High Parallel Computing of Reactive Particulate Flows in Complex Geometries

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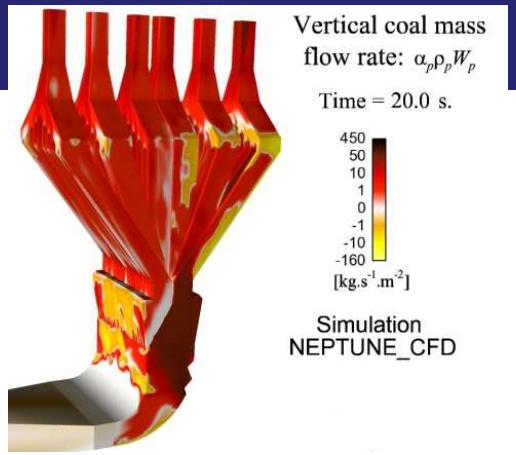
ACKOWNLEDGEMENTS

- A Multiscale Simulation-Based Design Platform for Cost-Effective **CO2 Capture Processes** using Nano-Structured Materials (**NanoSim**)

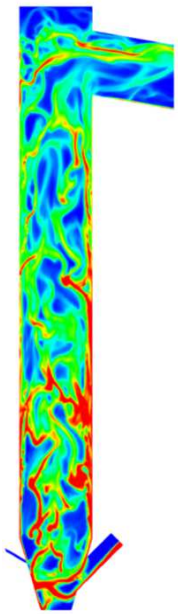
- Industrial steam generation with 100% carbon capture and insignificant efficiency penalty - Scale-Up of oxygen Carrier for **Chemical-looping** combustion using Environmentally SuStainable materials (**SUCCESS**)

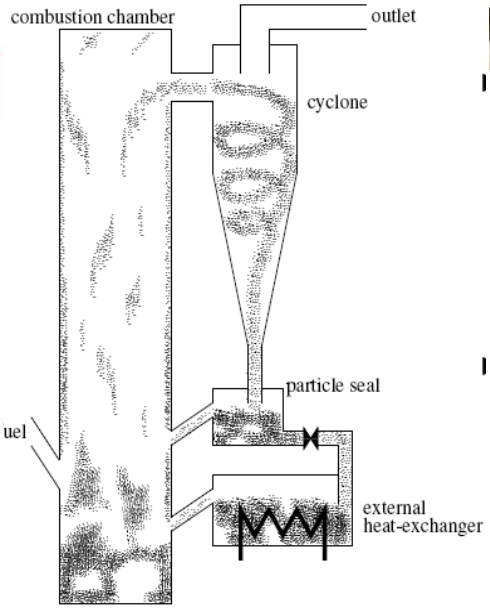
Prediction of industrial dispersed two-phase turbulent flow



Industrial applications:

- Coal fired furnaces
- CFB boilers
- Polymerization reactor
- FCC riser
- IC engine (liquid fuel injection)
- Solid rocket booster
- Separation
- ……



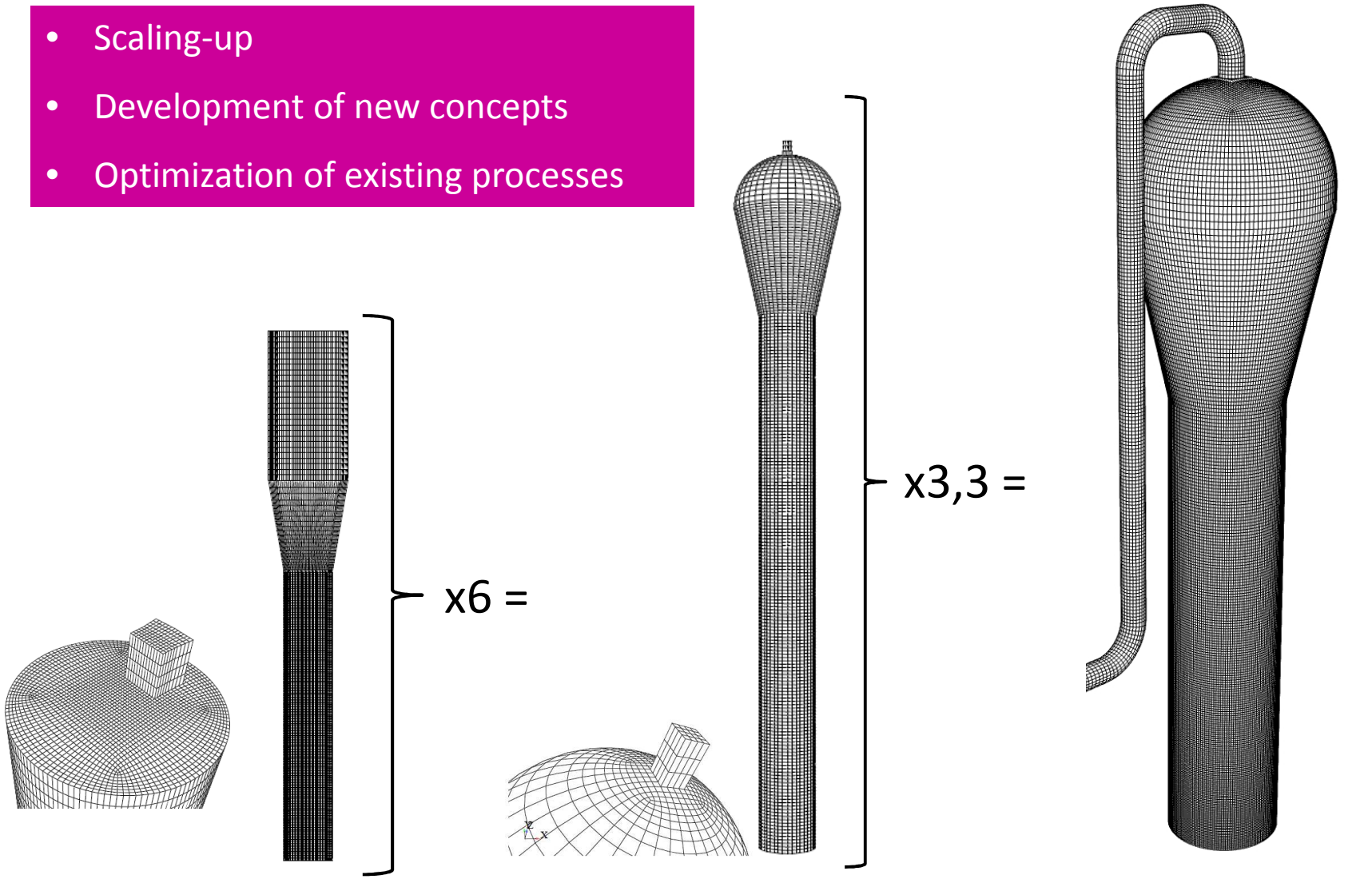


Turbulent two-phase flows:

- Fluid-particle interaction (mass, momentum and energy transfer)
- Particle-particle interaction (collision, agglomeration, attrition)
- Particle-wall interaction (inelastic bouncing with friction, deposition)

MOTIVATIONS

- Scaling-up
- Development of new concepts
- Optimization of existing processes



Mass balance equation

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \frac{\partial}{\partial x_j}(\alpha_k \rho_k U_{k,j}) = 0$$

Momentum balance equation

$$\alpha_k \rho_k \left[\frac{\partial U_{k,i}}{\partial t} + U_{k,j}\frac{\partial U_{k,i}}{\partial x_j}\right] = -\alpha_k \frac{\partial P_g}{\partial x_i} + \alpha_k \rho_k g_i + \sum_{q=g,p} I_{q\to k,i} - \frac{\partial \Sigma_{k,ij}}{\partial x_j}$$

