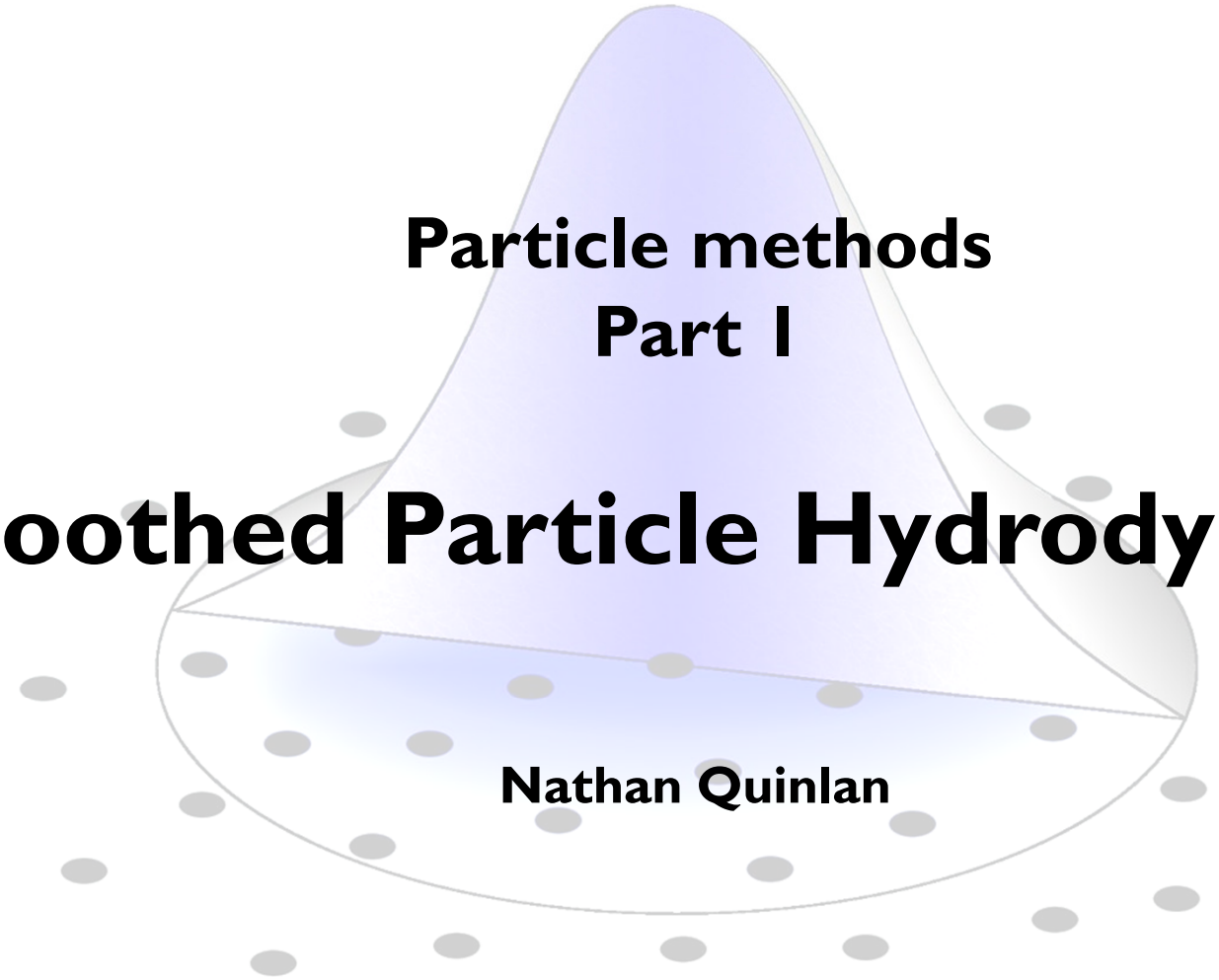


## Particle methods
## Part I

# Smoothed Particle Hydrodynamics

**Nathan Quinlan**

Mechanical Engineering

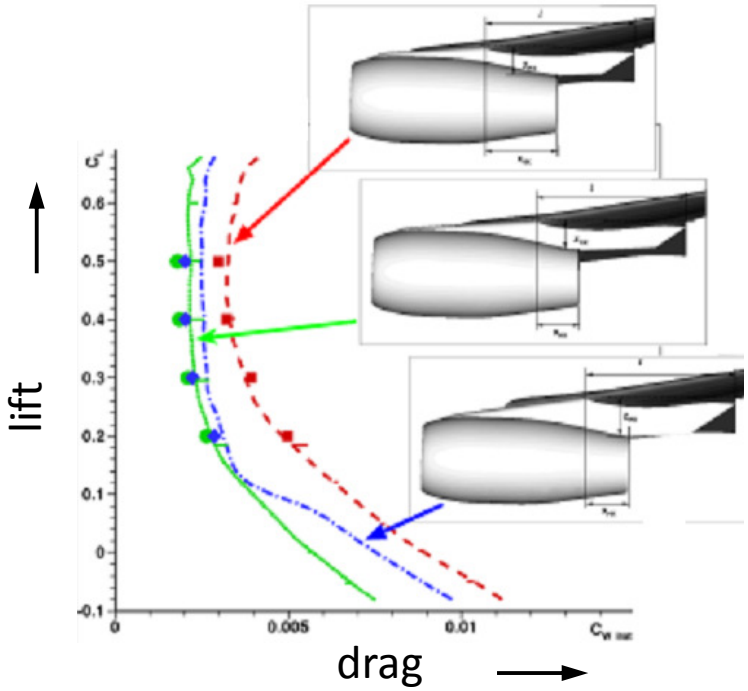
NUI Galway
OÉ Gaillimh

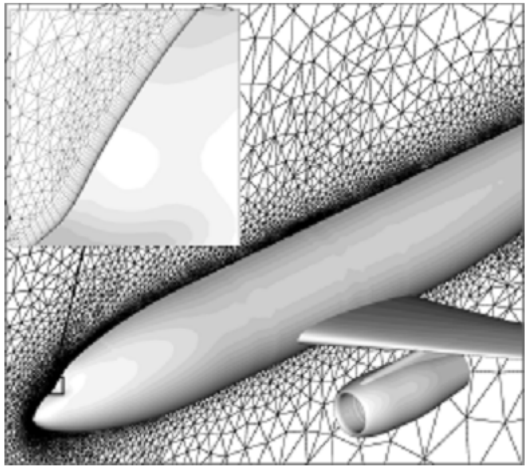
1: SPH

2: Truncation error and consistency of particle methods

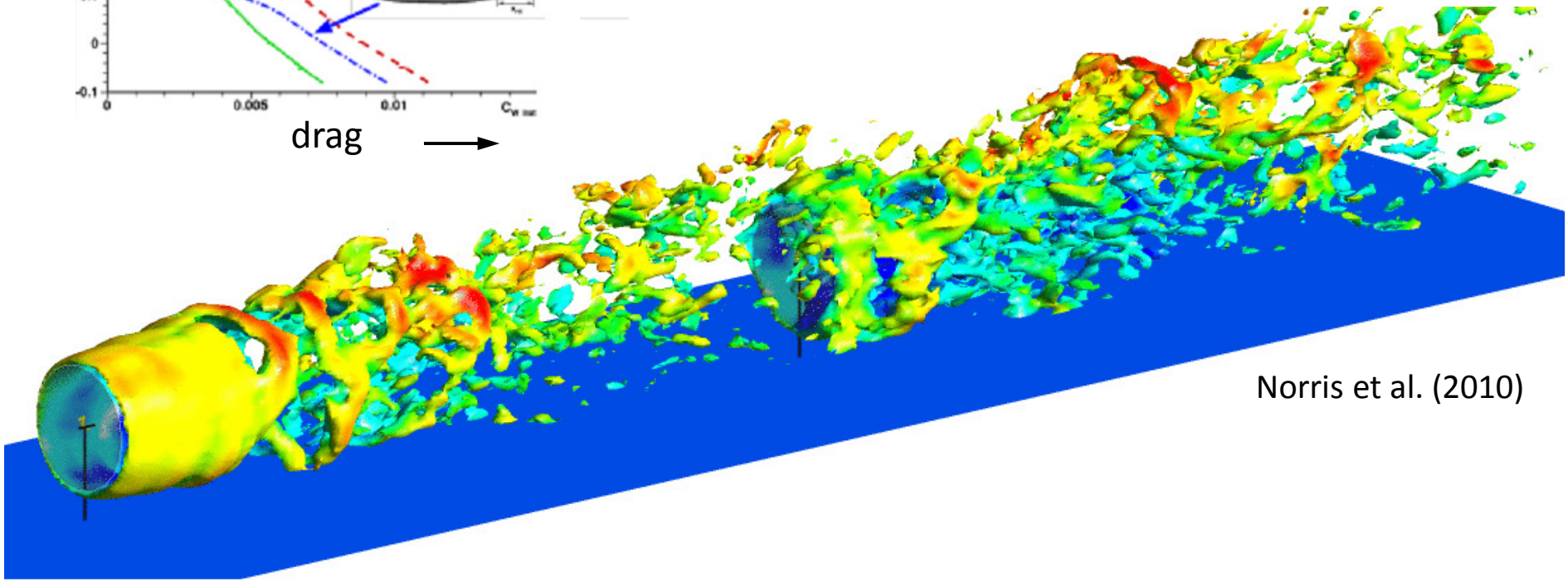
3: FVPM

# CFD is mature



Kroll et al. (2002)

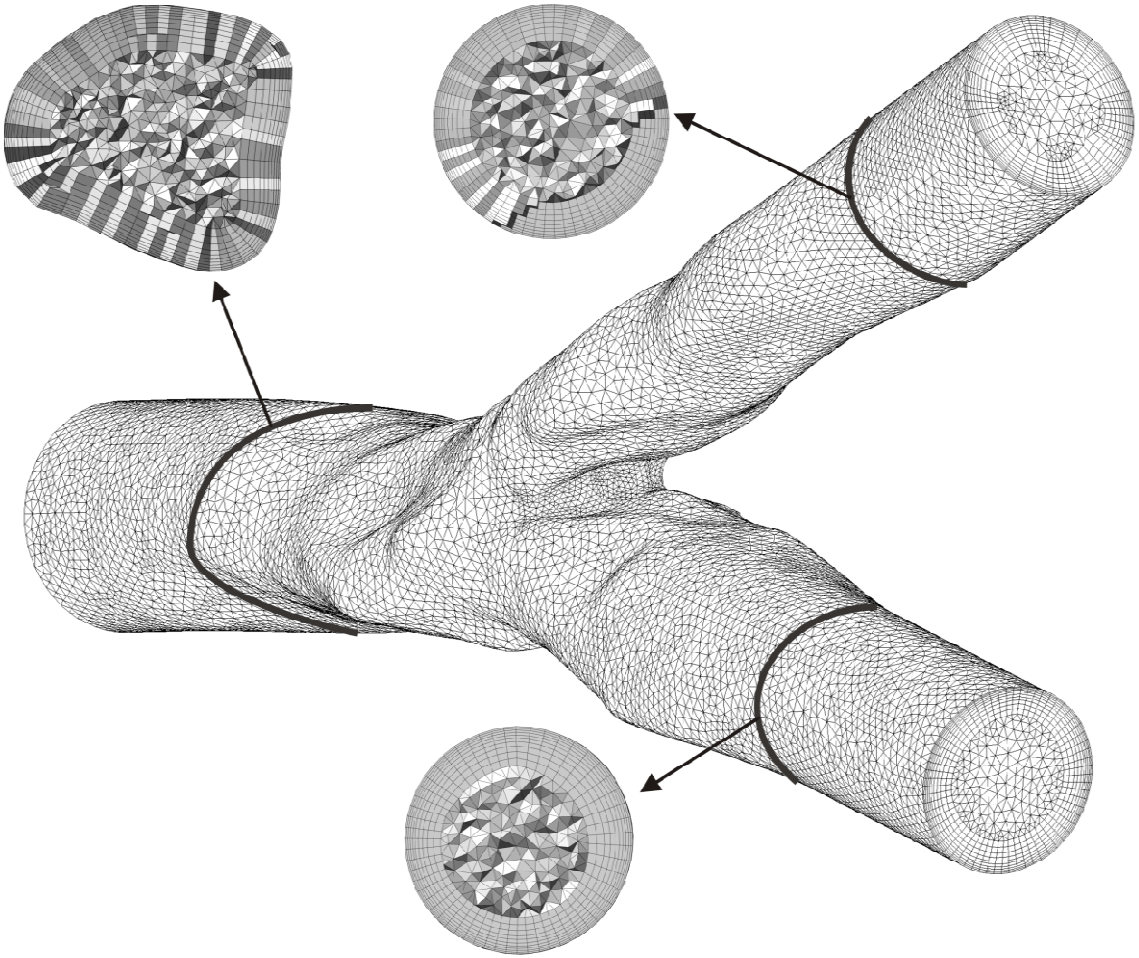


Norris et al. (2010)

