THE UNIVERSITY OF MAINE

# Asynchronous GPU-based DEM solver embedded in commercial CFD software with polyhedral mesh support

Alireza Kiani

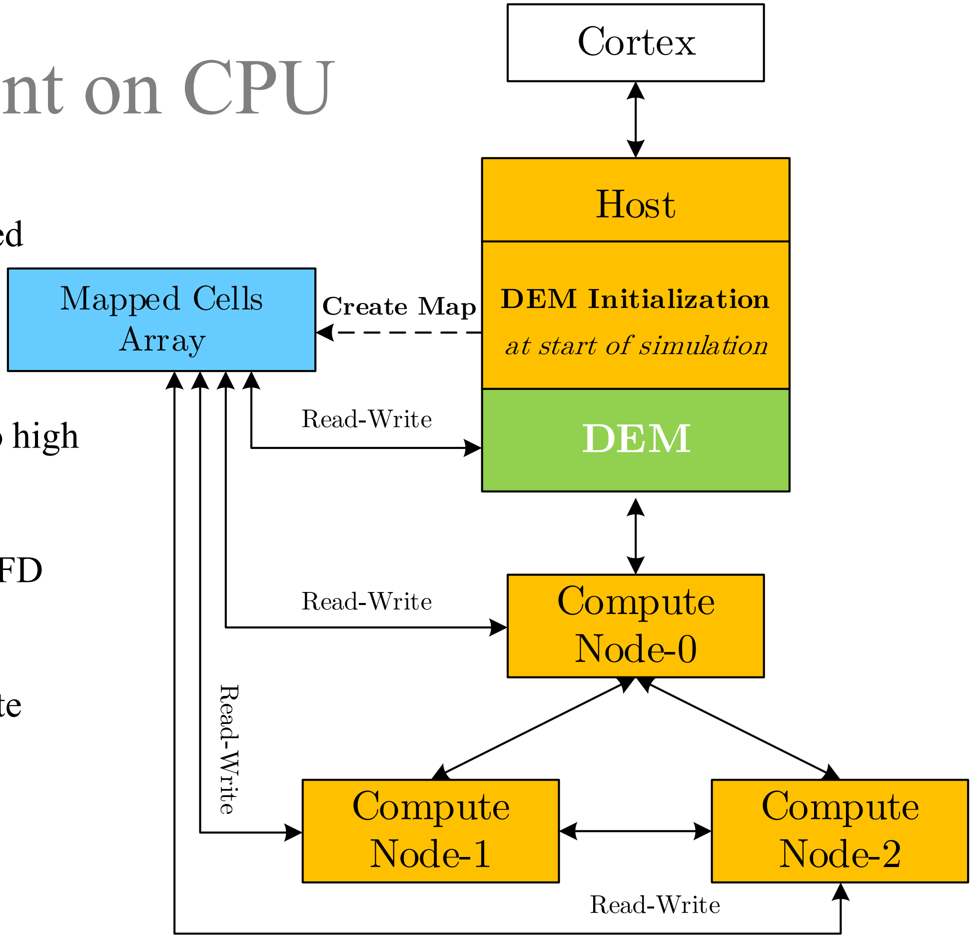
Dr. Justin Lapp

# Objectives

- Develop an in-house Discrete Element Method (DEM) Solver
- The object-oriented development of the DEM solver for particle-scale customization
- High computational speed for semi-industrial application
- Flexible in performing computation on complex geometries
- Seamless Coupling with reliable and well-developed CFD software

