A Hybrid Fictitious Domain-Immersed Boundary Method for the Direct Simulation of Heat and Mass Transport in Fluid-Particle Systems

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March 14 2016, LIGGGHTS and CFDEM coupling user meeting, Linz

Our Goal

Solving the transport equations in complex domains using a simple cartesian mesh

$$\frac{\partial u_i}{\partial x_i} = 0$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_j \partial x_j} + f_i^{IB}$$

$$\frac{\partial \theta}{\partial t} + \frac{\partial u_i \theta}{\partial x_i} = \frac{1}{Pe}\frac{\partial^2 \theta}{\partial x_i \partial x_i} + Q^{IB}$$

And boundary conditions...

Take into account the presence of rigid bodies inside the fluid domain

Immersed Boundary

The forcing term imposes the Dirichlet boundary condition at the immersed body surface*.

Fictitious Domain

The forcing term a imposes a rigidity condition inside the immersed body**.

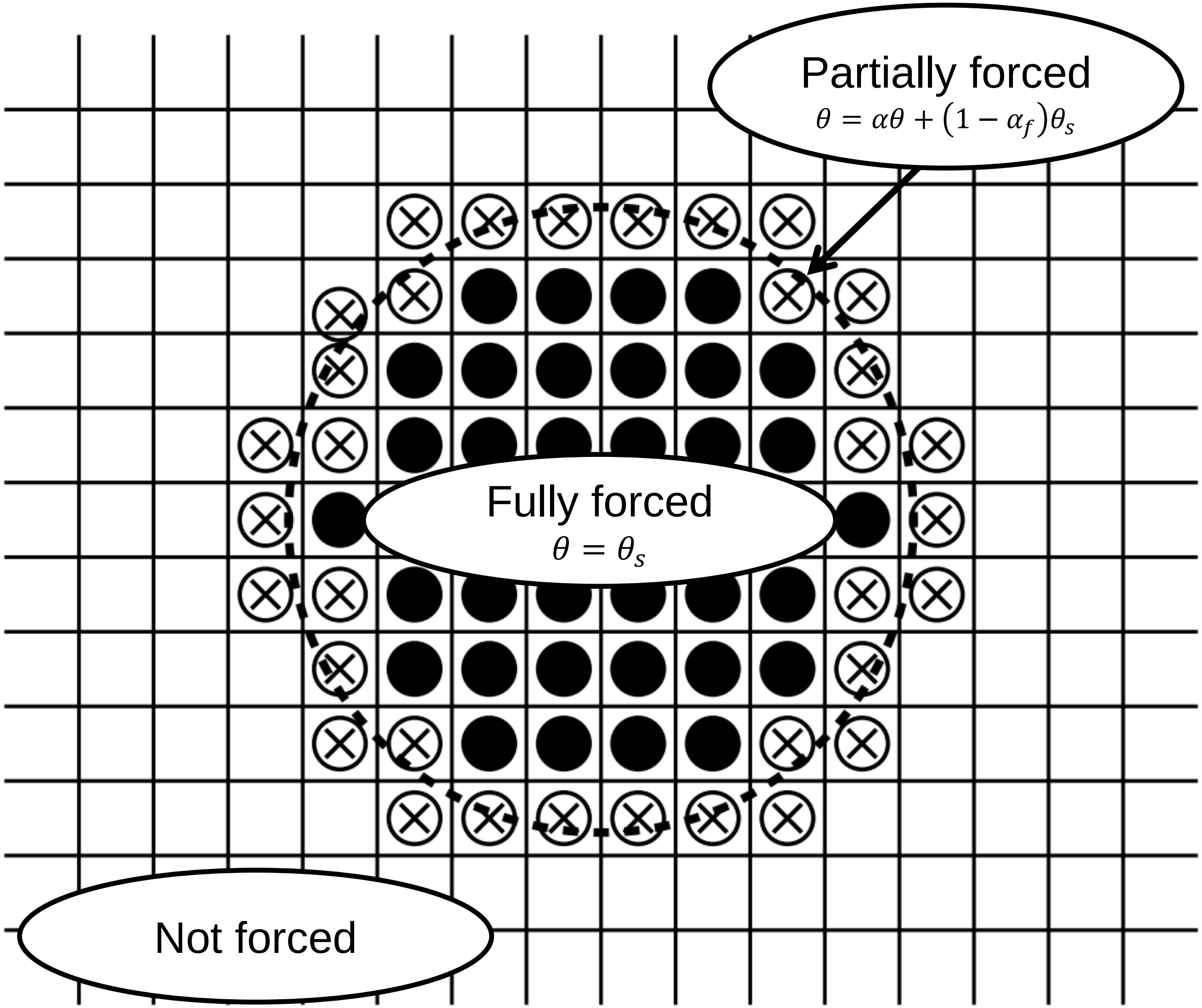
*Peskin C. , Flow patterns around heart valves: a numerical method, Journal of computational physics ,1971

**Smagulov S. , Fictitious domain method for the Navier-Stokes equations (in russian), Preprint CS SO USSR, N 68, 1979

Our Expectations

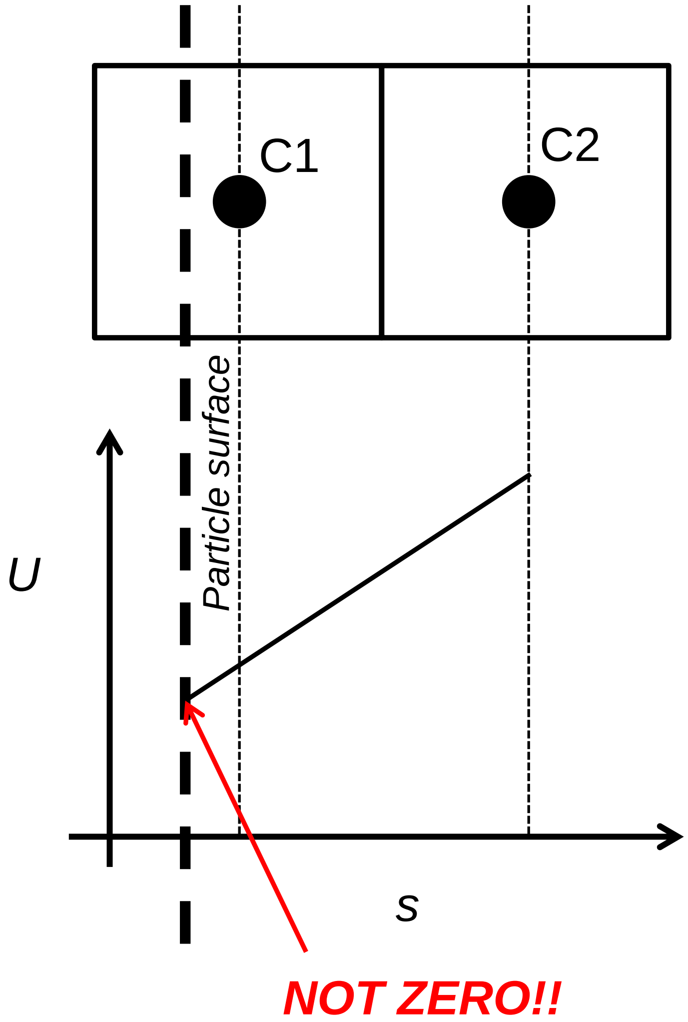
- ***Shape independence***: not effect of the shape
- **Consistency of source/forcing terms**: imposed forcing terms equivalent interphase exchange rates.
- ***Moving and static boundaries***
- ***Accuracy / Mass conservation*** : the mass inside the rigid body = const
- ***Performance & Scalability*** : linear speed-up

