω***)
- $C^1(R^n)$ at least



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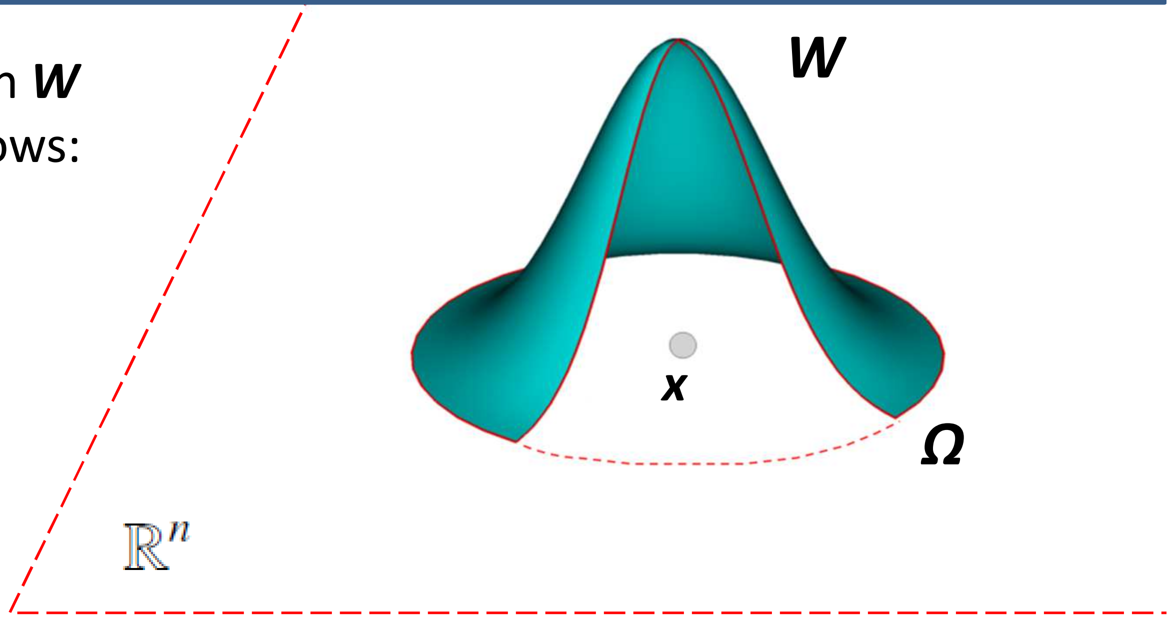
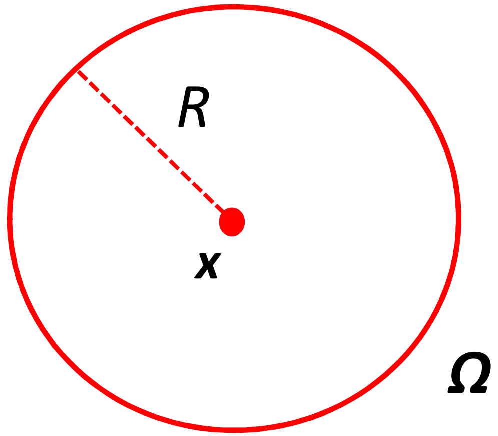


The kernel function has generally a bump-like shape:

- Gaussian-type
- Polinomial type (e.g. Wendland kernels)
- Spline kernels (e.g. Cubic/quintic splines)



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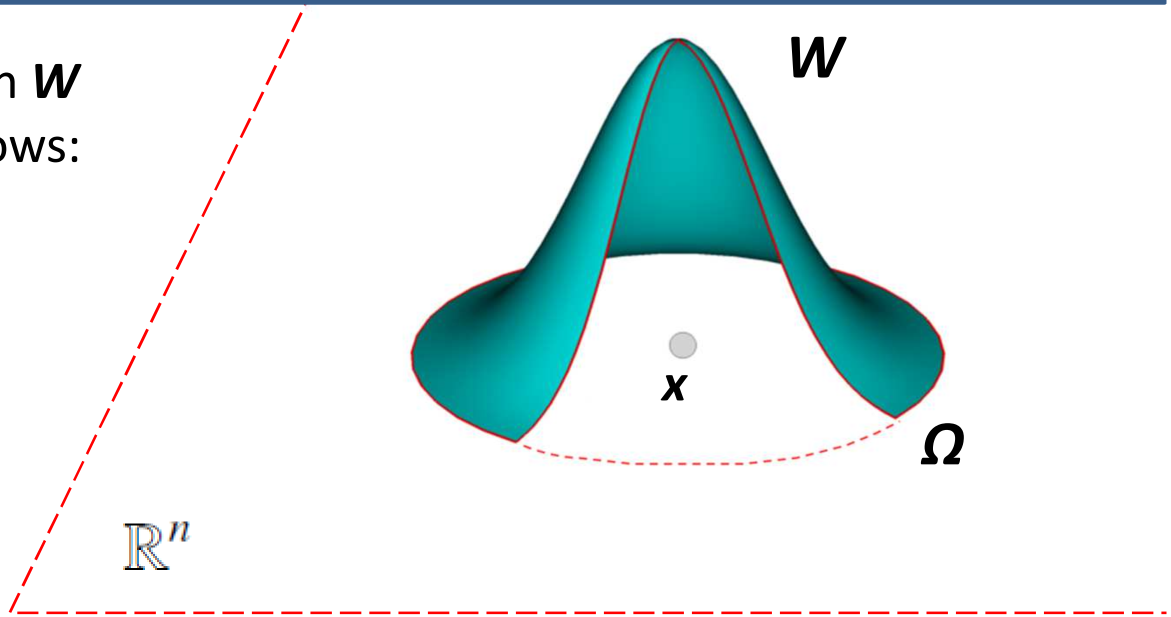


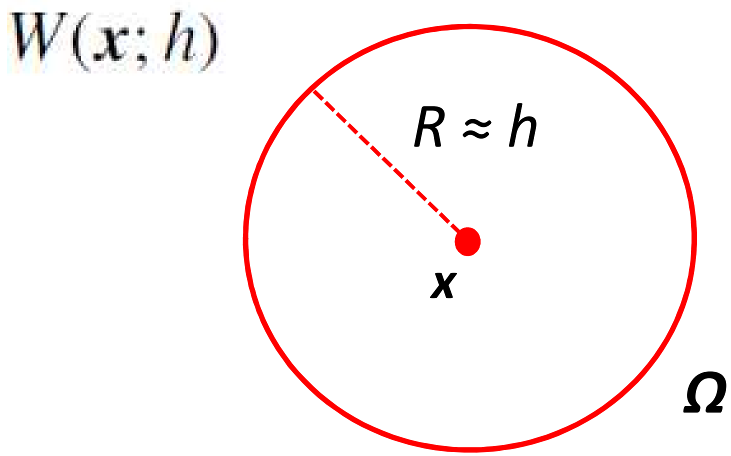
The kernel function is generally expressed

as a function of a reference length *h*,

called ***smoothing length***,

which is proportional to the radius *R*

of the kernel domain ***Ω***

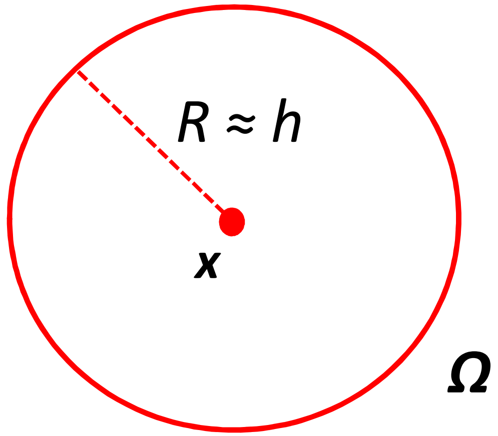


Smoothing

The kernel function is normalized to one, that is:

$$\int_{\Omega} W(\boldsymbol{x}; h)\, \mathrm{d}V^{*} = 1 \qquad h > 0$$

Consequently, the kernel function ***W*** preserves its «mass» inside the support ***Ω*** <u>for every choice of *h*</u>



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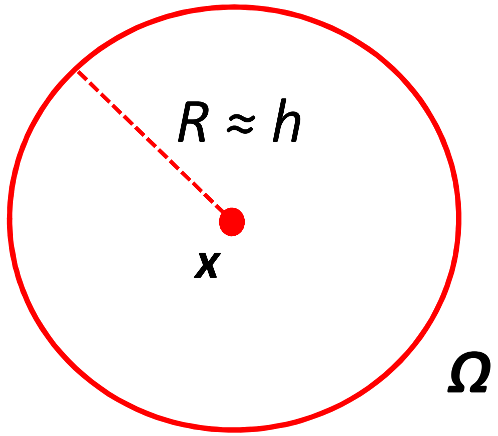

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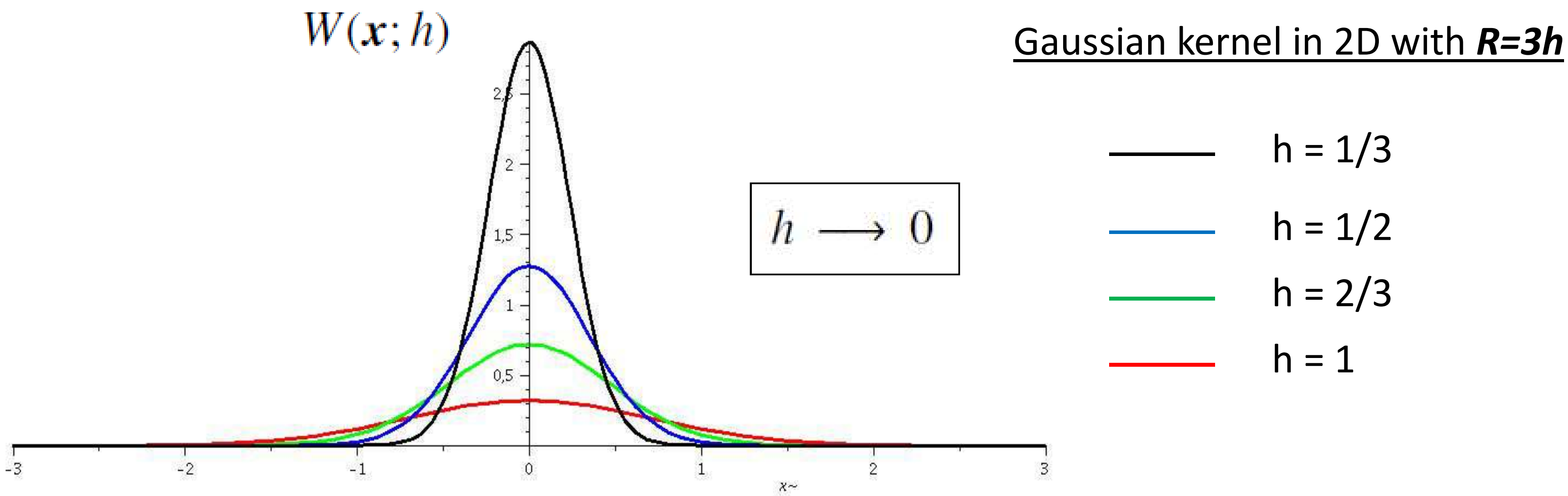
For *h* going to zero, the Kernel function shrinks to a point (<u>preserving its mass</u>)



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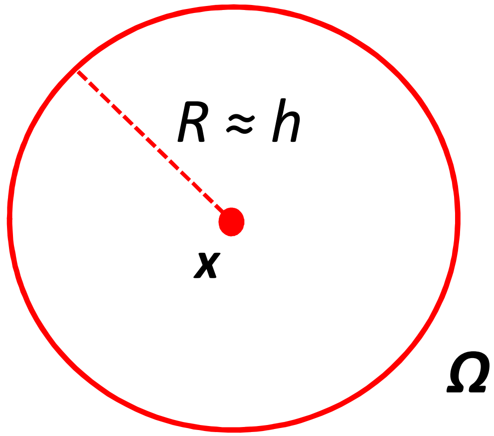
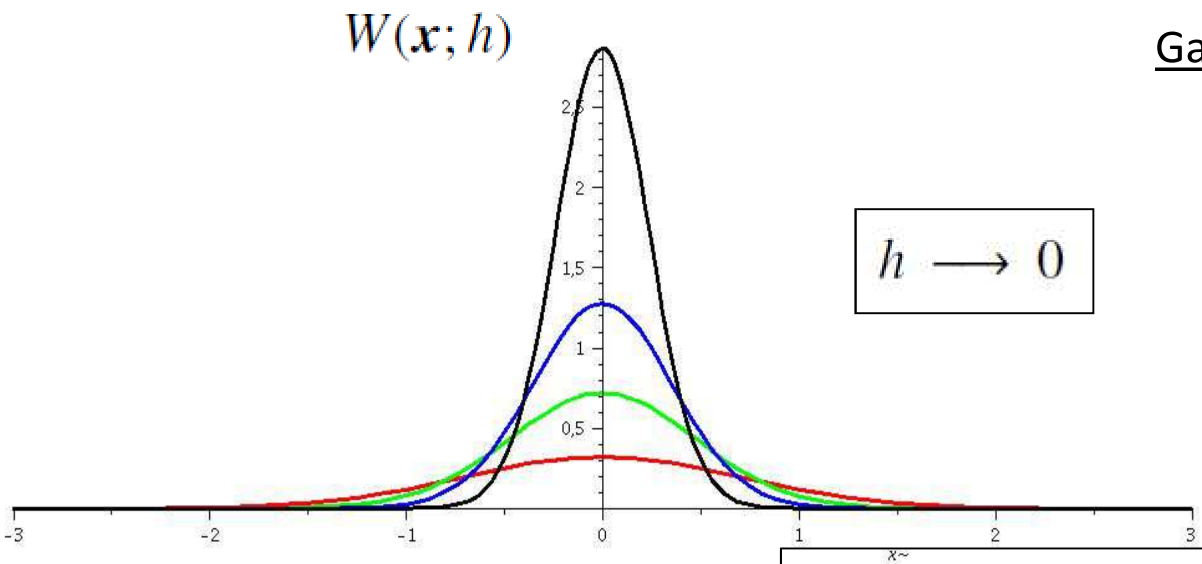


Consequently, the kernel function ***W*** preserves its «mass» inside the support ***Ω*** for every choice of *h*

For *h* going to zero, the Kernel function shrinks to a point (preserving its mass)



$$h \longrightarrow 0$$

Gaussian kernel in 2D with ***R=3h***

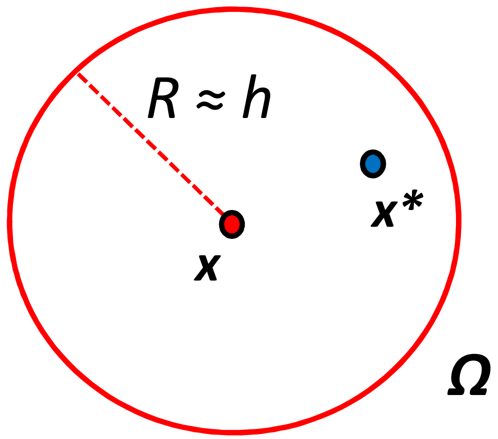
- h = 1/3 (black)
- h = 1/2 (blue)
- h = 2/3 (green)
- h = 1 (red)

***W* converges weakly to a Dirac function!**

Smoothing - continuum

The smoothing procedure is defined through a <u>*convolution integral*</u> with the kernel function ***W*** <u>*over the fluid domain* ***D***</u>

In particular, for a generic scalar function *f*, we define:



$$\langle f \rangle(\mathbf{x}) = \int_{\Omega \cap D} f(\mathbf{x}^*)\, W(\mathbf{x} - \mathbf{x}^*, h)\, \mathrm{d}V^*$$

the support ***Ω*** is centred at the point ***x*** and the integration is done on the variable ***x****

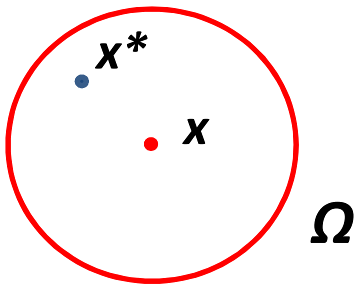
As a consequence of the properties of ***W***, we have:

- $W(\mathbf{x} - \mathbf{x}^*; h) = W(\mathbf{x}^* - \mathbf{x}; h)$
- $\nabla W(\mathbf{x} - \mathbf{x}^*; h) = -\nabla^* W(\mathbf{x} - \mathbf{x}^*; h)$

where ∇^* denotes differentiation with respect to ***x****

Smoothing - continuum

The simplest case is obtained for *f=1*



$$\Gamma(\boldsymbol{x}) = \int_{\Omega \cap D} W(\boldsymbol{x} - \boldsymbol{x}^*; h)\, \mathrm{d}V^*$$

This function takes into account how much "mass" of the fluid domain ***D*** is inside the kernel domain ***Ω***

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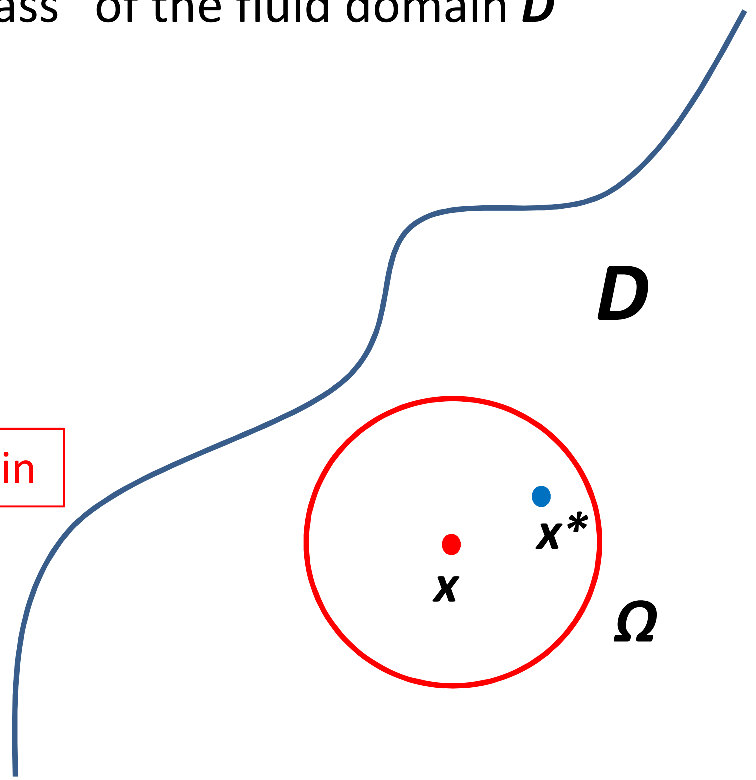
This function takes into account how much "mass" of the fluid domain ***D*** is inside the kernel domain ***Ω***

Since the kernel is normalized, we have:

$$\Gamma(\boldsymbol{x}) = 1 \qquad \text{if} \quad \Omega \subset D$$

All the «mass» is inside the fluid domain



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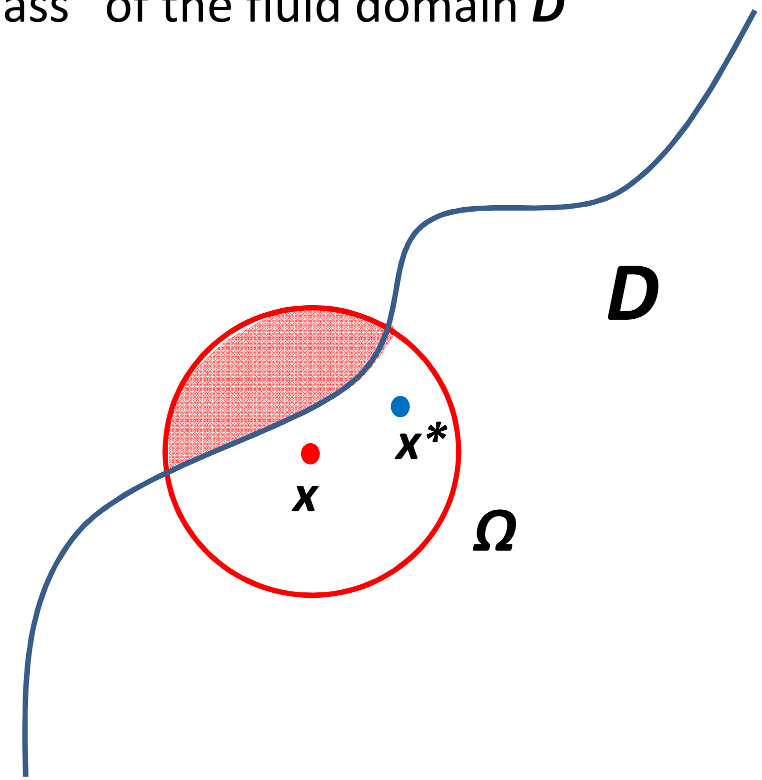
Since the kernel is normalized, we have:

$$\Gamma(\boldsymbol{x}) \;=\; 1 \qquad \text{if} \quad \Omega\subset D$$

$$\Gamma(\boldsymbol{x}) \;<\; 1 \qquad \text{if} \quad \Omega\cap D^c \neq \emptyset$$

