



Mesh-free Lagrangian modelling of fluid dynamics

David LE TOUZÉ, Ecole Centrale Nantes



CFD 2011, keynote lecture

Mesh-free Lagrangian methods in CFD

Smoothed-Particle Hydrodynamics (SPH)

Fast-dynamics free-surface flows

Multi-fluid flows

Fluid-Structure Interactions

HPC: massive interactive simulations

Mesh-free Lagrangian methods



Methods for discrete media

A « particle » is an atom, a molecule, a grain, etc.

Methods directly model laws of interaction between two elements

MD, DEM, DSMC...

Methods for continuous media

A « particle » is an elementary mass of considered continuous medium

Methods model local PDEs describing the medium mechanics/physics

SPH, MPS, FPM, RKPM...

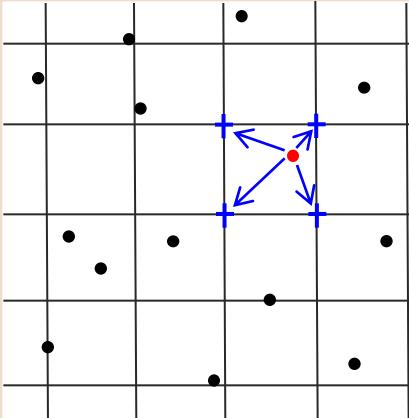
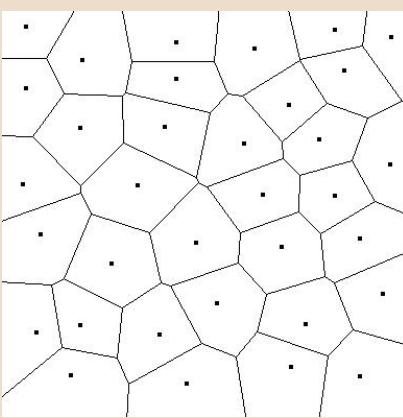
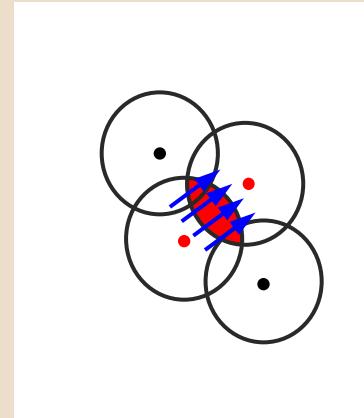
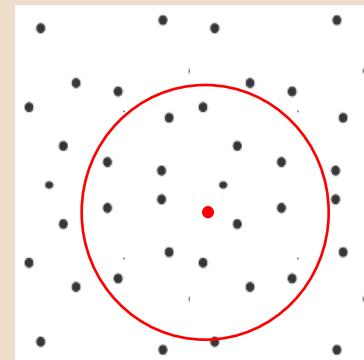
Numerically the discretized local equations can take the form of a Lagrangian set of material points (« particles »), implying intrinsic properties: conservation of linear and angular momenta, etc.

=> 2 complementary *numerical* visions:
standard discretized PDEs / particle system

Mesh-free Lagrangian methods for fluid dynamics



Mesh-free?

Projection	Tesselation	Face reconstruction	True mesh-free
			
PM...	PFEM	FVPM	SPH, MPS...

Mesh-free Lagrangian methods for fluid dynamics

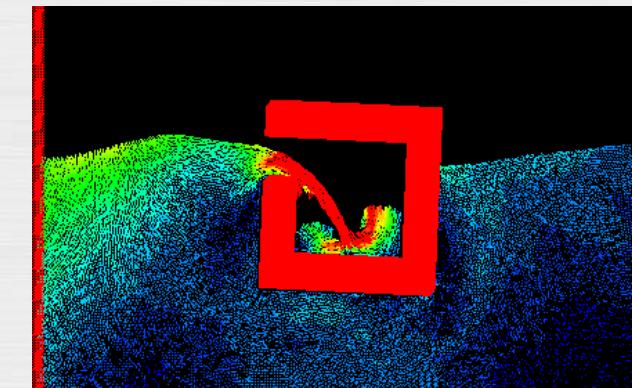


Mesh-free methods, for what purpose?

- to solve situations where meshes have difficulties:
very **large deformations** of the fluid domain / **large motions** of multi-bodies
(especially contact between 2 bodies in the flow)
- to avoid costly mesh generating/handling (human cost especially)

Lagrangian methods in fluid, for what purpose?

- to naturally and accurately follow **interfaces** deformations:
 - Complex free surfaces
 - Multi-fluid/-phase interfaces
 - Fluid-structure interfaces
- to solve **fast dynamics** flows: no convection term



Lagrangian meshless methods, NOT for what?

- for all problems where mesh-based methods are already reliable (e.g. high-Re turbulent flows, steady flow, etc.)



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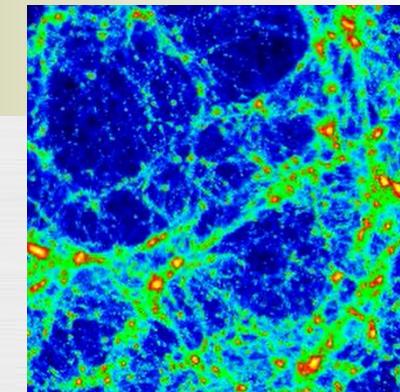
Fluid-Structure Interactions

HPC: massive interactive simulations

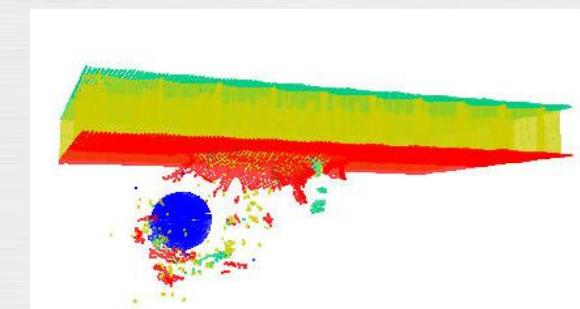
SPH method: origin



1977 : Gingold & Monaghan / Lucy: SPH
 application field: **astrophysics**
 methodological background: statistics



80's : mainly applied in **astrophysics**
 star formation, self-gravitating clouds, galactic shocks...
 then for modeling **structures**

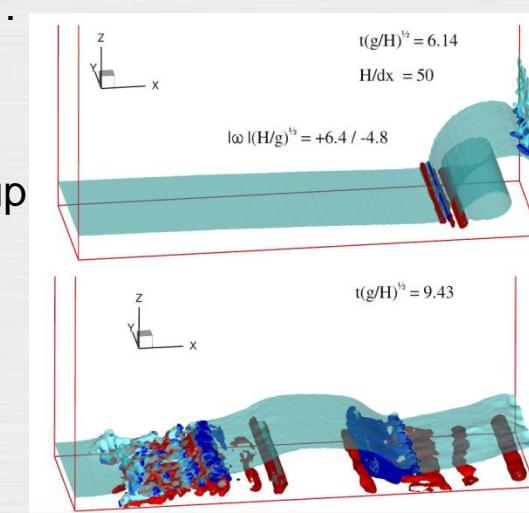


90's : astrophysics, structure;
 1994: **free-surface** SPH (Monaghan)

2000's : astrophysics, structure, **fluid dynamics**, polymers, surfactants, explosions, lava, porous media, geotechnical problems, biomechanics, metallurgy...

SPH in fluid dynamics

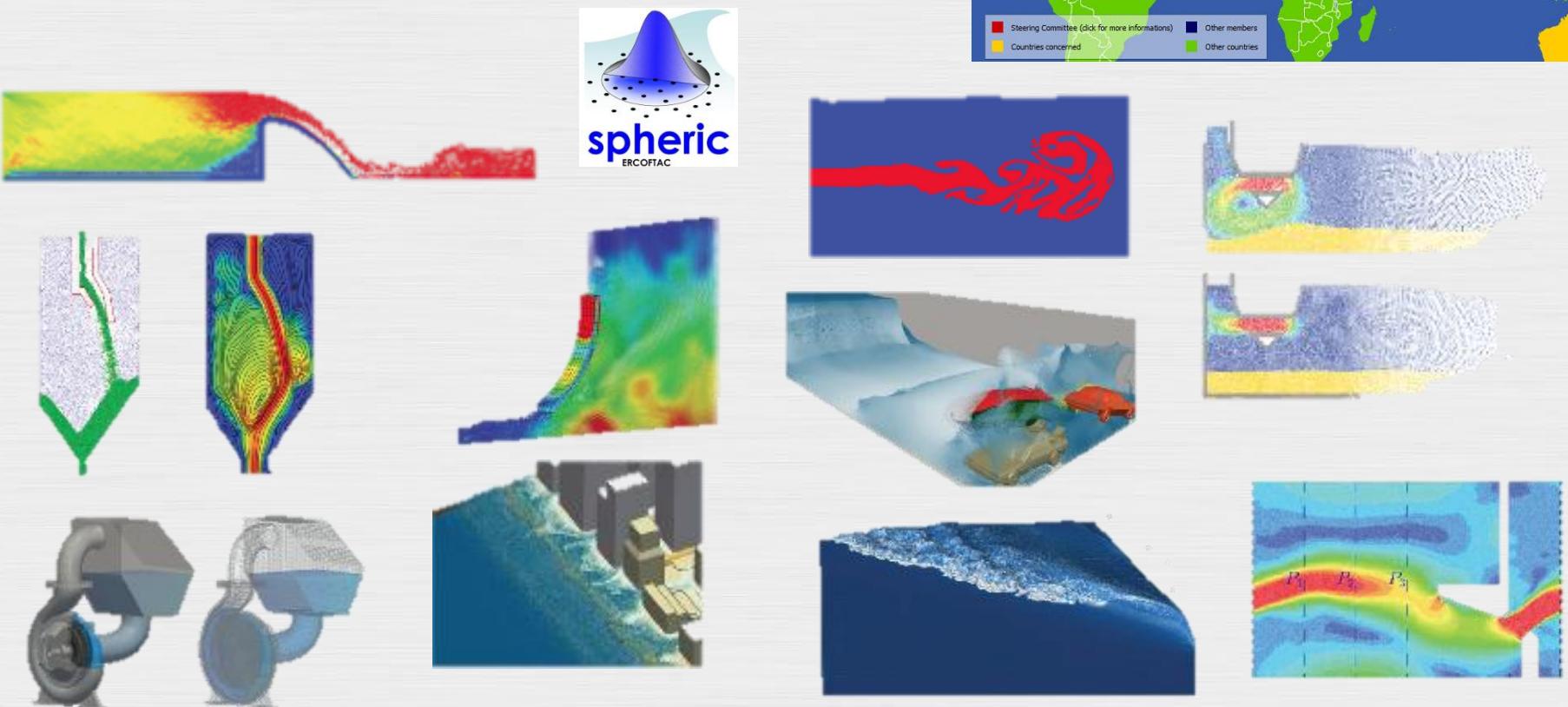
- **fast development:** **SPHERIC** ERCOFTAC Special Interest Group created in 2005, today: 91 international member entities
- a similar method (MPS) is also in fast development in Japan



SPH in the world



- **SPHERIC group** : 95 entities of 29 countries worldwide
Annual workshop, benchmarks, bibliography and job databases, codes...



SPH method: origin



Smoothed Particle Hydrodynamics

Regularizing
function

Mesh-free Lagrangian
method

Liquids in motion

A fluid dynamics problem numerically seen as a system of masses
(particles) using a regularizing function.

SPH method: characteristics

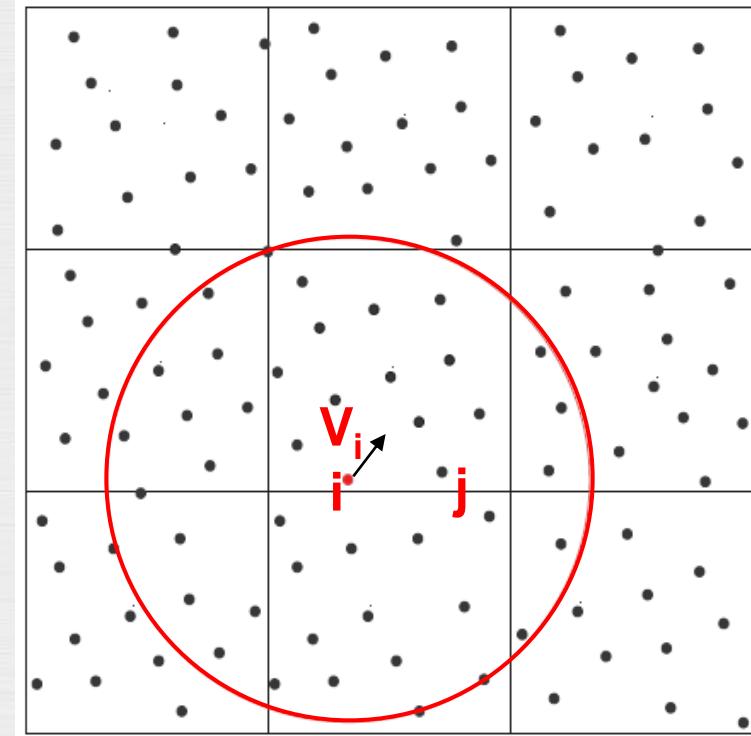
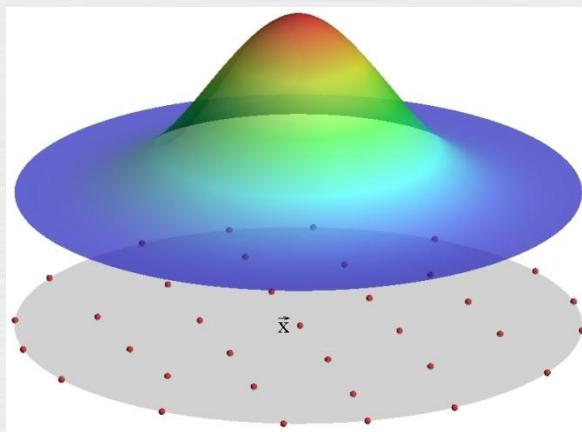


- **meshless**: no need for handling a mesh
- **explicit**: « easy » and efficient parallelization
- **Lagrangian**: no convective term modeling:
=> accurate for **fast dynamics** flows (violent impacts, shocks, explosions...)
- naturally handles large deformations of the domain:
 - large motion of (multi-)bodies
 - arbitrary complex free surface
- perfectly **non-diffusive interface**
- permits to include **different species** (materials, phases...) in a **monolithic way**

BUT

- enhanced versions are needed to get **accurate pressure fields**
- implementation of **boundary conditions** must be considered with great care
- convergence of SPH as usually used is not theoretically proved, heuristically: order 1

SPH method: principle



- Lagrangian formalism
- equations discretized within a compact zone of influence
- differential operators obtained from quantity values at the points included in this zone of influence

SPH method: discretization

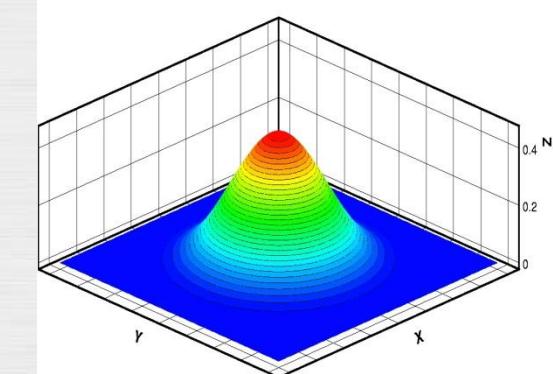


interpolation

convolution using a kernel W (~test fonction)

$$f(\vec{r}) \approx \int_D f(\vec{x})W(\vec{r} - \vec{x})d\vec{x}$$

$$W(q = \frac{|\vec{r}|}{h}) = C \begin{cases} \frac{2}{3} - q^2 + \frac{1}{2}q^3 & \text{if } 0 \leq q < 1 \\ \frac{1}{6}(2 - q)^3 & \text{if } 1 \leq q < 2 \\ 0 & \text{else} \end{cases}$$



interest

estimation of the gradient from the values of the considered quantity

$$\nabla f(\vec{r}) \approx \int_D \nabla f(\vec{x})W(\vec{r} - \vec{x})d\vec{x} = \int_D f(\vec{x}) \nabla W(\vec{r} - \vec{x})d\vec{x}$$

analytical

SPH discretization: weakly-compressible variant



Numerical scheme - inviscid here

fully explicit

- Euler equation
- Free-surface condition
- Initial conditions
- Compressible fluid

$$\frac{D\vec{v}}{Dt} = \vec{g} - \frac{\nabla p}{\rho}$$

$$p(\vec{x}, t) = 0 \text{ et } \frac{D\vec{x}}{Dt} = \vec{v}_{\partial\Omega} \quad \forall \vec{x} \in \partial\Omega$$

$$\vec{v}(\vec{x}, t_0) = \vec{v}_0 \text{ et } p(\vec{x}, t_0) = p_0$$

=> intrinsic
Colagrossi, Antuono,
Le Touzé,
Phys. Rev. E, 2009

$$\frac{D\rho}{Dt} = -\rho \operatorname{div}(\vec{v})$$

$$P - P_0 = \frac{\rho_0 c_0^2}{7} \left[\left(\frac{\rho}{\rho_0} \right)^7 - 1 \right]$$

$$\langle \nabla p_i \rangle = \sum_j (p + p_j) \omega_j \nabla W(\vec{x}_i - \vec{x}_j)$$

$$\langle \operatorname{div}(\vec{v}_i) \rangle = \sum_j (\vec{v}_j - \vec{v}_i) \omega_j \nabla W(\vec{x}_i - \vec{x}_j)$$

for compatibility (energy conservation)

chosen at the weak-cpr.
limit ($\text{Ma}=0.1$) when
simulating
incompressible flows
= pseudo-compressibility

