SPH - current and future challenges

DualSPHysics

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Overview

- Reminder of Smoothed Particle Hydrodynamics (SPH) key features
- Research and Applications now possible
- Current obstacles to quick development: formulation and sources of error
- SPHERIC & Grand Challenges
- How is the DualSPHysics group addressing these challenges

REMINDER

What is SPH?

Welcome to the amazing world of meshless methods

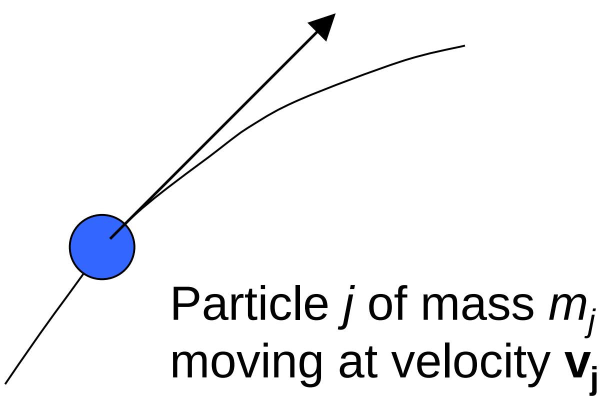
Meshless methods: Basic Idea of SPH

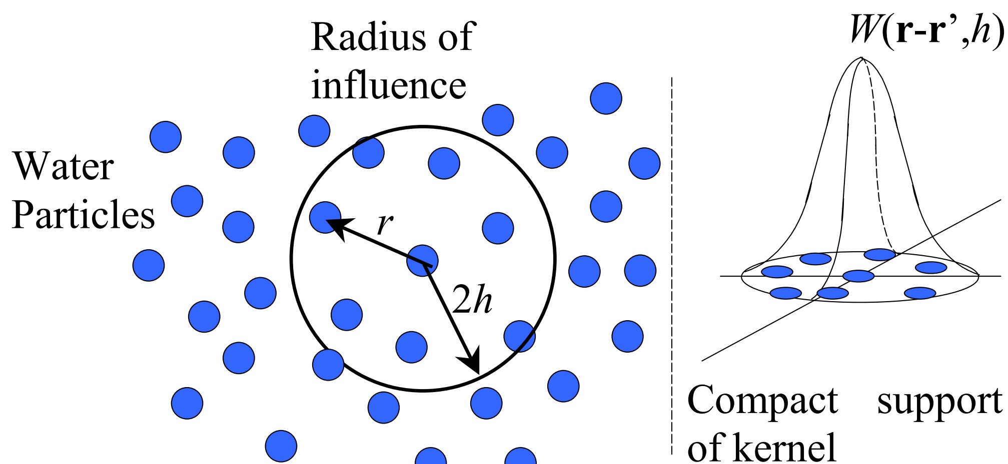
Meshless Our computation points are **particles** that now **move** according to governing dynamics , e.g. Navier-Stokes Equations

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

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

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





SPH Basics

- SPH describes a fluid by replacing its continuum properties with locally (smoothed) quantities at discrete Lagrangian locations ⇒ **meshless**

- SPH is based on integral interpolants invented in 1970s for astrophysics (Lucy 1977, Gingold & Monaghan 1977)

  (*W* is the smoothing kernel)

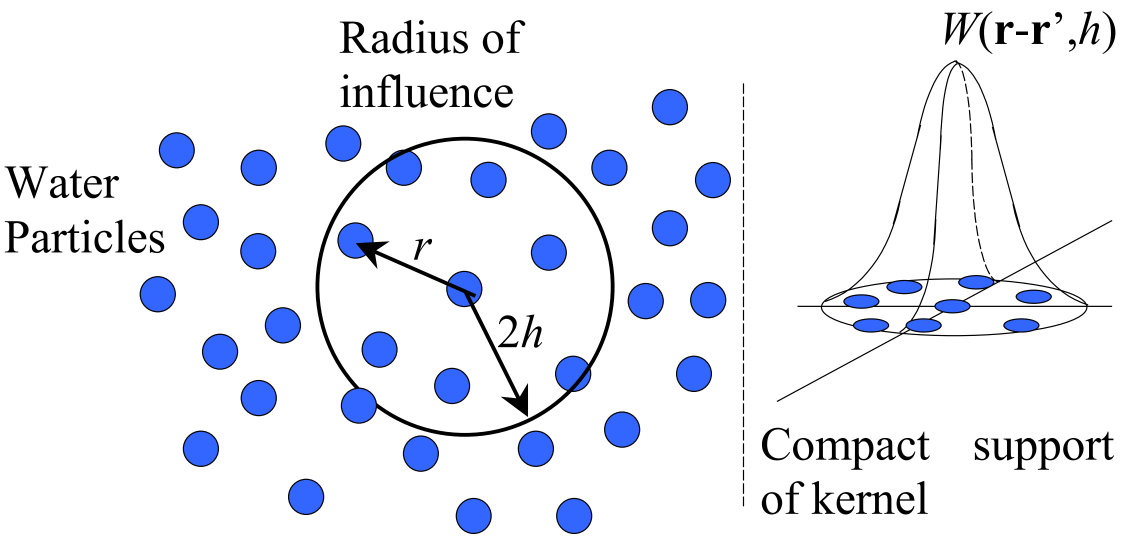
$$A(\mathbf{r}) = \int_{\Omega} A(\mathbf{r}')W(\mathbf{r}-\mathbf{r}',h)\,\mathrm{d}\mathbf{r}'$$

↓

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

- Governing equations can be approximated discretely by a summation

- Boundary conditions do not appear naturally in SPH



SPH Gradients

Consider the gradient of a integral interpolation.

(Like Finite Elements)

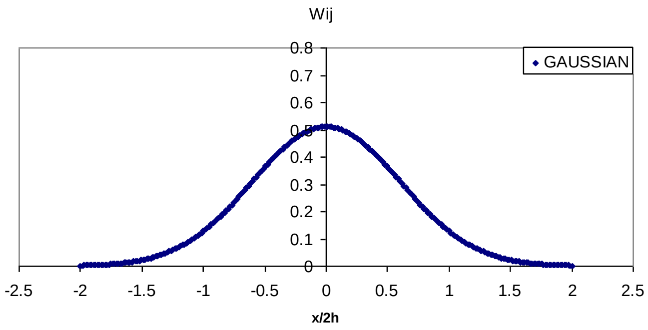
The definition of the integral interpolation is

$$\left\langle \frac{\partial A(x)}{\partial x} \right\rangle = \int_{-\infty}^{+\infty} \frac{\partial A(x')}{\partial x'} W(x - x', h) \, \mathrm{d}\, x'$$

But we cannot evaluate this because we don't know $\partial A / \partial x'$

So, after some algebra:

$$\left\langle \frac{\partial A(x)}{\partial x} \right\rangle \approx \sum_{j=1}^{N} A(x_j) \frac{\partial W(x - x_j, h)}{\partial x} \frac{m_j}{\rho_j}$$



This is **fantastic** since we specify the kernel and therefore know its gradient and can then easily calculate the gradient of **any scattered data**!!

Equations of Motion

- Navier-Stokes equations:

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

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

- Are recast in particle form as

(XSPH - Monaghan 1992)

$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = \mathbf{v}_i + \varepsilon\sum_j m_j\left(\frac{\mathbf{v}_{ji}}{\bar{\rho}_{ij}}\right)W_{ij}$$

$$\left(\frac{\mathrm{d}m_i}{\mathrm{d}t} = 0\right)$$

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = \sum_j m_j\left(\mathbf{v}_i - \mathbf{v}_j\right)\cdot\nabla_i W_{ij}$$

$$\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = -\sum_j m_j\left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right)\nabla_i W_{ij} + \sum_j m_j\frac{4\upsilon_o}{\rho_i + \rho_j}\frac{\mathbf{r}_{ij}\cdot\nabla_i W_{ij}}{r_{ij}^2 + 0.01h^2}\left(\mathbf{u}_i - \mathbf{u}_j\right) + \mathbf{F}_i$$

(I use *i* and *j* to denote different particles)

This is the classical WEAKLY COMPRESSIBLE SPH form, we will change this!

Equations of Motion

- Navier-Stokes equations:

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

- Are recast in

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$$\frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = \mathbf{v}_i + \varepsilon\sum_j$$

$$\left(\frac{\mathrm{d}m_i}{\mathrm{d}t} = 0\right)$$

$$\mathbf{u}_j\big) + \mathbf{F}_i$$

(I use *i* and *j* to den

Main points are that:

(i) we do not treat the **free surface**

(ii) No expensive meshing

(iii) SPH is Meshless & can therefore capture nonlinearity

This is the classical WEAKLY COMPRESSIBLE SPH form, we will change this!

WCSPH Examples
SPH for free-surface flows

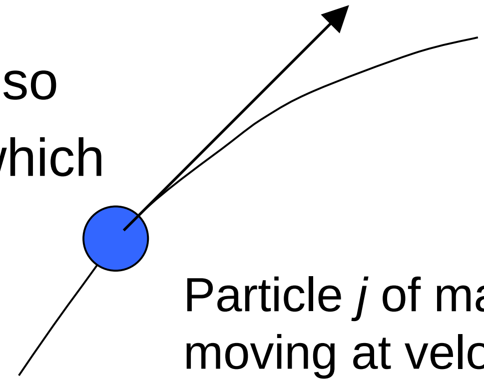
What can SPH offer?

What can SPH do that other models cannot?

What can SPH offer the simulation of free-surface flow?

SPH is a Lagrangian method

(a) Our computation points are the particles so we can track what happens to the particles which represent the water, the sediment, etc.



Particle *j* of mass m_j
moving at velocity $\mathbf{v_j}$

(b) This means we **avoid** the computation of the **nonlinear advection terms** within SPH

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

Only the RHS of our equations need SPH treatment

This makes nonlinear phenomena very easy to examine, in particular **FORMATION mechanisms**, eg. mixing …

DualSPHysics - What is it?

What is possible?

What is our aim?

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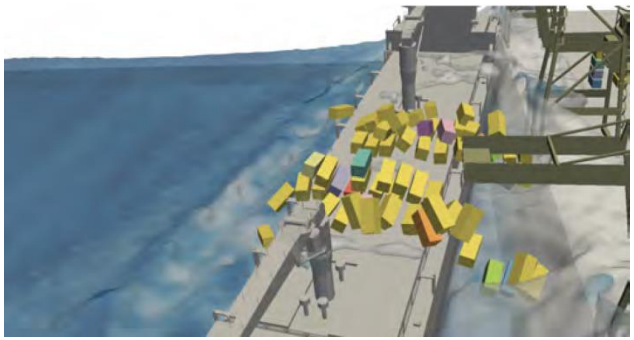
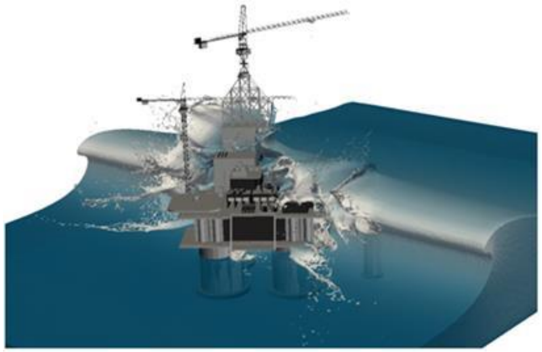
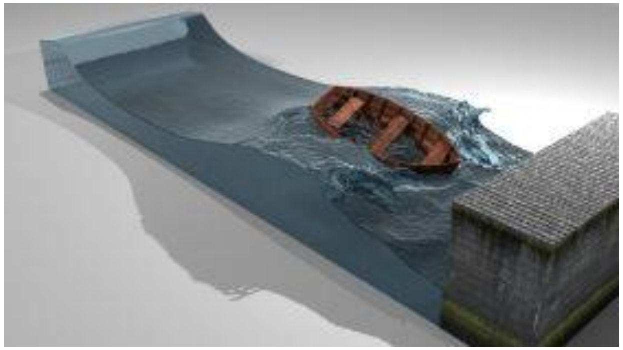
DualSPHysics Project:

