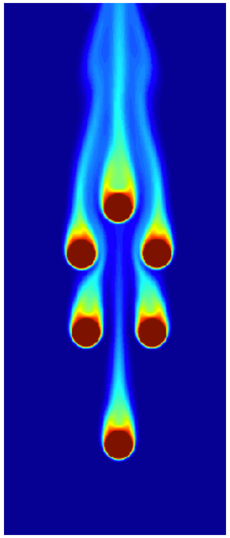
# A penalization method for DNS of weakly compressible reacting gas-solid flows

**Baptiste Hardy,** Juray De Wilde, Grégoire Winckelmans



**72nd APS-DFD, Tuesday, November 26th 2019. S28.00005**

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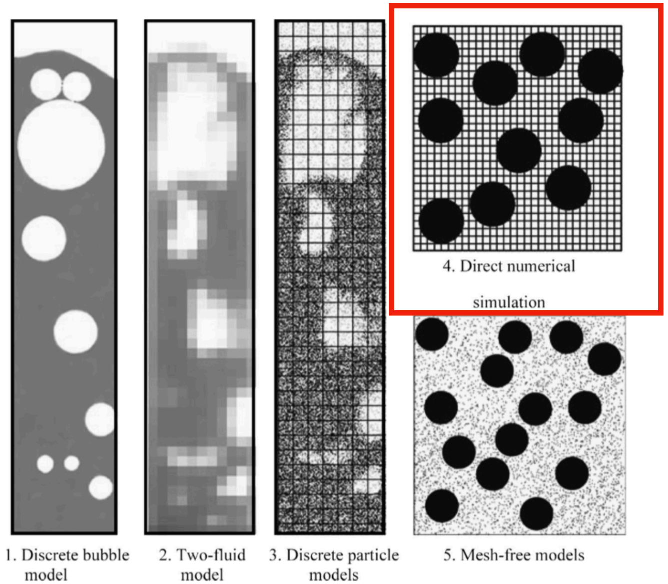
# Motivation

- Modeling strategies

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- Workable large-scale fluidized beds simulation:
  TFM or CFD-DEM
  = particle-unresolved models: $\Delta \gg d_p$

➡ Need for **closure laws**

- PR-DNS = powerful tool to build new closure laws from fundamental conservation principles

- Most PR-DNS work so far based on:
  - Gas-phase **incompressibility** approximation
  - **Uniform description** of the solid phase
- Applications : combustion of coke in FCC: very exothermic + gas expansion
  ➡ Density fluctuations at the particle surface
  ➡ **Weakly compressible** approximation.

# Solid phase treatment : penalization method

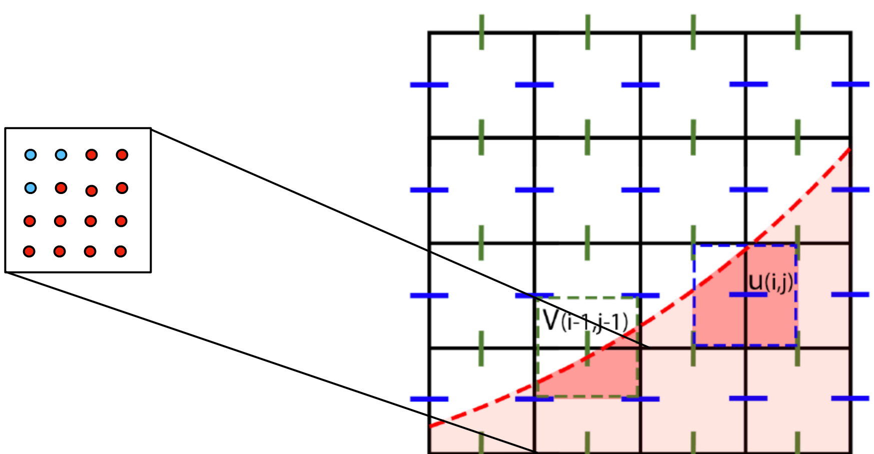
- Continuous-forcing method = impose no-slip boundary condition $\mathbf{u} = \mathbf{u}_s$ through an additional forcing term in Navier-Stokes momentum equation :

