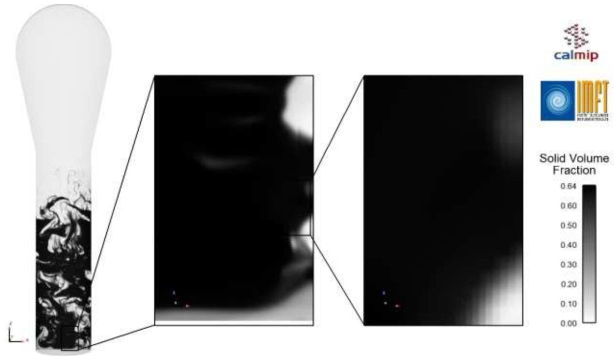
CALMIP : Mésochallenge 2018



JCAD'2018
Journées Calcul & données

Massively Parallel Numerical Simulation of Hydrodynamics and Transfers in a Polydispersed Reactive Gas-Particle Fluidized Bed at Industrial Scale

Hervé NEAU, Pascal FEDE, Renaud ANSART, Olivier SIMONIN
Université de Toulouse; Toulouse INP / CNRS / UPS – IMFT
Nicolas RENON, Pierrette BARBARESCO – *CALMIP*
Cyril BAUDRY, Nicolas MERIGOUX – *EDF R&D*

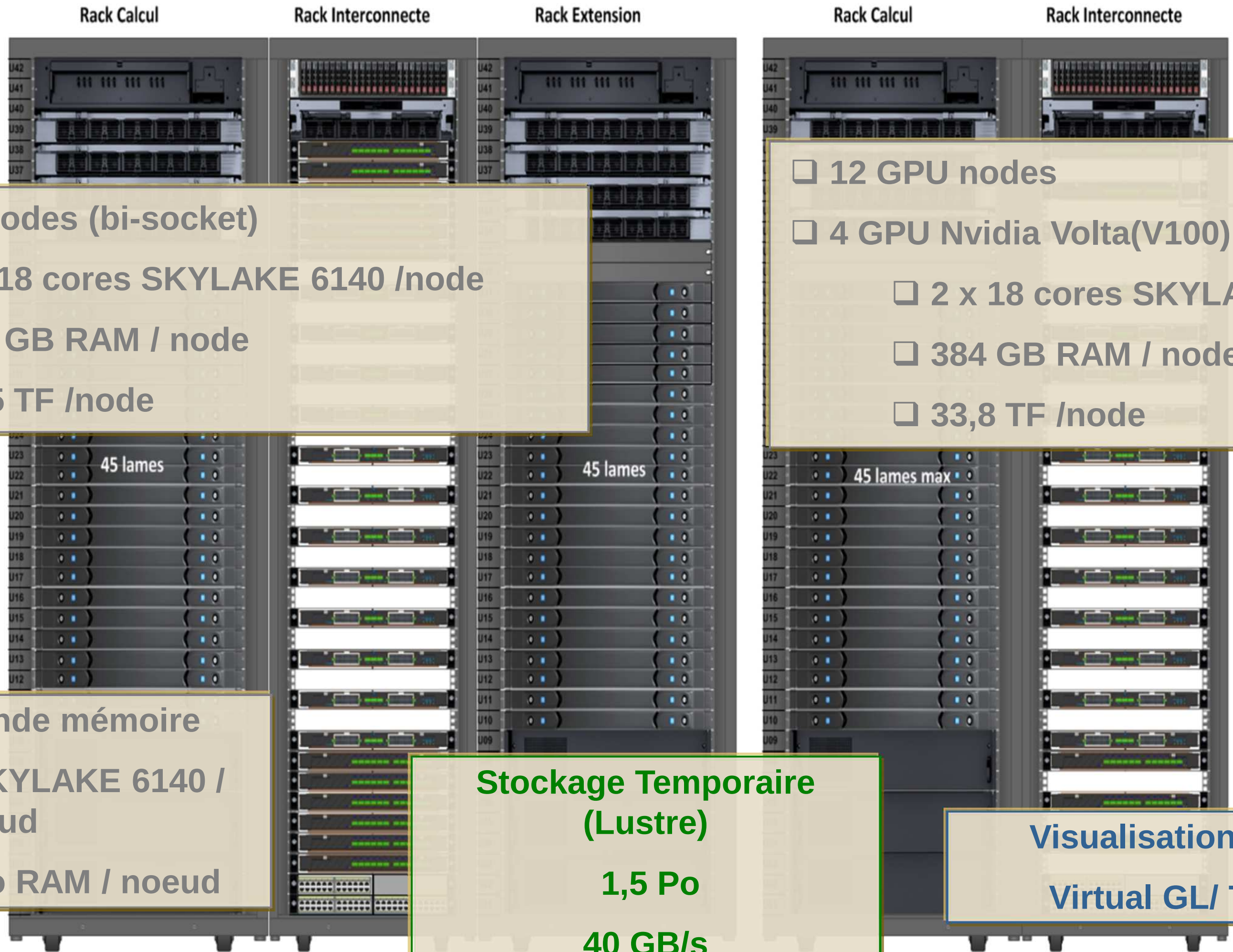
Présentation du système de calcul de CALMIP : OLYMPE

- Cluster Atos Bull SEQUANA X1000
- Nombre total de nœuds : **374**
- Nombre total de cores (Skylake 6140) : **13464**
- Nombre total Carte GPU (Nvidia V100) : **48**

- Téraflop Crête 1365 TF
- Conso Linpack : 199 Kw

- Calendrier
  - Mai 2018 : Installation (Bâtiment : Espace Clément Ader)
  - Juin-Juillet 2018 : Mésochallenges (4)
  - Juillet-Aout 2018 : Vérification de Service Régulier
  - Septembre 2018 : En production

« OLYMPE » : SYSTEME DE CALCUL CALMIP 2018-2022



- ❑ 360 SKL nodes (bi-socket)
  - ❑ 2 x 18 cores SKYLAKE 6140 /node
  - ❑ 192 GB RAM / node
  - ❑ 2,65 TF /node

- ❑ 12 GPU nodes
- ❑ 4 GPU Nvidia Volta(V100) / node
  - ❑ 2 x 18 cores SKYLAKE 6140 / node
  - ❑ 384 GB RAM / node
  - ❑ 33,8 TF /node

2 Nœuds grande mémoire

2 x 18 cores SKYLAKE 6140 / noeud

1536 Go RAM / noeud

Stockage Temporaire (Lustre)

1,5 Po

40 GB/s

Visualisation à distance:

Virtual GL/ Turbo VNC

OLYMPE : Mésochallenges CALMIP 2018

- **Principe :** mise à disposition d'Olympe pour relever un défi scientifique (et technique!)
- **Appel à projets** (contrainte technique : application scalable > 4096 cœurs)
  9 projets reçus => 4 projets sélectionnés

Spectroscopie in-silico de cyanines
Porteur : Michel Caffarel, LCPQ

Impact des fines échelles spatiales sur la dynamique océanique en Méditerranée
(JCAD) 2018)
Porteuse : Claude Estournel LA

Collision oblique de deux sphères dans un fluide visqueux
Porteuse : Annaïg Pedrono, IMFT

Simulation numérique massivement parallèle de l'hydrodynamique et des transferts d'un réacteur à lit fluidisé gaz-particule réactif polydisperse à l'échelle industrielle (>1 000 000 000 mailles)
Porteur : Hervé Neau, IMFT

Massively Parallel Numerical Simulation of Hydrodynamics and Transfers in a Polydispersed Reactive Gas-Particle Fluidized Bed at Industrial Scale

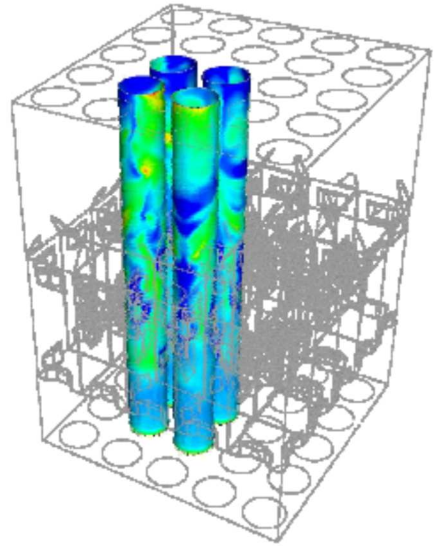
Fluidized beds are widely used in industry

- Polymerization of olefin
- Uranium fluorination
- Coal/biomass combustion (CO_2 capture/chemical looping)
- Production of pharmaceutical drugs
- …

The standard modeling Eulerian approach for industrial-scale geometries exhibits a sensitivity with respect to mesh size.

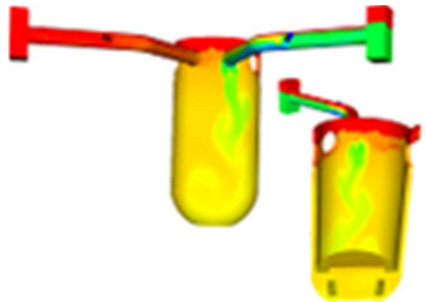
A First Worldwide Numerical Simulation of industrial fluidized bed with a very refined mesh using the whole new CALMIP supercomputer OLYMPE (Atos Bull SEQUANA X1000)

NEPTUNE_CFD code



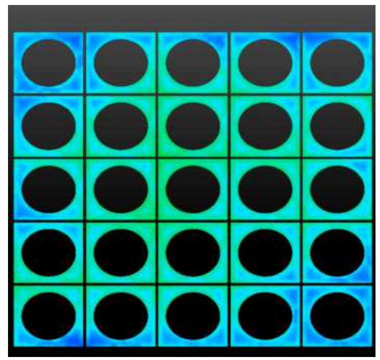
- **Finite Volume Eulerian multi-phase solver** developed jointly by EDF and CEA with financial support of IRSN and FRAMATOME, in the framework of the NEPTUNE project.