# CFD is mature

Images from Scaled Composites

# Classical CFD isn't perfect

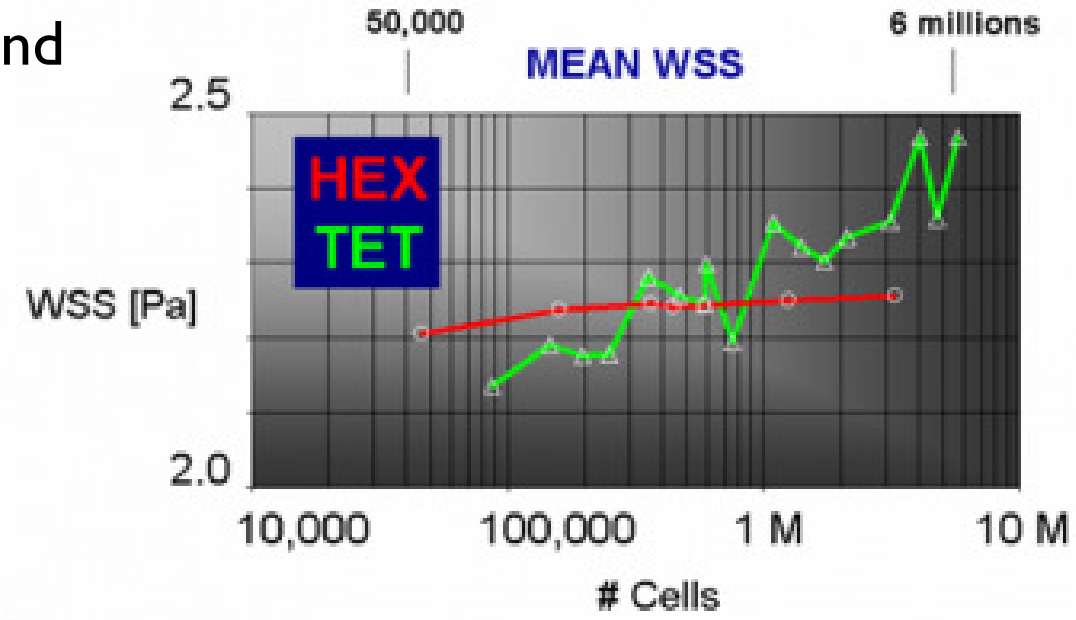


Geometry modelling and mesh generation is a slow, skilled task.

Heraty (2010)

# Classical CFD isn't perfect

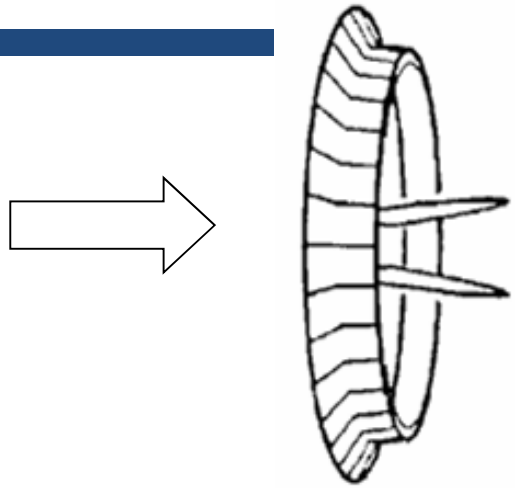
Results are mesh-sensitive and sometimes operator-dependent.

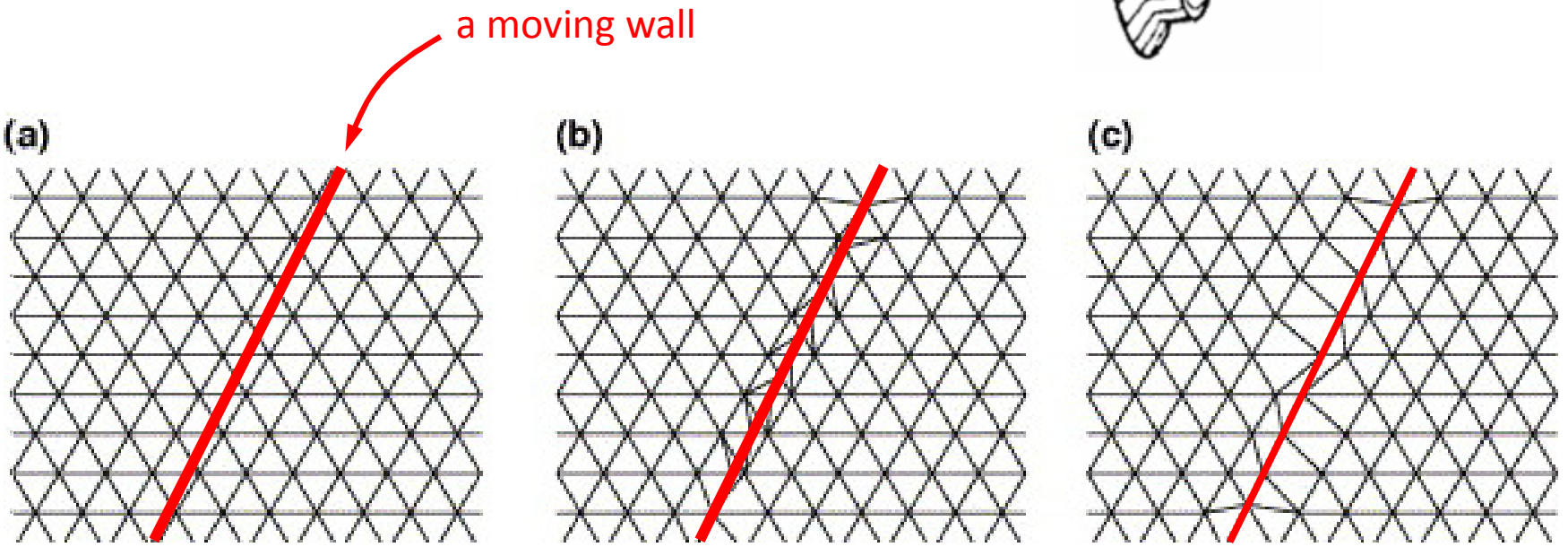



De Santis *et al*. (2010) Med. Biol. Eng. Comput.

# CFD isn't perfect

The mesh paradigm is not natural for moving walls.

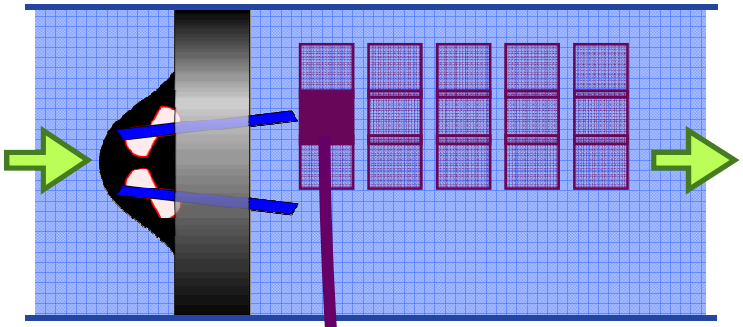




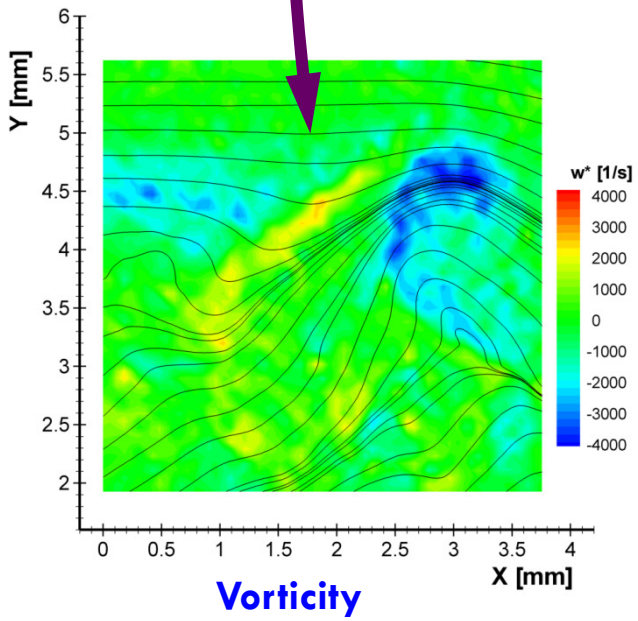

Van Loon *et al*. (2006) J. Comp. Phys.