Some «mass» is outside the fluid domain



Smoothing - continuum

$$\langle f \rangle(\boldsymbol{x}) = \int_{\Omega \cap D} f(\boldsymbol{x}^*)\, W(\boldsymbol{x} - \boldsymbol{x}^*, h)\, \mathrm{d}V^*$$

$$\Gamma(\boldsymbol{x}) = \int_{\Omega \cap D} W(\boldsymbol{x} - \boldsymbol{x}^*; h)\, \mathrm{d}V^*$$

A little more involved is the derivation of the smoothed gradient operator

Using integration by parts (and a careful modelling of boundary terms), it is possible to obtain the following approximation:

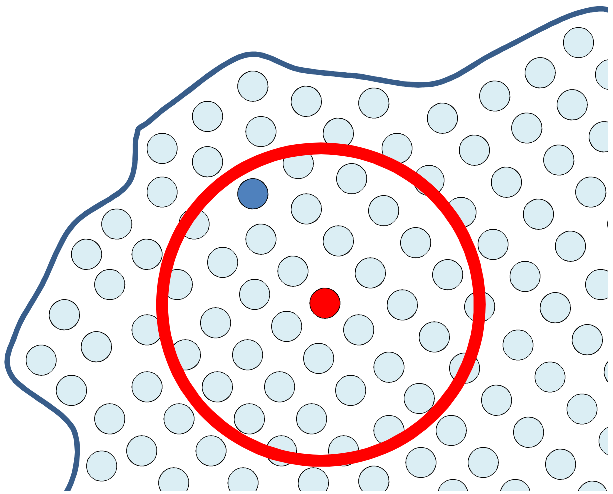
$$\langle \nabla f \rangle(\boldsymbol{x}) = \int_{\Omega \cap D} [\, f(\boldsymbol{x}^*) - f(\boldsymbol{x}) \,]\, \nabla W(\boldsymbol{x} - \boldsymbol{x}^*, h)\, \mathrm{d}V^* + \mathcal{O}(h)$$

Smoothing

The fluid domain is discretized in a finite number of particles that represent *elementary volumes of fluid* and transport the main physical quantities

Let us assume that the volumes V_i are known…

(these may be obtained through geometrical procedures basing on particle distribution or during the numerical simulation)



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Let us assume that the volumes V_i are known…

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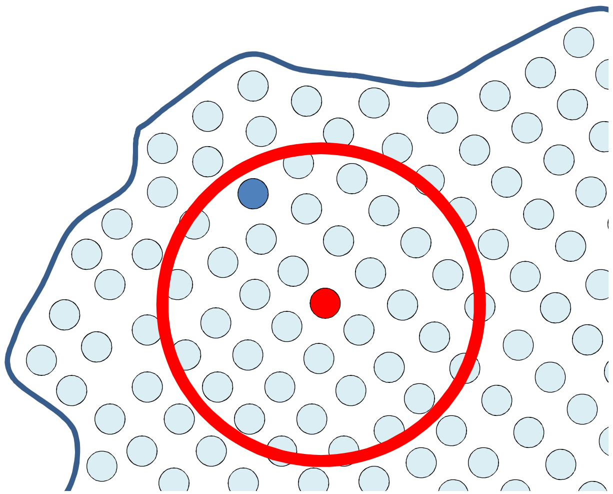
Then, we replace the integral over $\boldsymbol{\Omega}$ by summations over the neighbour particles

$$\Gamma(x) = \int_{\Omega \cap D} W(x - x^*; h)\, dV^*$$

$$\Gamma_i = \sum_{j \in \mathcal{N}_i} W_{i,j} V_j$$

$$W_{i,j} = W(\boldsymbol{x}_i - \boldsymbol{x}_j, h)$$

$$\mathcal{N}_i = \left\{ j \text{ such that } \|\boldsymbol{x}_i - \boldsymbol{x}_j\| \leq R \right\}$$



Smoothing

Similarly, we define:

$$\langle f\rangle(\boldsymbol{x}) = \int_{\Omega\cap D} f(\boldsymbol{x}^*)\, W(\boldsymbol{x}-\boldsymbol{x}^*, h)\, \mathrm{d}V^*$$

$$\langle f\rangle_i = \sum_{j\in\mathcal{N}_i} f_j\, W_{i,j}\, V_j$$

where $f_i = f(\boldsymbol{x}_i)$

$$\langle \nabla f\rangle(\boldsymbol{x}) = \int_{\Omega\cap D} [\, f(\boldsymbol{x}^*) - f(\boldsymbol{x})\,]\, \nabla W(\boldsymbol{x}-\boldsymbol{x}^*, h)\, \mathrm{d}V^*$$

$$\langle \nabla f\rangle_i = \sum_{j\in\mathcal{N}_i} \left(f_j - f_i \right) \nabla_i W_{i,j}\, V_j$$

where ∇_i represents differentiation with respect to $\boldsymbol{x}_i$

Hereinafter the symbol $\mathcal{N}_i$ in the summations is understood

Smoothing

What about the convergence of discrete operator towards the continuous ***smoothed*** operators?

increasing the number of particle in $\boldsymbol{\Omega}$ ⇒ decreasing $\boldsymbol{\Delta x/h}$

$\boldsymbol{\Delta x}$ *is the mean particle distance*

In any case….

- the convergence strongly depends on the way in which the particles are distributed (regular distributions are needed)
- even in the presence of regular particle distribution, the order of convergence is generally between 1 and 2

Smoothing

For the function, if $\boxed{\boldsymbol{x}_i \in \Omega \subset D}$ (i.e. inside the fluid domain)

discrete | **smoothed** (continuous) | **exact**

$$\langle f \rangle_i \xrightarrow{\frac{\Delta x}{h} \longrightarrow 0} \langle f \rangle(\boldsymbol{x}_i) \xrightarrow{h \longrightarrow 0} f(\boldsymbol{x}_i)$$

+ REGULAR PARTICLE DISTRIBUTIONS!

For regular distributions, the convergence to the exact solution is attained **if BOTH the parameters *Δx/h* and *h* go to zero*!*** (see, for example, Quinlan et al. 2006)

Smoothing

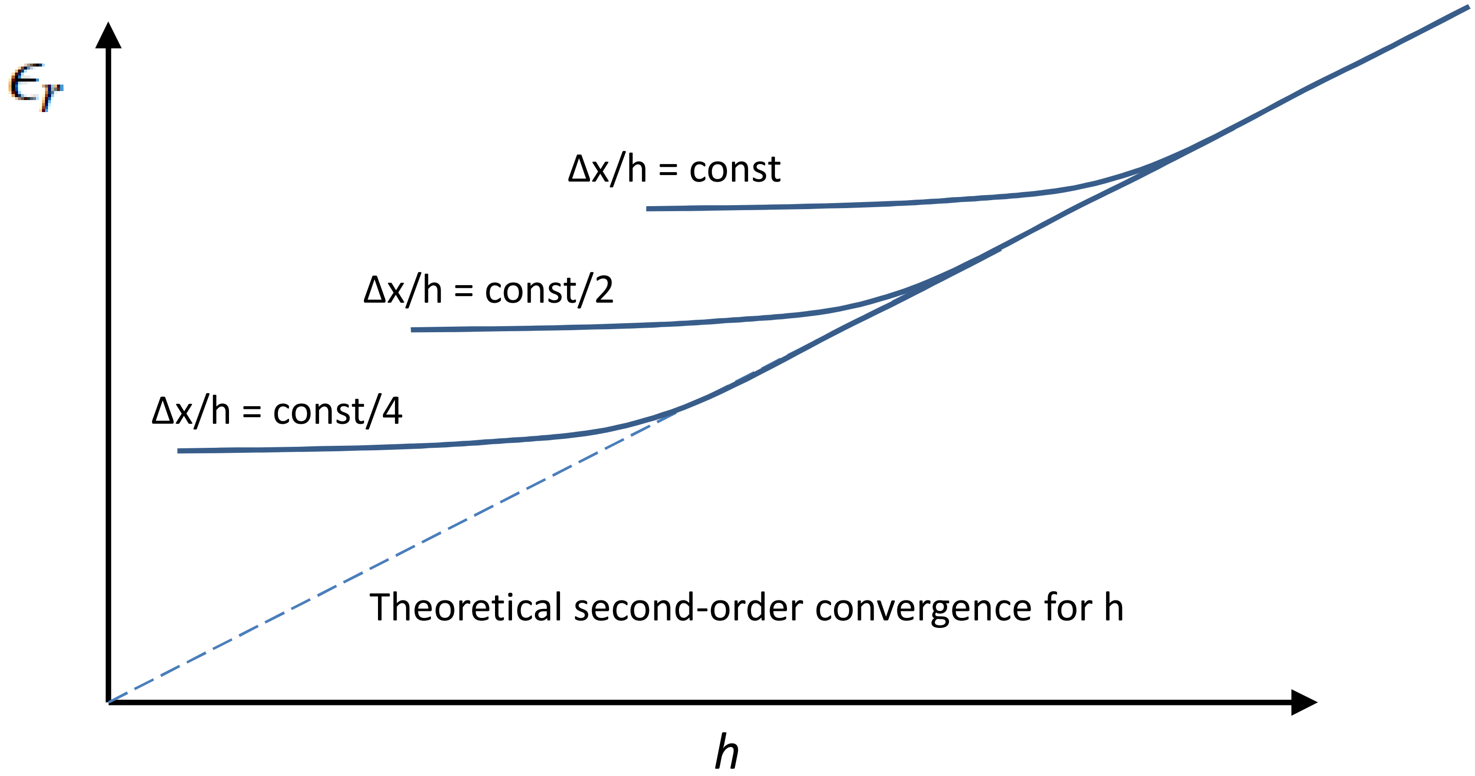
$$\epsilon_r = \| \langle f \rangle_i - f(\boldsymbol{x}_i) \|$$

For example, if we check the convergence

of the SPH by decreasing *h*

while *Δx/h* is fixed

(i.e. constant number of particles in ***Ω***)…



Smoothing

For $\boldsymbol{x}_i \in \Omega \subset D$ (i.e. inside the fluid domain)

for *Δx/h, h « 1* ....***and for regular distributions!***

$$\Gamma_i = \sum_j W_{i,j} V_j \simeq 1$$

$$\langle f \rangle_i = \sum_j f_j W_{i,j} V_j \simeq \Gamma_i f(\boldsymbol{x}_i)$$

$$\nabla \Gamma_i = \sum_j \nabla_i W_{i,j} V_j \simeq 0$$

$$\langle \nabla f \rangle_i = \sum_j \left(f_j - f_i \right) \nabla_i W_{i,j} V_j \simeq \Gamma_i \nabla f(\boldsymbol{x}_i)$$

The standard SPH

We are interested in the **SPH in the fluid dynamics field**….

Despite many fluids (like water) are modelled as incompressible, the SPH in its basic form relies on the hypotheses that ***the fluid is weakly-compressible*** (this will be clarified later)

It may be derived from the Navier-Stokes equations for compressible fluids:

$$\begin{cases} \dfrac{\mathrm{d}\rho}{\mathrm{d}t} = -\rho \nabla \cdot \boldsymbol{u} \\ \rho \dfrac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = \rho \boldsymbol{f} - \nabla p + \nabla \cdot \mathbb{V} \\ \dfrac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \boldsymbol{u} \qquad p = F(\rho) \end{cases}$$

Lagrangian derivatives

viscous component of the stress tensor

State equation for barotropic fluids

ρ is the fluid density,

$\boldsymbol{u}$ is the fluid velocity

p is the pressure field

f is a body force

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$$\begin{cases} \dfrac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\rho_i \langle \nabla \cdot \boldsymbol{u} \rangle_i \\[2ex] \rho_i \dfrac{\mathrm{d}\boldsymbol{u}_i}{\mathrm{d}t} = \rho_i \boldsymbol{f}_i - \langle \nabla p \rangle_i + \langle \nabla \cdot \mathbb{V} \rangle_i \\[2ex] \dfrac{\mathrm{d}\boldsymbol{x}_i}{\mathrm{d}t} = \boldsymbol{u}_i \qquad p_i = F(\rho_i) \end{cases}$$

the differential operators are substituted with their smoothed (and discrete) counterparts

The standard SPH

Divergence of the velocity…

$$\langle \nabla \cdot \boldsymbol{u} \rangle_i = \sum_j \left(\boldsymbol{u}_j - \boldsymbol{u}_i \right) \cdot \nabla_i W_{i,j} V_j$$

→ we need to find out the volumes!

Being a Lagrangian method, it is common practise in the standard SPH to associate a mass m_i to each particle and to maintain it constant during the flow evolution

→ $$\frac{\mathrm{d}m_i}{\mathrm{d}t} = 0$$ and $$V_i = \frac{m_i}{\rho_i}$$

It is also possible to define the volumes basing on geometrical considerations (e.g. particle distributions, Espaŋol & Revenga, 2003)

The standard SPH

$$\frac{\mathrm{d}m_i}{\mathrm{d}t} = 0$$

$$V_i = \frac{m_i}{\rho_i}$$

Generally….

- the SPH simulation is initialized by imposing
  a uniform particle distribution
  (or, at least, as regular as possible!)
  => **the volumes are *initially* uniform**

$$V_i\Big|_{t=t_0} = V_0 \quad \forall i$$

The standard SPH

$$\frac{dm_i}{dt} = 0$$

$$V_i = \frac{m_i}{\rho_i}$$

Generally….

- the SPH simulation is initialized by imposing a uniform particle distribution (or, at least, as regular as possible!)
  => **the volumes are *initially* uniform**

$$V_i\big|_{t=t_0} = V_0 \quad \forall i$$

- the density field is assigned as an initial condition (and generally it is not constant all over the fluid domain)
  => **the particles may have different masses**

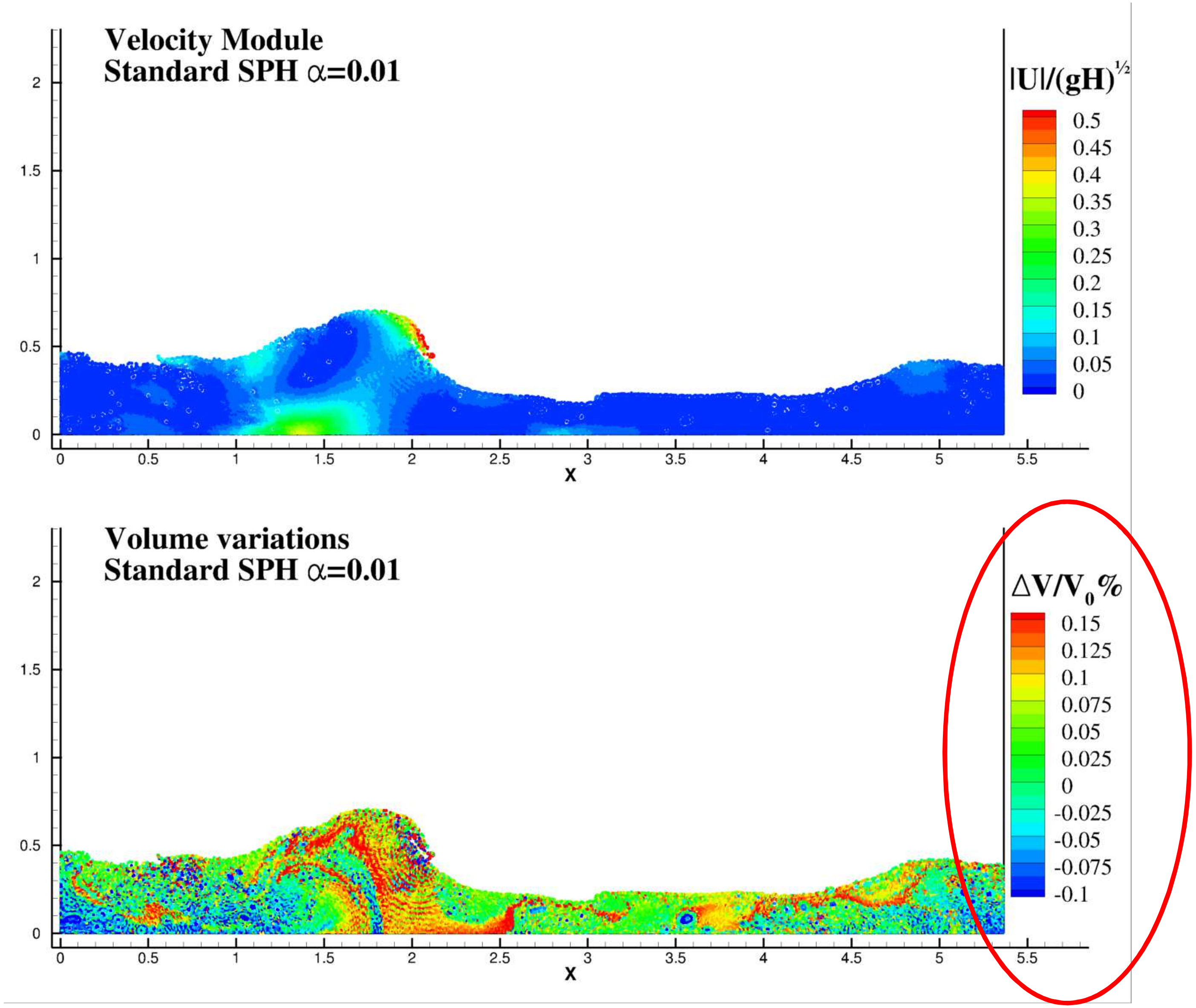
$$m_i = \rho_i\big|_{t=t_0} V_0$$

- During the simulation, the masses do not change while the density field evolves according to the physical equations
  => **volumes may evolve in a way that disregards the actual geometrical distribution of particles**

$$V_i(t) = \frac{m_i}{\rho_i(t)}$$

=> Reduced accuracy when intense density gradients occur!