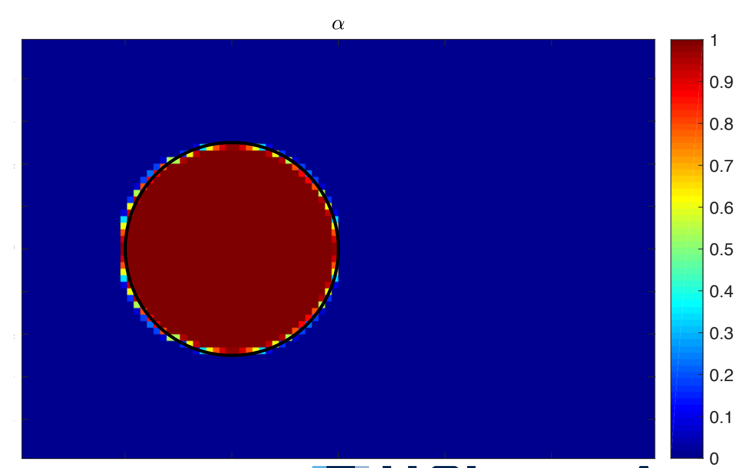
$$\frac{\partial}{\partial t}\left(\rho \mathbf{u}\right) + \nabla \cdot \left(\rho \mathbf{u}\mathbf{u}\right) = -\nabla \tilde{p} + \nabla \cdot \boldsymbol{\tau} + \mathbf{f}$$

Kajishima et al., IJHFF, 2002

$$\mathbf{f} = \alpha\rho\frac{(\mathbf{u}_s - \mathbf{u})}{\Delta t}$$

- Solid phase is tracked with a **solid volume fraction** $\alpha$
- Sub-divide each cell in sub-cells, check whether the sub-cell belongs to the body




Reproduced from *Luca Brandt's course, CISM, Udine, July 2019*

# Scalars treatment at particle boundary

What BC at the particle surface for temperature and species mass fractions ?

- **Case 1 : Uniform solid phase description = Dirichlet BC**
  - $T = T_s$ : uniform temperature over the particle
    (= equivalent to very large solid phase thermal conductivity)
  - Reaction $A \rightarrow B$ with $Y_A = 0,\ Y_B = 1$
    (= « infinitely » fast reaction, the surface of the particle is free of any reactant)

  ➡ **Penalize scalar transport equations similarly to momentum equation**

# Algorithm: Dirichlet BC at the surface of the particles

- Advance scalars : $Z = Y_k$ or $T$, with no forcing term

$$Z^* = Z^n + \Delta t \mathscr{F}(RHS^n, RHS^{n-1})$$

- Penalize scalars

$$q = \alpha \frac{(Z_s - Z^*)}{\Delta t}$$

$$Z^{n+1} = Z^* + \Delta t\, q$$

- Compute density from equation of state

$$\rho^{n+1} = \frac{p_0 \bar{W}^{n+1}}{R T^{n+1}}$$

- Compute velocity predictor

$$\mathbf{u}^* = \frac{1}{\rho^{n+1}} \left( \rho^n \mathbf{u}^n + \Delta t \mathscr{F}(\mathbf{RHS}^n, \mathbf{RHS}^{n-1}) \right)$$

- Penalize velocity

$$\mathbf{f} = \rho^{n+1} \alpha \frac{(\mathbf{u}_s - \mathbf{u}^*)}{\Delta t}$$

$$\mathbf{u}^{**} = \mathbf{u}^* + \frac{\Delta t}{\rho^{n+1}} \mathbf{f}$$

- Projection step

$$\nabla^2 \phi = \frac{1}{\Delta t} \left( \left( \frac{\partial \rho}{\partial t} \right) + \nabla \cdot \left( \rho^{n+1} \mathbf{u}^{**} \right) \right)$$

$$\mathbf{u}^{n+1} = \mathbf{u}^{**} - \Delta t \nabla \phi \,/\, \rho^{n+1}$$

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# Body Motion

- Hydrodynamic forces and torques evaluation :

$$\mathbf{F}_{f\to s} = \oint_{S_p} \boldsymbol{\sigma}\cdot\mathbf{n}\,ds \qquad\qquad \mathbf{T}_{f\to s} = \oint_{S_p} (\mathbf{r}\wedge\boldsymbol{\sigma})\cdot\mathbf{n}\,ds$$

$$= \int_{V_p} \nabla\cdot\sigma\,dv \qquad\qquad = \int_{V_p} (\mathbf{r}\wedge\nabla\cdot\boldsymbol{\sigma})\,dv$$

$$= \frac{d}{dt}\int_{V_p}\rho\mathbf{u}\,dv - \int_{V_p}\mathbf{f}dV \qquad\qquad = \frac{d}{dt}\int_{V_p}(\mathbf{r}\wedge\rho\mathbf{u})\,dv - \int_{V_p}(\mathbf{r}\wedge\mathbf{f})dV$$