# My motivation

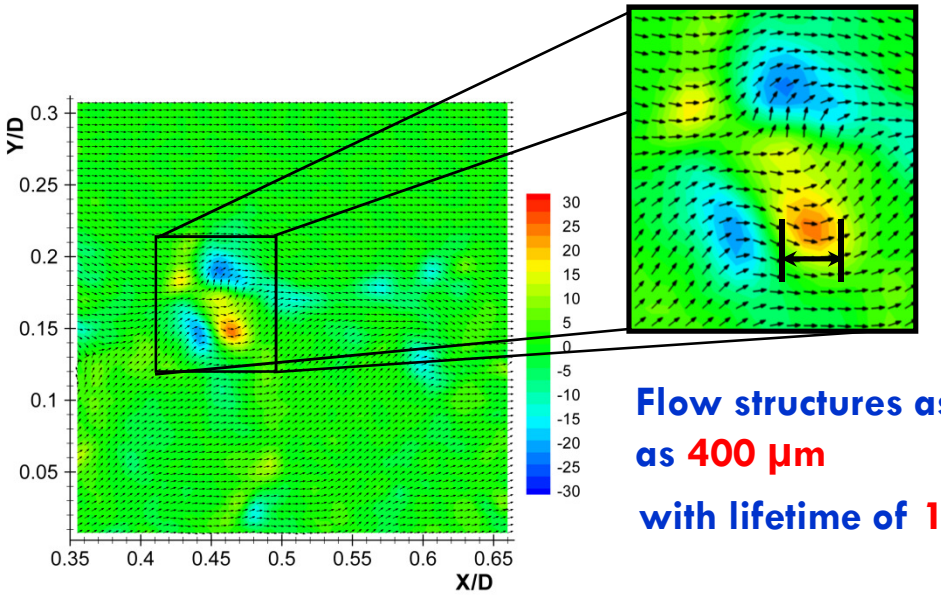
(Artificial) heart valves



flow




Vorticity




Flow structures as small as 400 µm with lifetime of 11 ms

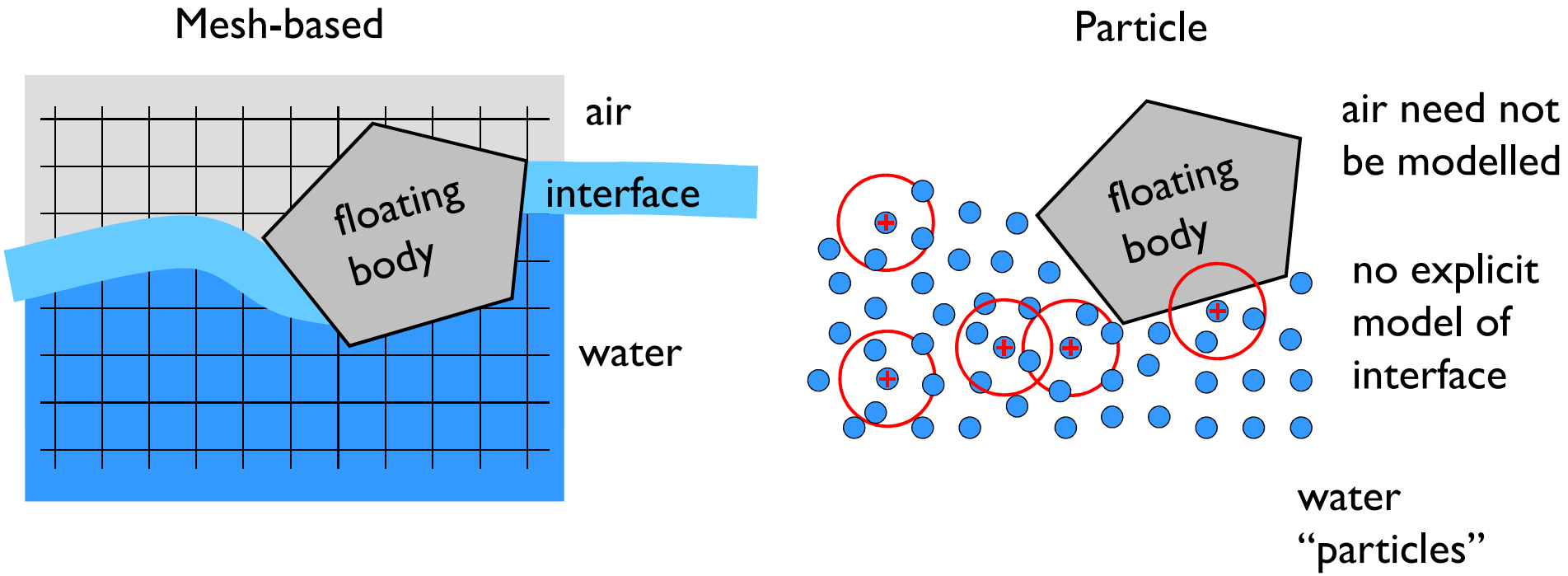
Bellofiore et al. (2011)

# My motivation

Aerosol generation

Aerogen

# The particle alternative



# What we want in a CFD method

- **mathematically** accurate and robust

  **consistency**
  **stability**
  **convergence**
  **conservation**

- **practically** accurate and robust

  **validation**

- walls, inlets and outlets
- free surfaces and phase interfaces
- non-uniform resolution
- adaptive resolution

# Smoothed Particle Hydrodynamics (SPH)

Astrophysics: 1977→

Monaghan and Gingold (1977), Lucy (1977)

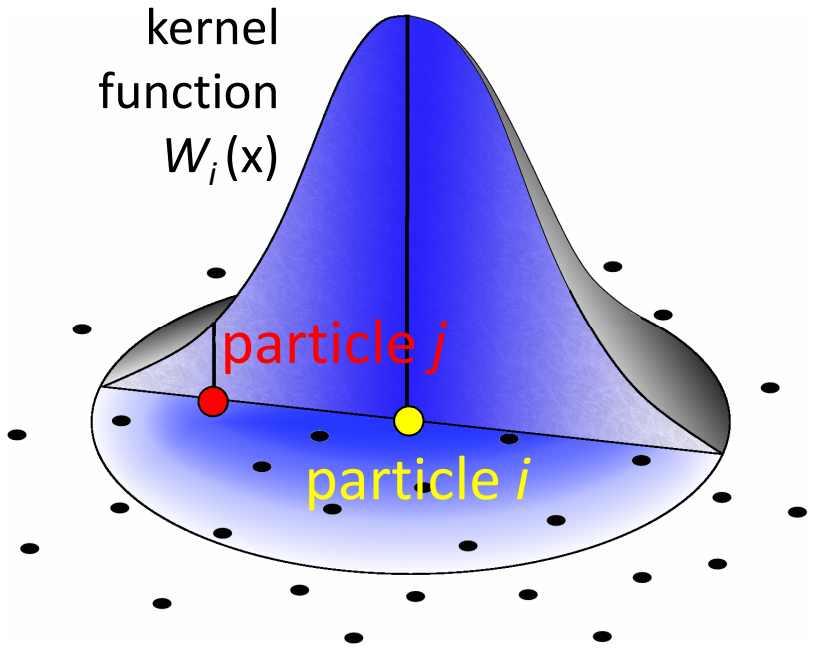
Solid Mechanics: c. 1990→

Libersky & Petshcek (1991)

Water waves: 1992→

Monaghan (1992)

Biomechanics: 2009→ in progress




A gradient at particle *i* is approximated using data at its neighbours.

$$\nabla\phi(\mathbf{x}_i) \cong \sum_j \phi(\mathbf{x}_j)\nabla W_i(\mathbf{x}_j)V_j$$

(a strong finite difference scheme)

Computational particles move with the flowing material (Lagrangian).

# Statement of the problem

Compressible Euler equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad \frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho \nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\rho} \nabla p = 0 \qquad \frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} + \frac{1}{\rho} \nabla p = 0$$

$$\frac{\partial}{\partial t} \begin{bmatrix} \rho \\ \rho u \\ \rho v \end{bmatrix} + \nabla \cdot \begin{bmatrix} \rho u & \rho v \\ \rho u^2 + p & \rho uv \\ \rho uv & \rho v^2 + p \end{bmatrix} = 0$$

A numerical method deals with solutions at a finite number of points $\mathbf{x}_i$.

We must approximate gradients (derivatives) based on those discrete values.

# The weak and the strong

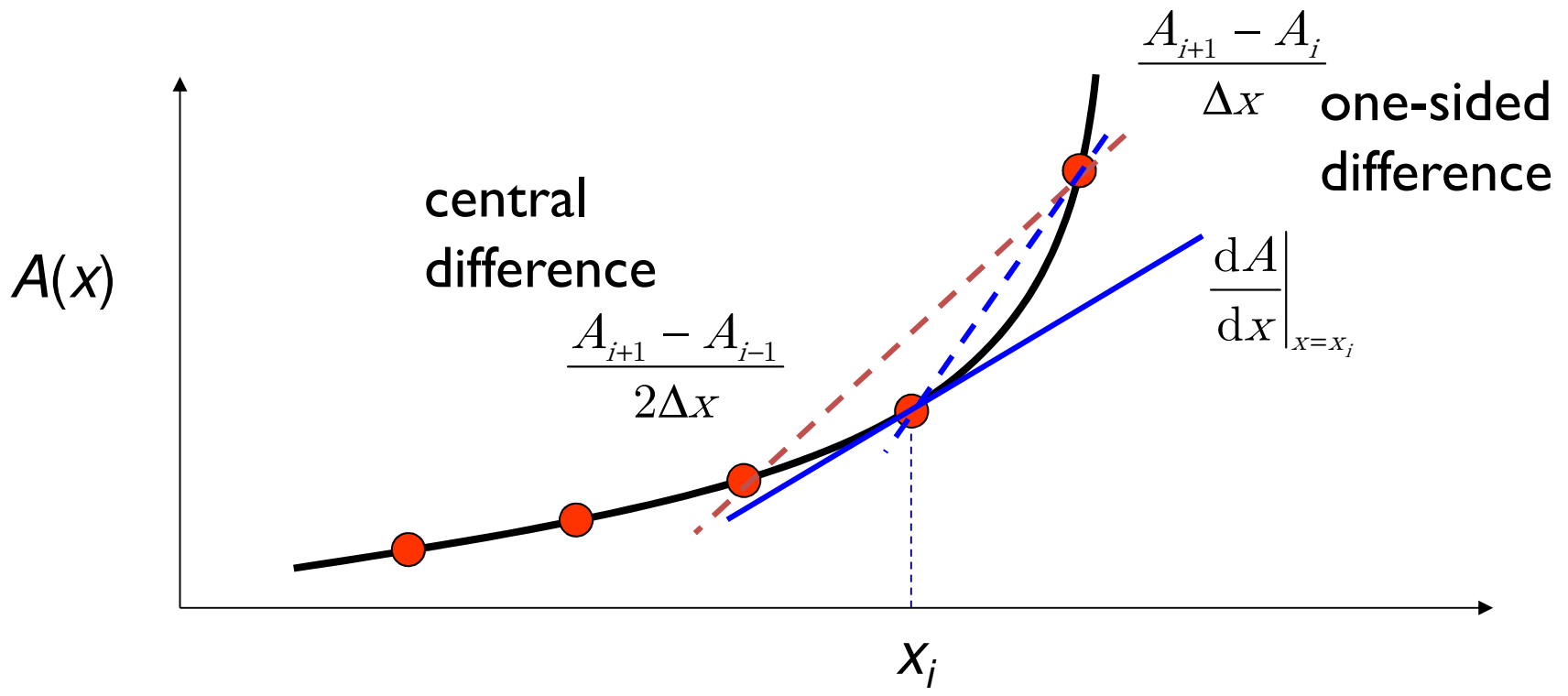
$$\frac{\partial \mathbf{u}}{\partial t} - \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\rho} \nabla p = 0$$

A **Strong** method requires solutions that satisfy (an approximate form of) the equation at every computed point

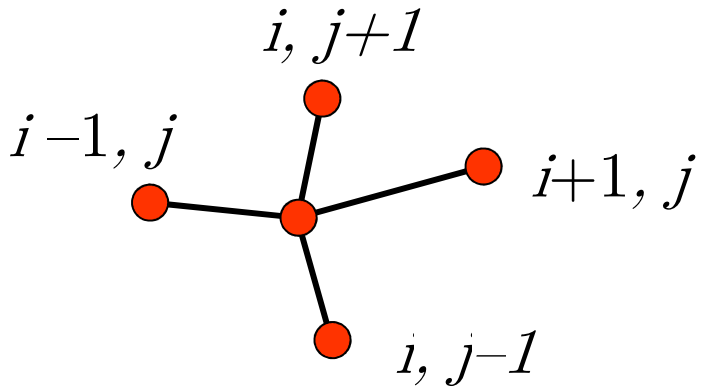
A **weak** method seeks solutions that satisfy the equations in some integral sense

$$\int_{\substack{some \\ region}} \left( \frac{\partial \mathbf{u}}{\partial t} - \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\rho} \nabla p \right) \mathrm{d}V = 0$$