- **Massively parallel code (MPI) to compute 3D reactive turbulent unsteady multiphase flows => HPC capabilities**
  C/C++, QT-Python graphical-user interface,
  parallel multi-grid solver, MPI I/O



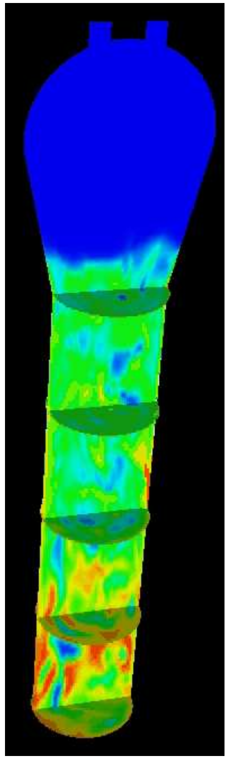
- **From laboratory-scale up to complex industrial-scale geometries**

- NEPTUNE_CFD is proprietary,
  based on open-sourced Code_Saturne



http://code-saturne.org

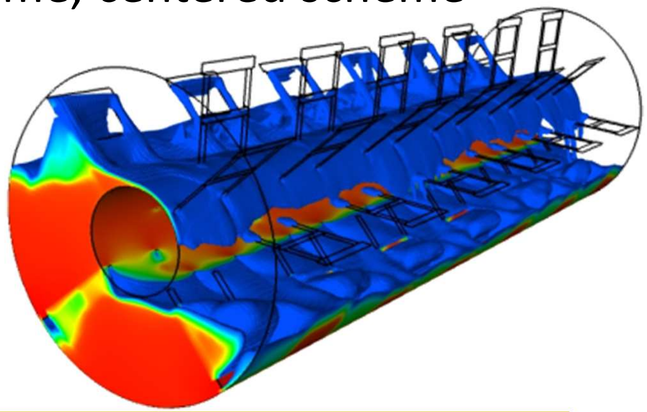
NEPTUNE_CFD@Toulouse



Pr. O. Simonin, Dr P. Fede, Dr R. Ansart, Dr E. Masi, Eng. H. Neau

- **Modeling approach**
  Unsteady multi-fluid modeling approach (N-Euler) developed and implemented by IMFT for **polydispersed particle-laden turbulent reactive flows** (turbulence, four-way coupling, polydispersed model, interfacial transfers and chemical reactions)

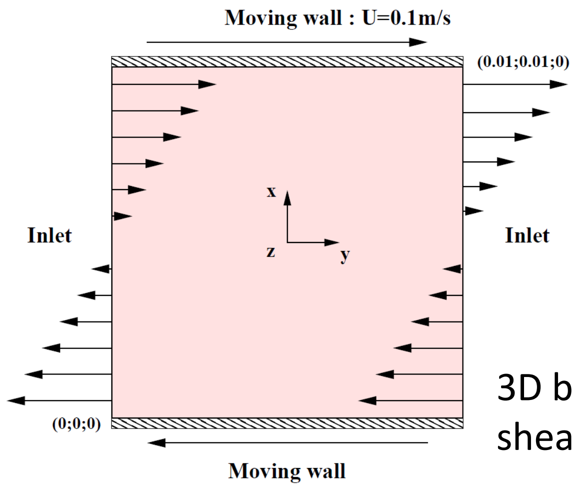
- **Numerical methods: semi-implicit solver**
  - **Massive Parallel** code: distributed-memory by domain decomposition (**MPI**)
    - parallel reading of meshes
    - parallel partitioning
    - MPI I/O
    - parallel multigrid solver for pressure
  - Numerical schemes
    - Time integration: 1^{st}-order fractional-step method
    - Spatial discretization: 2^{nd}-order unstructured finite-volume, centered scheme
  - Unstructured meshing:
    - Non-matching meshes
    - Rotating meshes



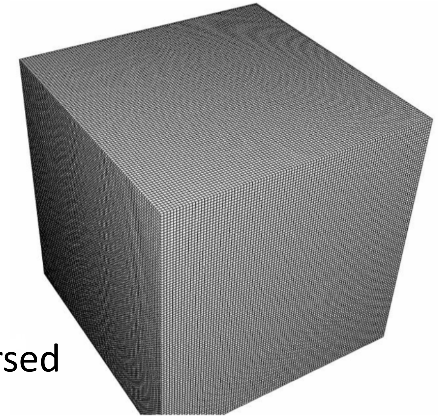
NEPTUNE_CFD parallel performances demonstrated up to 2,560 cores: super linear speedup

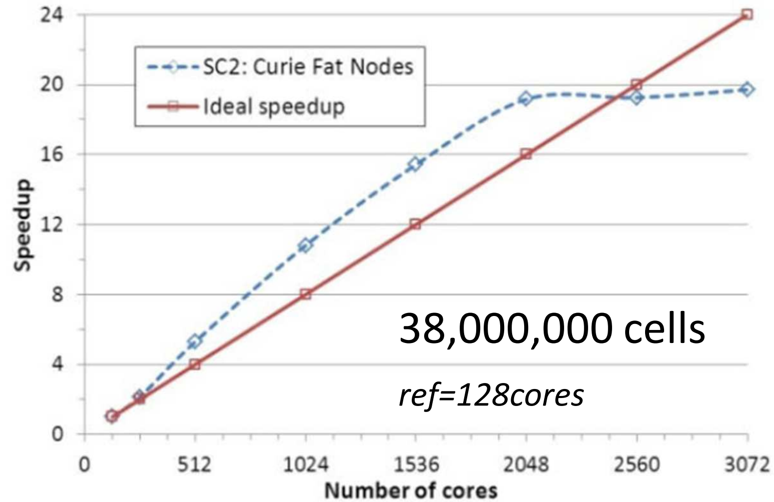
Neau H. et al., High performance computing (HPC) for the fluidization of particle-laden reactive flows, Fluidization XIV, 2013

Hamidouche Z. et al., Numerical Simulation of Multiphase Reactive Flows, Advances in Chemical Engineering, vol. 52, 2018



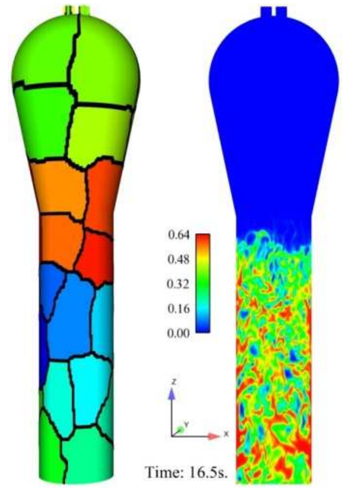
3D bidispersed shear flow





NEPTUNE_CFD massively parallel computation capabilities established up to **4,000 cores** during CALMIP Mesochallenge (2014) on a fluidized bed at industrial scale

Ideal speedup for number of cells per core over 25,000 cells



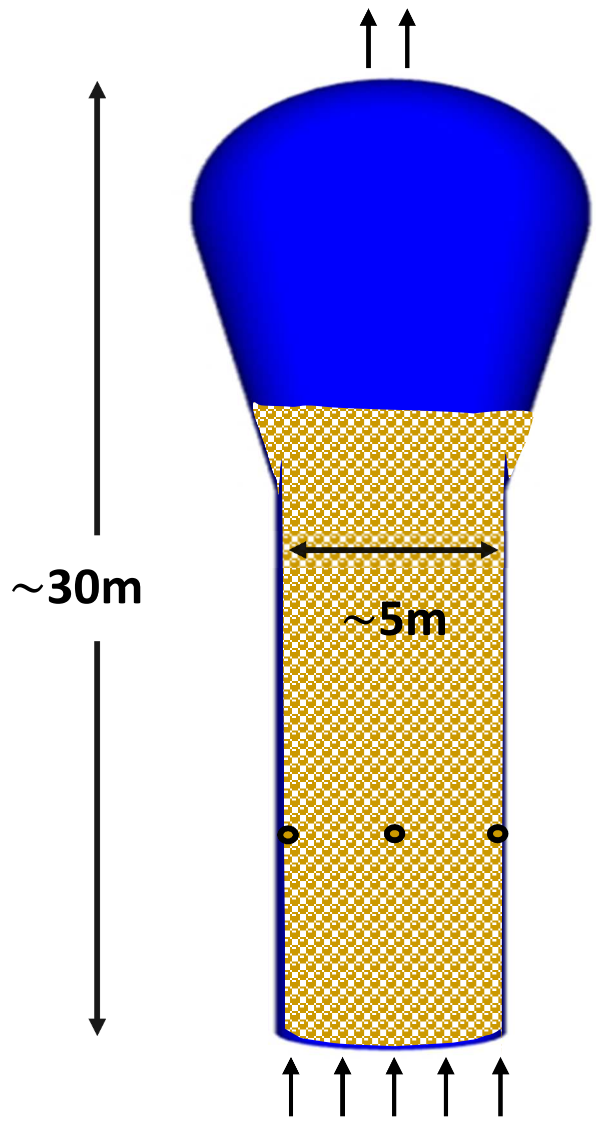
Gas-solid fluidized bed reactor

108,000,756 cells

Actual industrial geometry

- H~30m and D~5m
- Gas + 2 types of particles
- Injection of fine particles
- Heat transfers between gas and particles
- Exothermic reaction
- Multi-scale complex flow:

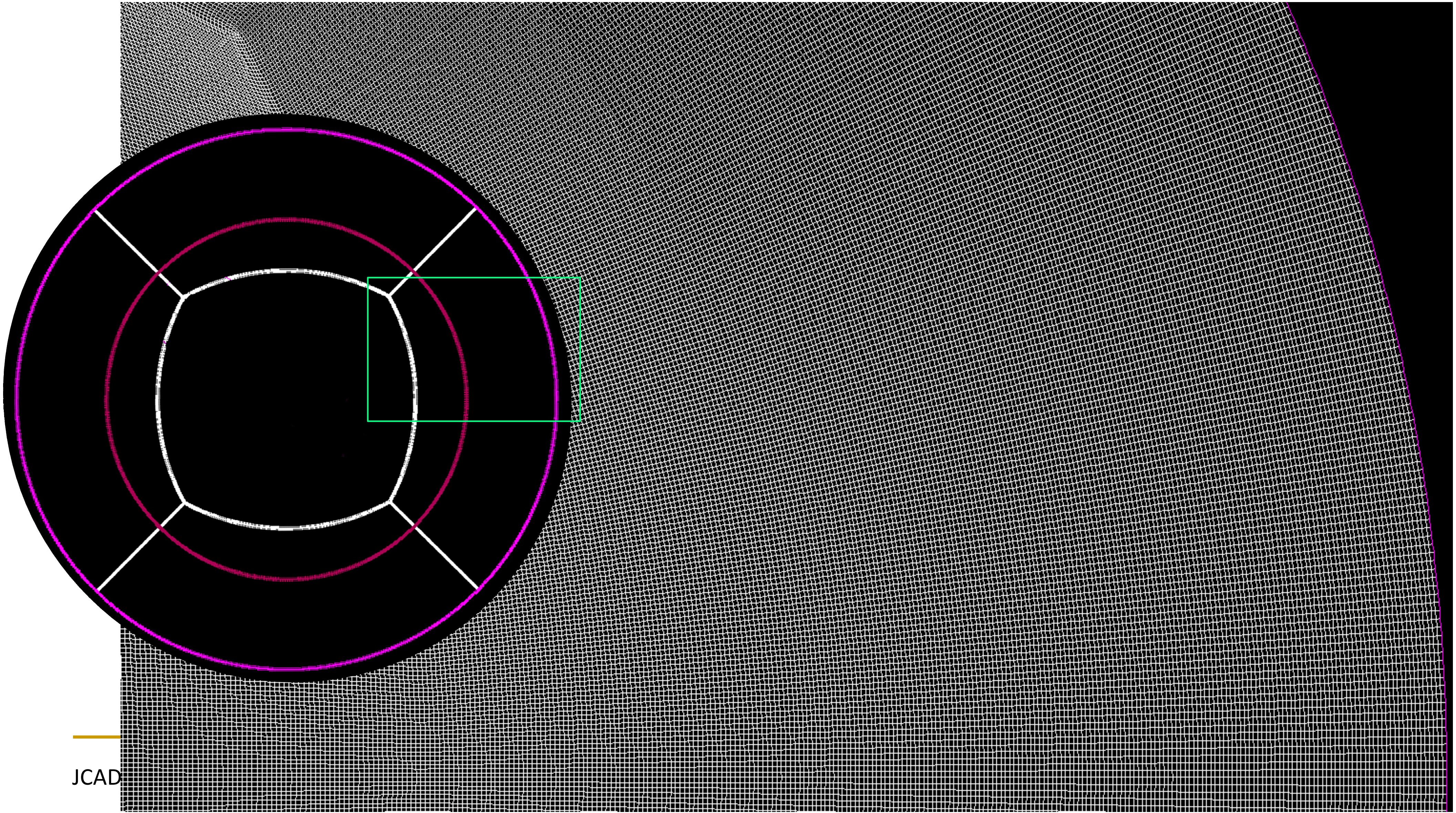
$$\frac{D_{reactor}}{d_{particles}} > 10^4$$



1st challenge: create the very large unstructured mesh

Simail mesher: creation of 5 pseudo-2D meshes (1 layer) - **850 cells over diameter**

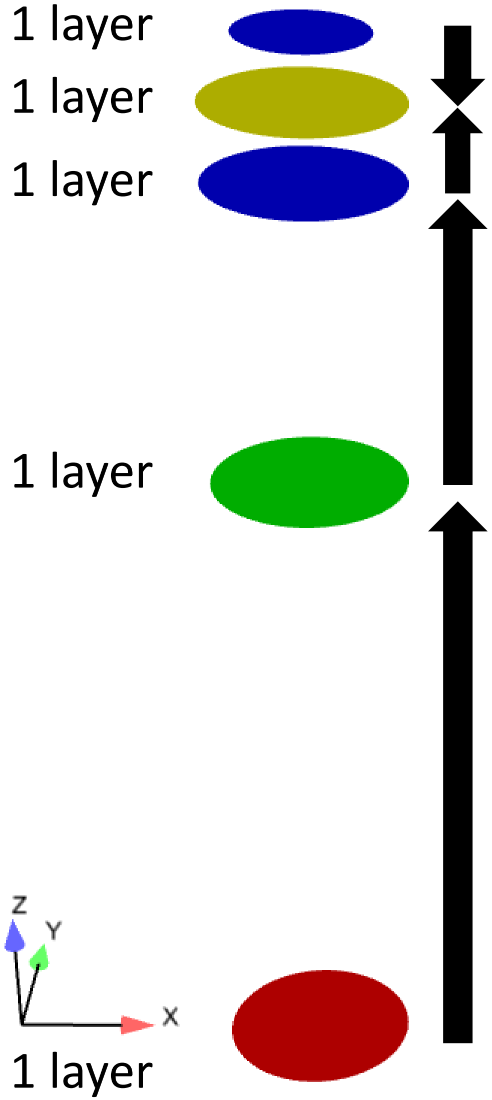
Extended O-grid meshes: 4 meshes with 476,928 hexahedral rectangular cells each
1 mesh with 253,184 hexahedral rectangular cells



1st challenge: create a very large unstructured mesh

Using **Code_Saturne** in preprocessing mode, (i) extrude 4 meshes and (ii) merge all meshes

90 nodes (2*12cores) on **Occigen/CINES** => 2160 cores - 3.9To - 5400s CPU per core



151 layers - expansion factor 1.0016

98 layers - expansion factor 1

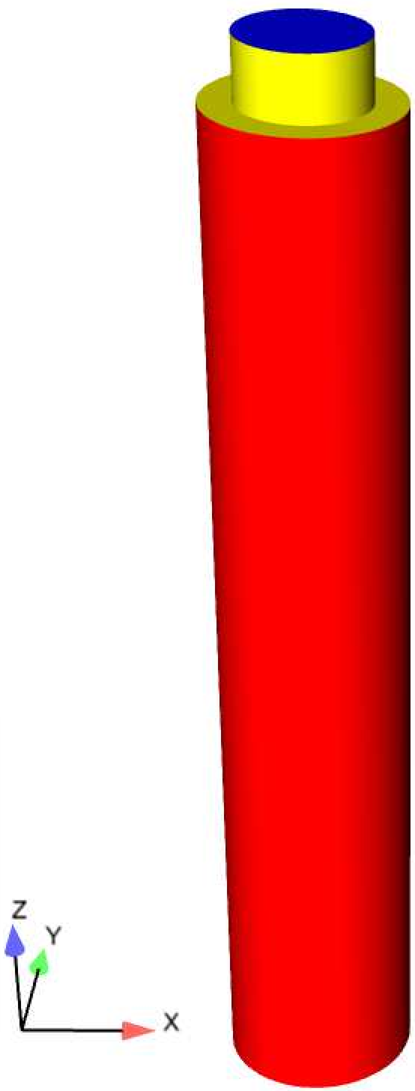
470 layers - expansion factor 1.0011

1450 layers - expansion factor 1

1,002,355,456 hexahedral cells

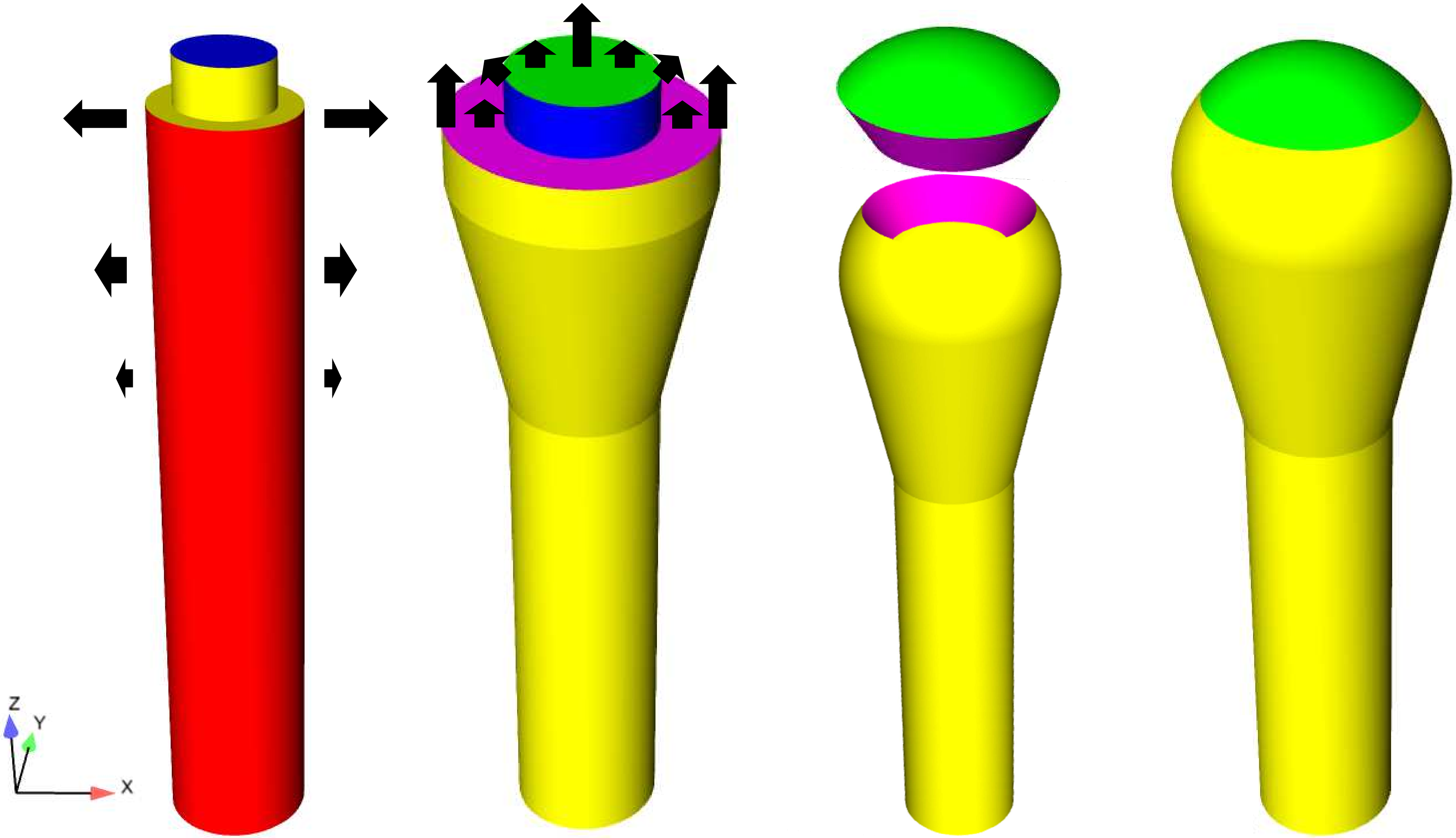
$\Delta_x \sim \Delta_y \sim \Delta_z \approx 5mm$