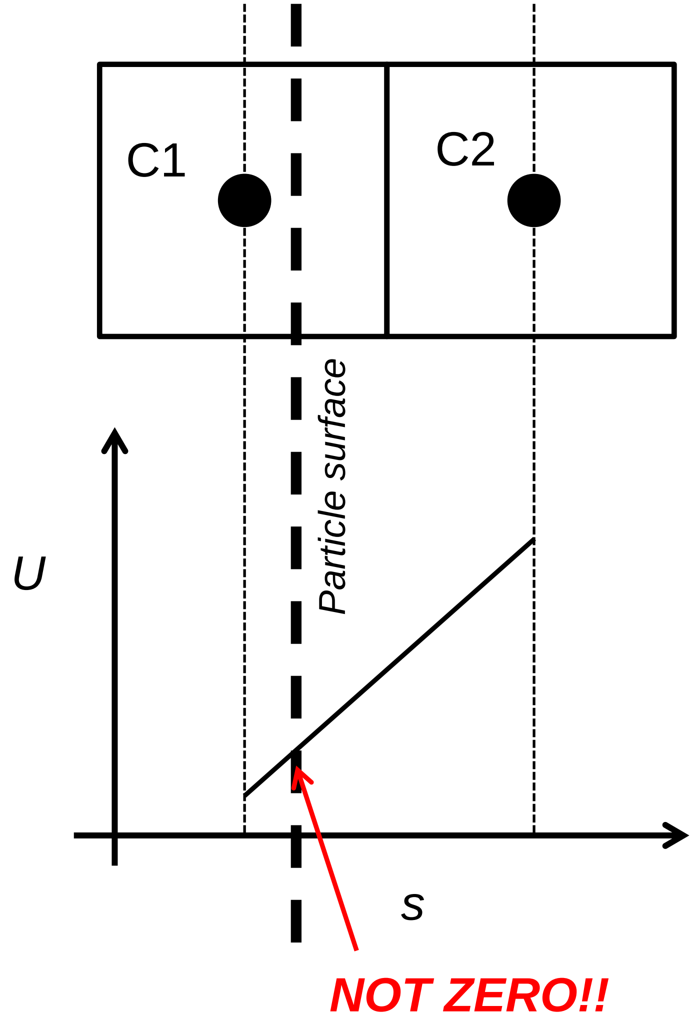
Standard CFDEMCoupling® IB solver*: forcing term



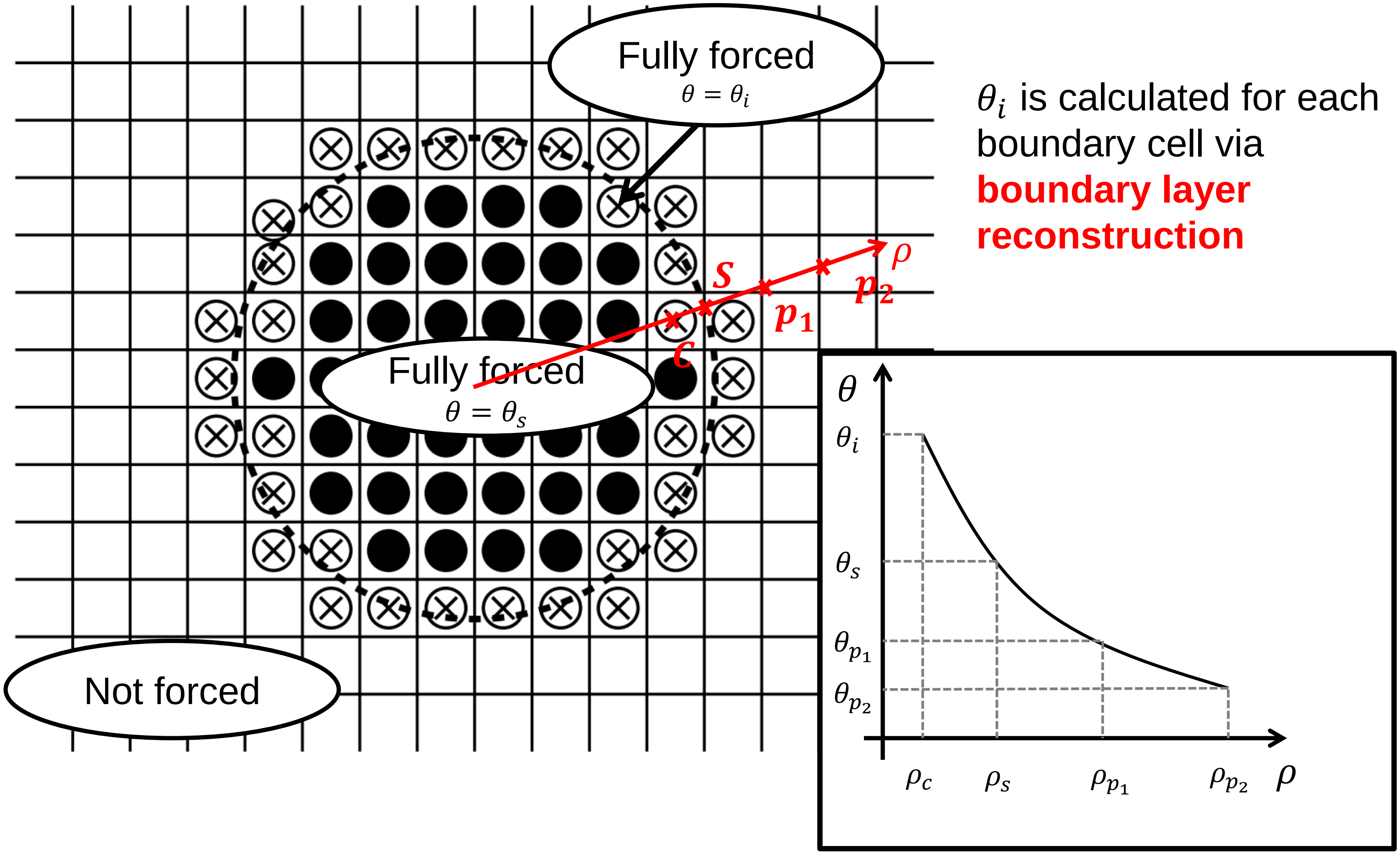
*Hager A. , Kloss C. , Goniva C. , Towards an efficient immersed bounday method within an open-source framework, Proc. Oof the 8° conf. On CFD in Oil and Gas, Metallurgical and Process Industries, 2011