# Finite differences on a mesh



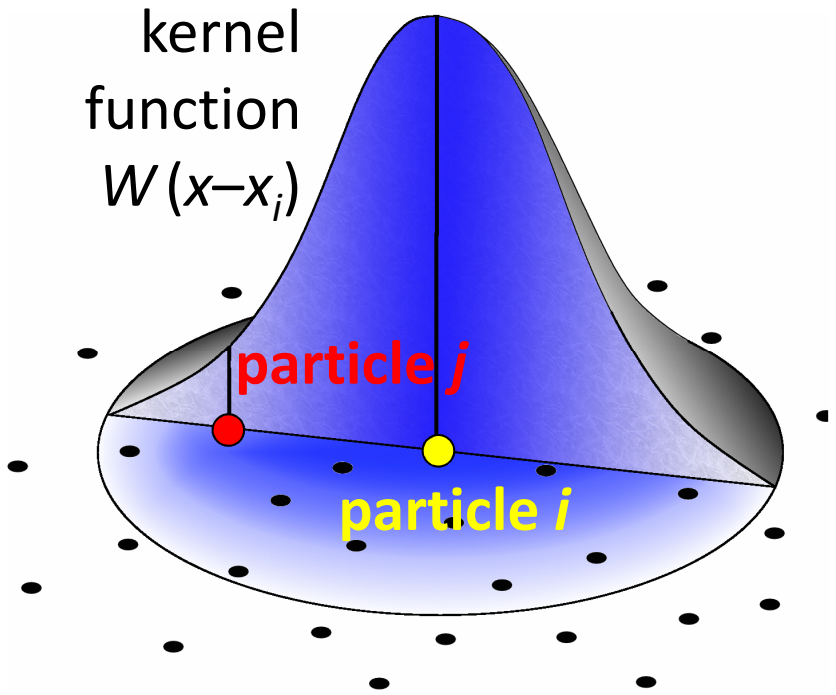

2D



# Without a mesh

Interpolation estimate of $A(x)$ at $x$:

$$\langle A(\mathbf{x}) \rangle = \sum_j A_j W(\mathbf{x} - \mathbf{x}_j) V_j$$




Gradient estimate:

$$\langle \nabla A(\mathbf{x}) \rangle = \sum_j A_j \nabla W(\mathbf{x} - \mathbf{x}_j) V_j$$

Gradient at $x = x_i$:

$$\langle \nabla A(\mathbf{x}) \rangle_{x=x_i} = \sum_j A_j \nabla_{x_i} W(\mathbf{x}_j - \mathbf{x}_i) V_j$$

# Some notation

$$\langle \nabla A_i \rangle = -\sum_j A_j \nabla W_{ij} V_j$$

SPH approximation to gradient of A(x) at $x = x_i$

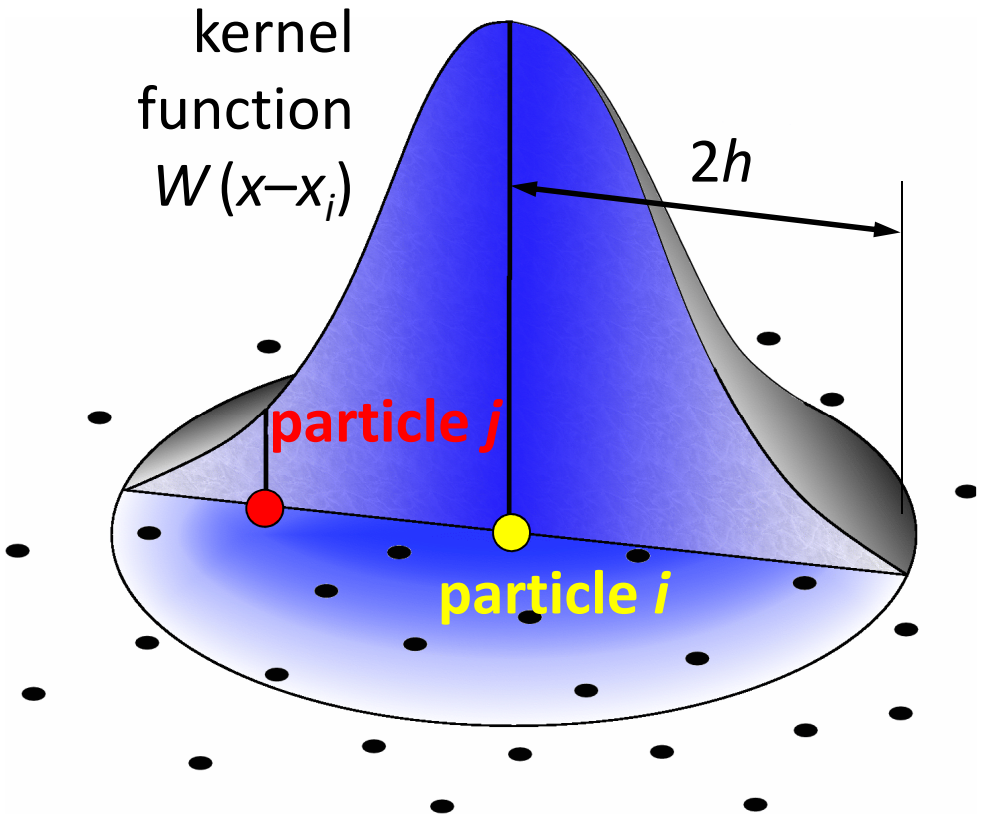
Gradient of kernel function centred on $x_i$, evaluated at $x = x_j$

# The kernel

$$W(\mathbf{x} - \mathbf{x}_i, h_i) \equiv W_i(\mathbf{x})$$

Centre particle

smoothing length




Typically:

- Compact support
- radius 2h
- Smooth
- Radially symmetric
- Normalised s.t. $\int W dV = 1$

# SPH continuity equations

Continuity

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho\nabla\cdot\mathbf{u} = 0$$

SPH grad $\rightarrow$

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} = -\rho_i \sum_j \nabla W_{ij}\cdot\mathbf{u}_j \frac{m_j}{\rho_j}$$

Alternatively:

$$\frac{\mathrm{d}\rho_i}{\mathrm{d}t} + \boldsymbol{\nabla}\cdot(\rho\mathbf{u}) - \mathbf{u}\cdot\nabla\rho = 0$$

$$\frac{d\rho_i}{dt} = -\sum_j \nabla W_{ij}\cdot\left(\rho_j\mathbf{u}_j - \mathbf{u}_i\rho_j\right)\frac{m_j}{\rho_j}$$

$$= -\sum_j \nabla W_{ij}\cdot\left(\mathbf{u}_j - \mathbf{u}_i\right)m_j$$

# SPH continuity equations

Another approach:
Calculate density by interpolation (smoothing )

$$\rho_i = \sum_j W_{ij}\rho_j \frac{m_j}{\rho_j} = \sum_j W_{ij} m_j$$

Differentiate wrt *t*:

$$\frac{d\rho_i}{dt} = \frac{d}{dt}\sum_j W(\mathbf{x}_j - \mathbf{x}_i)m_j = -\sum_j \nabla W_{ij} \cdot (\mathbf{u}_j - \mathbf{u}_i)m_j$$

The two forms of mass equation are equivalent if integrated exactly (Vaughan *et al.*, 2008).

Vaughan *et al.* (2008)

# SPH momentum equations

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}\boldsymbol{t}} + \frac{1}{\rho}\nabla p = 0$$

$$\frac{\mathrm{d}\mathbf{u}_i}{\mathrm{d}t} = -\frac{1}{\rho_i}\sum_j \nabla W_{ij} \cdot p_j \frac{m_j}{\rho_j}$$

Instead, use

$$\nabla\left(\frac{p}{\rho}\right) = \frac{1}{\rho}\nabla p - \frac{p}{\rho^2}\nabla\rho$$

This gives the most commonly used version of the SPH momentum equation:

$$\frac{D\mathbf{u}_i}{Dt} = \sum_b \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2}\right)\nabla W_{ij} m_j$$

# SPH momentum equations

Momentum equation:

$$\frac{d\mathbf{u}_a}{dt} = \sum_b \left( \frac{p_a}{\rho_a^2} + \frac{p_b}{\rho_b^2} \right) \nabla W_{ab} m_b$$

Force on *a* due to *b*: $$\left( \frac{p_a}{\rho_a^2} + \frac{p_b}{\rho_b^2} \right) \nabla W_{ab} m_a m_b$$

Force on *b* due to *a*: $$\left( \frac{p_a}{\rho_a^2} + \frac{p_b}{\rho_b^2} \right) \nabla W_{ba} m_a m_b = -\left( \frac{p_a}{\rho_a^2} + \frac{p_b}{\rho_b^2} \right) \nabla W_{ab} m_a m_b$$

The forces are equal and opposite if $W_a$ and $W_b$ are the same

→ **Conservation of momentum**

# SPH variants: ALE-SPH

Apply SPH to conservative form of Euler equations

$$\frac{d}{dt}(\omega_i \Phi_i) + \omega_i \sum_{j \in D_i} \omega_j 2 G_E(\phi_i, \phi_j) \nabla_i W_{ij} = \omega_i Q_V$$

Particle volume

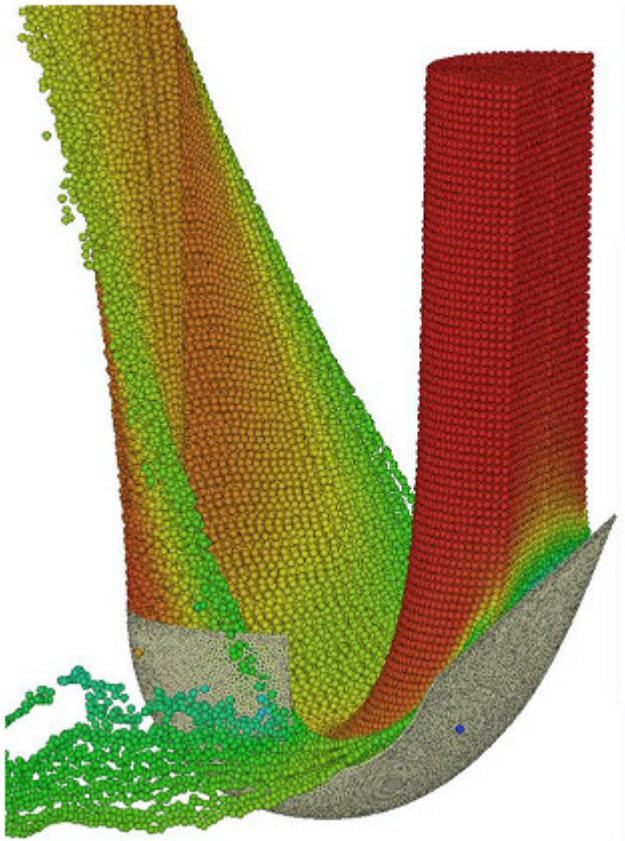
Conserved variables

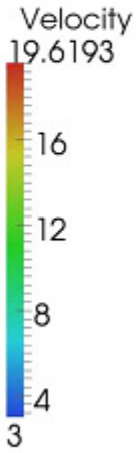
Godunov-type numerical flux function

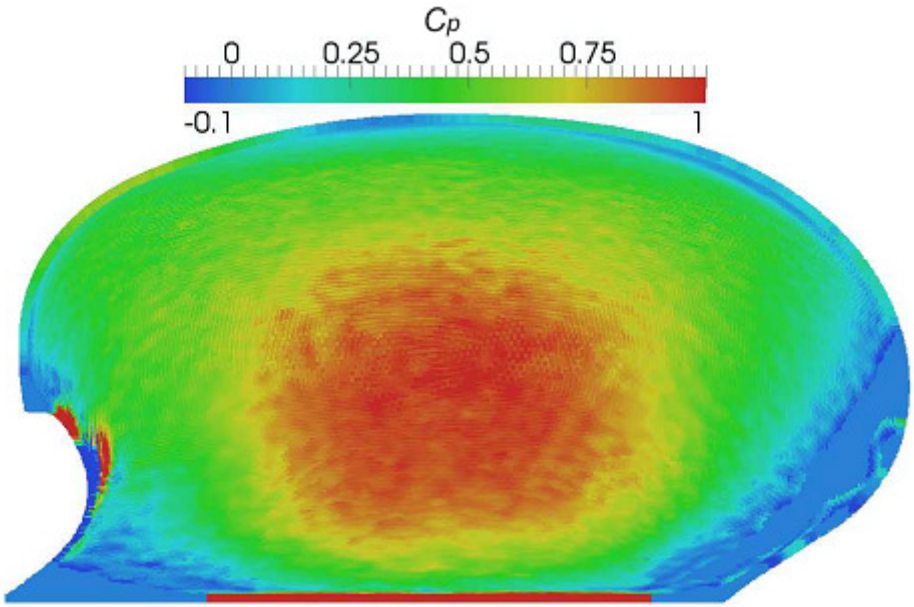
The "particles" are now control volumes, exchanging mass.
Particles are not particles anymore!

