PRESENTATION OF NEPTUNE_CFD SOLVER: ARCHITECTURE, SCHEMES, HPC, APPLICATIONS

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Solver NEPTUNE_CFD:
Parallelized unstructured code (MPI) solving unsteady Eulerian multi-fluid approach in turbulent and non-adiabatic flows

NEPTUNE_CFD is developed in the framework of the NEPTUNE project, financially supported by CEA/EDF/IRSN/AREVA for nuclear applications (liquid/vapor)
- Two-phase pressurized thermal shock
- Critical heat flux/ Departure from nucleate boiling

Academic collaboration : NEPTUNE_CFD developed and used by IMFT for dense or dilute particle-laden reactive flows simulations from the local scale up to industrial scale
NEPTUNE CFD: Navier-Stokes equations in the cases of 2D, 2D axisymmetric or 3D multiphase flows => C/C++, MPI, QT-Python GUI

Software architecture builds upon the HPC capabilities and I/O of the EDF open-source CFD code Code_Saturne (ready for Petascale computing systems)
Can be coupled with the SYRTHES code: transient thermal simulations in complex solid geometries

Unsteady Eulerian multi-fluid approach => mass, momentum, and energy mean transport equations solved for each phase and coupled through inter-phase transfer terms

- free surface
- droplet-laden
- bubbly or boiling
- particle-laden
- steady or unsteady
- laminar or turbulent
- incompressible or not
- isothermal or not

3D fully unstructured Finite Volume approach, with co-located arrangement for all variables (cell-center type)

Various mesh types which may be hybrid (containing several kinds of elements) and may have structural non-conformities (hanging nodes)

Parallel multi-grid solver (pressure)  MPI I/O
Parallel partitioning of mesh (PTScotch, ParMetis, ...) ...
Partial differential equations discretization:

Temporal discretization and solution algorithm: \(1^{\text{st}}\) order scheme

- original fractional step method using linear solvers or direct matrix inversion:
  - pressure: conjugated gradient or bi-cgstab
  - volume fraction: bi-cgstab or jacobi
  - velocity and enthalpy: jacobi
- momentum and energy equations coupled with the help of a pressure correction equation, within an iterative procedure (pressure-based approach)
- Algebraic multigrid solver for pressure

Spatial discretization: \(2^{\text{nd}}\) order centered scheme

- 3D fully unstructured Finite Volume approach, with co-located arrangement for all variables (cell-center type)
- arbitrary shaped cells including non-matching meshes
- gradient reconstruction method (consistency and precision for diffusive and advective fluxes)

Parallelism:

- distributed-memory by domain decomposition
  - MPI parallelization
  - automatic domain splitting
NEPTUNE_CFD’s high parallel computing performances for particle-laden reactive flows demonstrated with an excellent scalability up to 2,536 cores
Neau et Al., “High performance computing (HPC) for the fluidization of particle-laden reactive flows” Fluidization XIV Conference”, The Netherlands, 2013

NEPTUNE_CFD’s recent developments allow overtaking the code limitations: parallel partitioning of mesh, MPI I/O, parallel multi-grid solvers, ...

NEPTUNE_CFD is ready for massive parallel computing

38,000,000 cells
ref=128cores
Simulation of industrial particulate multi-phase turbulent flows

Industrial applications:
- Polymerization reactor (PE and PP)
- Chemical looping process (coal and gas)
- Transport of solid (dust control)
- Concentrating solar power system
- Coal fired furnaces
- Zircon chlorination reactor
- Uranium oxide fluorination reactor
- Biomass gasifier
- FCC riser
- Solid rocket booster
- Deposition of droplets or particles
- IC engine (liquid fuel injection)
...
Simulation of industrial particulate multi-phase turbulent flows

Physical mechanisms:
- Fluid-particle interaction
- Particle-particle interaction
- Particle-wall interaction

Modelling challenges:
- 3D unsteady flows (URANS or LES approaches)
- Poly-dispersed solid mixture
- Gaseous or heterogeneous combustion
- Granular flow regime transition
- Non-spherical particles
- Radiative transfer, electrostatic effects
...
NEPTUNE_CFD APPLICATIONS

Industrial applications:
- Coal fired furnaces
- CFB boilers
- Polymerization

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

Vertical coal mass flow rate: $\alpha_p\rho_p W_p$

Time = 20.0 s.

Simulation NEPTUNE_CFD

1 000 000 CPU h ⇔ 20s
12 000 cores
108 000 756 cells
Industrial applications:

- Polymerization
Industrial applications:

- Chemical looping

Mesh refinement

\[ \Delta x = 14 \text{cm} \]

\[ \Delta x = 10 \text{cm} \]

\[ \Delta x = 3 \text{cm} \]
Industrial applications: Concentrating solar power system
Development models:

- Sub-grid models for fluidized beds or circulating beds
Chemical reactor prototype with rotating parts

Solid Volume Fraction

Time = 0.054 s
Simulation NEPTUNE_CFD
NEPTUNE_CFD overall

HPC:
Solver ready for massive parallel computing

Feasibility demonstration of a fluidized bed reactor simulation at industrial scale using a mesh with more than 100 000 000 cells on a supercomputer with the solver NEPTUNE_CFD

Scientific:

• Gas/particle flow computing with a very refined mesh capturing small scales (cluster, bubbles, ...) which play a key role in momentum, heat, mass transfers and in chemical reactions

• Establish simulations of reference with numerical results independent of mesh refinement
  ▪ To analyze local mechanisms and to have a fine understood of local phenomenon
  ▪ To develop sub-grid models (macroscopic models) to run less CPU costing simulation with less refined meshes

• Take into account complexity of industrial configurations such as small injectors, internal heat exchangers, thin walls, ...

Applications:
Fit for large scale and complex industrial configurations in wide variety of fields: chemical engineering, bio- engineering, pharmaceutics, ...
Over the time, a unsteady reactive diphasic simulation requires 200 - 400 CPU h regardless the core number...
METHODOLOGY: multi-scale numerical approach

**Microscopic scale (~1mm)**
DNS, immersed boundary method

**Mesoscopic scale (~10cm)**
DNS/LES + Discrete Particle Simulation (DPS)

**Macroscopic scale (~10m)**
URANS/LES Euler-Euler

MeOx concentration field. NEPTUNE_CFD bi-solid prediction of the circulating fluidized bed coal combustion reactor (chemical looping fuel reactor)