Problem : incorrect reconstruction of the boundary field



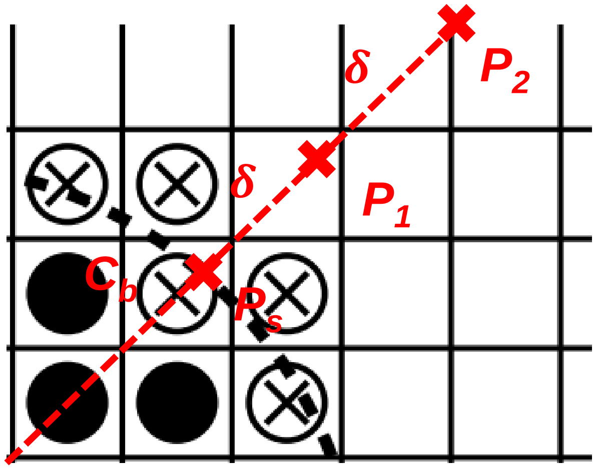


The Idea



θ_i is calculated for each boundary cell via **boundary layer reconstruction**

Hybrid Fictitious Domain / Immerse Boundary Method - HFD-IB



Field values are interpolated at P_1 and P_2 while the value at P_s is given.

Interpolated field values are, then, fitted using a 2nd order polynomial.

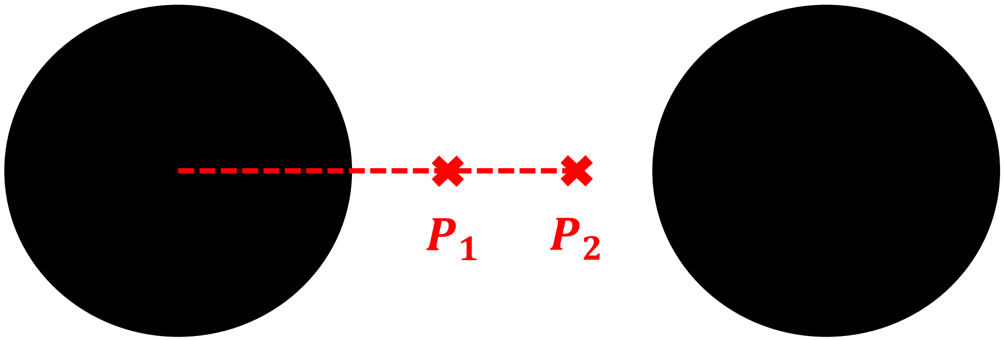
$$\boxed{\theta_i = a\sigma^2 + b\sigma + \theta_s}$$

$$a = \frac{\frac{(\theta_{P_1} - \theta_s)}{2} - (\theta_{P_2} - \theta_s)}{\delta^2}$$