SPH discretization: weakly-compressible variant



Stabilization

Method 1

last equations + artificial viscosity added to the pressure term

Method 2

use of a density diffusive term (proportional to a Rusanov flux) in the continuity equation

$$\frac{D\rho_i}{Dt} = -\rho_i \sum_j (\mathbf{u}_j - \mathbf{u}_i) \cdot \nabla_i W(\mathbf{r}_j) V_j + \delta h c_0 \sum_j \boldsymbol{\psi}_{ij} \cdot \nabla_i W(\mathbf{r}_j) V_j$$

Method 3

use of an ALE form (Vila, 1999) and of Riemann solvers between each pair of particles
(standard in FVM for compressible flows)

$$\begin{cases} \left. \frac{d\bar{x}_i}{dt} \right|_{v_0} = \bar{v}_{0i} \\ \left. \frac{d\omega_i}{dt} \right|_{v^0} = \sum_{j \in P(\Omega)} \omega_i \omega_j (\bar{v}_{0j} - \bar{v}_{0i}) \cdot \nabla_i W_{ij} \\ \left. \frac{d\omega_i \bar{\phi}_i}{dt} \right|_{v^0} + \sum_{j \in P(\Omega)} \omega_i \omega_j \underbrace{(\bar{F}_i - \bar{\phi}_i \otimes \bar{v}_{0i} + \bar{F}_j - \bar{\phi}_j \otimes \bar{v}_{0j})}_{\text{given by the Riemann problem solution}} \cdot \nabla_i W_{ij} = \omega_i \bar{S}_i \end{cases}$$

SPH discretization: incompressible variant



Numerical scheme - viscous here

semi-implicit

$$\frac{Du}{Dt} = -\frac{1}{\rho} \nabla p + v \nabla^2 u + F$$

$$\nabla \cdot u = 0$$

$$u_i^* = u_i^n + v \nabla^2 u_i^n + F_i^n \Delta t$$

$$r_i^* = r_i^n + \Delta t u_i^*$$

$$\rho_i^* = \sum_j m_j \omega_{ij}$$

Pressure Poisson Equation

$$\nabla \cdot \left(\frac{1}{\rho} \nabla p^{n+1} \right)_i = \frac{1}{\Delta t} \nabla \cdot u_i^* \quad \text{or} \quad \nabla \cdot \left(\frac{1}{\rho} \nabla p^{n+1} \right)_i = \frac{\rho_0 - \rho_i^*}{\rho_0 \Delta t^2}$$

ISPH_DF

ISPH_DI

$$u_i^{n+1} = u_i^* - \frac{\Delta t}{\rho} \nabla p_i^{n+1}$$

$$r_i^{n+1} = r_i^n + \Delta t \left(\frac{u_i^{n+1} + u_i^n}{2} \right)$$

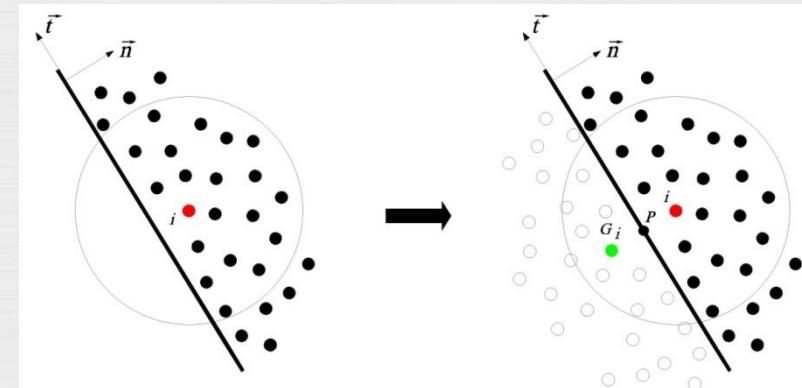
- Solved by standard incompressible solvers (pre-conditioned Bi-CGStab...)
- Need for correctly imposing free-surface conditions

Solid boundaries handling: **ghost particles**

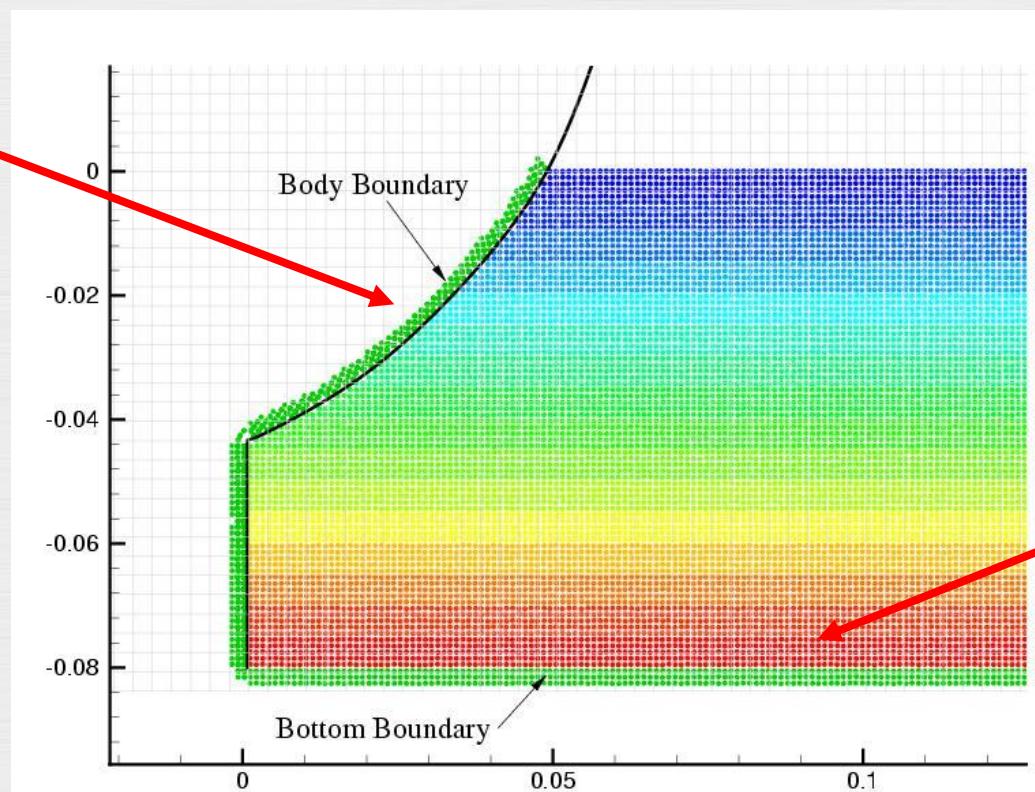


principle

solid BCs are imposed thanks to mirrored particles



'ghost'
particles



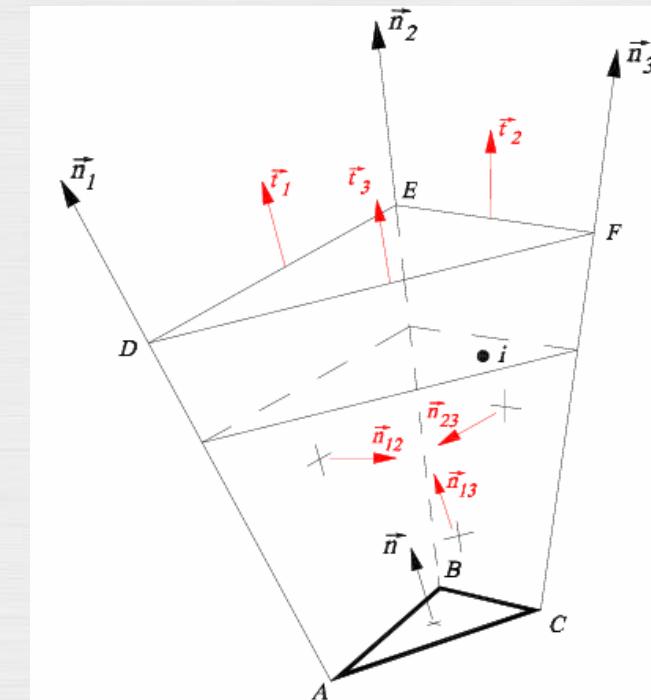
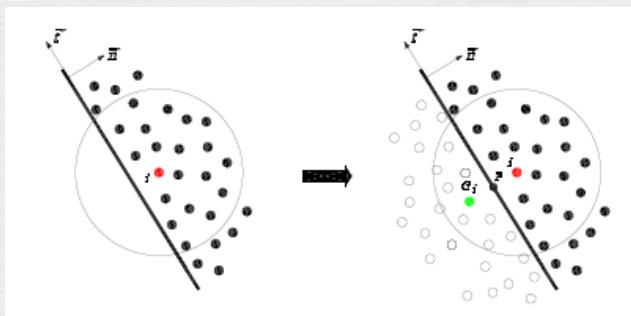
$$\begin{aligned} V_{G_{in}} &= 2V_{pn} - V_{in} \\ V_{G_{it}} &= V_{pt} \end{aligned}$$

fluid
particles

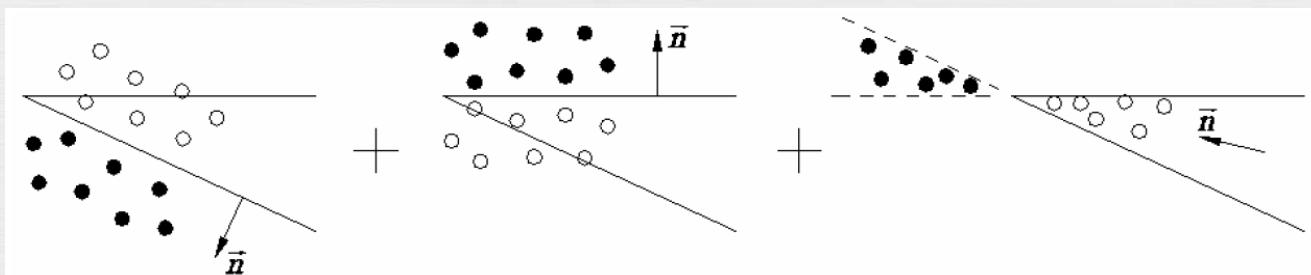
Solid boundaries handling: ghost particles



- 3D generic technique
 - from any surface (e.g. IGES format)



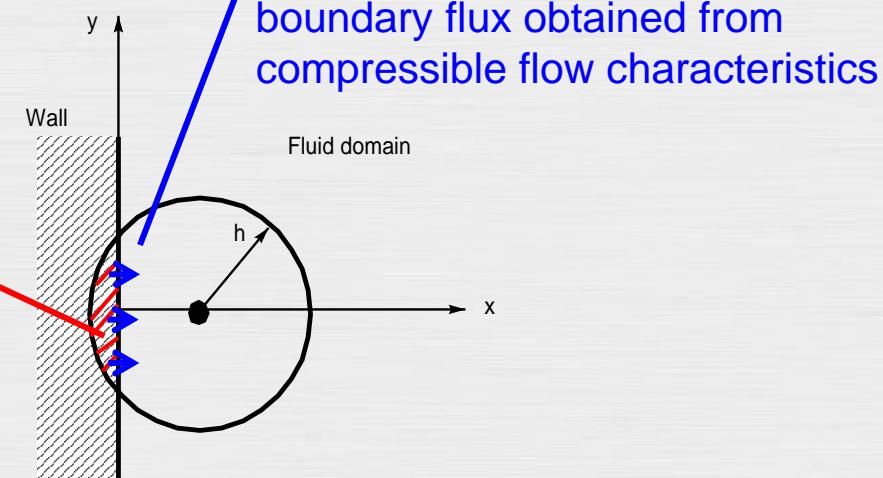
- Exact only for a flat panel, **difficulties with geometrical singularities**, especially sharp edges



Solid boundaries handling: normal flux method

$$\begin{cases} \left. \frac{d\bar{x}_i}{dt} \right|_{v_0} = \bar{v}_{0i} \\ \left. \frac{d\omega_i}{dt} \right|_{v^0} = \frac{1}{\gamma_i} \sum_{j \in P(\Omega)} \omega_i \omega_j (\bar{v}_{0j} - \bar{v}_{0i}) \cdot \nabla_i W_{ij} + \frac{1}{\gamma_i} \sum_{j \in P(\partial\Omega)} \omega_i s_j (\bar{v}_{0j} - \bar{v}_{0i}) \cdot \bar{n}_j W_{ij} \\ \left. \frac{d\omega_i \bar{\phi}_i}{dt} \right|_{v^0} + \frac{1}{\gamma_i} \sum_{j \in P(\Omega)} \omega_i \omega_j (\bar{F}_i + \bar{F}_j) \cdot \nabla_i W_{ij} + \frac{1}{\gamma_i} \sum_{j \in P(\partial\Omega)} \omega_i s_j (\bar{F}_i + \bar{F}_j) \cdot \bar{n}_j W_{ij} = \omega_i \bar{S}_i \end{cases}$$