$\Delta_x * \Delta_y * \Delta_z \approx 0.125cm^3$

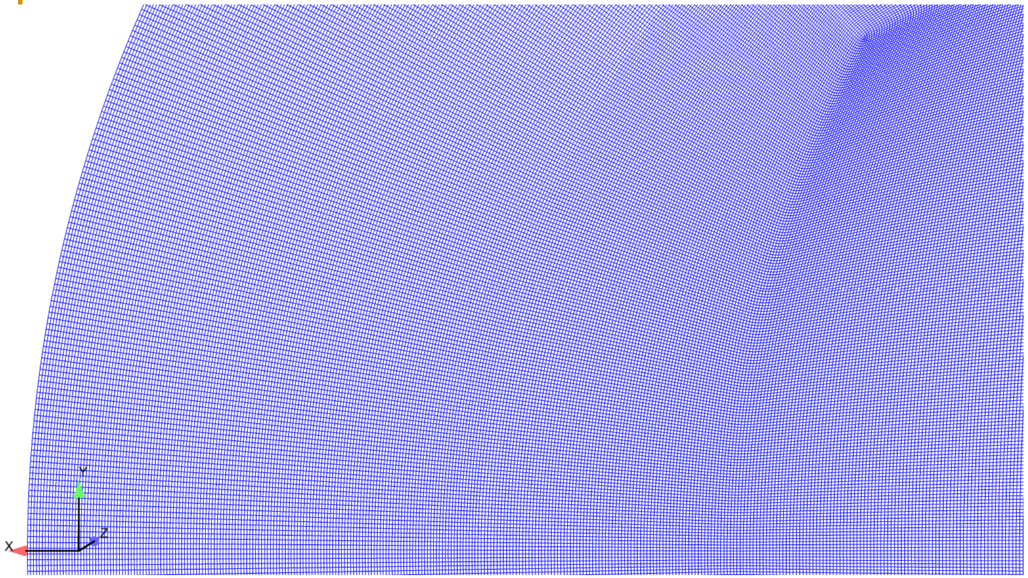


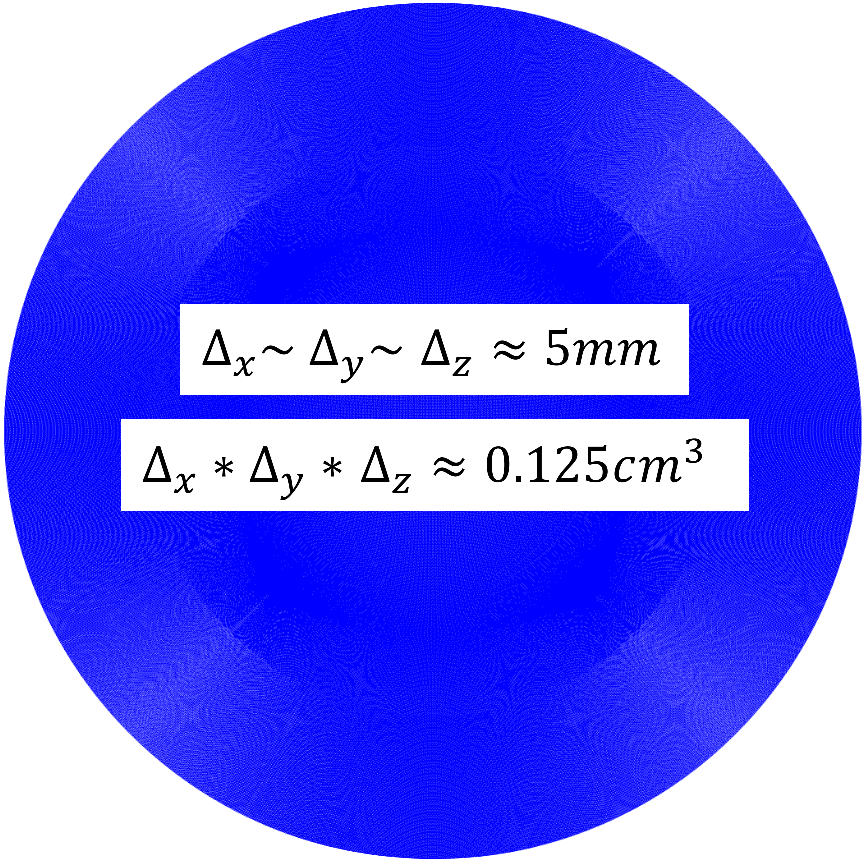
1st challenge: create a very large unstructured mesh

Using **Code_Saturne**, in preprocessing mode, modify the geometry: (i) dilatation, (ii) coordinates transformations to create the 2 parts of the bulb and (iii) final merge



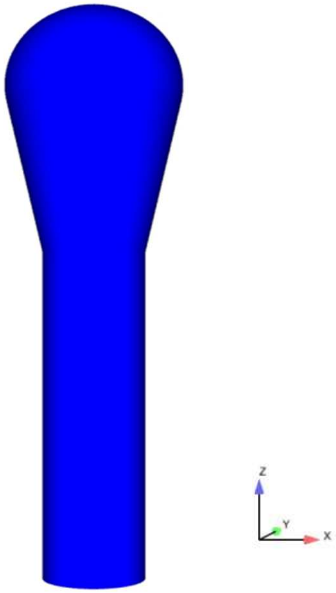
1^{st} challenge: create a very large unstructured mesh

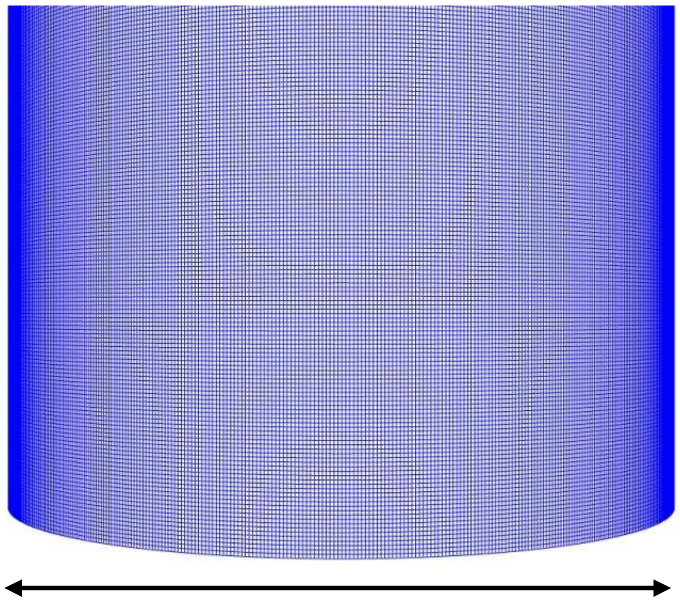




$\Delta_x \sim \Delta_y \sim \Delta_z \approx 5mm$

$\Delta_x * \Delta_y * \Delta_z \approx 0.125cm^3$





$\approx 850\ \Delta_x$

Binary Final Mesh: 209 Go

1,002,355,456 hexahedrons

3,008,918,880 faces

1,004,210,878 nodes

generated with Simail/Code_Saturne

Human time: 4 weeks

2nd challenge: Domain partitioning

Objective: create partitioning before run from 2,160 up to 13,032 cores

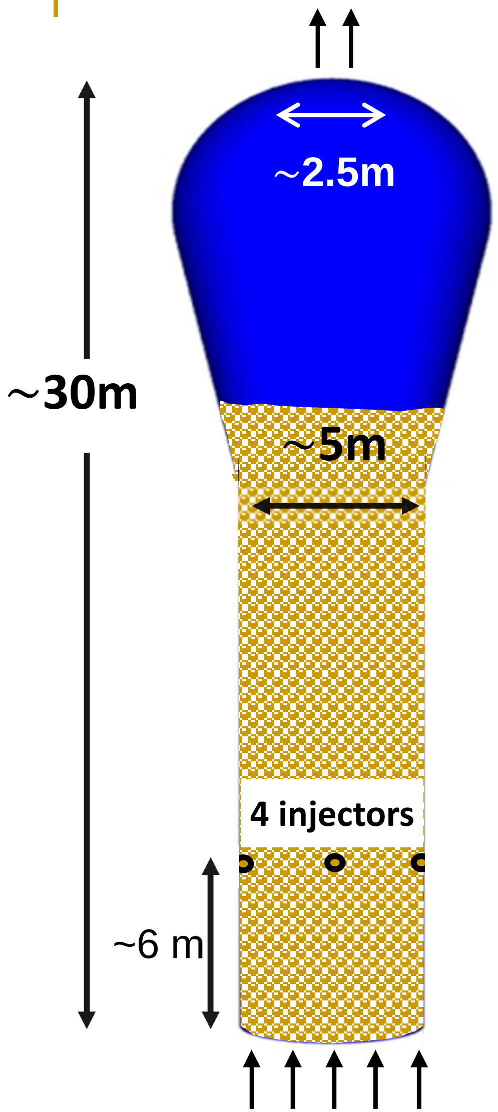
	PT-SCOTCH	ParMETIS	Morton curve	Hilbert curve	Block
Stability	Only on a limited number of cores even to create a lot of domains otherwise crash	No (mesh too big? Too much domains to create?)	yes	yes	yes
CPU time efficiency	No slower than using old supercomputer (ATOS-Bull doesn't solve this problem) 5x slower than Morton curve	--	yes	yes	no
Domain unbalance	~20% * Random seed algorithm	--	<<1% *	<<1%	~10%
Neighboring unbalance	Excellent (5-23)	--	Good (10-43)	Good	Bad
Ghost cell unbalance	Very good (31200-63700)	--	Good (54270-116000)	Good	Bad
Computation CPU time	Good	--	Good	Good	--

Final choice: Morton curve

*: creating 11520 domains

Outlet

Relative pressure = 0Pa



Fluidization inlet

- Gas inlet: V_f=0.6 m/s (Q_f=210 kg/s), T_{in}=50°C
- Large/fine particles: wall

Case description

Gas/Powder properties	Gas	Large part.	Fine part.
Density (kg/m^3)	22	850	850
Viscosity x10^{-5} (Pa.s)	1.54	--	--
Mean diameter (µm)	--	1600	80
Initial solid mass (kg)	--	100,000	0
Restitution coefficient	--	0.9	0.9
Specific heat (J/kg/K)	1728.65	2000	2000
Thermal conductivity W/m/K	0.04	--	--

