COMETE – Mid-term Meeting
Institute of Fluid Mechanics and Heat Transfer, TU Wien

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WP1
Smoothed Particle Hydrodynamics (SPH) for simulation of multiphase flows

Eleonora Spricigo
Advisors: Jacek Pozorski & Michał Olejnik
Institute of Fluid Flow Machinery
Polish Academy of Sciences
(IMP PAN)
Gdańsk, Poland

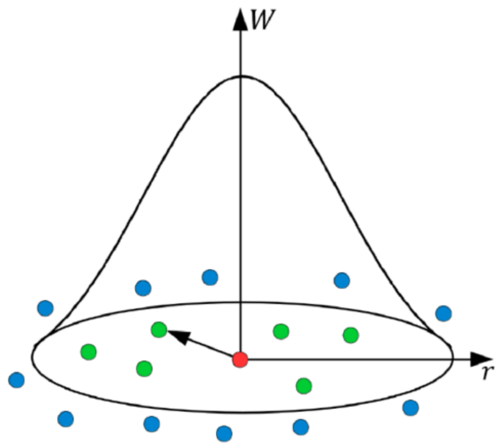
I hold my Bachelor's and Master's degree in mechanical engineering at University of Udine (Italy).

In July 2019 I joined MSCA-ITN-EID COMETE as a Ph.D. student at IMP PAN, a research institute in Gdańsk (Poland).

2. Basics of SPH

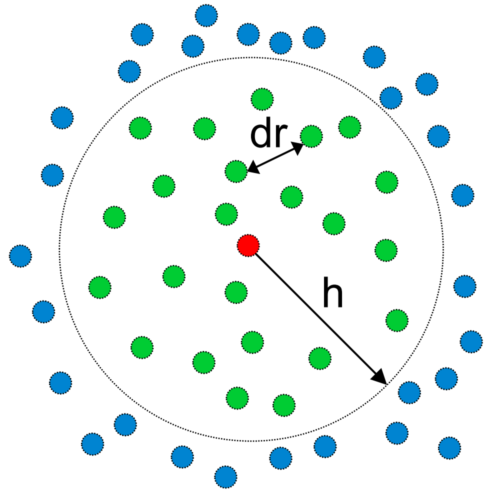
Smoothed

Regularizing functions used (smoothed Dirac delta).



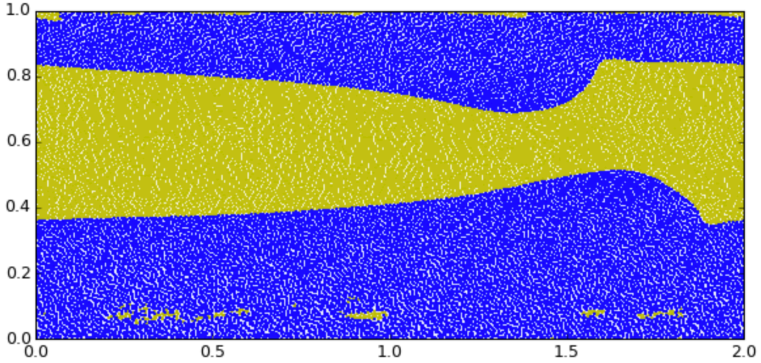
Particle

Particle approach: advection treated exactly mass conserved.



Hydrodynamics

Originally developed for astrophysical simulations: Lucy(1977), Monaghan and Gingold (1977).
Only later used for fluid flow.



2. Basics of SPH

Continuous

Discrete

Any scalar or vector field:

$$\widehat{A}(\mathbf{r}) = \int_{\Omega} A(\mathbf{r}')W(\mathbf{r}-\mathbf{r}',h)d\mathbf{r}' \longrightarrow \langle A\rangle(\mathbf{r}) = \sum_b A(\mathbf{r}_b)W(\mathbf{r}-\mathbf{r}_b,h)\Omega_b$$

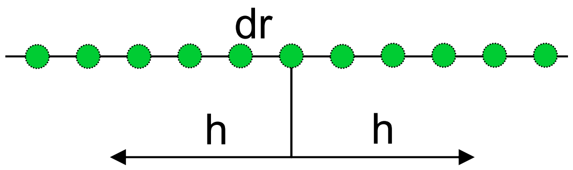
$$\widehat{\nabla A}(\mathbf{r}) = \int_{\Omega} \nabla A(\mathbf{r}')W(\mathbf{r}-\mathbf{r}',h)d\mathbf{r}' \longrightarrow \langle \nabla A\rangle_a = \sum_b A_b \nabla_a W_{ab}(h)\Omega_b$$

3. Accuracy considerations

The purpose was to write a python code able to approximate a 1D analytical function using the SPH method.