The standard SPH



The standard SPH

About the pressure gradient….

$$\langle \nabla p \rangle_i = \sum_j (p_i + p_j) \nabla_i W_{i,j} V_j$$

- **preserves linear and angular momenta**
- the work along the free surface is null ***in an integral sense***, namely

$$\int_{\partial D} p\,(\boldsymbol{u} \cdot \boldsymbol{n})\,\mathrm{d}S = 0$$

Advantages:

- if we set *p=0* along the FS at the initial time, the SPH does a null work along the FS (in an integral sense) during the subsequent evolution
- in comparison to the incompressible SPH variants, there is no need to impose *p=0* along the FS during the evolution

The standard SPH

Almost done…

$$\begin{cases} \dfrac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\rho_i \sum_j (\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot \nabla_i W_{i,j} V_j \\ \rho_i \dfrac{\mathrm{d}\boldsymbol{u}_i}{\mathrm{d}t} = \rho_i \boldsymbol{f}_i - \sum_j (p_j + p_i) \nabla_i W_{i,j} V_j + \langle \nabla \cdot \mathbb{V} \rangle_i \\ \dfrac{\mathrm{d}\boldsymbol{x}_i}{\mathrm{d}t} = \boldsymbol{u}_i \qquad p_i = F(\rho_i) \end{cases}$$

Viscous term (Monaghan & Gingold,1983)

$$\langle \nabla \cdot \mathbb{V} \rangle_i = K \sum_j \frac{(\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot (\boldsymbol{x}_j - \boldsymbol{x}_i)}{\|\boldsymbol{x}_j - \boldsymbol{x}_i\|^2} \nabla_i W_{i,j} V_j$$

$K > 0$

Symmetric => cons. linear momentum

+

Radial => cons. angular momentum

$$\sum_i \boldsymbol{u}_i \cdot \langle \nabla \cdot \mathbb{V} \rangle_i V_i \le 0$$ **=> purely dissipative term!**

The standard SPH

$$\langle \nabla \cdot \mathbb{V} \rangle_i = K \sum_j \frac{(\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot (\boldsymbol{x}_j - \boldsymbol{x}_i)}{\|\boldsymbol{x}_j - \boldsymbol{u}_i\|^2} \nabla_i W_{i,j} V_j$$

To stabilize and regularize the simulations of "inviscid" flows

$$K = \begin{cases} \alpha\, h\, c_0\, \rho_0 \\ n\,(n+2)\,\mu \end{cases}$$

ARTIFICIAL VISCOSITY $\alpha = 0.01 - 0.1$

c_0 is the sound velocity (to be defined later)

ρ_0 is the reference density value

PHYSICAL VISCOSITY μ is the dynamical viscosity

n is the number of spatial dimensions

$$\langle \nabla \cdot \mathbb{V} \rangle_i \simeq 2\mu \nabla (\nabla \cdot \boldsymbol{u}) + \mu \nabla^2 \boldsymbol{u} \qquad \text{for} \quad h \ll 1\,, \quad \frac{\Delta x}{h} \ll 1\,,$$

and regular particle distributions

The standard SPH

If the viscosity is set to zero, the standard SPH preserves the **sum of kinetic energy , potential energy (if any) and** ***reversible*** **internal energy**

$$\mathcal{E}_k + \mathcal{E}_p + \mathcal{E}_c = constant$$

$$\mathcal{E}_k = \sum_i m_i \frac{\|\boldsymbol{u}_i\|^2}{2} \qquad \mathcal{E}_p = -\sum_i m_i \phi_i \qquad \mathcal{E}_c = \sum_i m_i \int_{\rho_0}^{\rho_i} \frac{p(s)}{s^2} ds$$

If the viscosity is included in the scheme, in agreement with the second law of thermodynamics , we have:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathcal{E}_k + \mathcal{E}_p + \mathcal{E}_c\right) = \mathcal{P} \leq 0$$

Power due to dissipation

The standard SPH - weak-compressibility

Up to now, the SPH equations represent a generic compressible fluid

$$\begin{cases} \dfrac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\rho_i \displaystyle\sum_j (\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot \nabla_i W_{i,j} V_j \\[2ex] \rho_i \dfrac{\mathrm{d}\boldsymbol{u}_i}{\mathrm{d}t} = \rho_i \boldsymbol{f}_i - \displaystyle\sum_j (p_j + p_i) \nabla_i W_{i,j} V_j + K \sum_j \frac{(\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot (\boldsymbol{x}_j - \boldsymbol{x}_i)}{\|\boldsymbol{x}_j - \boldsymbol{x}_i\|^2} \nabla_i W_{i,j} V_j \\[2ex] \dfrac{\mathrm{d}\boldsymbol{x}_i}{\mathrm{d}t} = \boldsymbol{u}_i \qquad p_i = F(\rho_i) \end{cases}$$

The fluid is barotropic, then the pressure field is derived from the knowledge of the density field

The signals (e.g. pressure waves) move with a finite velocity, which is called ***sound velocity c(ρ)***

$$c^2(\rho) = \frac{\mathrm{d}p}{\mathrm{d}\rho} = \frac{\mathrm{d}F(\rho)}{\mathrm{d}\rho}$$

The standard SPH - weak-compressibility

For the problems we want to simulate (e.g. water),
the physical sound velocity is much larger than the fluid velocity

$\Rightarrow$ nearly incompressible fluids **(small density variations)!**

=> **we can linearize the state equation around a reference density value** $\boldsymbol{\rho_0}$

$$p = F(\rho) \quad \longrightarrow \quad p = c_0^2\,(\rho - \rho_0) \quad \text{where} \quad c_0 = c\,(\rho_0)$$

Generally for free-surface flows ρ_0 is the density along the FS (where $p=0$)

The standard SPH - weak-compressibility

The time step of the SPH is approximately

$$\Delta t \simeq \frac{h}{c_0}$$

Unfortunately, we cannot use the physical sound velocity otherwise the time step of the simulation (which depends on the inverse of c_0) would be too small!

$$c_0 = 10 \max\left(U_{max} \, , \sqrt{\frac{\Delta p_{max}}{\rho_0}} \right)$$

where U_{max} and p_{max} are the maximum expected velocity and pressure

The above constraint guarantees that the density variations maintains below 1% during the evolution, that is:

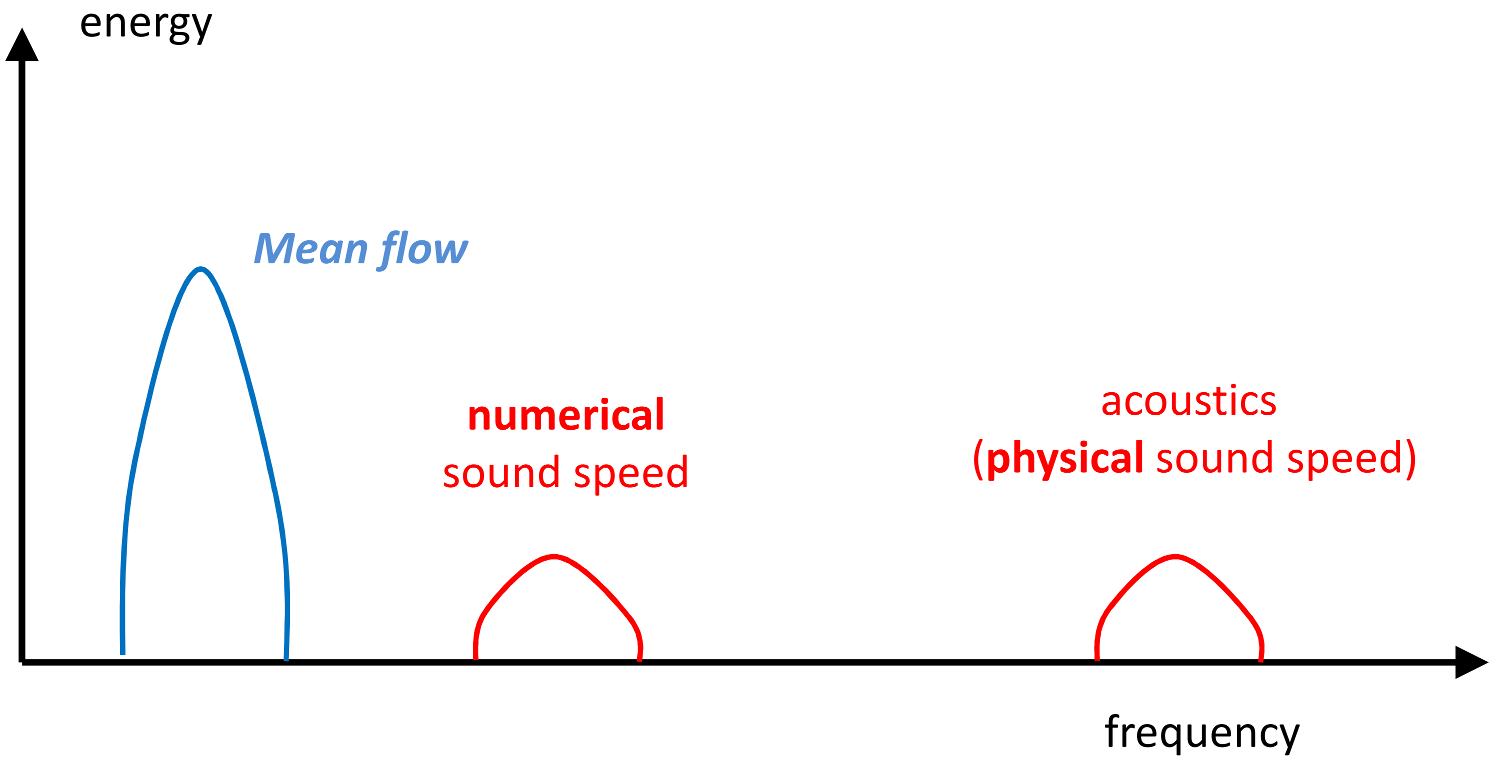
$$\left| \frac{\Delta \rho}{\rho} \right| \leq 0.01$$

Weakly-compressibility assumption

The standard SPH - weak-compressibility

In fact, the use of a ***numerical sound velocity*** is not a problem…

…at least for the phenomena we want to simulate!



The standard SPH - weak-compressibility

Finally…. ***the standard SPH scheme***

$$\begin{cases} \dfrac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\rho_i \displaystyle\sum_j (\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot \nabla_i W_{i,j} V_j \\[2ex] \rho_i \dfrac{\mathrm{d}\boldsymbol{u}_i}{\mathrm{d}t} = \rho_i \boldsymbol{f}_i - \displaystyle\sum_j (p_j + p_i) \nabla_i W_{i,j} V_j + K \sum_j \dfrac{(\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot (\boldsymbol{x}_j - \boldsymbol{x}_i)}{\|\boldsymbol{x}_j - \boldsymbol{x}_i\|^2} \nabla_i W_{i,j} V_j \\[2ex] \dfrac{\mathrm{d}\boldsymbol{x}_i}{\mathrm{d}t} = \boldsymbol{u}_i \qquad p_i = c_0^2 (\rho_i - \rho_0) \qquad V_i = m_i / \rho_i \end{cases}$$

- ✓ **Conservation of mass**
- ✓ **Conservation of linear and angular momenta**
- ✓ **If *K=0*, conservation of (kinetic + potential + internal)**

(see, for example, Monaghan 2005)

The standard SPH - weak-compressibility

The standard SPH:

PROS:

✓ explicit scheme => **good for parallelization (e.g. 3D simulations)**

✓ Implicit fulfilment of the free-surface boundary conditions

=> **good for simulations with complex interface deformations/fragmentations**

CONS:

➢ large sound speed => **small time step**

➢ weakly-compressible fluid => **acoustic noise**

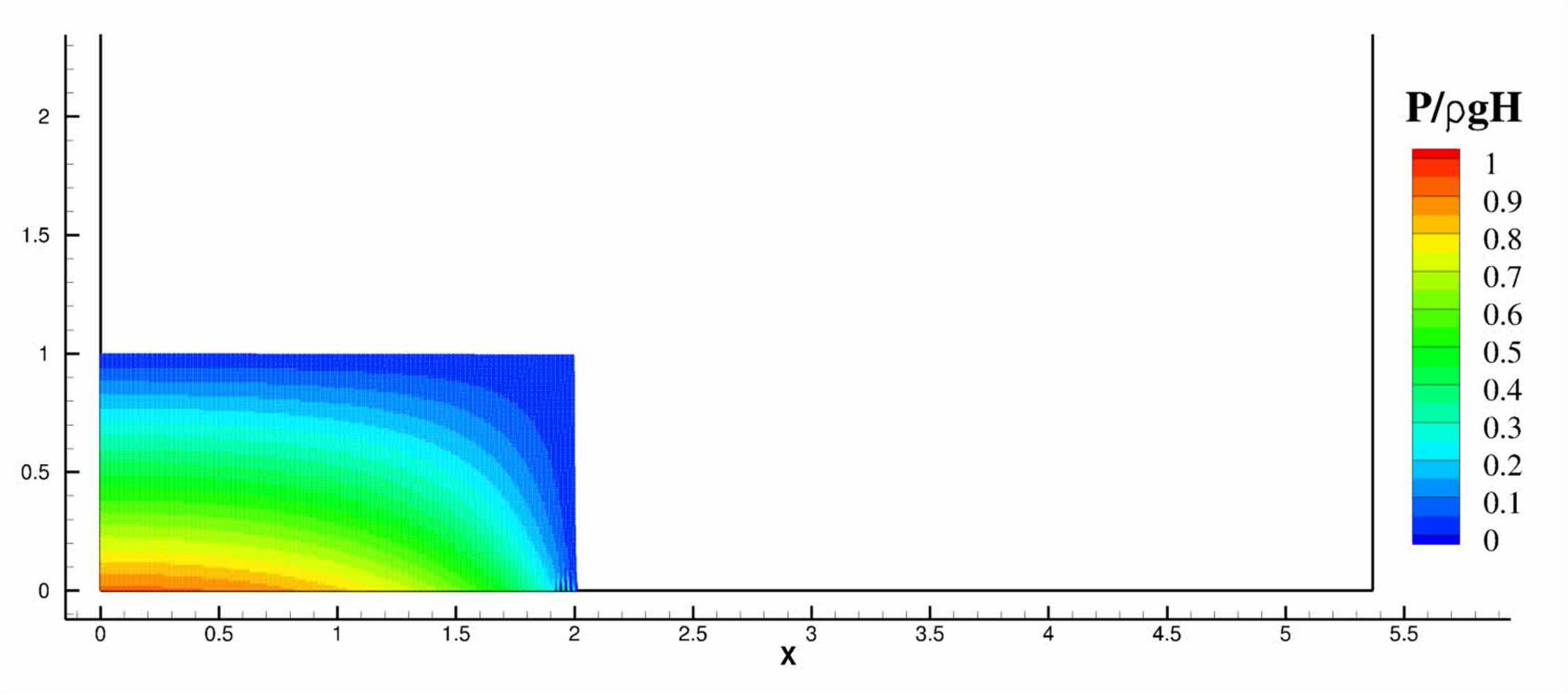
➢ central-explicit scheme (+ nonlinearities) => **spurious numerical noise**

numerical schemes to reduce/avoid the spurious numerical noise

The standard SPH - noise in the pressure field

Generally, the velocity field and particle positions are good….

What about other relevant quantities like pressure?



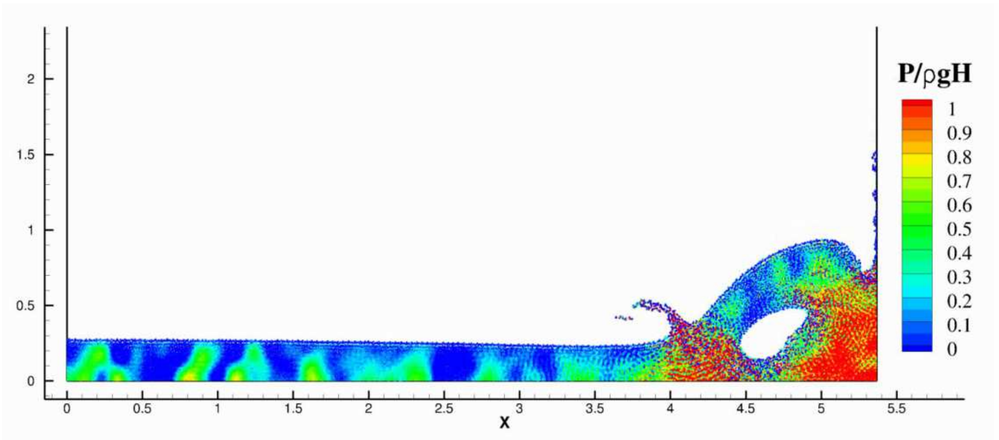
Dam-break flow: “inviscid fluid” simulated with artificial viscosity (***α=0.01***)

The standard SPH - noise in the pressure field

Kinematics is correct, but pressure field is noisy!

Main sources of noise on the pressure field:

- Numerical scheme: centred + explicit



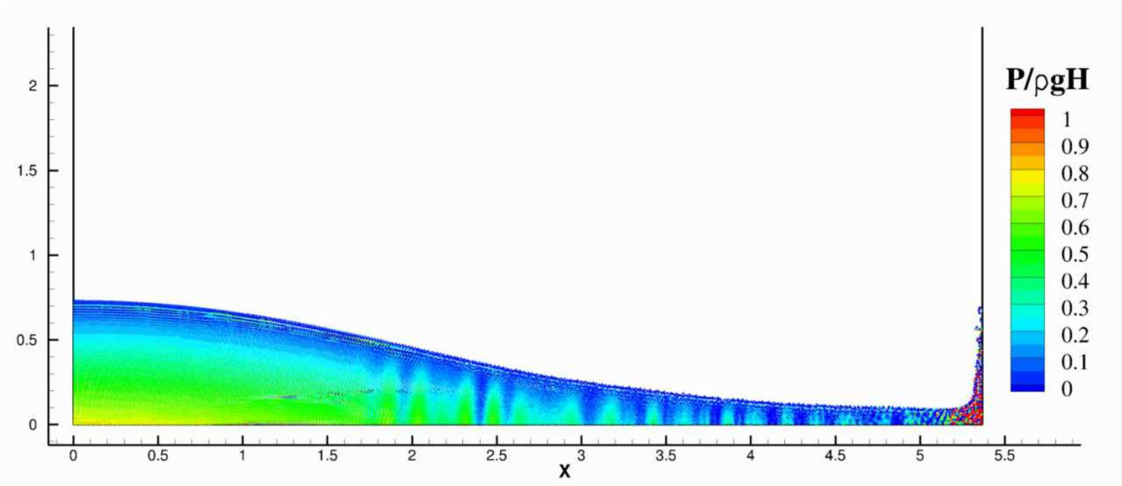
The standard SPH - noise in the pressure field

Kinematics is correct, but pressure field is noisy!

Main sources of noise on the pressure field:

- Numerical scheme: centred + explicit

- Physical model: acoustic waves

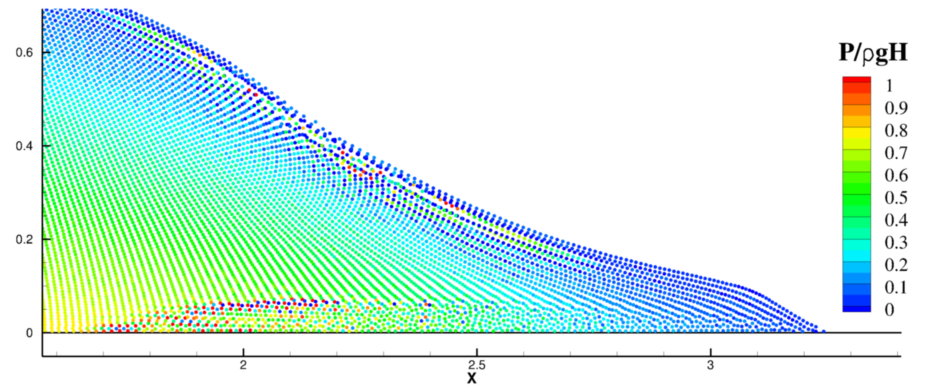


The standard SPH - noise in the pressure field

Kinematics is correct, but pressure field is noisy!

Main sources of noise on the pressure field:

- Numerical scheme: centred + explicit
- Physical model: acoustic waves
- Lagrangian character:
  particle resettlement



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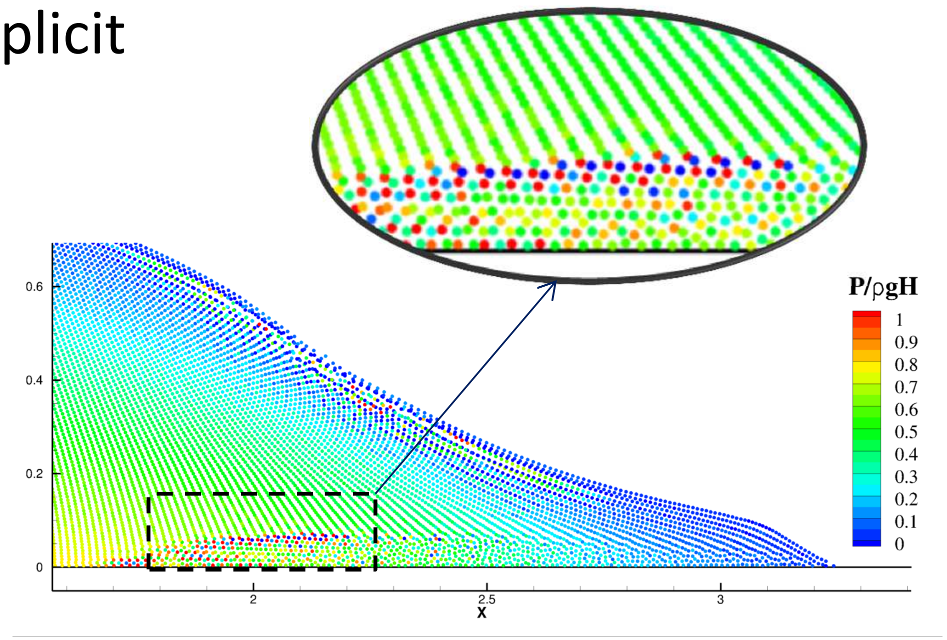

The standard SPH - noise in the pressure field

Kinematics is correct, but pressure field is noisy!