compensates
missing part of the
kernel support

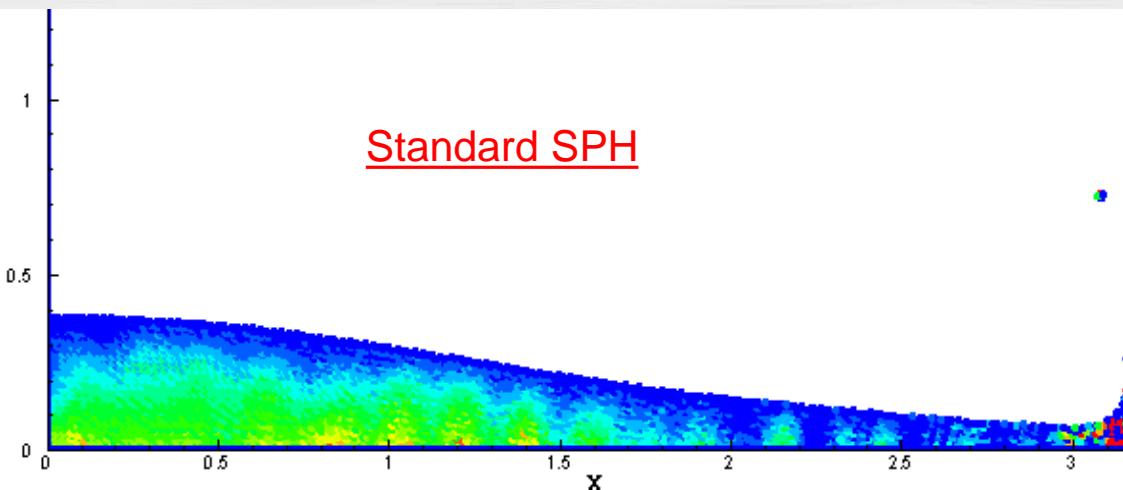


- Fully general technique

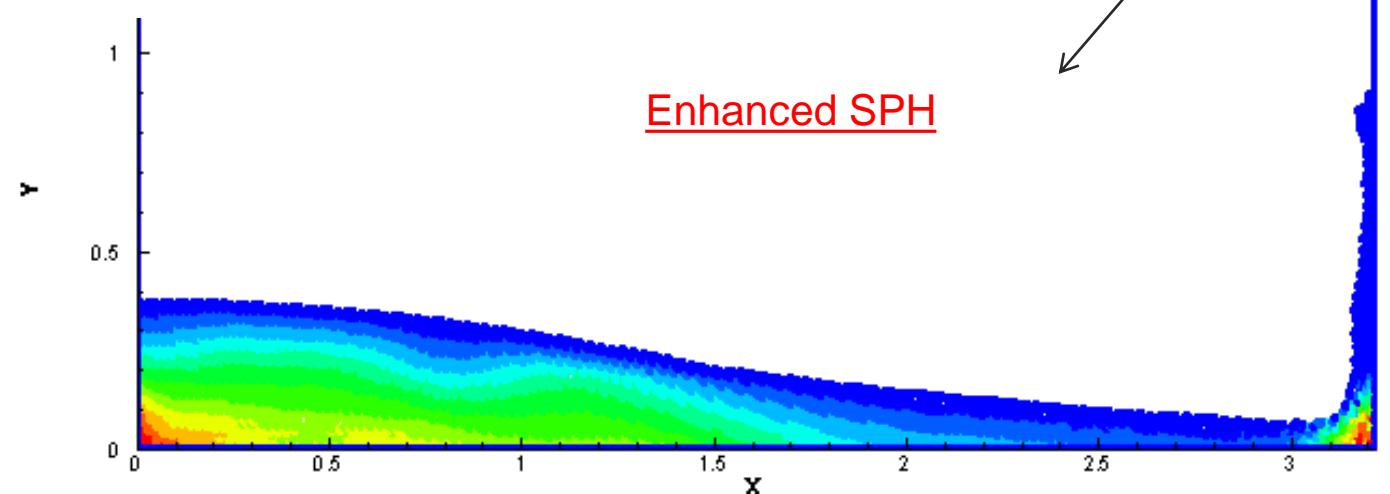
SPH solver: accuracy



Pressure field quality



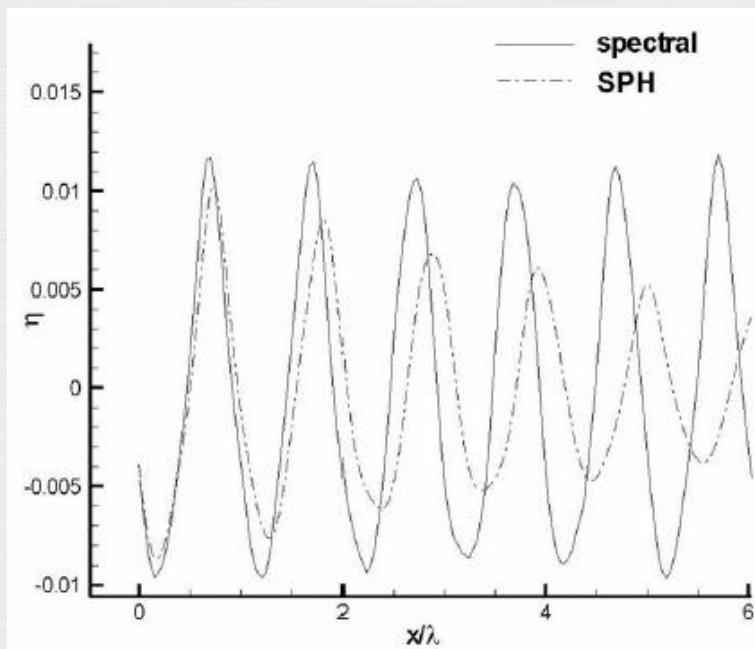
Use of density
diffusive term, or
Riemann solver ,or
incompressible
variant...



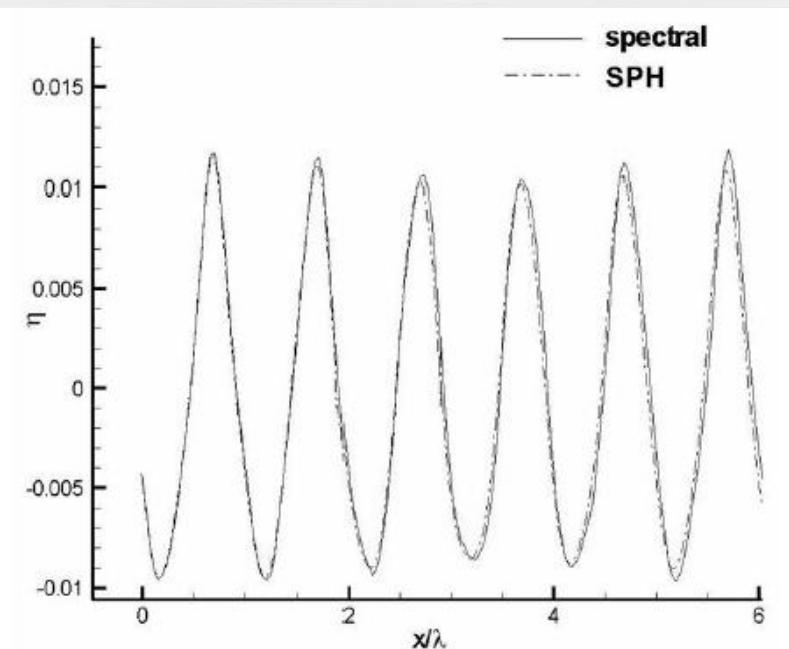
SPH solver: accuracy



Accuracy test: gravity wave propagation



Standard SPH



Enhanced SPH

Additional use of kernel renormalization to get order-1 completeness

The solver SPH-flow



SPH-flow

SPH-flow solver

Model core

- 3D
- specific tools to **enhance model accuracy** (Riemann solver, kernel renormalisation...)
- **variable-size particle** algorithm (equivalent to mesh refinement)
- generalized ghost technique for modeling **any 3D solid boundary**
- 6-dof bodies
- efficient **parallel** model
- **inflow/outflow** conditions implemented

Extensions of the model

- **fluid-structure** coupling
- **multifluid** flows
- **Navier-Stokes**: viscous flow + turbulence modeling
- **wave-structure** interaction ; shallow-water SPH model ; ...

Three key points

- accuracy
- HPC
- validation



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Fast-dynamics free-surface flows

Multi-fluid flows

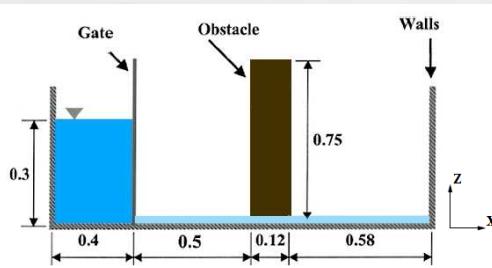
Fluid-Structure Interactions

HPC: massive interactive simulations

Fast dynamics free surface flows: validation

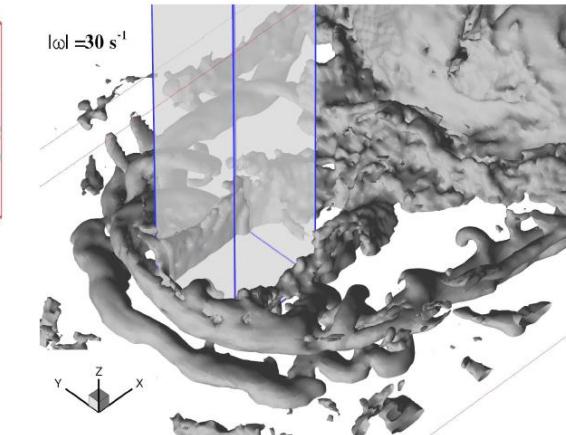
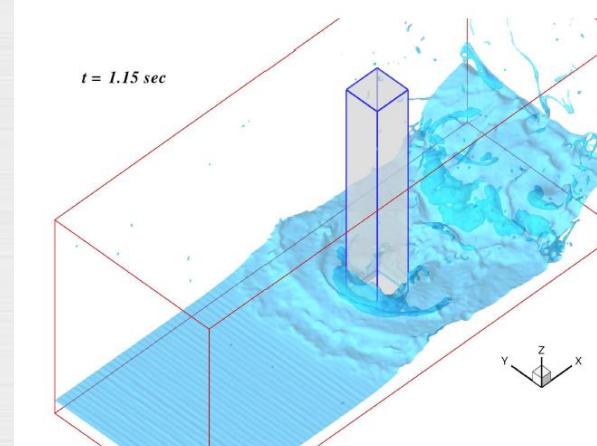


Validation on dam breaking test cases

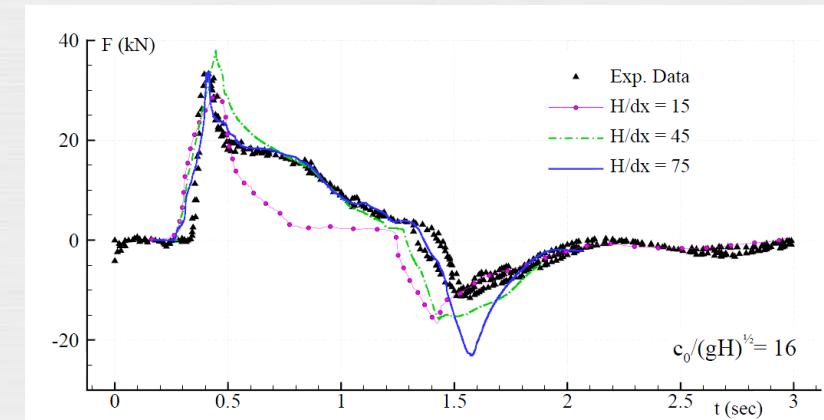
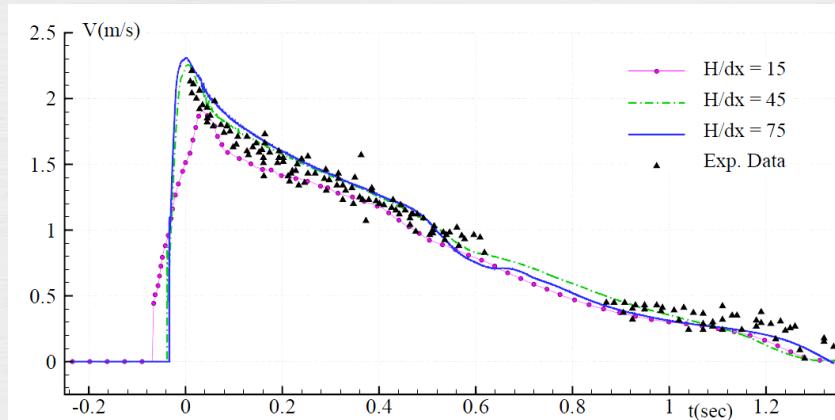


with 80,000 particles only =>

with 1 million particles =>



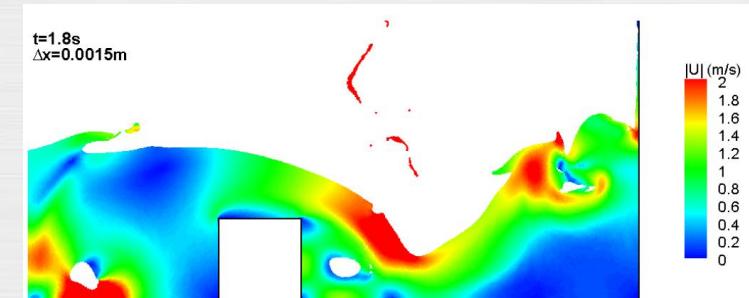
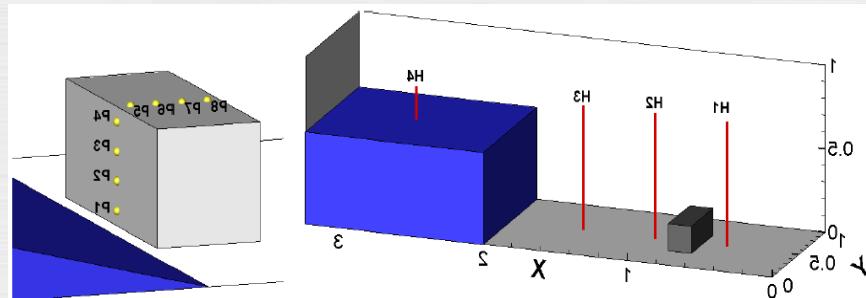
Good prediction of velocity and forces :



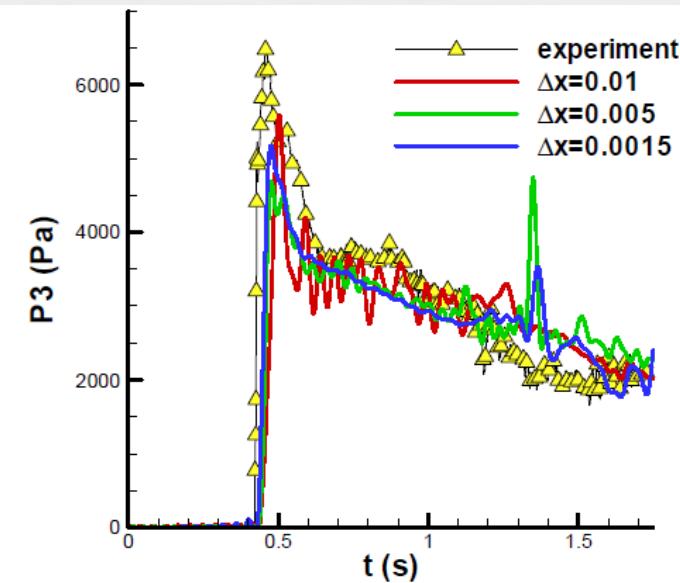
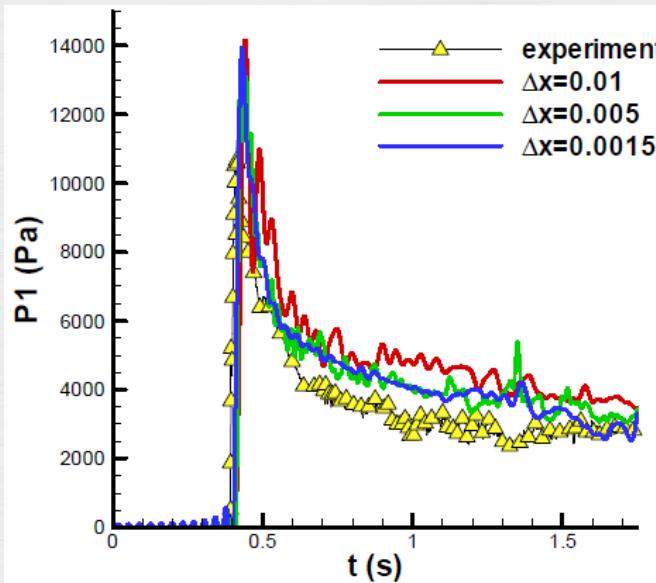
Fast dynamics free surface flows: validation



Validation on dam breaking test cases



- Good prediction of local loads:



Fast dynamics free surface flows: naval applications



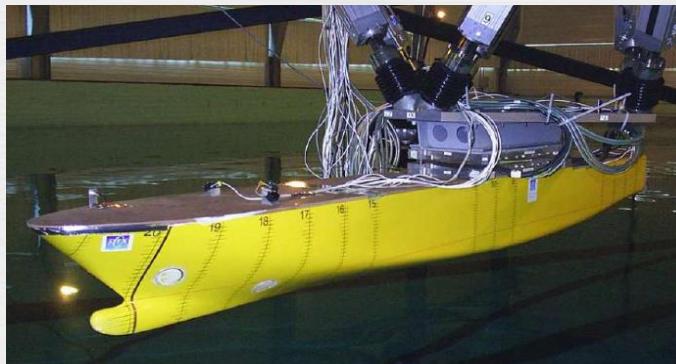
SPH-flow



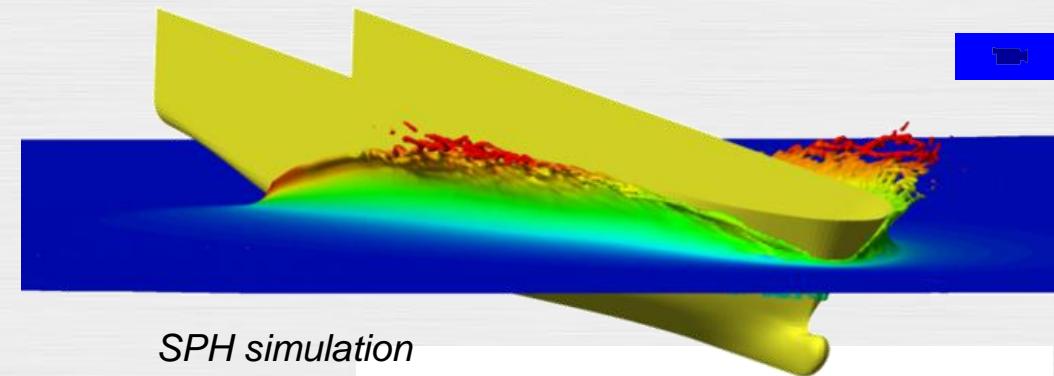
HydrOcean

Slamming impact

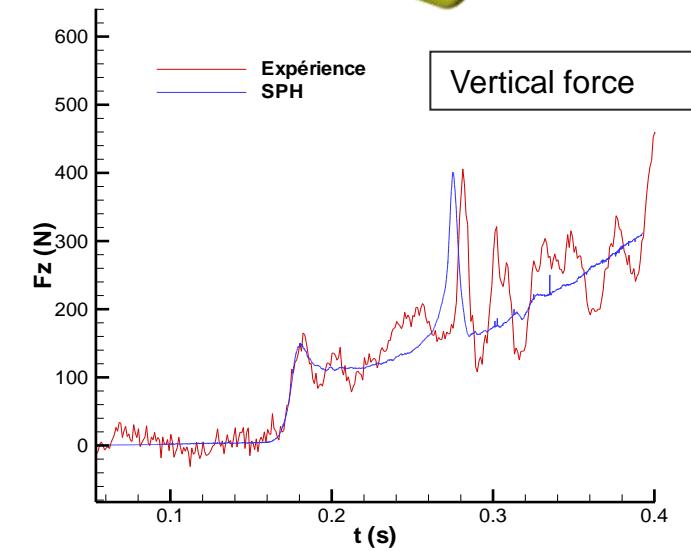
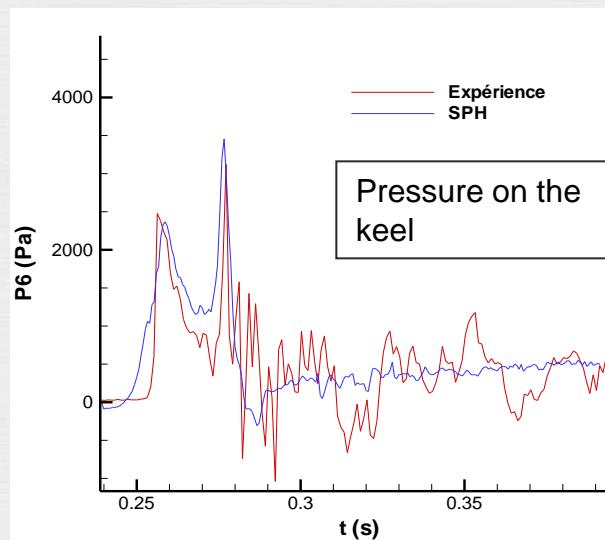
Maruzewski et al., J. Hydraul. Res. 48, 2010



Experiment (ECN wave tank)



SPH simulation



Vertical force

- 3 million particles
- 6m/s impact
- 250m long ship at real scale

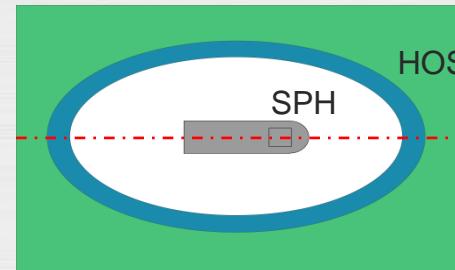
Fast dynamics free surface flows: naval applications

SPH-flow

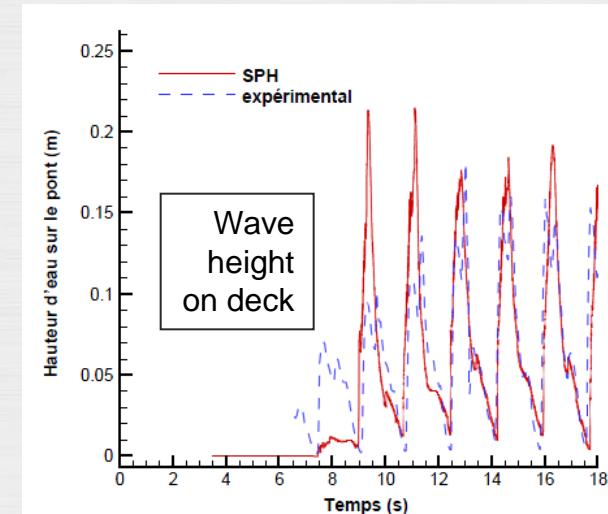
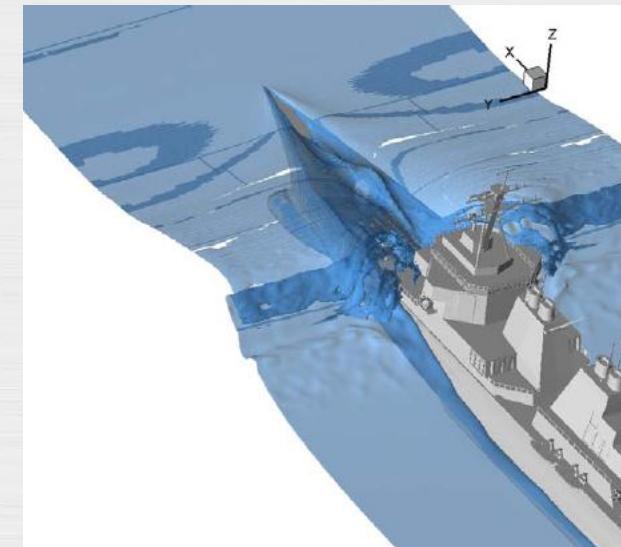
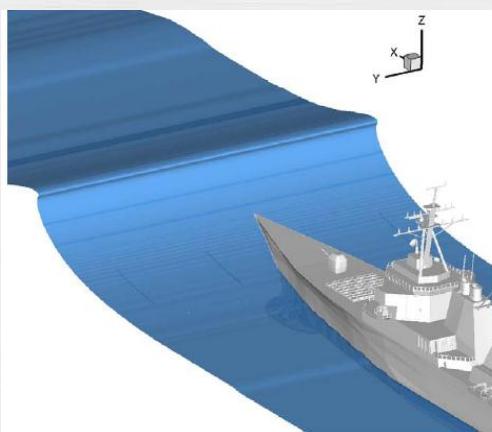
- FPSO in severe sea state
coupling strategy:



Violent wave-structure interactions



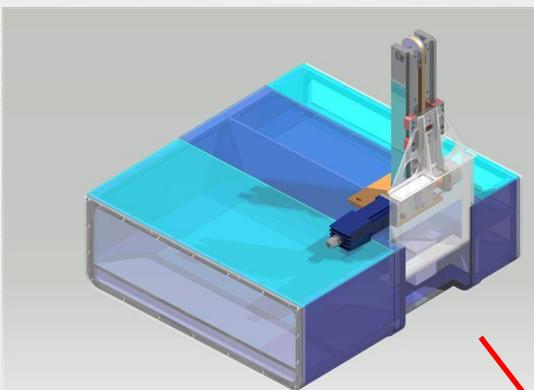
- Fregate facing a dimensioning wave



Fast dynamics free surface flows: naval applications

SPH-flow

- Flooding

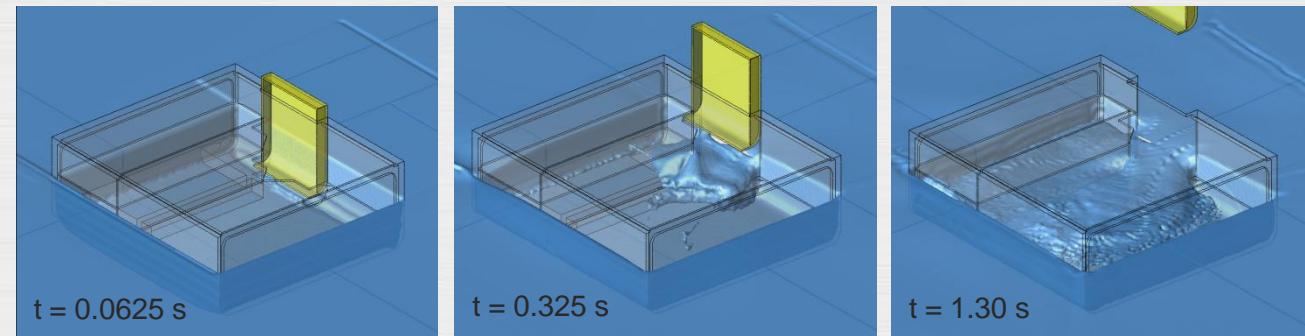


Experiment in the ECN tank

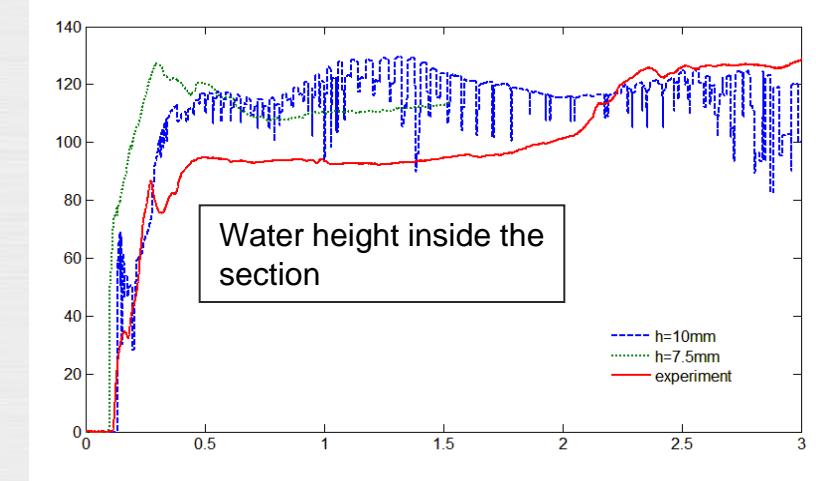


Other naval applications

SPH calculation



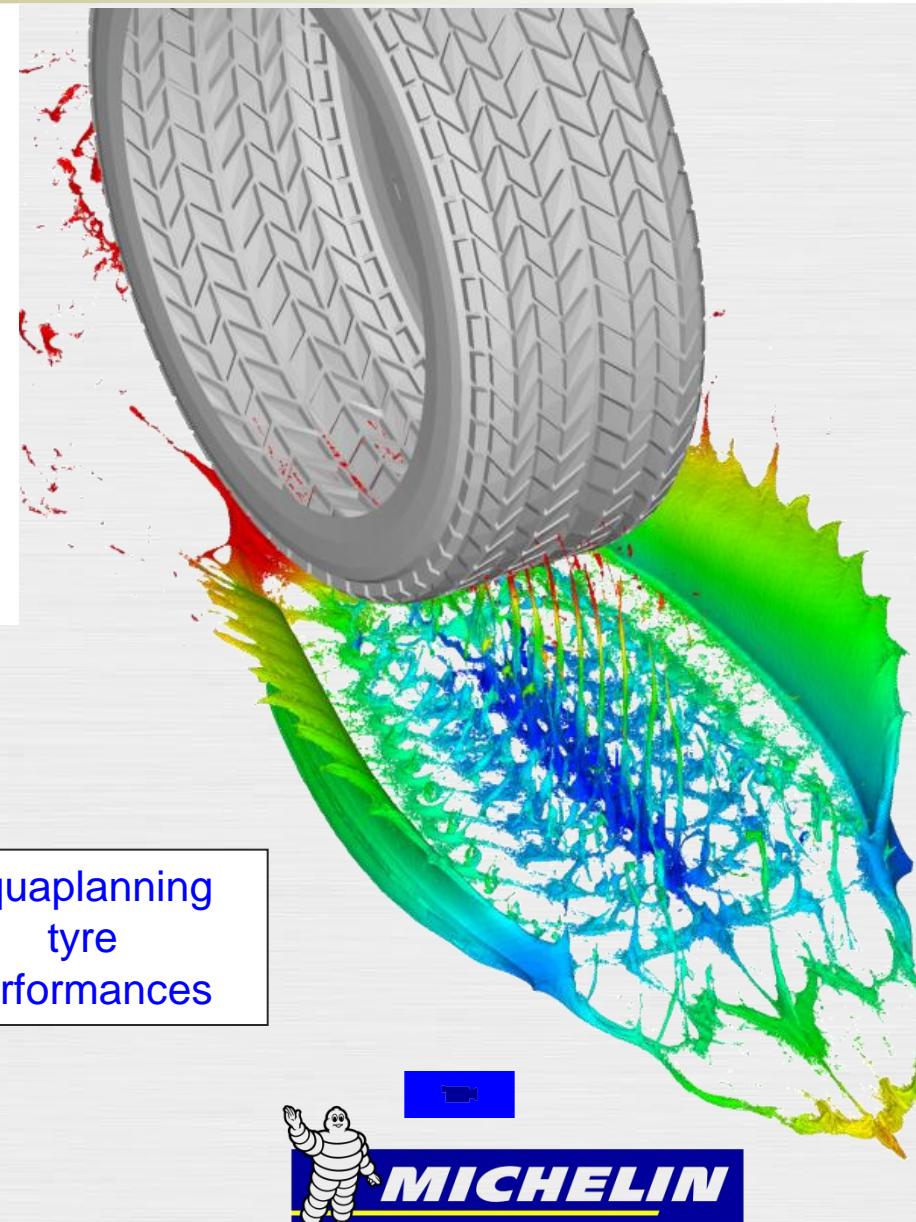
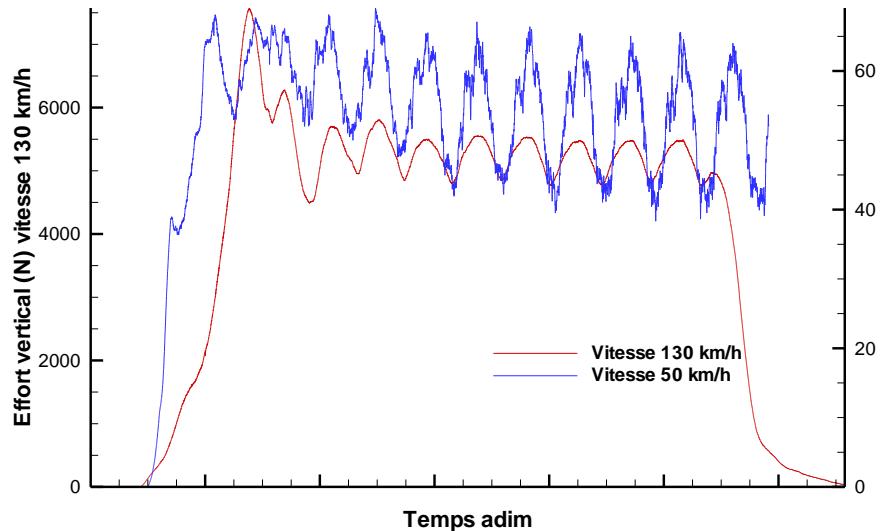
Miship Ro-Ro ferry
section flooding



Water height inside the
section

- Fast ship

Fast dynamics free surface flows: tyre aquaplaning



- very complex geometry
- 6 million particles
- 130 km/h and 50 km/h velocity
- 1cm-thick layer of water
- tyre deformations imposed

Fast dynamics free surface flows: other demonstrative applications

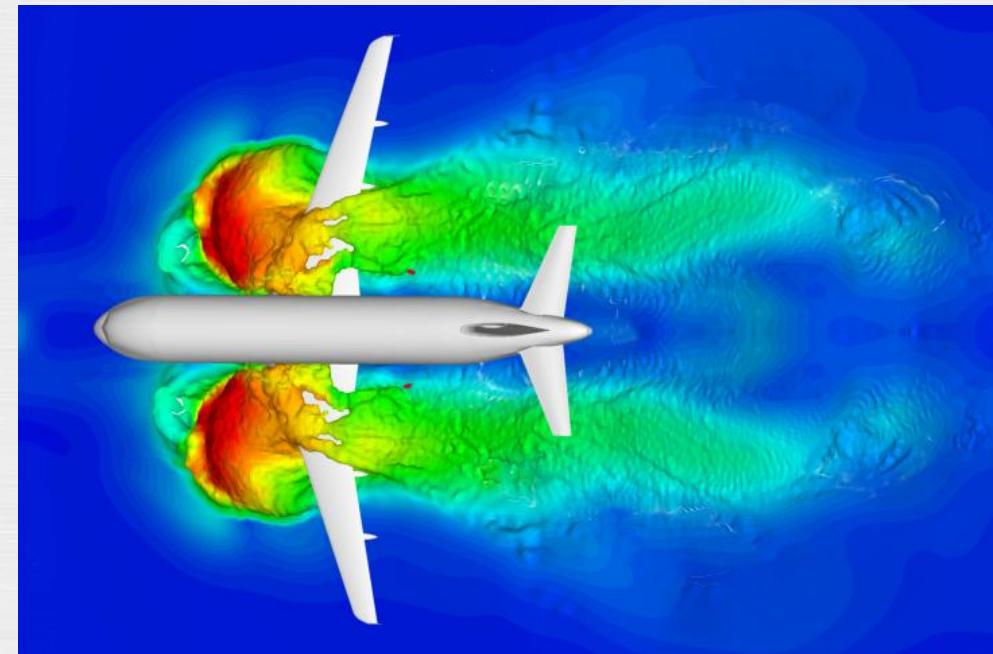


SPH-flow

- 11° initial trim angle
- 65 m/s initial velocity
- Air effects neglected
- 3 DOF (X, Z and θ)
- 6,000,000 particles