The most immediate example is the one-dimensional Wendland kernel

$$W(\mathbf{r},h) = C\begin{cases}\Phi(q) & for\ q > 1 \\ 0 & otherwise\end{cases} \quad q = |\mathbf{r}|/h$$



$$\text{1D, } \mathbf{r} = f(x)\,, \quad C = \frac{5}{4}, \quad \Phi(q) = (1-q)^3(1+3q)$$

But SPH approximation should stay below the analytical function

$$\langle f(x_i)\rangle \leq f(x_i)$$

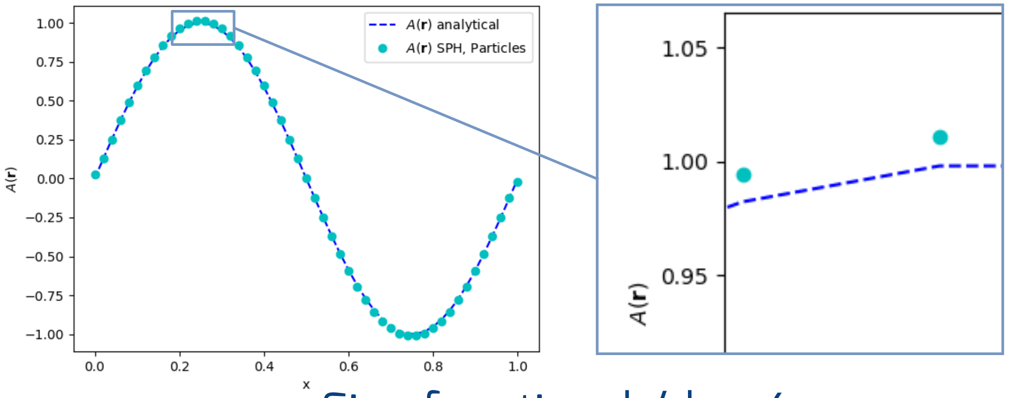
Proof:

$$\int_\Omega W(r')\,dr' = 1 \;\Rightarrow\; \sum_j W_{ij}\Omega_j \cong 1$$

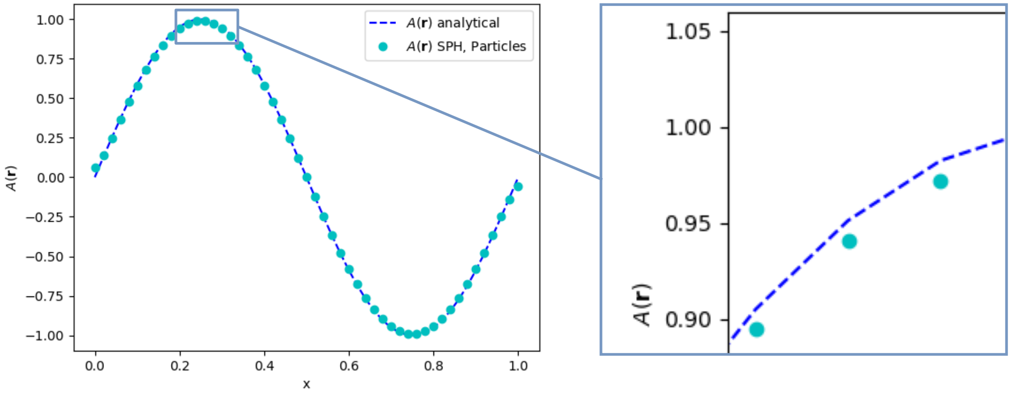
$$\forall\, j\ st\ f(x_j) \leq f(x_i)$$

$$\langle f(x_i)\rangle = \sum_j f(x_j)W_{ij}\Omega_j \leq \sum_j f(x_i)W_{ij}\Omega_j = f(x_i)\sum_j W_{ij}\Omega_j \cong f(x_i)$$

