COMETE – Kick-off Meeting
Institute of Fluid Mechanics and Heat Transfer, TU Wien

October 22nd, 2019

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

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Layout of presentation

1. Aims of my PhD
2. Basics of SPH
3. What I have done so far
   a. Accuracy cosiderations
   b. Surface tension modeling
4. Next-term work

1. Aims of my PhD

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

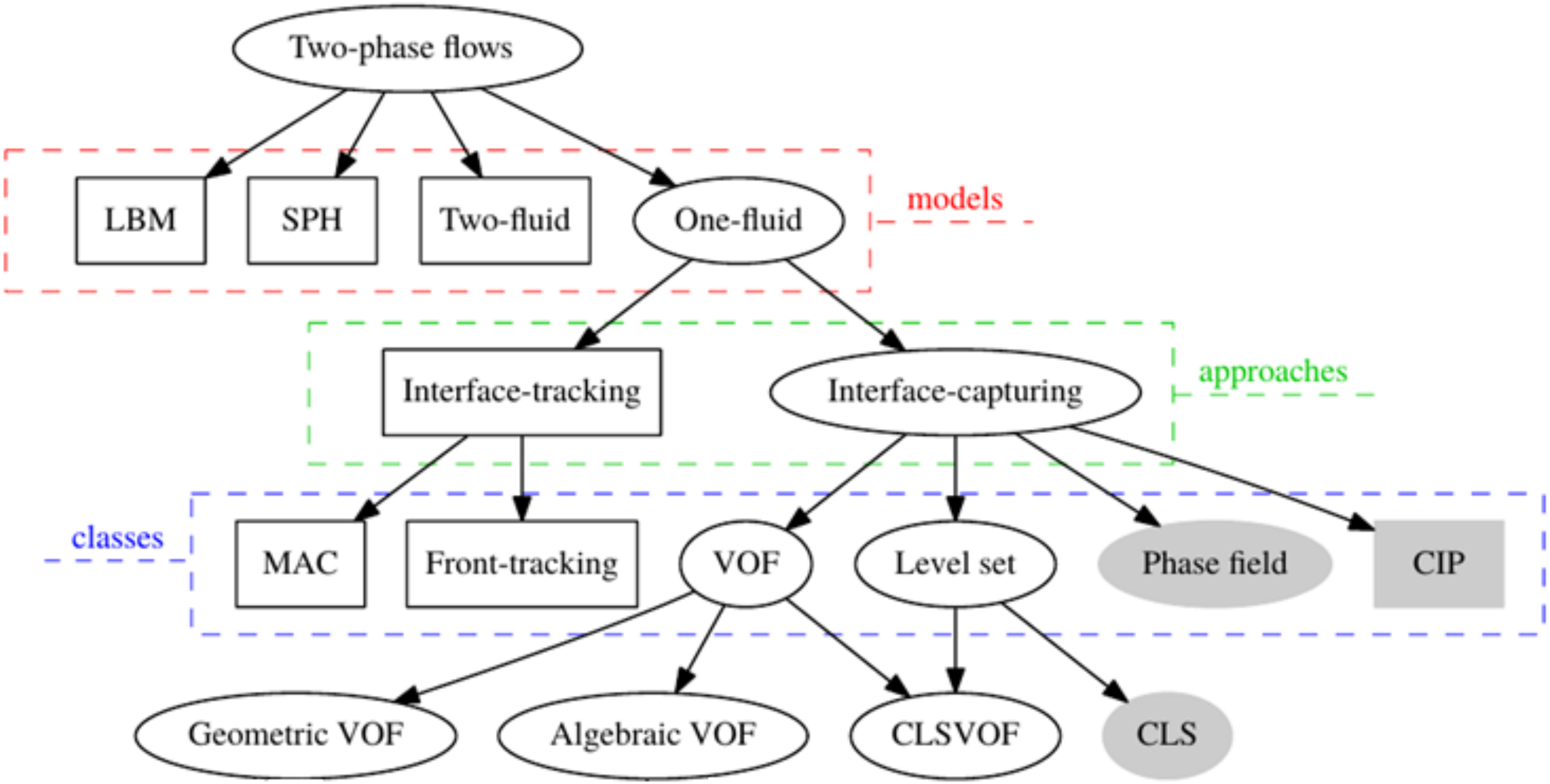
- to upgrade the existing in-house code, starting with improving the interface description and mitigating the occurrence of the micro-mixing phenomena;

- to 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;

- to work on the applications of the SPH approach to industrial cases, for example three phase flow, i.e. two fluids separated by a variable-shape interface plus a disperse solid phase.

2. Basics of SPH

Classification of numerical methods for two-phase flow

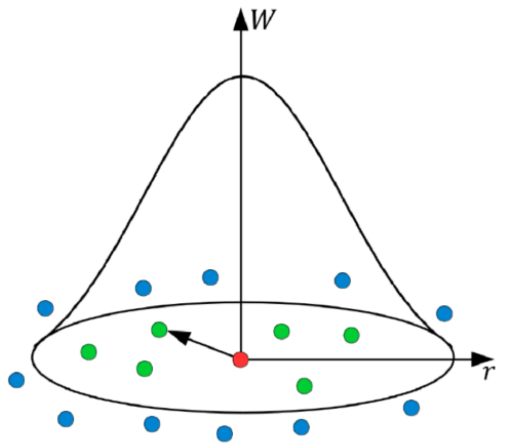


[S. Mirjalili, S.S. Jain, M.S. Dodd, CTR, 2017]

2. Basics of SPH

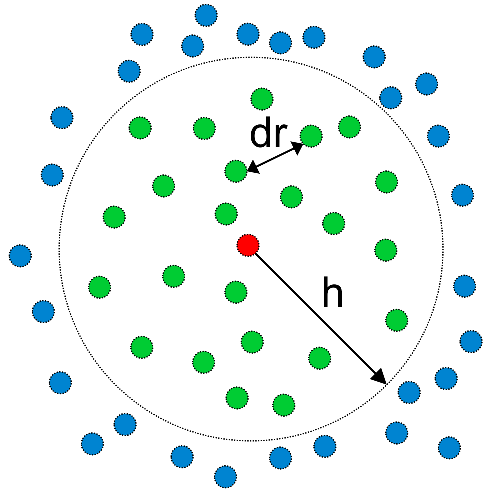
Smoothed

Regularizing functions used (smoothed Dirac delta).



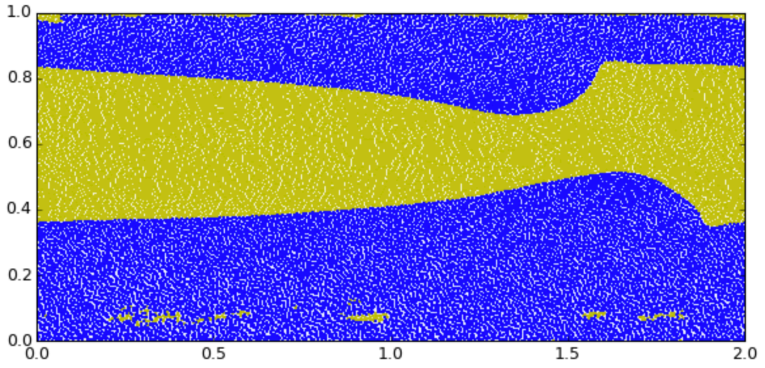
Particle

Particle approach: advection treated exactly, mass conserved.



Hydrodynamics

Liquid in motion developed for astrophysical simulations: Lucy(1977), Monaghan and Gingold (1977).