Aeronautics: aircraft ditching



Energy: offshore wind turbines



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Multiphase flow modelling: method 1



- Modification of the standard formulation to preserve density of each phase

$$\langle \rho_i \rangle = \frac{\sum_{j \in \mathcal{X}} dm_j W_j(\mathbf{x}_i)}{\Gamma_i^{\mathcal{X}}}; \Gamma_i^{\mathcal{X}} = \sum_{k \in \mathcal{X}} W_k(\mathbf{x}_i) dV_k; p_i = \frac{c_{0\mathcal{X}}^2 \rho_{0\mathcal{X}}}{\gamma_{\mathcal{X}}} \left[\left(\frac{\langle \rho_i \rangle}{\rho_{0\mathcal{X}}} \right)^{\gamma_{\mathcal{X}}} - 1 \right]; \forall \mathbf{x}_i \in \mathcal{X}$$

$$\begin{cases} \frac{D \log \mathcal{J}_i}{Dt} = \sum_j (\mathbf{u}_j - \mathbf{u}_i) \cdot \frac{\nabla W_j(\mathbf{x}_i)}{\Gamma_i} dV_j; & \Gamma_i = \sum_k W_k(\mathbf{x}_i) dV_k \\ \frac{D \mathbf{u}_i}{Dt} = -\frac{1}{\rho_i} \sum_j \left(\frac{p_i}{\Gamma_i} + \frac{p_j}{\Gamma_j} \right) \nabla W_j(\mathbf{x}_i) dV_j + \mathbf{F}_V + \mathbf{F}_S + \mathbf{F}_B & ; \quad \frac{D \mathbf{x}_i}{Dt} = \mathbf{u}_i \end{cases}$$

- Continuous Surface Stress surface tension modelling

$$\mathbf{F}_{Si}^{xy} = \sigma \kappa \delta_I \mathbf{n}_I$$

$$\begin{cases} \mathbf{T}_{Si}^{xy} = \sigma^{xy} \frac{1}{|\nabla C_i|} \left(\frac{1}{d} |\nabla C_i|^2 - \nabla C_i \otimes \nabla C_i \right) \\ \mathbf{F}_{Si}^{xy} = \operatorname{div}(\mathbf{T}_{Si}^{xy}) \quad \forall i \in \chi \end{cases}$$

Multiphase flow modelling: method 2



- In the Riemann-solver ALE formulation, prevent any mass flux through the interface

$$\frac{d(x_i)}{dt} = v_0(x_i, t)$$

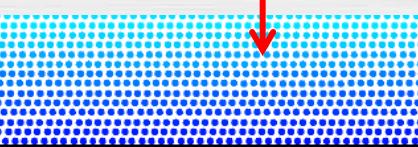
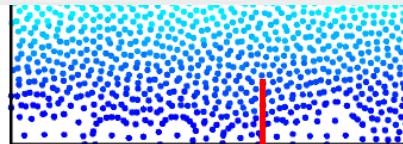
$$\frac{d(\omega_i \rho_i)}{dt} + \omega_i \sum_{j \in D_i} \omega_j 2 \rho_{E,ij} \cancel{v_{E,ij} - v_0(x_{ij}, t)} \cdot \nabla_i W_{ij} = 0$$

$$\frac{d(\omega_i \rho_i v_i)}{dt} + \omega_i \sum_{j \in D_i} \omega_j 2 \left[\rho_{E,ij} v_{E,ij} \otimes \cancel{v_{E,ij} - v_0(x_{ij}, t)} + p_{E,ij} \right] \cdot \nabla_i W_{ij} = \omega_i \rho_i g$$

Multiphase flow modelling: **laminar flow validation**

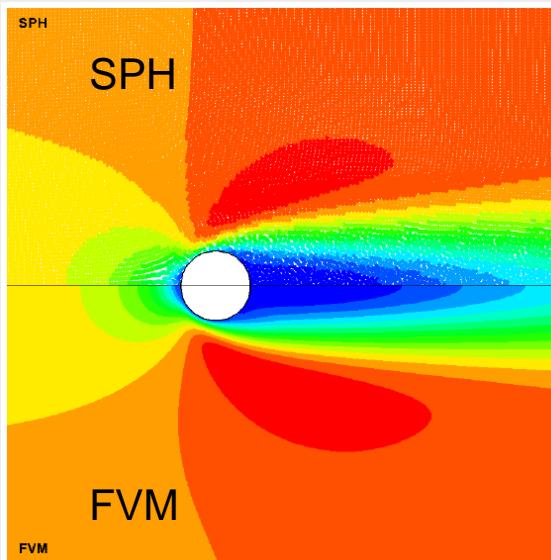


- Application of ghost viscous condition only on the pressure gradient term to preserve the hyperbolicity of the system inviscid part (De Leffe et al., Proc. 6th SPHERIC workshop, 2011)



$$\begin{aligned} \frac{dE}{dt} = & - \sum_{i \in P(\Omega)} \sum_{j \in P(\Omega) \cup P(\partial\Omega)} m_i m_j \left(\frac{\bar{p}_j \bar{v}_i}{\rho_j^2} + \frac{\bar{p}_i \bar{v}_j}{\rho_i^2} + \frac{1}{2} \Pi_{ij} (\bar{v}_i + \bar{v}_j) \right) \cdot \nabla_i W_{ij} \\ = & \Delta E + \Delta E^\Pi \end{aligned}$$

- Validation on flow past cylinder at Re=200



	Strouhal	C _d
SPH	2.0	1.47
Experiment	1.9	1.3

experiment by Tritton (1959)

Multiphase flow modelling: validations



Rayleigh-Taylor instabilities

collaboration with CNR-INSEAN (Rome)

Grenier et al., *J. Comput. Phys.*, 2009

Fast convergence on the interface shape
thanks to Lagrangian nature of SPH

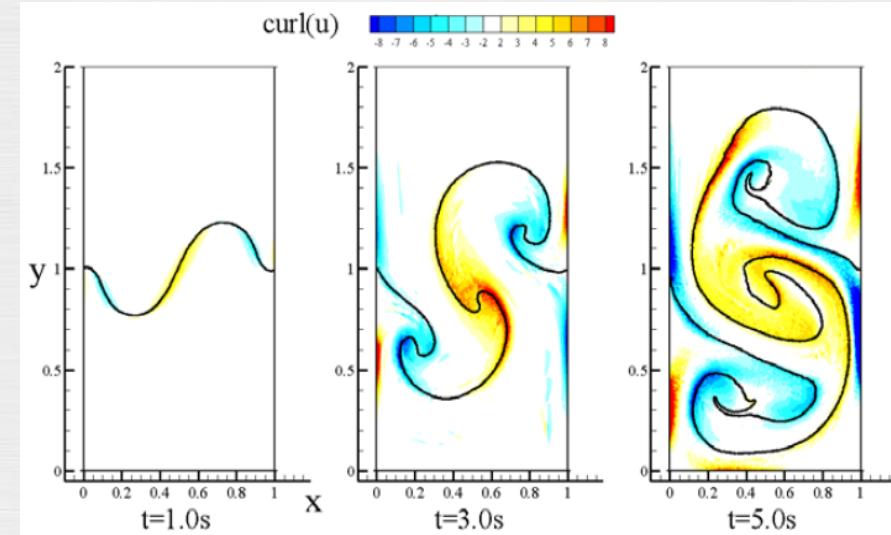
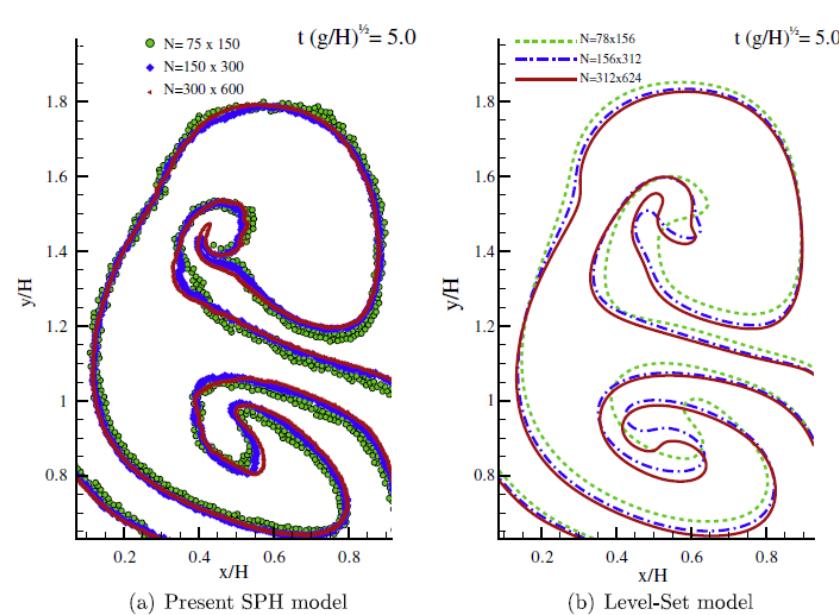


Figure 5: Vorticity of the present SPH formulation.

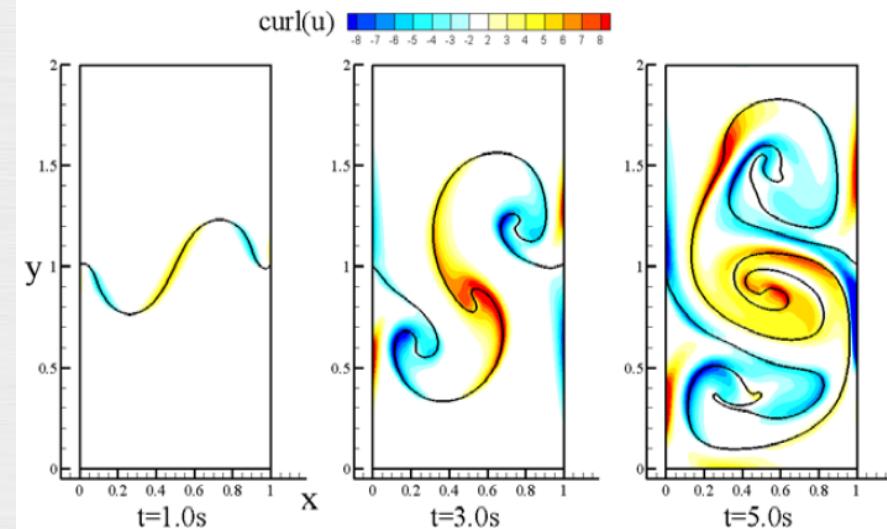
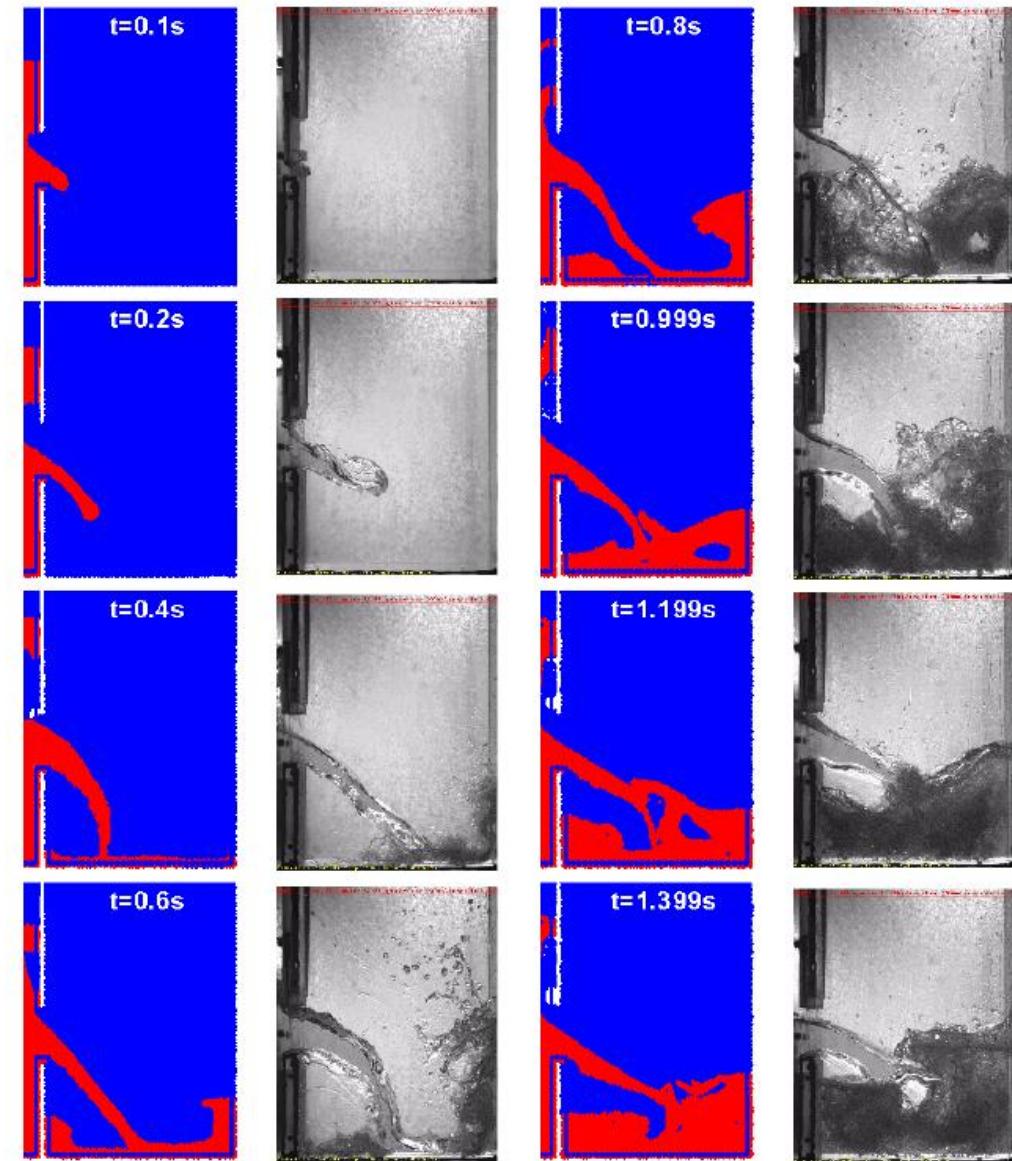


Figure 6: Vorticity of the NS-LS formulation.