Sine function, h/dr = 2



Sine function, h/dr = 4



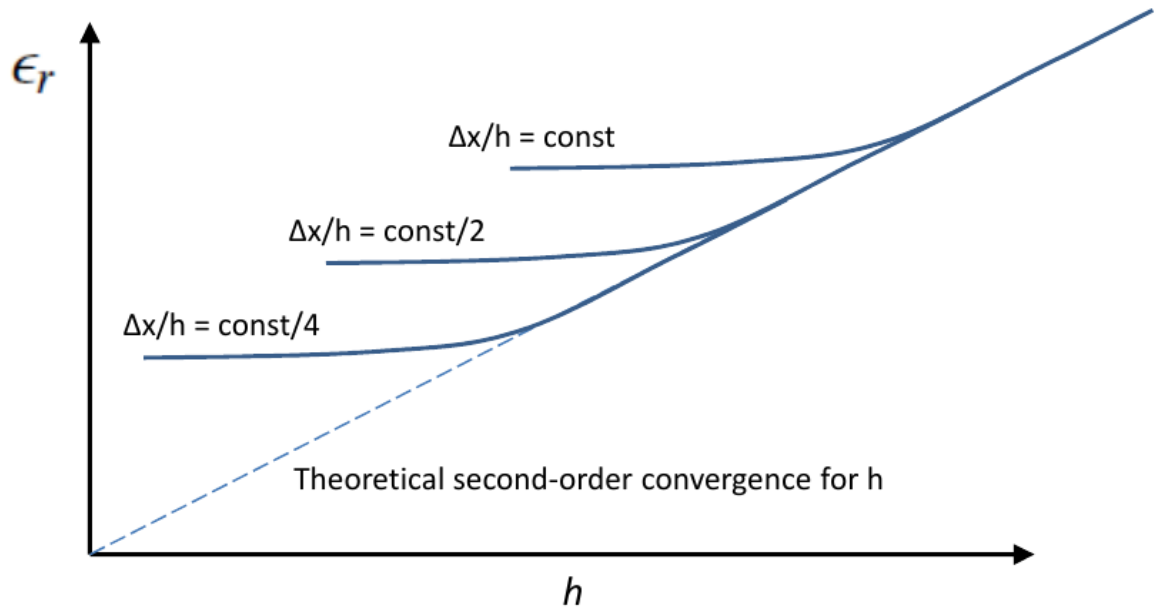
[W. Dehnen, H. Aly, MNRAS, 2012]

3. Accuracy considerations

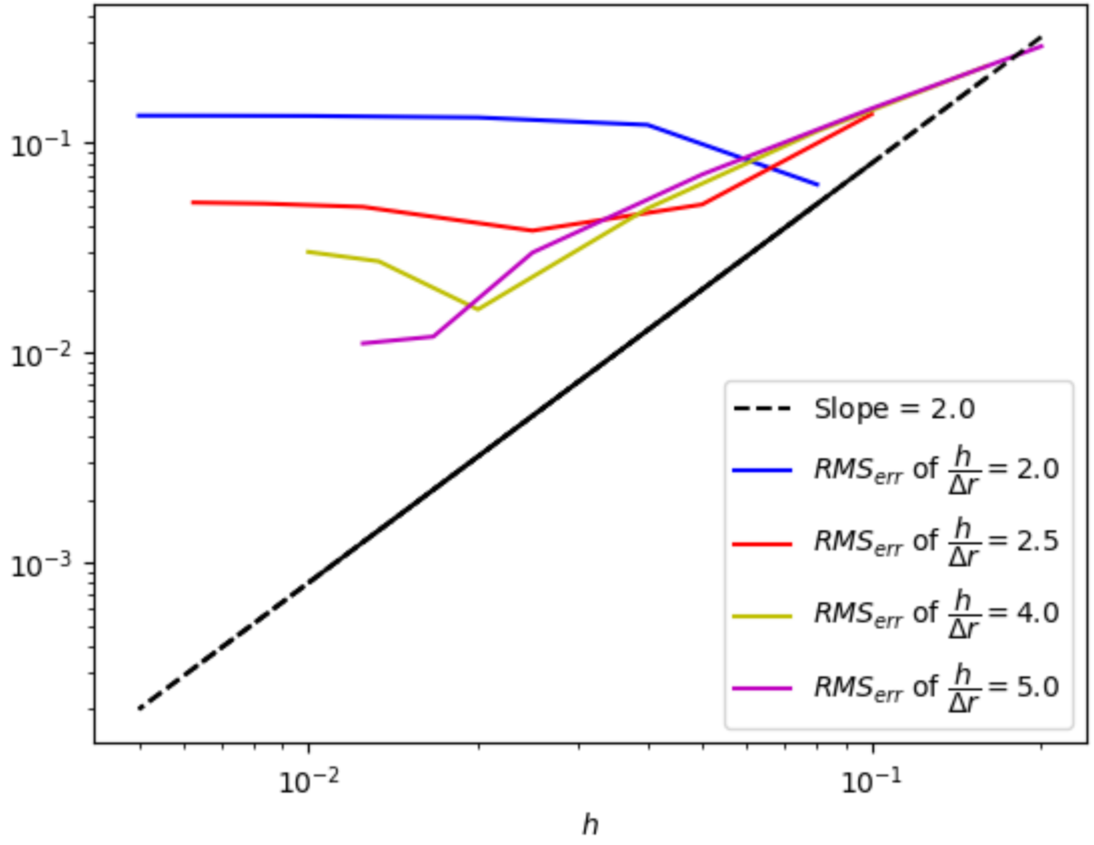
1D Approximation error: from theory… …to computation