2. Basics of SPH

Continuous

Discrete

Any scalar or vector field:

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

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

2. Basics of SPH

Governing equations

SPH representation

Continuity equation

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

$$\left\{ \begin{array}{l} \varrho_a = m_a \sum_b W_{ab}(h) = m_a \Theta_a \\ \dfrac{d\varrho_a}{dt} = \varrho_a \sum_b \mathbf{u}_{ab} \cdot \nabla_a W_{ab}(h) \Omega_b \end{array} \right.$$

Advection

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

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

Momentum equation

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\varrho} \nabla p + \nu \nabla^2 \mathbf{u} + \mathbf{g}$$

$$\left\{ \begin{array}{l} \dfrac{d\mathbf{u}_a}{dt} = \mathbf{F}_a + \sum_b \mathbf{F}_{ab}^{\text{interact}} \\ \langle \nu \nabla^2 \mathbf{u} \rangle = \dfrac{1}{m_a} \sum_b \dfrac{2\mu_a \mu_b}{\mu_a + \mu_b} \left(\dfrac{1}{\Theta_a^2} + \dfrac{1}{\Theta_b^2} \right) \dfrac{\mathbf{r}_{ab} \cdot \nabla_a W_{ab}(h)}{r_{ab}^2 + \eta^2} \mathbf{u}_{ab} \\ \left\langle \dfrac{\nabla p}{\varrho} \right\rangle_a = \dfrac{1}{m_a} \sum_b \left(\dfrac{p_a}{\Theta_a^2} + \dfrac{p_b}{\Theta_b^2} \right) \nabla_a W_{ab}(h) \end{array} \right.$$

3. What I have done so far: Accuracy considerations

The purpose

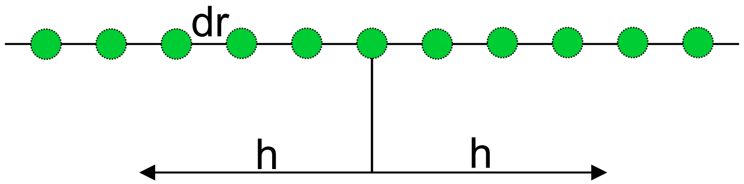
Write a python code able to approximate a 1D analytical function using the SPH method

Equations

The most immediate example is the one-dimensional Wendland kernel

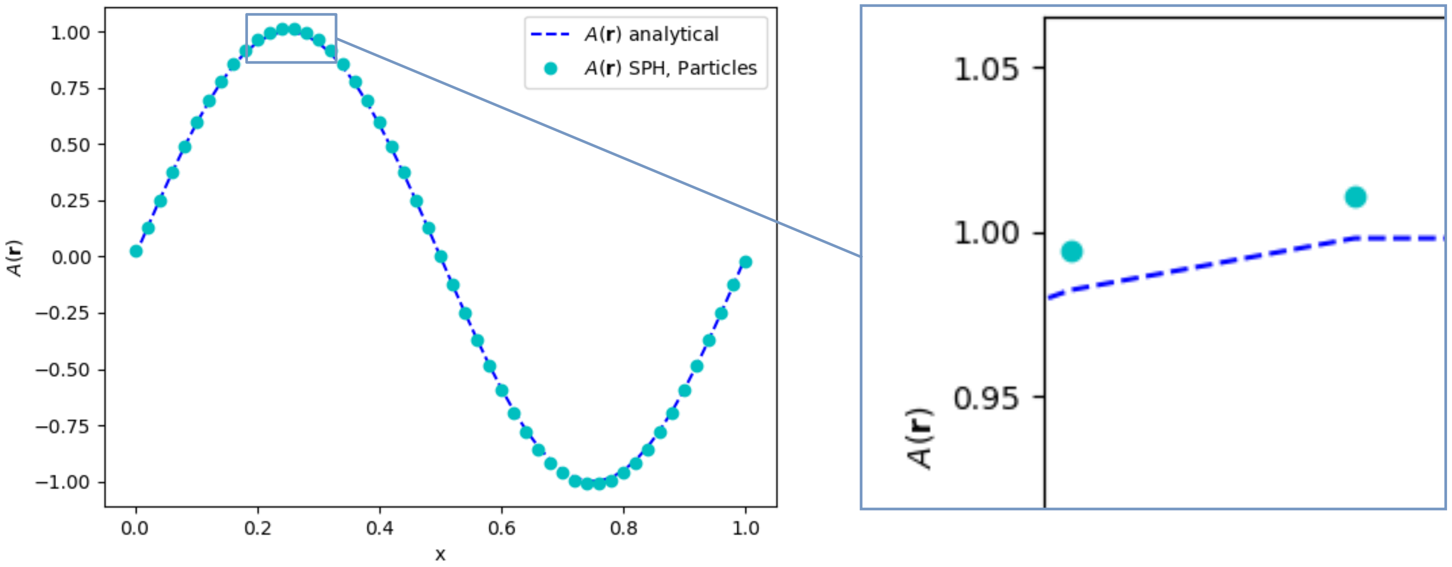
$$W(\boldsymbol{r}, h) = C \begin{cases} \Phi(q) & for\ q > 1 \\ 0 & otherwise \end{cases} \qquad q = |\boldsymbol{r}|/h$$

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

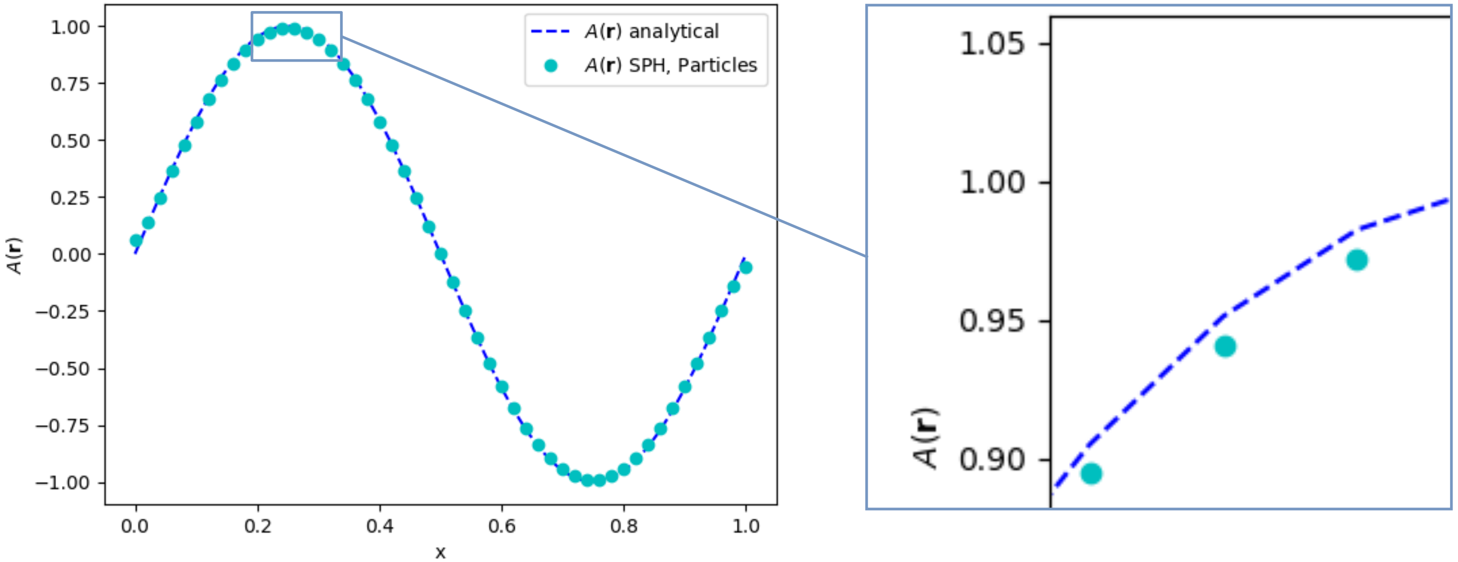


[W. Dehnen, H. Aly, MNRAS, 2012]

Sine function, h/dr = 2



Sine function, h/dr = 4



3. What I have done so far: Accuracy considerations

What we notice

By modifying the value of h/dr the values of SPH approximation may stay above or below the analytical function