- Body motion solver

$$\mathbf{u}_p^{n+1} = \mathbf{u}_p^n + \frac{1}{\rho_p V_p}\left\{\left(\int_{V_p}\rho\,\mathbf{u}\,dv\right)^n - \left(\int_{V_p}\rho\,\mathbf{u}\,dv\right)^{n-1}\right\} - \frac{\Delta t}{\rho_p V_p}\int_{V_p}\mathbf{f}^n\,dv + \frac{\Delta t}{\rho_p V_p}\mathbf{F}^n_{coll} + \Delta t\left(1 - \frac{\int \rho^n\,dv}{\rho_p V_p}\right)\mathbf{g}$$

$$\boldsymbol{\Omega}_p^{n+1} = \boldsymbol{\Omega}_p^n + \frac{1}{\rho_p J_p}\left\{\left(\int_{V_p}(\mathbf{r}\wedge\rho\,\mathbf{u})\,dv\right)^n - \left(\int_{V_p}(\mathbf{r}\wedge\rho\,\mathbf{u})\,dv\right)^{n-1}\right\} - \frac{\Delta t}{\rho_p J_p}\int_{V_p}(\mathbf{r}\wedge\mathbf{f}^n)\,dv + \frac{\Delta t}{\rho_p J_p}\mathbf{T}^n_{coll}$$

$$\mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \frac{\Delta t}{2}\left(\mathbf{u}_p^{n+1} + \mathbf{u}_p^n\right)$$

$$\boldsymbol{\theta}_p^{n+1} = \boldsymbol{\theta}_p^n + \frac{\Delta t}{2}\left(\boldsymbol{\Omega}_p^{n+1} + \boldsymbol{\Omega}_p^n\right)$$

$$\Rightarrow \mathbf{u}_s^{n+1}(\mathbf{x}) = \mathbf{u}_p^{n+1} + \boldsymbol{\Omega}_p^{n+1}\wedge(\mathbf{x} - \mathbf{x}_p^{n+1})$$

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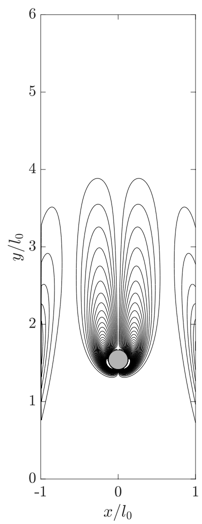
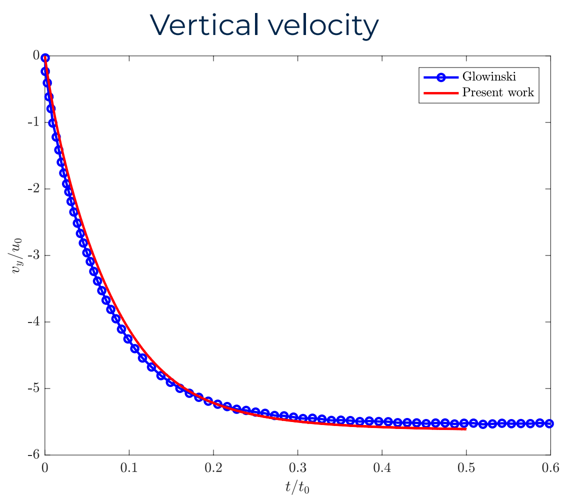
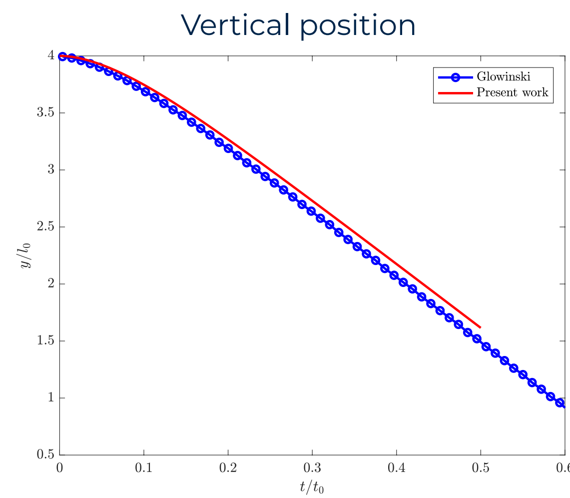
# Validation: cold flow