Main sources of noise on the pressure field:

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- Physical model: acoustic waves
- Lagrangian character:
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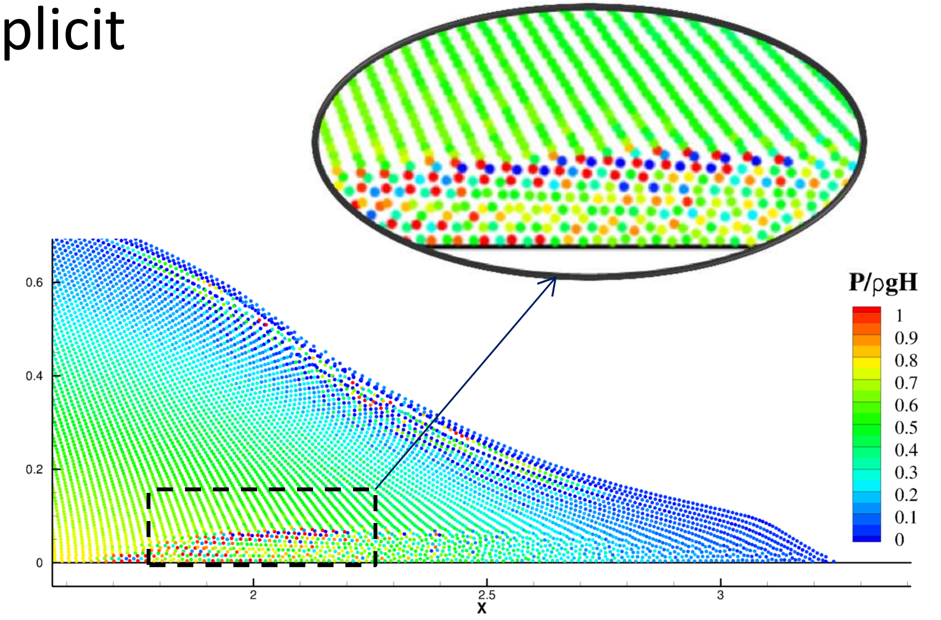
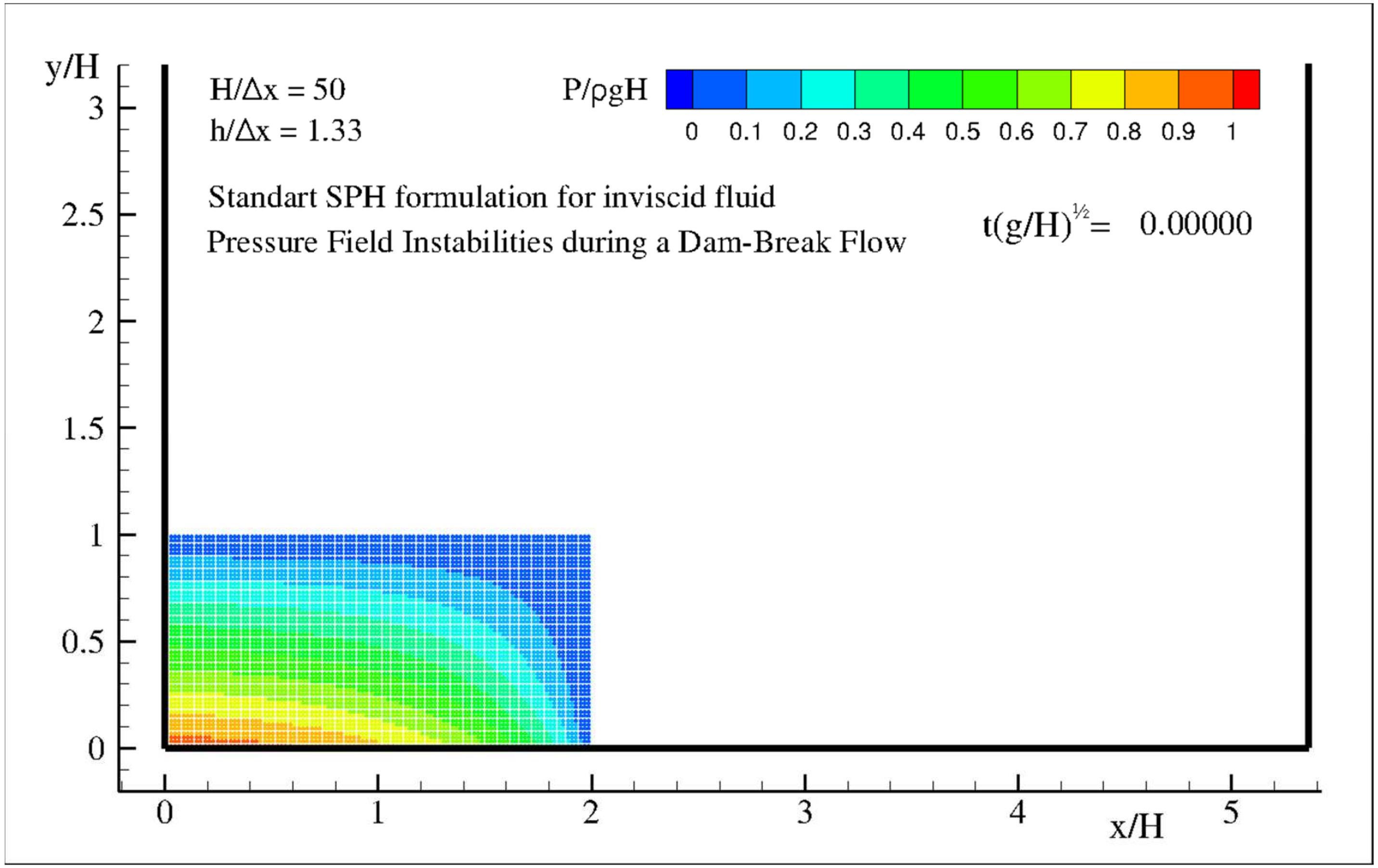


All the three aspects are strictly linked!

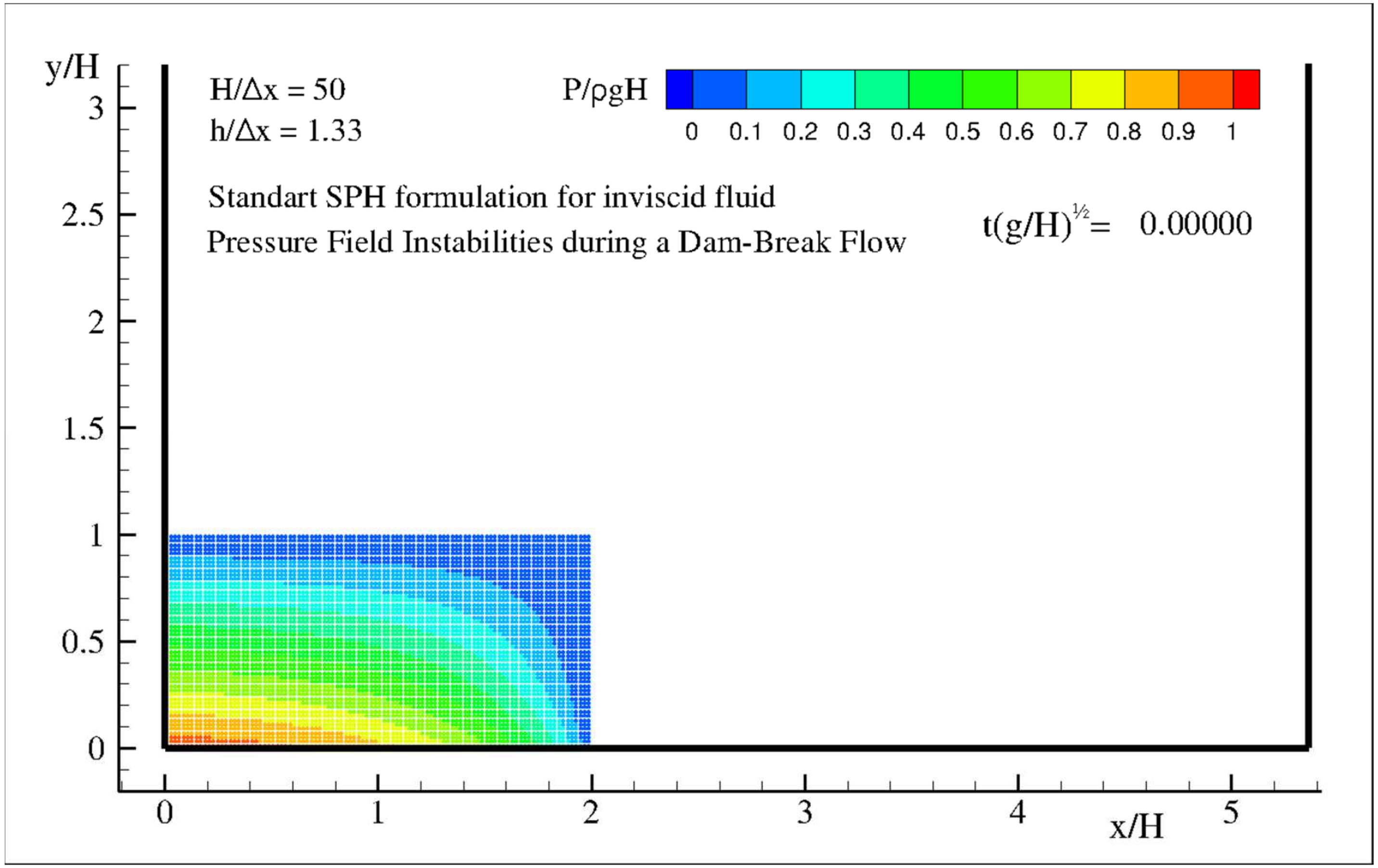
The standard SPH - noise in the pressure field

An example:
simulation of dam-break **without** artificial viscosity (***α=0***)



The standard SPH - noise in the pressure field

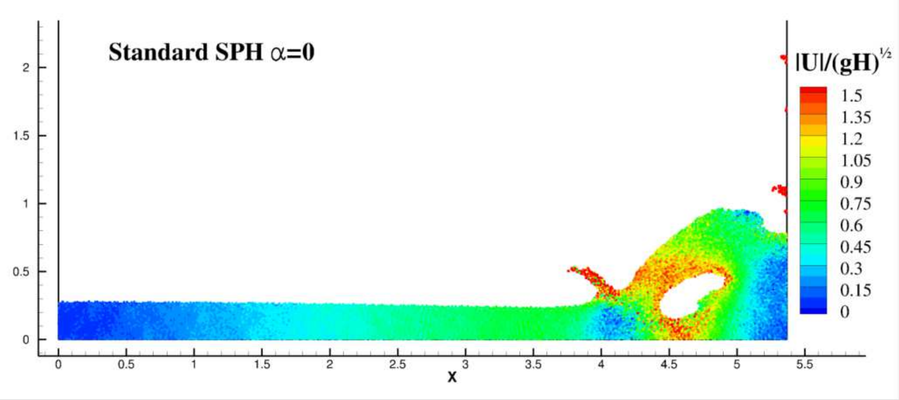
Remember the scheme relies on conservation:
errors goes in internal energy!

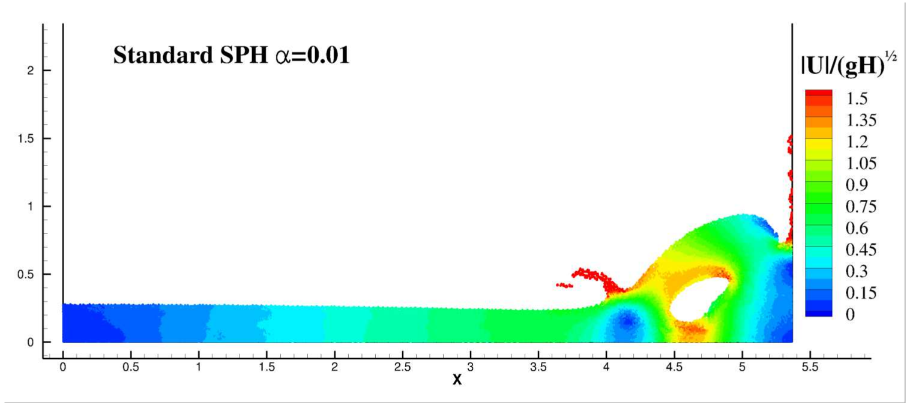


The standard SPH - noise in the pressure field

The effect of the artificial viscosity is to add diffusion inside the momentum equation

Velocity Field





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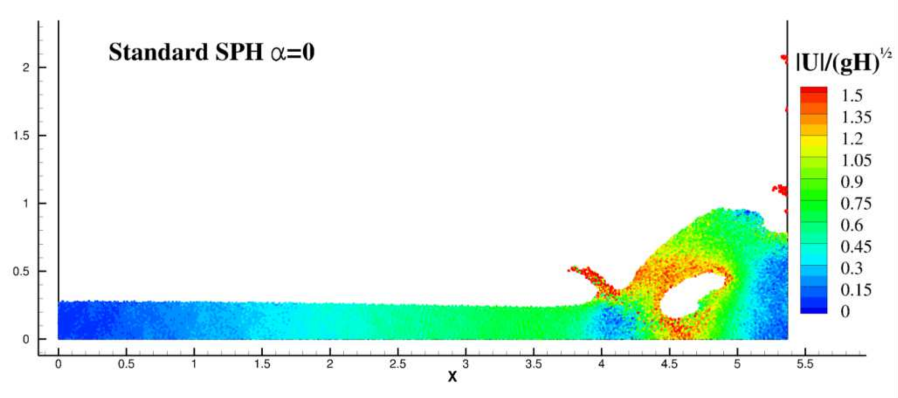
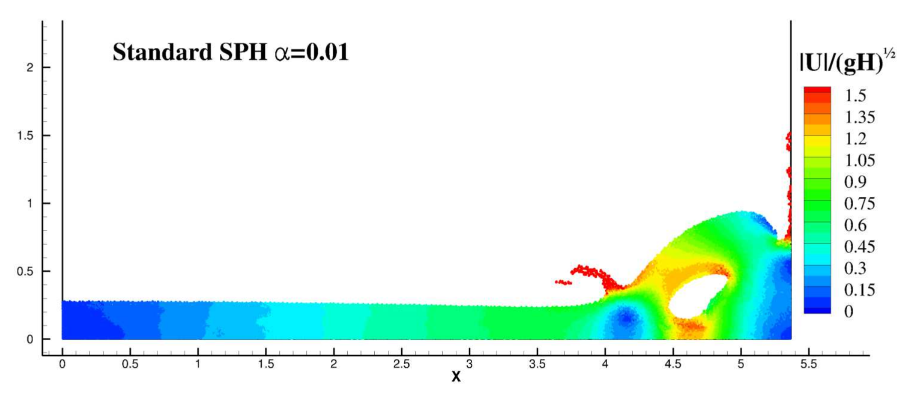
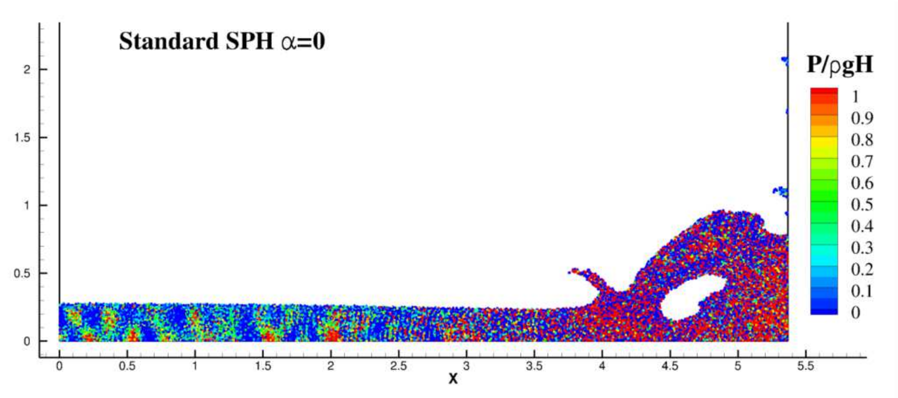
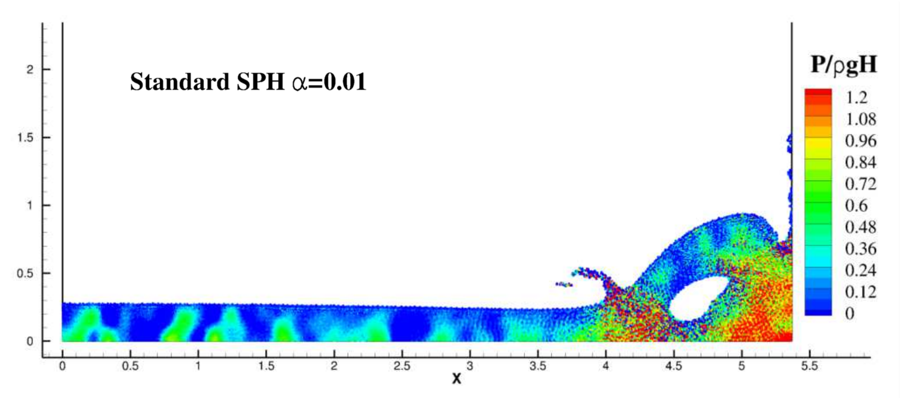




Pressure Field





The standard SPH - noise in the pressure field

The effect of the artificial viscosity is to add diffusion inside the momentum equation

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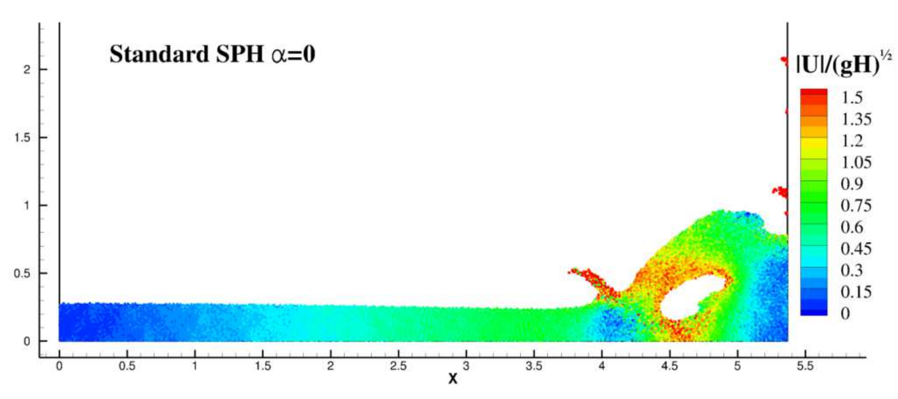
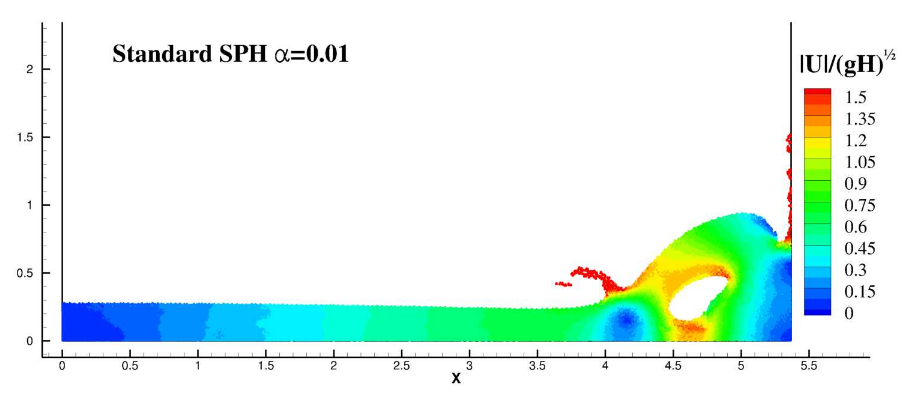
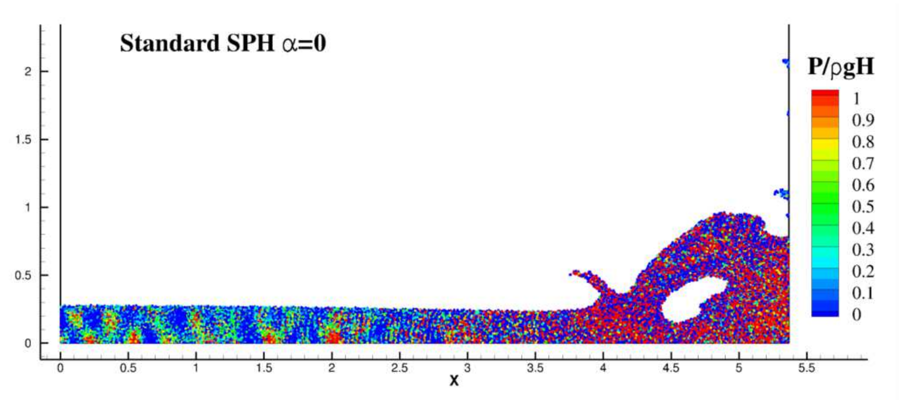
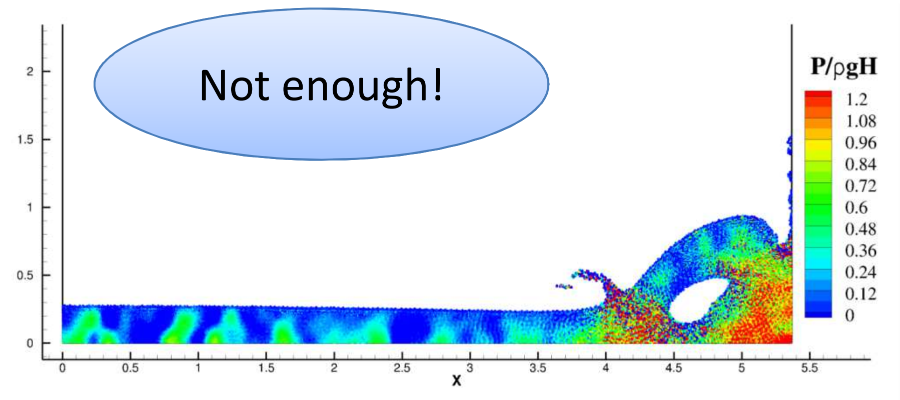