Multiphase flow modelling: validations



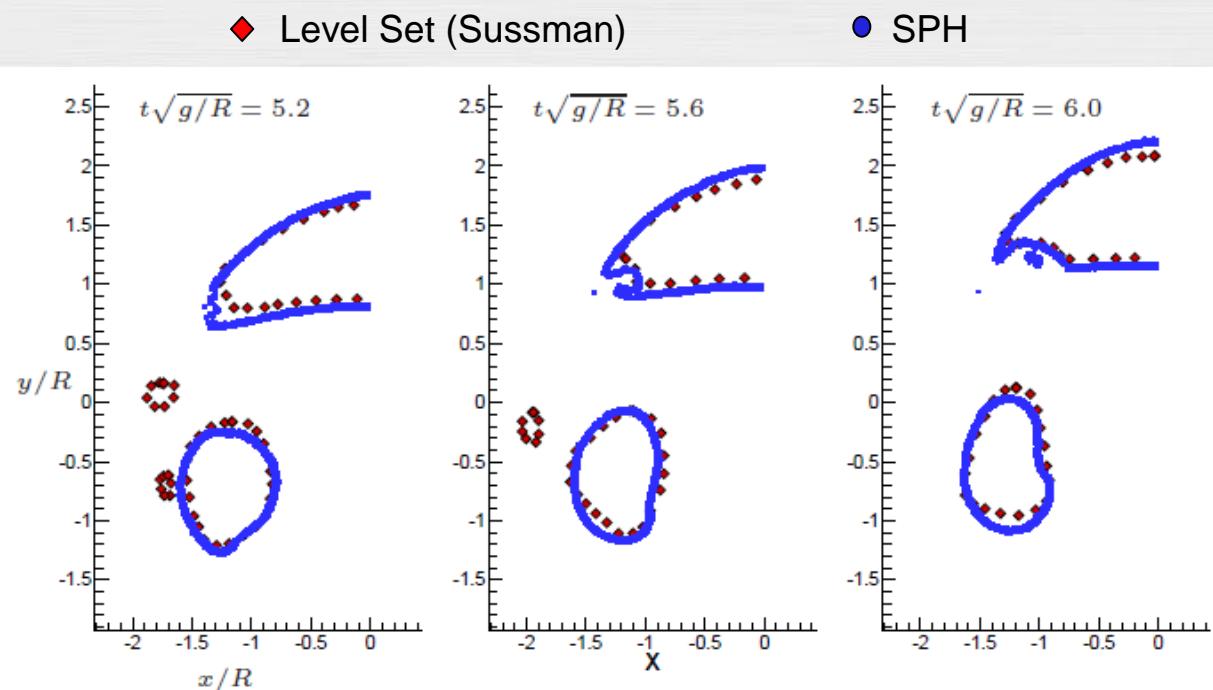
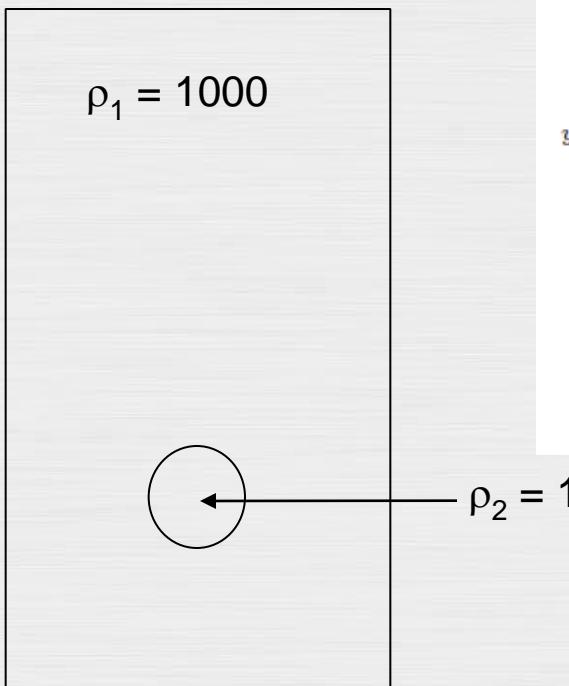
Flooding
experiment
(made in ECN)
comparison



Bubbly flows: isolated bubble



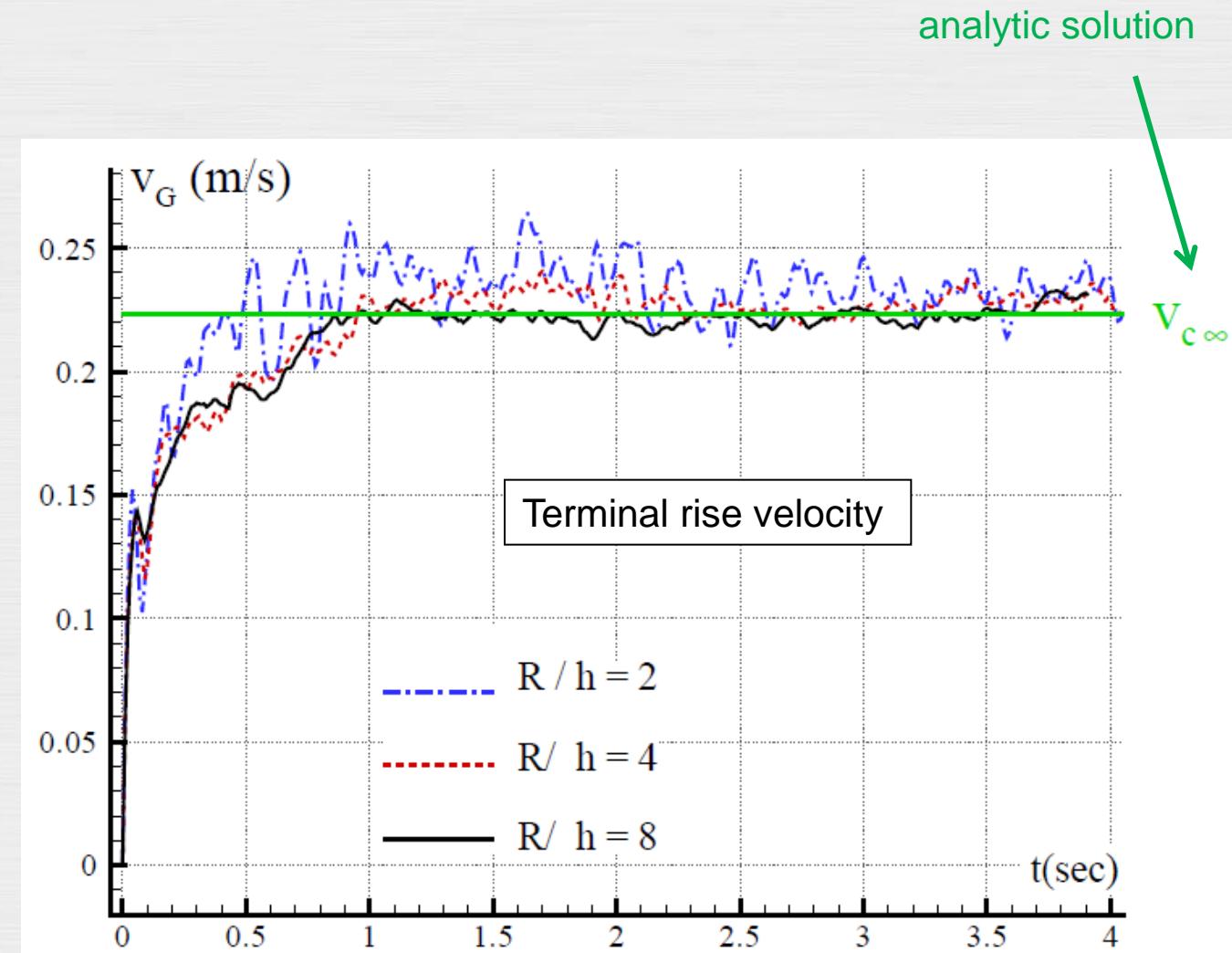
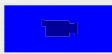
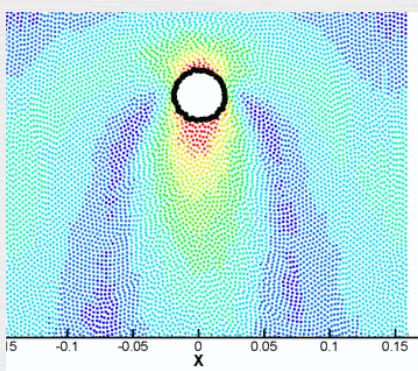
Large Bond number
bubble rise



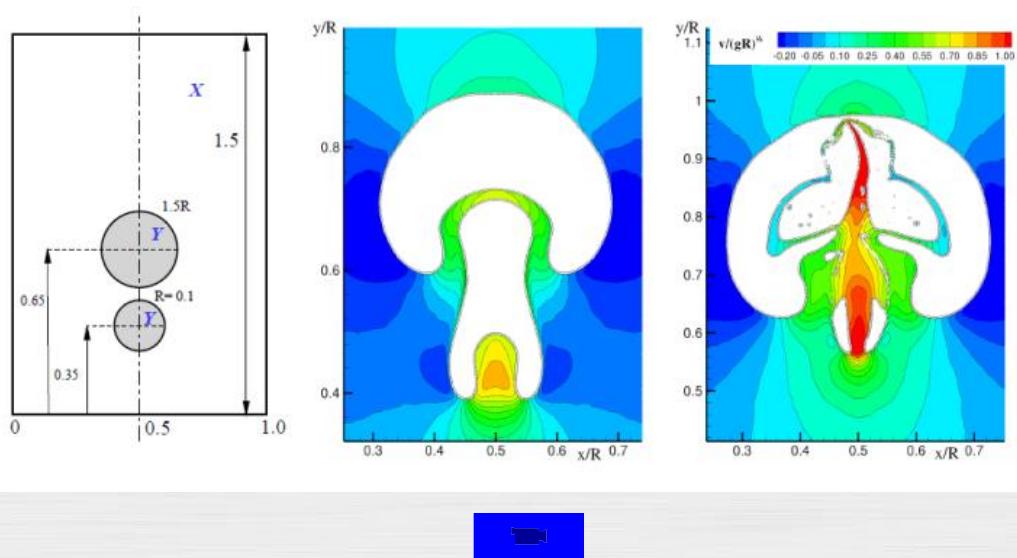
Bubbly flows: isolated bubble



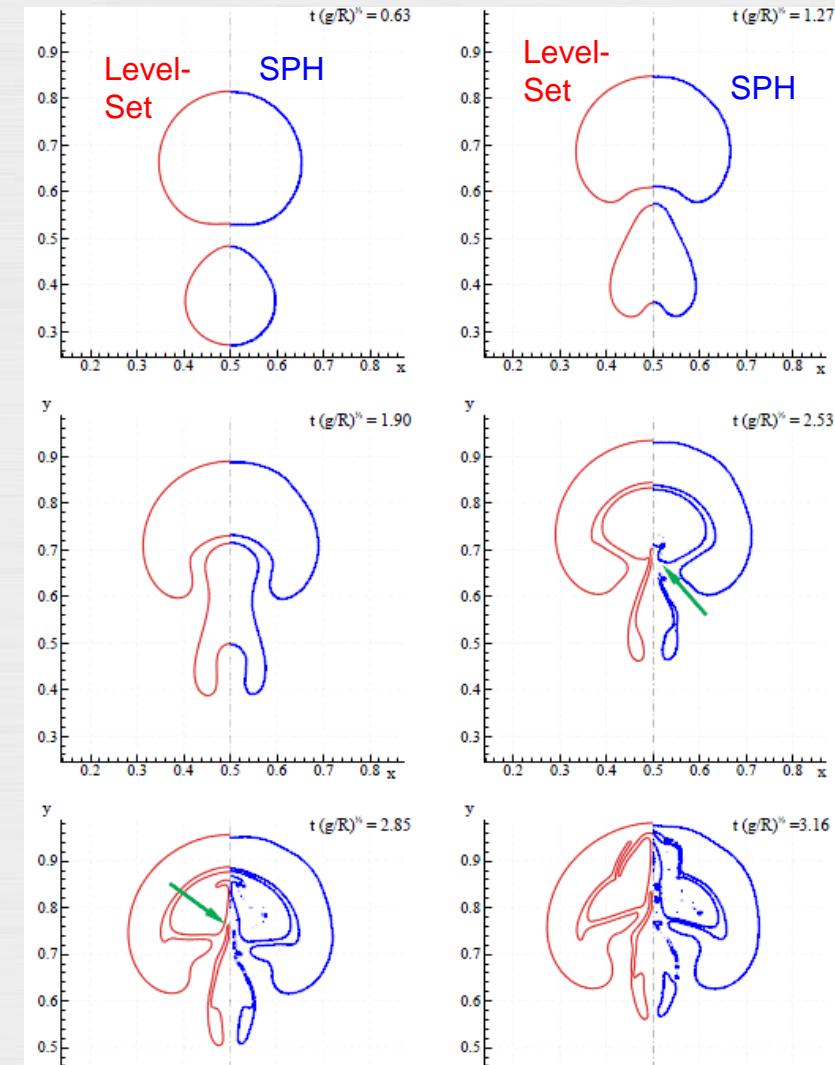
Small Bond number
bubble rise



Bubbly flows: two-merging bubbles



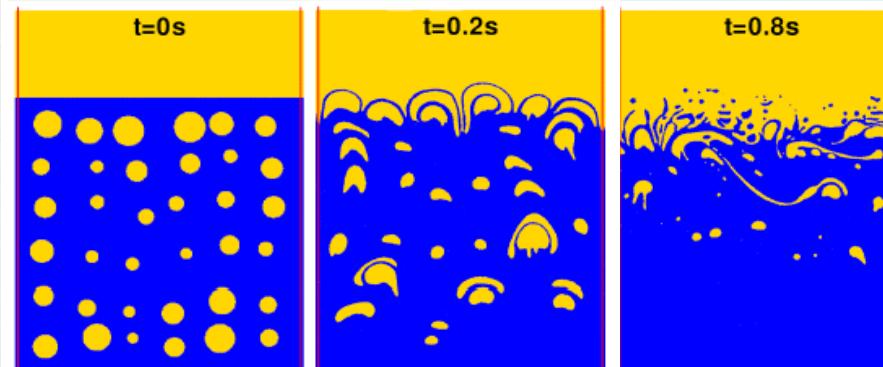
Infinite Bond number and density ratio = 10



Bubbly flows: water-oil separation



collaboration with CNR-INSEAN (Rome)



Infinite Bond number

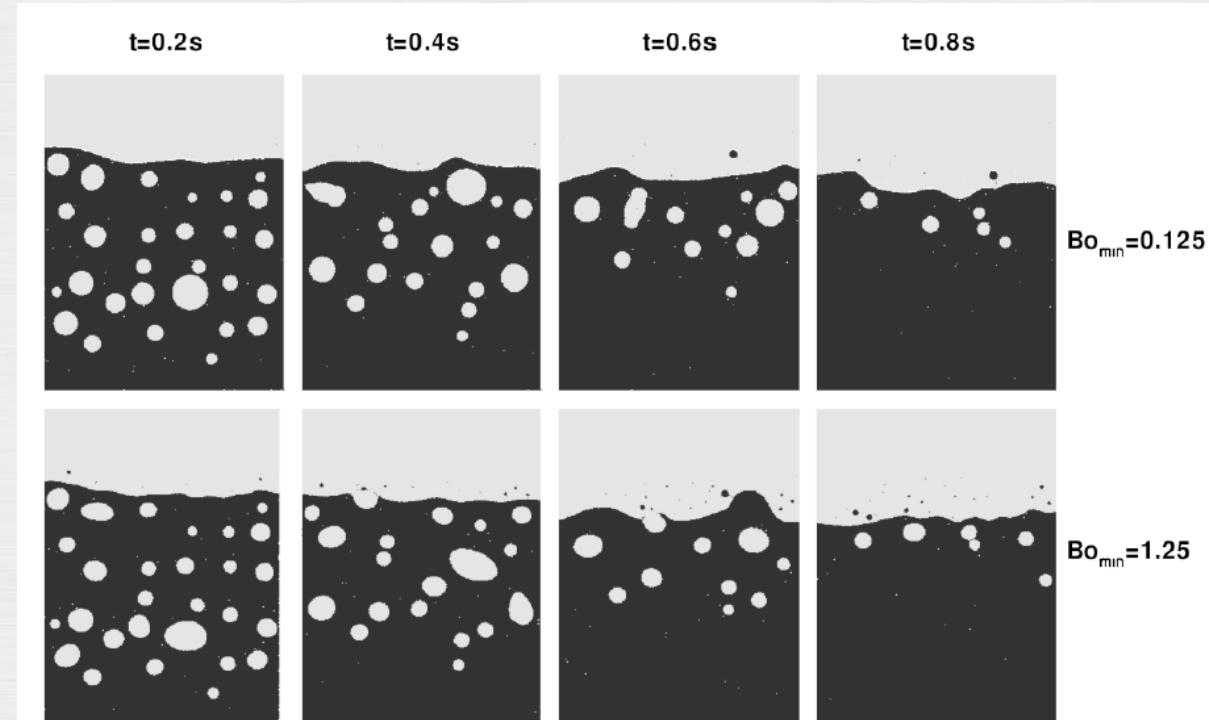
$$Bo_{min} = 0.1$$

$$Bo_{min} = 1$$

naive gravity separator



Saipem





Mesh-free Lagrangian modelling of fluid dynamics

David LE TOUZÉ, Ecole Centrale Nantes



CFD 2011, keynote lecture

Mesh-free Lagrangian methods in CFD

Smoothed-Particle Hydrodynamics (SPH)

