An Efficient Parallel Solver for LES-DEM Simulation of Fluidized Bed

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Contents

Research context

Context and objectives

Particle-laden flows are omnipresent...

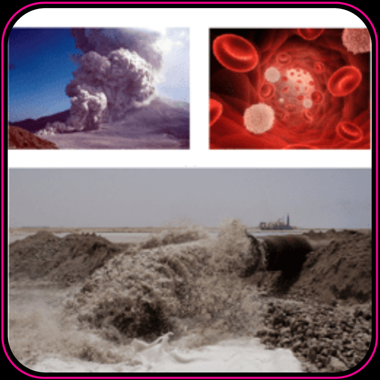
→ Industry: biomass combustion, chemical industry, pharmaceutical, ...

→ Research: study of sedimentation, snow avalanche, and rheology.

... and still raise numerous questions

→ Experiments: measurement implementation.

→ Scale-up from lab-scale to industrial scale is a troublesome endeavor[1].



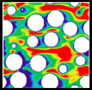
Objectives of the present study

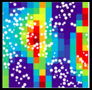
- Develop Parallel Eulerian–Lagrangian solver for 3D simulation of fluidized bed.
- Assess CFD-DEM capability to predict the instantaneous motion of particles.

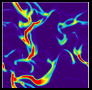
[1] Rüdisüli, M., Schildhauer, T. J., Biollaz, S. M., & van Ommen, J. R. (2012). Scale-up of bubbling fluidized bed reactors–A review. Powder Technology, 217, 21-38.

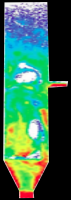
DEM–LES for fluidized bed

Fluidized bed: A numerical problem









Micro-scale	Meso-scale	Macro-scale
DNS	CFD-DEM TFM	MP-PIC Filtered-TFM EMMS

- ✔ Moderate numerical cost
- ✔ Multi-scale access

➡ **Euler-Lagrange approach**

- ✔ Large-eddy simulation
- ✔ Discrete element method

Discrete-element method (DEM)

Newton's second law

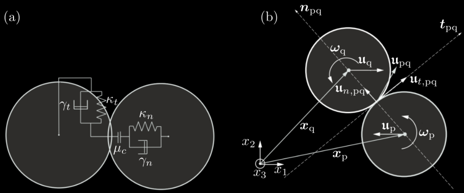
$$
\begin{cases}
m_{\mathrm{p}} \dfrac{\mathrm{d}\mathfrak{u}_{\mathrm{p},i}}{\mathrm{d}t} = \mathfrak{f}^{\mathrm{inter}}_{\mathrm{p},i} + \mathfrak{f}^{\mathrm{col}}_{\mathrm{p},i} + m_{\mathrm{p}}\,\mathfrak{g}_i, \quad \text{with} \quad \dfrac{\mathrm{d}x_{\mathrm{p},i}}{\mathrm{d}t} = \mathfrak{u}_{\mathrm{p},i} & \text{(1a)} \\
\mathscr{I}_{\mathrm{p}} \dfrac{\mathrm{d}\omega_{\mathrm{p},i}}{\mathrm{d}t} = \mathscr{M}^{\mathrm{drag}}_{\mathrm{p},i} + \mathscr{M}^{\mathrm{col}}_{\mathrm{p},i} & \text{(1b)}
\end{cases}
$$

$$
\mathfrak{f}^{\mathrm{inter}}_{\mathrm{p},i} \approx \mathscr{V}_{\mathrm{p}} \partial_j \tau_{ij} + \mathfrak{f}^{\mathrm{drag}}_{\mathrm{p},i} \approx -\mathscr{V}_{\mathrm{p}} \partial_i \mathfrak{p}^{\copyright} + \mathfrak{f}^{\mathrm{drag}}_{\mathrm{p},i}
$$

- Particle mass $m_{\mathrm{p}} = \pi \varrho_{\mathrm{p}} d_{\mathrm{p}}^3 / 6$
- Particle-particle and particle-wall repulsion force $\mathbf{f}^{\mathrm{col}}_{\mathbf{p}}$
- Force exerted on a single particle p by the surrounding fluid $\mathfrak{f}^{\mathrm{inter}}_{\mathrm{p}}$
- Drag and collision moments $\mathscr{M}^{\mathrm{drag}}_{\mathrm{p},i}$ and $\mathscr{M}^{\mathrm{col}}_{\mathrm{p},i}$

Collision modelling

- ✔ Particle-particle and particle-wall collisions are modeled using the **A**daptive **C**ollision **T**ime **M**odel (**ACTM**)[2]



[2] Kempe, T., & Fröhlich, J. (2012). Collision modelling for the interface-resolved simulation of spherical particles in viscous fluids. Journal of Fluid Mechanics, 709, 445-489.