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

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**)…



Number of particles= [25, 50, 100, 200, 300, 400]
Variable h/Δr = [2.0, 2.5, 4.0, 5.0]
1D particle arrangement



[M. Antuono, TU Delft, 2019]

4. Our work on the modeling: governing equations

Continuity equation

$$\frac{d\varrho}{dt} = -\varrho \nabla \cdot \mathbf{u}$$

$$\begin{cases} \varrho_a = m_a \sum_b W_{ab}(h) = m_a \Theta_a \\ \frac{d\varrho_a}{dt} = \varrho_a \sum_b \mathbf{u}_{ab} \cdot \nabla_a W_{ab}(h) \Omega_b \end{cases}$$

Advection

$$\frac{d\mathbf{r}}{dt} = \mathbf{u} \qquad \frac{d\mathbf{r}_a}{dt} = \mathbf{u}_a$$

Momentum equation

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\varrho}\nabla p + \frac{1}{\varrho}\nabla \cdot \tau + \mathbf{f}_b + \frac{1}{\varrho}\mathbf{f}_{st}$$

Where the pressure gradient is approximated as

$$\left\langle \frac{\nabla p}{\varrho} \right\rangle_a = \frac{1}{m_a} \sum_b \left(\frac{p_a}{\Theta_a^2} + \frac{p_b}{\Theta_b^2} \right) \nabla_a W_{ab}(h)$$

We want to enhance the model of the interface:
so our work is focused on surface tension and viscosity force

$$\mathbf{f}_{st} = \mathbf{f}_s \delta_s \qquad \mathbf{F}_\nu = \frac{1}{\varrho}\nabla \cdot \tau$$

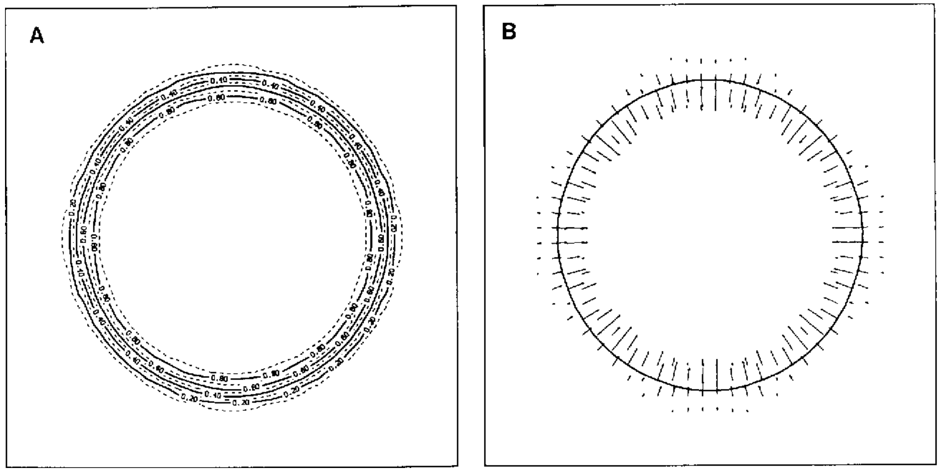
5. Surface tension force: the model

Continuum surface force (CSF)

surface force per unit volume

$$\mathbf{f}_{st} = \mathbf{f}_s \delta_s \qquad \delta_s = |\mathbf{n}|$$

$$\mathbf{f}_s = \sigma \kappa \hat{\mathbf{n}}$$ where $$\hat{\mathbf{n}} = \frac{\mathbf{n}}{|\mathbf{n}|} = \frac{\nabla c}{|\nabla c|} \qquad \kappa = -\nabla \cdot \hat{\mathbf{n}}$$



[J.U. Brackbill and al., JCP, 1992]

From Hu & Adams…

$$\tilde{c}_a = \sum_b c_b W_{ab}(h) \Omega_b$$

$$\kappa_a = \sum_b (\hat{\mathbf{n}}_a - \hat{\mathbf{n}}_b) \cdot \nabla_a W_{ab}(h)$$