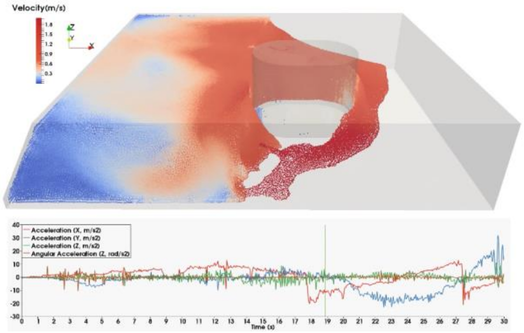
THE community open-source SPH code

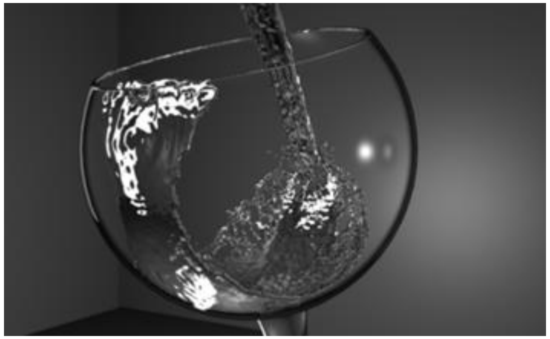
Runs on multi-core CPU or GPU using WCSPH

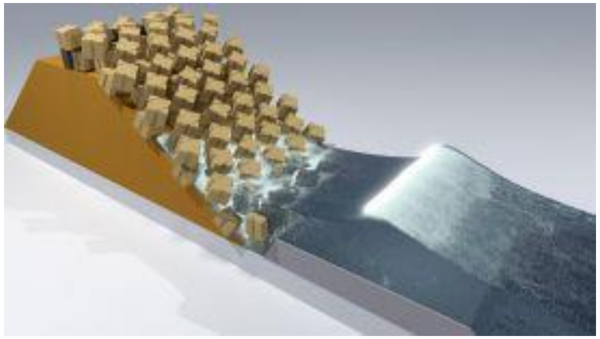








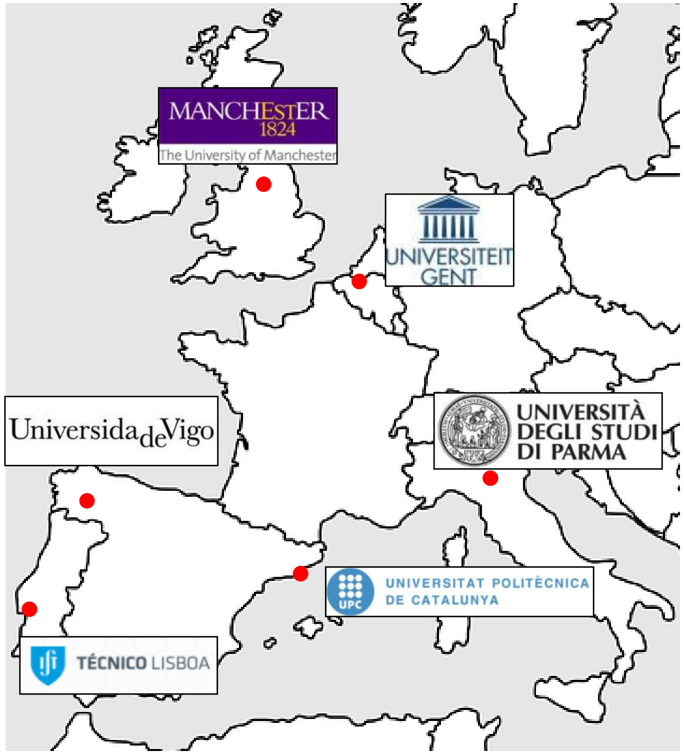




http://www.dual.sphysics.org

DualSPHysics Project:

- University of Manchester
- University of Vigo (Spain)
- University of Parma (Italy)
- University of Lisbon (Portugal)
- University of Ghent (Belgium)



Websites

- Free open-source **SPHysics** code:

  http://www.sphysics.org

  http://www.dual.sphysics.org

Downloaded 30,000+ times: Open-source plug & play SPH code for free-surface flow

DualSPHysics Project:

Annual Users Workshops – 60 people attending

4th Users Workshop

Oct 2018, Lisbon, Portugal

Our overall aim

We're trying to create state-of-the-art SPH software to fulfil several objectives:

1. SPH software that's useful for engineers, industry and fundamental research

2. State-of-the-art **validated** SPH formulations to simulate complex physics: *L2-error norm convergence*

3. Open-source so that's open to researchers to improve & expand

4. Does not require expensive & massive HPC resources

5. Easy to use for applications with different physics

At Manchester, birthplace of the industrial revolution, we collaborate a lot with industry (EDF, National Nuclear Laboratory, BAE Systems).

DualSPHysics

Example applications at Manchester:

- Fuel tank sloshing

- Tsunamis

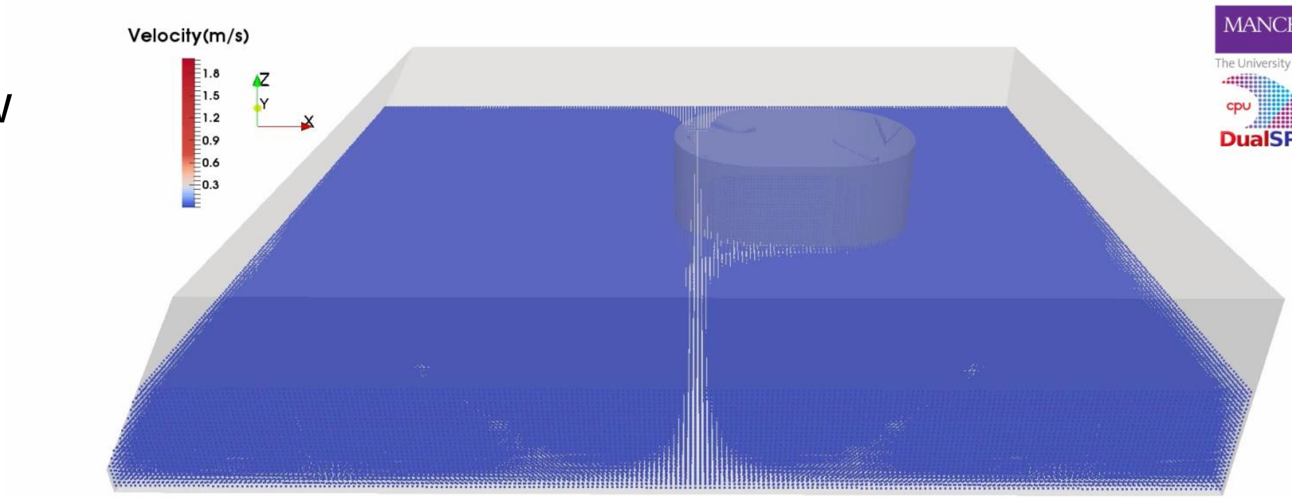
Fuel-tank sloshing with Leading Motorsport Company

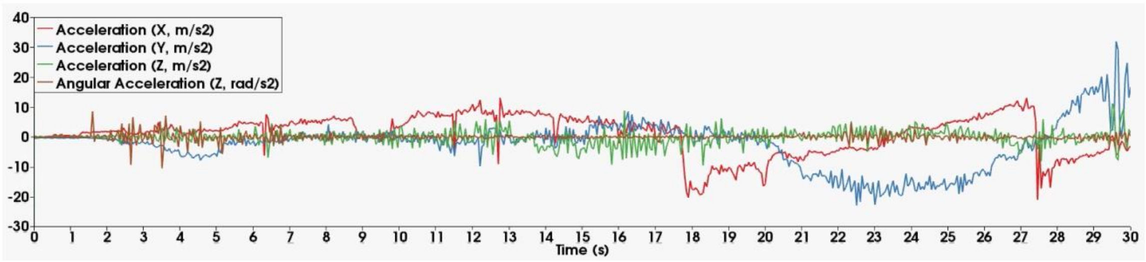
Real engineering problems are now accessible

Only allowed to show highly simplified geometry

Accelerations are up to 5*g*

Comparisons with in-tank footage were close.





Longshaw & Rogers (2015), Advances Engineering Software

Funded by Knowledge Transfer Account (KTA), *now the IAA*

SPH free-surface Applications

Application: Large-scale Flooding Impact

Pringgana et al. 2016, Cunningham et al. 2015

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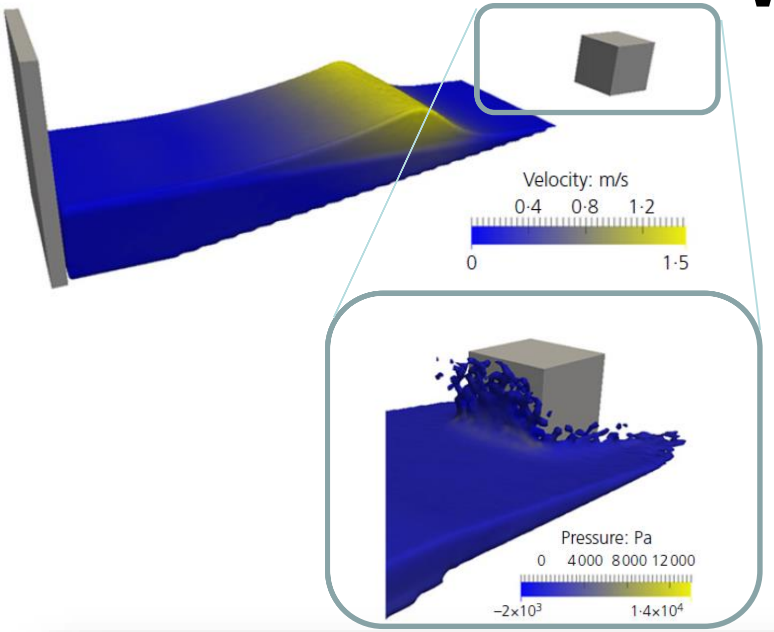
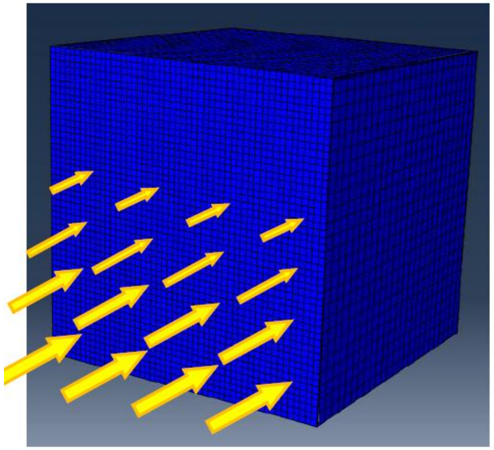
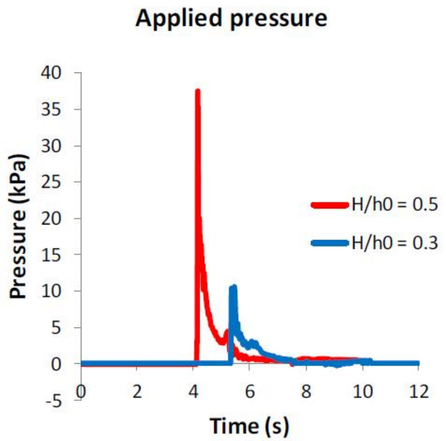
Tsunami-structure interaction modelling with SPH