Pressure Field





The diffusive approach

Since the spurious noise mainly affects the density/pressure fields, a possible strategy is to add a diffusive term inside the continuity equation:

$$\begin{cases} \dfrac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\rho_i \sum_j (\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot \nabla_i W_{i,j} V_j + \delta \, h \, c_0 \, \mathcal{D}_i \\ \rho_i \dfrac{\mathrm{d}\boldsymbol{u}_i}{\mathrm{d}t} = \rho_i \boldsymbol{f}_i - \sum_j (p_j + p_i) \nabla_i W_{i,j} V_j + K \sum_j \dfrac{(\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot (\boldsymbol{x}_j - \boldsymbol{x}_i)}{\|\boldsymbol{x}_j - \boldsymbol{x}_i\|^2} \nabla_i W_{i,j} V_j \\ \dfrac{\mathrm{d}\boldsymbol{x}_i}{\mathrm{d}t} = \boldsymbol{u}_i \qquad p_i = c_0^2 (\rho_i - \rho_0) \qquad V_i = m_i / \rho_i \end{cases}$$

where δ is a dimensionless parameter and

$$\mathcal{D}_i = 2 \sum_j \boldsymbol{\psi}_{i,j} \cdot \nabla_i W_{i,j} V_j$$

the specific form of $\boldsymbol{\psi}_{i,j}$ characterizes the diffusive scheme at hand

The diffusive approach

The vector $\psi_{i,j}$ has to be **symmetric**, that is

$$\psi_{i,j} = \psi_{j,i} \quad \Longrightarrow \quad \sum_i \mathcal{D}_i V_i = 0$$

This ensures the consistency of the integral form of the continuity equation (e.g. consistency with the equation of mass conservation)

with diffusion | without diffusion

$$\underbrace{\sum_i \left[\frac{\mathrm{d}\rho_i}{\mathrm{d}t} + \rho_i \langle \nabla \cdot \boldsymbol{u} \rangle_i - \delta\, h\, c_0\, \mathcal{D}_i \right]}_{\text{with diffusion}} V_i = \underbrace{\sum_i \left[\frac{\mathrm{d}\rho_i}{\mathrm{d}t} + \rho_i \langle \nabla \cdot \boldsymbol{u} \rangle_i \right]}_{\text{without diffusion}} V_i$$

$$\simeq \int_D \left[\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \nabla \cdot \boldsymbol{u} \right] \mathrm{d}V = 0$$

The diffusive approach

$$\psi_{i,j} = (\rho_j - \rho_i)\frac{(\boldsymbol{x}_j - \boldsymbol{x}_i)}{\|\boldsymbol{x}_j - \boldsymbol{x}_i\|^2}$$

Molteni & Colagrossi (2009)

$$\psi_{i,j} = (\rho_j - \rho_i)\frac{(\boldsymbol{x}_j - \boldsymbol{x}_i)}{2h\,\|\boldsymbol{x}_j - \boldsymbol{x}_i\|}$$

Ferrari et al. (2009)

$$\boxed{\mathcal{D}_i \simeq \nabla^2 \rho_i}$$

but they are inconsistent close to the free surface **(no hydrostatic solution!)**

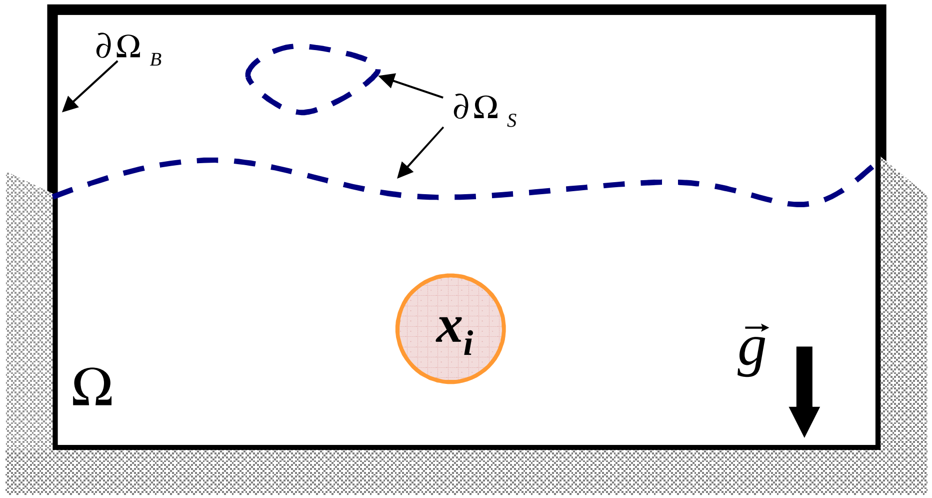
The diffusive approach

For example, let us consider the diffusive term by Molteni & Colagrossi (2009)

$$2\sum_i (\rho_j - \rho_i)\frac{(\boldsymbol{x}_j - \boldsymbol{x}_i)}{\|\boldsymbol{x}_j - \boldsymbol{x}_i\|^2}\cdot \nabla_i W_{ij} V_j = 2\,\nabla\rho_i \cdot \nabla\Gamma_i + \Gamma_i \Delta\rho_i + \mathcal{O}(h)$$

$$\Gamma_i = \sum_j W_{i,j} V_j \simeq 1$$

$$\nabla\Gamma_i = \sum_j \nabla_i W_{i,j} V_j \simeq 0$$



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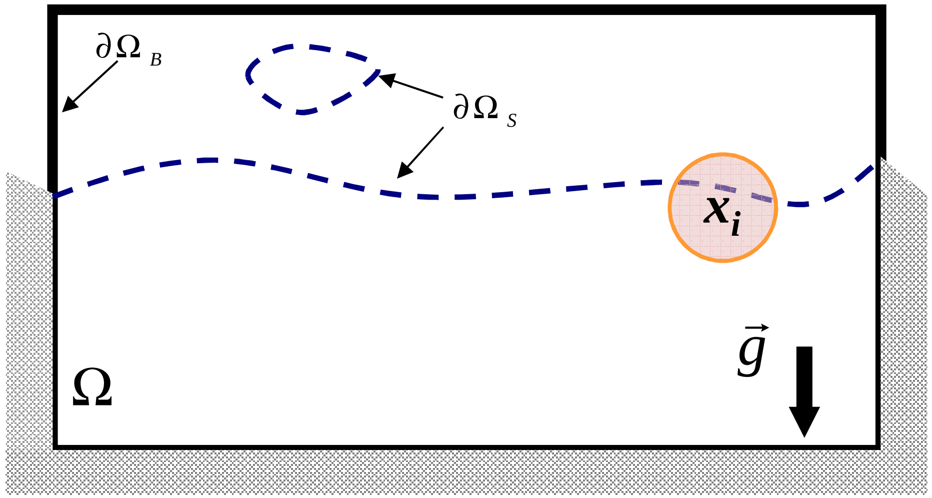
$$2\sum_i (\rho_j - \rho_i)\frac{(\boldsymbol{x}_j - \boldsymbol{x}_i)}{\|\boldsymbol{x}_j - \boldsymbol{x}_i\|^2}\cdot \nabla_i W_{ij} V_j = 2\nabla\rho_i \cdot \nabla\Gamma_i + \Gamma_i \Delta\rho_i + \mathcal{O}(h)$$

$$\Gamma_i = \sum_j W_{i,j} V_j < 1$$

$$\nabla\Gamma_i = \sum_j \nabla_i W_{i,j} V_j \simeq \mathcal{O}\left(h^{-1}\right)$$

A spurious term appears close to the free surface!



The diffusive approach

To avoid such an inconsistency, Antuono et al. (2010) defined the following form:

$$\psi_{i,j} = \left[(\rho_j - \rho_i) - \frac{1}{2} \left(\langle \nabla \rho \rangle_j^L + \langle \nabla \rho \rangle_i^L \right) \cdot (\boldsymbol{x}_j - \boldsymbol{x}_i) \right] \frac{(\boldsymbol{x}_j - \boldsymbol{x}_i)}{\| \boldsymbol{x}_j - \boldsymbol{x}_i \|^2}$$

- this formulation is consistent close to the free surface
- the diffusive term converges to zero if h goes to zero

Inside the fluid domain

$$\mathcal{D}_i \simeq \frac{h^2}{12} \mathbb{B}_{jkpq} \left(\frac{\partial^4 \rho_i}{\partial x_j \partial x_k \partial x_p \partial x_q} \right)$$

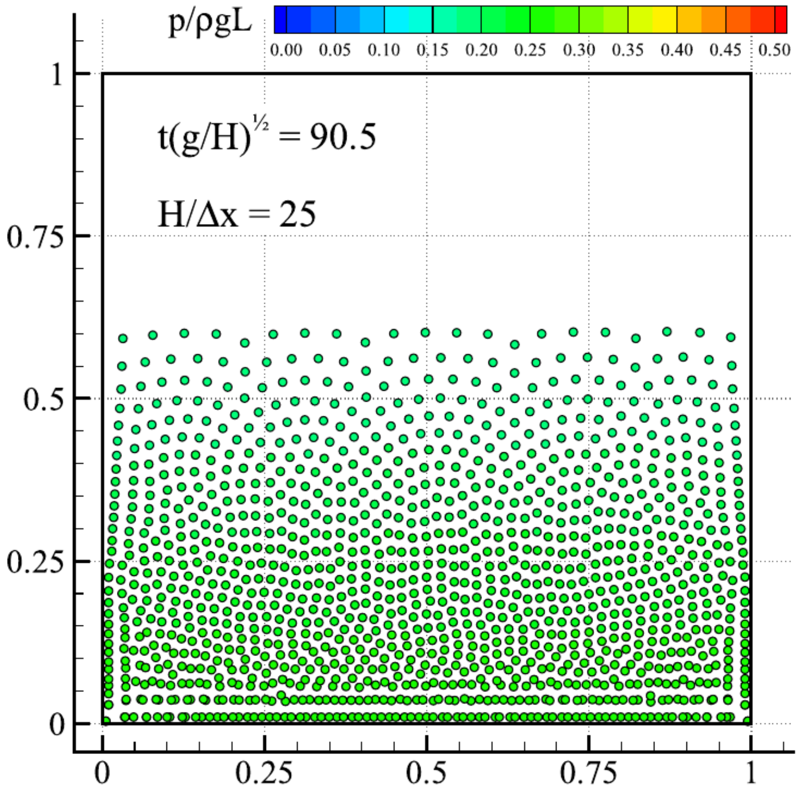
The latter scheme is called δ-SPH scheme

The diffusive approach

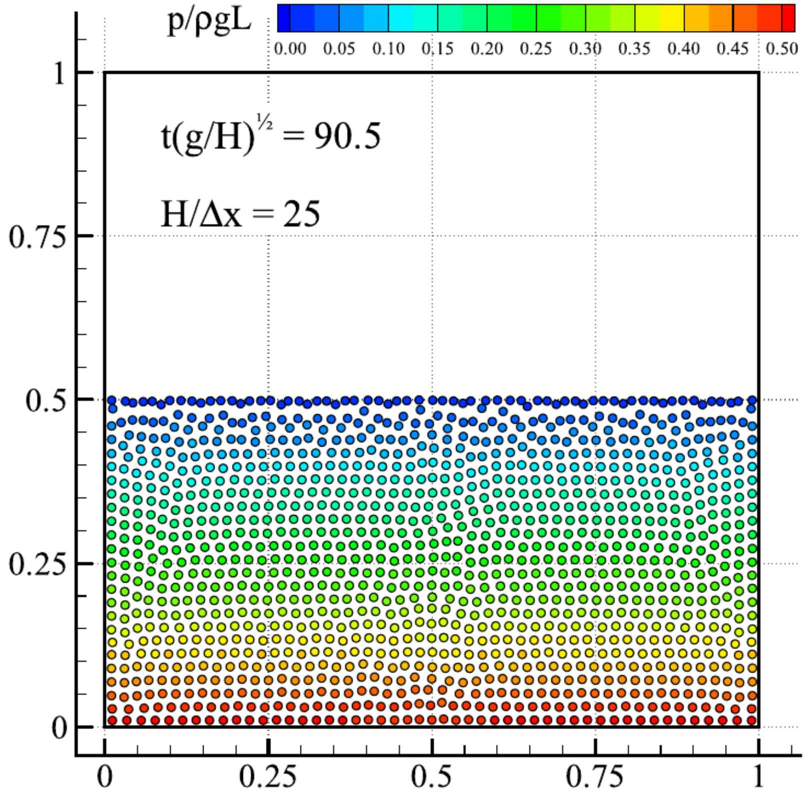
Hydrostatic test

Molteni & Colagrossi (2009)

$$\psi_{ij} = 2\,(\rho_j - \rho_i)\;\frac{(\boldsymbol{r}_j - \boldsymbol{r}_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^2}$$



δ-SPH

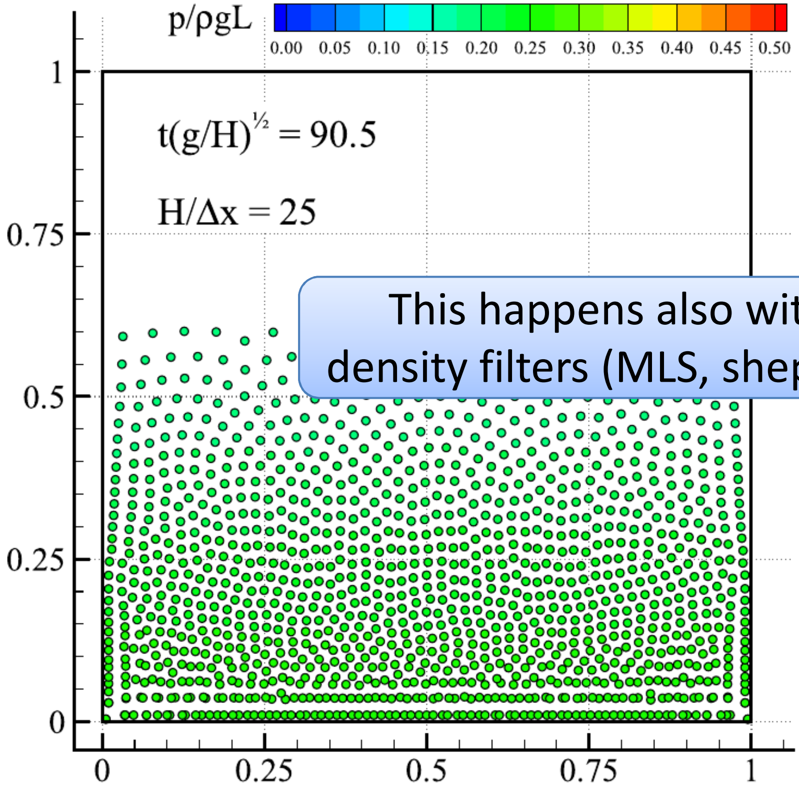


The diffusive approach

Hydrostatic test

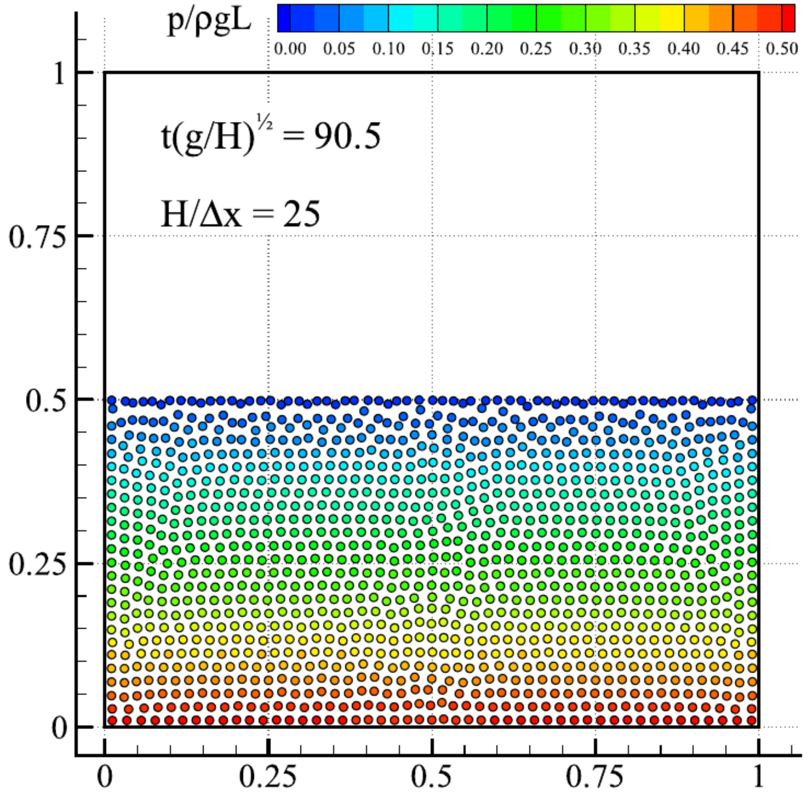
Molteni & Colagrossi (2009)

$$\psi_{ij} = 2\,(\rho_j - \rho_i)\,\frac{(\boldsymbol{r}_j - \boldsymbol{r}_i)}{|\boldsymbol{r}_j - \boldsymbol{r}_i|^2}$$



This happens also with density filters (MLS, shepard)