Gas-particle momentum transfer

$$I_{g\to p,i} = -I_{p\to g,i} = -\alpha_p \rho_p \frac{V_{r,i}}{\tau_{gp}^F}$$

$$\begin{cases} \dfrac{1}{\tau_{gp}^F} = \dfrac{3}{4}\dfrac{\rho_g}{\rho_p}\dfrac{\langle|\mathbf{v}_r|\rangle}{d_p} C_D & \text{particle relaxation time} \\ Re_p = \dfrac{\alpha_g d_p \langle|\mathbf{v}_r|\rangle}{\nu_g} & \text{particle Reynolds number} \\ V_{r,i} = U_{p,i} - U_{g,i} & \text{mean gas-particle relative velocity} \end{cases}$$

Particle-particle momentum transfer

$$I_{q\to p,i} = -\frac{m_p m_q}{m_p + m_q}\frac{1+e_c}{2}\frac{n_p}{\tau_{pq}^c} H_1(z)\left(U_{p,i} - U_{q,i}\right)$$

$$\frac{1}{\tau_{pq}^c} = 4 n_q g_0 \pi d_{pq}^2 H_0(z)\sqrt{\frac{2}{3\pi} q_r}$$

Effective solid stress modeling

$$\Sigma_{p,ij} = \left[P_p - \lambda_p \frac{\partial U_{p,m}}{\partial x_m}\right]\delta_{ij} - \mu_p\left[\frac{\partial U_{p,i}}{\partial x_j} + \frac{\partial U_{p,j}}{\partial x_i} - \frac{2}{3}\frac{\partial U_{p,m}}{\partial x_m}\delta_{ij}\right]$$

$$\mu_p = \alpha_p \rho_p (\nu_p^{kin} + \nu_p^{col}) \begin{cases} \nu_p^{kin} = \left[\frac{1}{2}\tau_{gp}^F \frac{2}{3} q_p^2 \left(1 + \hat{\alpha}_p g_0 \Phi_c\right)\right] \times \left[1 + \frac{\tau_{gp}^F}{2}\frac{\sigma_c}{\hat{\tau}_p^c}\right]^{-1} \\ \nu_p^{col} = \frac{4}{5}\hat{\alpha}_p g_0 (1+e_c)\left[\nu_p^{kin} + \hat{d}_p\sqrt{\frac{2}{3}\frac{q_p^2}{\pi}}\right] \end{cases}$$

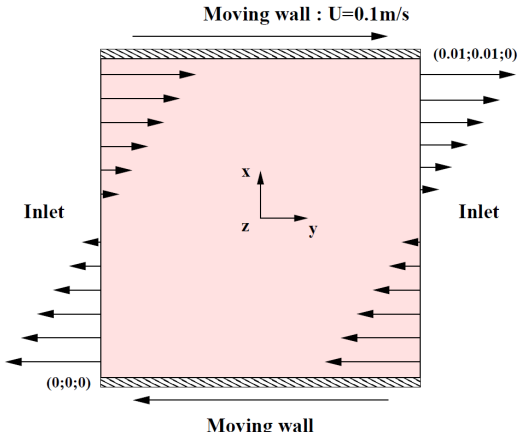
Polydispersion (Batrak et al., 2005)

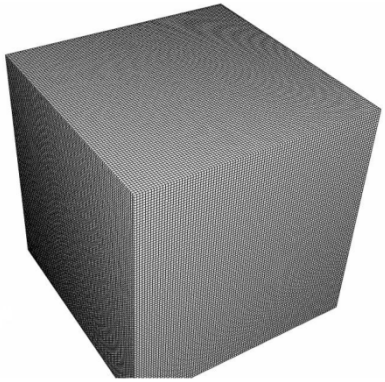
$$\hat{\alpha}_p = \sum_{q\neq p} \alpha_p \frac{2m_q}{m_p + m_q}\left[\frac{d_{pq}}{d_q}\right]^3 \qquad \hat{d}_p = \frac{1}{\hat{\alpha}_p}\sum_{q\neq p}\alpha_q \frac{d_{pq}^4}{d_q^3}\frac{2m_q}{m_p+m_q} \qquad \frac{1}{\hat{\tau}_p^c} = \sum_{q\neq p}\frac{2m_q}{m_p+m_q}\frac{1}{\tau_{pq}^c}$$

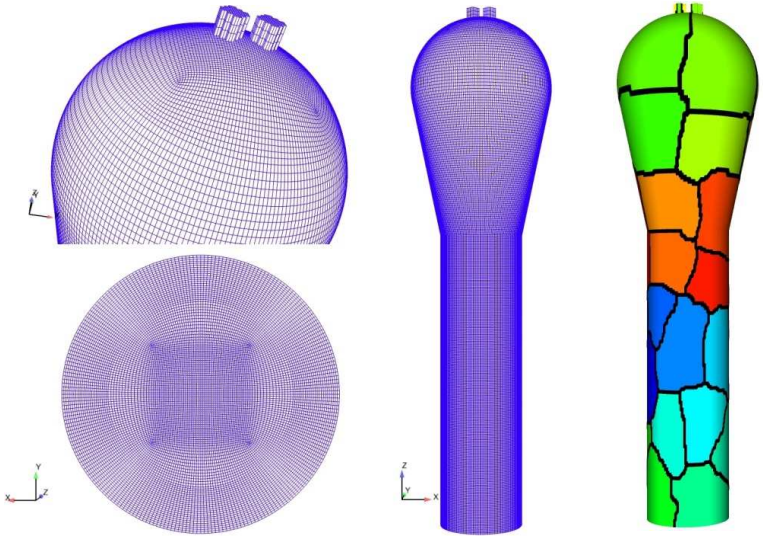
Turbulence modeling

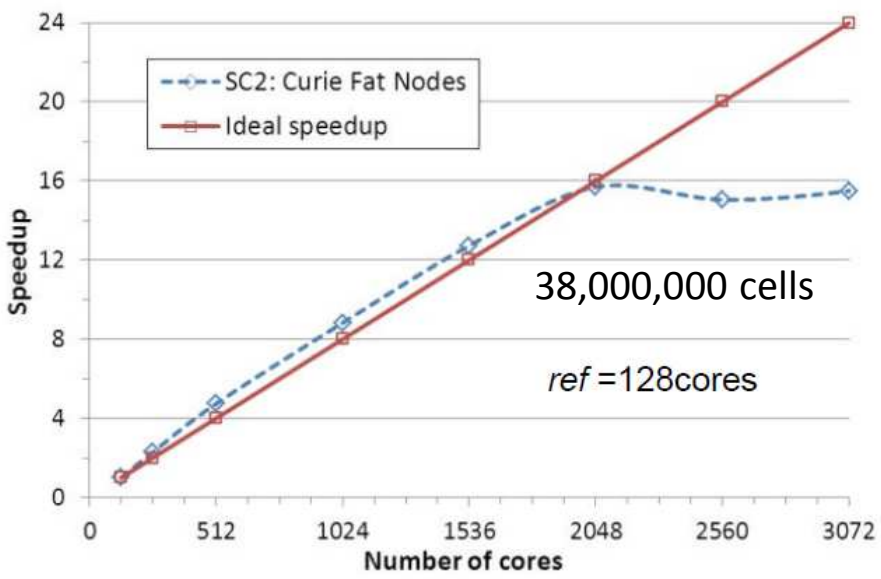
- Laminar for the gas or k-epsilon
- Equation on the random kinetic energy for each particle class q_p^2 (polydisperse model)