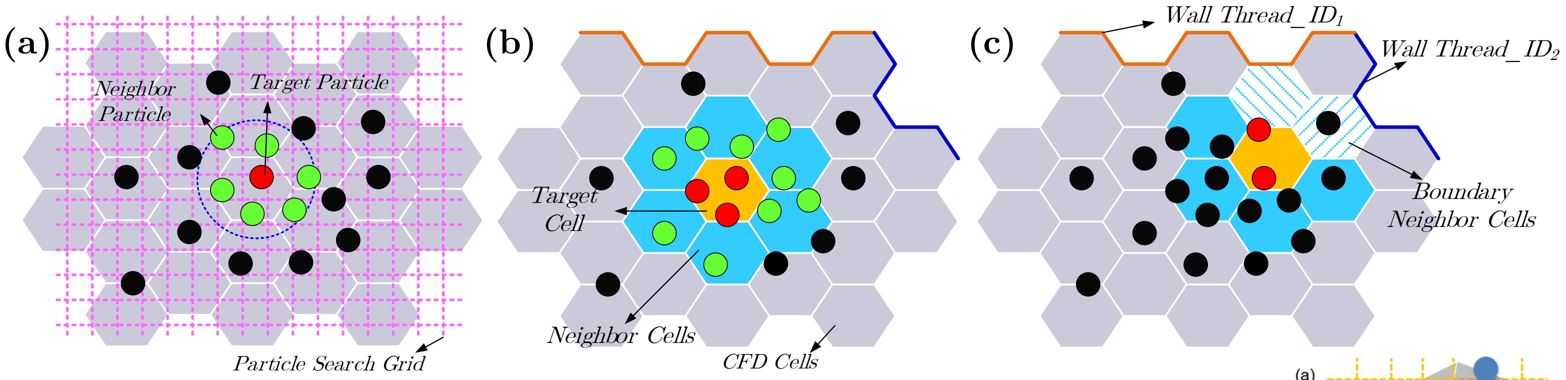
# Coupling with ANSYS Fluent on CPU

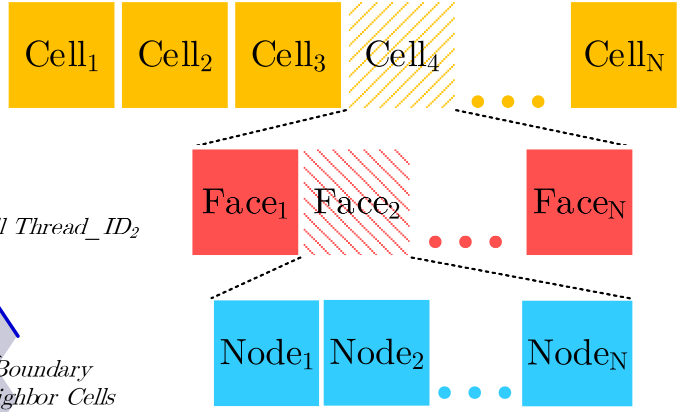
- The solver must be compatible with ANSYS Fluent User Defined Function (UDF)
  - **The solver is developed in C language**
- To compensate the slow computations of the DEM solver due to high number of particles, it is parallelized over CPU cores
- The CFD and the DEM solver read the geometry and cells by CFD software
- The DEM solver requires access to the CFD cell in each compute node during the simulation time
  - **Memory Mapping**



# Data Structure

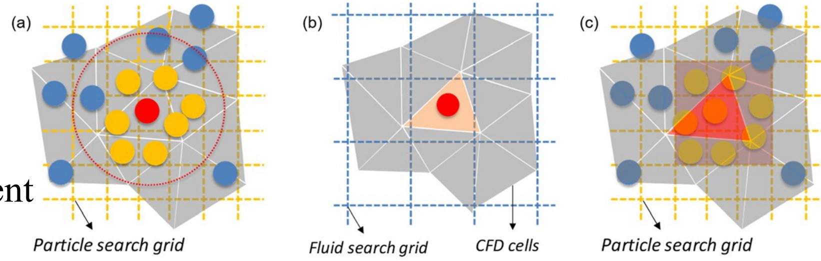
- Another challenge: Using 2 grids for particles, and cells requires high amount of memory on GPU!
  - Solution: Use the CFD cells geometry.