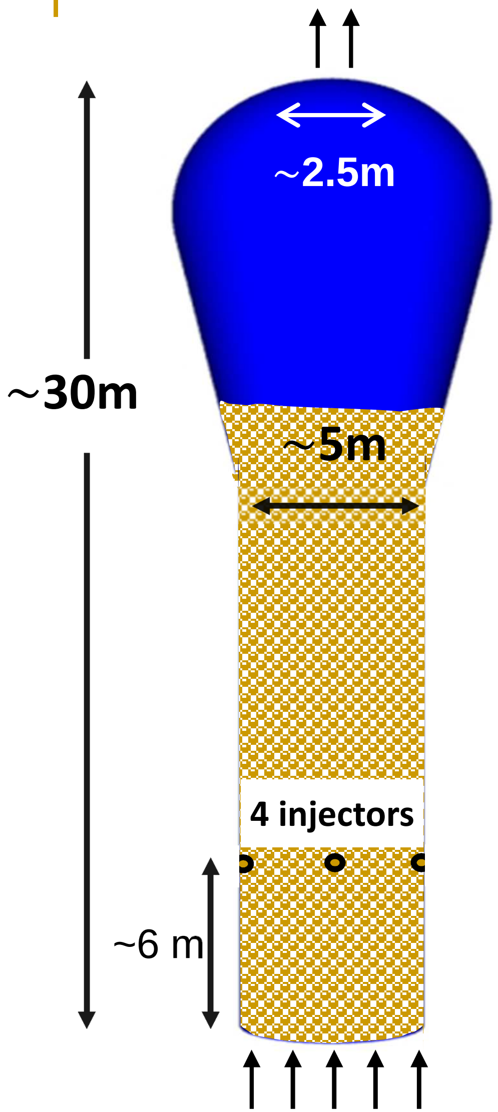
Injection of gas and fine particles through 4 injectors of ~0.03 m²

- Gas inlet: Q_{inj_gas}=21.5 kg/s (i.e. 77.3 t/h), T_{inj_gas} = 50°C
- Fine particles inlet: Q_{inj_fine}=0.2 kg/s (i.e. 720 kg/h), T_{inj_fine} = 50°C
- Large particles: wall

Wall boundary conditions (zero flux for enthalpy)

- Gas: wall with friction
- Large/fine particles: wall with no slip condition

Case description



Initialization parameters

- Mass of large particles = 100,000 kg (if z<18m, $\alpha_{large\ part.}$=0.402)
- Mass of fine particles = 0 kg
- Gas and large/fine particles temperature = 100°C

Operating point

- Exothermic reaction: $Q_{reaction}$ = 20MW
- Input temperature: T_{in} = 50 °C
- Expected outlet temperature: $T_{out} \approx$ 100°C

Physical models

- **Turbulence** (Four way coupling)**:** Gas ⇔ k-ε - Particles ⇔ q_p-q_{fp}
- **Drag: Wen & Yu** for particles
- **Large and fine particle interactions:** frictional model, granular model, kinetic model and polydispersed model
- **Thermal transfers:** gas / large, gas / fine

Thermal source terms: Fine particles 30 x more reactive than larges

- Large particles: $TS_{large} = \alpha_{large} * \rho_{large} * Q_{reaction}/M_{large}$
- Fine particles: $TS_{fine} = \alpha_{fine} * \rho_{fine} * Q_{reaction}/M_{large} * 30$

Principal metrics

- Hexahedral unstructured mesh: **1,002,355,456 cells**
- Binary mesh size: **209 Go**
- True industrial geometry: H~30m and D~5m => V~**600** $\boldsymbol{m^3}$
- Reading time for mesh, partitioning and restart file in NEPTUNE_CFD: **13 minutes**
- Checkpoint Restart file size: **1.34 To**

- Post-processing: Generated data size (EnSight Gold binary) over 600 time steps => ~**10 To**
  - saving 10 variables on all mesh elements every 25ms => 2.5 Po
  - Data saved only on 12 selected thick planes and cylinders and external surface
- Whole generated data (restart files, …): ~**120 To**

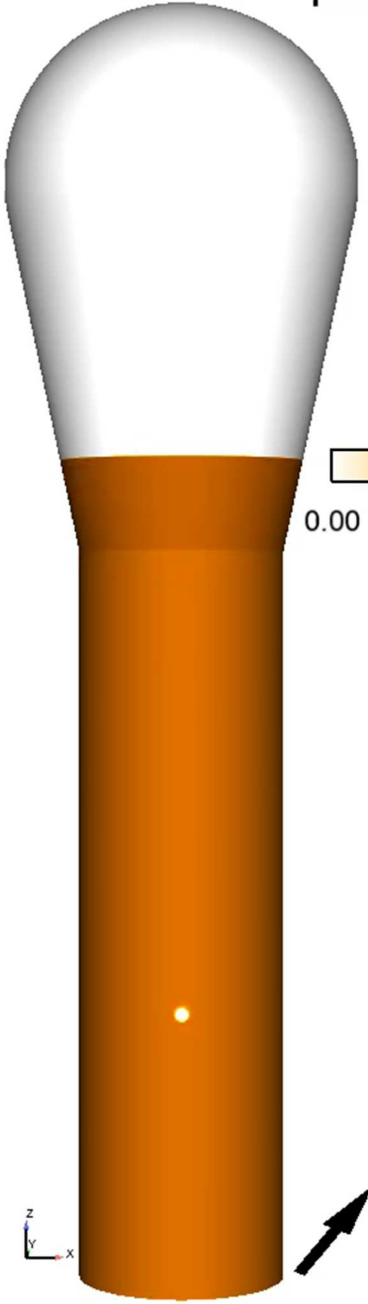
- **NEPTUNE_CFD V4.0.1 + Compiler Intel 18.2 + IntelMPI 18.21**
  21 coupled PDE solved for each time step

Runs from 60 nodes (2,160 cores) up to 362 nodes (13,032 cores) during 2018 summer

- **5 millions of CPU hours ⇔ 15 days (elapsed time) ⇔ 16.5s of physical time**
- 88,349 iterations with ~55s CPU per iteration using 120 nodes (4320 cores – 1/3 Olympe)

Industrial Scale Bidispersed Reactive Fluidized Bed Reactor

100 tonnes of particles - D~5m - H~30m - Unstructured Mesh: 1,002,355,456 cells



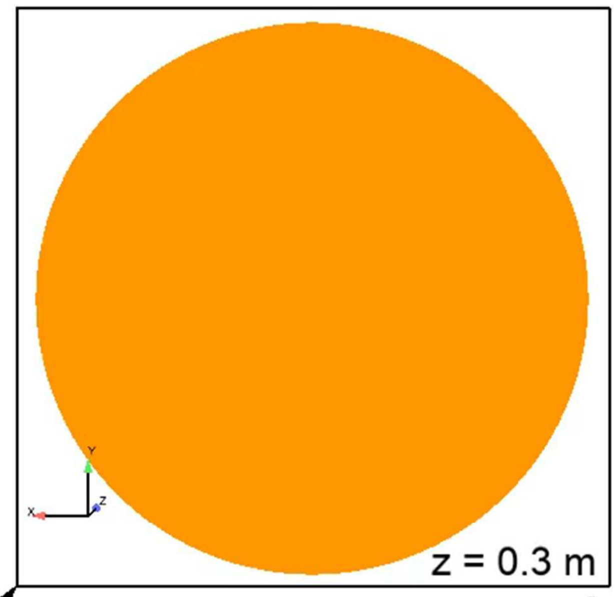
NEPTUNE_CFD HPC at CALMIP

HPC Center: 13 032 cores

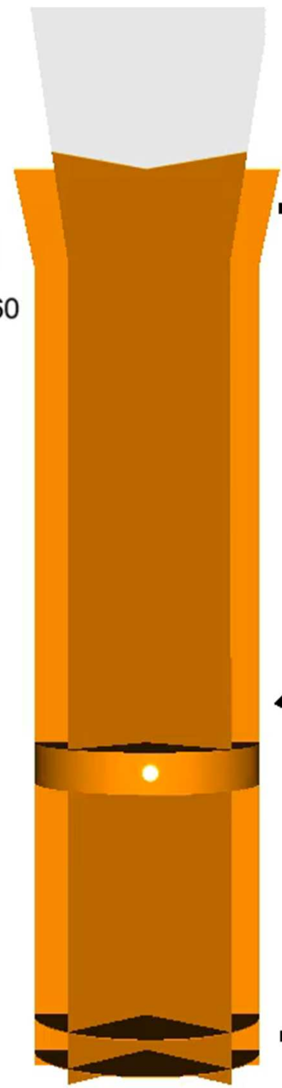
Skylake 6140 2.3GHz

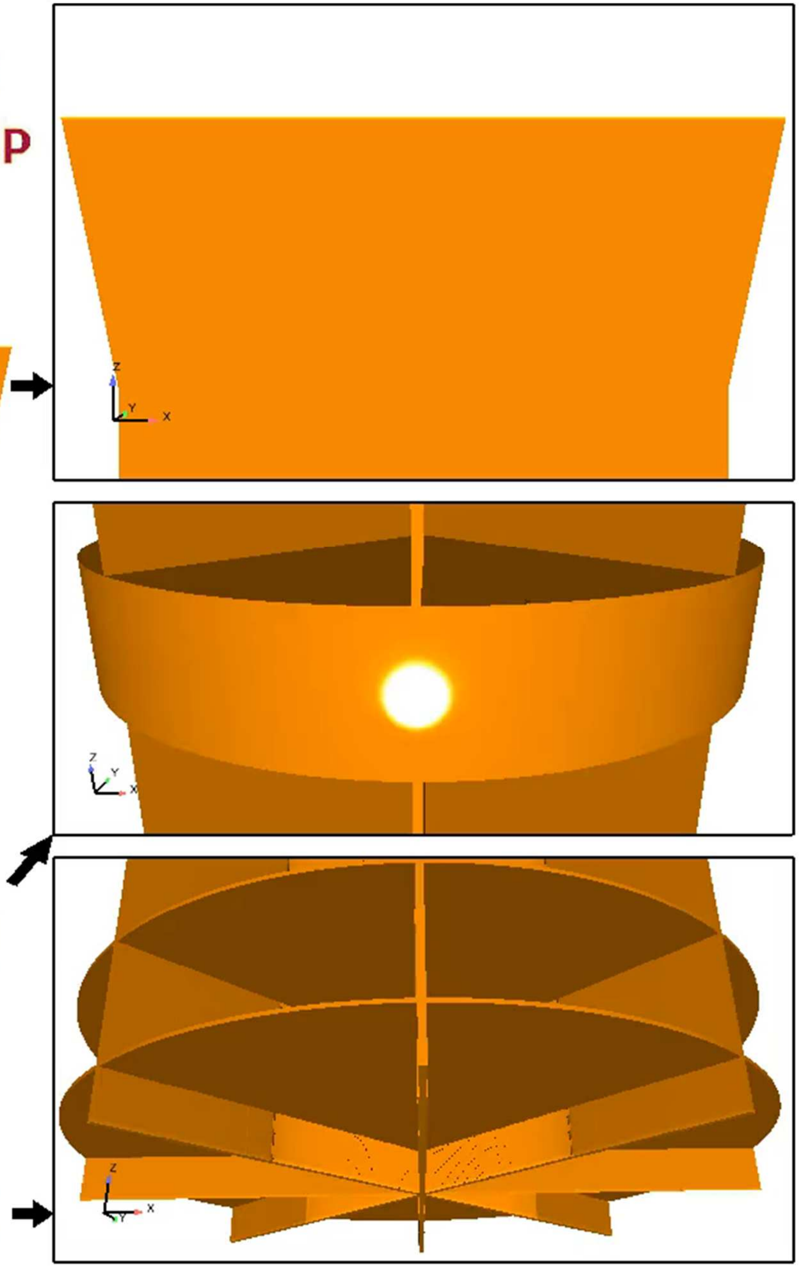
Solid Volume Fraction

0.00 0.10 0.20 0.30 0.40 0.48 0.52 0.56 0.60



Time = 0.03s.