Fast-dynamics free-surface flows

Multi-fluid flows

Fluid-Structure Interactions

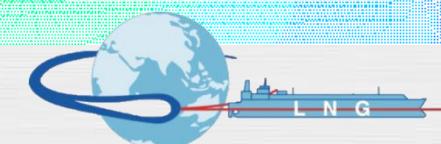
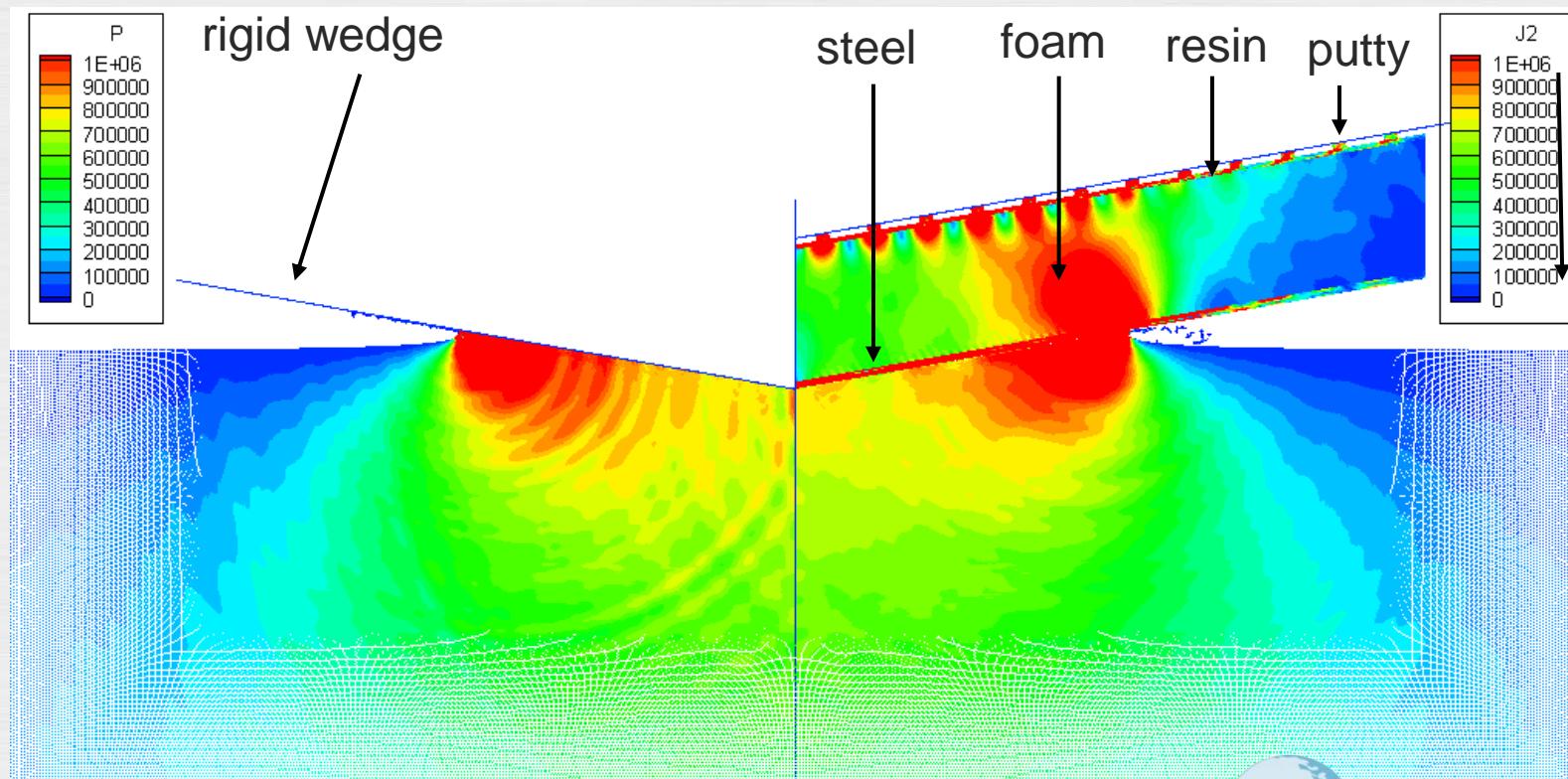
HPC: massive interactive simulations

Fluid-Structure coupling: SPH monolithic coupling



Principle:

- each particle has its own continuous medium local equations
- mass fluxes through the interface are prevented, as for multiphase method 2

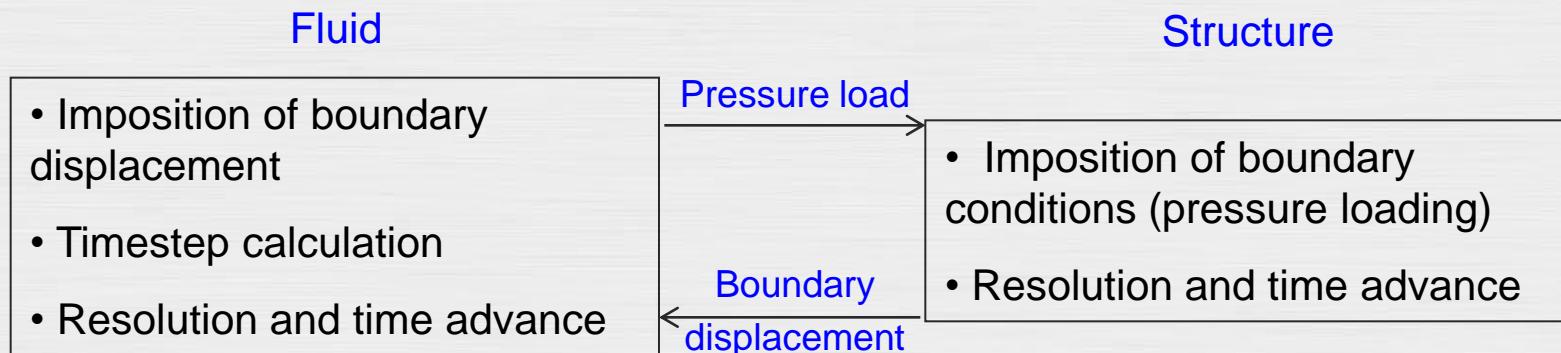


Fluid-Structure coupling: SPH-FEM strategy



SPH-FEM coupling

- Weak coupling strategy, at each substep of Runge-Kutta 4



- Timestep of FSI simulations is based on SPH timestep (very small)
- In practice, several processors are used to compute flow evolution while only one is used for solid mechanics
- FEM solver is fast and its computation time is masked by the flow solver => scalability of SPH-Flow code is unaffected

Fluid-Structure coupling: SPH-FEM strategy



Advantages of SPH-FEM coupling

- FEM is an accurate and fast method to simulate structures behaviour under pressure loads
- SPH method easily handles fragmentations and reconnections of free surface
- No free-surface tracking method is needed
- No specific treatment is needed at the fluid-structure interface



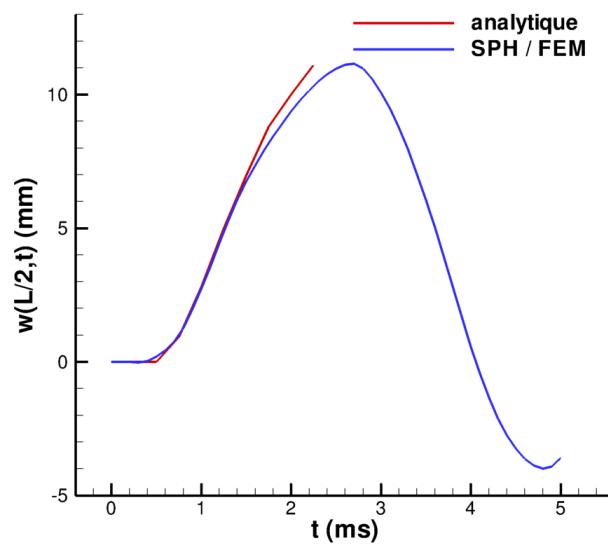
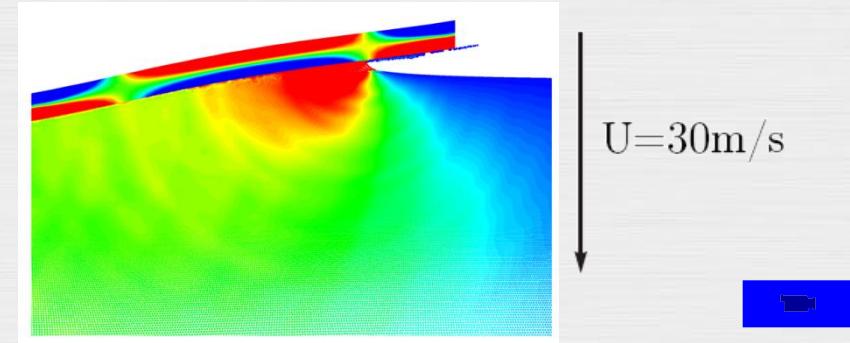
SPH-FEM coupling: validation test cases



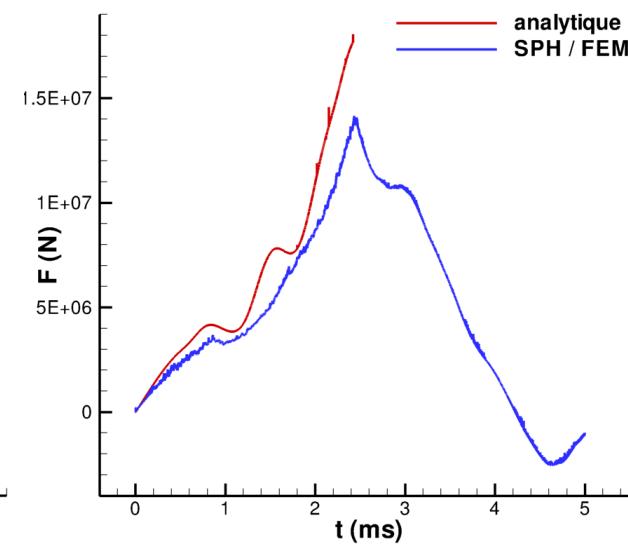
Fourey et al., submitted to Comput. Meth. Appl. Mech. Engng.

Half-wedge hydroelastic impact

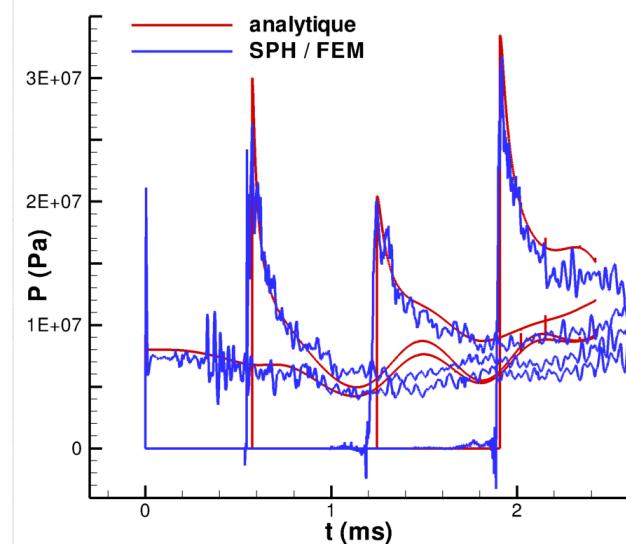
- Aluminium beam
- High velocity impact
- Motion of the beam is prescribed at its two ends



Beam deflection at mid point



Total vertical force

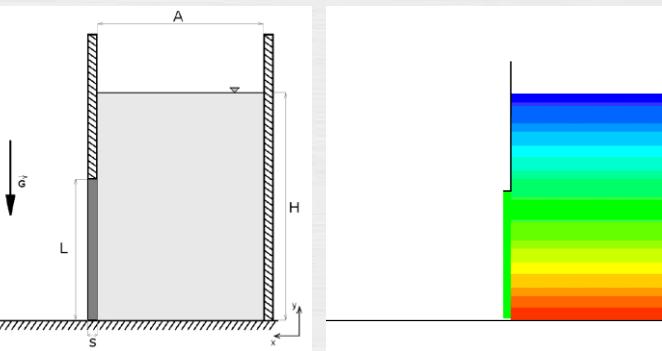


Pressure probe measurements

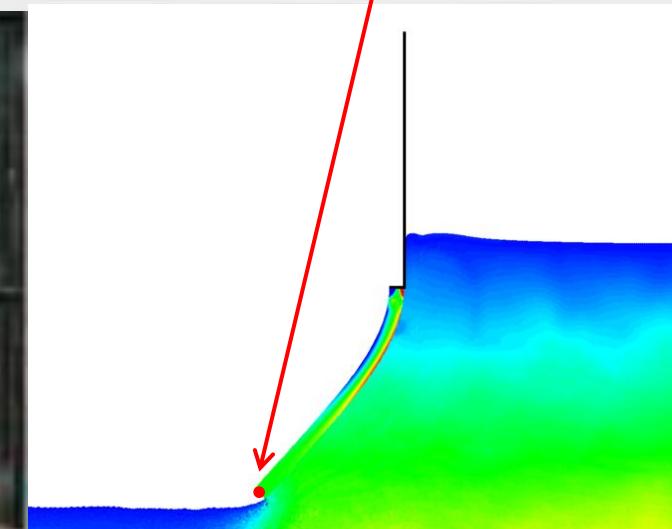
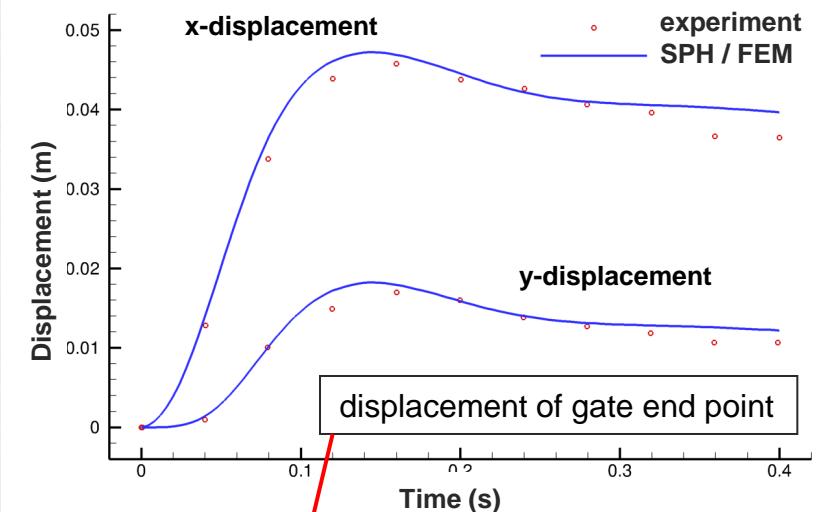
SPH-FEM coupling: validation test cases



Water exit under an elastic gate



Fourey et al., submitted to Comput. Meth. Appl. Mech. Engng.