Advantages:

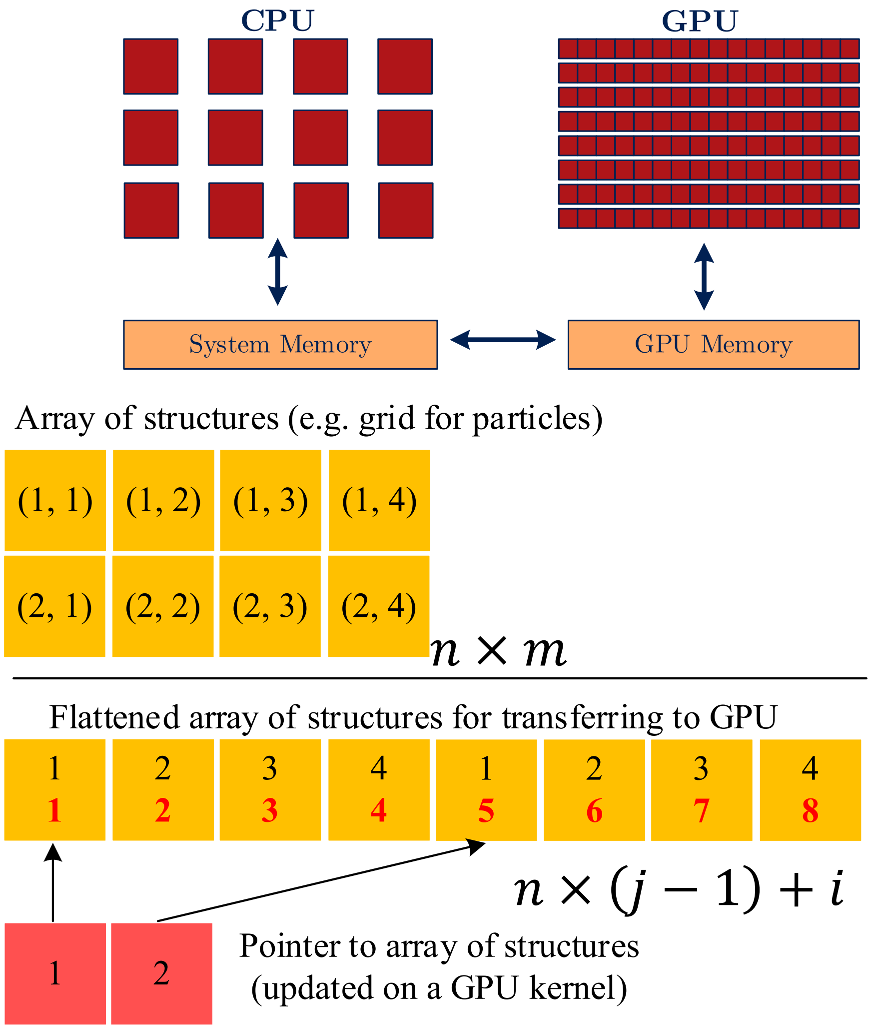
- Consumes much less memory
- Compatibility with any type of mesh
- The DEM and CFD can read the mesh from the same source, ANSYS Fluent (in-house UDF functions are required for the reading mesh)




He et al. 2020

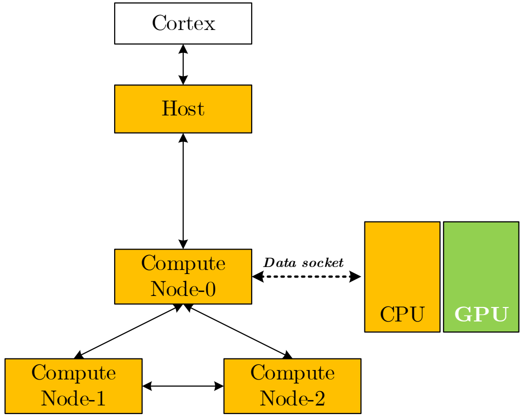
# Memory Management

- ❑ To make the solver compatible with GPU, the 3D grid for particles needs to be transferred to GPU memory.
  - There is no built-in function in NVIDIA CUDA for transferring 3D array of structures.
  - Flattening the 3D array then transferring to GPU.
  - By allocating and updating the pointer on the GPU kernel, the array can be treated as a 3D array.
- ❑ All the functions must be parallelized to be compatible with the GPU architecture.
- ❑ The goal is to make data transfer between GPU and CPU memories minimal for optimal performance.