…to Adami, Hu & Adams

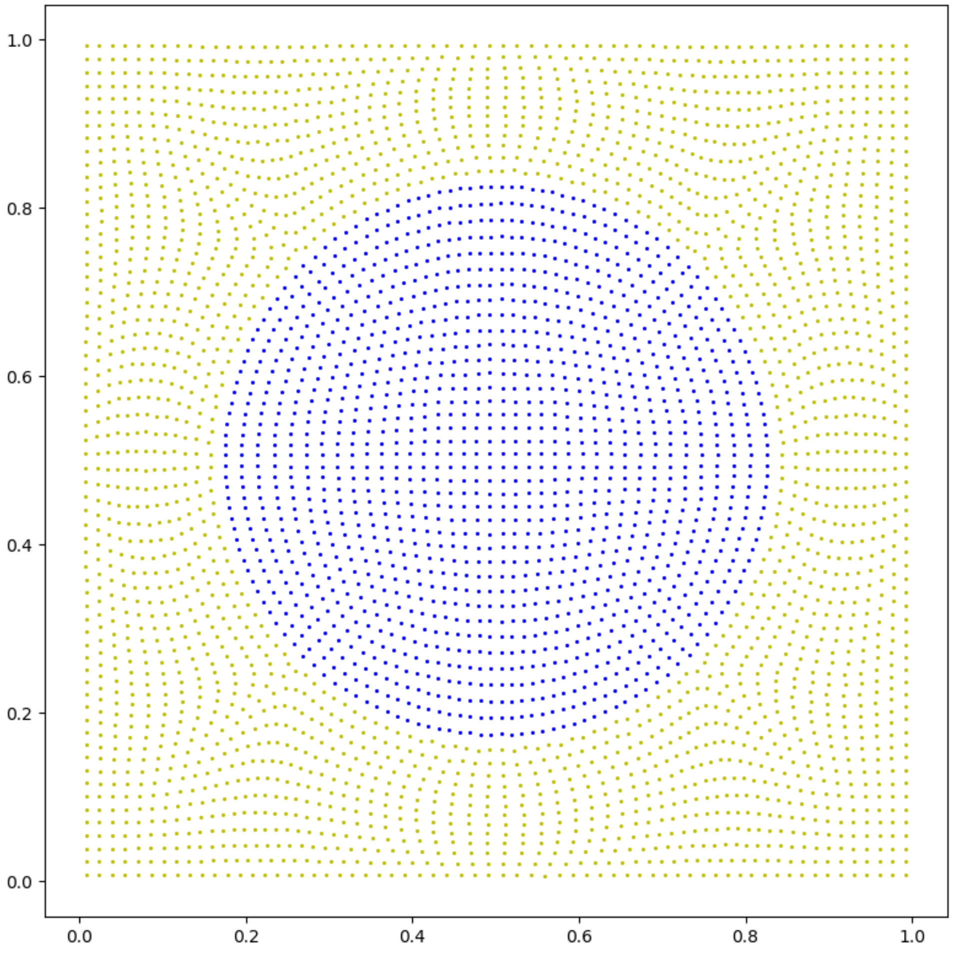
$$\tilde{c}_{ij} = \frac{\rho_j}{\rho_i + \rho_j} c_i^i + \frac{\rho_i}{\rho_i + \rho_j} c_j^i$$

where c_l^k is 1 if the k^{th} particle doesn't belong to the phase of particle l, otherwise 0

$$\nabla \cdot \varphi_i = d \frac{\sum_j \varphi_{ij} \cdot \boldsymbol{e}_{ij} \frac{\partial W}{\partial r_{ij}} V_j}{\sum_j r_{ij} \frac{\partial W}{\partial r_{ij}} V_j} r^2$$