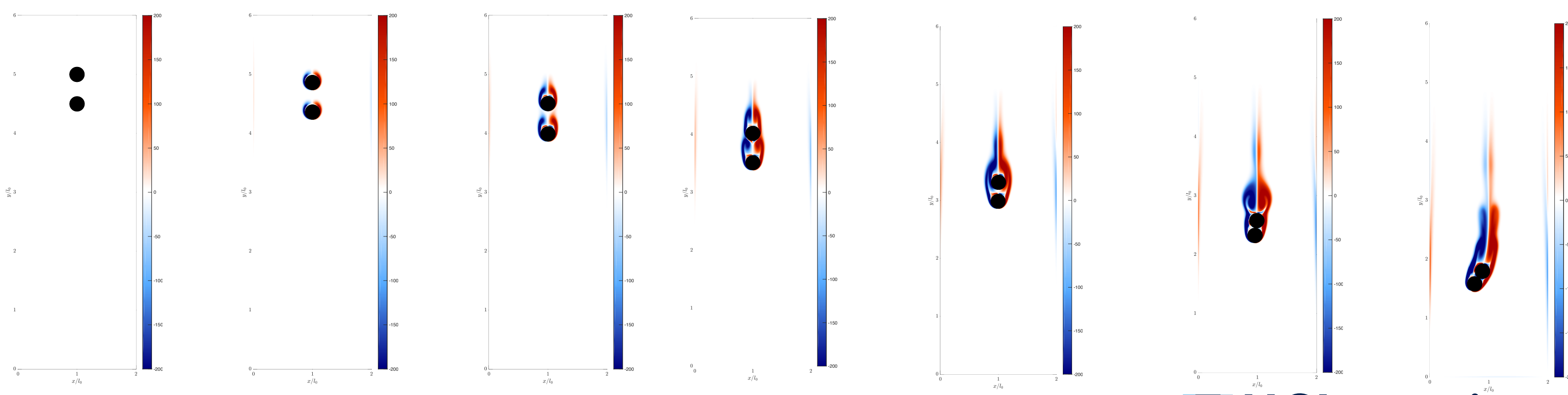
- Sedimentation of a particle in a closed cavity




- Drafting-Kissing-Tumbeling





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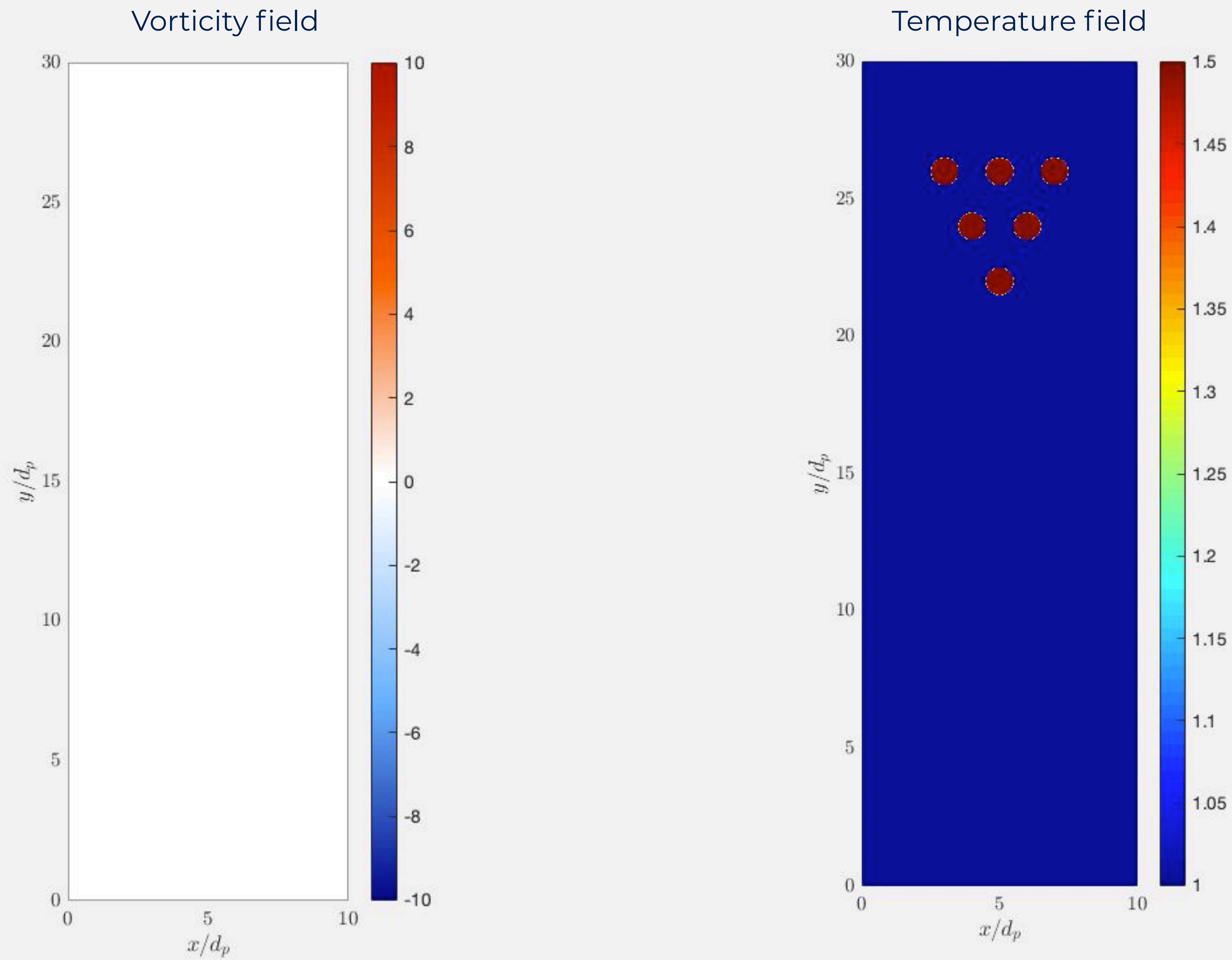
# Sedimentation of 5 particles with fixed temperature