But SPH approximation should stay below the analytical function

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

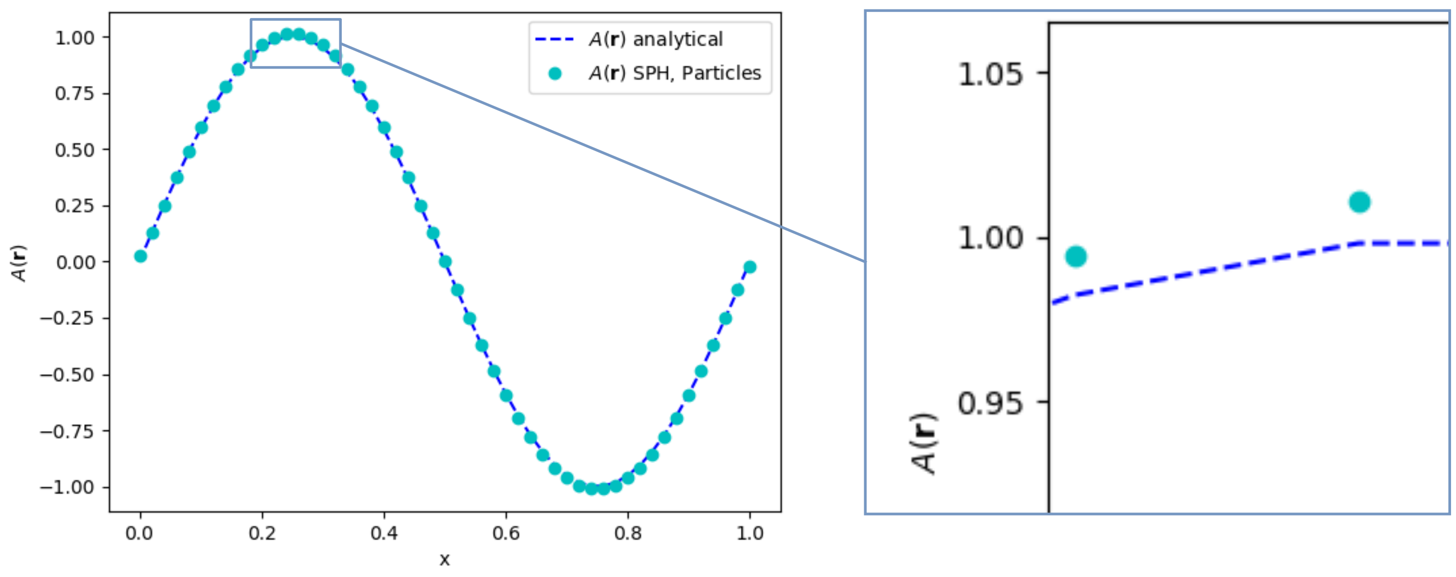
Proof

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

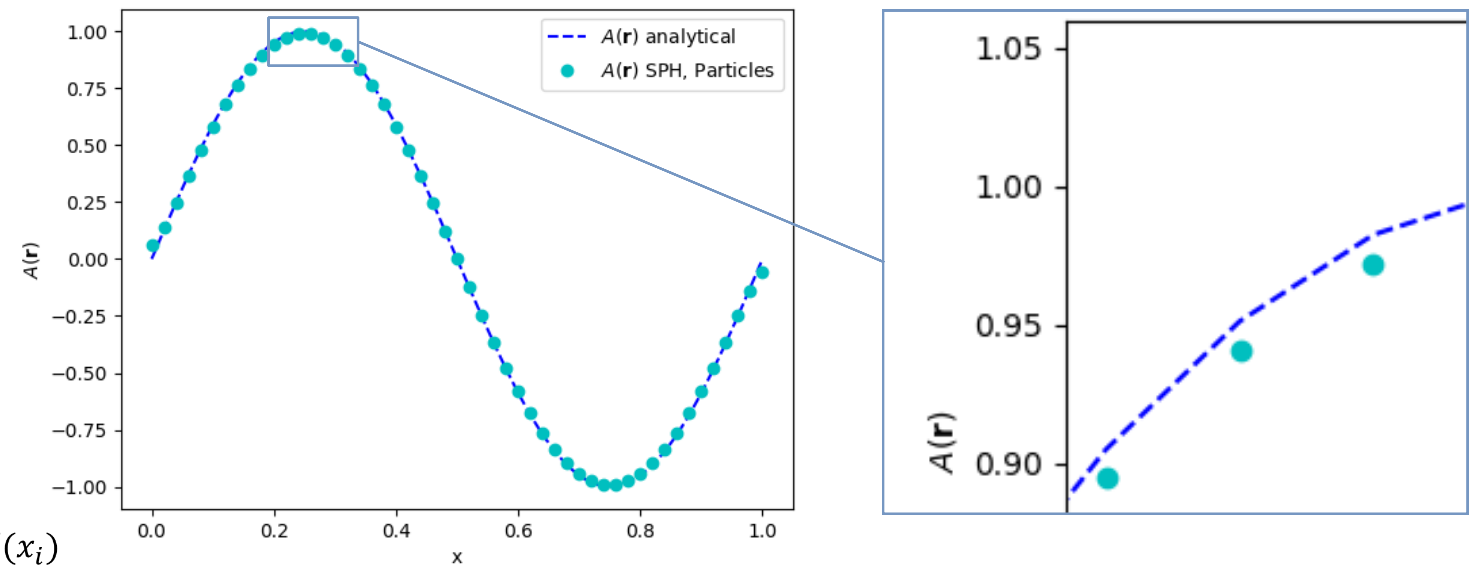
$$\forall\, j \; st \; f(x_j) \leq f(x_i)$$

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

Sine function, h/dr = 2

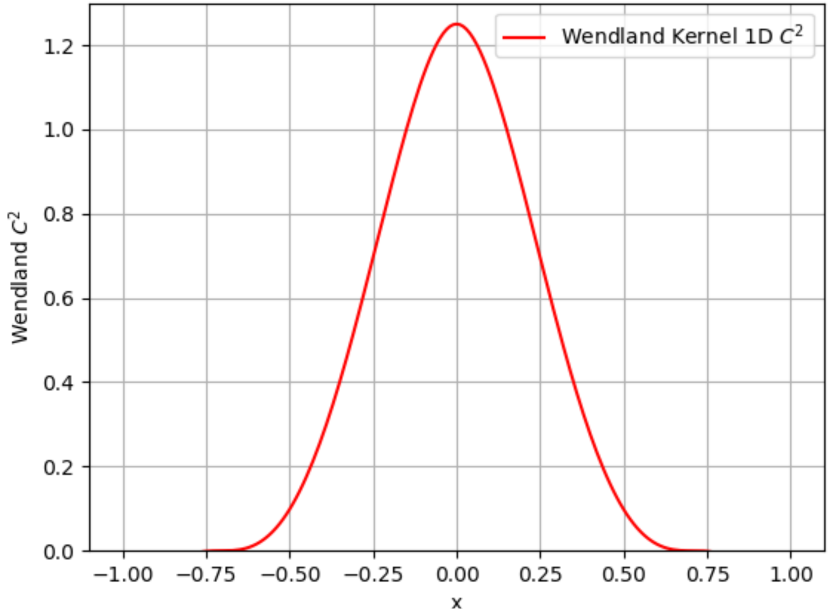


Sine function, h/dr = 4



3. What I have done so far: Accuracy considerations

1D Kernel



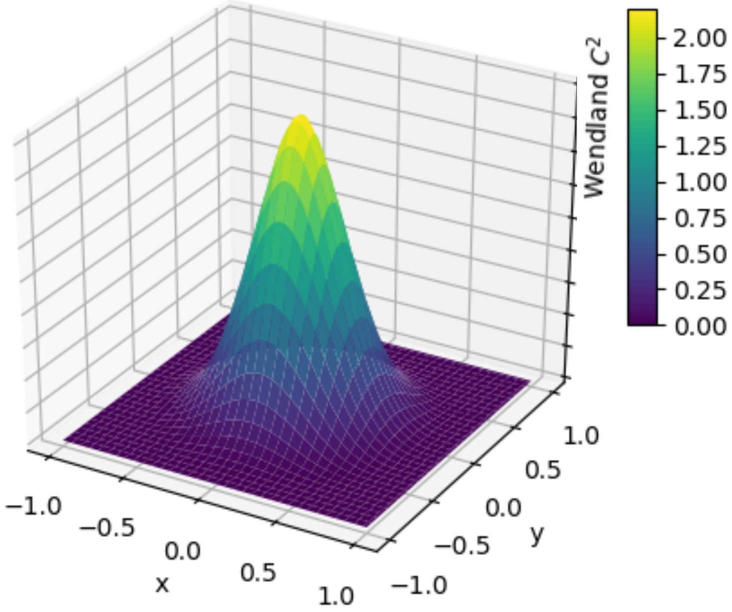
$$W(\boldsymbol{r},h) = C\begin{cases}\Phi(q) & for\ q > 1\\ 0 & otherwise\end{cases}$$