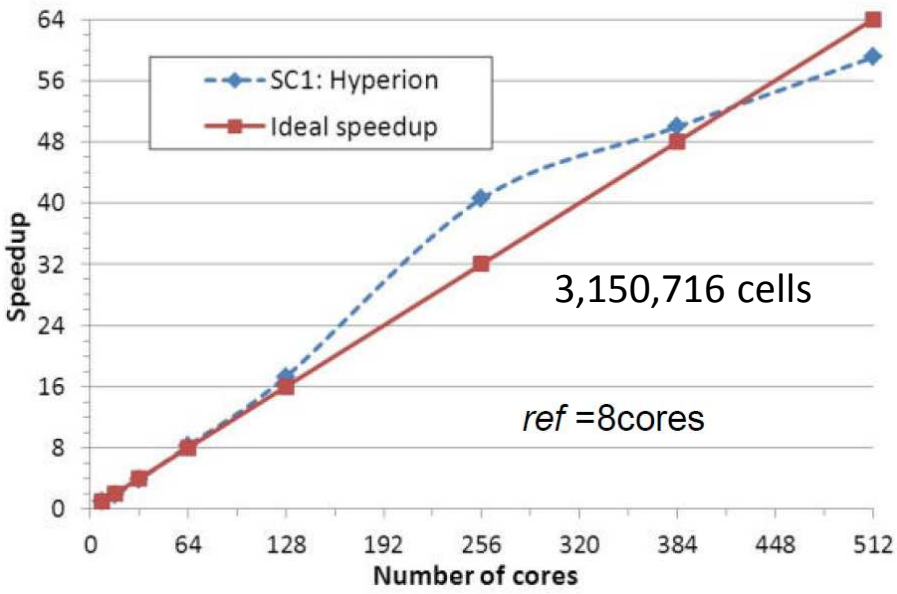
NEPTUNE_CFD computation efficiency:



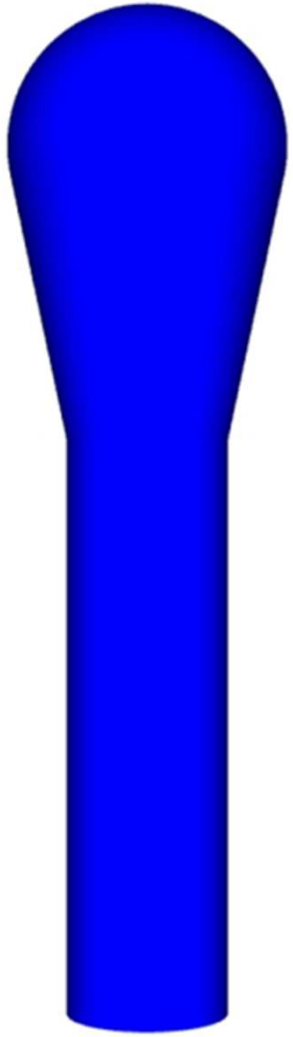


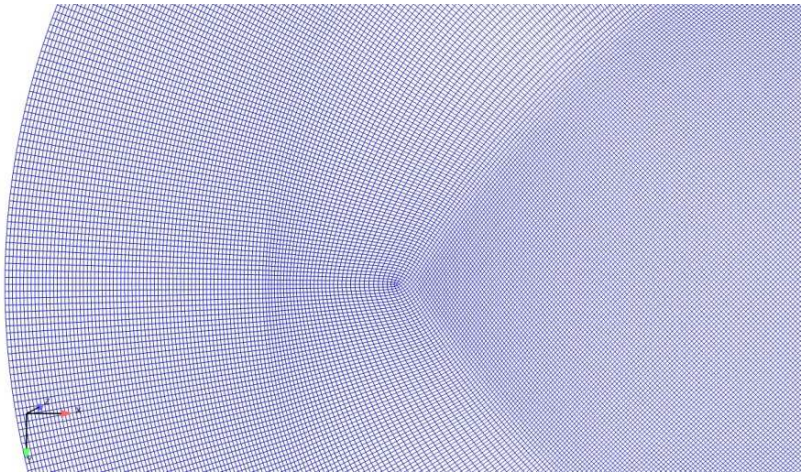


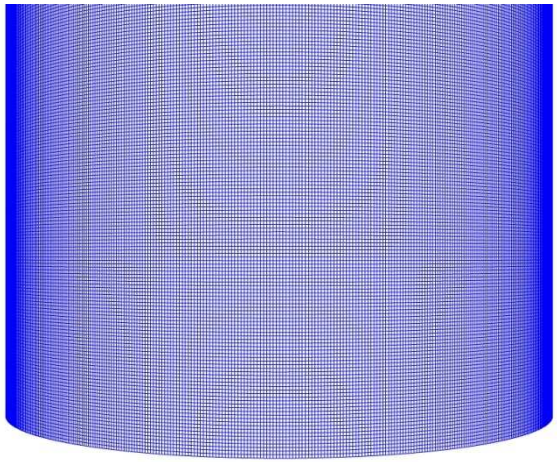




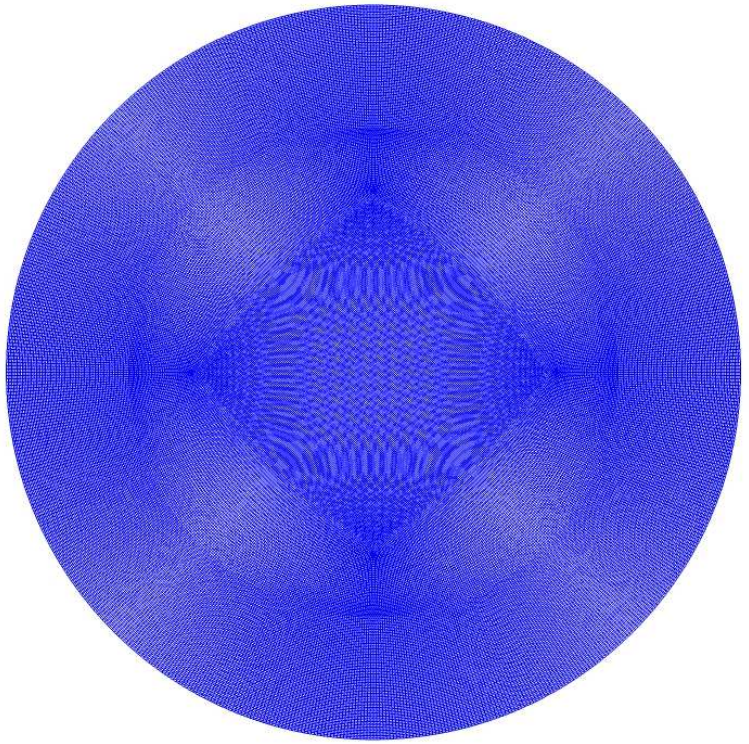
NEPTUNE_CFD computation efficiency:







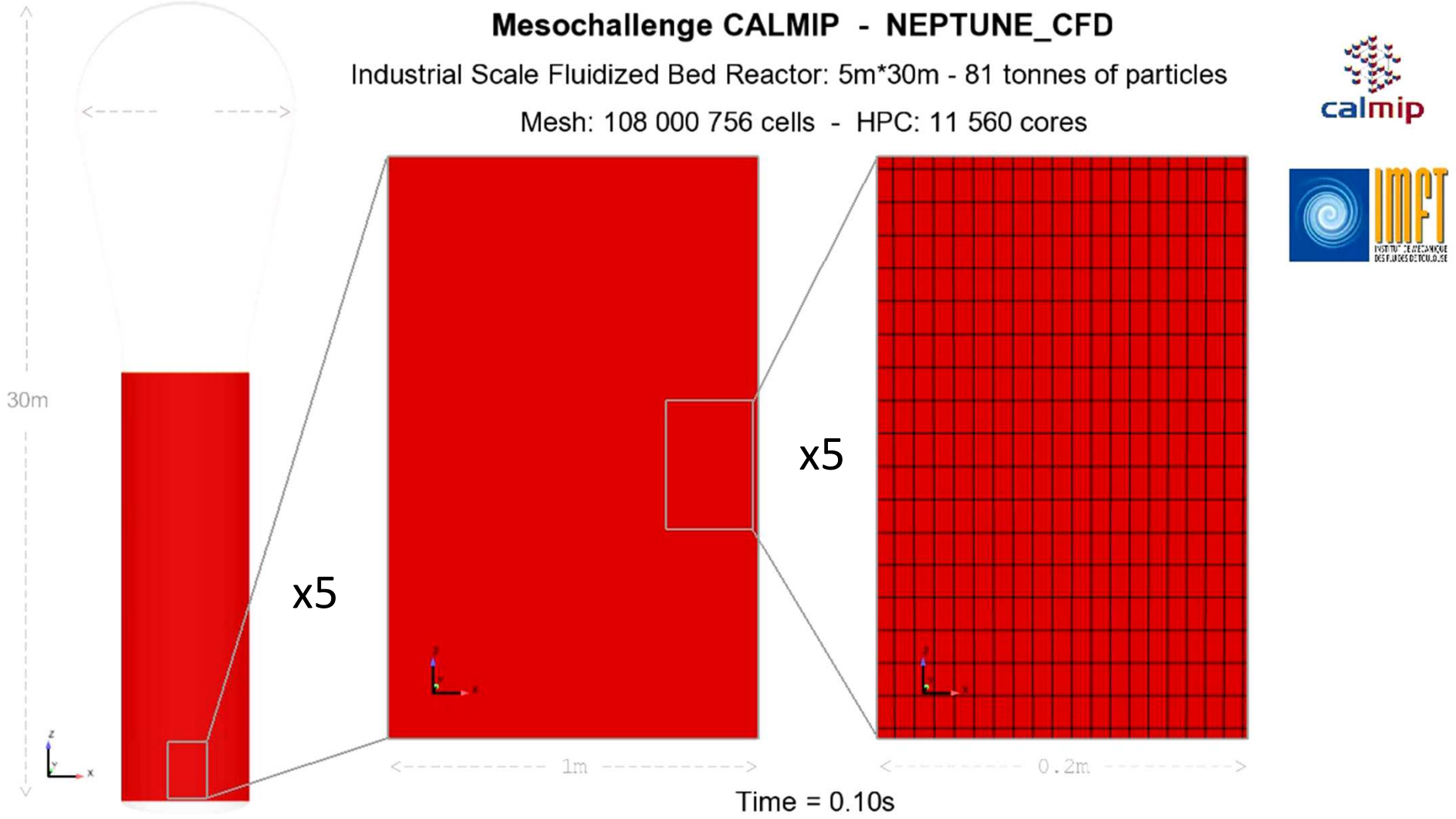
$\approx 500\ \Delta_x$



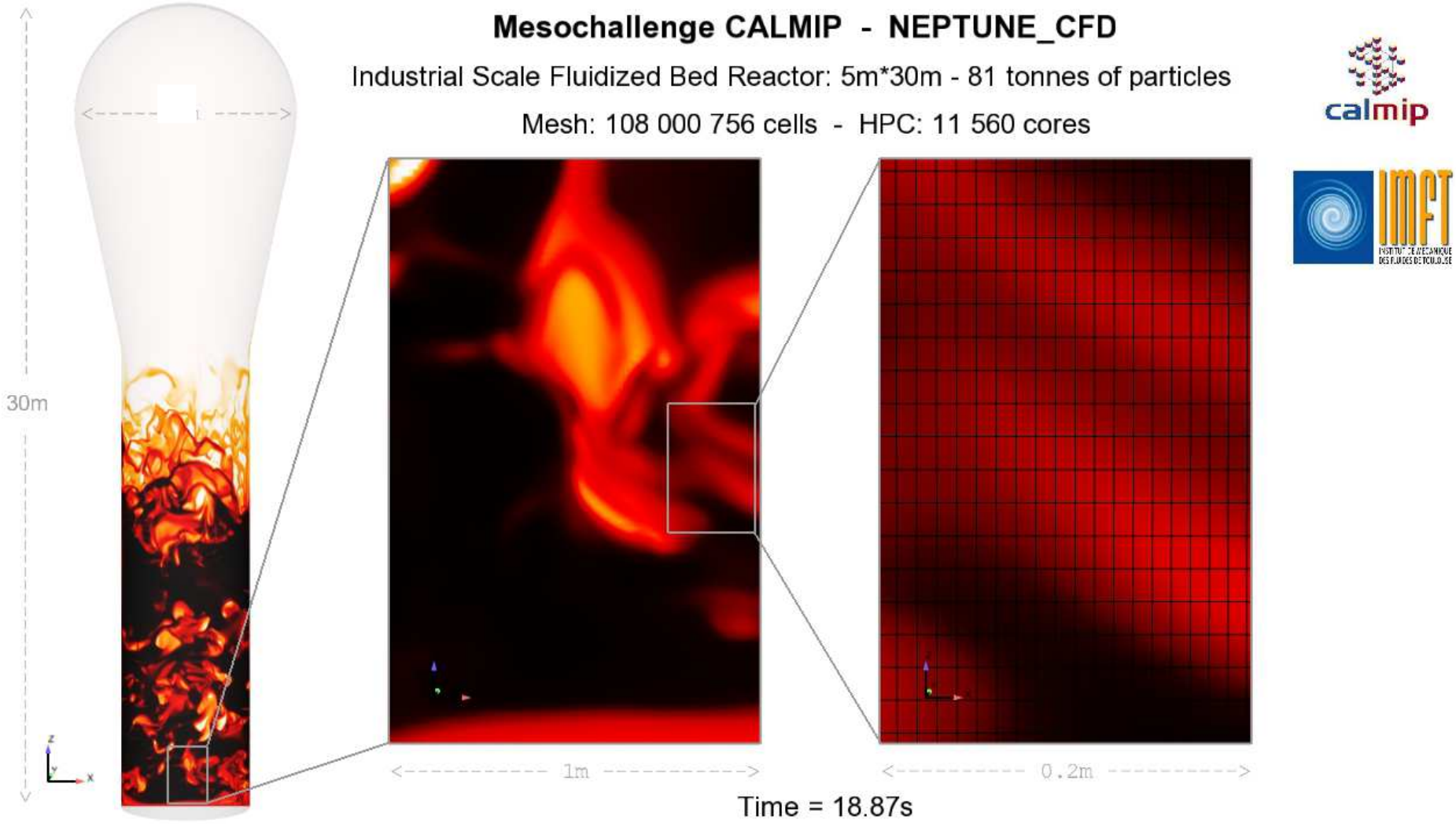
Full mesh ≈ 100,000,000 cells

$\Delta_x \approx \Delta_y \approx \Delta_z \approx 1cm^3$

NEPTUNE_CFD computation efficiency:



NEPTUNE_CFD computation efficiency:



Why performing such a massive simulation?