$$b = \frac{4(\theta_{P_1} - \theta_s) - (\theta_{P_2} - \theta_s)}{2\delta}$$

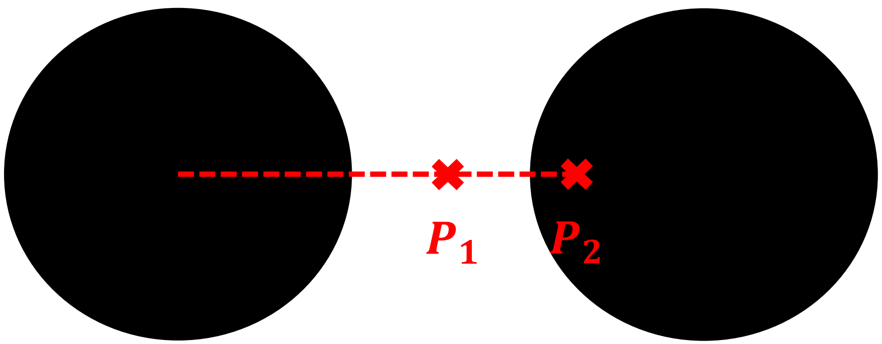
$$\sigma = \rho_c - \rho_s$$

Adaptive order of accuracy



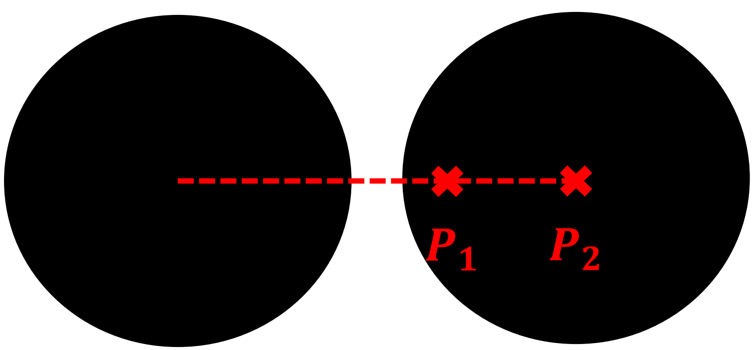
Second order reconstruction

$$\theta_i = a\sigma^2 + b\sigma + \theta_s$$



First order reconstruction

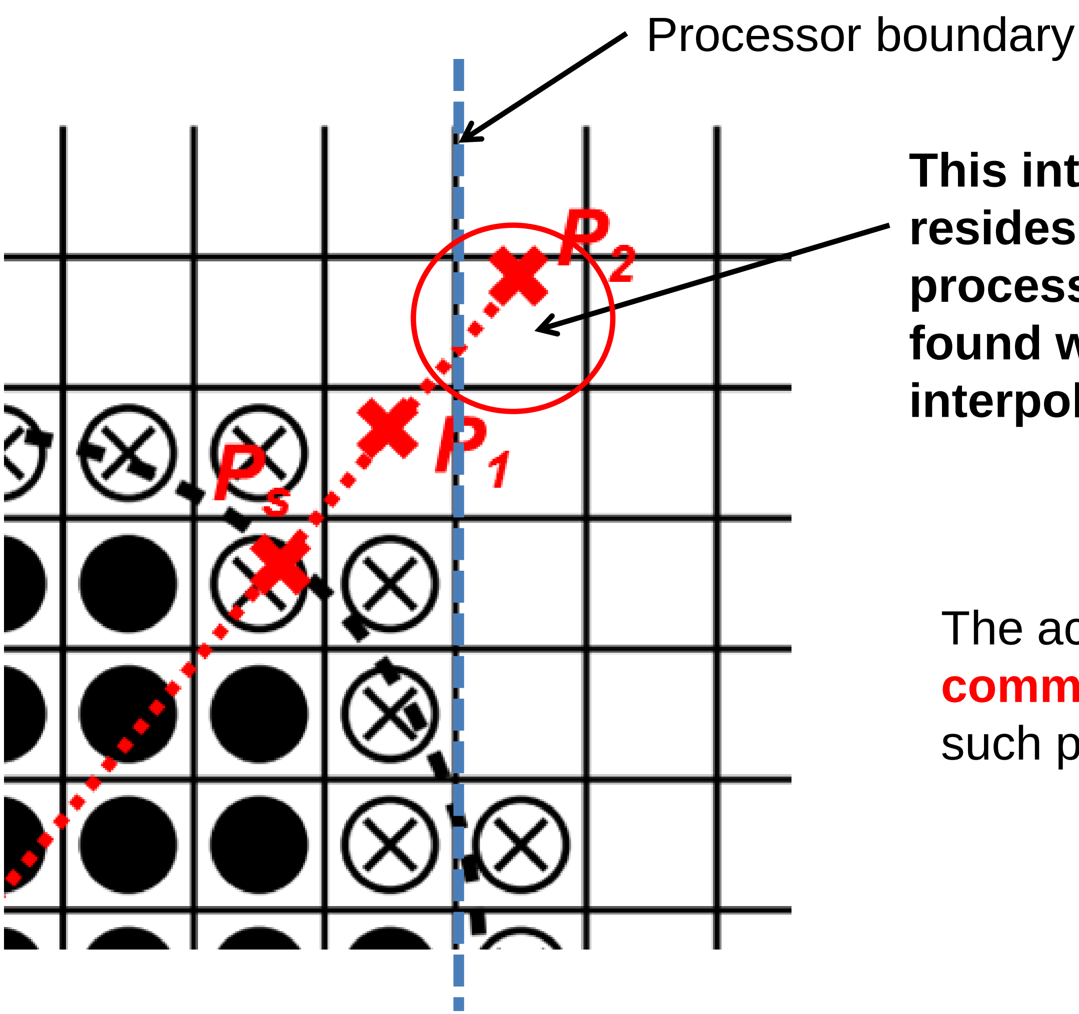
$$\theta_i = a\sigma + \theta_s \qquad a = \frac{(\theta_{P_1} - \theta_s)}{\delta}$$



Zero order reconstruction

$$\theta_i = \theta_s$$

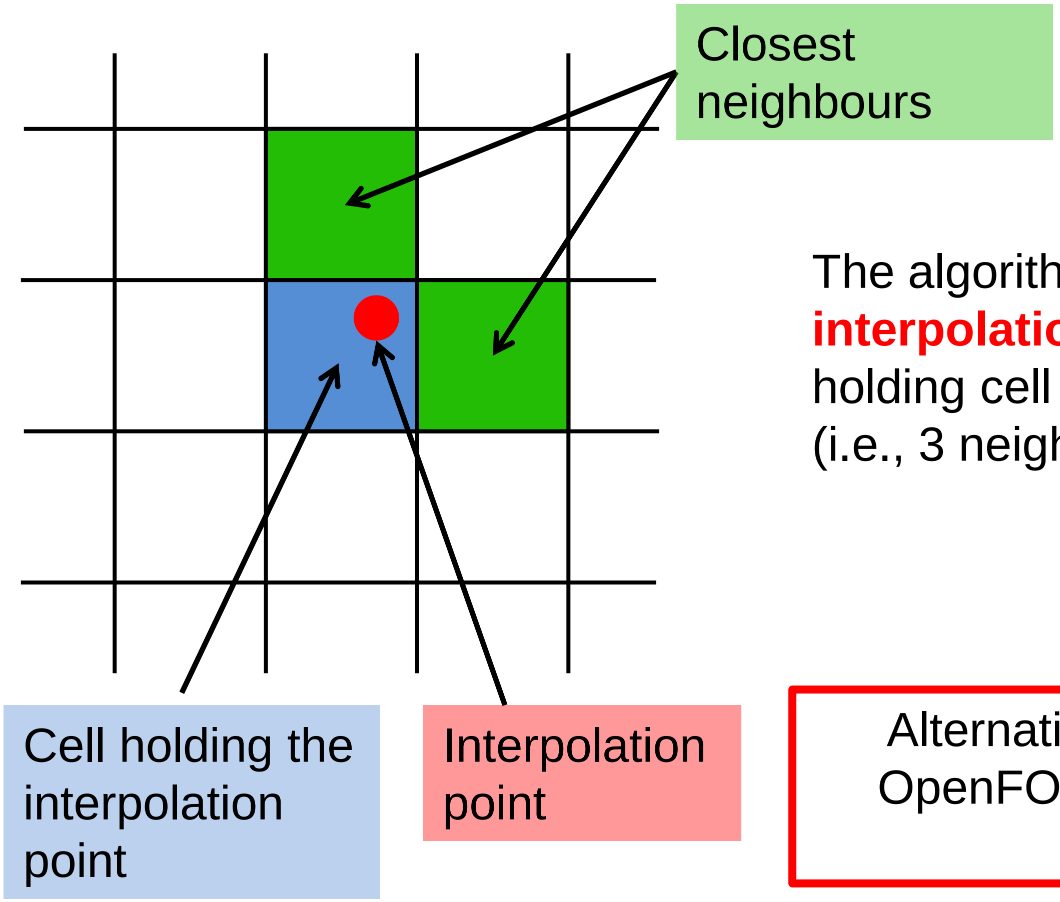
The issue with decomposed domains



This interpolation cell resides on a different processor and it will not be found when computing the interpolation points for P_s