$$q = |\boldsymbol{r}|/h$$

$$1\text{D}, \quad \boldsymbol{r} = f(x)\,, \quad C = \frac{5}{4}\,,$$

$$\Phi(q) = (1-q)^3(1+3q)$$

2D Kernel



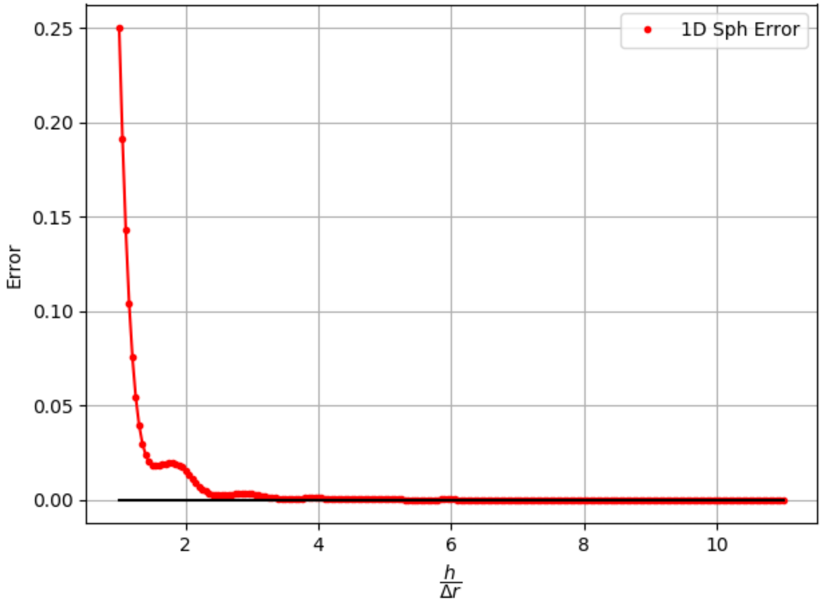
$$\text{W}(\boldsymbol{r},h) = C\begin{cases}\Phi(q) & for\ q > 2\\ 0 & otherwise\end{cases}$$

$$q = |\boldsymbol{r}|/h$$

$$2\text{D}, \quad r = f(x,y)\,, \quad C = \frac{7}{4\pi h^2}$$

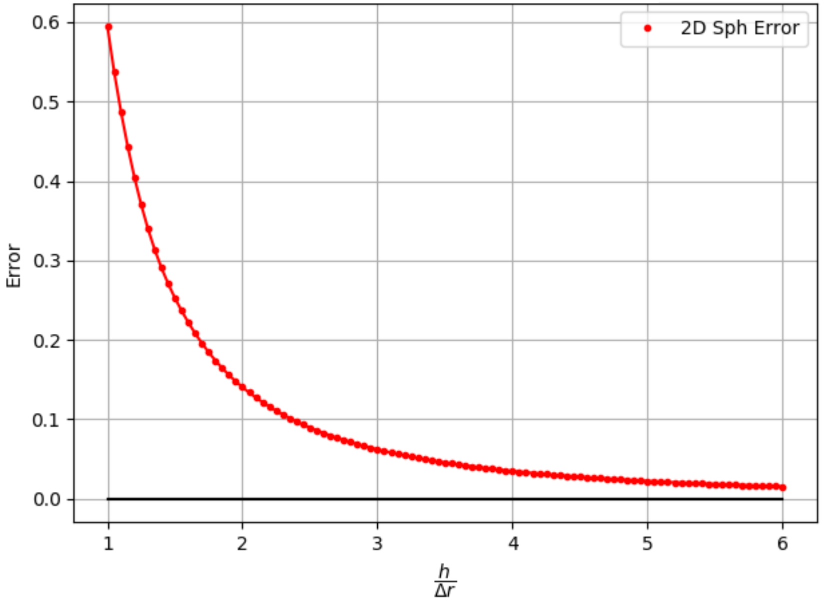
$$\Phi(q) = (1-(q/2))^4(1+2q)$$

[M. Olejnik, PhD thesis, 2019]