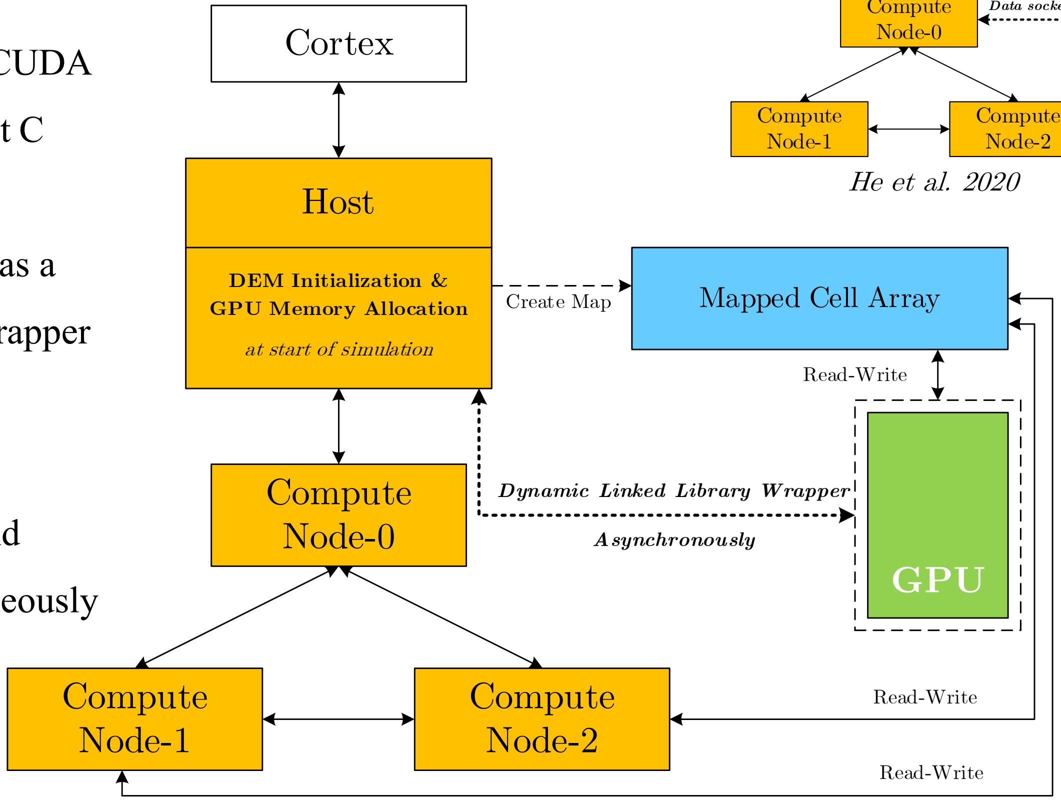


# Asynchronous Dynamic-Linked Library

- The compiler of the DEM solver is NVIDIA CUDA which is incompatible with the ANSYS Fluent C compiler.
- Thus, the DEM solver is compiled by CUDA as a Dynamic-Linked Library (DLL) which is a wrapper for the solver.
- The DEM is executed asynchronously as an external function in UDF so that both CPU and GPU compute fluid and solid phases simultaneously for optimum performance.