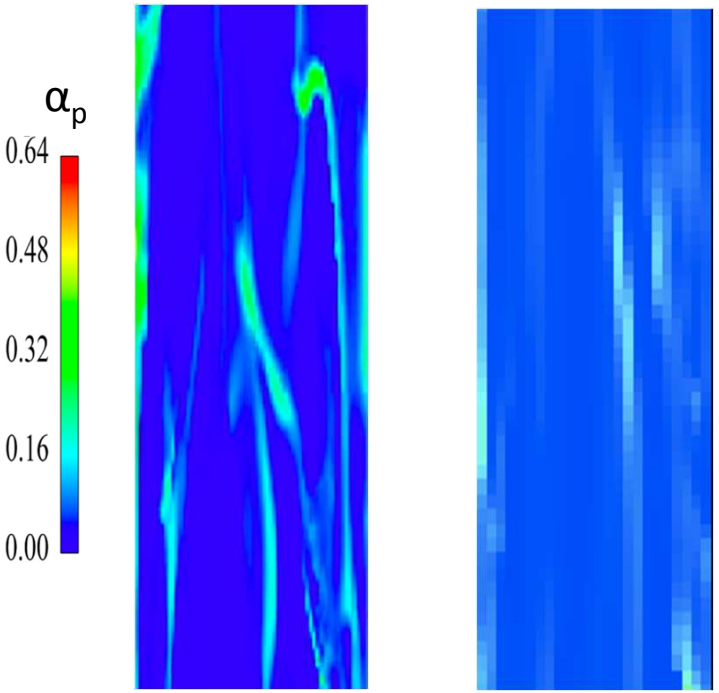
→ Not only to do nice videos

What can be learn from such a numerical simulation?

- Understanding of the local gas-particle interactions

- Development of filtered approach

HOW TO ANALYZE/MODEL THE EFFECT OF SUBGRID SOLID STRUCTURE



Fine grid

Δ=1 cm

Coarse grid

Δ=10 cm

Numerical simulation of large-scale industrial CFB

↓

Limitation of computational resources leads to use relatively too coarse mesh for detailed prediction of the meso-scale structure

↓

Bad prediction of the meso-scale structures

↓

Dramatic influence on bed hydrodynamics (solid flux, bed height, …)

Mesh independent results useful for:

- understanding/modelling of the effect of meso-scale solid structures
- model validation

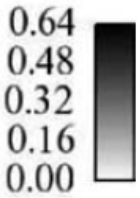
Development of an approach allowing to perform numerical simulation with a reasonable mesh

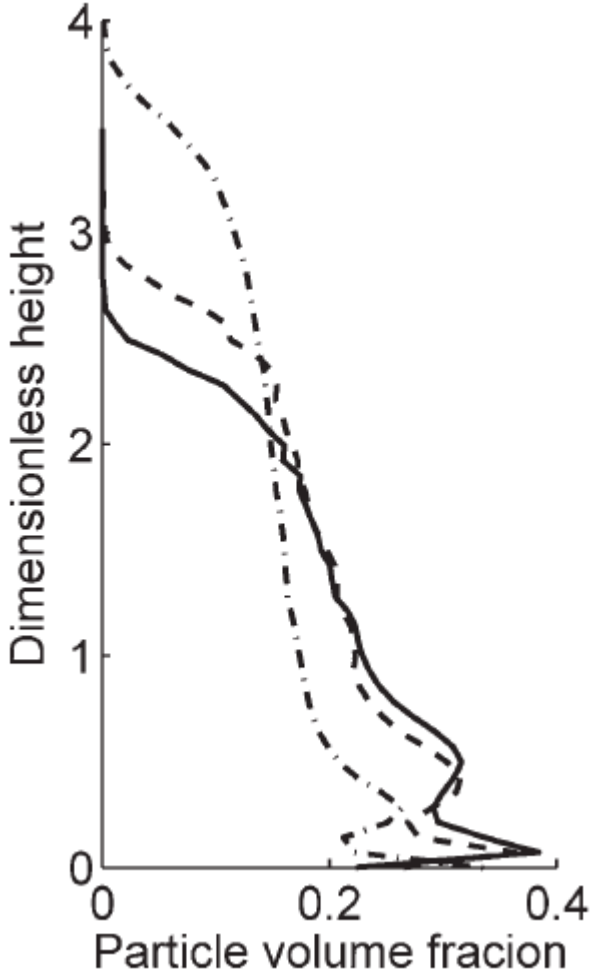
2D DENSE FLUIDIZED BED

Mesh ind. results

Without sgs model

With sgs model





PERIODICAL CIRCULATING FLUIDIZED BED

Fr^{-1} = 0.032
(128 × 128×1024=16,777,216)

Fr^{-1} = 0.128
(32× 32×256=262,144)

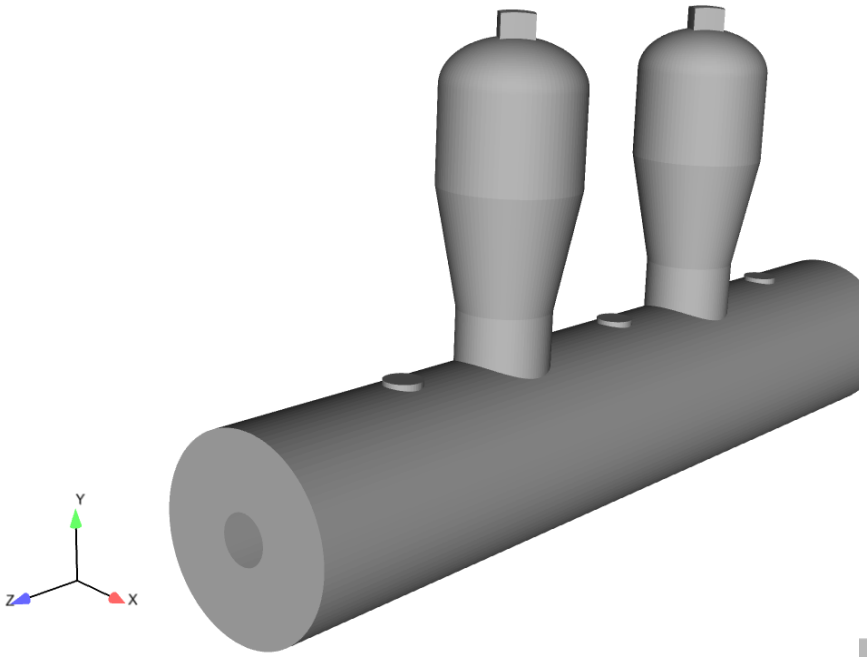
Fr^{-1} = 0.128
(32× 32×256=262,144)

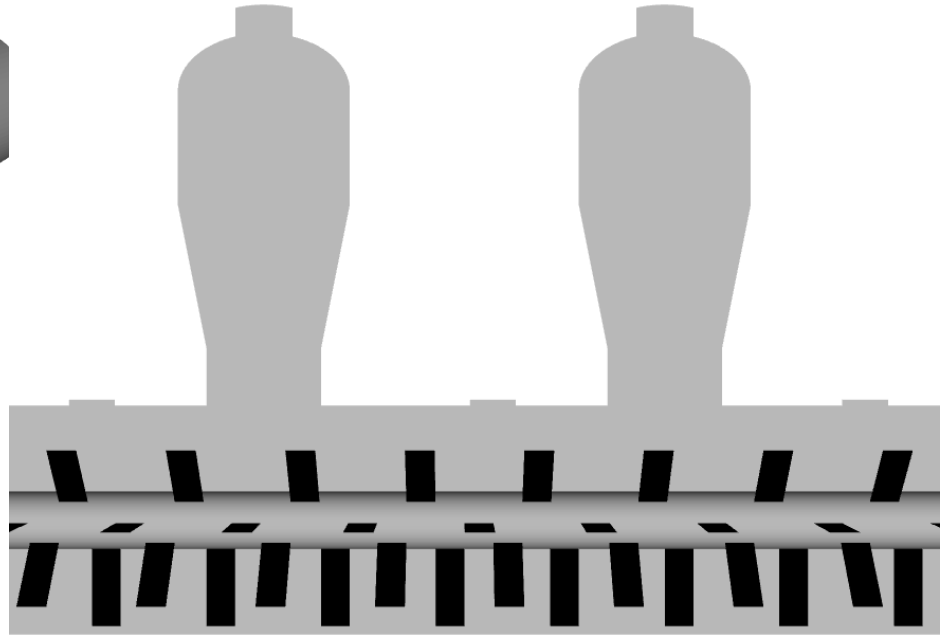
With Subgrid model

More complex geometries

POLYPROPYLENE POLYMERIZATION REACTOR

Geometry from Soares, J. B., & McKenna, T. F. (2013). Polyolefin Reaction Engineering. John Wiley & Sons