The actual algorithm features a **communication scheme** to avoid such problem

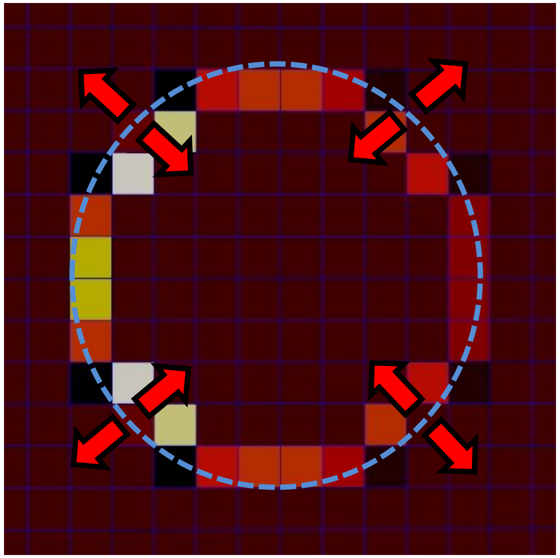
The issue with decomposed domains



The algorithm performs a **linear interpolation** using values from the holding cell and the **closest neighbours** (i.e., 3 neighbours in 3D).

Alternatively, it is possible to use OpenFOAM® built-in interpolation schemes

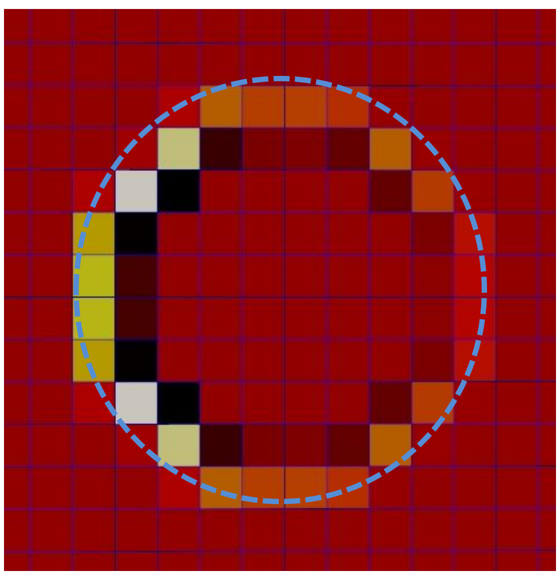
θ_i



The imposed scalar field is constant inside the particle (i.e., the value in the body) and calculated at the particle surface cells.

However, the diffusion process would happen towards both the fluid and the solid!

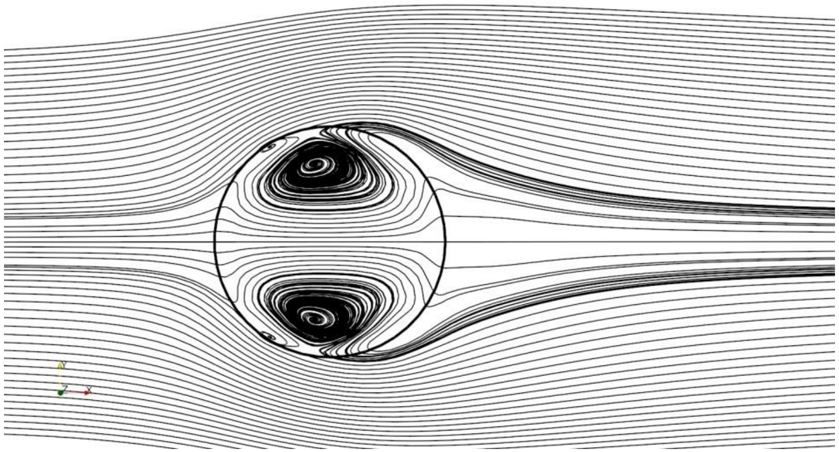
Q_{IB}



Imposing a fixed temperature inside the immersed body allows to automatically compensate the internal fluxes

The total source term is consistent with the solid-fluid exchange process

Flow field handling



Boundary forcing induces a flow inside the immersed body (problem: **viscous dissipation**).

Imposing rigidity would force the flow outside the immersed body producing a «banana shaped» recirculation at its surface.

Thus, we:

- just use **boundary forcing** (no rigidity is imposed!)
- **Full immersed boundary**
- A theoretical work by **Sabetghadam*** is suggesting that the fluid inside the particles behaves like an **inviscid flow**

** Sabetghadam F. , An analytical framework for the imposition of a rigid immersed surface on the incompressible Navier-Stokes equation, ArXiv e-prints, 2014*

Summary of equations

$$\frac{\partial u_i}{\partial x_i} = 0$$ *Continuity*

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re}\frac{\partial^2 u_i}{\partial x_j \partial x_j} + I_s f_i^{IB}$$ *Navier-Stokes*

$$\frac{\partial \theta}{\partial t} + \frac{\partial u_i \theta}{\partial x_i} = \frac{1}{Pe}\frac{\partial^2 \theta}{\partial x_i \partial x_i} + (I_i + I_s) Q^{IB}$$ *Scalar transport*