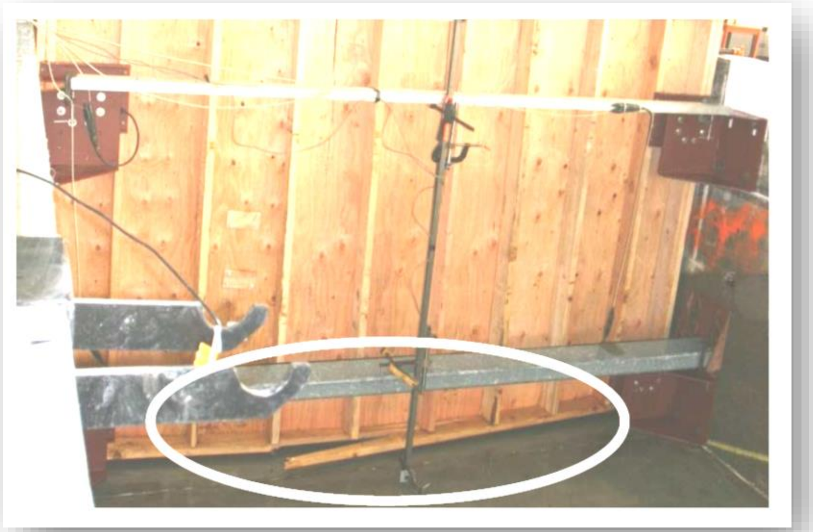


FE model mesh size and applied loads



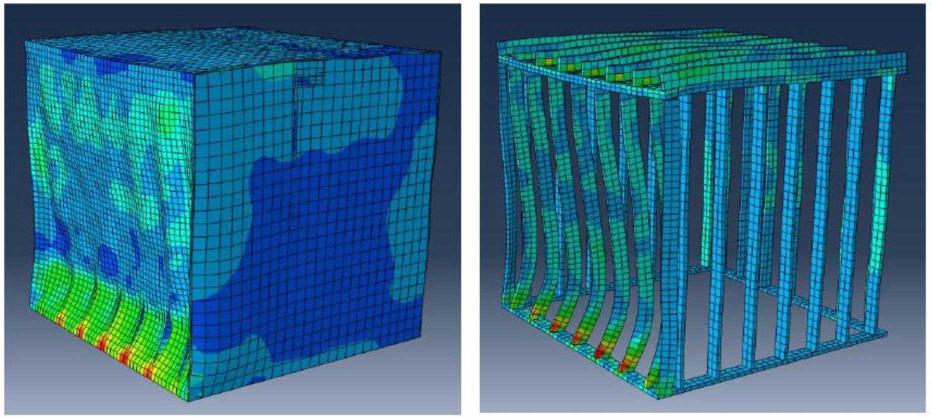


Example of load (pressure) time histories at lowest level



Linton *et al*. (2012)

Stress on structure's components



Let me remind you of the most common question I receive

While pointing to possibly the most impossible application in their industry, someone asks:

“Can SPH/DualSPHysics/SPHERIC do this?”

SPH looks easy right?

SPH attractive features:

- List of particles – easy to vectorize & “embarrassingly parallel”.
- Particles interact with each other using weighting functions with a compact support
- Meshless and Lagrangian so many of the complicated algorithms can be avoided
- Formulations are generally simpler than other computational techniques

Why aren’t things easy and straightforward to implement in SPH and DualSPHysics?

Why SPH is NOT easy

1. The numbers of particles needed for real applications is large (10^8+) so hardware acceleration is required (GPUs)

2. Sources of Error

3. Physics of applications are some of the most complicated and beyond other simulation techniques

SPH Sources of error

1. **Mollification Error**

2. **Discretisation Error**

3. **Summation Error**

4. **Others (Equation of State, time integration)**

SPH Fundamentals: Mollification Error

The SPH Integral Interpolation

We actually start from a delta function interpolation:

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

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

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

where < · > is the integral SPH averaged quantity and h is the **SMOOTHING LENGTH** (more later on this).

(Qu: What's the difference?)

SPH Fundamentals: Mollification Error

The SPH Integral Interpolation

We actually start from a delta function interpolation:

Using a weighting function, we have to choose:

(i) Our kernel function

(ii) Size (support) of *W*,

(iii) Smoothing length

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SPH Sources of error

1. Mollification Error
2. **Discretisation Error**
3. Summation Error
4. Others (Equation of State, time stepping, etc.)

SPH Basics – Discretisation error

- SPH describes a fluid by replacing its continuum properties with locally (smoothed) quantities at discrete Lagrangian locations ⇒ **meshless**

- SPH is based … invented in 1… (Lucy 1977, G…

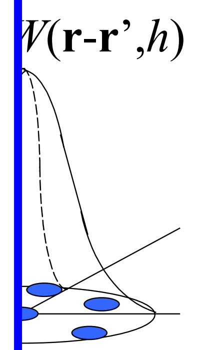
$)\mathrm{d}\mathbf{r}'$

(*W* is the smo…

$)\frac{m_j}{\rho_j}$

- Governing e… approximated… summation

- Boundary co… appear natur…



In going from **continuous** to the **discrete** we have to choose:

(i) Our particle size *dp*

(ii) Ratio of Smoothing length to particle size, *h/dp*

We have to worry about CONVERGENCE

SPH Sources of error

1. Mollification Error
2. Discretisation Error
3. **Summation Error**
4. Others (Equation of State, time stepping, etc.)

SPH ACCURACY

Do you remember the **axioms of SPH**?

Partition of unity

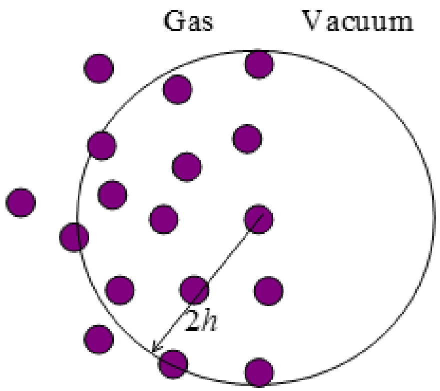
$$(i) \qquad \int_{\Omega} W(\mathbf{r}-\mathbf{r}', h)\, \mathrm{d}\Omega = 1$$

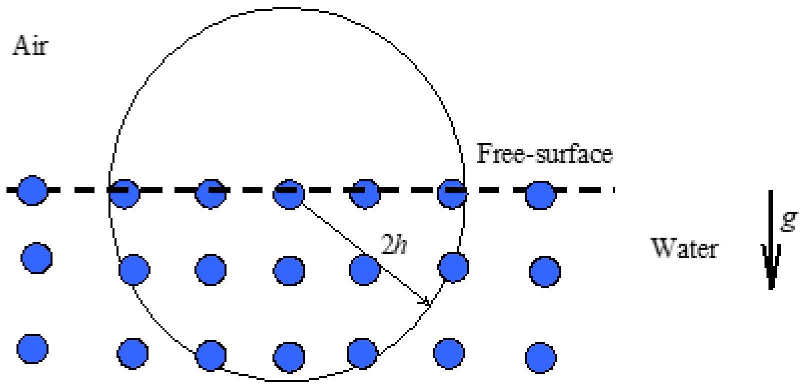
In the discrete domain, this SHOULD be equivalent to:

$$\sum_j W(\mathbf{r}-\mathbf{r}_j, h)\frac{m_j}{\rho_j} = 1$$

I ask you when this is not satisfied and what happens?

Incomplete support





Here are examples of such a case, and of course the accuracy suffers, leading to maybe bad results, or **numerical instability**

ACCURACY OF THE SPH FORMULATION

So, just how accurate is the SPH Calculation??

Let's do some basic analysis.

Here I quote Monaghan (2005) section 2.4, equations (2.35 & 2.36):

Starting with the integral interpolant in one dimension where $A_{\mathrm{I}}(x)$ is the SPH or interpolated value

$$A_{\mathrm{I}}(x) = \int A(x')W(x - x')\,\mathrm{d}x' = A(x) + \int \left(A(x') - A(x)\right)W(x - x')\,\mathrm{d}x'$$

The error can be estimated by a Taylor series expansion of $A(x')$.

SPH ACCURACY

Assuming the kernel is an even (symmetric) function, the interpolant gives:

$$A_I(x) = A(x) + \frac{\sigma h^2}{2} \frac{d^2 A(x)}{d x^2}$$

where σ is a constant depending on the kernel. The integral interpolant, therefore, gives at least a **second-order interpolation O(h^2)**.

And this is BEFORE we discretise and run a simulation. So the order of convergence is generally lower than 2!

(I will return to this later)

SPH Sources of error

1. **Mollification Error**

2. **Discretisation Error**

3. **Summation Error**

4. **Others (Equation of State, time integration)**

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Modelling Fluids with SPH

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SPH for Fluids: Compressible or Incompressible?

So when solving conservation of mass and momentum:

$$\frac{d\rho}{dt} + \rho\nabla \cdot \boldsymbol{u} = 0 \qquad \rho\frac{\boldsymbol{du}}{dt} = -\nabla p + \mu\nabla^2\boldsymbol{u}$$

question is whether to model compressibility present. Two options for near-incompressible fluids:

- **Strict Incompressibility** –easier mathematically but creates PPE matrix

$$\nabla \cdot \boldsymbol{u} = 0 \quad \rightarrow \quad \nabla \cdot \left(\frac{1}{\rho}\nabla p^{n+1}\right)_i = \frac{1}{\delta t}\nabla \cdot \mathbf{u}_i^* \quad \rightarrow \quad \mathbf{AX} = \mathbf{b}$$

- **Weak Compressibility** – more difficult to do accurately with more unknowns, e.g. extra equation linking pressure to density - *an equation of state*:

$$p = f(\rho, T, S, \ldots) \qquad p = \frac{c_o^2 \rho_w}{\gamma}\left(\left(\frac{\rho}{\rho_w}\right)^\gamma - 1\right)$$

- Both have advantages & disadvantages

DualSPHysics uses Weakly compressible SPH (WCSPH), but there are problems with pressure …

$$p = \frac{c_0^2 \rho_0}{\gamma}\left[\left(\frac{\rho}{\rho_0}\right)^7 - 1\right] \rightarrow$$ pressure $p \; \alpha \; \rho^7$