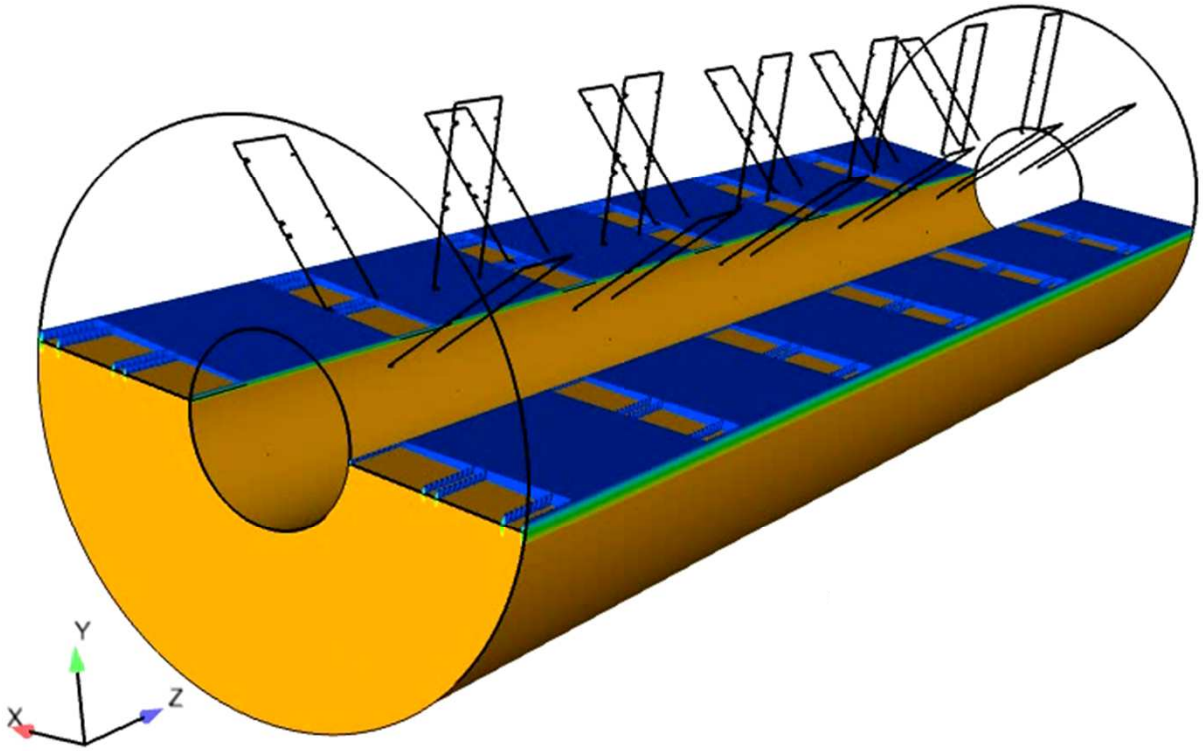
First approach

In a first approach the domes have not been considered then the symetry of the geometry allows to solve the equation in a rotating frame

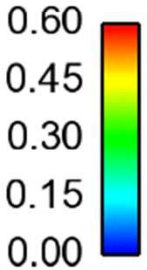
- Add coriolis and centrifugal forces in gas and solid momentum equations
- Projection of the gravity
- Rotating moving walls with imposed velocity