Large-eddy simulation (LES)

Filtered NS equations

$$\begin{cases} \partial_t \left(\theta_{\mathfrak{f}} \overline{\varrho_{\mathfrak{f}}}\right) + \partial_i \left(\theta_{\mathfrak{f}} \overline{\varrho_{\mathfrak{f}}} \widetilde{\mathfrak{u}_{\mathfrak{f},i}}\right) = 0, & \text{(2a)} \\ \partial_t \left(\theta_{\mathfrak{f}} \overline{\varrho_{\mathfrak{f}}} \widetilde{\mathfrak{u}_{\mathfrak{f},i}}\right) + \partial_j \left(\theta_{\mathfrak{f}} \overline{\varrho_{\mathfrak{f}}} \widetilde{\mathfrak{u}_{\mathfrak{f},i}} \widetilde{\mathfrak{u}_{\mathfrak{f},j}}\right) = -\partial_j \overline{\mathfrak{p}} + & \\ \partial_j \left(\overline{\tau_{ij}} + \overline{\tau_{ij}}^{\mathrm{SGS}}\right) + \theta_{\mathfrak{f}} \overline{\varrho_{\mathfrak{f}}} \mathfrak{g}_i + \mathscr{F}_i^{\mathrm{inter}} & \text{(2b)} \end{cases}$$

$$\mathscr{F}^{\mathrm{inter}} = \sum_{p=1}^{\mathcal{N}_{\mathrm{p}}} \xi(|\boldsymbol{x} - \boldsymbol{x}_p|)\, \mathbf{f}_p^{\mathrm{inter}}$$

- where $\theta_{\mathfrak{f}}$, $\varrho_{\mathfrak{f}}$, and $\mathfrak{u}_{\mathfrak{f}}$ are the fluid-phase volume fraction, density, and velocity, respectively.
- The force $\mathbf{f}_{\mathrm{p}}^{\mathrm{inter}}$ exerted on a single particle p by the surrounding fluid is related to the interphase exchange term

Subgrid-scale modelling

- ✔ The volume-filtered stress tensor

$$\overline{\tau_{ij}} = \mu \left[\partial_i \overline{\mathfrak{u}_{\mathfrak{f},j}} + \partial_j \overline{\mathfrak{u}_{\mathfrak{f},i}} - \frac{2}{3} \partial_i \overline{\mathfrak{u}_{\mathfrak{f},i}} \delta_{ij}\right] + \mathscr{R}_{\mu,ij}$$

- ✔ Effective viscosity μ^* to account for enhanced dissipation

$$\mathscr{R}_{\mu,ij} \approx \mu^* \left[\partial_i \overline{\mathfrak{u}_{\mathfrak{f},j}} + \partial_j \overline{\mathfrak{u}_{\mathfrak{f},i}} - \frac{2}{3} \partial_i \overline{\mathfrak{u}_{\mathfrak{f},i}} \delta_{ij}\right]$$

- ✔ SGS eddy viscosity

$$\mu^{\mathrm{SGS}} = \overline{\varrho} \left(C^{\mathrm{SGS}} \Delta\right)^2 \sqrt{2 \overline{S}_{ij} \overline{S}_{ji}}$$

Some Numerical details

- Projection method based on fractional time steps developed by Chorin [3] and improved by Kim & Moin [4].
  - ✔ Fourth-order central scheme is used for the spatial integration
  - ✔ Third-order accurate semi-implicit Crank-Nicolson scheme is employed for time integration.
- Poison equation is solved using the **Livermore's Hypre library** with the PCG (pre-conditioned conjugate gradient) method.
- The normalized drag force coefficients $\mathbb{F}$ are modeled using **Tenneti's model** [5]

$$\mathbb{F}^{\mathtt{TENNETI}}\left(\theta_{\mathfrak{f}}, \mathrm{Re}_{\mathrm{p}}\right) = \mathbb{F}^{\mathtt{WY}}\left(\theta_{\mathfrak{f}}, \mathrm{Re}_{\mathrm{p}}\right)\theta_{\mathfrak{f}}^{1.65} + \theta_{\mathfrak{f}}\mathbb{F}_1^{\mathtt{TENNETI}}\left(\theta_{\mathfrak{f}}\right) + \theta_{\mathfrak{f}}\mathbb{F}_2^{\mathtt{TENNETI}}\left(\theta_{\mathfrak{f}}, \mathrm{Re}_{\mathrm{p}}\right)$$