and Accuracy of SPH summation

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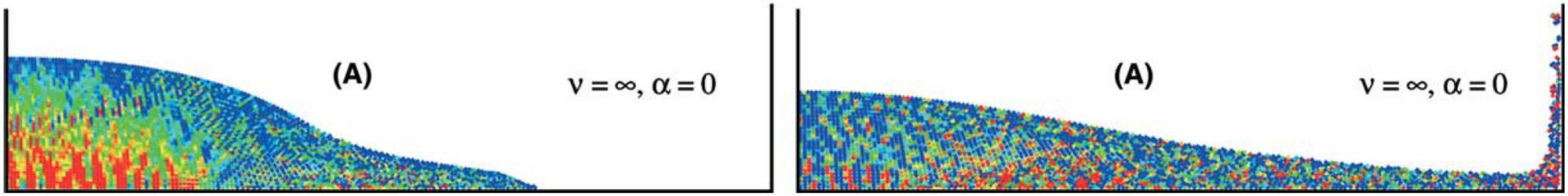
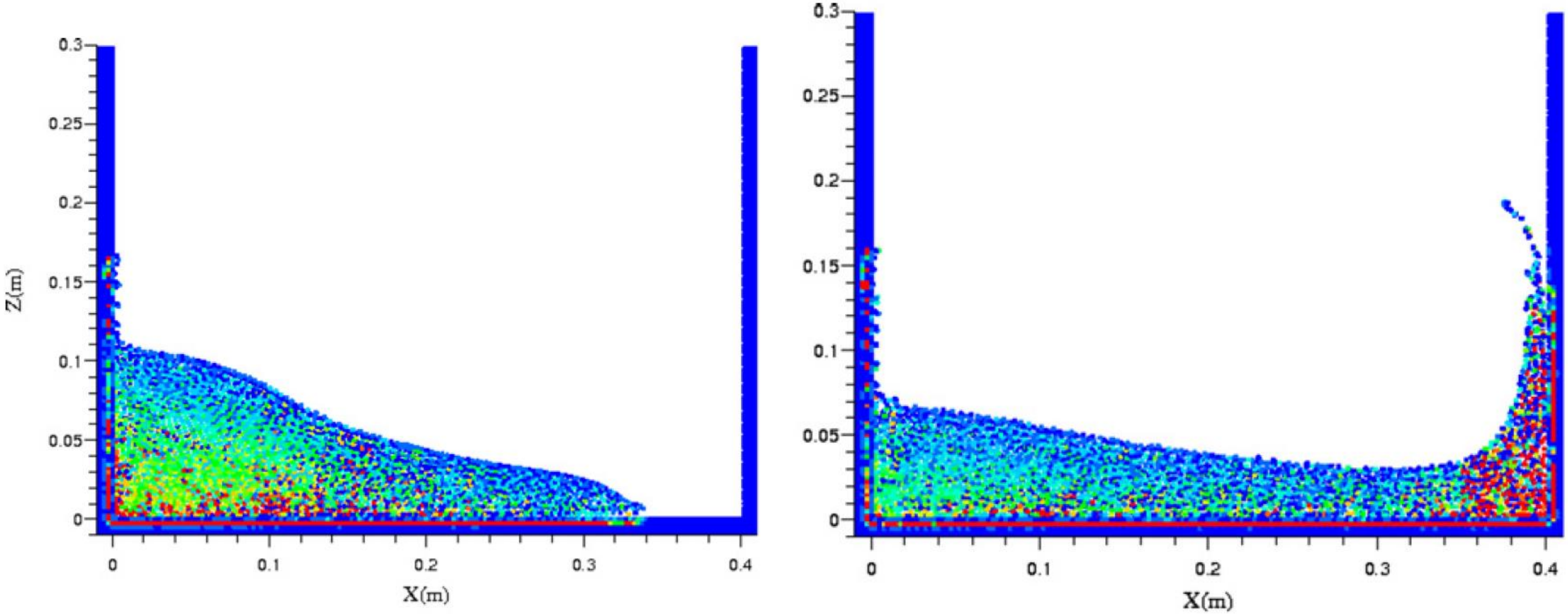
WCSPH Pressure Oscillations & Noise

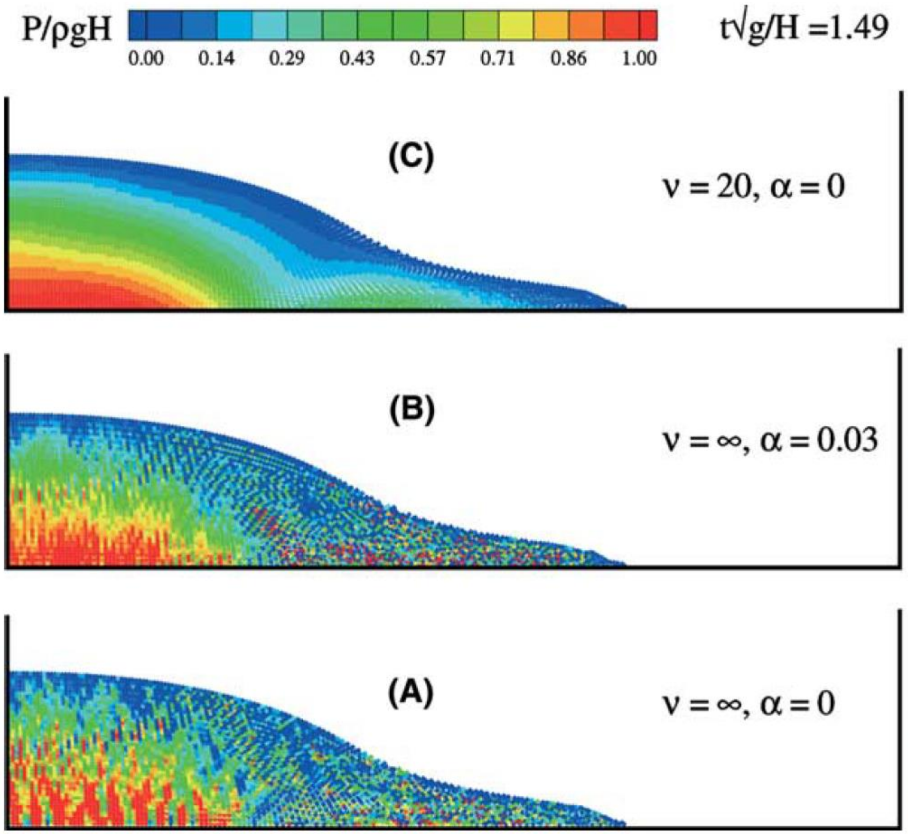


(Colagrossi & Landrini, 2003)

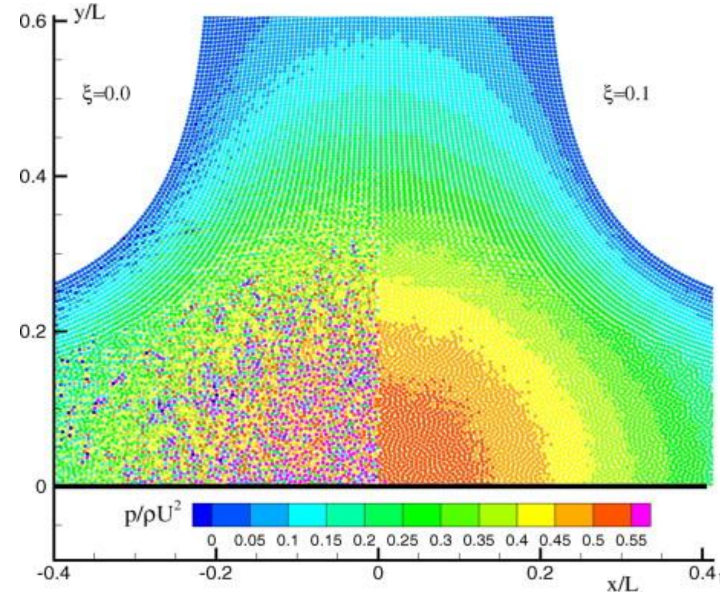


(Lee et al., 2008)

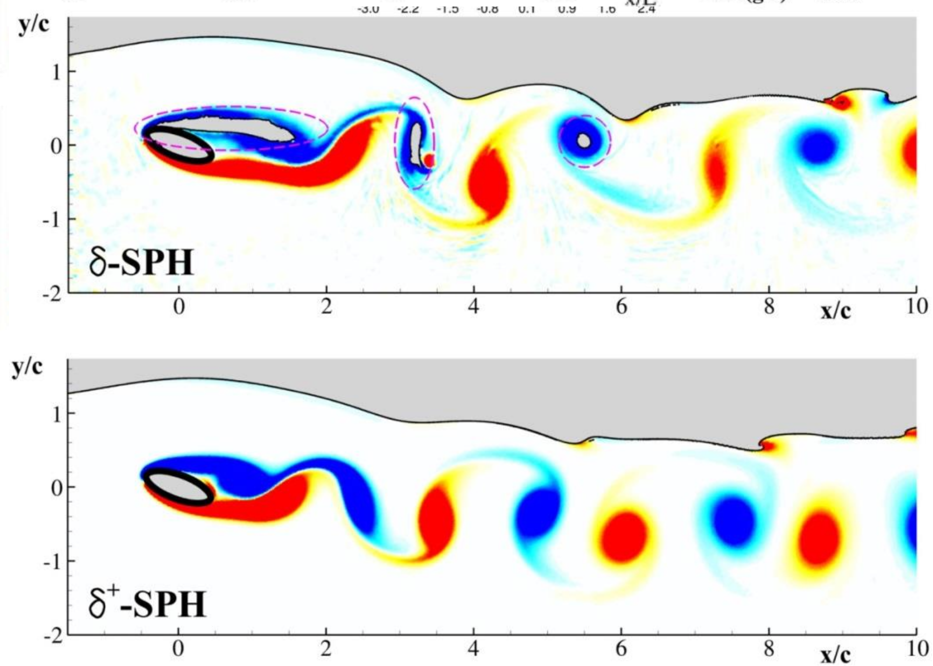
WCSPH with/without extra treatments



With/without Shepard filter & artificial viscosity(Colagrossi & Landrini 2003)



With/without Delta-SPH (Molteni & Colagrossi 2009)



With/without shifting (Sun et al, 2017)

All these problems in SPH on their own might appear simple

They show themselves in particle instabilities (pairing, energy evolution)

Together they are very challenging!

SPHERIC Grand Challenges

What is SPHERIC?

What are the Grand Challenges?

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SPHERIC

International Research Initiative:

https://spheric-sph.org

- Founding members

- Steering Committee

- Webmasters
  BDR: 2005-2015
  AJC: 2015 -

-Chair (2015 - 2020)

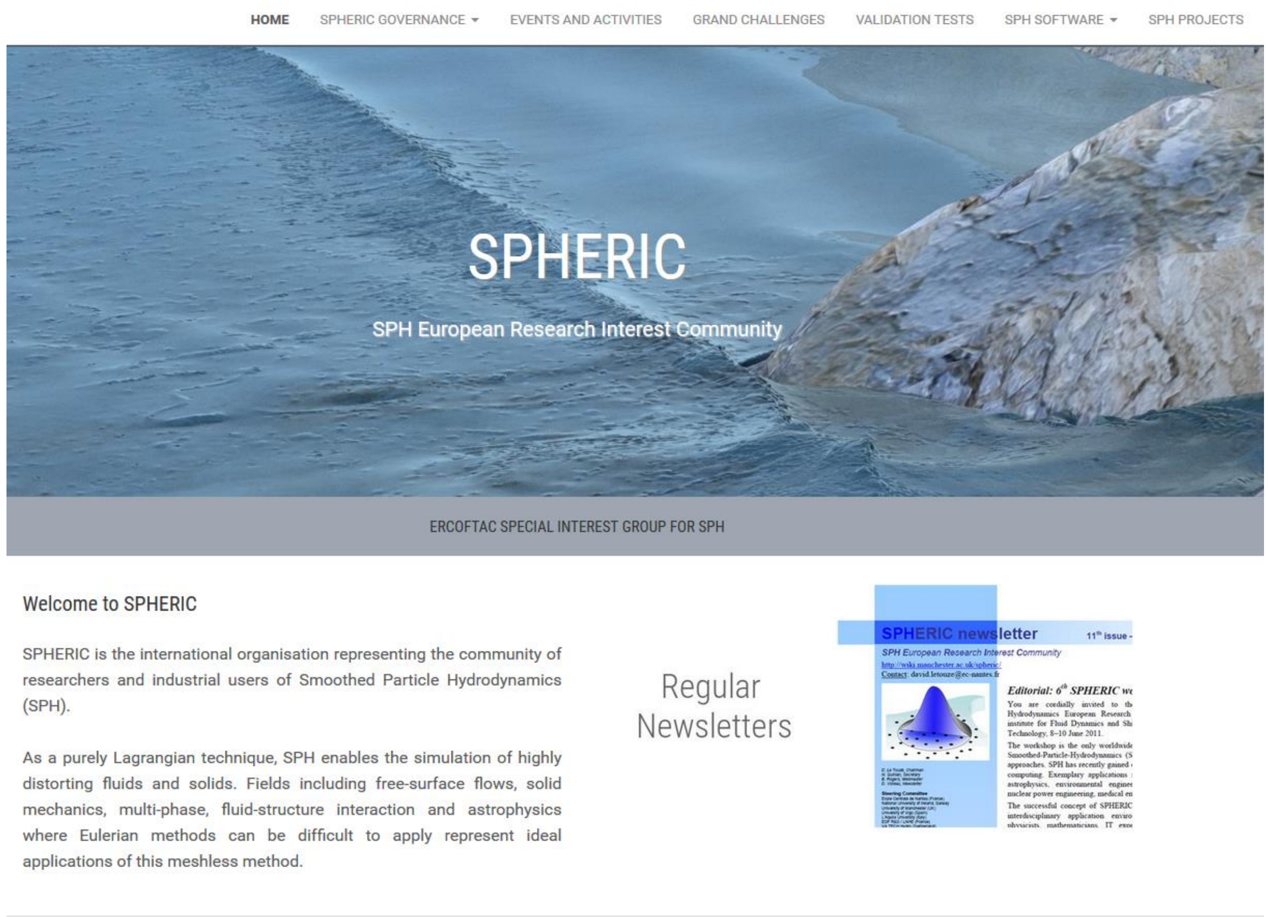
  -13 International Workshops

  -2019 Exeter

  -2020 Harbin

  -2020 NYC

  -Training Day



- 75 Institutions are members: universities, government research labs & industrial companies