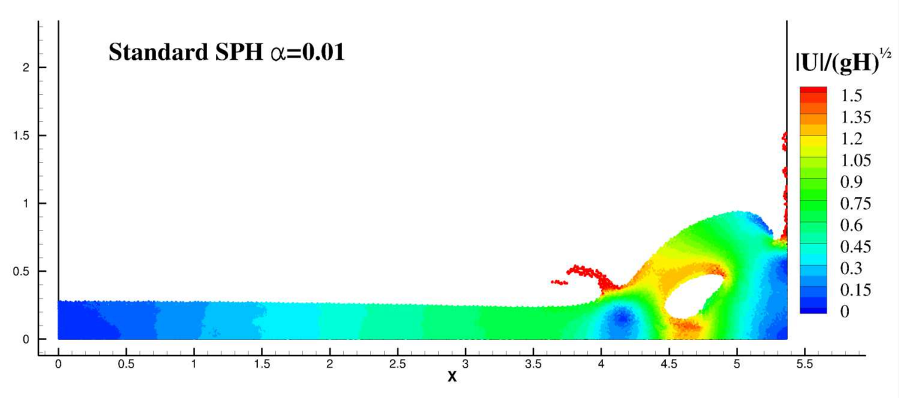
δ-SPH

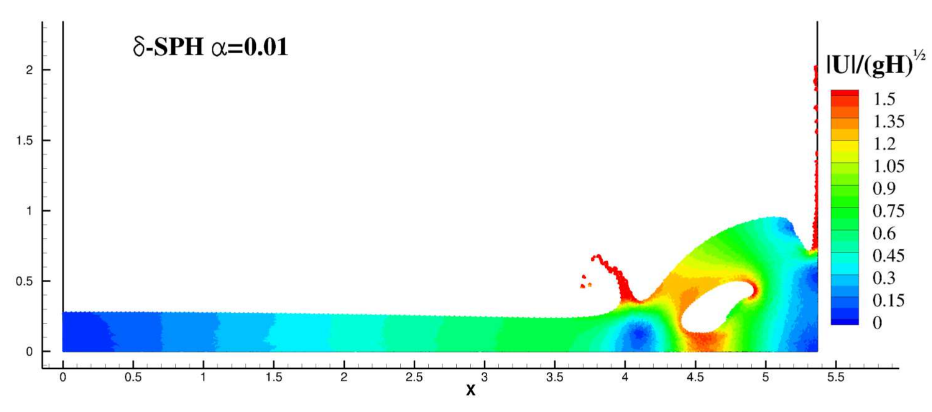


The diffusive approach

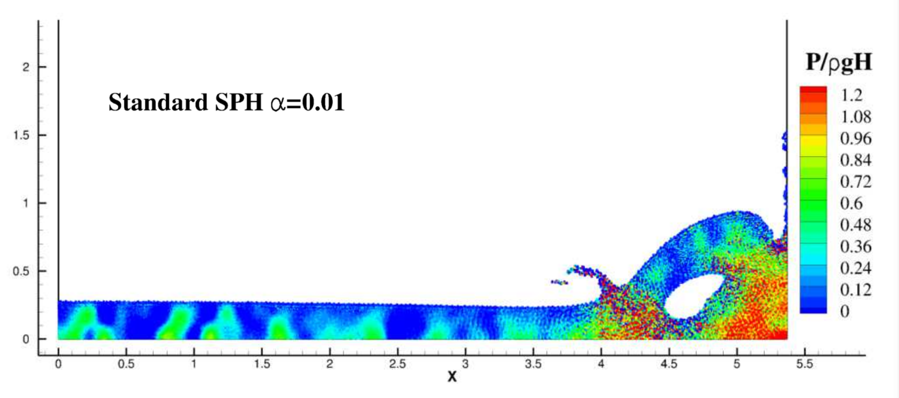
Comparison with standard SPH

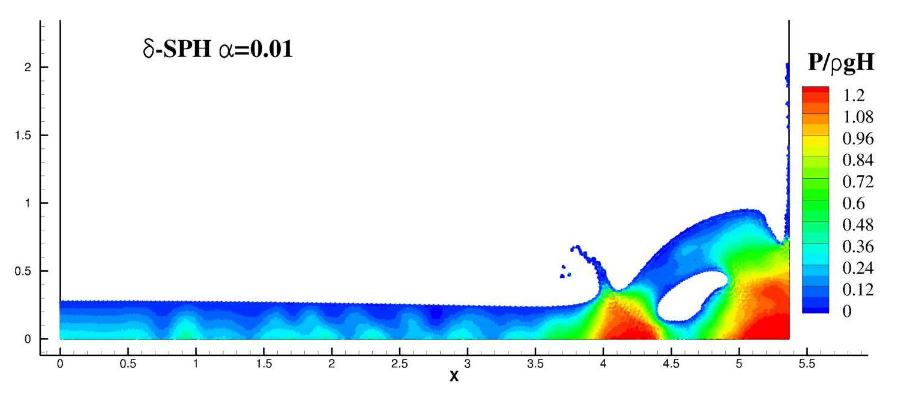
Velocity Field



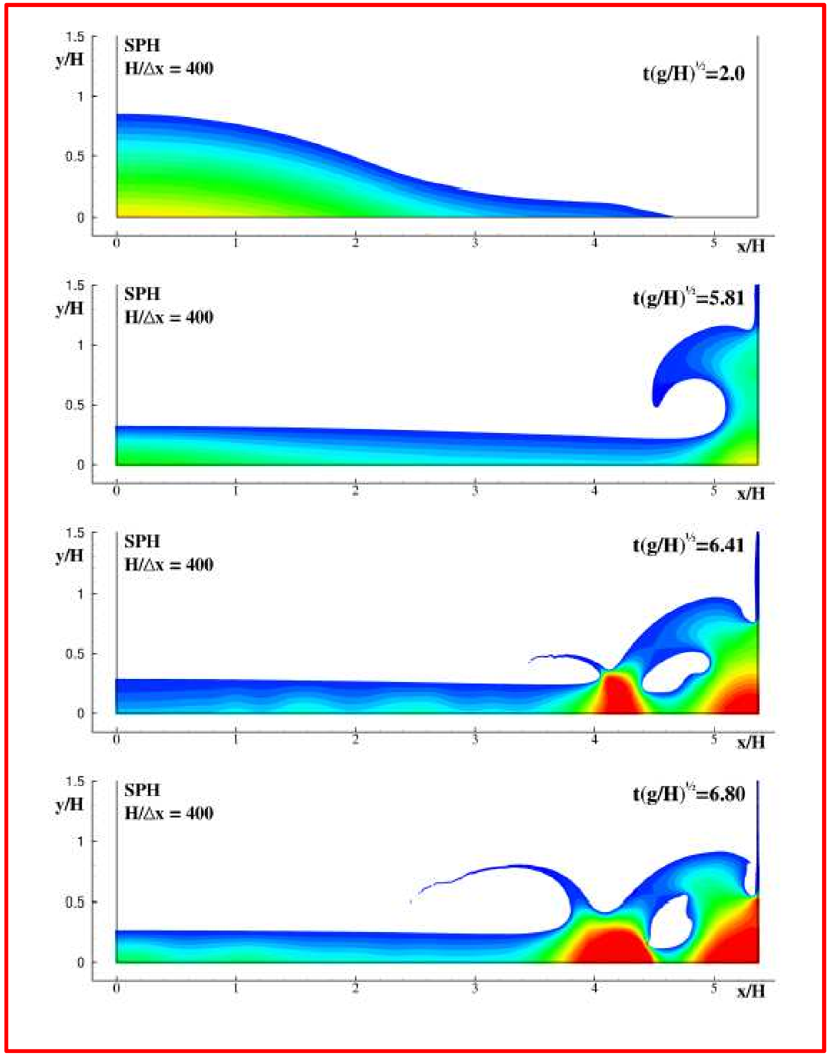


Pressure Field

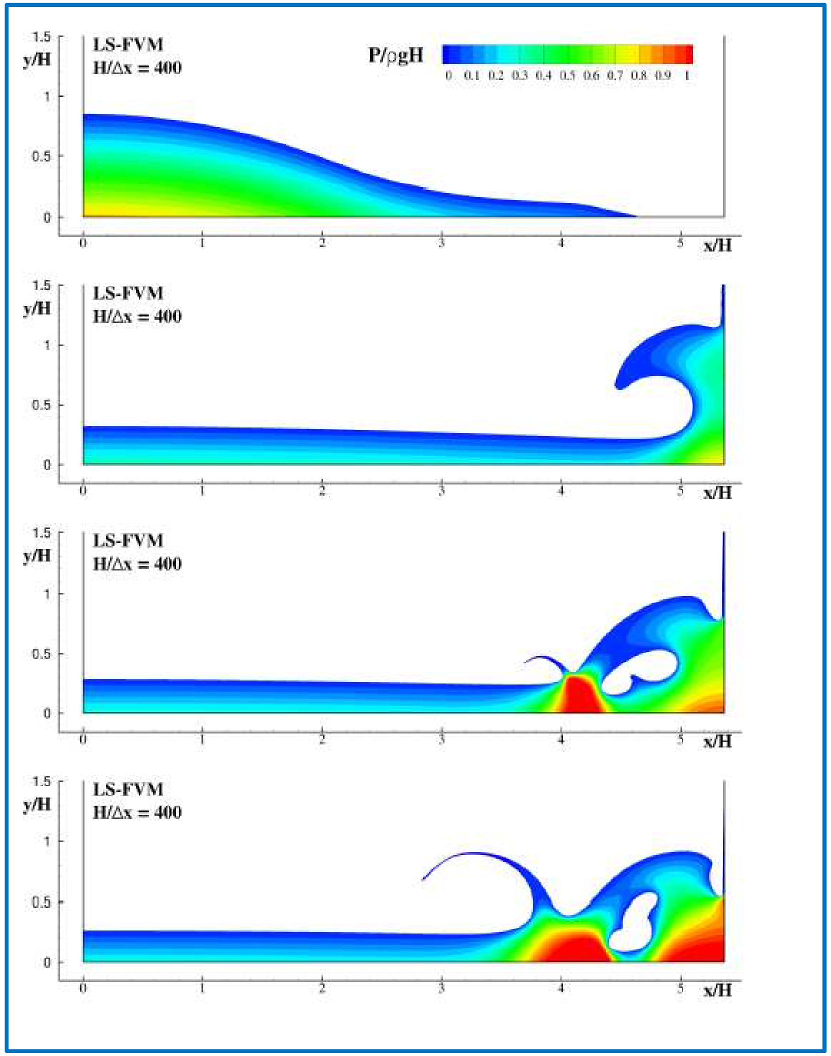




The diffusive approach



Weakly-Compressible δ-SPH



Incompressible FVM

The δ-SPH scheme

$$
\begin{cases}
\dfrac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\rho_i \sum_j (\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot \nabla_i W_{i,j} V_j + \delta\, h\, c_0\, \mathcal{D}_i \\[2ex]
\rho_i \dfrac{\mathrm{d}\boldsymbol{u}_i}{\mathrm{d}t} = \rho_i \boldsymbol{f}_i - \sum_j (p_j + p_i) \nabla_i W_{i,j} V_j + K \sum_j \dfrac{(\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot (\boldsymbol{x}_j - \boldsymbol{x}_i)}{\|\boldsymbol{x}_j - \boldsymbol{x}_i\|^2} \nabla_i W_{i,j} V_j \\[2ex]
\dfrac{\mathrm{d}\boldsymbol{x}_i}{\mathrm{d}t} = \boldsymbol{u}_i \qquad p_i = c_0^2 (\rho_i - \rho_0) \qquad V_i = m_i / \rho_i
\end{cases}
$$

where δ is a dimensionless parameter and

$$
\mathcal{D}_i = 2 \sum_j \boldsymbol{\psi}_{i,j} \cdot \nabla_i W_{i,j} V_j
$$

$$
\boldsymbol{\psi}_{i,j} = \left[(\rho_j - \rho_i) - \frac{1}{2} \left(\langle \nabla \rho \rangle_j^L + \langle \nabla \rho \rangle_i^L \right) \cdot (\boldsymbol{x}_j - \boldsymbol{x}_i) \right] \frac{(\boldsymbol{x}_j - \boldsymbol{x}_i)}{\| \boldsymbol{x}_j - \boldsymbol{x}_i \|^2}
$$

The δ-SPH scheme

The δ-SPH maintains all the conservation properties of the standard SPH scheme

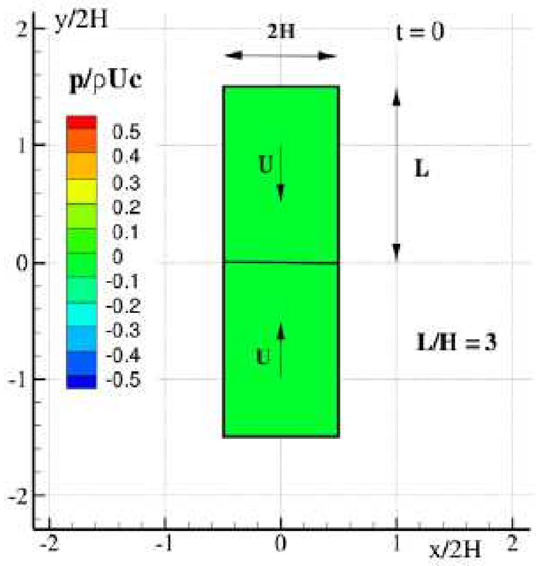
- ✓ **Conservation of mass**
- ✓ **Conservation of linear and angular momenta**
- ✓ **If *K=0*, conservation of (kinetic + potential + internal)**

(see, for example, Antuono et al. 2015)

The dimensionless parameter δ varies in a narrow range of values that depends on the ratio ($\Delta x/h$) and on the spatial dimensions (see Antuono et al. 2012)

(δ=0.1 is a reliable choice in 2D simulations)

The δ-SPH scheme – an example of application



acoustic waves

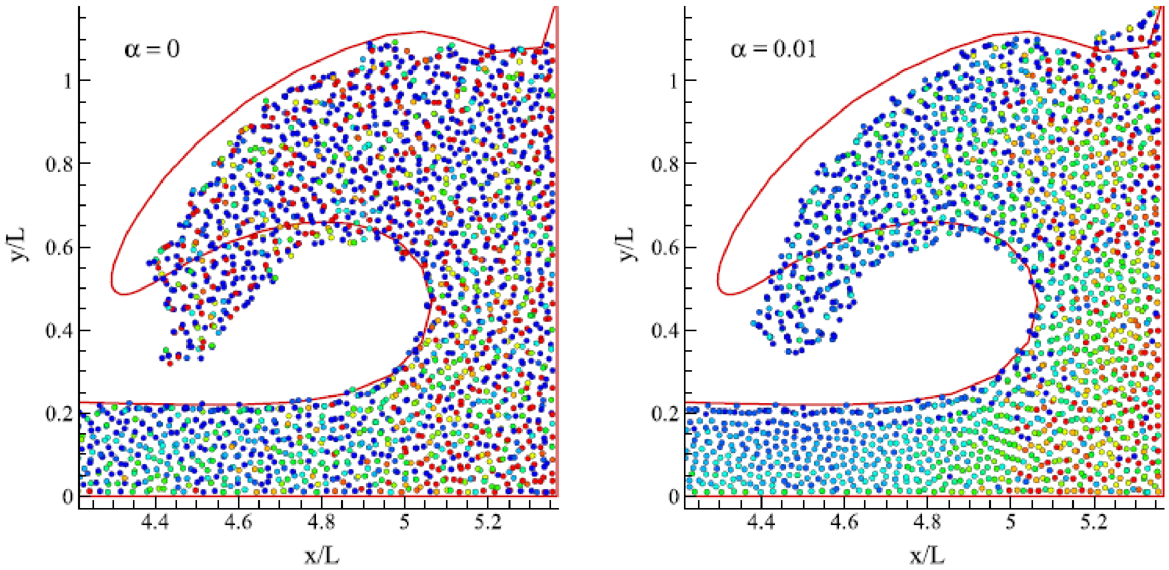
nonlinear wave-wave interaction

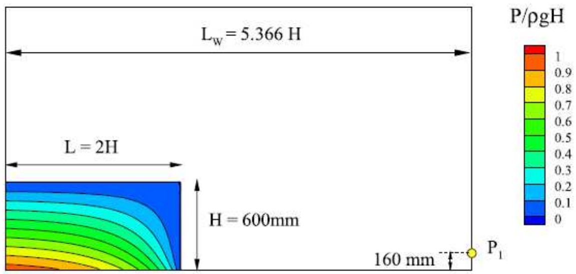
spurious high-frequency noise

Fig. 14. The impact of two rectangular fluid patches: sketches of the evolution. The upper part of the fluid domain is given by the δ-SPH while the lower part is obtained by using the standard SPH.

Simulation of a dam break flow

Standard SPH
(with and without artificial viscosity)





Simulation of a dam break flow

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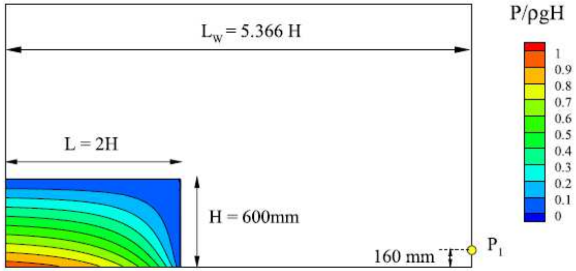
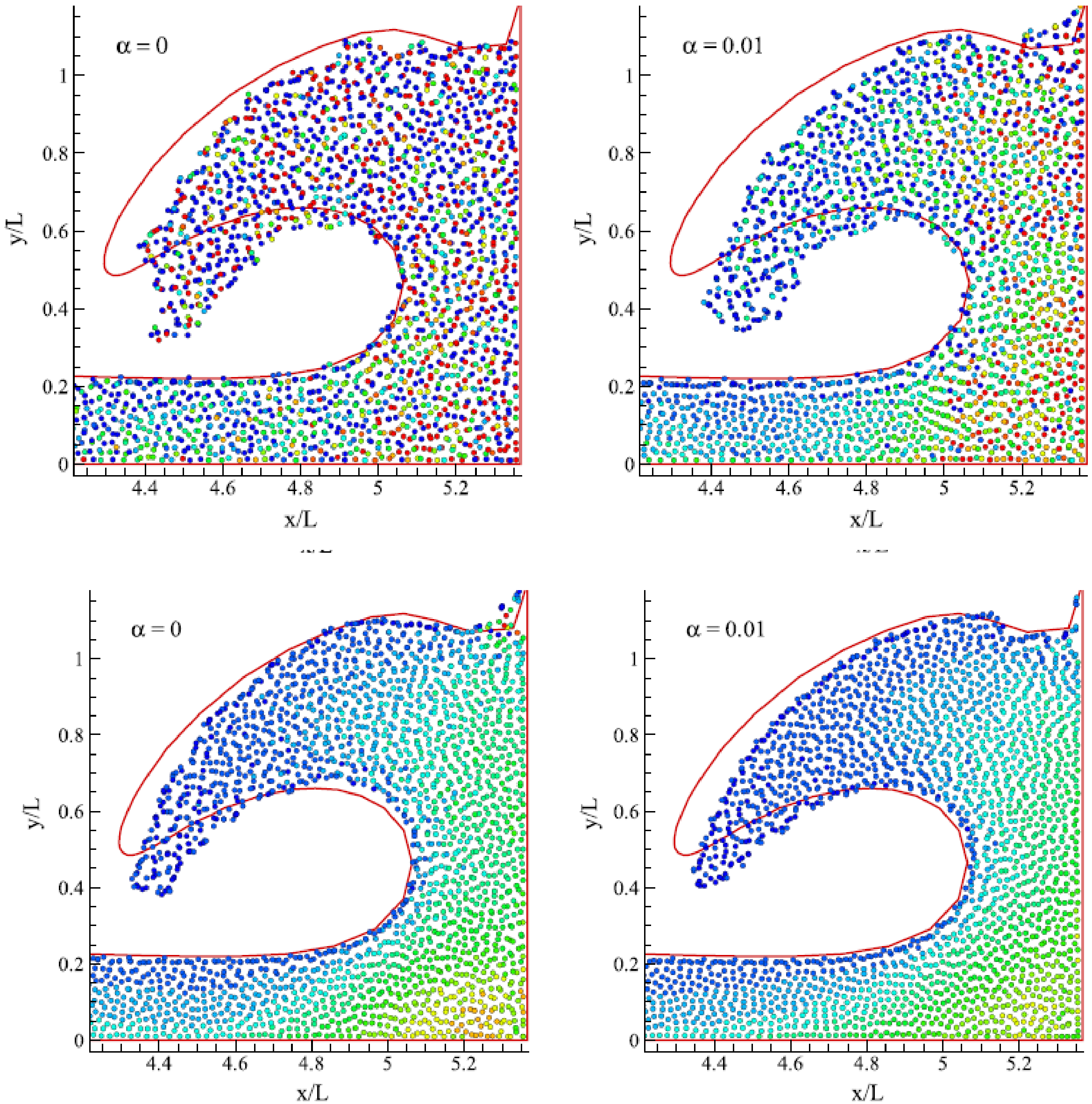




δ-SPH
(with and without artificial viscosity)

The δ-SPH scheme – numerical details

$$\psi_{i,j} = \left[(\rho_j - \rho_i) - \frac{1}{2}\left(\langle\nabla\rho\rangle_j^L + \langle\nabla\rho\rangle_i^L \right) \cdot (\boldsymbol{x}_j - \boldsymbol{x}_i) \right] \frac{(\boldsymbol{x}_j - \boldsymbol{x}_i)}{\|\boldsymbol{x}_j - \boldsymbol{x}_i\|^2}$$

- An additional loop is needed in order to calculate renormalized gradients

$$\langle\nabla\rho\rangle_i^L = \sum_j (\rho_j - \rho_i)\, \boldsymbol{L}_i\, \nabla_i W_{ij}\, V_j \qquad \boldsymbol{L}_i = \left[\sum_j (\boldsymbol{r}_j - \boldsymbol{r}_i) \otimes \nabla_i W_{ij}\, V_j \right]^{-1}$$