1D error

$$err = \sum_j W_{ij}\Omega_j - 1$$



2D error

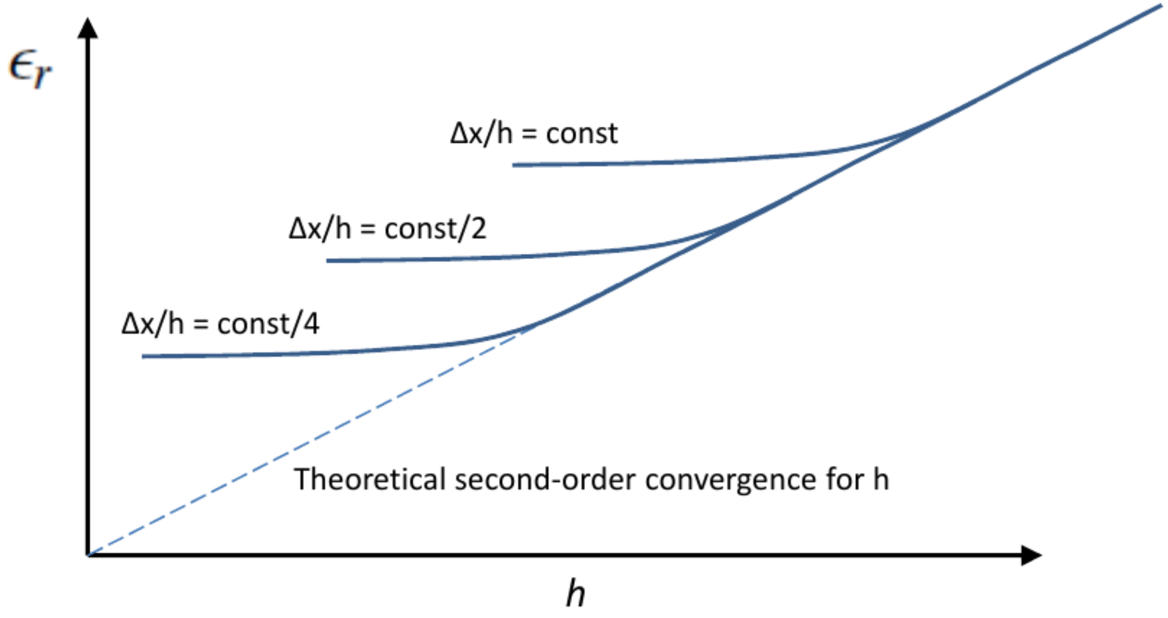
$$err = \sum_j W_{ij}\Omega_j - 1$$

3. What I have done so far: Accuracy considerations

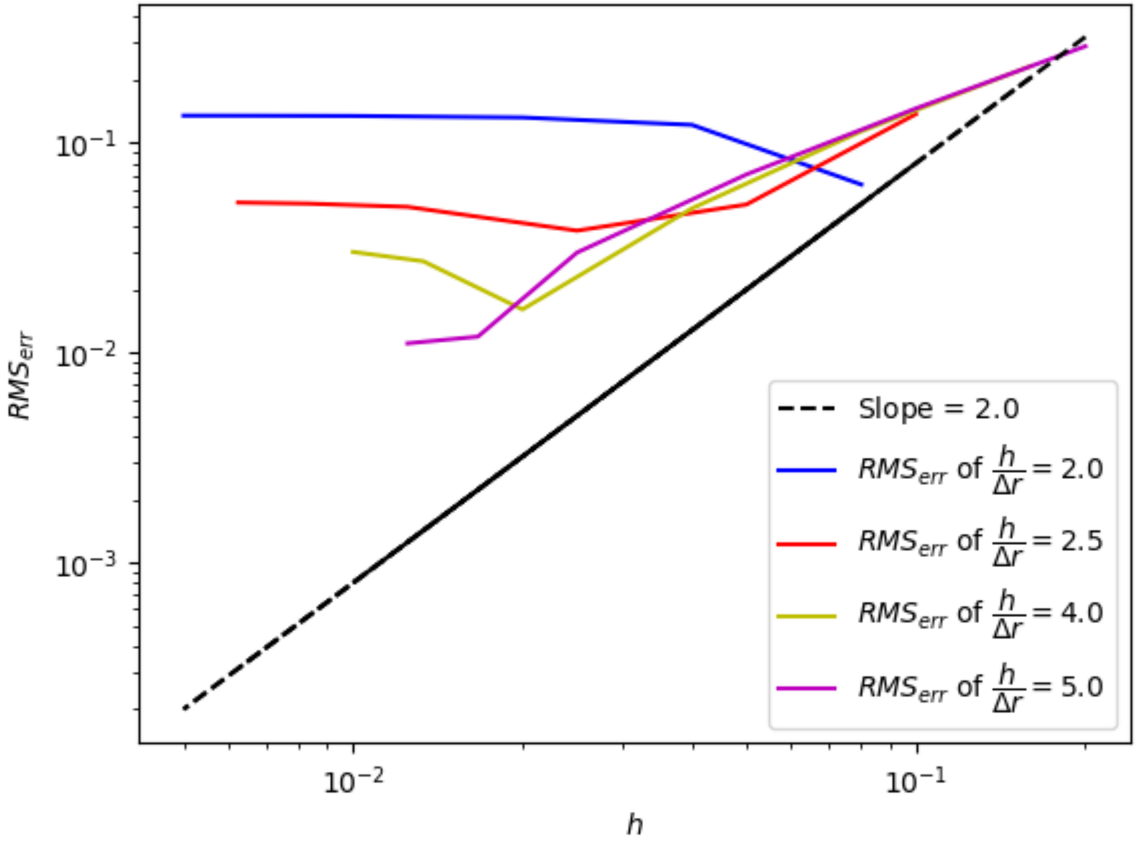
1D Approximation error: from theory… …to computation

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

For example, if we check the convergence of the SPH by decreasing h while $\Delta x/h$ is fixed (i.e. constant number of particles in $\boldsymbol{\Omega}$)…



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

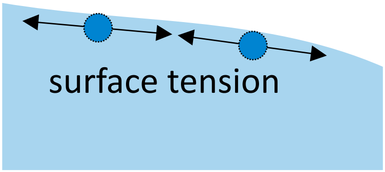


[M. Antuono, TU Delft, 2019]

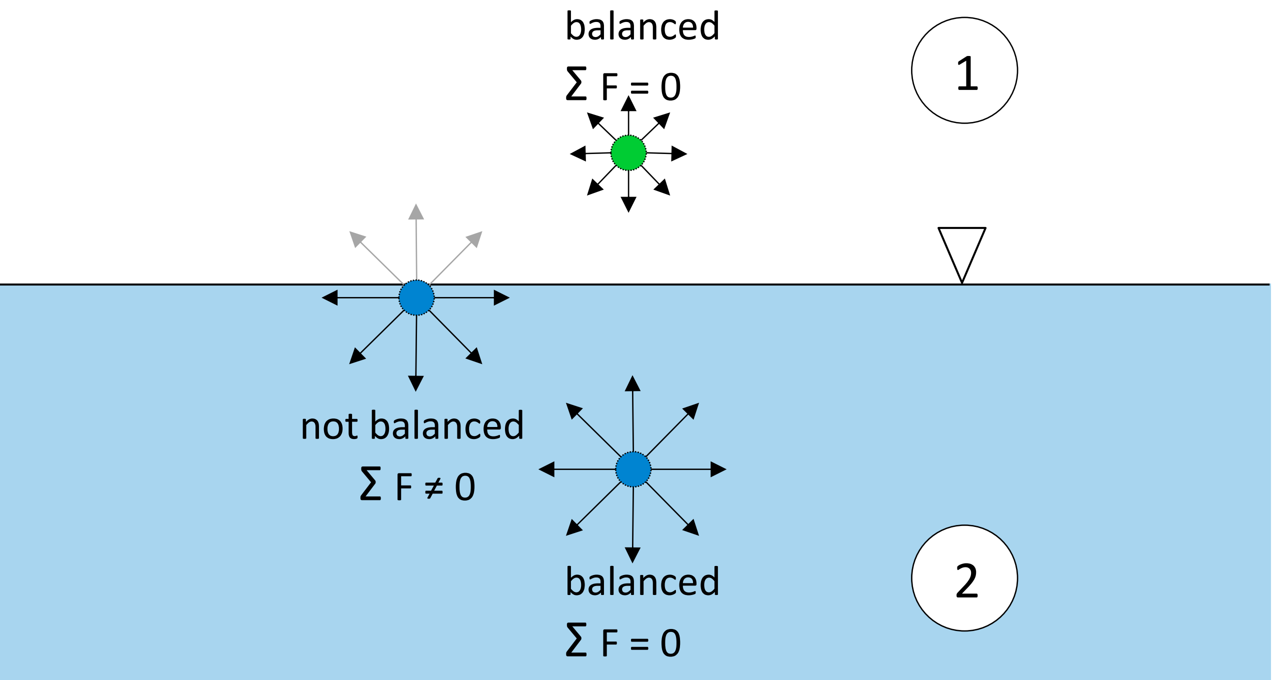
3. What I have done so far: Surface tension modeling

Basics

Material property of a fluid-fluid (1-2) interface whose origins lie in the different attractive intermolecular forces acting in the two phases

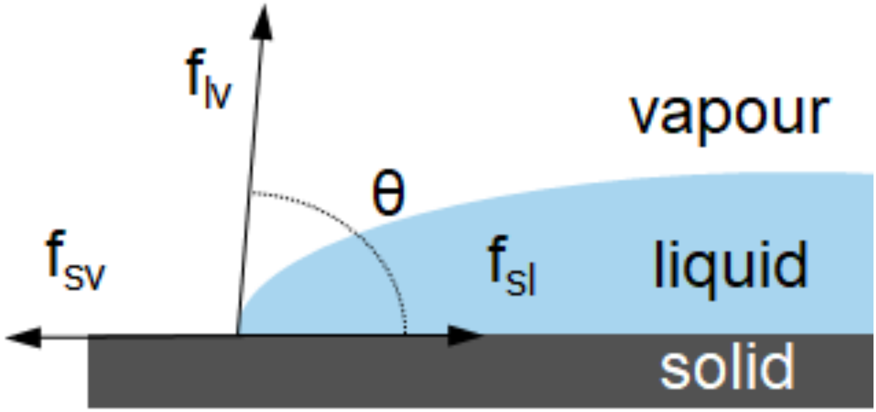


Surface of any liquid behaves as it is covered by a stretched membrane



Wettability

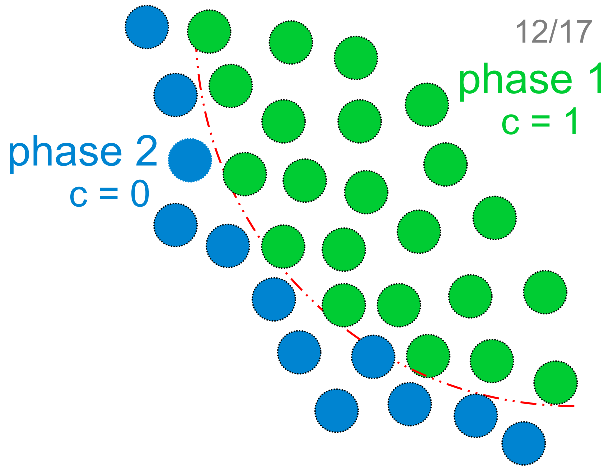
Forces	**Cohesive**: forces of attraction acting between the molecules of same types
	Adhesive: forces of attraction acting between the molecules of different types



The Young-Laplace formula $p_1 - p_2 = f\left(\frac{1}{R_1} + \frac{1}{R_2}\right)$

[L. D. Landau, E. M. Lifschitz, 1987]

3. What I have done so far: Surface tension modeling



Continuum surface force (CSF)