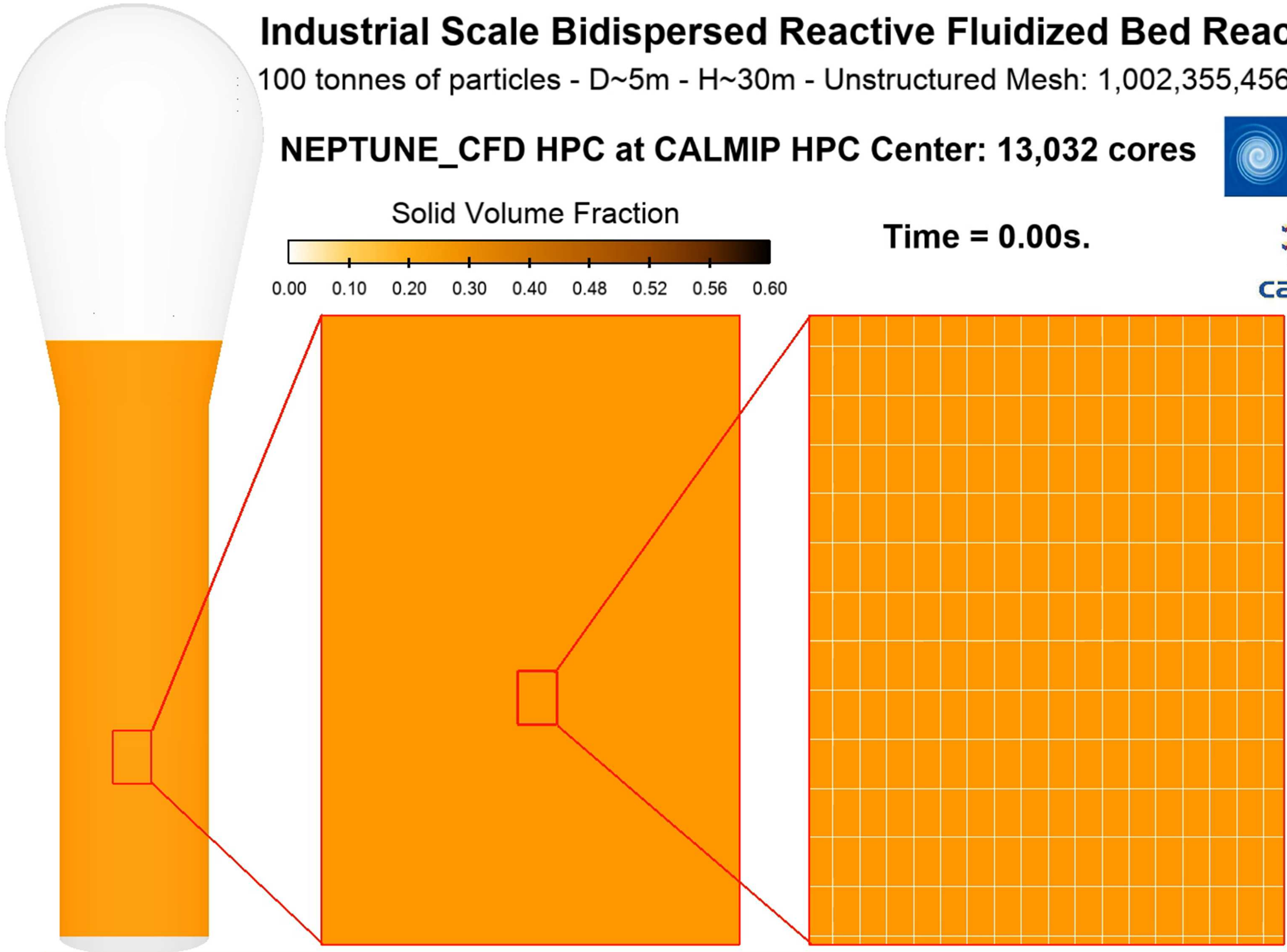




Industrial Scale Bidispersed Reactive Fluidized Bed Reactor

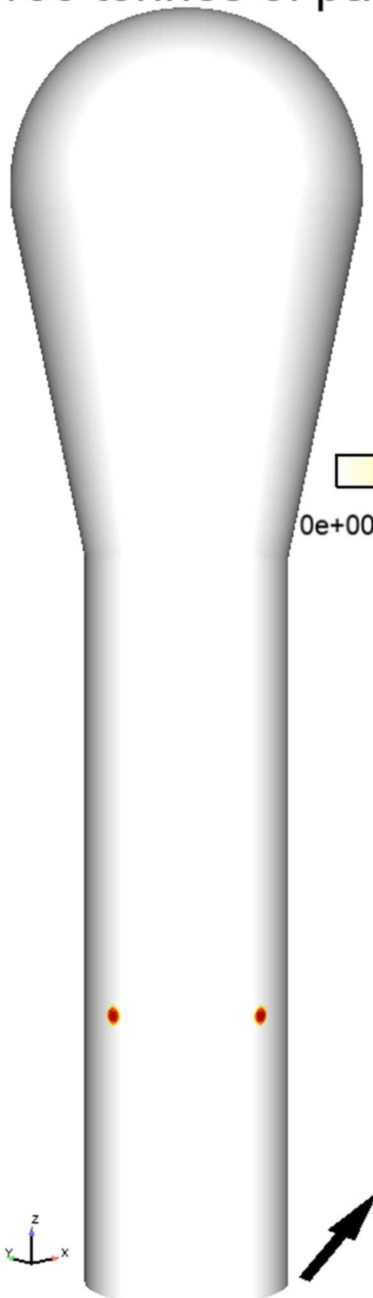
100 tonnes of particles - D~5m - H~30m - Unstructured Mesh: 1,002,355,456 cells