- However when using higher-order time integrators (e.g. RK4) this cost can be drastically reduced through a “frozen” diffusion

The δ-SPH scheme – numerical details

The discrete scheme can be represented as follows:

$$\frac{\mathrm{d}\boldsymbol{w}}{\mathrm{d}t} = \boldsymbol{Q}(\boldsymbol{w}) + \boldsymbol{D}(\boldsymbol{w})$$

where ***D(w)*** contains the diffusive term

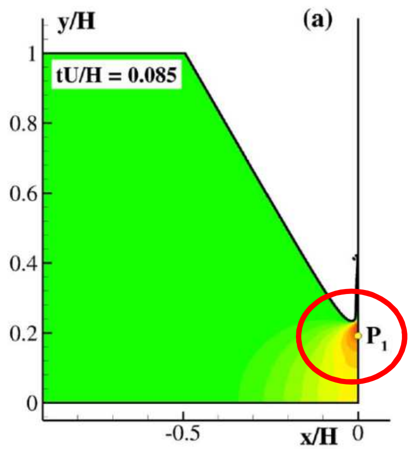
The RK 4-th order ***with frozen diffusion*** reads:

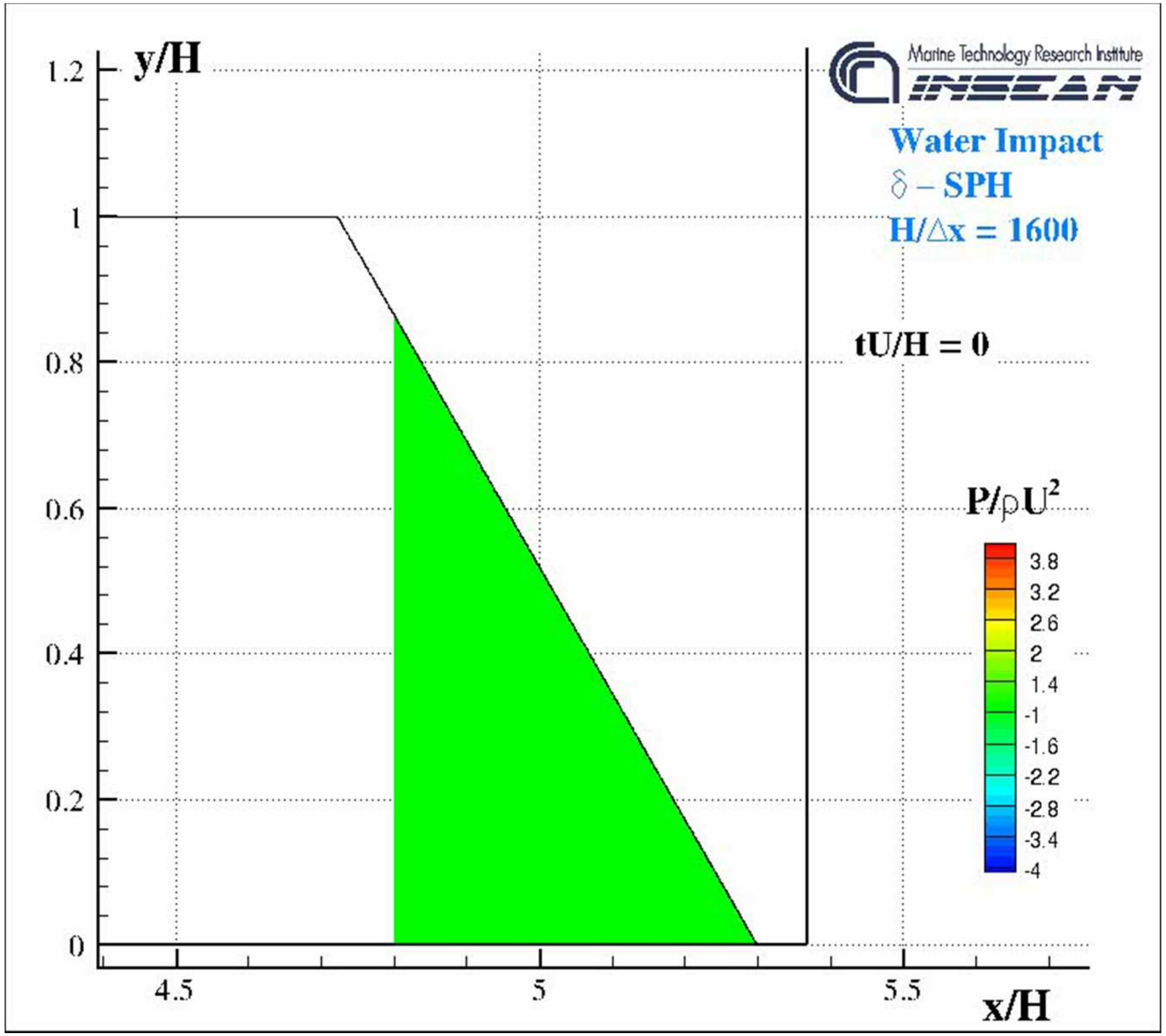
$$\begin{cases} \boldsymbol{w}^{(0)} = \boldsymbol{w}^{n} \\ \boldsymbol{w}^{(1)} = \boldsymbol{w}^{(0)} + \boldsymbol{Q}\left(\boldsymbol{w}^{(0)}\right) \Delta t/2 + \boldsymbol{D}\left(\boldsymbol{w}^{(0)}\right) \Delta t/2 \\ \boldsymbol{w}^{(2)} = \boldsymbol{w}^{(0)} + \boldsymbol{Q}\left(\boldsymbol{w}^{(1)}\right) \Delta t/2 + \boldsymbol{D}\left(\boldsymbol{w}^{(0)}\right) \Delta t/2 \\ \boldsymbol{w}^{(3)} = \boldsymbol{w}^{(0)} + \boldsymbol{Q}\left(\boldsymbol{w}^{(2)}\right) \Delta t + \boldsymbol{D}\left(\boldsymbol{w}^{(0)}\right) \Delta t \\ \boldsymbol{w}^{(4)} = \boldsymbol{w}^{(0)} + \left[\boldsymbol{Q}\left(\boldsymbol{w}^{(0)}\right) + 2\,\boldsymbol{Q}\left(\boldsymbol{w}^{(1)}\right) \right. \\ \qquad \left. +2\,\boldsymbol{Q}\left(\boldsymbol{w}^{(2)}\right) + \boldsymbol{Q}\left(\boldsymbol{w}^{(3)}\right) \right] \Delta t/6 + \boldsymbol{D}\left(\boldsymbol{w}^{(0)}\right) \Delta t \\ \boldsymbol{w}^{n+1} = \boldsymbol{w}^{(4)}. \end{cases}$$

The δ-SPH scheme – convergence

Impinging jet

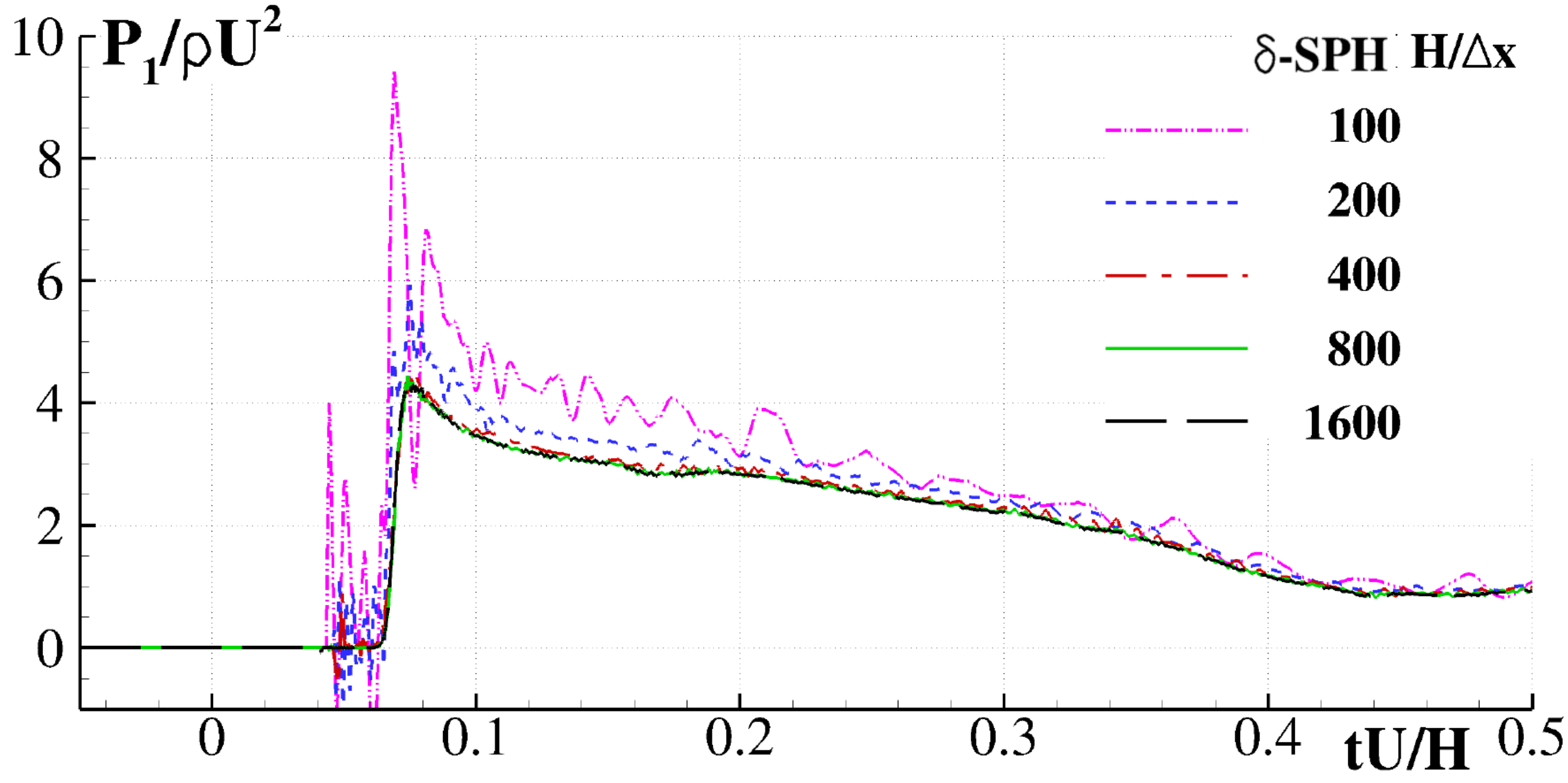
Water wedge impact against a wall





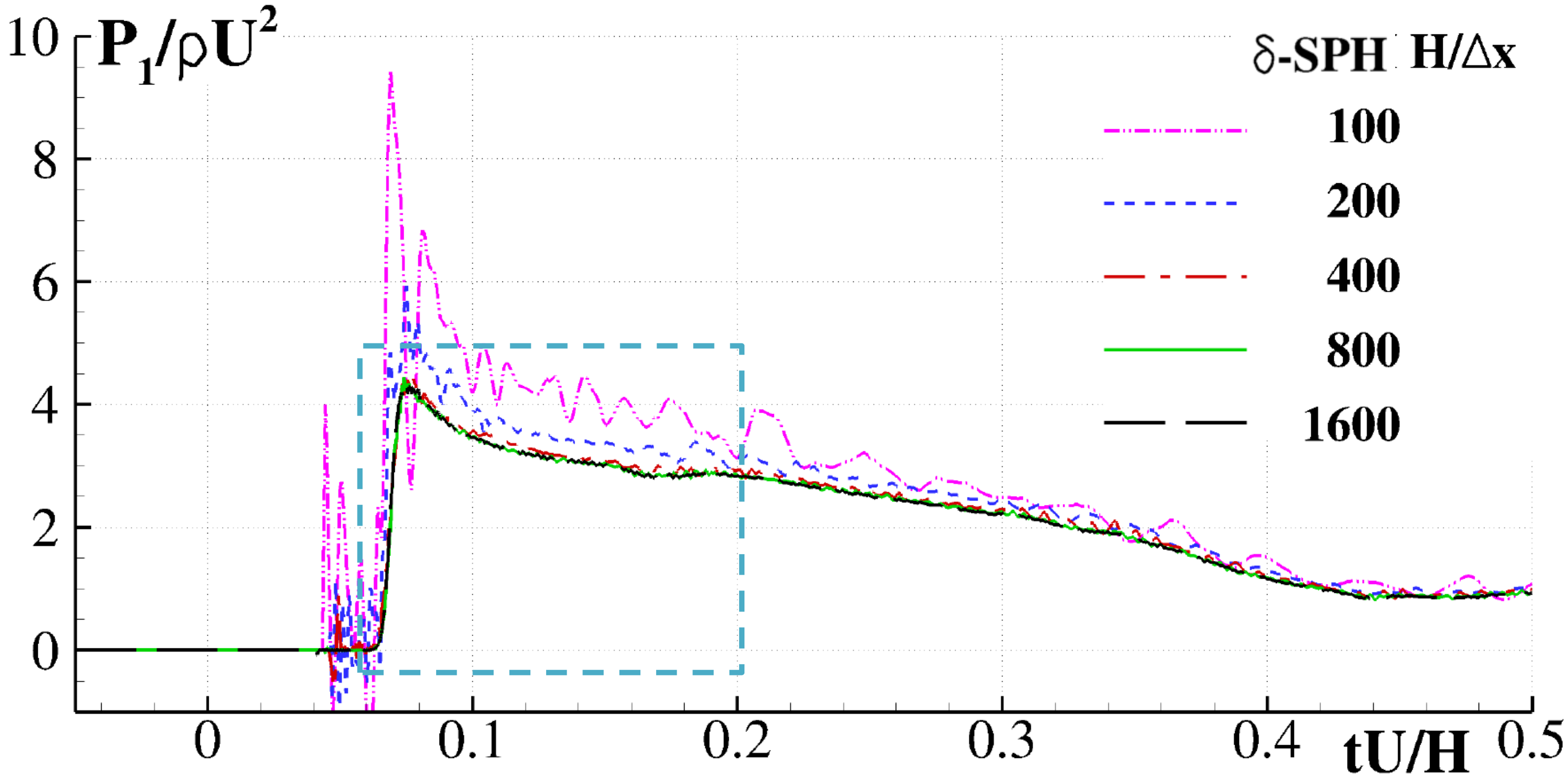
The δ-SPH scheme – convergence

Pressure signals at probe P1



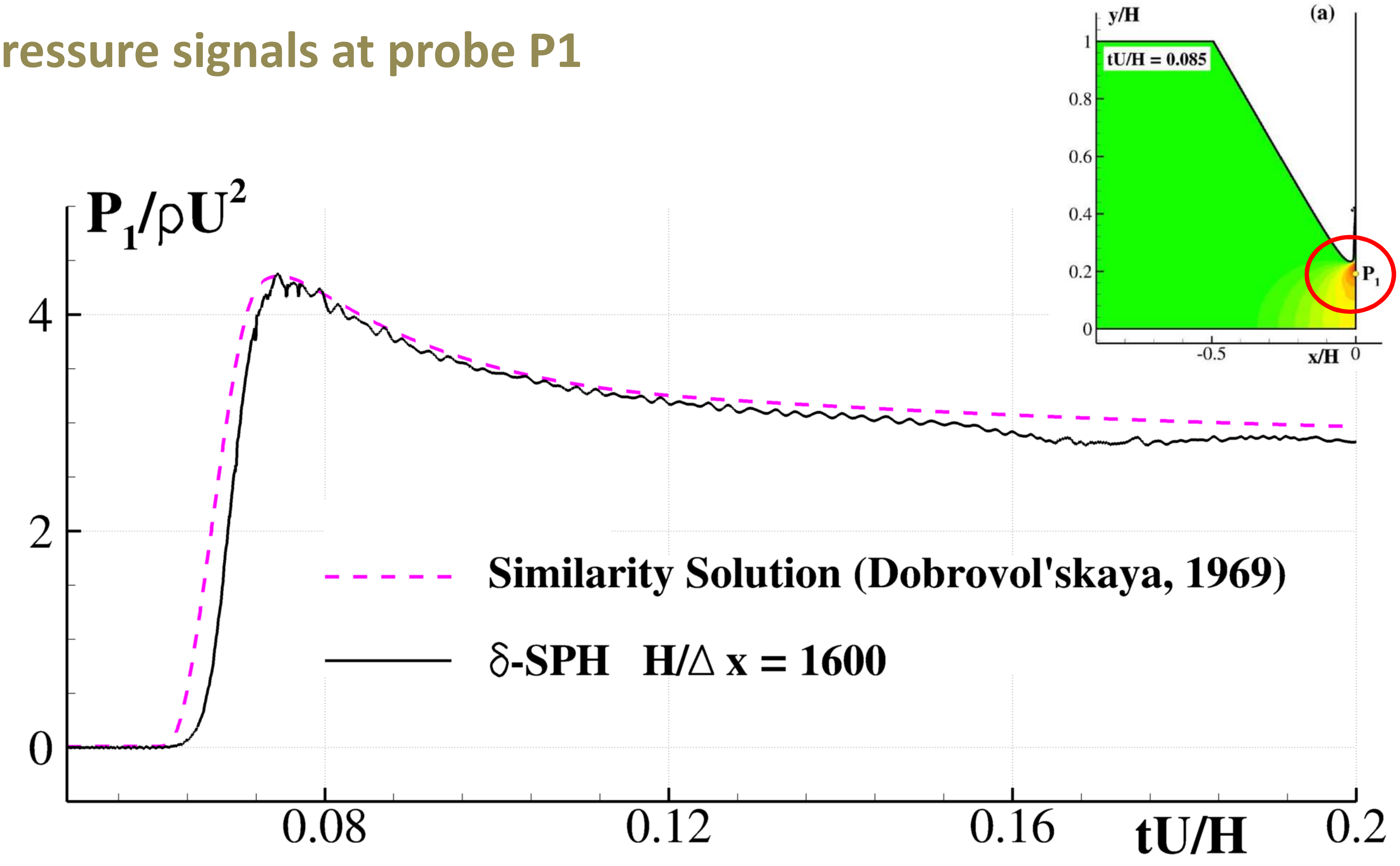
The δ-SPH scheme – convergence

Pressure signals at probe P1



The δ-SPH scheme – convergence

Pressure signals at probe P1



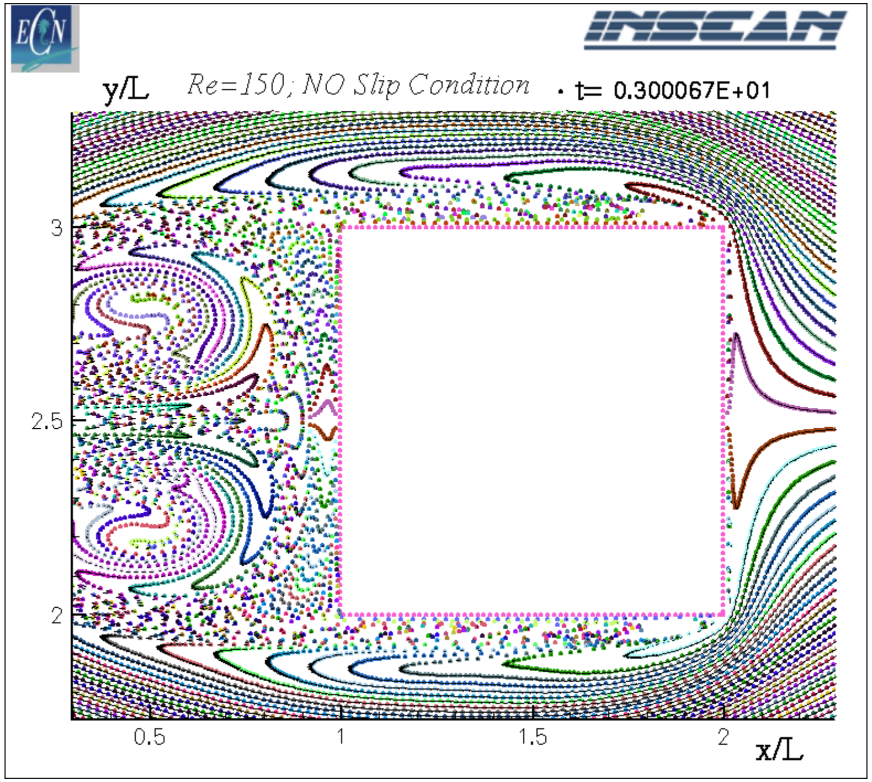
The δ-SPH scheme – recent and future developments