Vila (1999)
Marongiu *et al.* (2010)

# Pelton turbine





Marongiu *et al.*, 2010

# SPH variants: δ-SPH

Dissipative terms of order *h*

$$\boldsymbol{\psi}_{ij} = 2(\rho_j - \rho_i)\frac{\mathbf{r}_{ji}}{|\mathbf{r}_{ij}|^2}$$

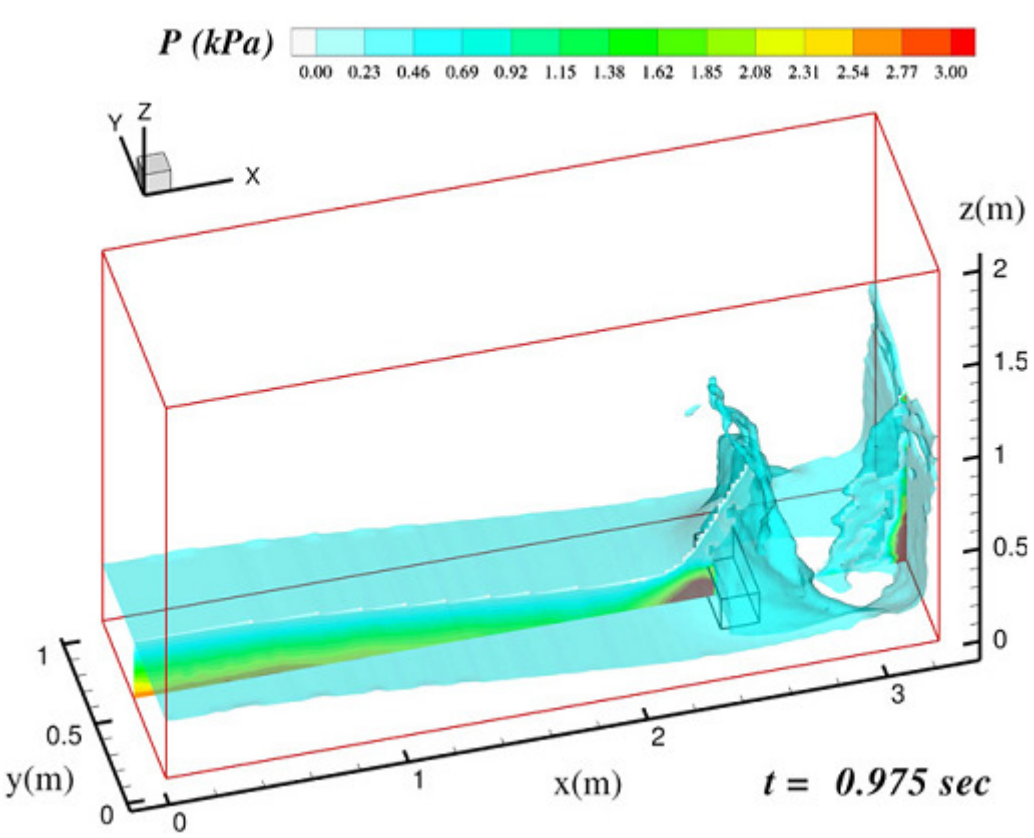
$$\frac{D\rho_i}{Dt} = -\rho_i \sum_j (\boldsymbol{u}_j - \boldsymbol{u}_i)\cdot\nabla_i W(\boldsymbol{r}_j)\,\mathrm{d}V_j + \xi h c_0 \sum_j \boldsymbol{\psi}_{ij}\cdot\nabla_i W(\boldsymbol{r}_j)\,\mathrm{d}V_j,$$

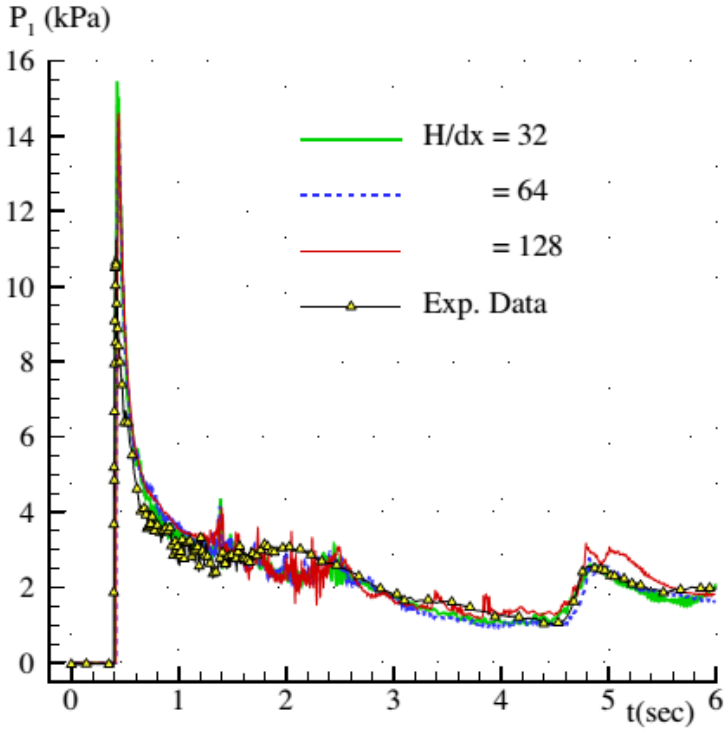
$$\rho_i \frac{D\boldsymbol{u}_i}{Dt} = -\sum_j (p_j + p_i)\nabla_i W(\boldsymbol{r}_j)\,\mathrm{d}V_j + \rho_i \boldsymbol{f}_i + \alpha h c_0 \rho_0 \sum_j \pi_{ij}\nabla_i W(\boldsymbol{r}_j)\,\mathrm{d}V_j,$$

$$\pi_{ij} = \frac{(\boldsymbol{u}_j - \boldsymbol{u}_i)\cdot\mathbf{r}_{ji}}{|\mathbf{r}_{ij}|^2}$$

Antuono et al. (2010)