Additional relations

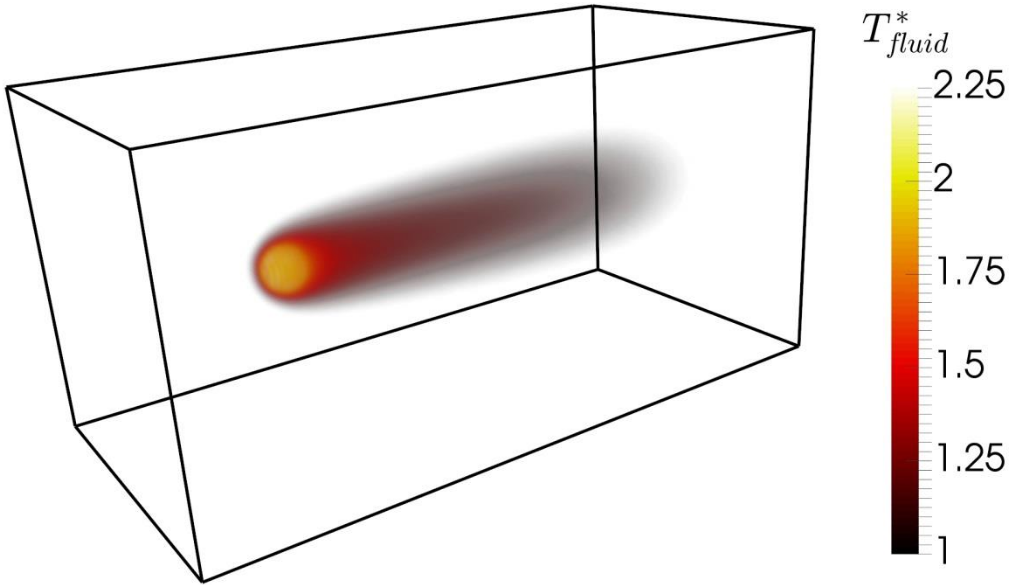
I_i *is 1 if the cell is completely inside the particle, 0 otherwise.*

I_s *is 1 if the cell is partially inside the particle, 0 otherwise.*

f_i^{IB} *is calculated following Blais et al.**

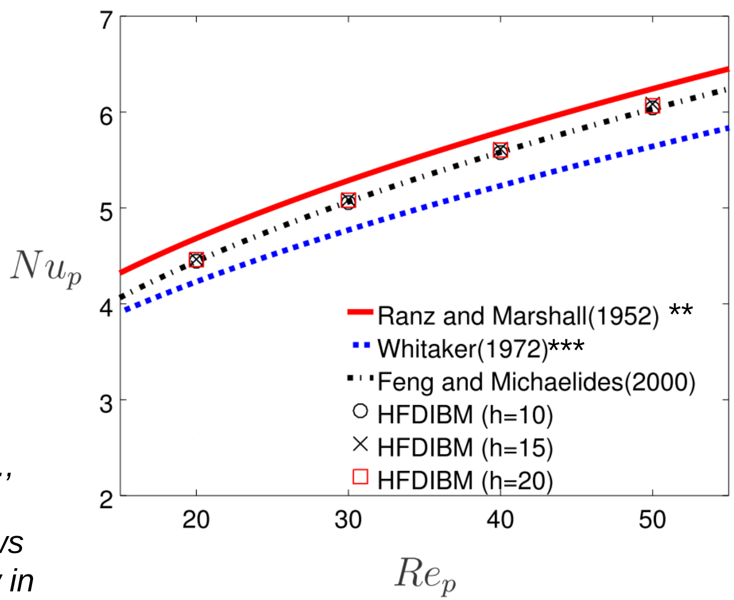
$Q^{IB} = A\theta^{IB} - H$ *Where A and H refer to the respective operators in OpenFOAM® **and θ^{IB} is the imposed value according to the IB scheme.*

**Blais B. , Lassaigne M. , Goniva C. , A semi-implicit immersed boundary method and its applications to viscous mixing, Computers and Chemical Engineering, 2016*
***openfoamwiki.net/index.php/OpenFOAM_guide/H_operator*

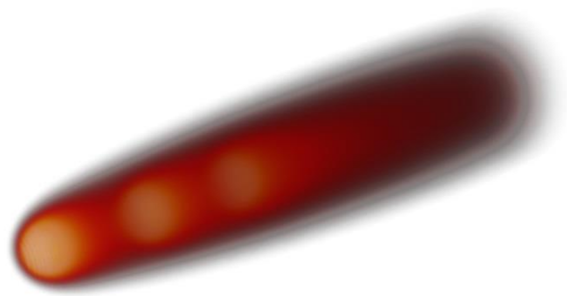


Forced convection past a steady sphere

Agreement with existing correlations, in particular with the latest work of **Feng and Michaelides***



**Feng Z. , Michaelides E. A numerical study on the transient heat transfer from a sphere at high Reynolds and Peclet numbers, International Journal of Heat and Mass transfer, 2000*
***Ranz W. , Marshall W. , Evaporation from drops, Chem. Eng. Prog., 48, 141-146, 1952*
**** Whitaker S. , Forced convection heat transfer correlations for flows in pipes, past flat plates, single cylinders, single spheres and for flow in packed beds and tube bundles, AICHE J., 1972*

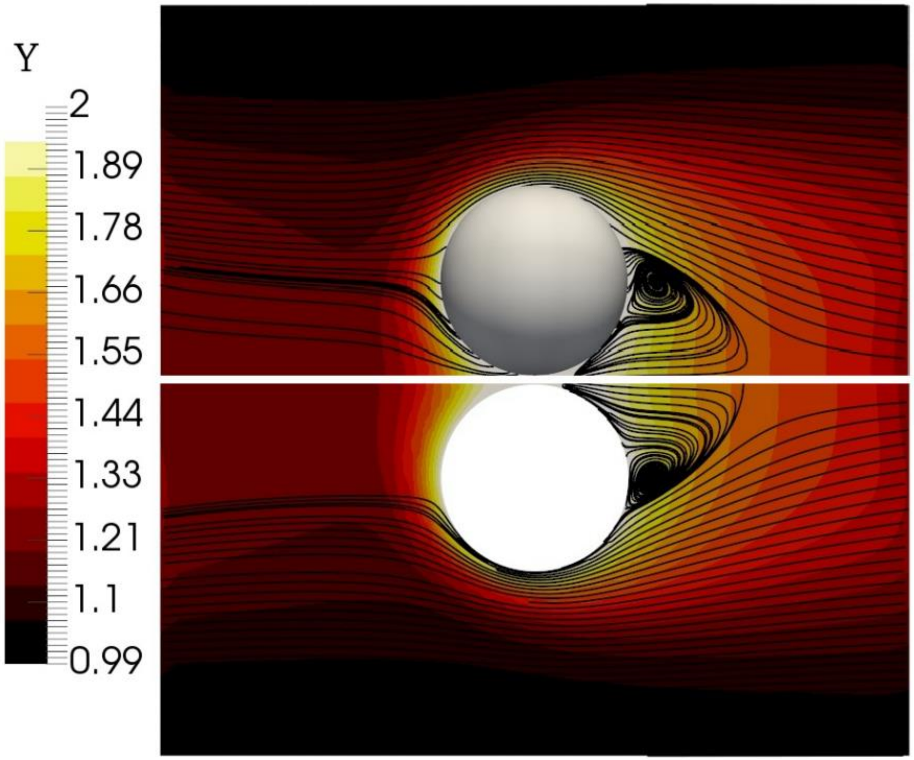


Forced convection past a chain of three spheres

- Deviations from literature are comparable (or even lower) to the deviations obtained by Tavassoli et al.***