ROTATING FRAME

Solid Volume Fraction



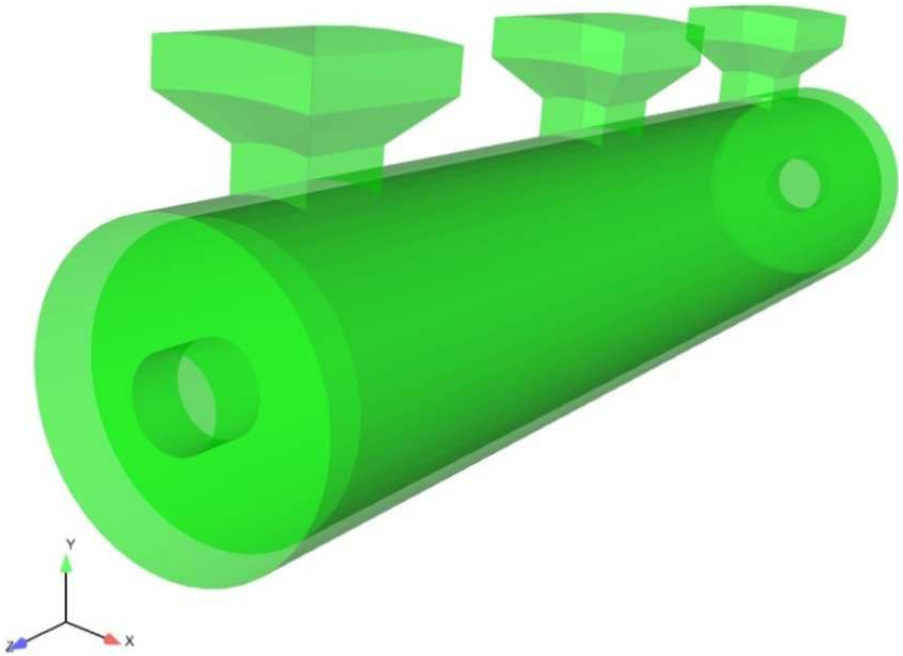
Time = 0.001s

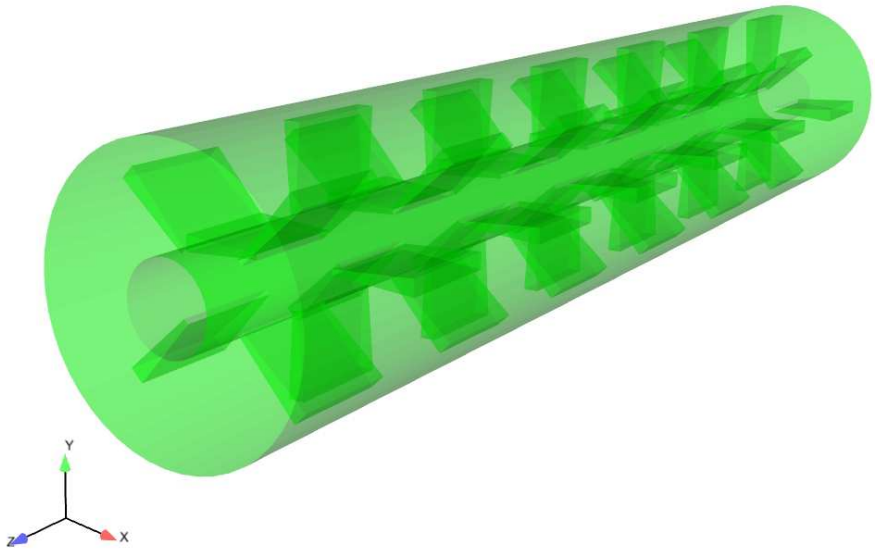


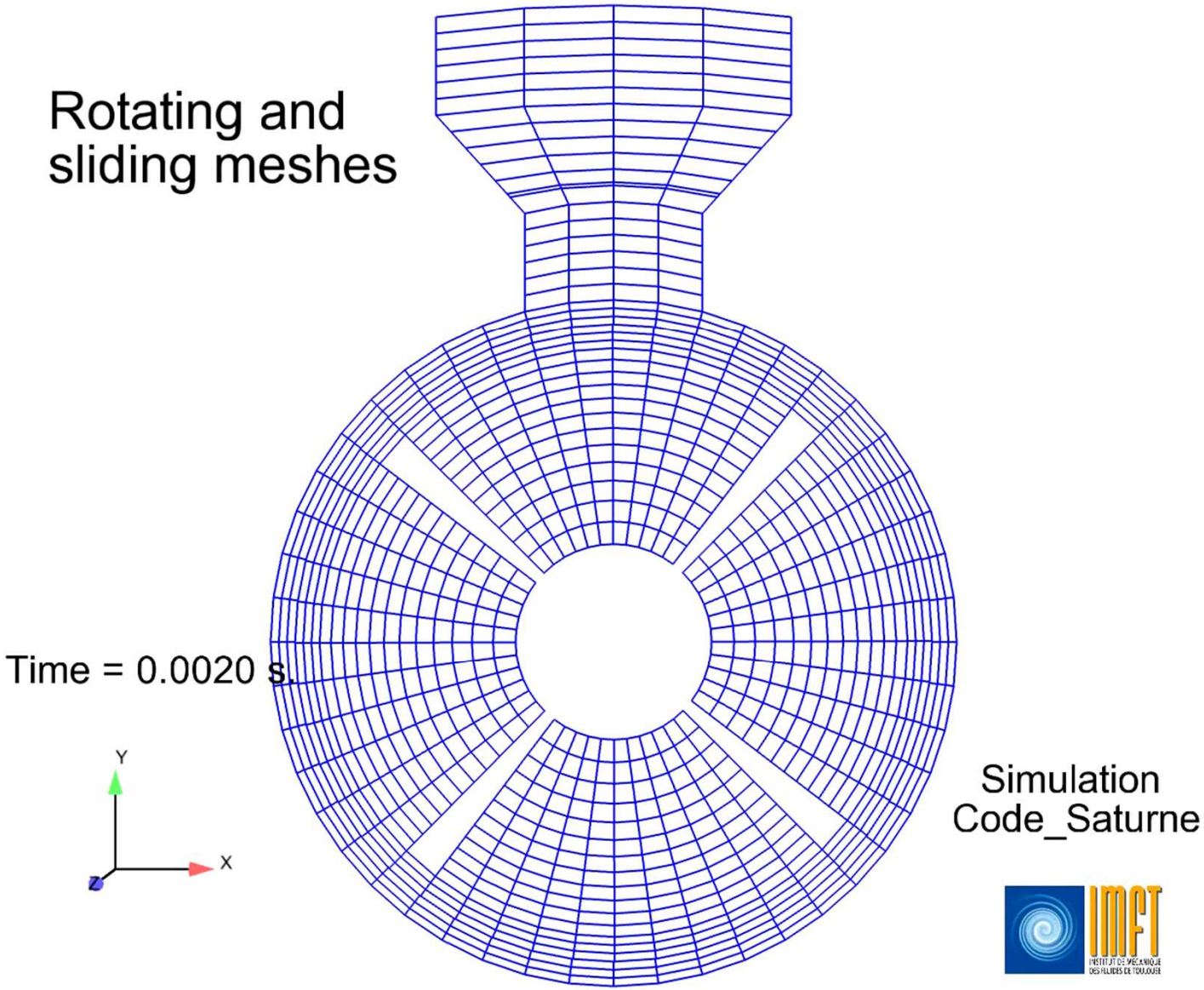
Simulation
NEPTUNE_CFD

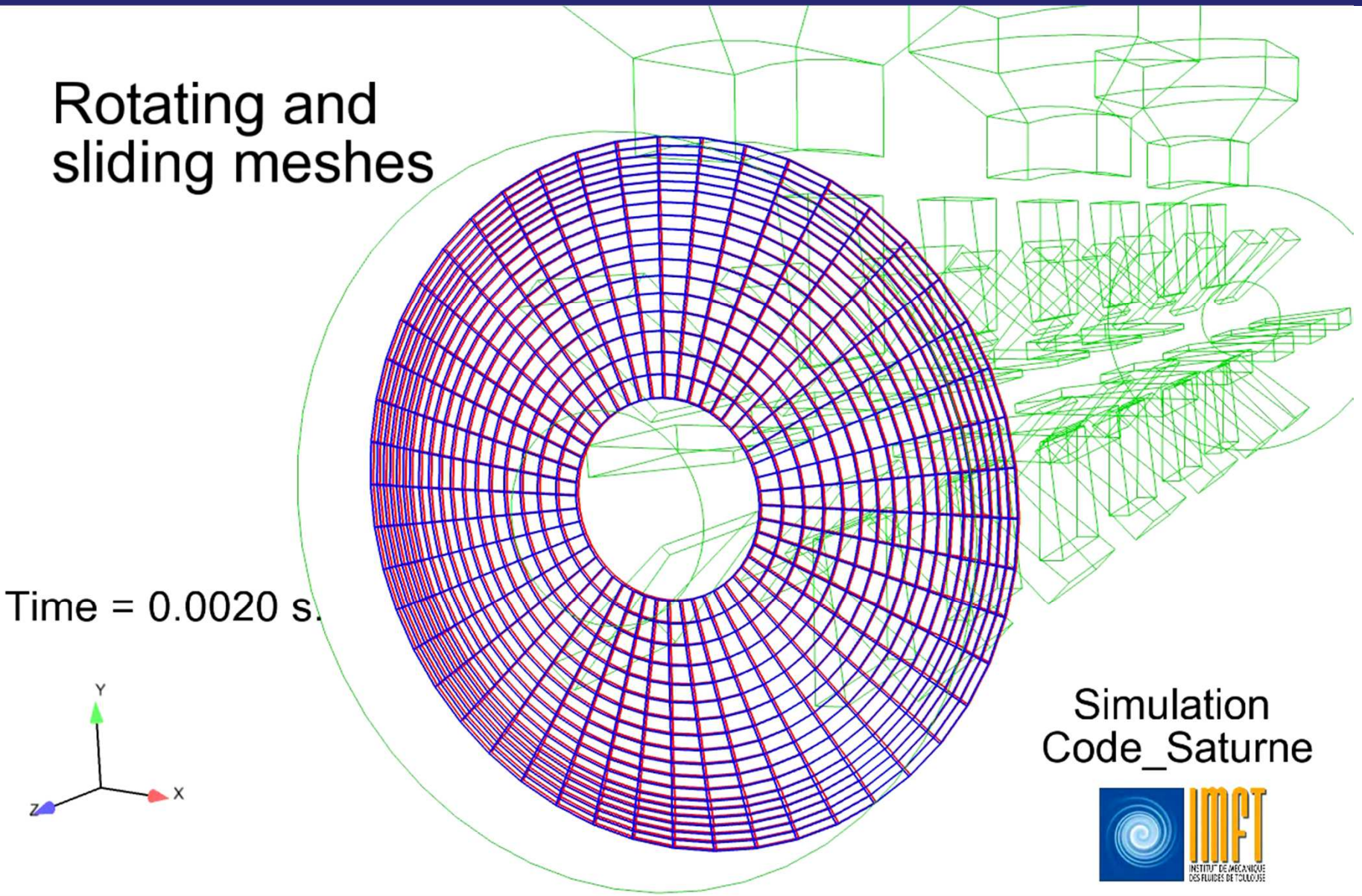
With the domes the first approach cannot be used, then an hybrid method has been developed.