Key Issues in SPH: SPHERIC Grand Challenges & then some

1. **GC#1: Convergence, consistency and stability**– this is still in development
2. **GC#2: Boundary conditions** – probably the worst culprit of all problems for free-surface flow
3. **GC#3: Adaptivity** – efficient simulations are key for engineering application
4. **GC#4: Coupling to other models** – taking advantage of the benefits of 2 models
5. **GC#5: Applicability to industry** – industrial engineering applications can be extremely difficult and will remain so for a long time

- **Formulation** for simulation involving many complex physics – SPH is good & bad, the right method: OTHER METHODS?
- **Multi-phase physics**: Phase change
- **Turbulence** – a very difficult topic in its own right is yet to receive comprehensive investigation

SPHERIC Grand Challenges

How is the DualSPHysics Group addressing these Challenges?

GC#1: Stability Shifting – 2009 & 2012

Improved accuracy brings new problems!

- After each time step, particles are shifted slightly to maintain a uniform concentration loosely based on Fick's law of diffusion

$$\delta \mathbf{r}_s = -D' \nabla C$$

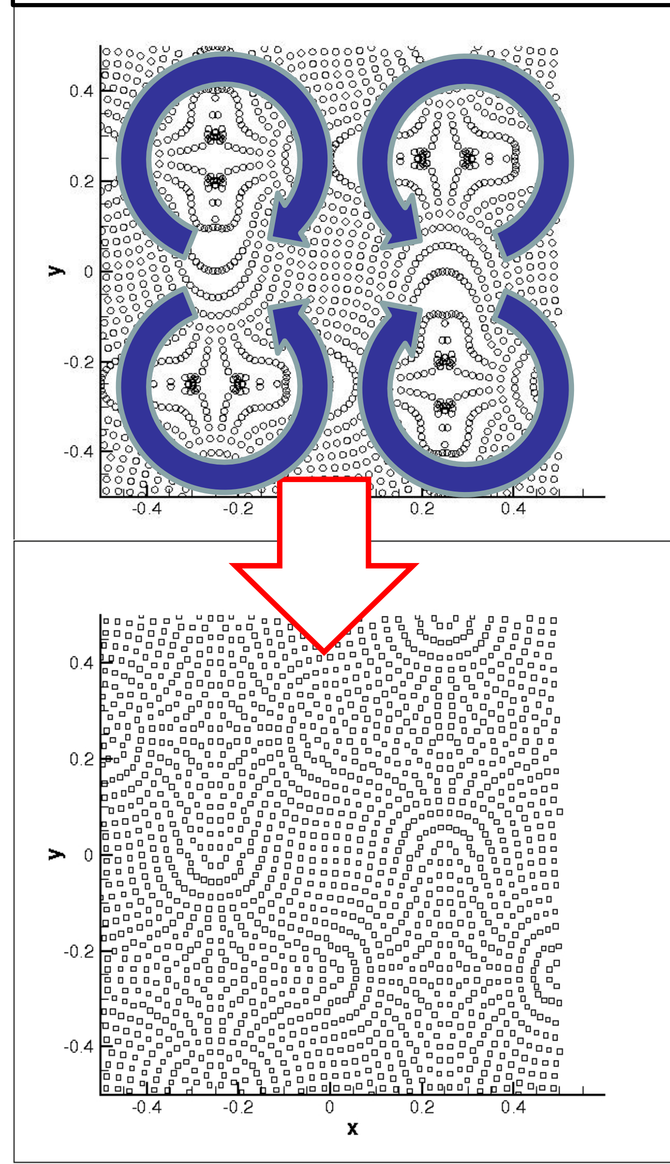
- Shifted particle velocities are corrected by interpolation

- Stable accurate solution (with no artificial viscosity as commonly used in WCSPH)

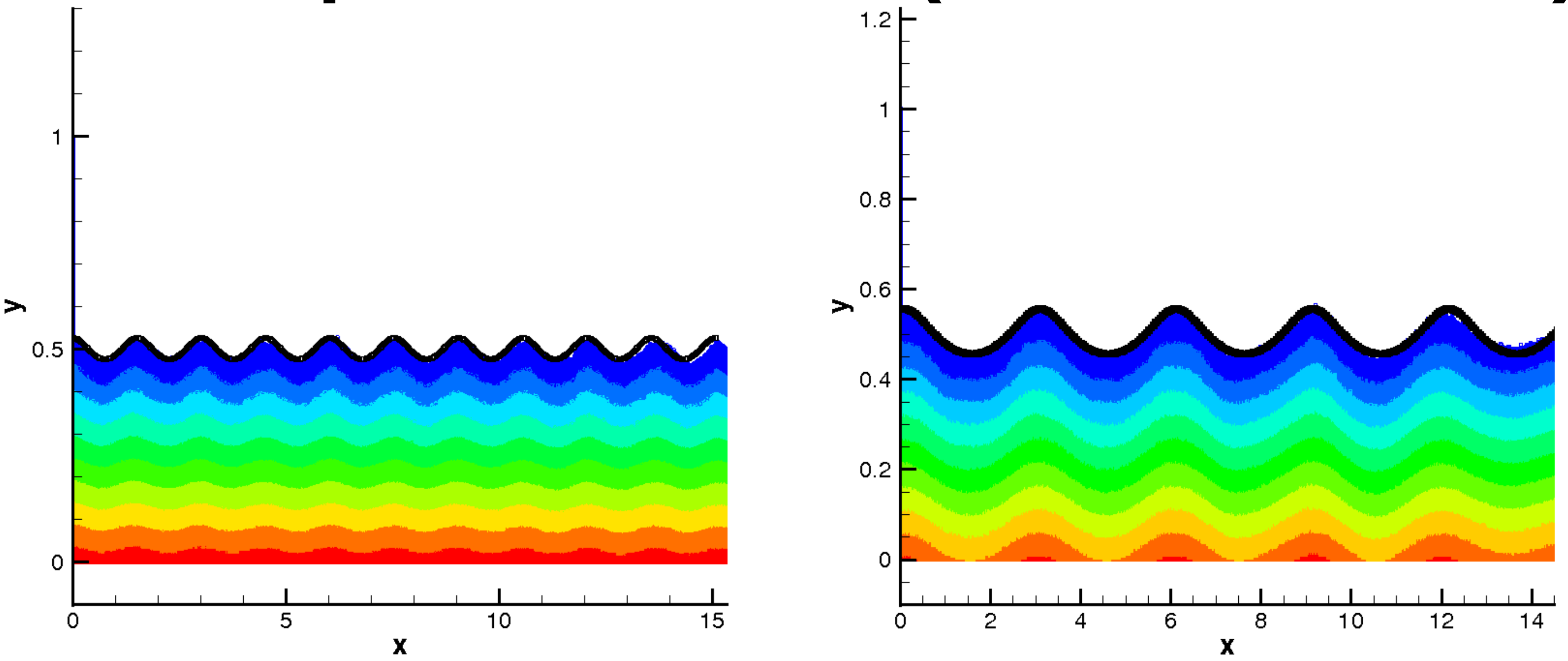
- Near free surface diffusion rates are restricted normal to the free surface (n)

$$\delta \mathbf{r}_s = -\mathcal{D}\left(\frac{\partial C}{\partial s}\mathbf{s} + \alpha\left(\frac{\partial C}{\partial n} - \beta\right)\mathbf{n}\right)$$

Taylor-Green Counter Rotating Vortices



Improvement in wave propagation using Incompressible SPH (Lind *et al*. 2012)



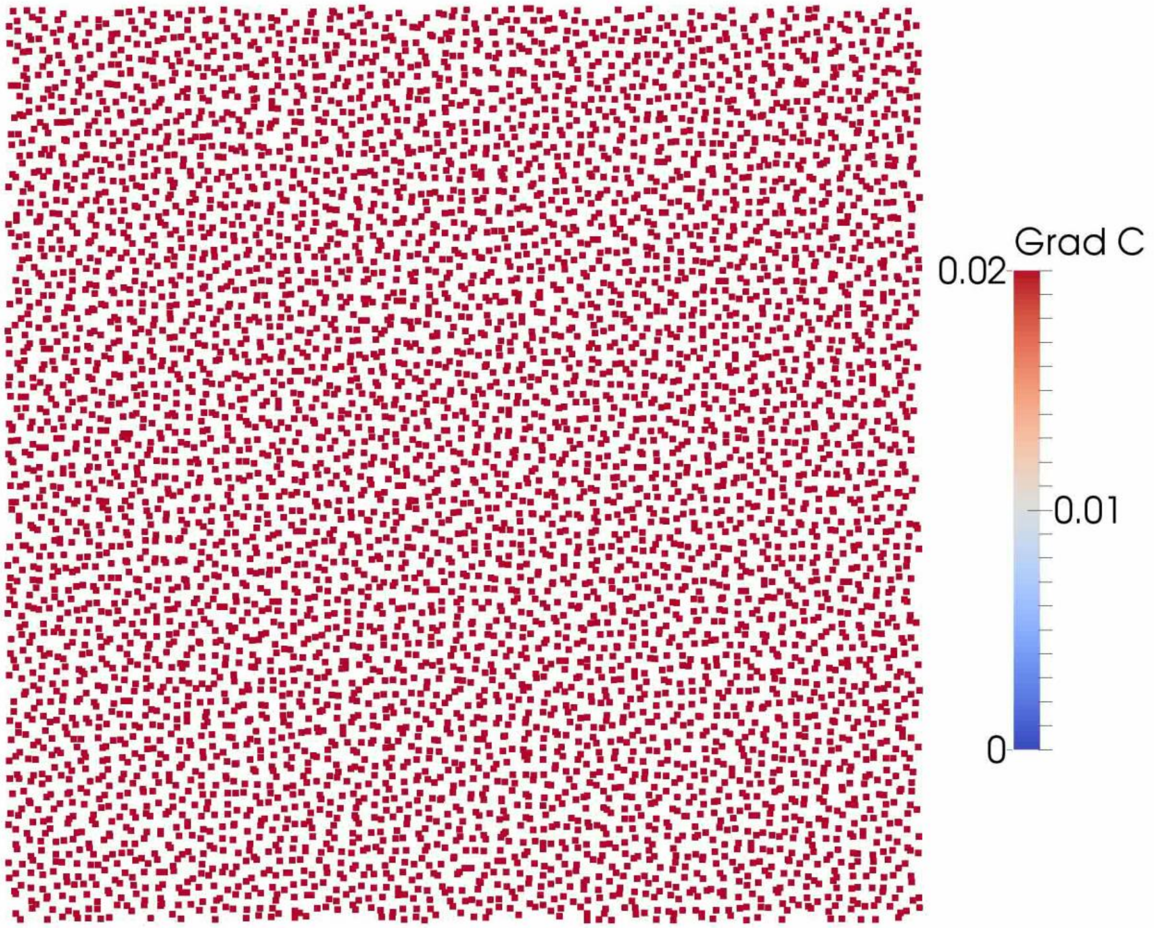
Comparison of wave propagation along a channel (including pressure contours) with free-surface predictions of SAWW (bold black line).
(a) Wave height *H = 0.05m at t = 19.5s. (b) Wave height H = 0.1m at t = 9.75s.*

As we saw WCSPH would struggle to do this.