NEPTUNE_CFD HPC at CALMIP HPC Center: 13,032 cores



Industrial Scale Bidispersed Reactive Fluidized Bed Reactor

100 tonnes of particles - D~5m - H~30m - Unstructured Mesh: 1,002,355,456 cells

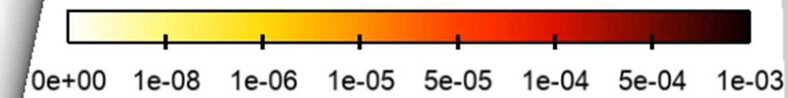


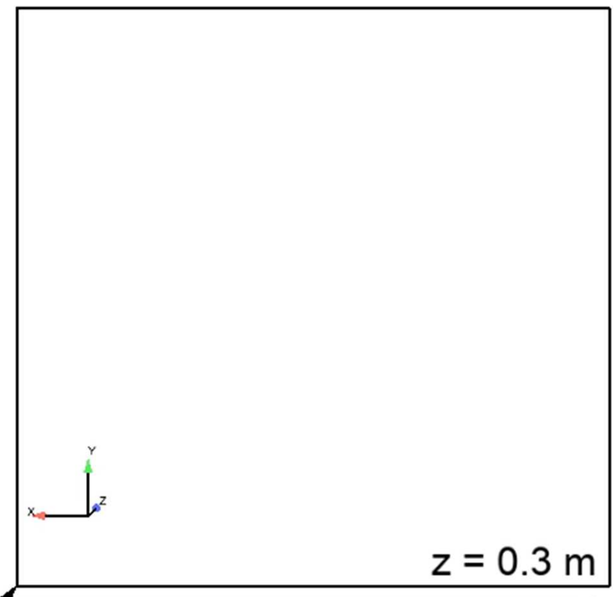
NEPTUNE_CFD HPC at CALMIP

HPC Center: 13 032 cores

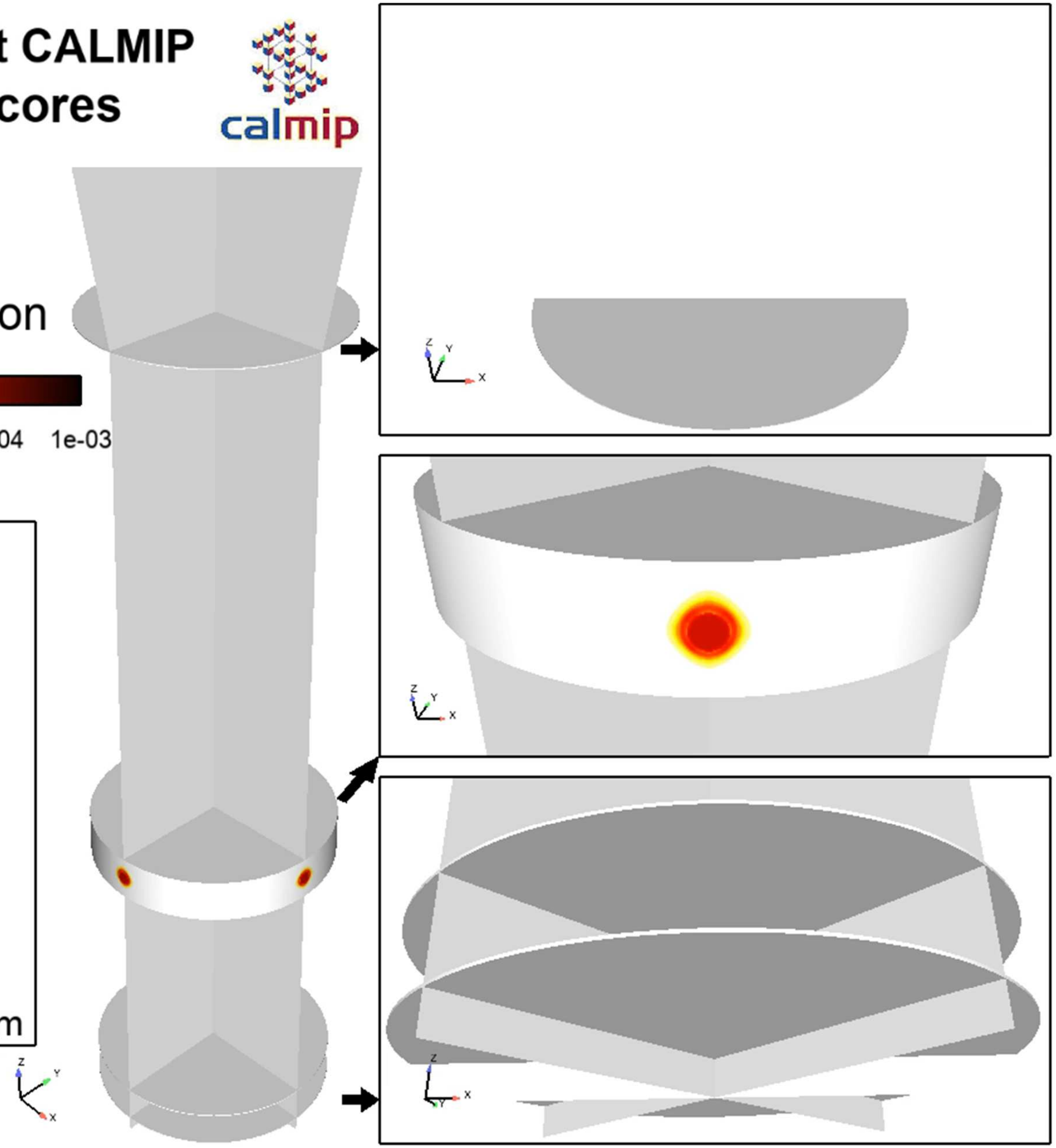
Skylake 6140 2.3GHz

Fine Solid Volume Fraction



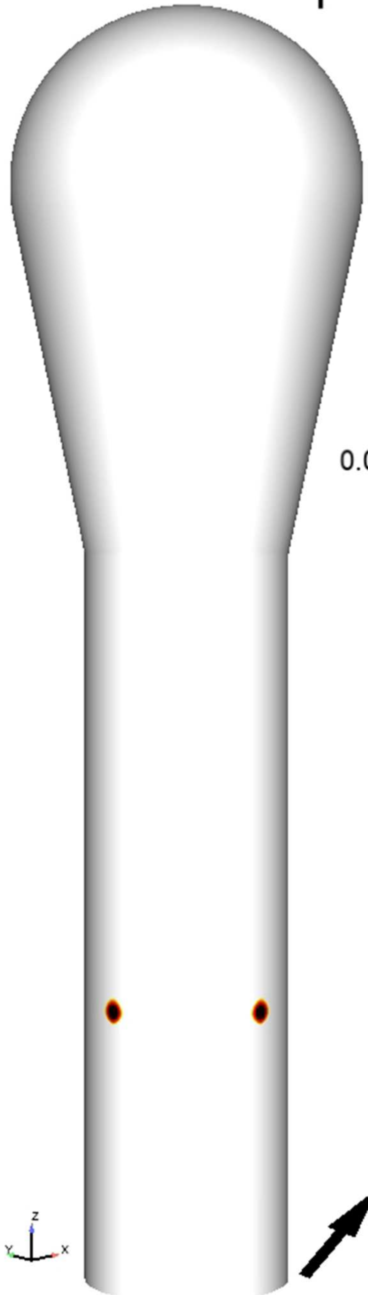


Time = 0.03s.

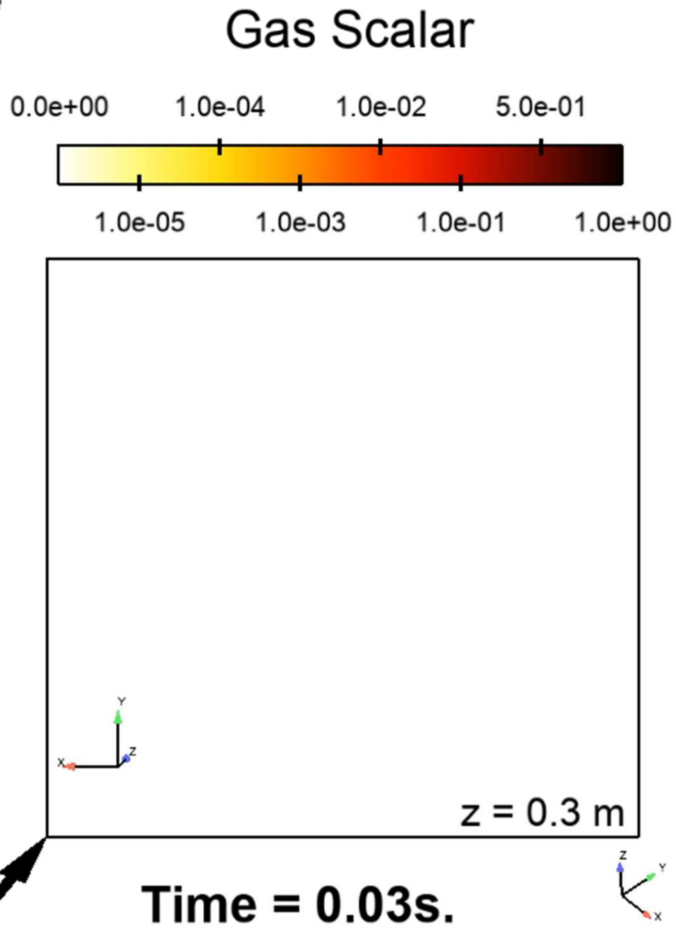


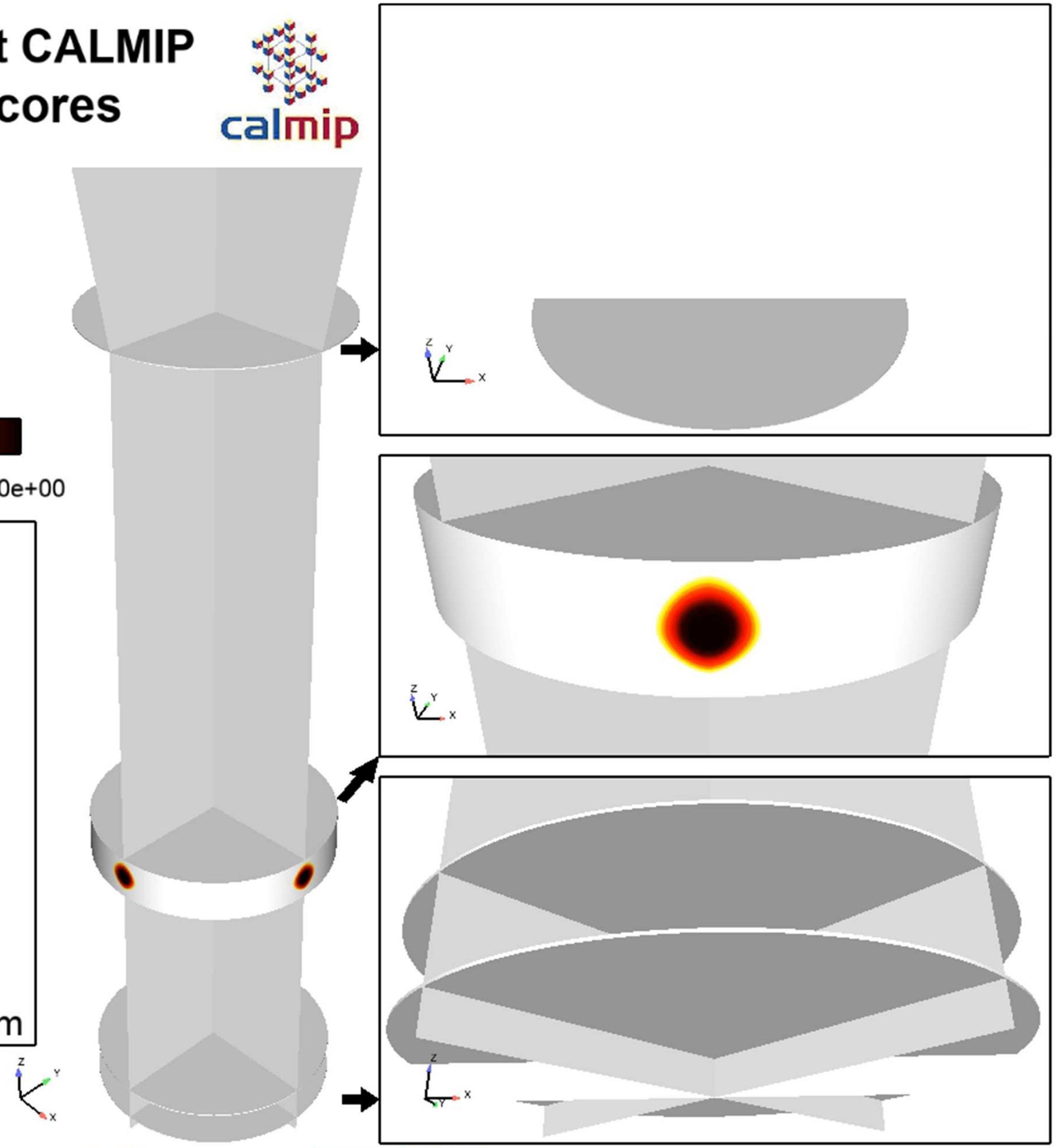
Industrial Scale Bidispersed Reactive Fluidized Bed Reactor