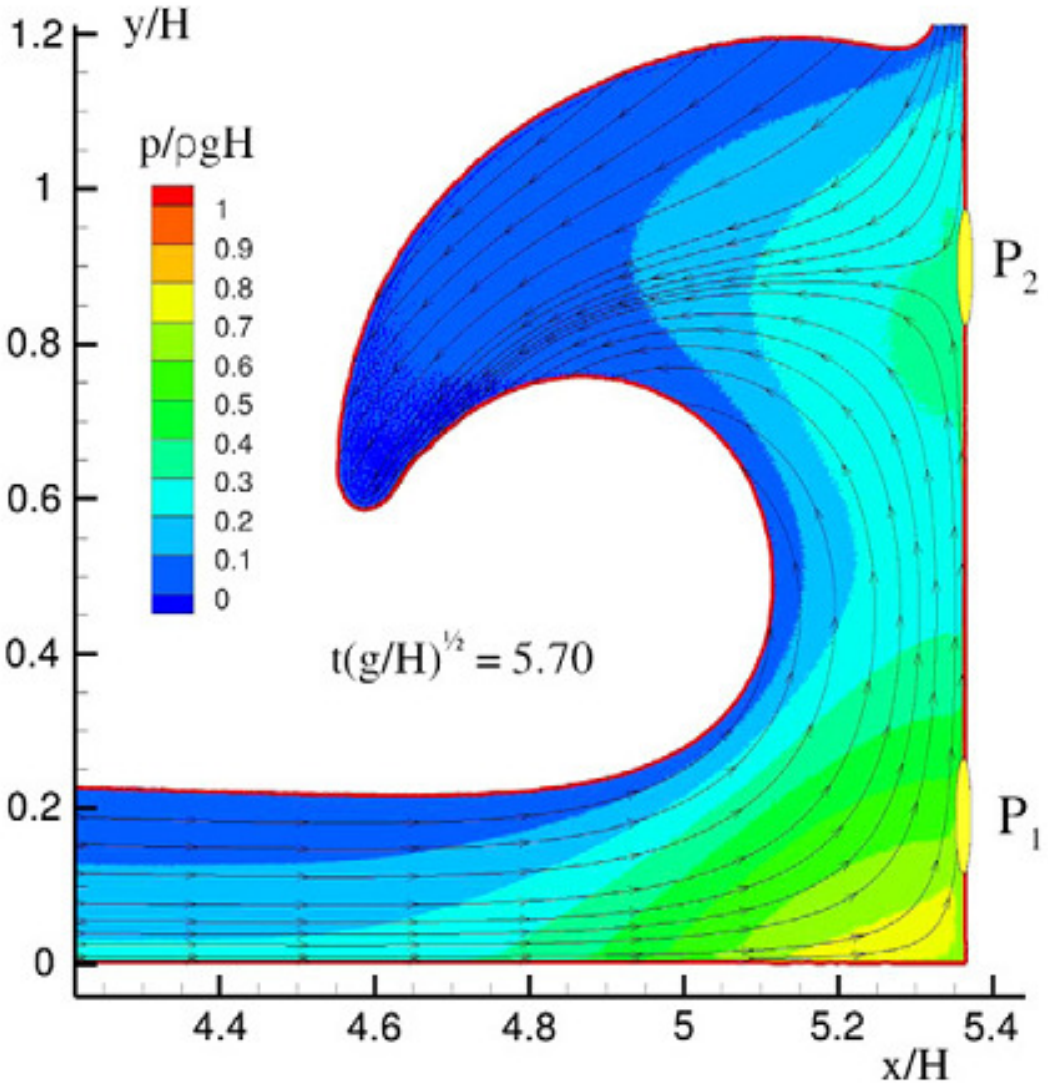
# SPH variants: δ-SPH



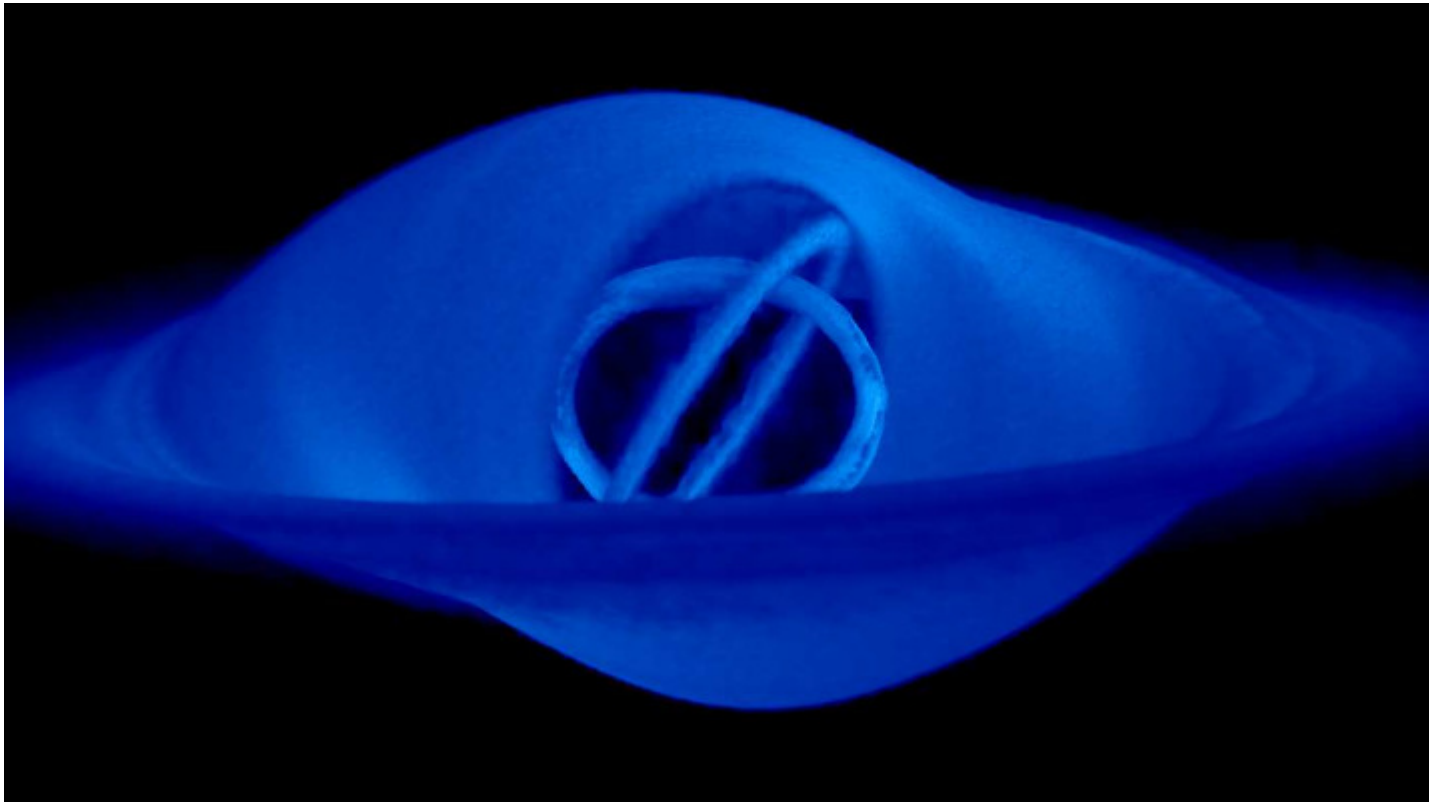

Marrone et al. (2011)

# SPH variants: δ-SPH



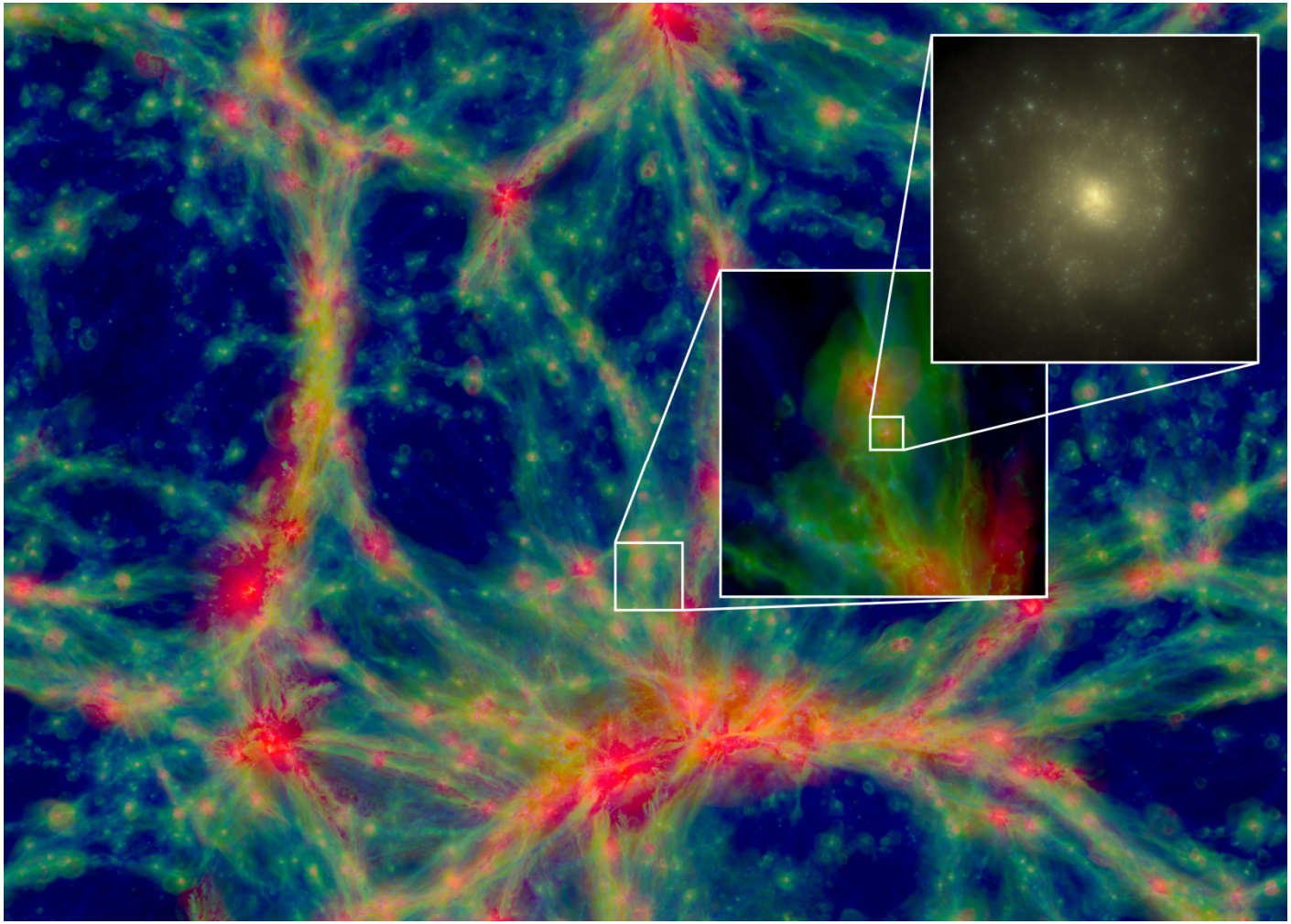

Marrone et al. (2011)

# Boundary conditions in SPH



Black hole accretion
Nixon et al (2012)

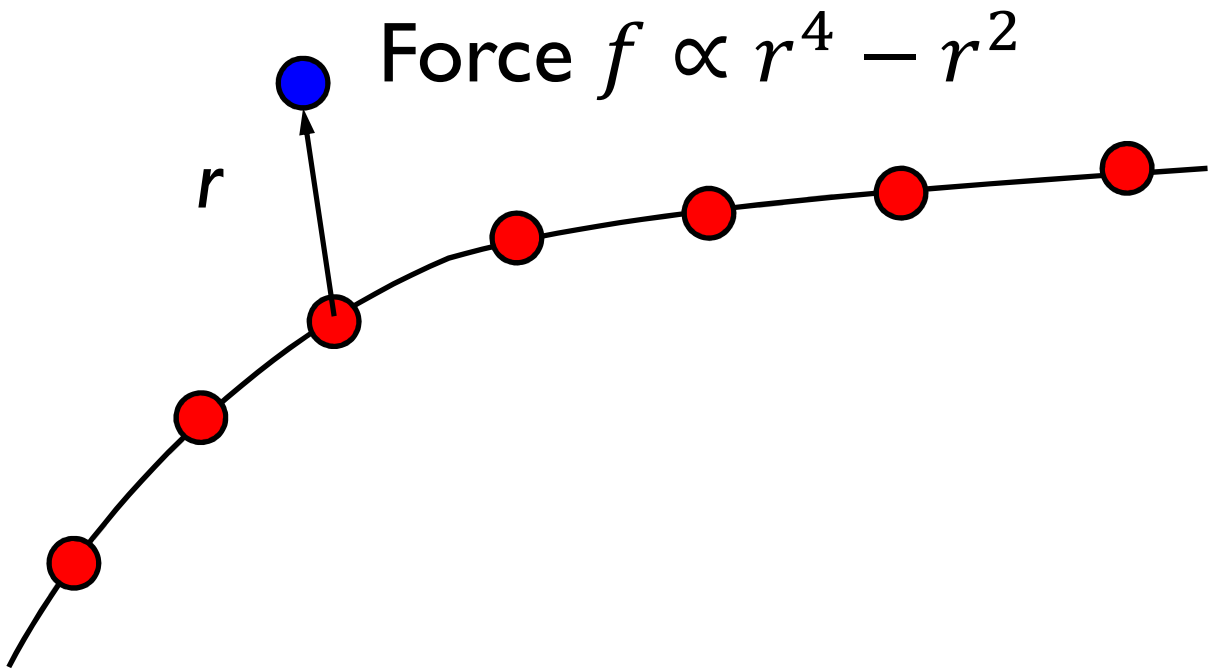
# Boundary conditions in SPH



Galaxy formation
Schaller et al (2015)