Improved Formulations: Iterative shifting

→ GC#1: Convergence, consistency and stability

Vacondio et al. (2017)



GC#5: Application to Industry

The need for :

- **Multi-Phase Modelling**
- **Variable resolution → GC#3: Adaptivity**
- **Coupling → GC#4: Coupling**

Multi-Phase SPH

Mokos *et al*. (2015, 2017) : WATER + GAS

Fourtakas & Rogers (2016) : WATER + SEDIMENT

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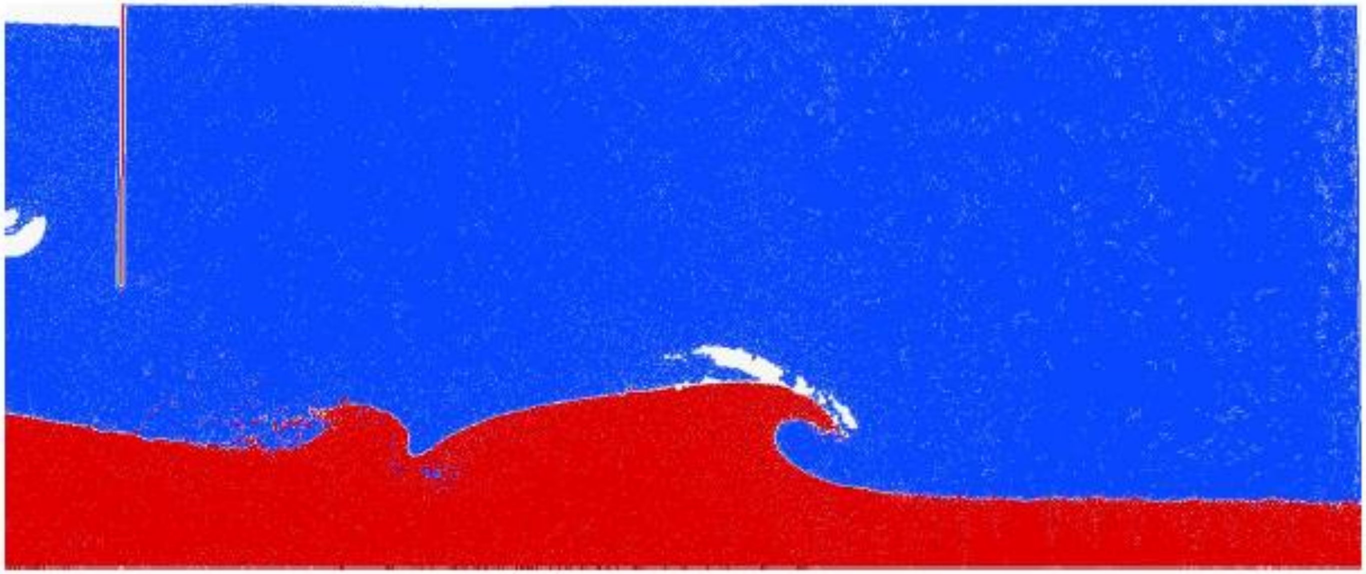
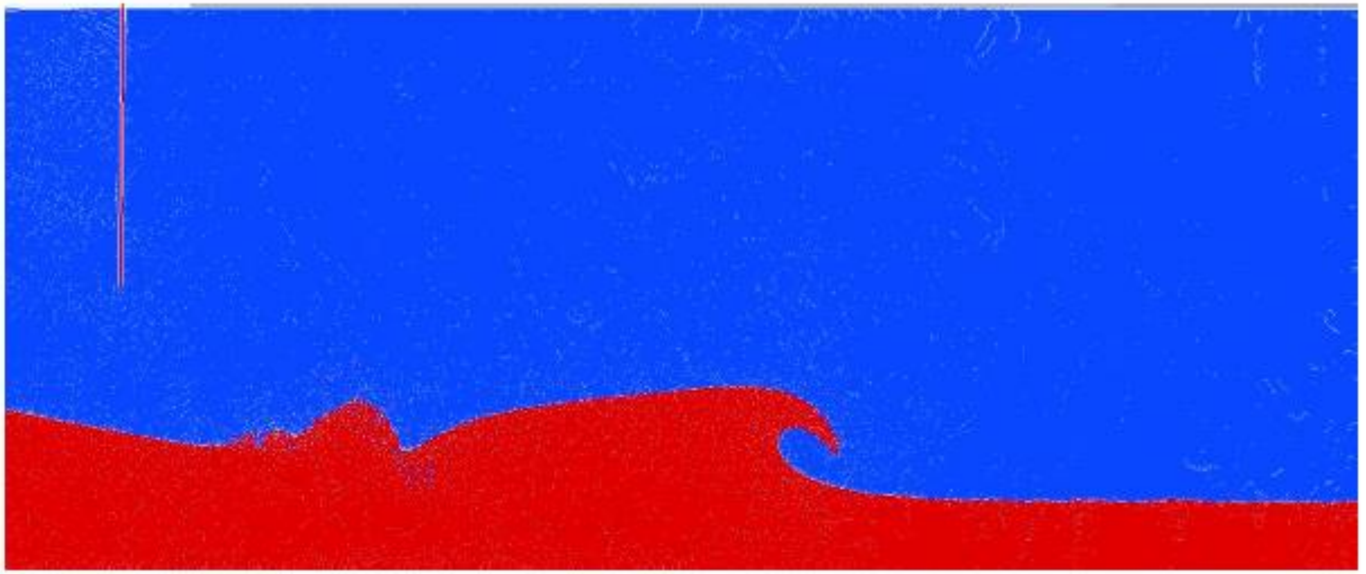
Wet Dam Break

Original multi-phase model



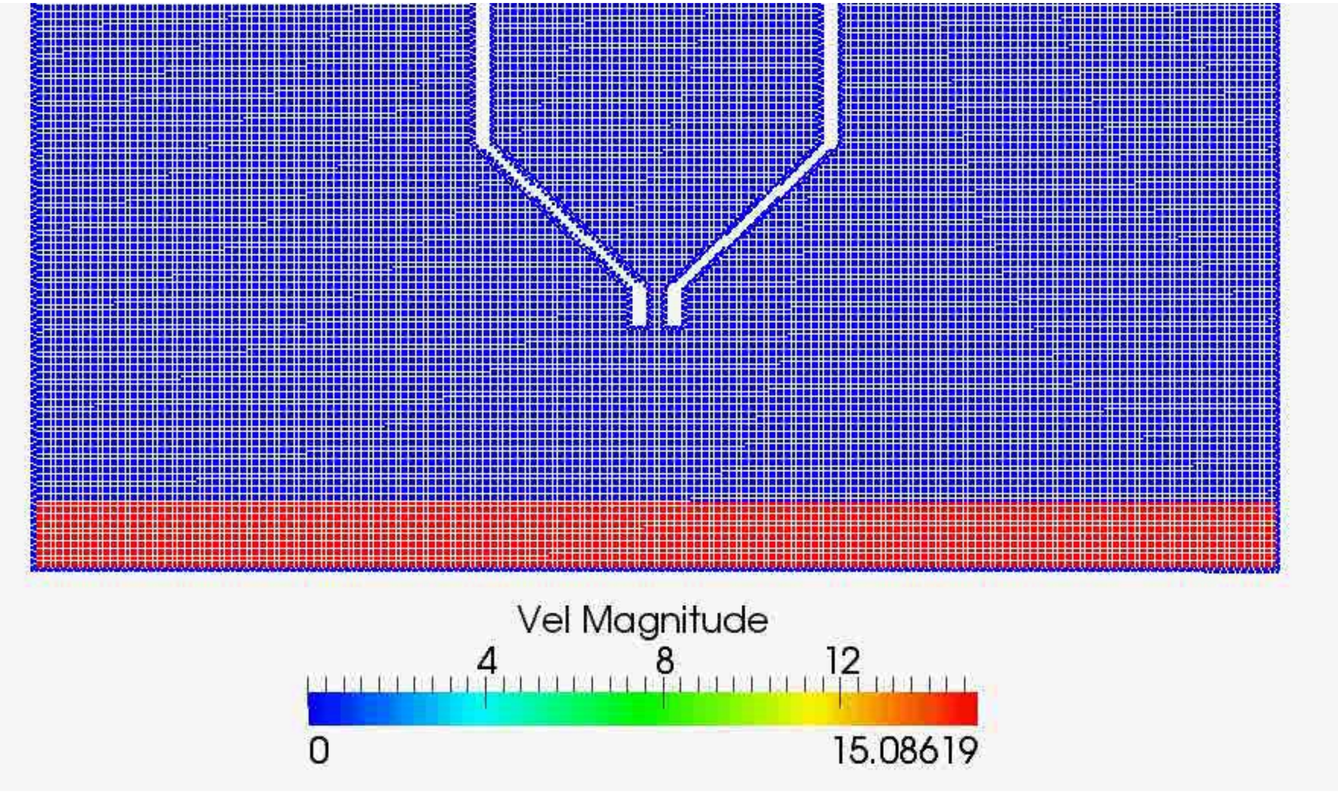
Multi-phase shifting



Nuclear Applications: mixing

Submerged jet impinging on sediment

- Configuration
  - $\rho_s = 1.54\ \rho_w$
  - $\mu_s^{cr} = 5x10^3\ \mu_w$
  - Cohesive sediment
  - 60 000 particles



Fourtakas & Rogers (2016), Advances Water Resources

Efficient SPH simulations

Dynamically varying the particle size

Vacondio et al. (2013, 2016) CMAME

→ **GC#3: Adaptivity**

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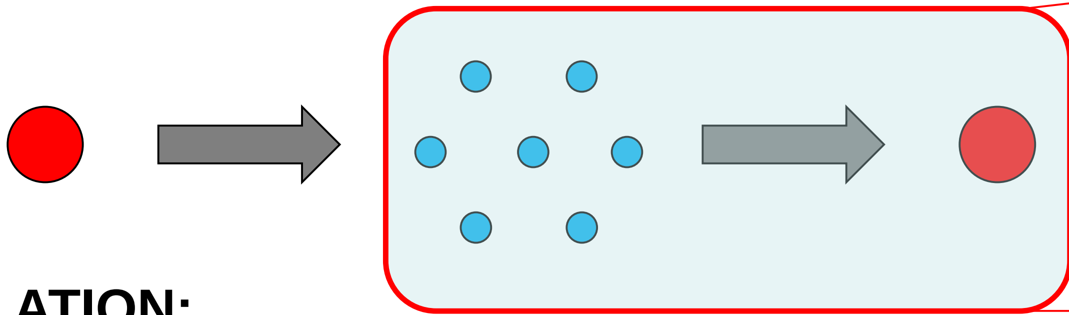
Dynamic Particle Refinement