5. Surface tension force: square to droplet deformation

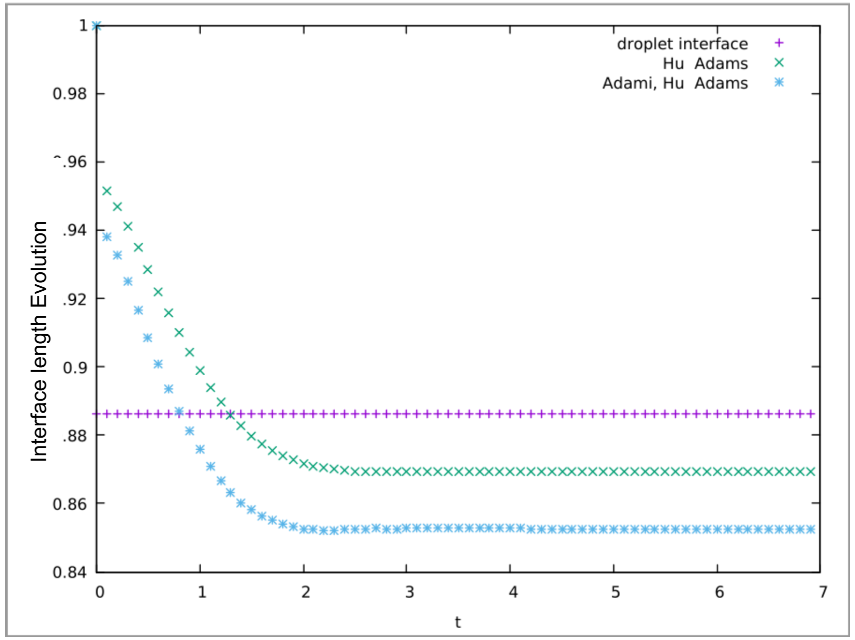
Density ratio = 1000

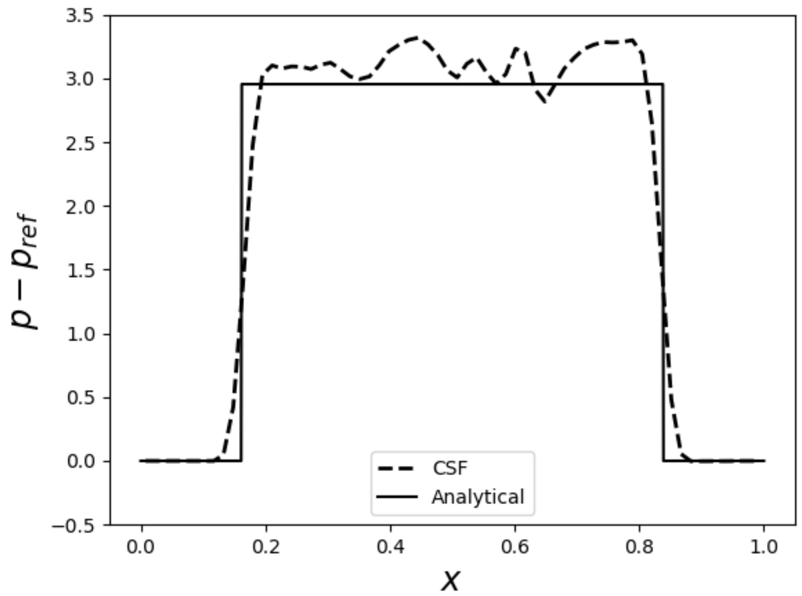


$$\frac{\rho_1}{\rho_2} = 1000$$
$$c_1 = 1$$
$$c_2 = 0$$
$$\frac{\mu_1}{\mu_2} = 1$$

Interface length:

$$S = \int_\Omega \delta(\mathbf{x}) \mathrm{d}\Omega$$





6. Viscous force: proposal of a new formulation

$$\mathbf{F}_\nu = \frac{1}{\varrho}\nabla\cdot\tau$$

Constitutive law $\tau = \mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)$

Hu and Adams (2006)

$$\frac{d\mathbf{u}_a}{dt} = \frac{1}{m_a}\sum_b \frac{2\mu_a\mu_b}{\mu_a+\mu_b}\left(\frac{1}{\theta_a^2}+\frac{1}{\theta_b^2}\right)\frac{1}{r_{ab}+\eta}\frac{\partial W}{\partial r_{ab}}\mathbf{u}_{ab}$$

Where $\theta_b(\mathbf{r}) = \sum_b W(\mathbf{r}-\mathbf{r}_b, h)$

Violeau (2012)

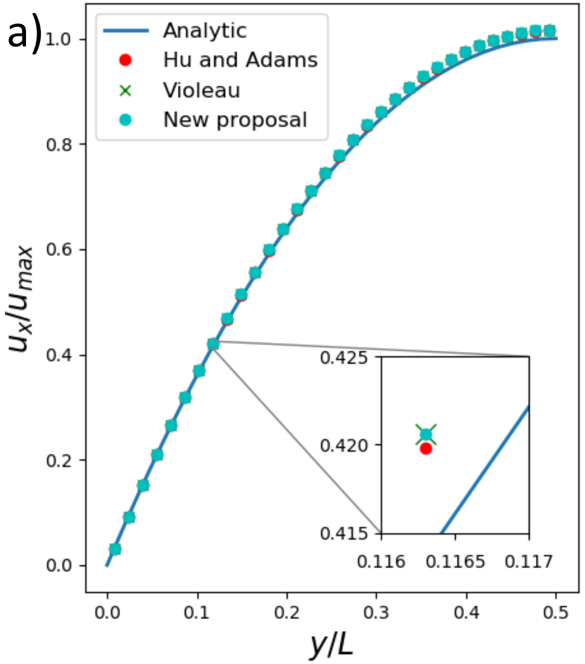
$$\frac{d\mathbf{u}_a}{dt} = -\sum_b \frac{\mu_a+\mu_b}{2}\left(\frac{-m_b}{\rho_a\rho_b}\right)\frac{1}{r_{ab}+\eta}\frac{\partial W}{\partial r_{ab}}[(n+2)(\mathbf{u}_{ab}\cdot\mathbf{e}_{ab})\mathbf{e}_{ab}+\mathbf{u}_{ab}]$$