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  ➡ **Penalize scalar transport equations similarly to momentum equation**

- **Case 2 : Coupled heat and mass transfer (CHMT) between fluid/solid phases**

  ➡ Continuity of the scalar function + **fluxes** at the interface
  - $T_f = T_s$ (but not known a priori)
  - $Y_{k,f} = Y_{k,s}$ (but not known a priori)
  - $\mathbf{q}_f = \mathbf{q}_s \Leftrightarrow \kappa_f \dfrac{\partial T_s}{\partial \mathbf{n}} = \kappa_f \dfrac{\partial T_f}{\partial \mathbf{n}}$
  - $\mathbf{j}_{A,f} = \mathbf{j}_{A,s} \Leftrightarrow D_{A,s} \left.\dfrac{\partial (Y_A \bar{W})}{\partial \mathbf{n}}\right|_s = D_{A,f} \left.\dfrac{\partial (Y_A \bar{W})}{\partial \mathbf{n}}\right|_f$

  ➡ **Need to modify the diffusion operator to account for discontinuities in transport coefficients**

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# Sharp interface method for CHMT

- 1-D illustration: possible discontinuity in first derivative
- 2-D :

$$a_\Gamma = f^+ - f^- = [f]_\Gamma = 0$$

Continuous function

$$b_{\Gamma_x} = \beta^+ f_x^+ - \beta^- f_x^- = [\beta f_x]_\Gamma$$

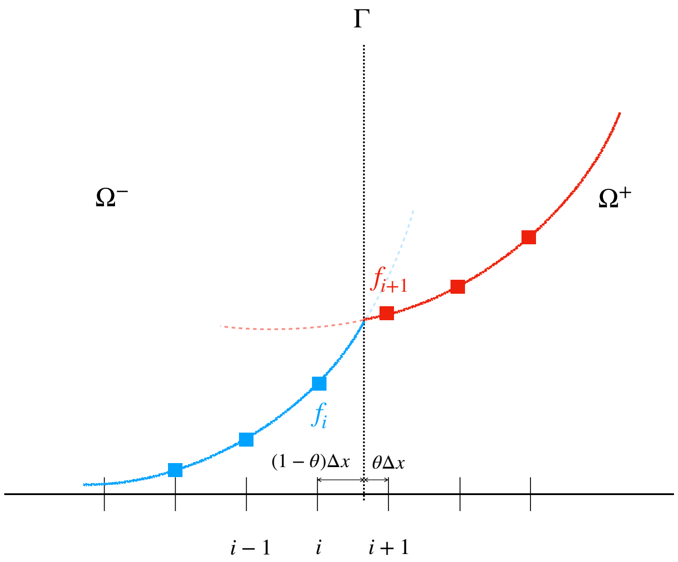
$$b_{\Gamma_y} = \beta^- f_y^+ - \beta^- f_y^- = [\beta f_y]_\Gamma$$

- Finite difference framework : we need information on jumps along cartesian coordinates:

Continuous flux

$$b_{\Gamma,x} = \cancel{b_{\Gamma,n}} n_x - b_{\Gamma,s} n_y = -b_{\Gamma,s} n_y$$

$$b_{\Gamma,y} = \cancel{b_{\Gamma,n}} n_y + b_{\Gamma,s} n_x = b_{\Gamma,s} n_x$$




- Modification of the diffusion operator when an interface is identified

$$\nabla \cdot (\beta \nabla f) = \left[ \beta_{i+1/2,j} \left( \frac{f_{i+1,j} - f_{i,j}}{\Delta x} \right) - \beta_{i-1/2,j} \left( \frac{f_{i,j} - f_{i-1,j}}{\Delta x} \right) \right] \Big/ \Delta x$$

$$+ \left[ \beta_{i,j+1/2} \left( \frac{f_{i,j+1} - f_{i,j}}{\Delta y} \right) - \beta_{i,j-1/2} \left( \frac{f_{i,j} - f_{i,j-1}}{\Delta y} \right) \right] \Big/ \Delta y - \left( F^x + F^y \right)$$

with additional terms depending on the jump conditions: $F_x(a_\Gamma, \mathbf{b}_\Gamma), F_y(a_\Gamma, \mathbf{b}_\Gamma)$.