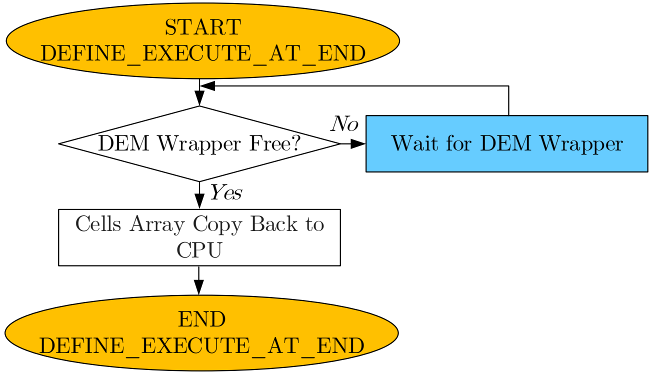

*He et al. 2020*

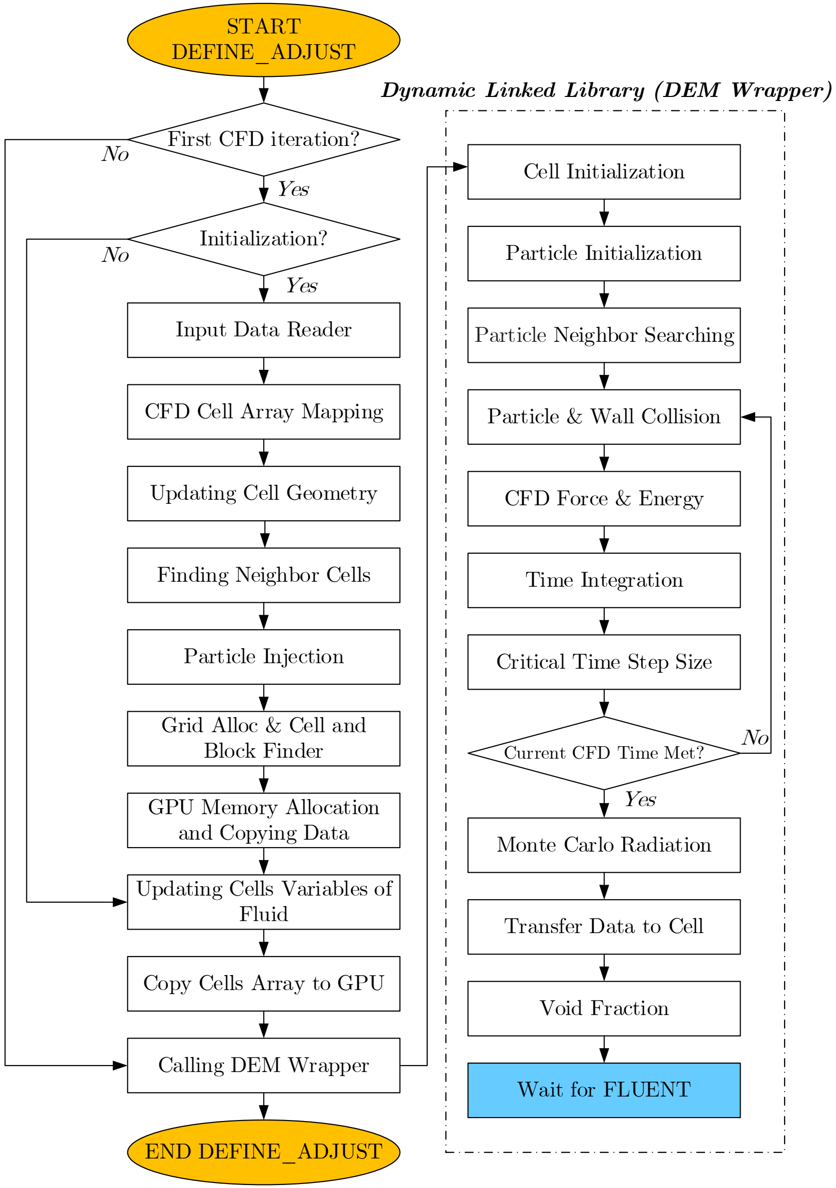


1865 THE UNIVERSITY OF MAINE

# Algorithm

- The figure demonstrates the algorithm of the CFD-DEM solver.
- The functions of the GPU-based DEM Solver wrapped in the DLL are shown inside the dotted line.
- All of the DEM solver functions including fluid-solid interactions for momentum and heat transfer are executed on GPU.
- At the end of each CFD time step, the CFD and DEM solvers wait for each other to finish their job.