Parma & Manchester were the first to propose a solution to this problem

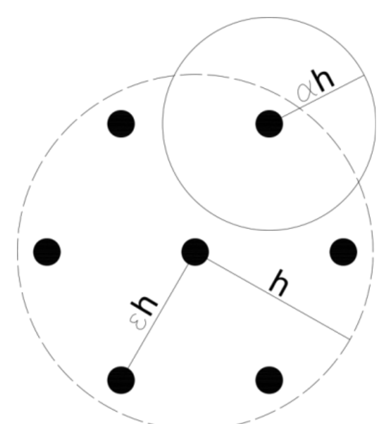
FORMULATION:

- Particle splitting and coalescing procedures for Navier-Stokes equations
- WCSPH <u>variationally consistent</u> scheme with *h*-variable
- New smoothing length h_M is obtained by **enforcing zero density error**

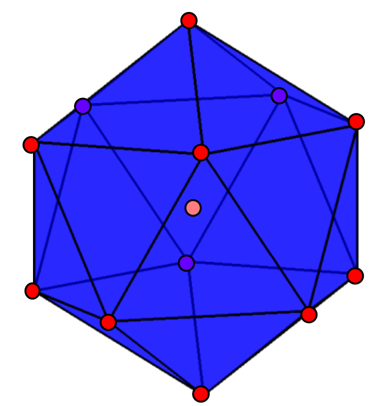
Particle Splitting: Optimal splitting patterns

(Vacondio et al. 2013, 2016)

2D: Hexagon



3D: Icosahedron

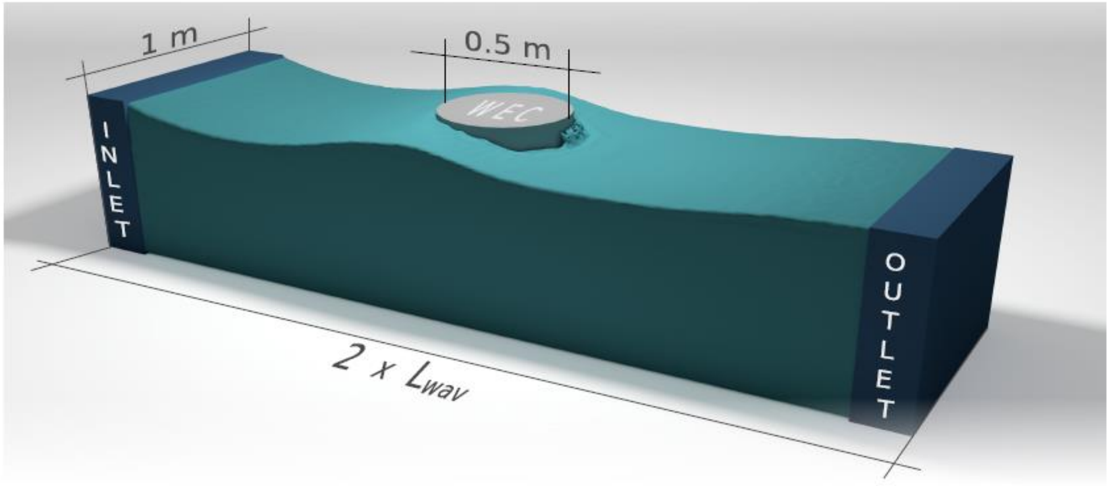


GC#4: Coupling

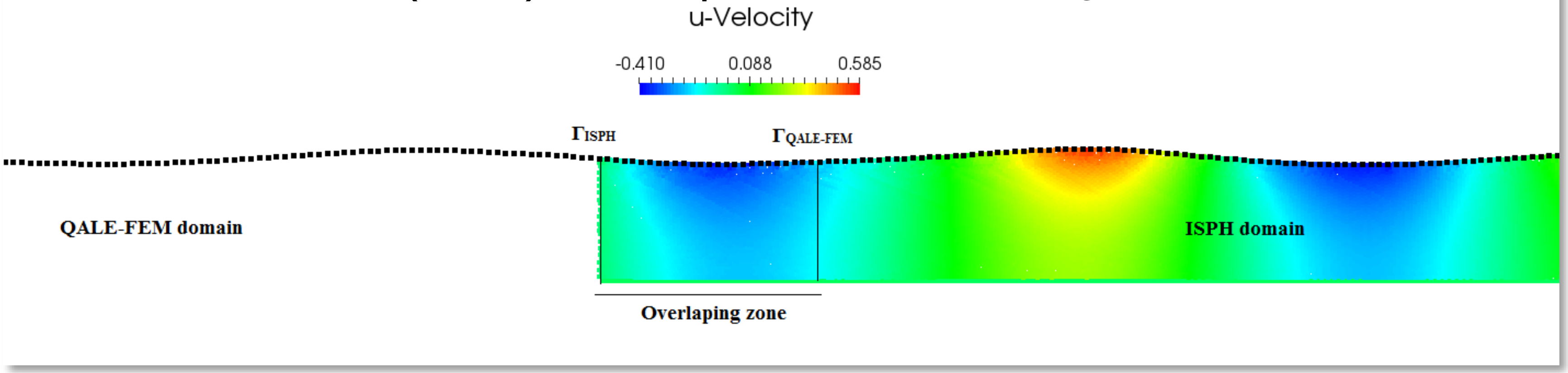
Verbrugghe et al. (2018):

DualSPHysics + OceanWave3D

see also Altomare et al. (2018)



Fourtakas et al. (2018): Incompressible SPH + QALE-FEM



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Coupling – Assessment?

Some good work has been achieved, BUT

The main problem is that there is no general methodology for coupling.

Why?

Mainly because coupling depends on the boundary conditions which are an open problem

Improved formulations …

Improved formulations: Incompressible SPH

Incompressible SPH (ISPH) accelerated on a GPU

Chow et al. (2018) CPC

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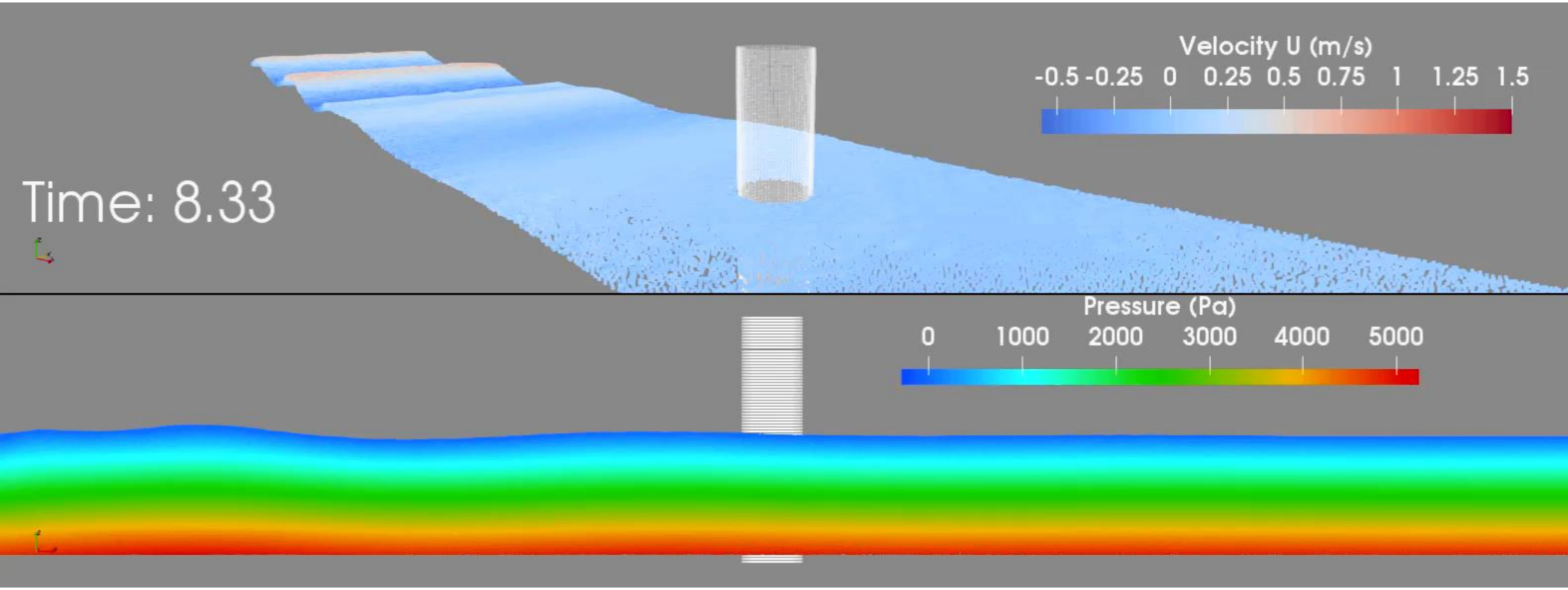
Focused wave group breaking on cylinder

$$F15 : H = 0.22\ m, f_p = 0.82\ Hz\ \textit{(Breaking)}$$

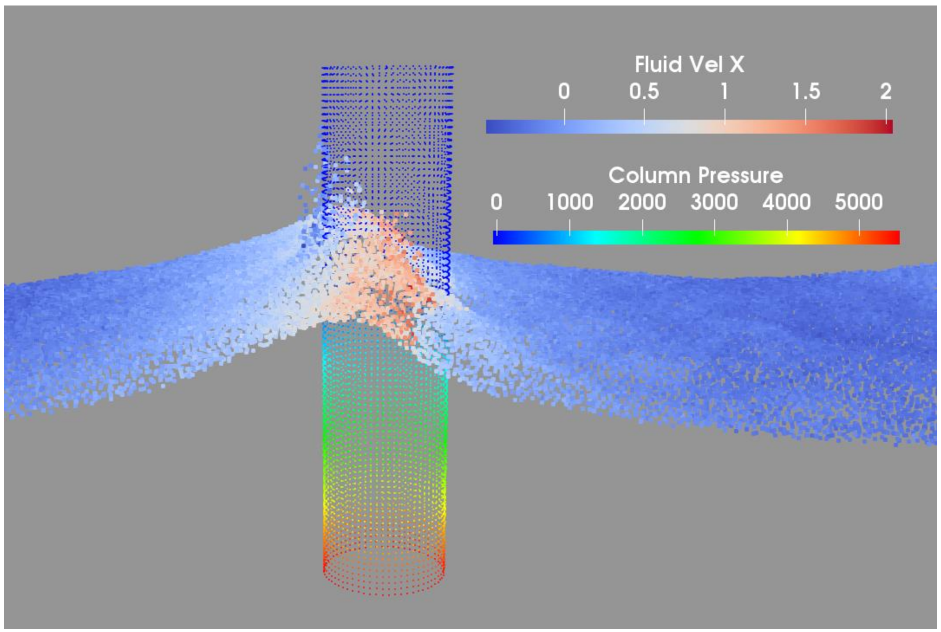


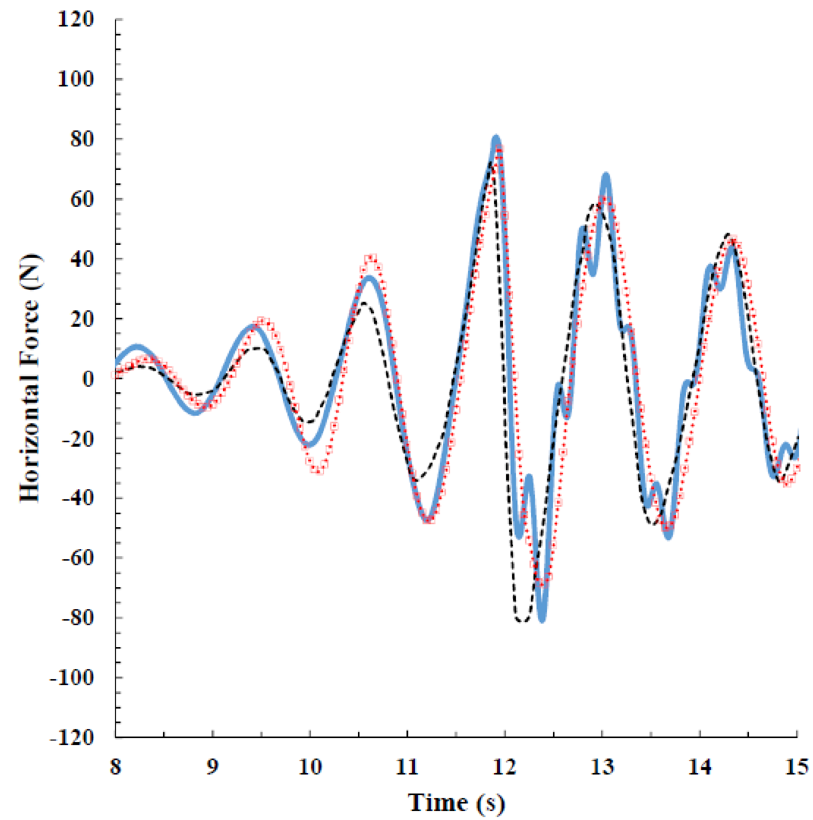
Pressure field is NOISE-FREE

GPU acceleration gives speedups of 20-30 over single CPU

Horizontal force on column data extraction

$$F_x = \sum_i P_i dp^2 \frac{(x_c - x_i)}{\sqrt{(x_c + x_i)^2 + (y_c - y_i)^2}} \qquad column\ centre = (x_c, y_c)$$