with

$$\begin{cases} \mathbb{F}_1^{\mathtt{TENNETI}}\left(\theta_{\mathfrak{f}}\right) = \dfrac{5.81(1-\theta_{\mathfrak{f}})}{\theta_{\mathfrak{f}}^3} + \dfrac{0.48(1-\theta_{\mathfrak{f}})^{1/3}}{\theta_{\mathfrak{f}}^4} \\ \mathbb{F}_2^{\mathtt{TENNETI}}(\theta_{\mathfrak{f}}, \mathrm{Re}_{\mathrm{p}}) = (1-\theta_{\mathfrak{f}})^3 \mathrm{Re}_{\mathrm{p}}\left[0.95 + \dfrac{0.61(1-\theta_{\mathfrak{f}})^3}{\theta_{\mathfrak{f}}^3}\right] \end{cases}$$

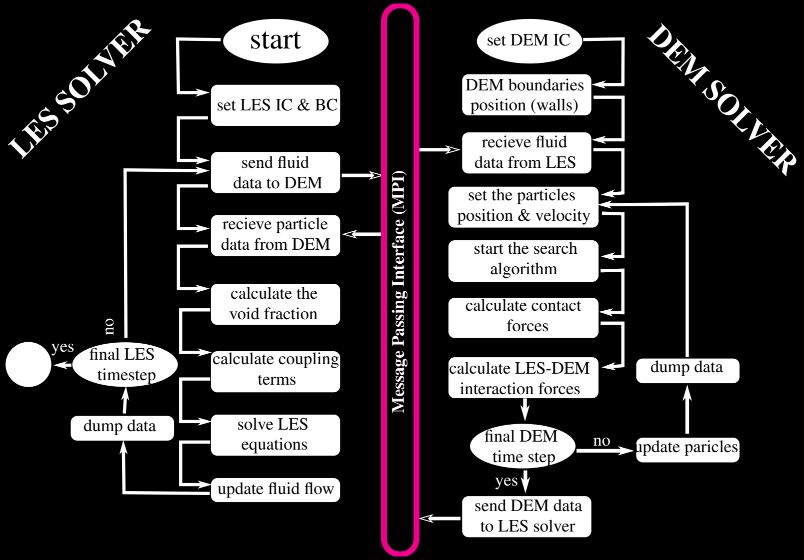
[3] Chorin, A. J. (1968). Numerical solution of the Navier-Stokes equations. Mathematics of computation, 22(104), 745-762.

[4] Kim, J., & Moin, P. (1985). Application of a fractional-step method to incompressible Navier-Stokes equations. Journal of computational physics, 59(2), 308-323.

[5] Tenneti, S., Garg, R., & Subramaniam, S. (2011). Drag law for monodisperse gas–solid systems using particle-resolved direct numerical simulation of flow past fixed assemblies of spheres. International journal of multiphase flow, 37(9), 1072-1092.