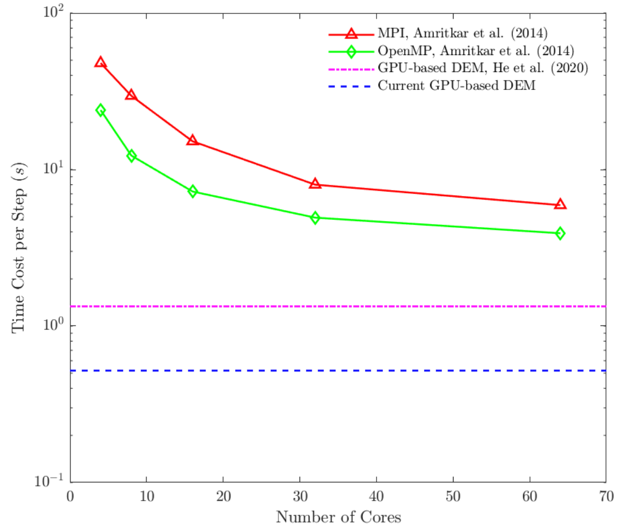



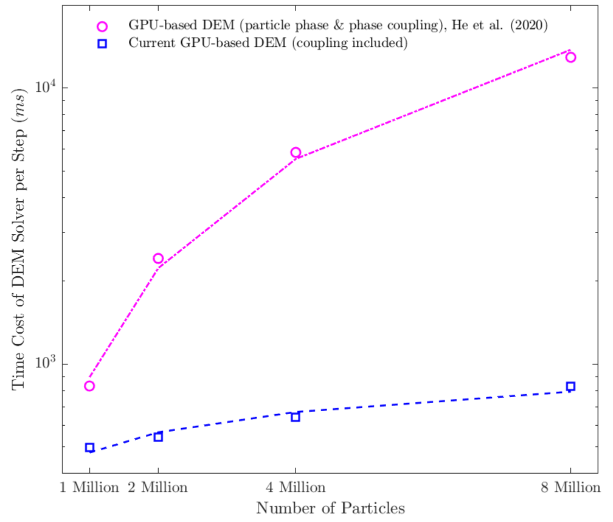
THE UNIVERSITY OF MAINE 1865

# Performance

- The average eclipsed time of each time step of the current GPU-based DEM solver compared to Amritkar and Tafti MPI and OpenMP and He et al. GPU-based DEM solver for **1.3** millions of particles (Amritkar et al. study).

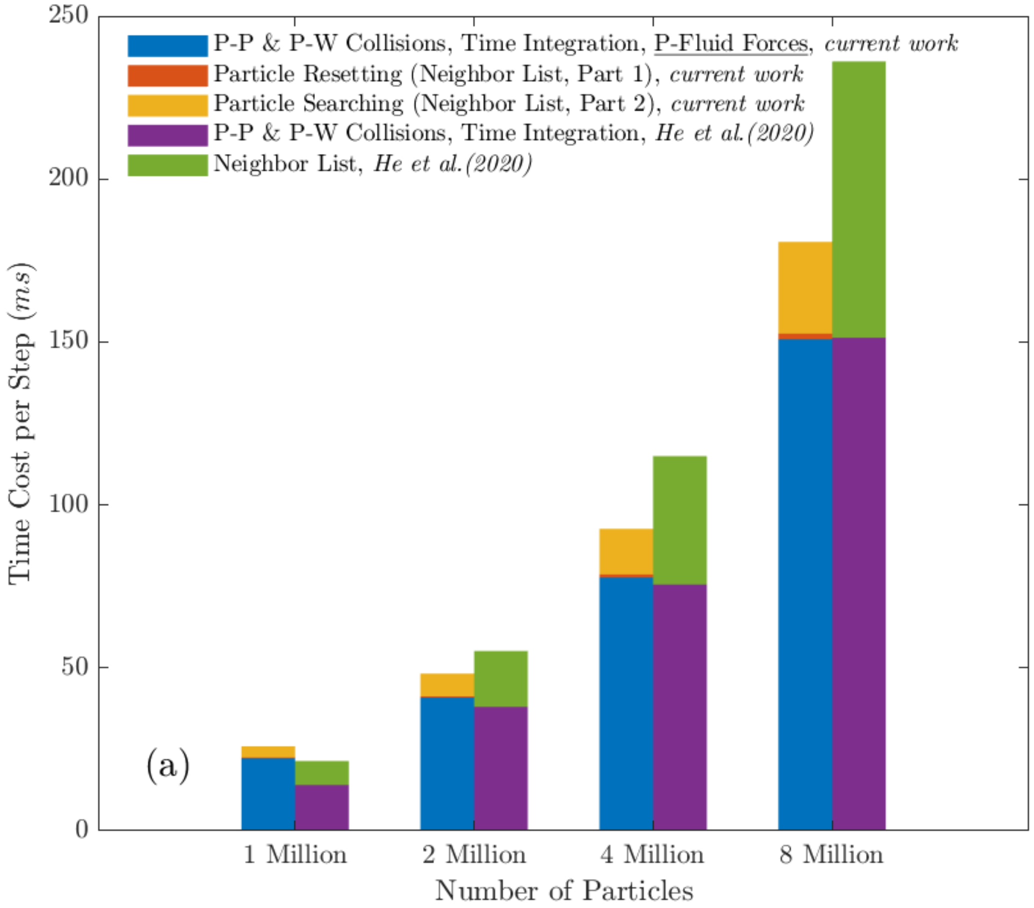
- The average eclipsed time cost of the DEM solver for each time step for the GPU-based DEM solver of He et al. and the current GPU-based DEM solver for **1.0**, **2.0**, **4.0**, and **8.0** millions of particles.