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

$\mathbf{f}_{st} = \mathbf{f}_s \delta_s$ surface force per unit volume

$\delta_s = |\mathbf{n}|$ suitably chosen surface delta function

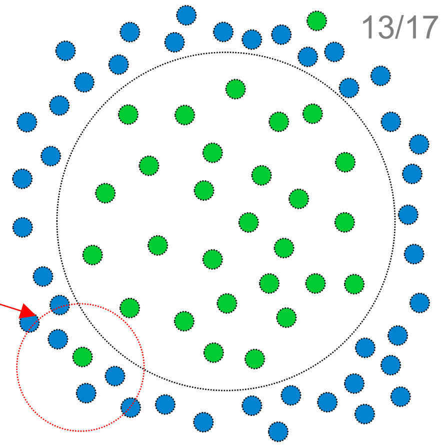
$\mathbf{f}_s = \sigma \kappa \hat{\mathbf{n}}$ surface force per unit area

$\hat{\mathbf{n}} = \frac{\mathbf{n}}{|\mathbf{n}|} = \frac{\nabla c}{|\nabla c|}$ unit vector normal to the interface

$\kappa = -\nabla \cdot \hat{\mathbf{n}}$ local curvature of the interface

σ: surface tension coefficient

3. What I have done so far: Surface tension modeling



$$\mathbf{f}_s = \sigma \kappa \hat{\mathbf{n}}$$

$$\hat{\mathbf{n}} = \frac{\mathbf{n}}{|\mathbf{n}|} = \frac{\nabla c}{|\nabla c|}$$

From Hu & Adams...

Smoothed color function

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

Surface normal vector

$$\mathbf{n_a} = \sum_b (\tilde{c}_b - \tilde{c}_a) \nabla_a W_{ab}(h) \Omega_b$$

Curvature

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

...to Adami, Hu & Adams

Color indicator

$$c_l^k = \begin{cases} 1, & \text{if the kth particle doesn't belong to the phase of particle } l \\ 0, & \text{if the kth particle belongs to the phase of particle } l \end{cases}$$

Color function

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

Surface normal vector

$$\nabla c_i = \frac{1}{V_i} \sum_j [V_i^2 + V_j^2] \tilde{c}_{ij} \frac{\partial W}{\partial r_{ij}} \boldsymbol{e}_{ij}$$

Curvature

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

[S. Adami, X.Y. Hu, N.A. Adams, JCP, 2019]

3. What I have done so far: Surface tension modeling

Square-to-droplet deformation

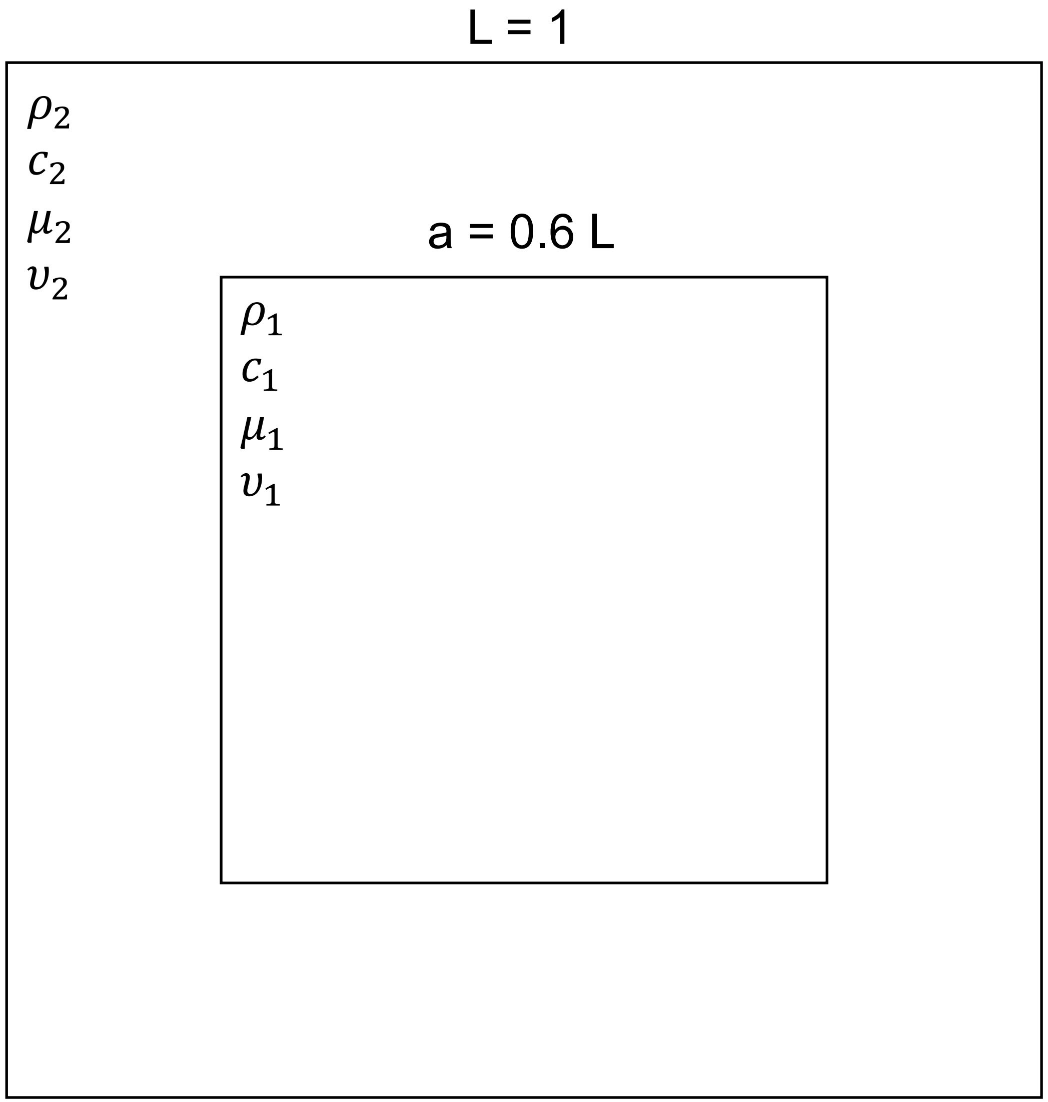
$$S = \int_{\Omega} \delta(\mathbf{x}) \mathrm{d}\Omega$$

Simple method of tracking interface length/area:
Ω contains two phases
S is the interphase length/area
δ(***x***) is a function misureing contribution towards interface at point ***x***