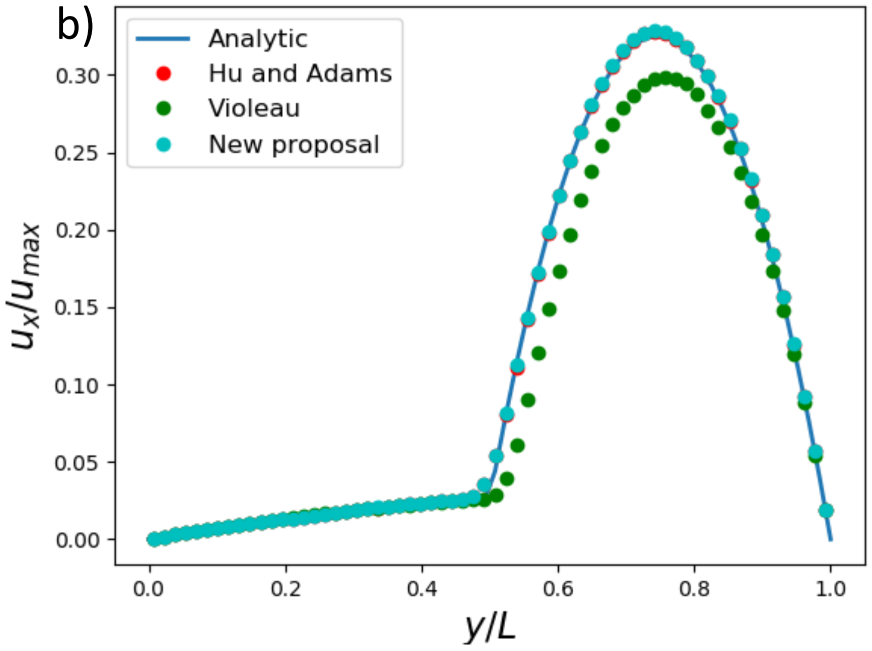
New proposal

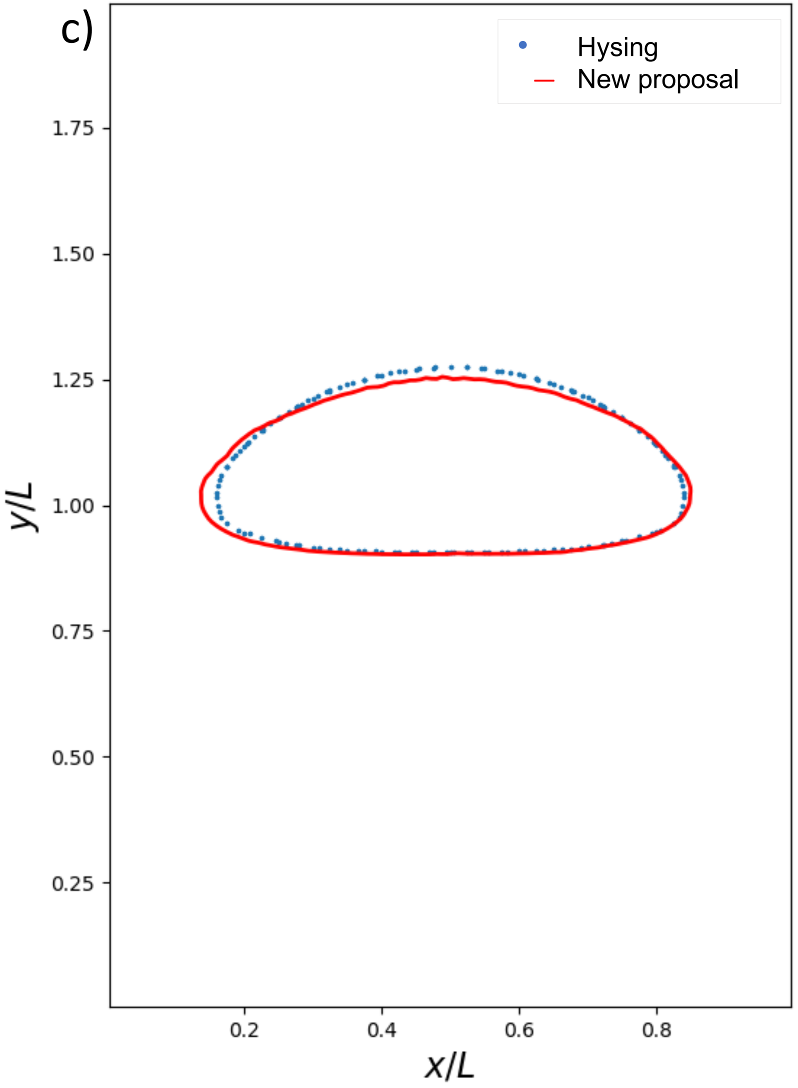
$$\frac{d\mathbf{u}_a}{dt} = -\sum_b \frac{2\mu_a\mu_b}{\mu_a+\mu_b}\left(\frac{-m_b}{\rho_a\rho_b}\right)\frac{1}{r_{ab}+\eta}\frac{\partial W}{\partial r_{ab}}[(n+2)(\mathbf{u}_{ab}\cdot\mathbf{e}_{ab})\mathbf{e}_{ab}+\mathbf{u}_{ab}]$$