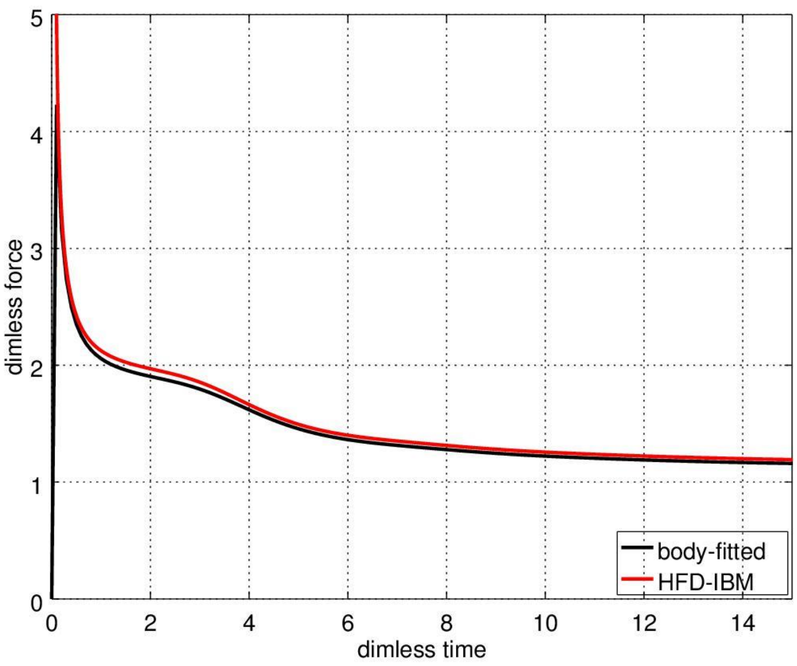
	HFDIBM Maheshwari*	HFDIBM Ramachandran**	Tavassoli Maheshwari	Tavassoli Ramachandran
Sph. 1 d=2	**0.35%**	2.1%	**4.1%**	2.5%
Sph. 2 d=4	**6.8%**	**6.8%**	**8.3%**	7.2%
Sph. 3 d=4	6.7%	**7.4%**	6.7%	**7.5%**

**Mashewari A. ,Chhabra R., Biswas G. , Effect of blockage on drag and heat transfer fom a single sphere and an in-line array of three spheres, powder technology, 168, 74-83, 2006*
***Rachmadran R., Kleinstreurer C., Wang T., Forced convection heat transfer of interacting spheres, Numerical Heat Transfer, 15°, 471-487, 1989*
**** Tavassoli H. , Kriebitzsch S., Vand der Hoef M, Kuipers J.A.M , Direct numerical simulation of particulate flow with heat transfer, International journal of multiphase flow 57, 29-37, 2013*



Two close spheres – direct comparison with body fitted DNS

The Nusselt number differs by less than 3%

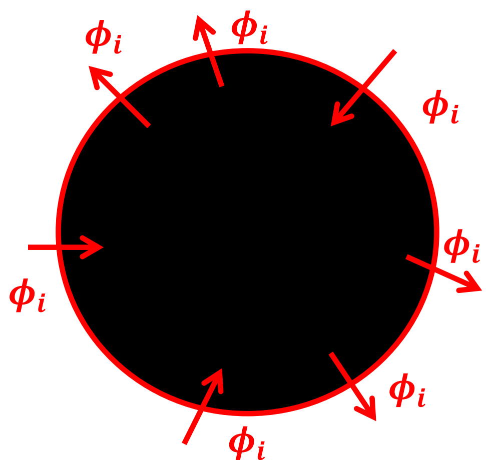


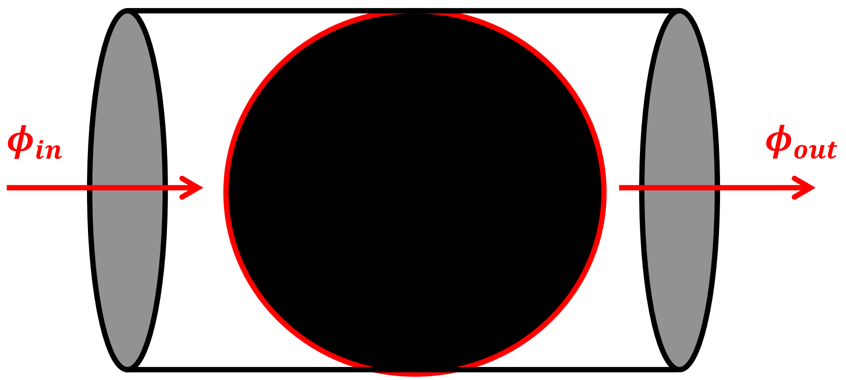
Slight overprediction of the dimensionless force but similar trend

An approach to evaluate the level of “sealing”

$$\sigma = 1 - \frac{\phi_{tot}}{\phi_{max}}$$

Sigma quantifies the **amount of fluid passing through the particle boundary** with respect to the maximum possible fluid amount.