δ(***x***) could be length of normal vector |$\boldsymbol{n}_a$|

$$S \simeq \sum_{a}^{N} |\mathbf{n}_a| \frac{m_a}{\varrho_a}$$

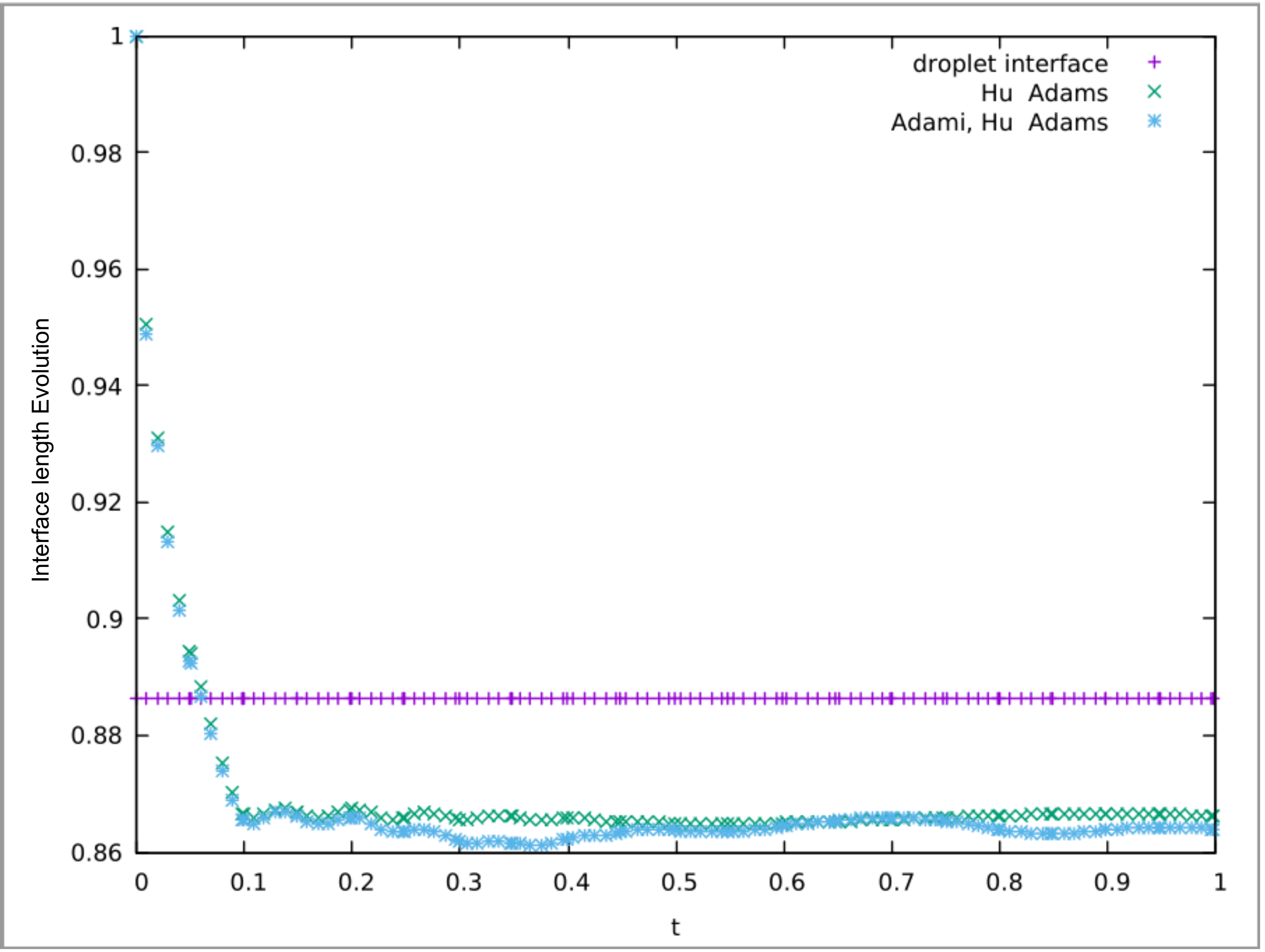
Domain



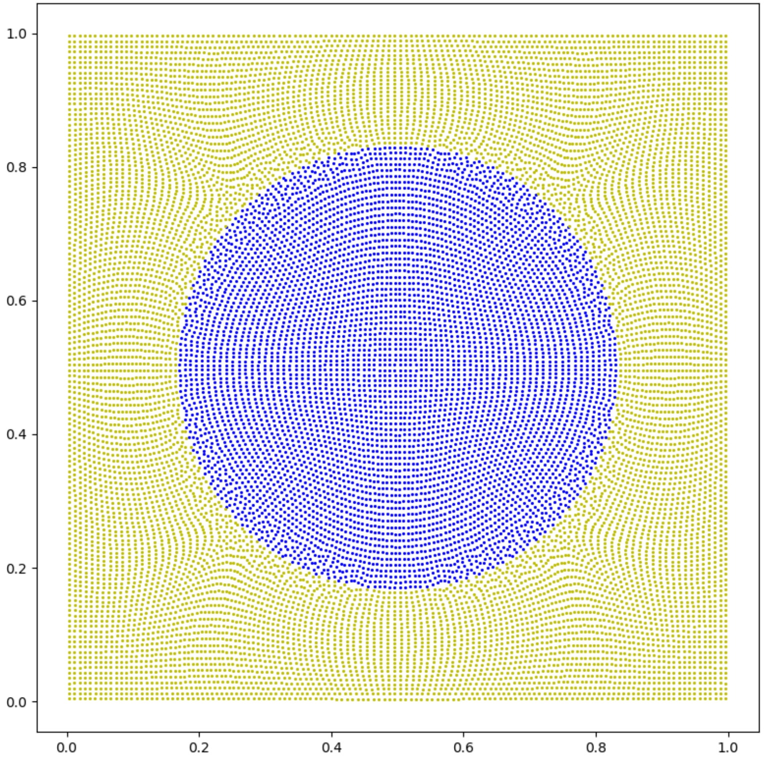
[M. Olejnik, PhD work, 2019]

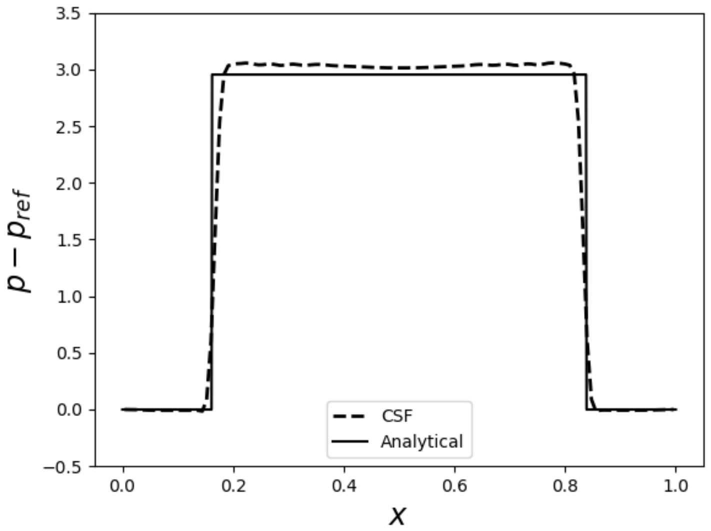
3. What I have done so far: Surface tension modeling

Density ratio = 1



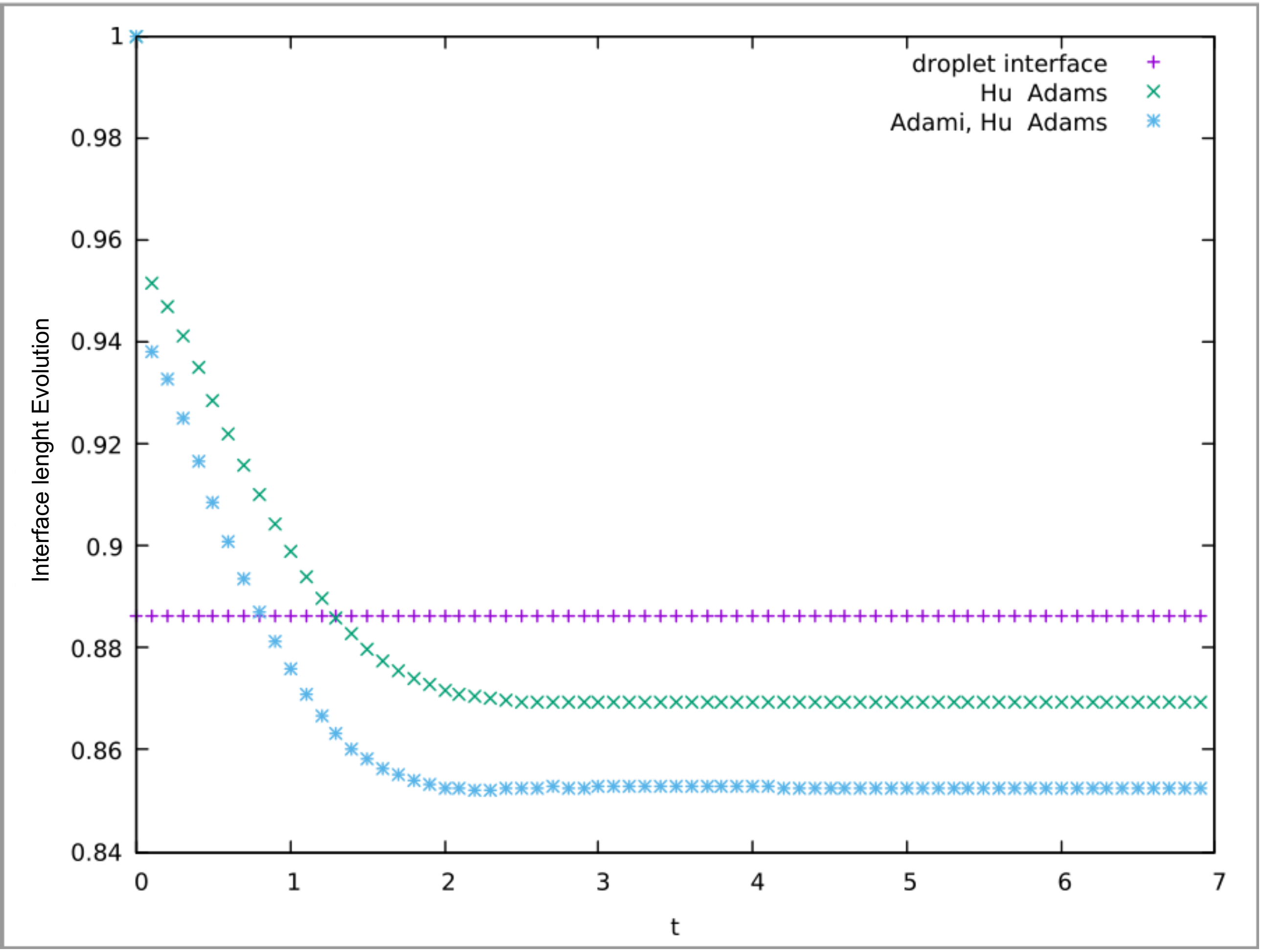
$$\frac{\rho_1}{\rho_2} = 1$$
$$c_1 = 1$$
$$c_2 = 0$$
$$\frac{\mu_1}{\mu_2} = 1$$