100 tonnes of particles - D~5m - H~30m - Unstructured Mesh: 1,002,355,456 cells



NEPTUNE_CFD HPC at CALMIP
HPC Center: 13 032 cores
Skylake 6140 2.3GHz

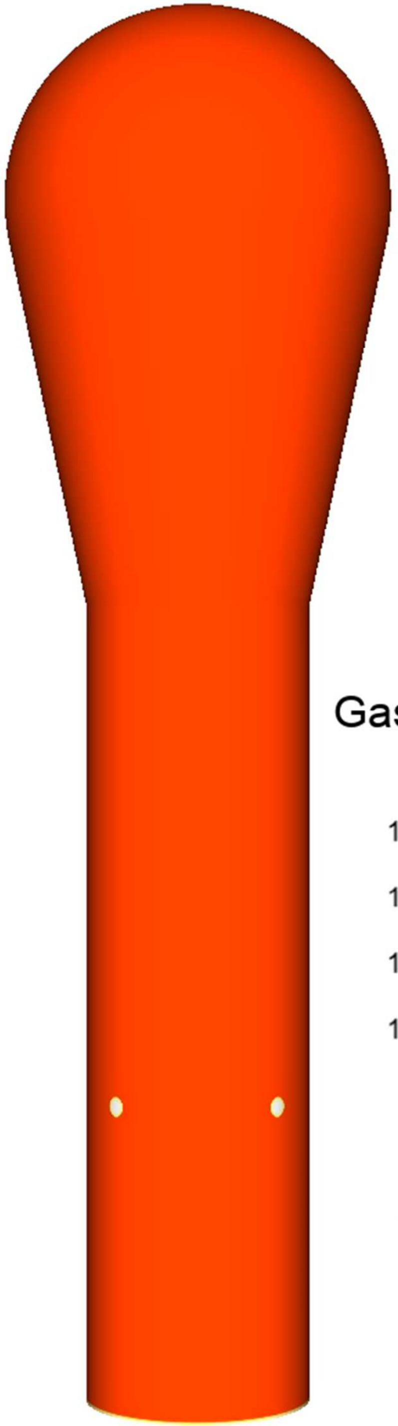


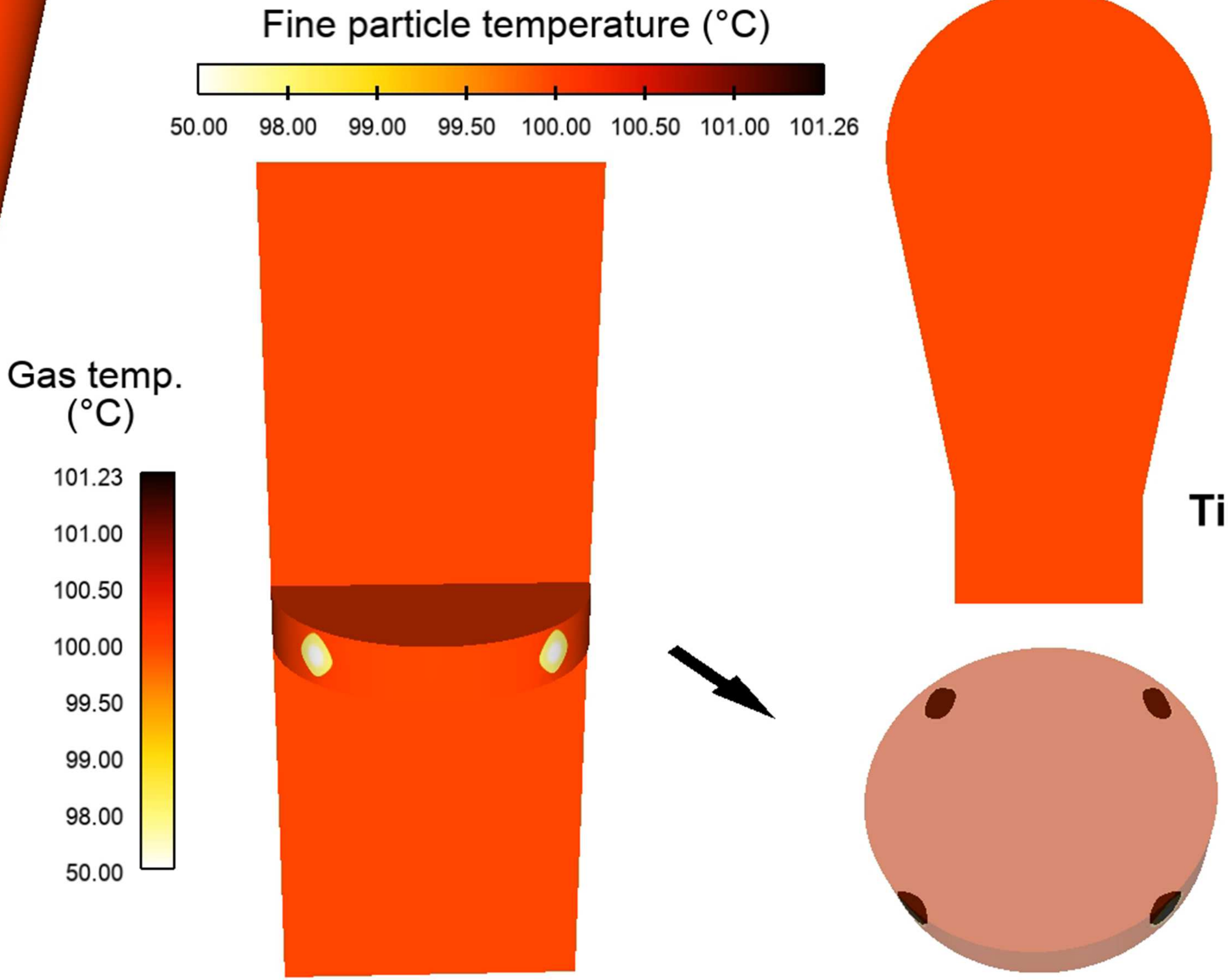


Industrial Scale Bidispersed Reactive Fluidized Bed Reactor

100 tonnes of particles - D~5m - H~30m - Unstructured Mesh: 1,002,355,456 cells

NEPTUNE_CFD HPC at CALMIP HPC Center: 13,032 cores





CALMIP 2018 NEPTUNE_CFD Mesochallenge overview

A **Worldwide Premiere highly-detailed** Numerical Simulation of **industrial reactive fluidized-bed** using the **whole new CALMIP supercomputer** OLYMPE (Atos Bull SEQUANA)

=> Challenge tackled thanks to very **efficient parallel software, NEPTUNE_CFD** and **fine meshing** (more than 1 000 000 000 elements) and advanced physical models

Operating challenges:

- Occurring **hardware failures:** unresponsive nodes, data recovery, …
- Handling large-cluster **MPI issues:** fine tuning for ALLREDUCE operations through env. variables

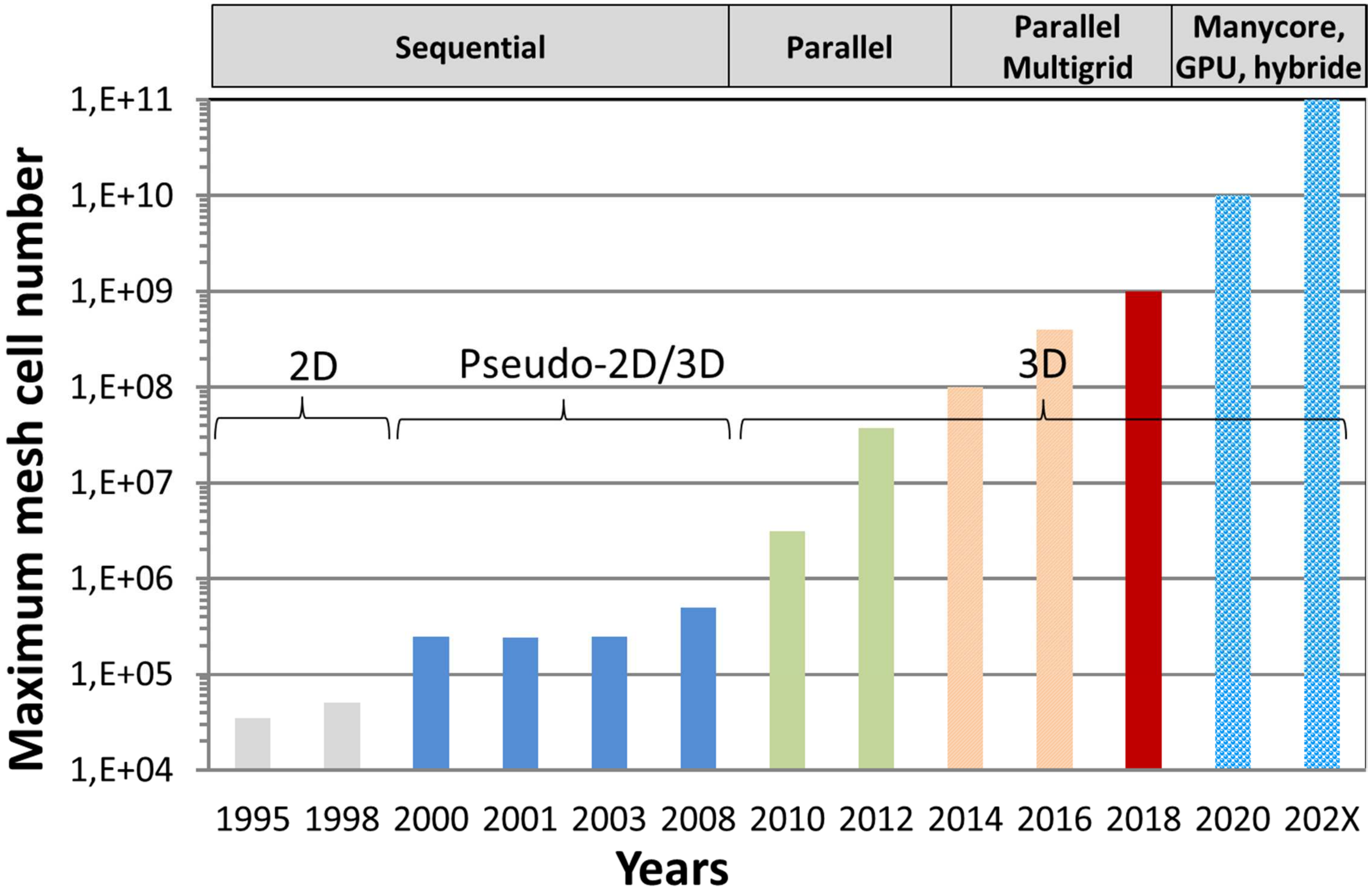
Academic and industrial interests:

- **Simulation of gas-particle flows with fine meshing (small scales)**
  Model predictions highly sensitive to small-scale structures (particle clusters, « pockets », …) due to their major impact on local mechanisms: mass, momentum and heat transfer, chemical reactions
- **Accounting for industrial complex geometries:** *e.g.* centimeter-scale injectors in large-volume
- **Generating reference simulation sets:**
  Simulation results insensitive to mesh refinements at industrial scales
  - Local phenomenon analysis, accurate understanding of local mechanisms
  - Development of sub-mesh relevant models: aiming at lower-cost simulation with coarser meshes while encompassing local phenomenon

Prospects

Big Mesochallenge on CALMIP: “Grand challenge” candidate on national centers or Prace

Next step (dec-2018) EDF Grand challenge on their new super computer with 40,000 cores



Benchmark: maximum mesh size for { **20s** unsteady reactive gas-particle simulation / **2 weeks simulation time** }