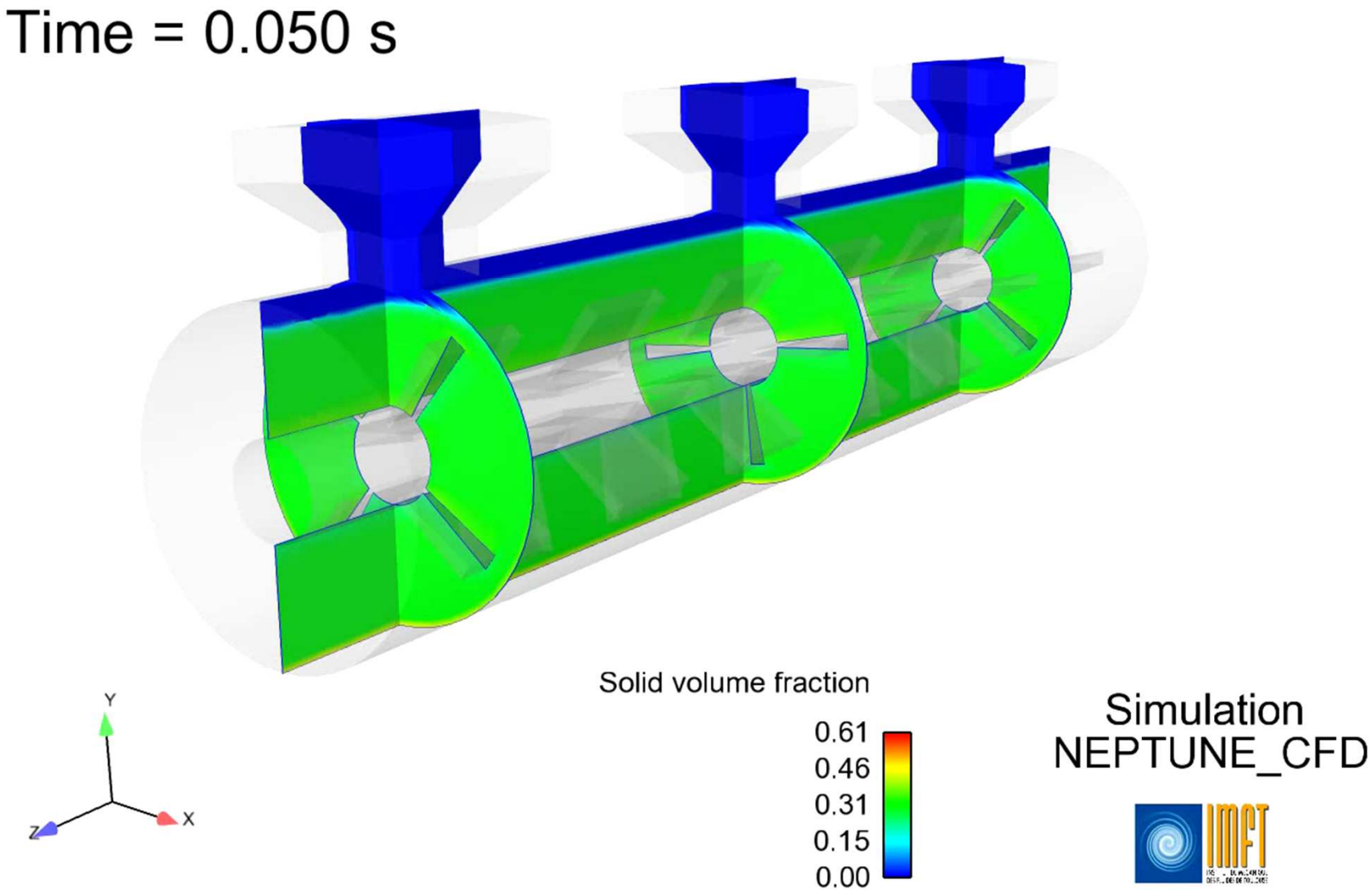
- Two meshes are used: one static (stator) and one rotating (rotor)
- Real-time non-coincidence mesh joining



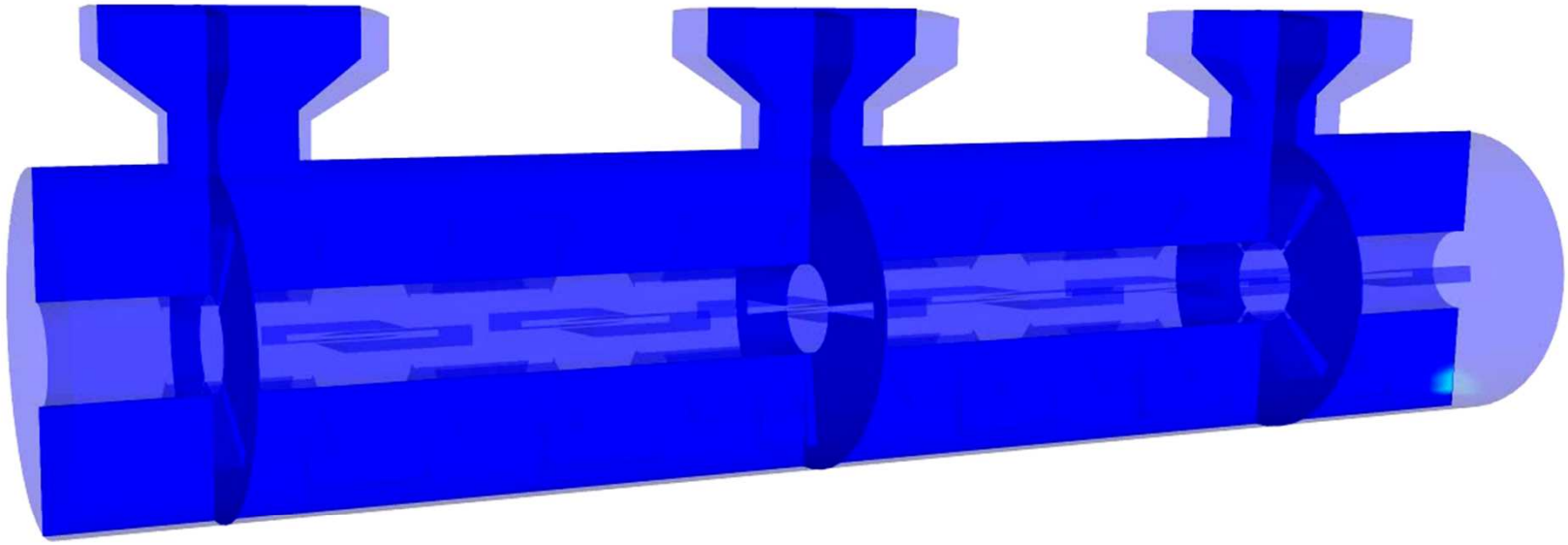


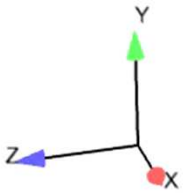

Rotating and
sliding meshes
Time = 0.0020 s.
Y
X
Z
Simulation
Code_Saturne


Rotating and
sliding meshes
Time = 0.0020 s.
Y
X
Z
Simulation
Code_Saturne


Time = 0.050 s
Y
Z
X
Solid volume fraction
0.61
0.46
0.31
0.15
0.00
Simulation
NEPTUNE_CFD

Time = 0.050 s





Scalar
1.00
0.75
0.50
0.25
0.00

Simulation
NEPTUNE_CFD

CONCLUSIONS

- Numerical simulation of dense fluidized bed of an industrial scale geometry is possible up to 100 millions of cells
  - This allows to understand the local gas-particle interactions
  - These are “reference simulations” for model development (filtered approach)

- Rotating mesh opens the doors for the numerical simulation of horizontal reactor for polypropylene polymerization
  - Method validation is still in progress (rotating drum)
  - Needs model for frictional effects

- Additional physics