Shao et al., IJHMT, 2012
Sulaiman et al., Chem Eng. Sc., 2019

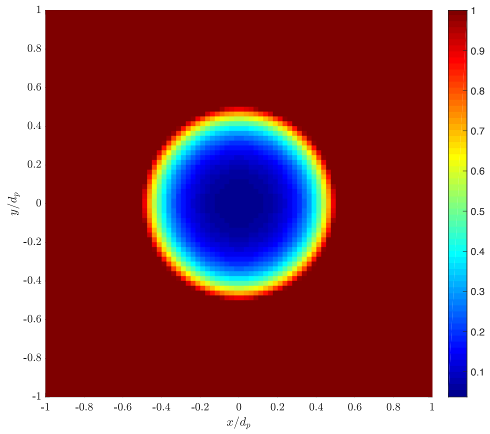
# Validation: sharp interface for CHMT

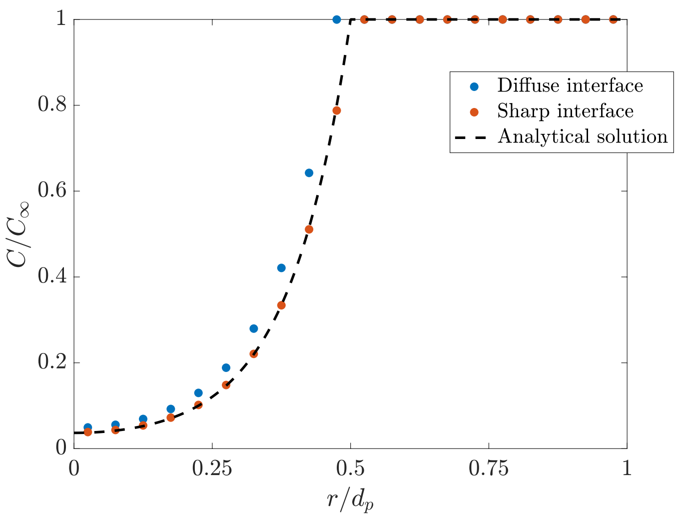
- Steady-state reaction-diffusion in a cylindrical particle

$$\nabla_r \cdot \left(D_s \nabla_r C\right) - kC = 0, \text{ with } C(r = R) = C_\infty$$

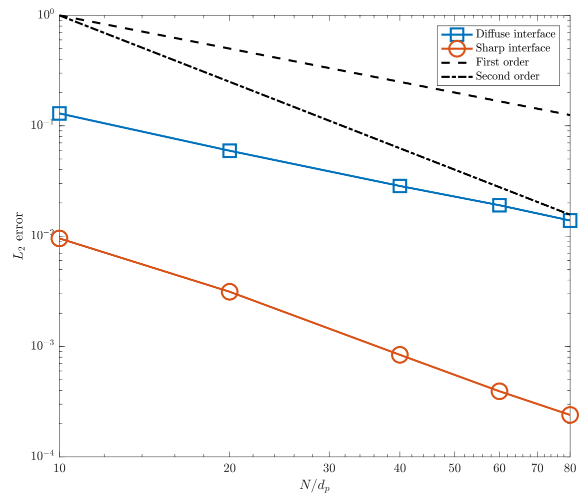
- Analytical solution :

$$\frac{C(r)}{C_\infty} = \frac{J_0\left(i\sqrt{Da}\frac{r}{d_p}\right)}{J_0\left(i\frac{\sqrt{Da}}{2}\right)}, \text{ with } Da = \frac{d_p^2 k}{D_s}.$$