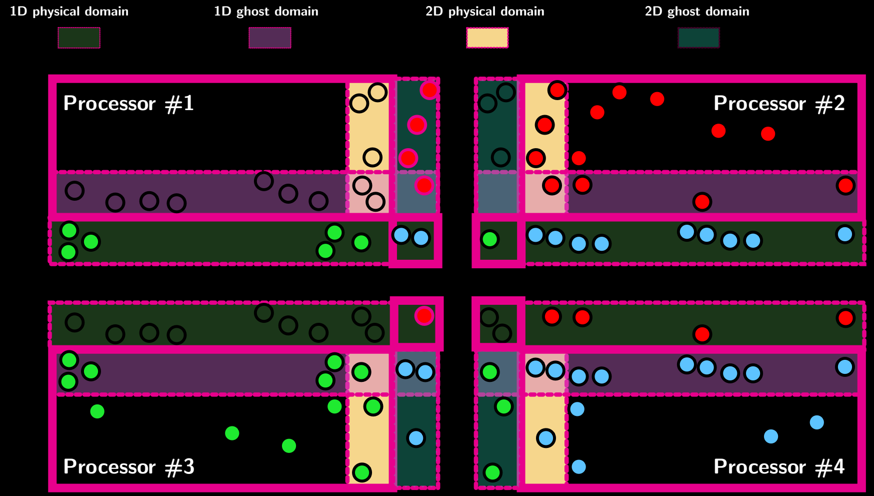
Parallelism management

Parallelization strategy



Parallelization strategy

➥ Schematic view of two-dimensional decomposition of particles with 4 processors



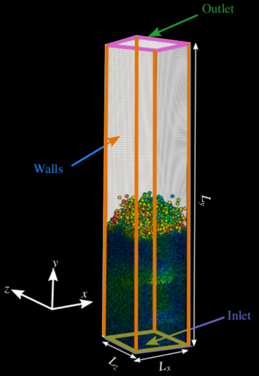
Parallel processing and data-structure update

```
begin
    Reconstruct: label Particle ℙ
    hotpart false
    Create an empty list 𝒮
    if contour particle label changes at sub-domaine boundary then
        activate particle as a hot particle; hotpart ← true
    end
    Ghost mappings: Particle
    if there is any hot ghost particle then
        add it as a seed to the list 𝒮
    end
    Global: reduce operation on hotpart
    while hotpart do
        Reconstruct label Particle ℙ using flood fill from the seeds in 𝒮
        Empty: 𝒮
        Ghost mappings: Particle
        if there is any hot ghost particle then
            add it as a seed to the list 𝒮
        end
    end
end
```

Small scale bubbling fluidized bed

Small scale bubbling fluidized bed: Numerical setup

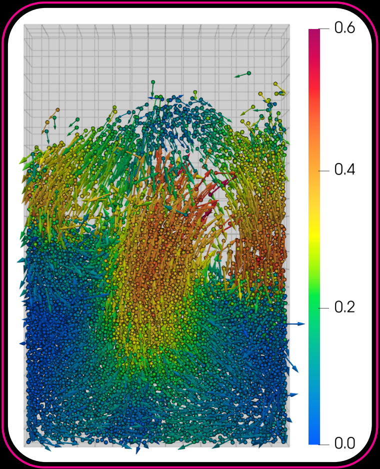
Properties	Müller *et al.*[6]	Van Wachem *et al.*[7]
Fluid phase		
Fluid density ϱ_f [kg/m^3]	1.2	1.28
Fluid viscosity μ [Pa·s]	1.8×10^{-5}	1.7×10^{-5}
Superficial gas velocity u_∞ [m/s]	0.6 – 0.9	0.9
Solid phase		
Number of particle	9240	4080
Particle diameter d_p [mm]	1.20	1.545
Particle density ϱ_p [kg/m^3]	1000	1150
Inter-particle restitution coefficient e_{dry}	0.98	0.90
Particle-wall restitution coefficient e_{dry}	0.98	0.90
Inter-particle restitution coefficient μ_c	0.1	0.3
Particle-wall friction coefficient μ_c	0.1	0.3
Geometry and Mesh		
Bed $L_x \times L_y \times L_z$ [mm^3]	$44 \times 288 \times 10$	$90 \times 450 \times 8$
Grid number $\mathcal{N}_x \times \mathcal{N}_y \times \mathcal{N}_z$	$16 \times 120 \times 4$	$33 \times 168 \times 3$
Non-dimensional parameters		
Particle Reynolds number $\mathcal{R}e_p$	48, 72	104.7
Stokes number $\mathcal{S}t$	2.66 – 4	5.81
Archimedes number $\mathcal{A}r$	6.27×10^4	1.84×10^5
Galileo number $\mathcal{G}a$	250.41	429.03



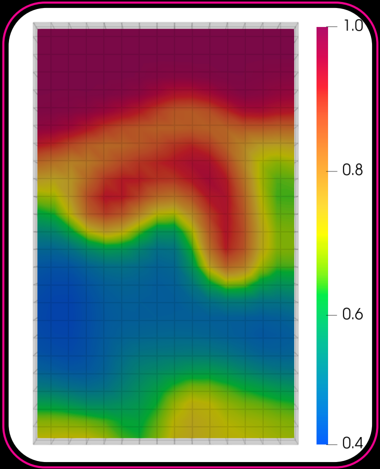
[6] Müller, C. R., Holland, D. J., Sederman, A. J., Scott, S. A., Dennis, J. S., & Gladden, L. F. (2008). Granular temperature: comparison of magnetic resonance measurements with discrete element model simulations. Powder Technology, 184(2), 241-253.