[E. Spricigo et al.,KKMP2020, submitted]

6. Viscous force: Test cases







a) Steady-state single-phase Poiseuille flow

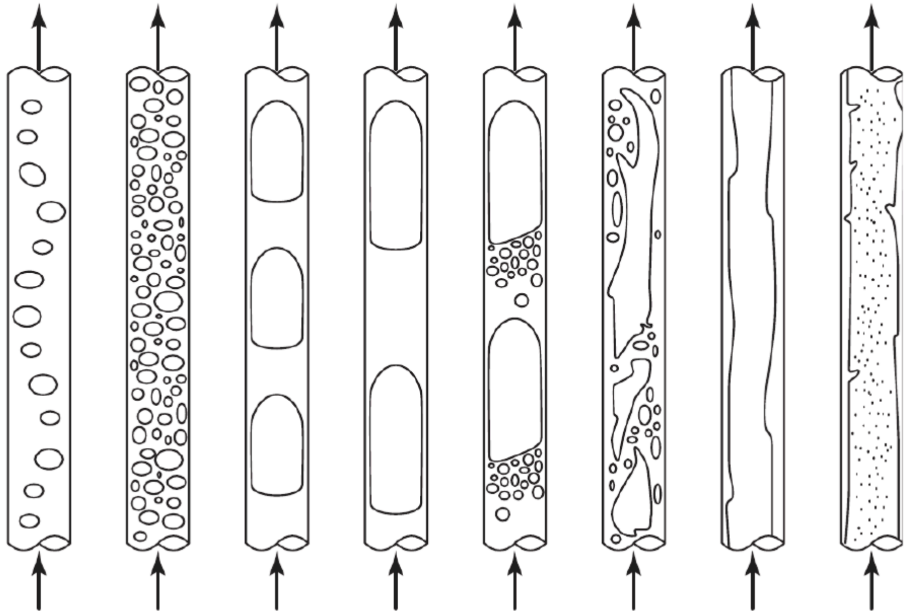
b) Steady-state two-phase Poiseuille flow (ν_1/ν_2=100) (Grenier 2013, Bird1924)

c) Rising bubble (first case Hysing 2009)

4. Next-term work and impact of the action on my future career

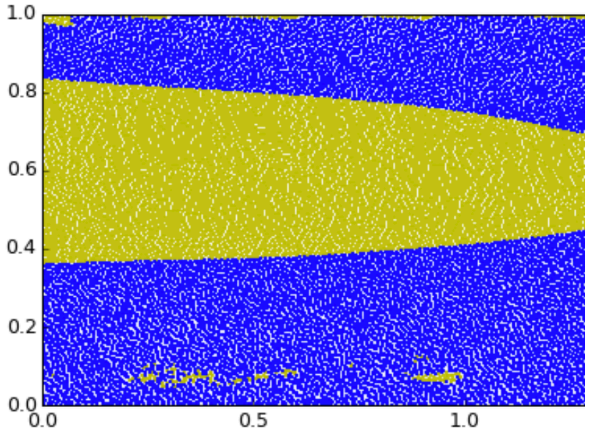
This project goals to contribute to the ongoing efforts in multiphase SPH:

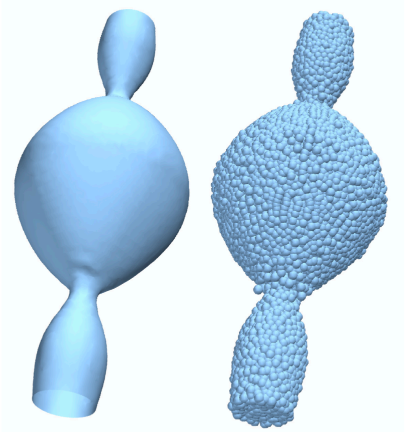
1. upgrade the code existing in-house code, starting with improving variable viscosity formulation, the interface description and mitigating the occurrence of the micro-mixing phenomena
2. improve the physical modelling, carrying out further work based on what has already been done in the PhD of Olejnik (2019) about two-phase flow behavior in a channel and different flow regimes, moving on to 3D simulations;
3. assess the SPH approach in applications, some of them to be defined jointly with the industrial partner of the project (ESTECO, Italy)



Many are the expectations on my future after this project, but the most relevant are:

- Broaden my perception of industrial flow cases and apply my knowledge to some of them;
- Go deep in fluid flows physical modeling and enhance my coding ability;
- improve my soft skills, especially learn how to:
  carry on research, manage the work time, work in an international team.





[M. Olejnik, PhD thesis, 2019]

Thanks