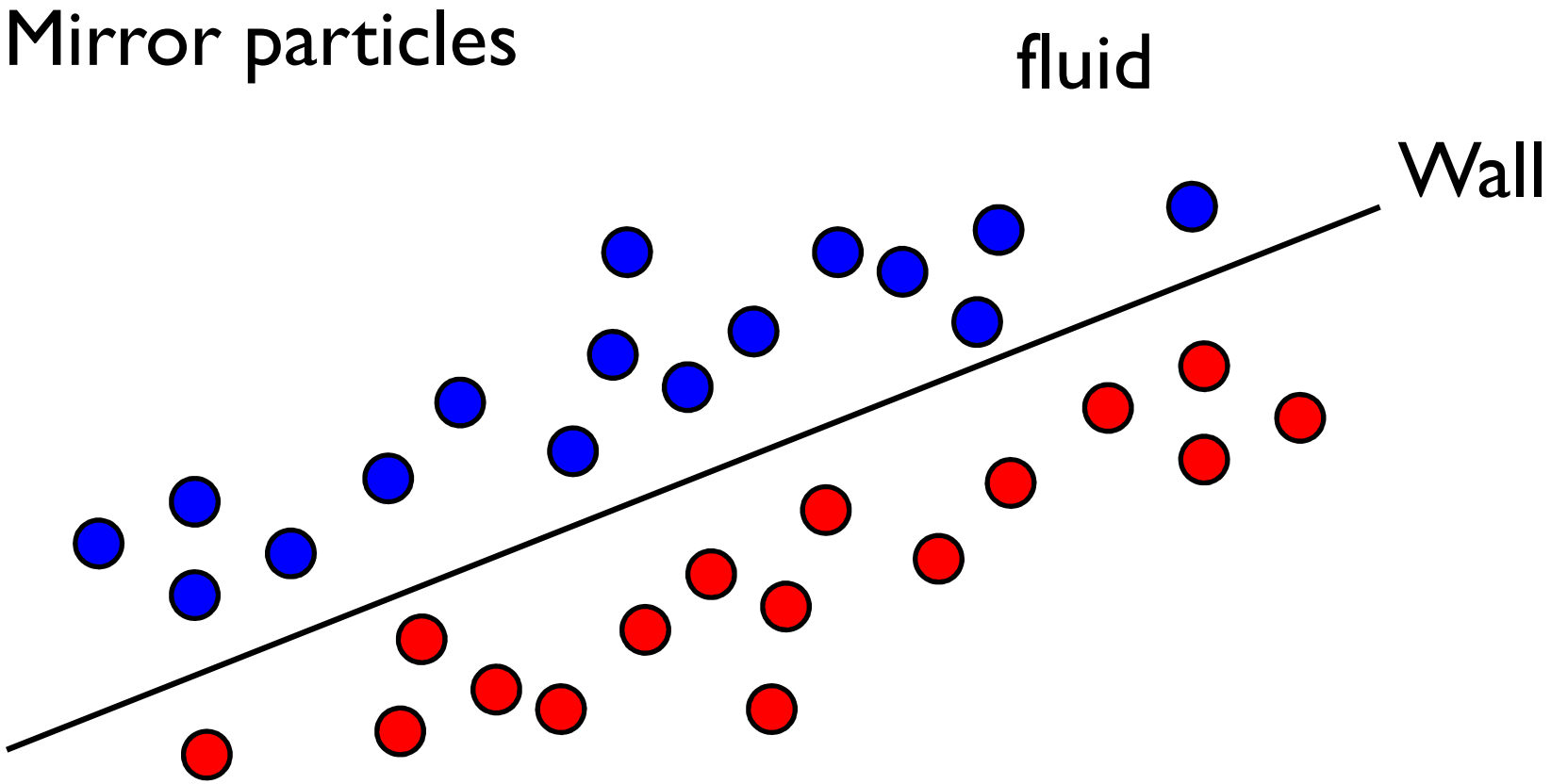
# Boundary conditions in SPH

## Repulsive wall particles




Monaghan (1994)

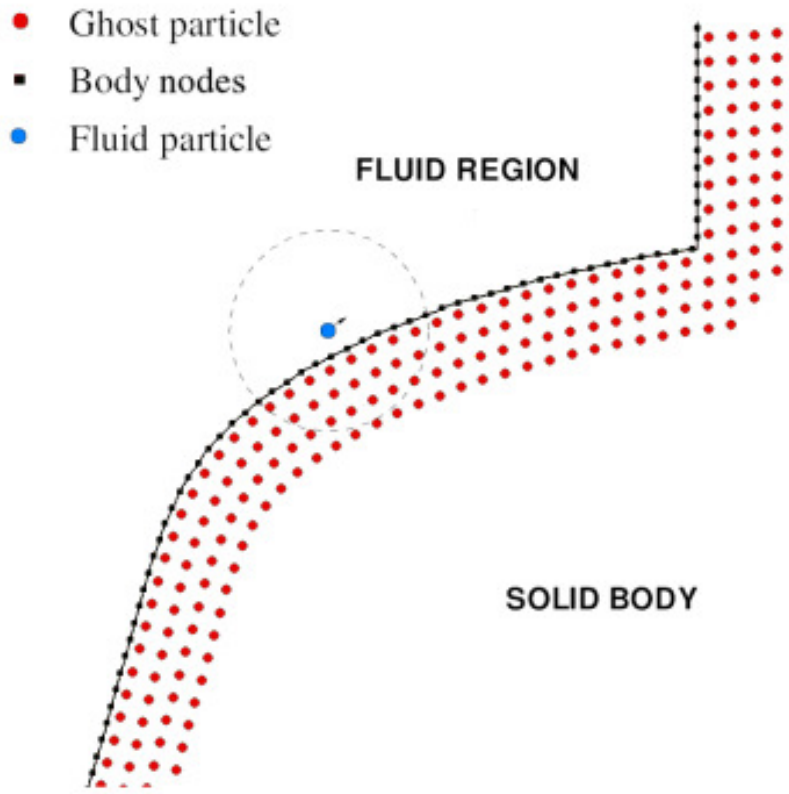
# Boundary conditions in SPH

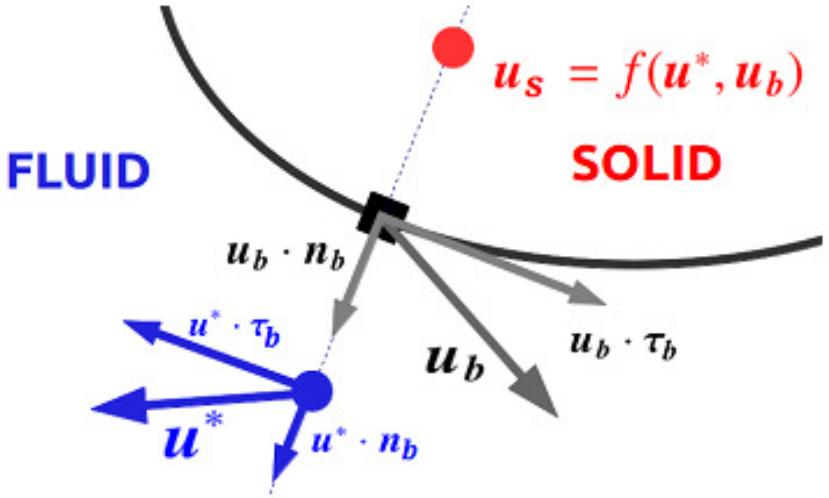


# Boundary conditions in SPH

## Ghost particles

Bouscasse et al. (2013)

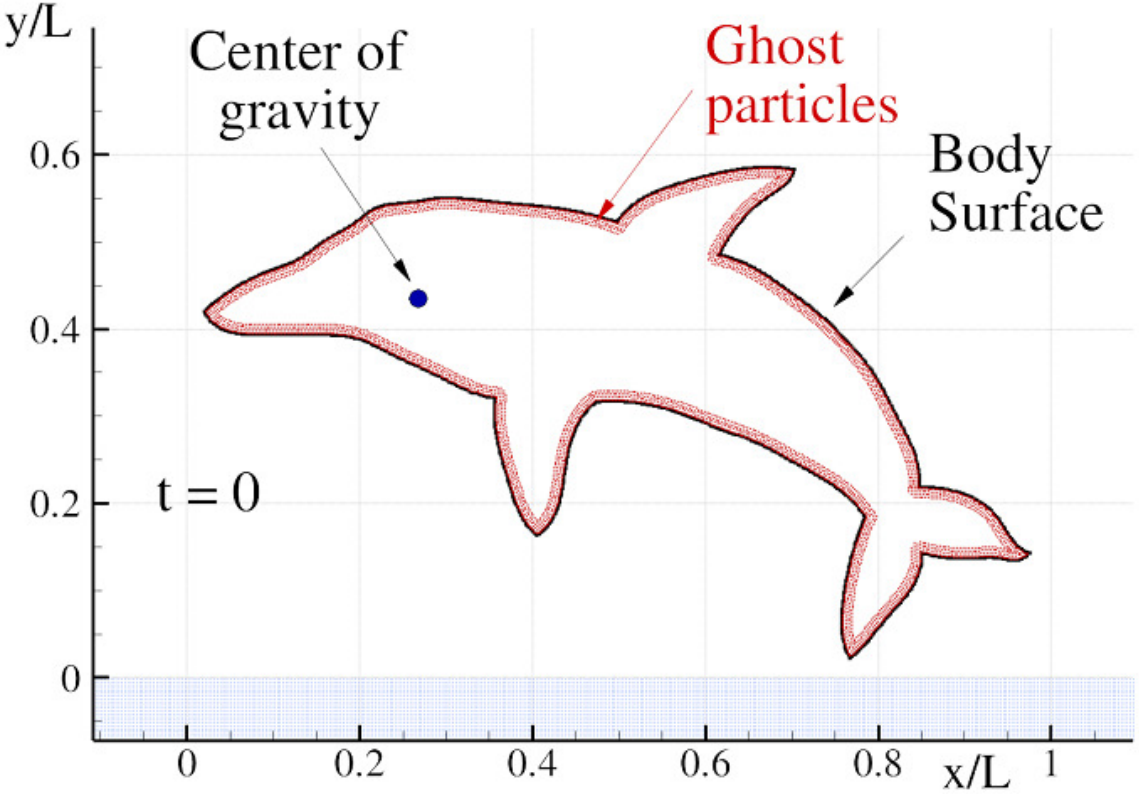


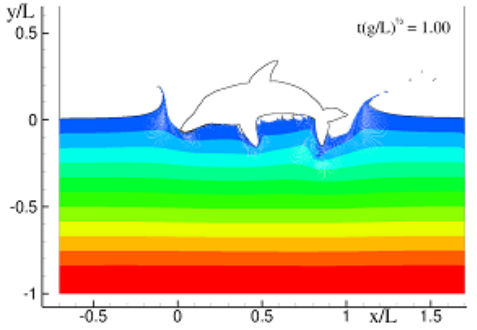



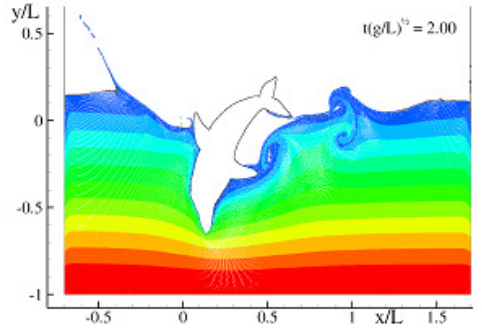

- Mirror **u,** $p$ etc from fluid particles into wall
- Interpolate onto ghosts of ghosts in fluid

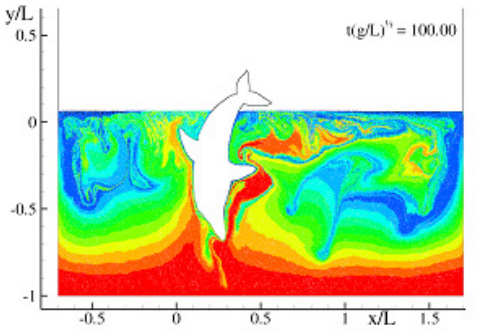
# Boundary conditions in SPH

Bouscasse et al. (2013)