[7] Van Wachem, B. G. M., Van der Schaaf, J., Schouten, J. C., Krishna, R., & Van den Bleek, C. M. (2001). Experimental validation of Lagrangian–Eulerian simulations of fluidized beds. Powder Technology, 116(2-3), 155-165.

Small scale bubbling fluidized bed: Qualitative analysis

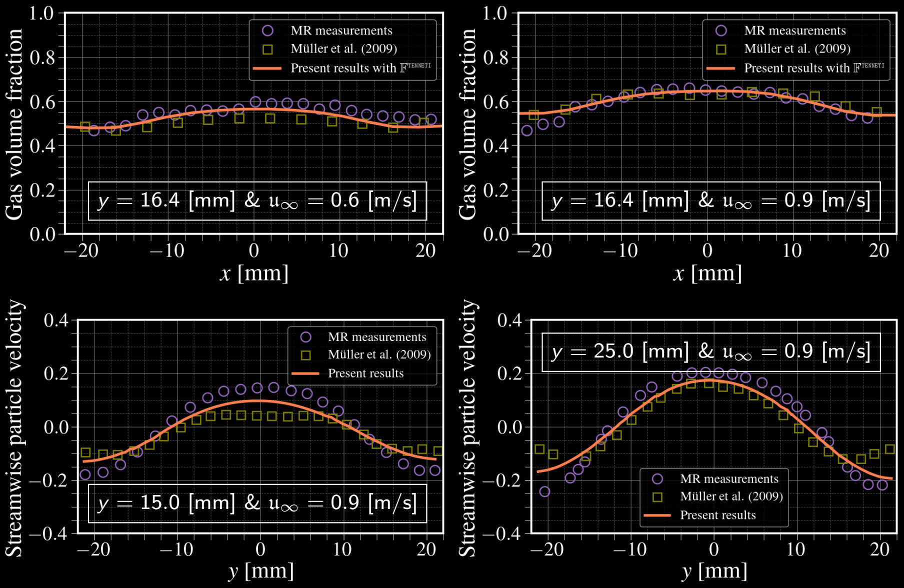


Instantaneous snapshots of the particle flow dynamic



a slice of the contours of the gas volume fraction

Small scale bubbling fluidized bed: Quantitative analysis



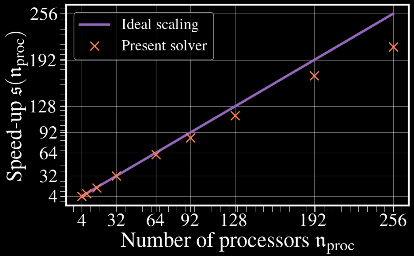
Parallel performance

Parallel performance on ASCC cluster

- A rectangular fluidized bed of 8 million particles and of dimensions $0.1 \times 0.4 \times 0.1$ [m^3].
- Uniform mesh is used with the cell size of 1.0 [mm], resulting in a total of 4 million cells in the LES grid.

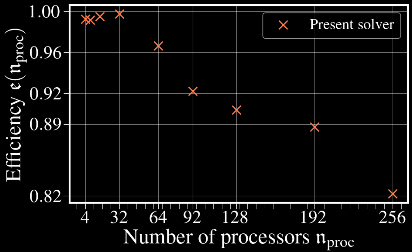
➽ Speedup factor

$$\mathfrak{s}(\mathfrak{n}_{proc}) = \frac{\text{Time(Serial)}}{\text{Time}(\mathfrak{n}_{proc})}$$



➽ Efficiency

$$\mathfrak{e}(\mathfrak{n}_{proc}) = \frac{\text{Time(Serial)}}{\mathfrak{n}_{proc}\,\text{Time}(\mathfrak{n}_{proc})}$$



Conclusion and perspectives

Few conclusions and many perspectives

- Conclusions
  - ✔ A new solver coupling DEM and LES using parallelization strategies is developed.
  - ✔ A thoroughly verification is performed.
  - ✔ The results are agreeably compared with available measurements data.
  - ✔ Good stability and high performance of the parallelization strategy.
- Perspectives
  - ➝ Implementation of the particles feature complex geometries with a wide range of size distributions.
  - ➝ Consideration of heat transfer model.
  - ➝ Hybrid MPI/OpenMP or MPI/GPU framework.
  - ➝ And so many other things to do ...

Thanks for tuning in!
Please leave comments & questions

Acknowledgments
African SuperComputing Center