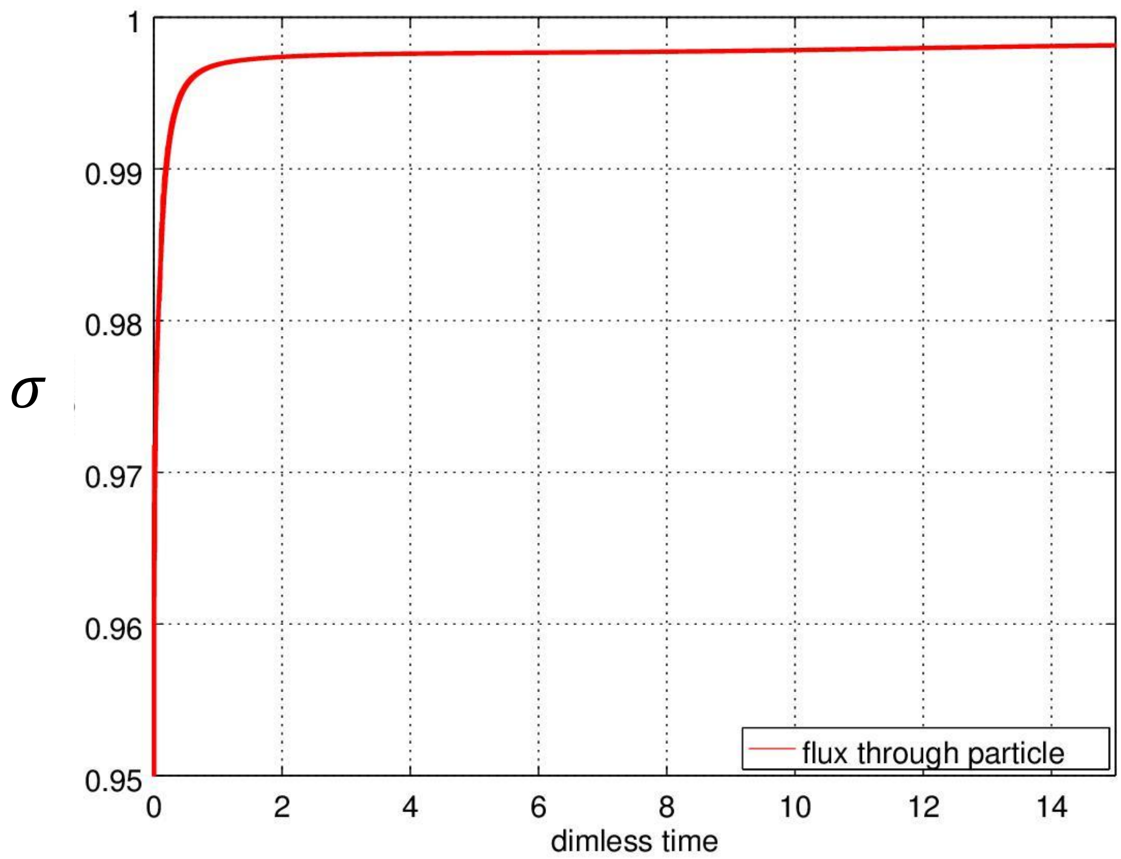
$$\phi_{tot} = \sum_i |\phi_i|$$

$$\phi_{max} = |\phi_{in}| + |\phi_{out}|$$

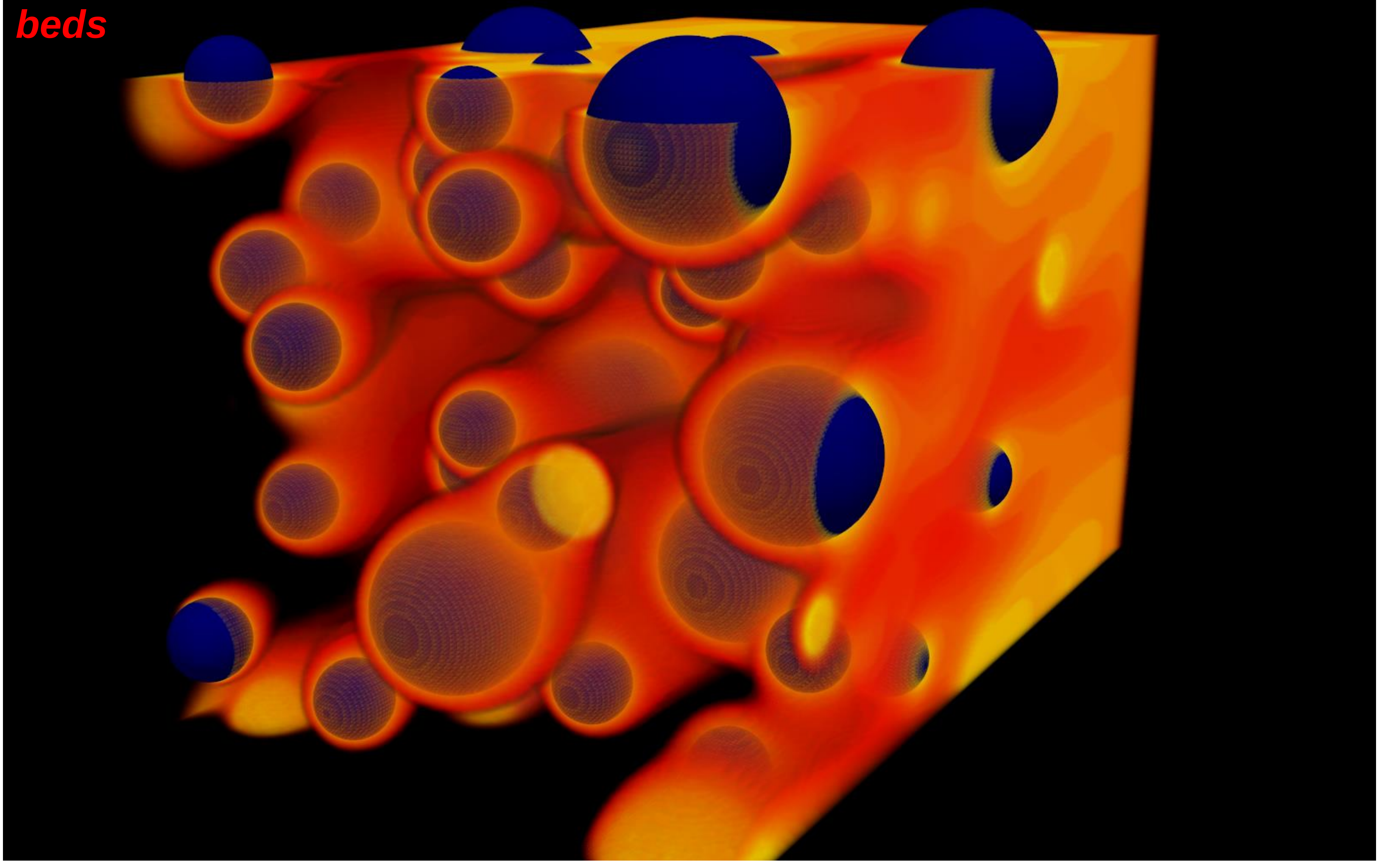
An approach to evaluate the level of “sealing”

This metric reveals that **the particle surface is blocking more than 99.5%** of the incoming flow

- *Re = 30*
- *15 cells per particle diameter*
- *Fully periodic domain*



Application to heat and mass transfer in poly-disperse particle beds



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