Concentration profile, $D = 20h, Da = 100$

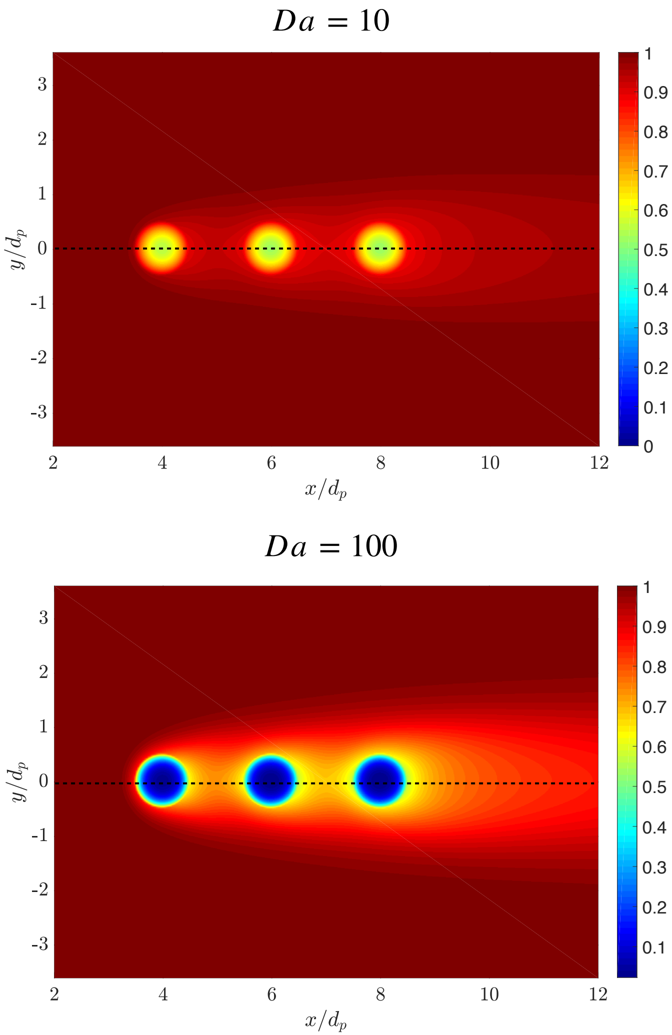



Evolution of the $L_2$ error

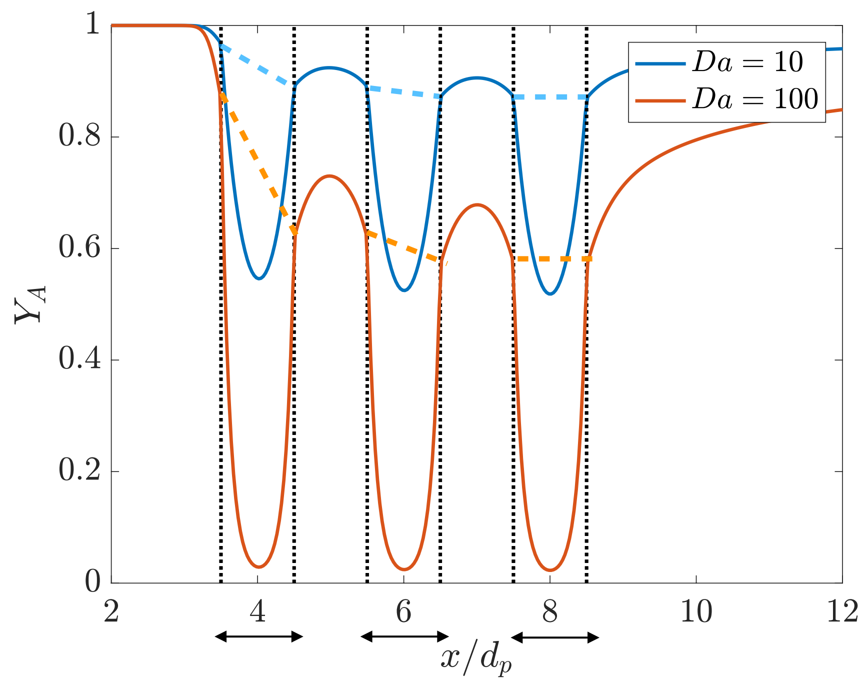
# Application: 3-inline catalytic particles