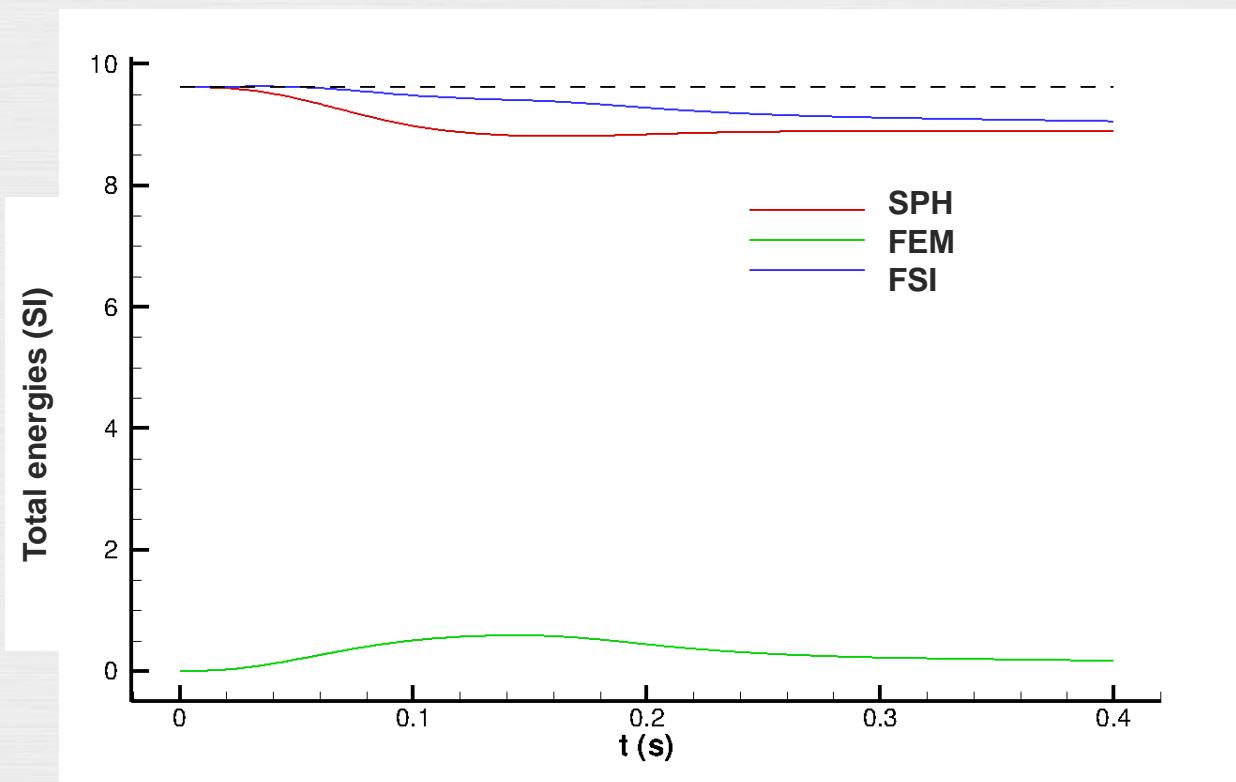


SPH-FEM coupling: validation test cases



Water exit under an elastic gate

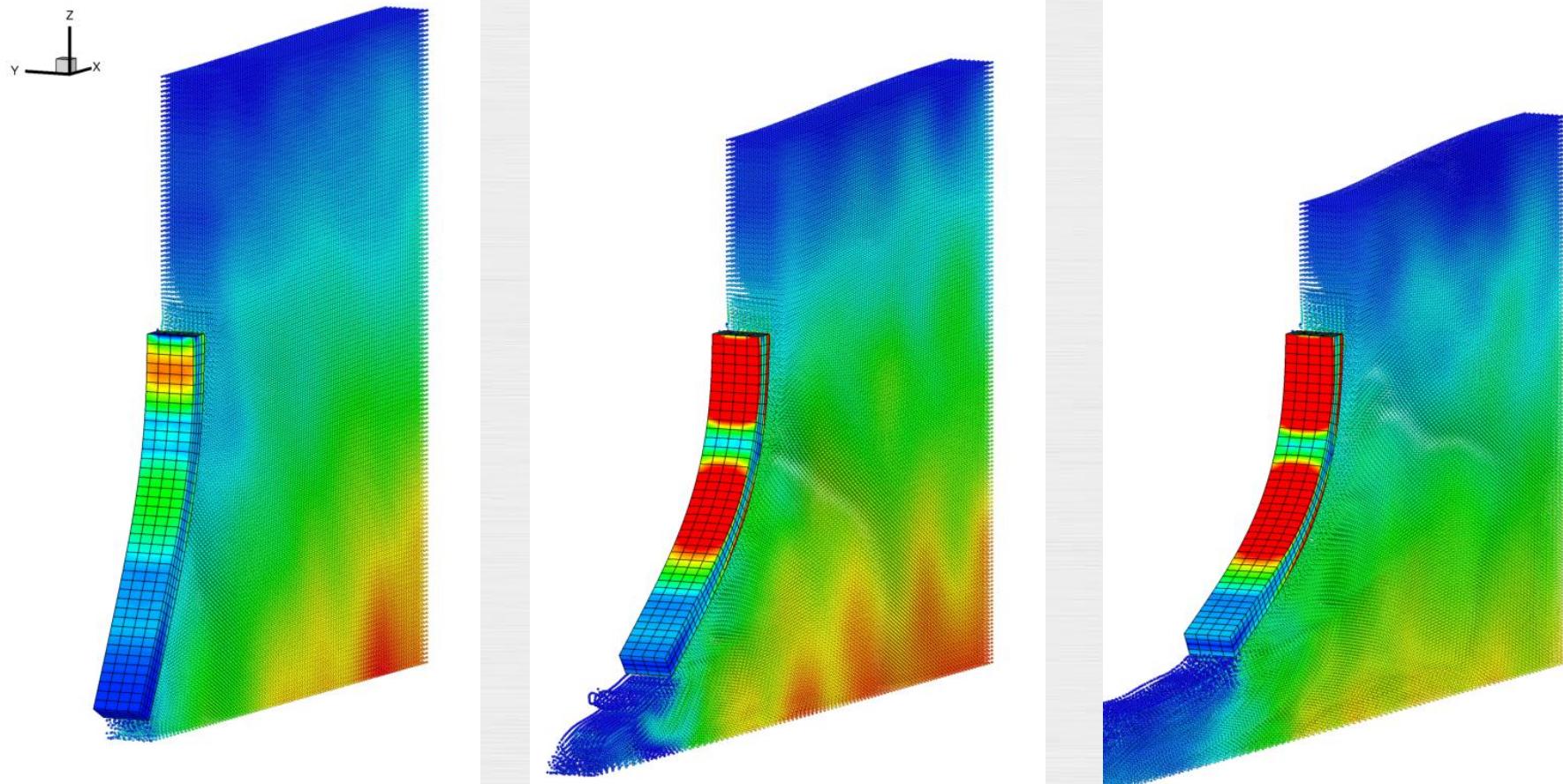
- Total energy evolution for the FSI simulation:



SPH-FEM coupling: three-dimensional extension

SPH-flow

3D water exit under an elastic gate

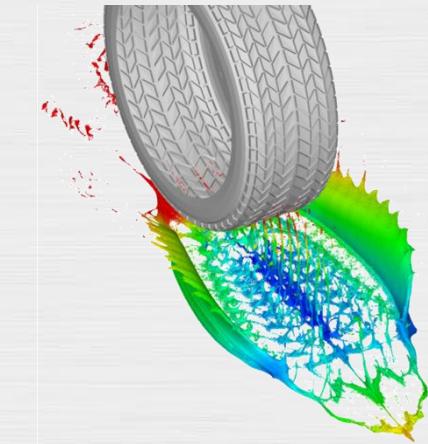
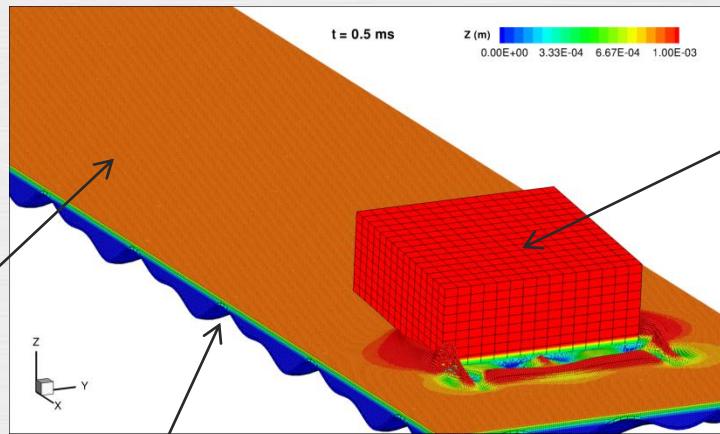


SPH-FEM coupling: Example of industrial application

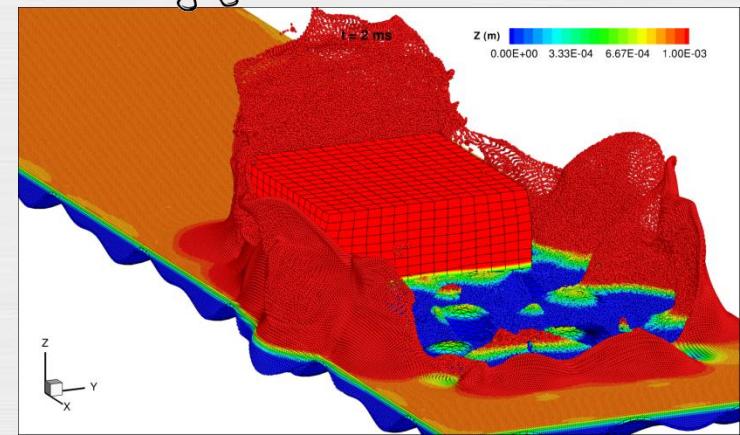
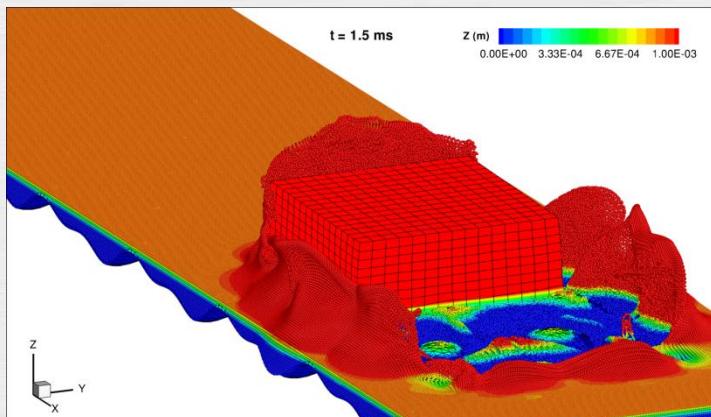
SPH-flow

Tyre deformation when rolling on a wet rough road

still water



collaboration
with Michelin





Mesh-free Lagrangian modelling of fluid dynamics

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CFD 2011, keynote lecture

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Smoothed-Particle Hydrodynamics (SPH)

Fast-dynamics free-surface flows

Multi-fluid flows

Fluid-Structure Interactions

HPC: massive interactive simulations

FP7 European project NextMuSE: SPH & HPC



Initialize

(CAD geometry, no mesh)

Compute

(continuously)

Analyze

(on the fly)

Render

(immersive)

Update

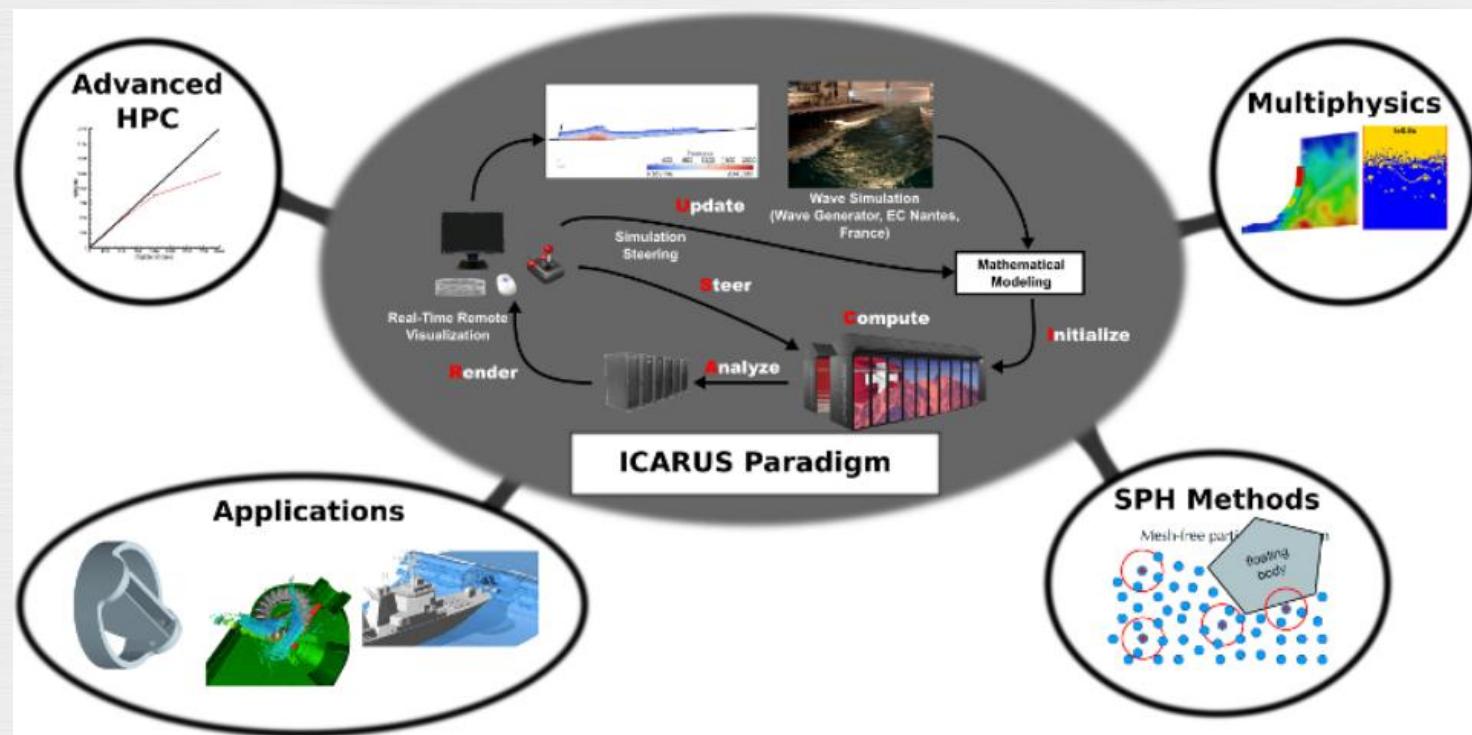
(interactive)

Steer

(interactive)



<http://nextmuse.cscs.ch>

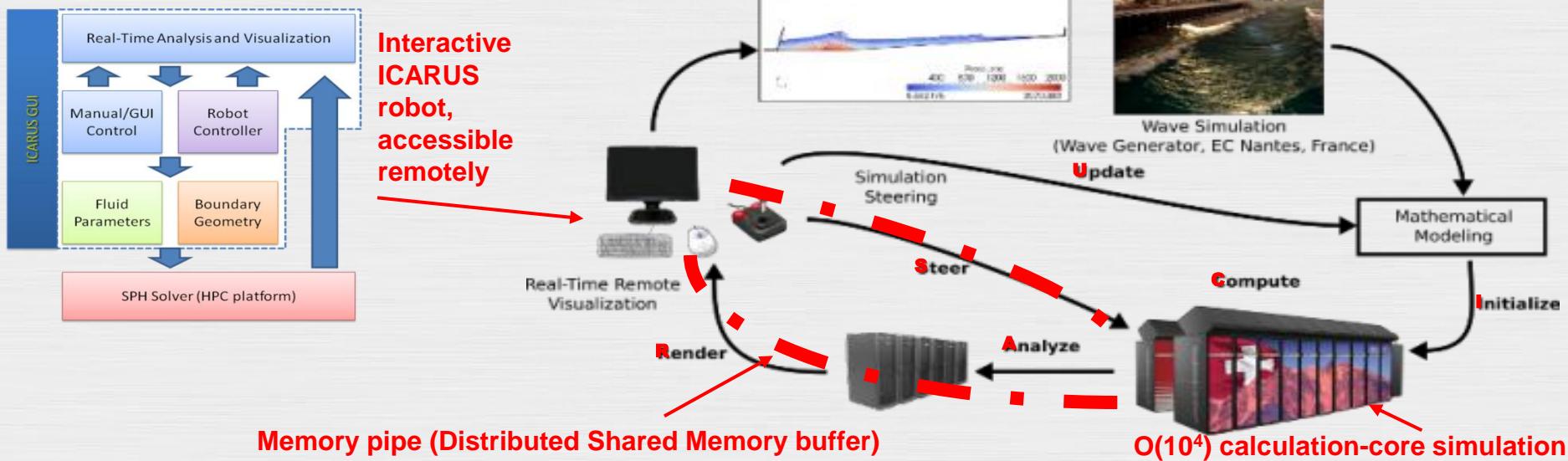
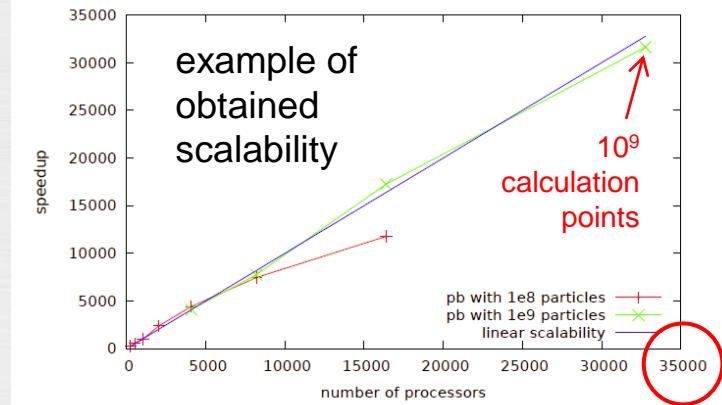


FP7 European project NextMuSE: SPH & HPC



High-performance (HPC) flexible simulation environment

- Immersive environment ICARUS:
visualization, analysis, steering of geometry/parameters
simulation runs on a massively-parallel architecture
- Optimization of the method on modern architectures:
« manycore » CPUs (MPI/OpenMP) and hybrid GPGPU/CPU



Conclusion



- Research on mesh-free Lagrangian methods is growing fast and they are reaching industrial maturity on some problems
- These methods can represent a valuable alternative where mesh-based methods find their limits
- They are well suited to:
 - fast dynamics problems, especially with free-surface
 - multi-species/multiphase problems with interfaces: multi-fluid, fluid-structure...for which they are simple and accurate
- These methods could probably be used more in the oil & gas industry (presently mainly applied to ocean engineering in this industrial field)