Being Lagrangian is a double-edged sword…

Particles distribution becomes non-uniform → **larger errors!**

This occurs when:

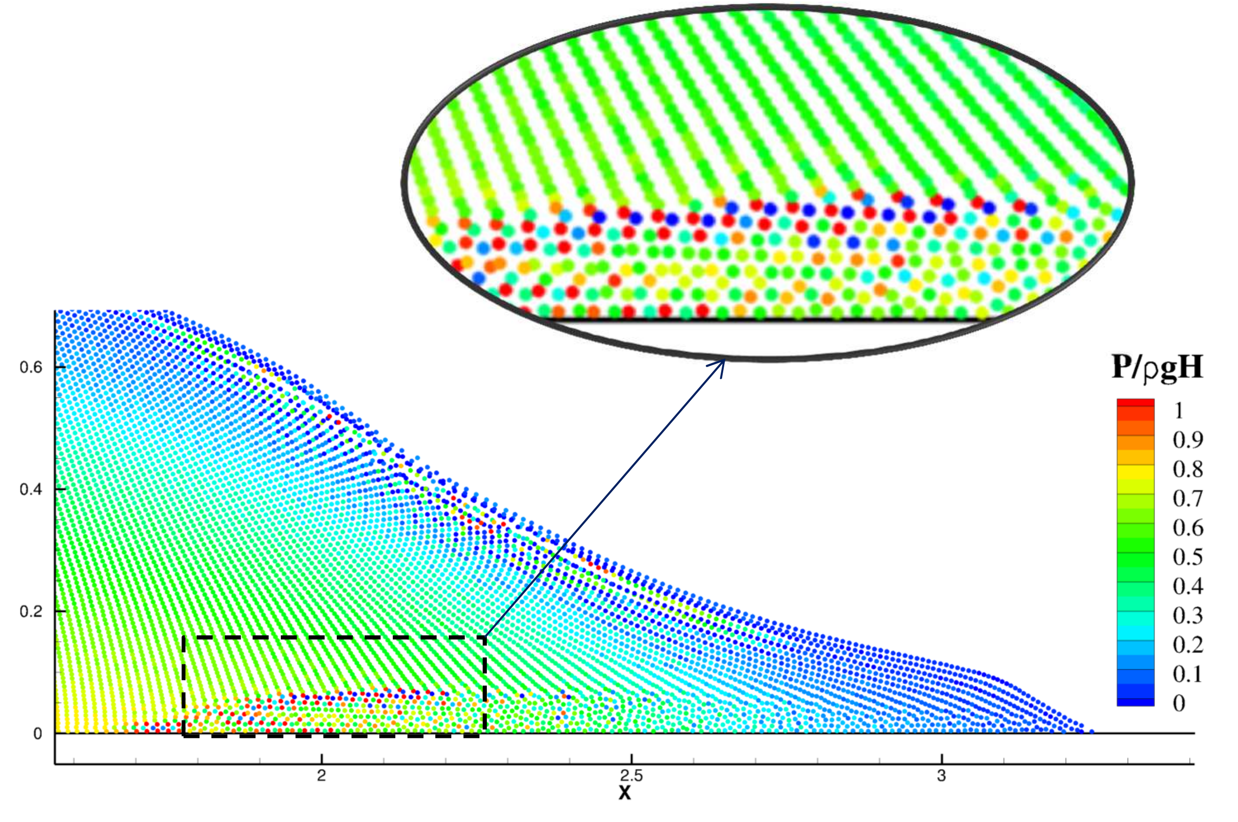
- increasing diffusion (Riemann)
- Increasing accuracy (e.g. interpolation order)
- simulating high shear regions



Eulerian solver with Lagrangian tracers

The δ-SPH scheme – recent and future developments

SPH has a self-rearrangement mechanism (<u>when *p* is positive</u>!)



but this induces however numerical noise and energy dissipation!!

The δ-SPH scheme – recent and future developments

further insight….

$$\langle \nabla p \rangle_i = \sum_j (p_j + p_i)\, \nabla_i W_{i,j}\, V_j = \sum_j (p_j - p_i)\, \nabla_i W_{i,j}\, V_j + 2\, p_i \nabla \Gamma_i$$

standard formula for the gradient (e.g. divergence of the velocity)

$$\nabla \Gamma_i = \sum_j \nabla_i W_{i,j}\, V_j$$

$\nabla \Gamma_i$ points towards the «voids» in the fluid domain

- if $p_i > 0$, the term $p_i \nabla \Gamma_i$ tends to reduce the disorder in the particle distribution

  → **«implicit particle packing»**

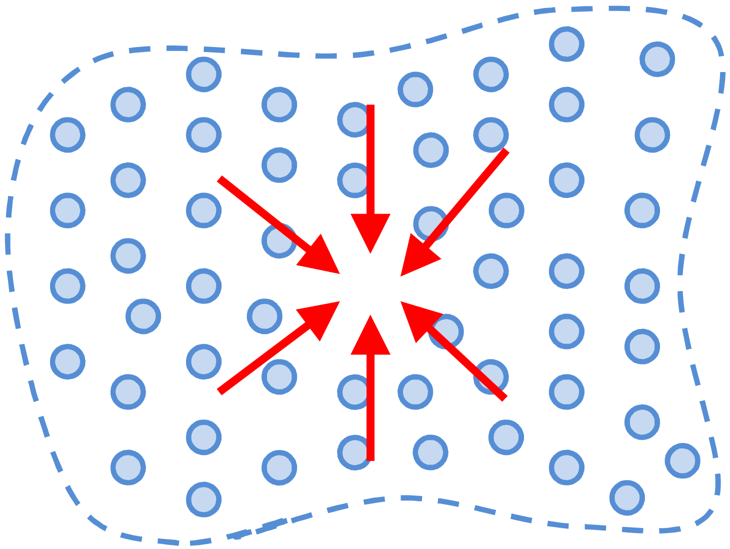
- if $p_i < 0$, the term $p_i \nabla \Gamma_i$ tends to increase the disorder in the particle distribution

  → **tensile instability**

The δ-SPH scheme – recent and future developments

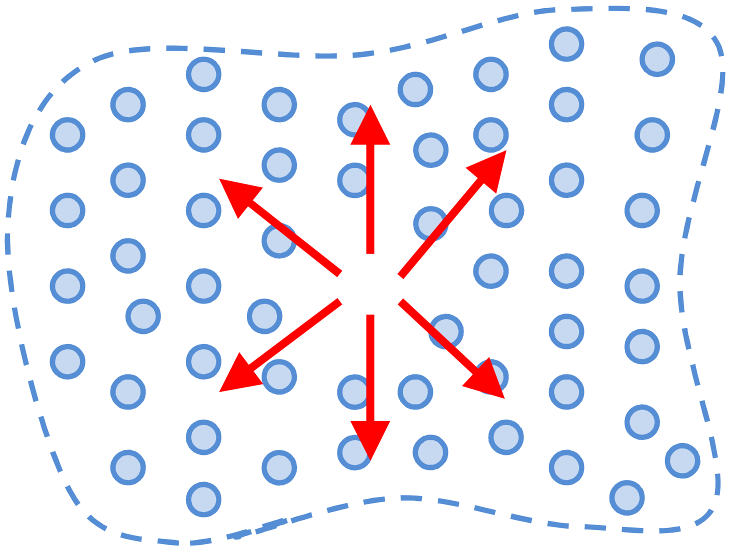
Inside the momentum equation, the contribution from this term is $-2\,p_i\,\nabla\Gamma_i$

$p_i > 0$



regularizing

$p_i < 0$



increasing disorder

The δ-SPH scheme – recent and future developments

Onset of tensile instability

Negative pressure regions

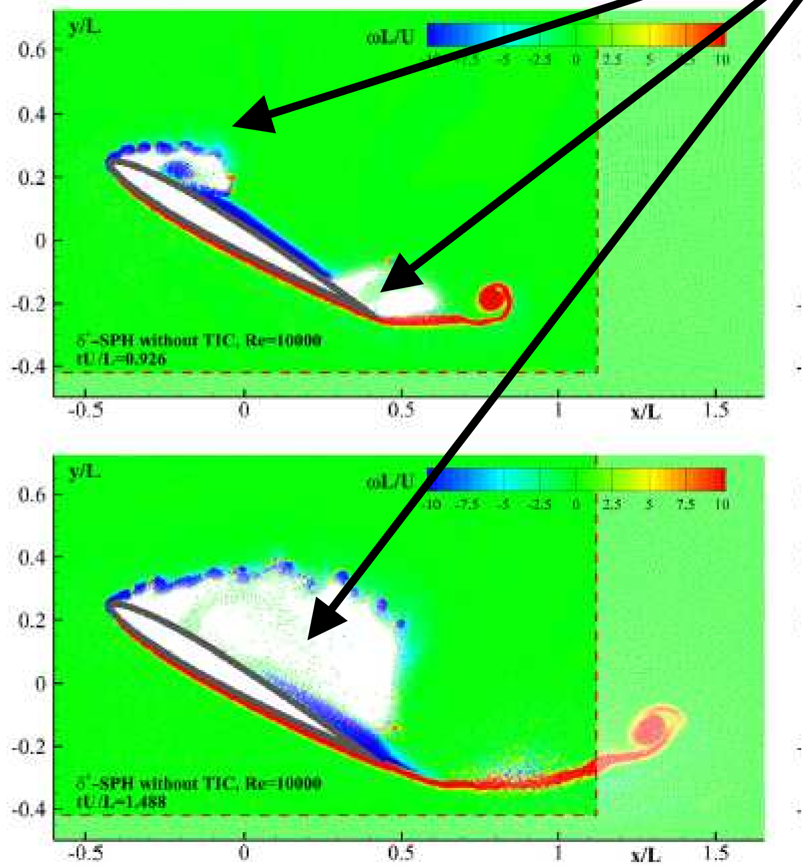


Fig. 1. Flow around a NACA0010 profile, $\alpha = 30°$, Re = 10,000. Snapshots of the δ^{+}-SPH solutions without (left) and with (right) Tensile Instability Control.

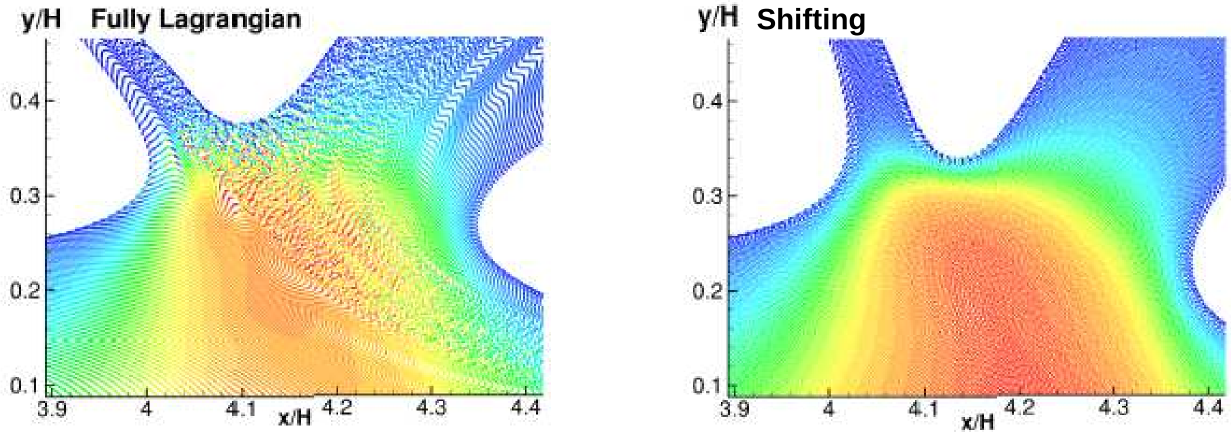
With tensile instability control

The δ-SPH scheme – recent and future developments

The idea is to put a term similar to $-2\,p_i\,\nabla\Gamma_i$ with $p_i > 0$ directly in the particle position update:
“particle shifting” (*Nestor et al. JCP 2009, Lind et al. JCP 2012*)

$$\begin{cases} \boldsymbol{r}_i^* = \boldsymbol{r}_i + \delta\boldsymbol{r}_i \\ \delta\boldsymbol{r}_i := -\mathrm{CFL}\cdot\mathrm{Ma}\cdot(2\,h_{ij})^2 \cdot \sum_j \nabla_i W_{ij}\, V_j \end{cases}$$

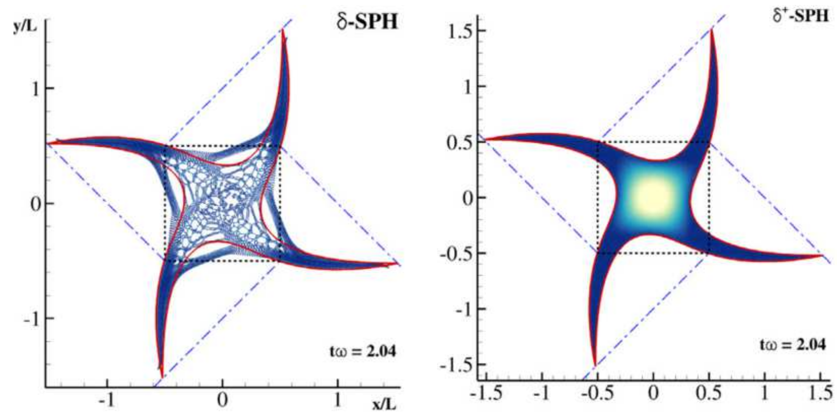
$$\nabla\Gamma_i = \sum_j \nabla_i W_{i,j}\, V_j$$



The δ-SPH scheme – recent and future developments

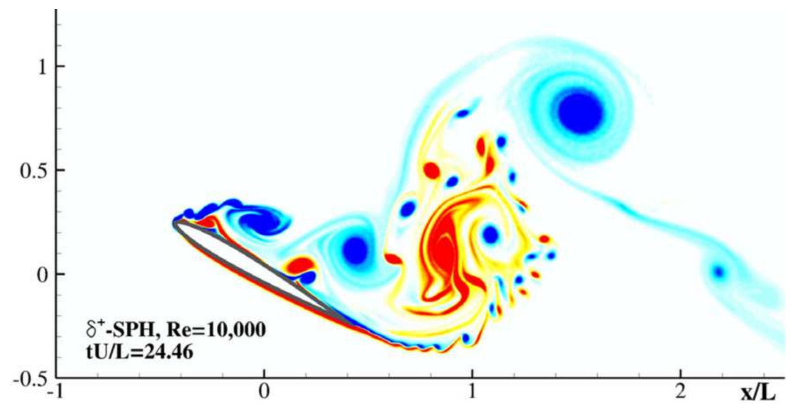
- Increasing accuracy through particle shifting technique: the δ^+-SPH

Rotating square patch
Sun et al. CMAME 2016



- Tensile instability control

Airfoil in stall configuration
at Re=10000
Sun et al. CPC 2018



The δ-SPH scheme – recent and future developments

- Arbitrary Lagrangian Eulerian framework for δ-SPH

- δ-SPH for multi-phase flows

- Large Eddy Simulation perspective for δ-SPH

Di Mascio et al. (2017)
Meringolo et al. (2018)

The δ-SPH scheme – recent and future developments

The viscous term in the momentum equation and the diffusive term in the continuity equation are interpreted as closures in the **LES framework**

=> *dynamic choice of coefficients using the velocity deformation tensor*

$$\begin{cases} \dfrac{D\rho_i}{Dt} = -\rho_i \sum_j (\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot \nabla_i W_{ij} V_j + h c_0 \sum_j \delta_{ij} \mathcal{D}_{ij} \cdot \nabla_i W_{ij} V_j, \\ \dfrac{D\boldsymbol{u}_i}{Dt} = \boldsymbol{g}_i - \dfrac{1}{\rho_i} \sum_j \big(p_i + p_j\big) \nabla_i W_{ij} V_j + h c_0 \dfrac{\rho_0}{\rho_i} \sum_j \alpha_{ij} \pi_{ij} \nabla_i W_{ij} V_j, \\ \dfrac{D\boldsymbol{r}_i}{Dt} = \boldsymbol{u}_i, \qquad p_i = c_0^2 (\rho_i - \rho_0). \end{cases}$$

$$\delta_{ij} = 2\,\frac{\delta_i\,\delta_j}{\delta_i + \delta_j}, \qquad \delta_i = \frac{\nu_i^\delta}{c_0\,h}, \qquad \nu_i^\delta = (C_\delta\, l_{LES})^2\, \|\mathbb{D}\|_i\,,$$

The δ-SPH scheme – recent and future developments

The viscous term in the momentum equation and the diffusive term
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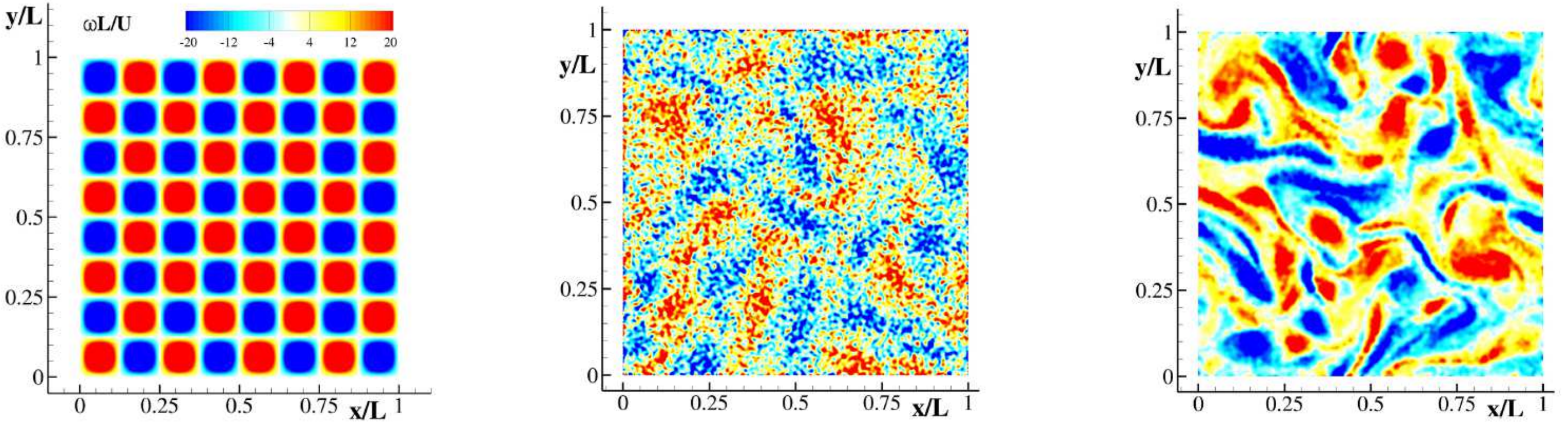
$$\begin{cases} \dfrac{D\rho_i}{Dt} = -\rho_i \sum_j (\boldsymbol{u}_j - \boldsymbol{u}_i) \cdot \nabla_i W_{ij} V_j + h c_0 \sum_j \delta_{ij} \mathcal{D}_{ij} \cdot \nabla_i W_{ij} V_j, \\ \dfrac{D\boldsymbol{u}_i}{Dt} = \boldsymbol{g}_i - \dfrac{1}{\rho_i} \sum_j \big(p_i + p_j\big) \nabla_i W_{ij} V_j + h c_0 \dfrac{\rho_0}{\rho_i} \sum_j \alpha_{ij} \pi_{ij} \nabla_i W_{ij} V_j, \\ \dfrac{D\boldsymbol{r}_i}{Dt} = \boldsymbol{u}_i, \qquad\qquad p_i = c_0^2 (\rho_i - \rho_0). \end{cases}$$

$$\alpha_{ij} = \alpha + 2 \frac{\alpha_i \alpha_j}{\alpha_i + \alpha_j}, \quad \alpha = \frac{K \mu}{c_0 h \rho_0}, \qquad \alpha_i = \frac{K \nu_i^T}{c_0 h}. \qquad \nu_i^T = (C_s l_{LES})^2 \|\mathbb{D}\|_i ,$$

The δ-SPH scheme – recent and future developments

Two-dimensional freely-decaying turbulence: $Re_l = 125{,}000$



Initial vorticity field
(2D vortex pattern)

DNS by using SPH
(insufficient resolution)

LES-SPH
(same resolution,
correct modelling of
large vortex structures)

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Thank you
for
your attention!