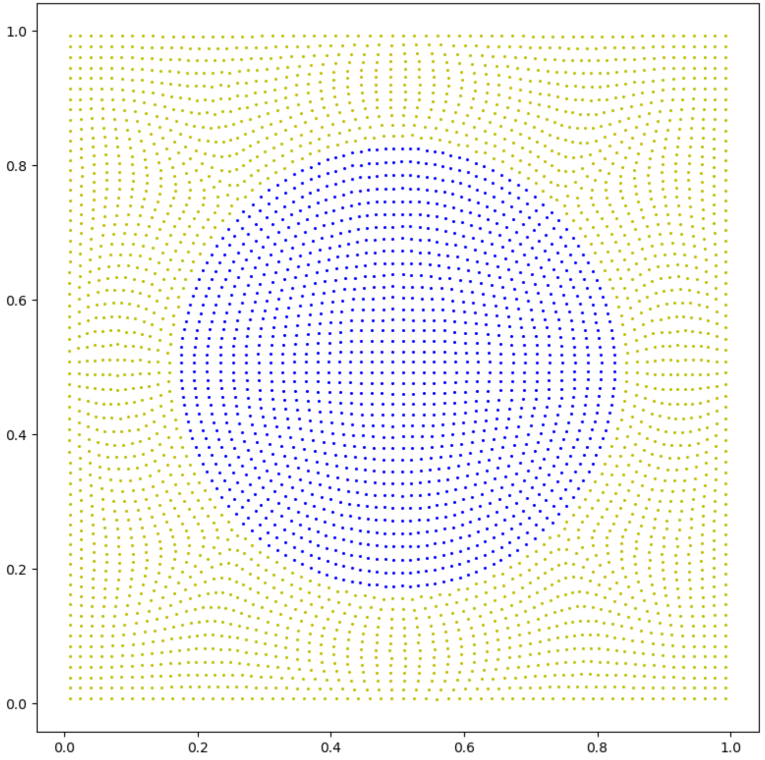


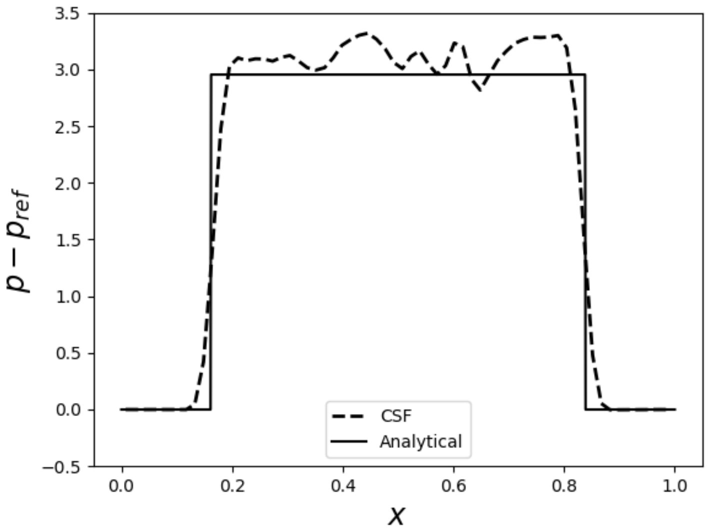
3. What I have done so far: Surface tension modeling

Density ratio = 1000



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





4. Next-term work

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

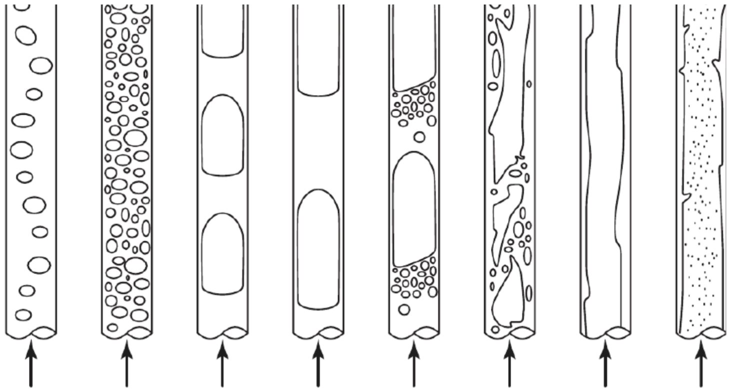
1. upgrade the code: improve the interface description and decrease the occurrence of the micro-mixing phenomena, move on to 3D simulations

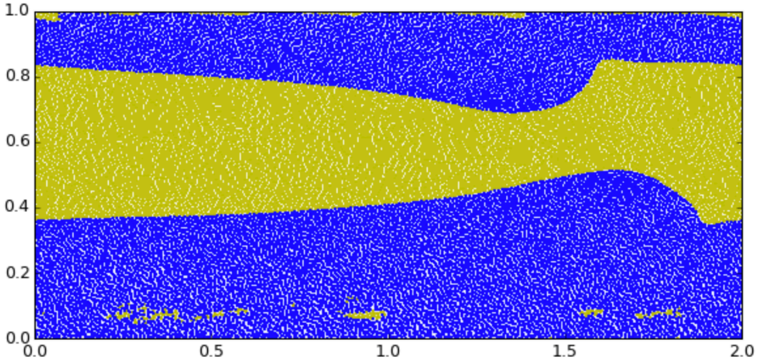
2. improve the physical modelling: three phase flow, i.e. two fluids separated by a variable-shape interface plus a disperse solid phase;

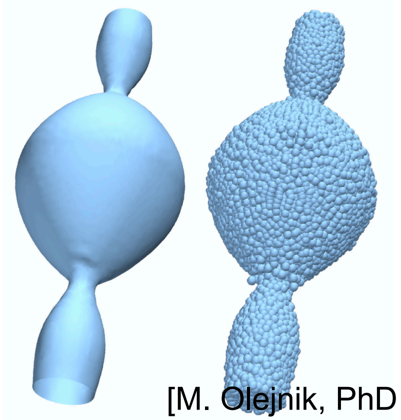
3. assess the SPH approach in applications, some of them to be defined jointly with the industrial partner of the project (Esteco, Italy)

4. later in 2020, we plan to prepare a manuscript of journal publication with the results of points (2) or (3) above

5. anticipated conference, workshop attendance, courses, and/or seminar presentation:
   - 24th Fluid Mechanics Conference, 1-3 July 2020, Rzeszów, Poland
   - Multiphase Flow Conference and Short Course at Helmholtz-Zentrum Dresden Rossendorf (HZDR), November 2020, Dresden, Germany
   - CISM, VKI advanced courses for general CFD knowledge, to widen my perspective on possible future career path







[M. Olejnik, PhD thesis, 2019]

Thanks