(c) F14: $f_p = 0.82$ Hz, $H = 0.14$ m (breaking)

Experiment — Lind et al. — ISPH on the GPU

SPH high-order accuracy

Nasar et al. (2018) SPHERIC Galway

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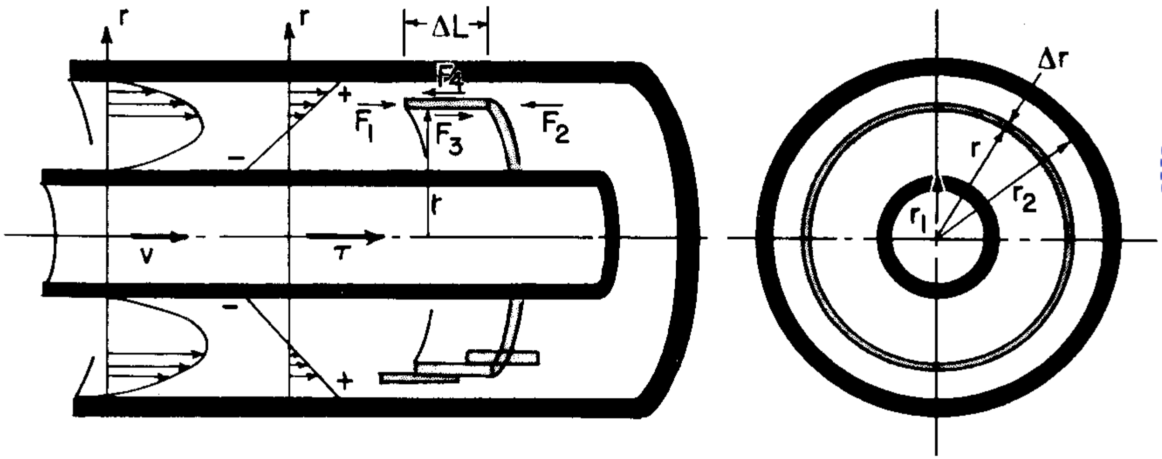
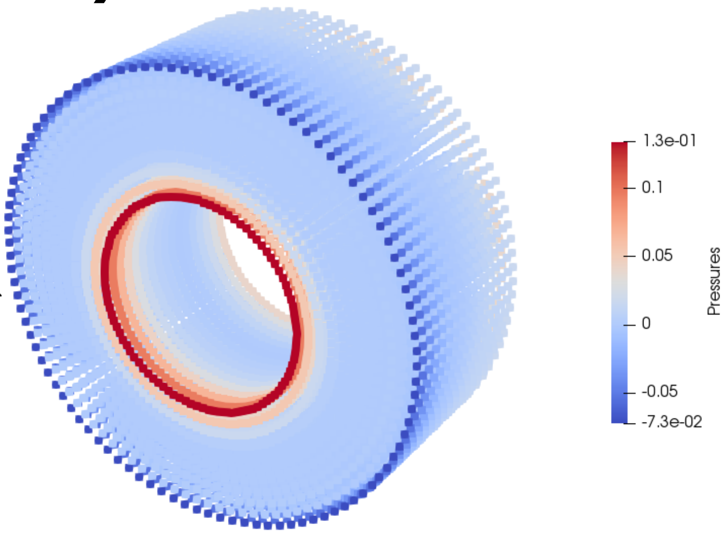
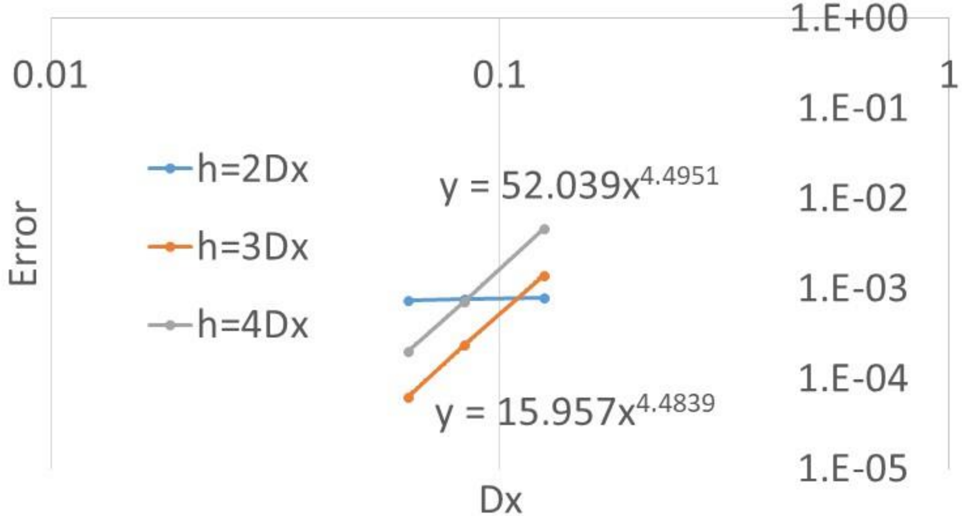
Eulerian ISPH for HIGH-ORDER CONVERGENCE (Nasar *et al.* 2018)

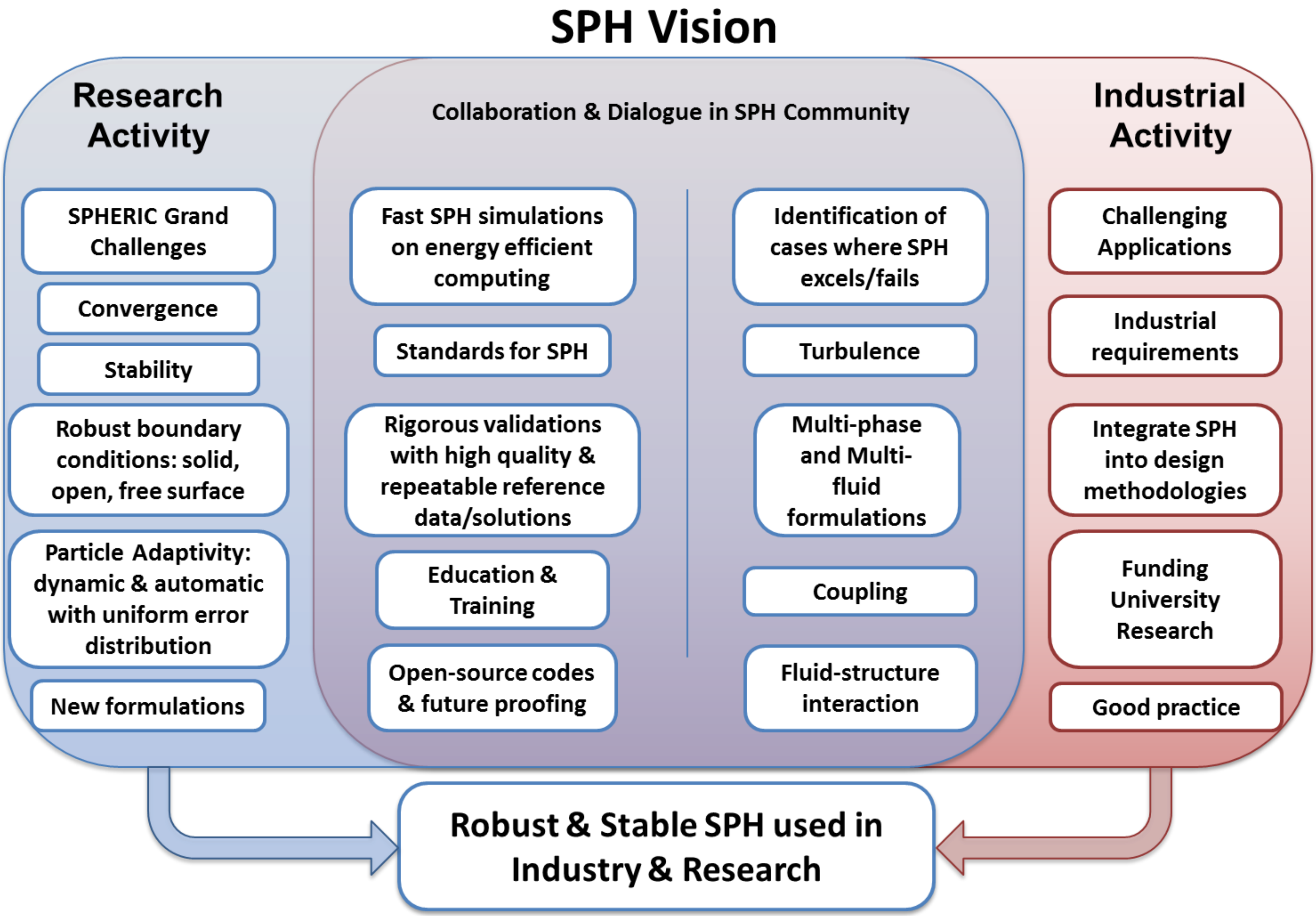




Convergence study for kernel interpolations with wall BC extrapolation but analytical solution for fluid;
Error=$L_2^{norm\ (Fluid\ only)}$

4^{th} to 5^{th}-order convergence!!!





Violeau & Rogers (2016), “SPH for free-surface flow: past, present and future”, *Journal of Hydraulic Research.*

Conclusions

- Huge number of applications: large to small scale
- There are lots of very difficult elements to SPH which prevent quick progress
- Developing DualSPHysics is NOT EASY (and I haven't discussed coding!!)
- SPHERIC & Future challenges
- The DualSPHysics project is working hard both to open the door of accessibility but also trying to solve some of the hardest challenges in CFD right now.

Thank you

Acknowledgments

- U-Man: Peter Stansby, Steve Lind, George Fourtakas, Abouzied Nasar
- U-Vigo: Alex Crespo, Jose Dominguez, Moncho Gomez-Gesteira
- U-Parma: Renato Vacondio FHR: Corrado Altomare

Websites

- Free open-source
- **SPHysics** codes:

http://www.sphysics.org

http://www.dual.sphysics.org

SPH@Manchester https://sph-manchester.weebly.com

@SPH_Manchester

International SPH organisation:

SPH research and engineering international community = SPHERIC

http://spheric-sph.org

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