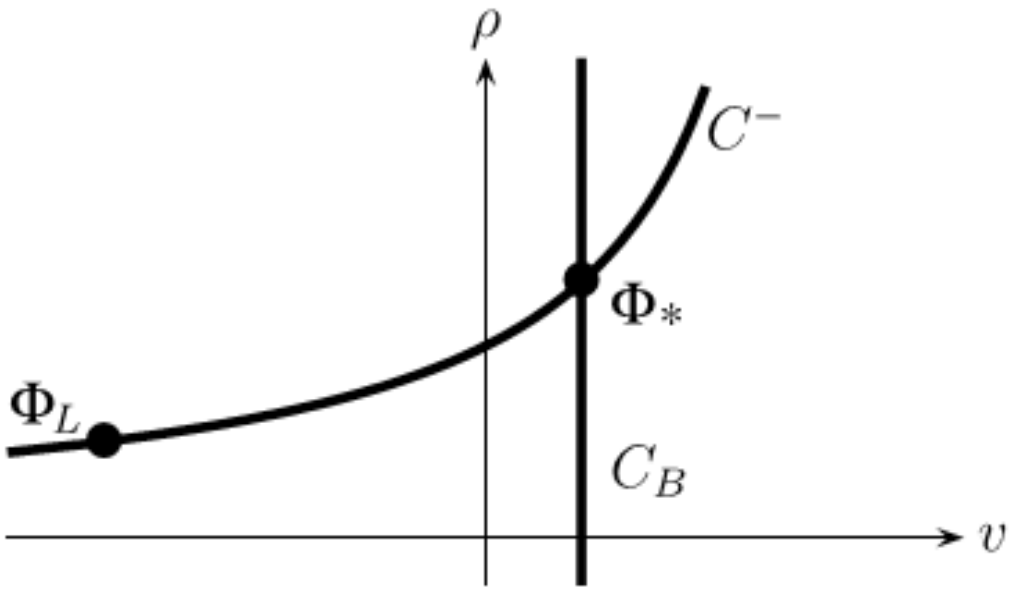



# Boundary conditions in SPH

Partial Riemann

- Consider acoustic wave from fluid particle to boundary



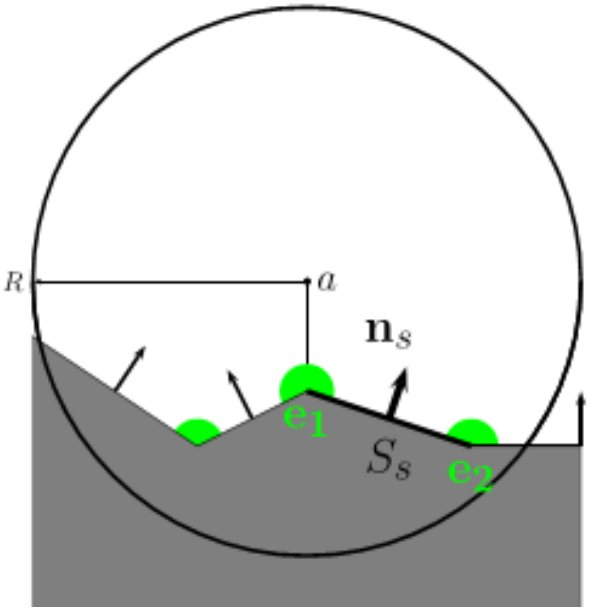

Marongiu et al. (2010)

# Boundary conditions in SPH

Analytical

- Define volume normalisation near boundary
- Incorporate into SPH operators

$$\gamma_a \equiv \int_{\Omega \cap \Omega_a} w\left(\mathbf{r}' - \mathbf{r}_a\right) \mathrm{d}V'$$




$$\rho_a \simeq \frac{1}{\gamma_a} \sum_{b \in \mathcal{F}} m_b w_{ab}$$

$$\widetilde{\mathbf{Grad}}_a\{A_b\} \equiv \frac{\rho_a}{\gamma_a} \sum_{b \in \mathcal{F}} m_b \left(\frac{A_a}{\rho_a^2} + \frac{A_b}{\rho_b^2}\right) \nabla w_{ab} - \frac{\rho_a}{\gamma_a} \sum_{s \in \mathcal{S}} \left(\frac{A_a}{\rho_a^2} + \frac{A_s}{\rho_s^2}\right) \rho_s \nabla \gamma_{as}$$

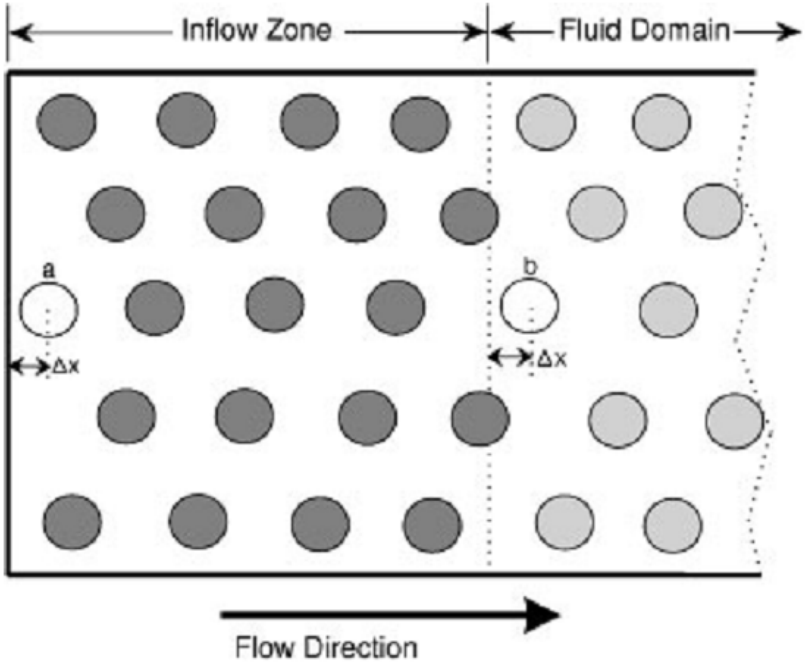
Ferrand et al. (2013), Mayrhofer et al. (2014)

Kulasegaram et al. (2004)

# Boundary conditions in SPH

Inlets and outlets

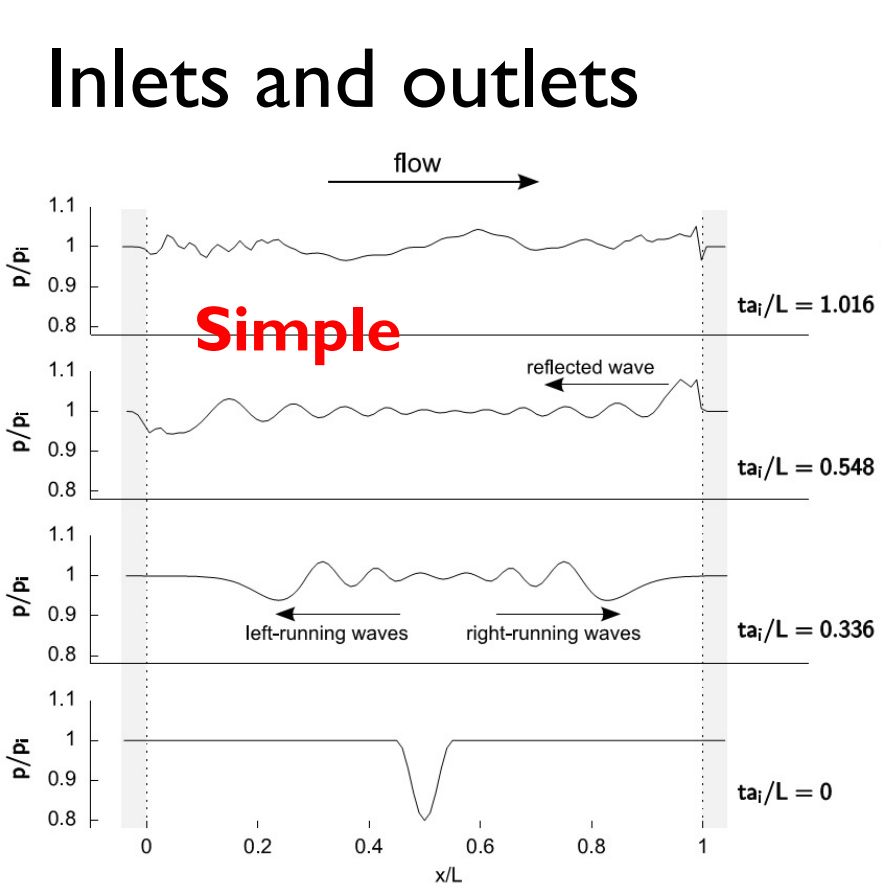
- Buffer zone of semi-active particles
- For non-reflecting boundary conditions, Riemann invariants

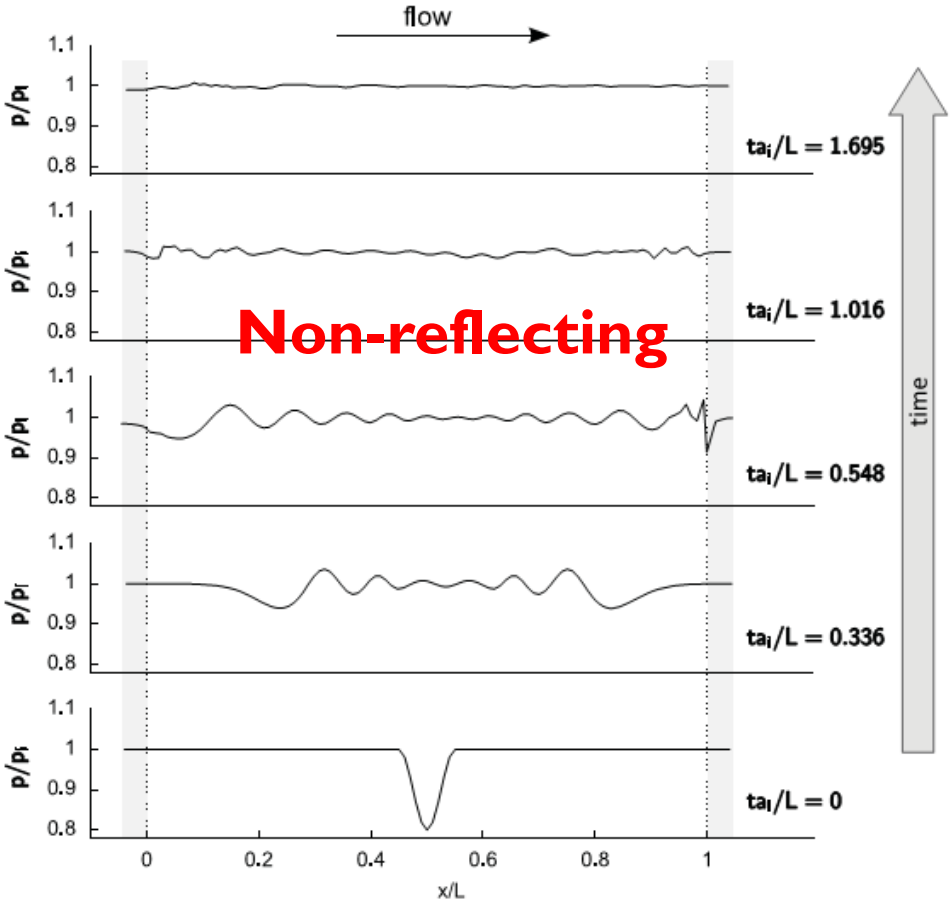


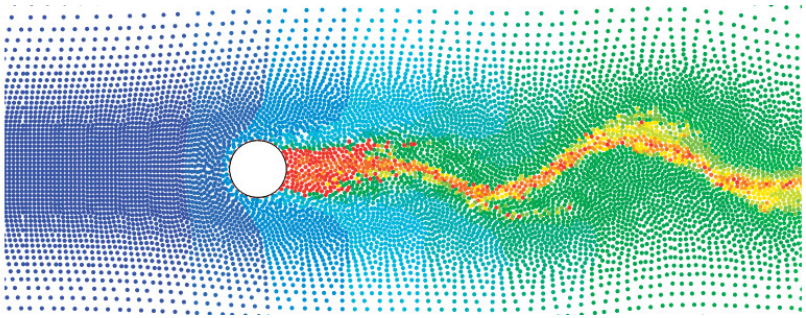

Lastwika et al. (2008)

# Boundary conditions in SPH

## Inlets and outlets



Lastwika et al. (2008)

# An alternative view

## Lagrangian mechanics (Hamiltonian) – Price

$$\left.\frac{\partial A}{\partial x}\right|_{x=x_a} \cong -\sum_b A(x_b)\frac{\partial W(x_b - x_a)}{\partial x_b}\Delta x_b$$

Lagrangian of the particle set

$$L = \sum_b m_b \left[\frac{1}{2}v_b^2 - u(\rho, s)\right]$$

The $+\frac{p}{\rho^2}$ form emerges naturally

The only numerics in the proof is the density estimate

This is a system of particles – SPH is incidental

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