Catalytic reaction $A \rightarrow B$, $Re_p = 40$, $Sc = 0.7$, $D_f/D_s = 10$

Reactant mass fraction field




Longitudinal mass fraction profile

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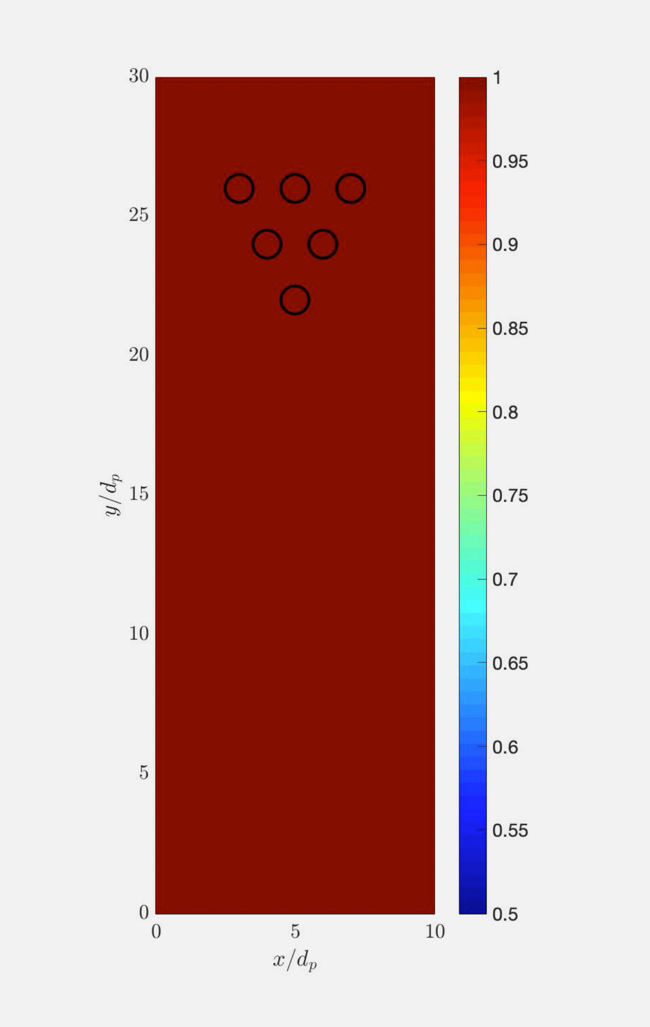
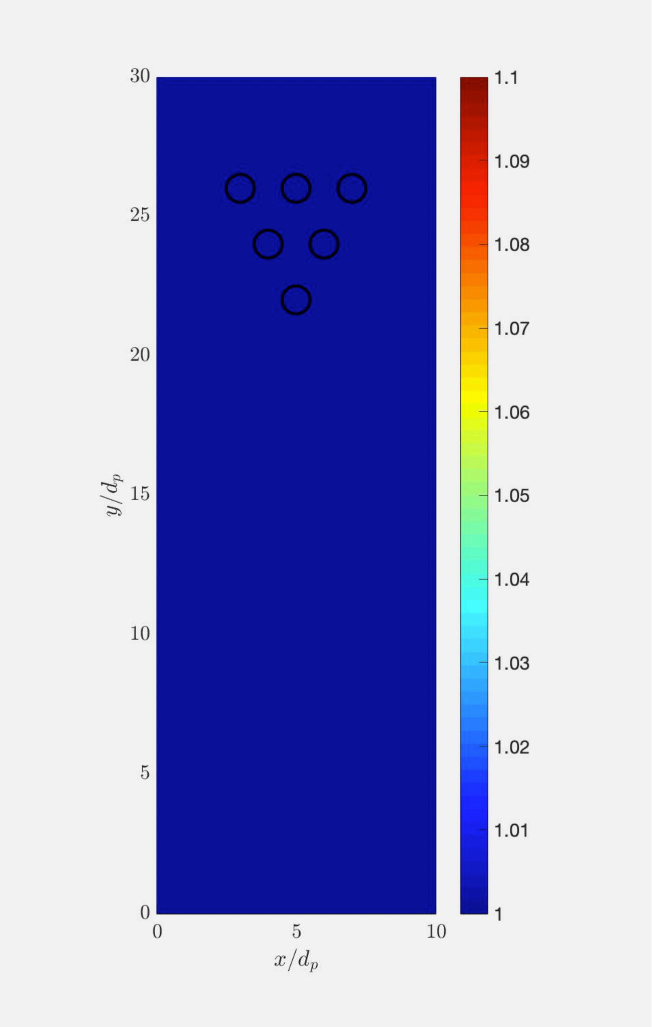
# Sedimentation of 5 particles with coupled heat and mass transfer

Reactant mass fraction field




Temperature field

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# Conclusion

- Original combination of the penalization method and the weakly compressible approximation
- Validation of the numerical method
- Applications: particulate flows with chemical reactions and various boundary conditions:
  - Fixed temperature / composition
  - Coupled heat and mass transfer between phases
- Current extension to 3D

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# Acknowledgments


- Baptiste Hardy is a Research Fellow of the Fonds de la Recherche Scientifique - FNRS, under grant FC 23583
- The present research benefited from computational resources made available on the Tier-1 supercomputer of the Fédération Wallonie-Bruxelles, infrastructure funded by the Walloon Region under the grant agreement n°1117545.
- Computational resources have been provided by the Consortium des Équipements de Calcul Intensif (CÉCI), funded by the Fonds de la Recherche Scientifique de Belgique (F.R.S.-FNRS) under Grant No. 2.5020.11 and by the Walloon Region.


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