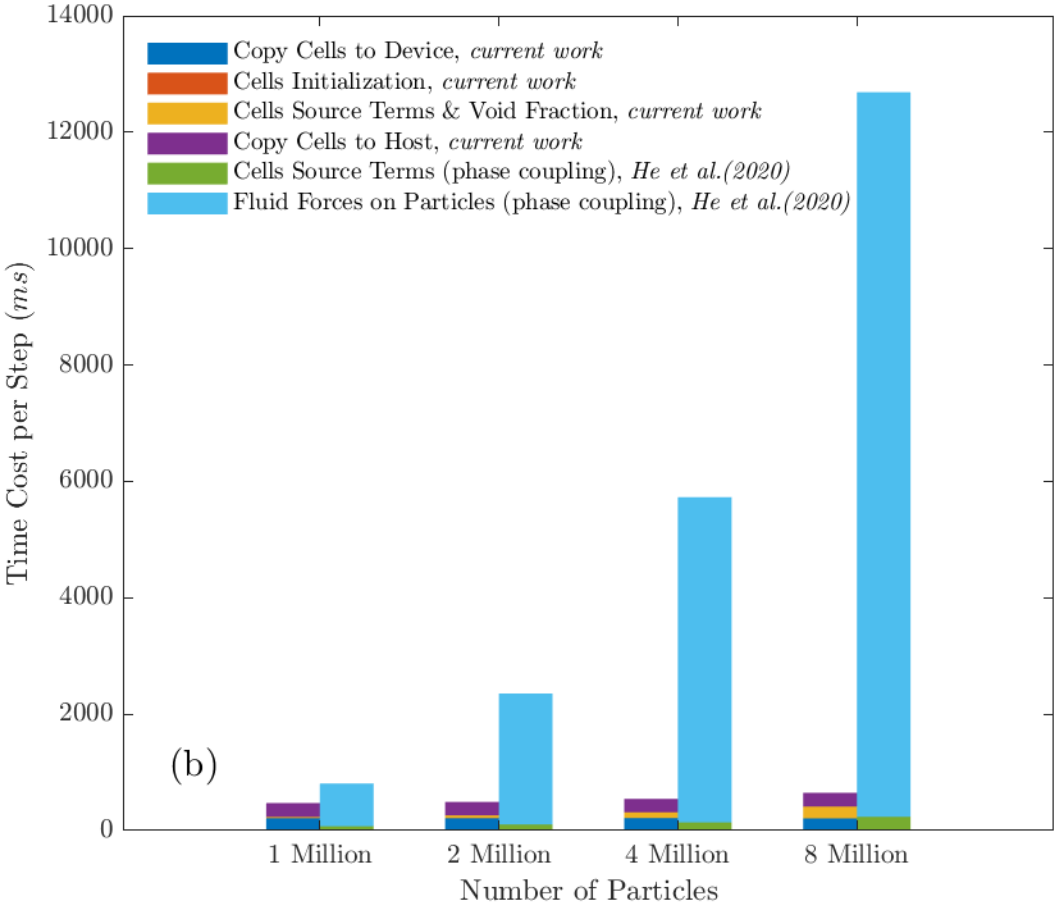
# Performance, Overall

- The average eclipsed time of the particle-particle and particle-wall collision, time integration, and neighbor list functions. The particle-fluid force calculation is integrated into the collision function. However, particle-fluid force calculation is part of phase coupling in the He et al. solver.



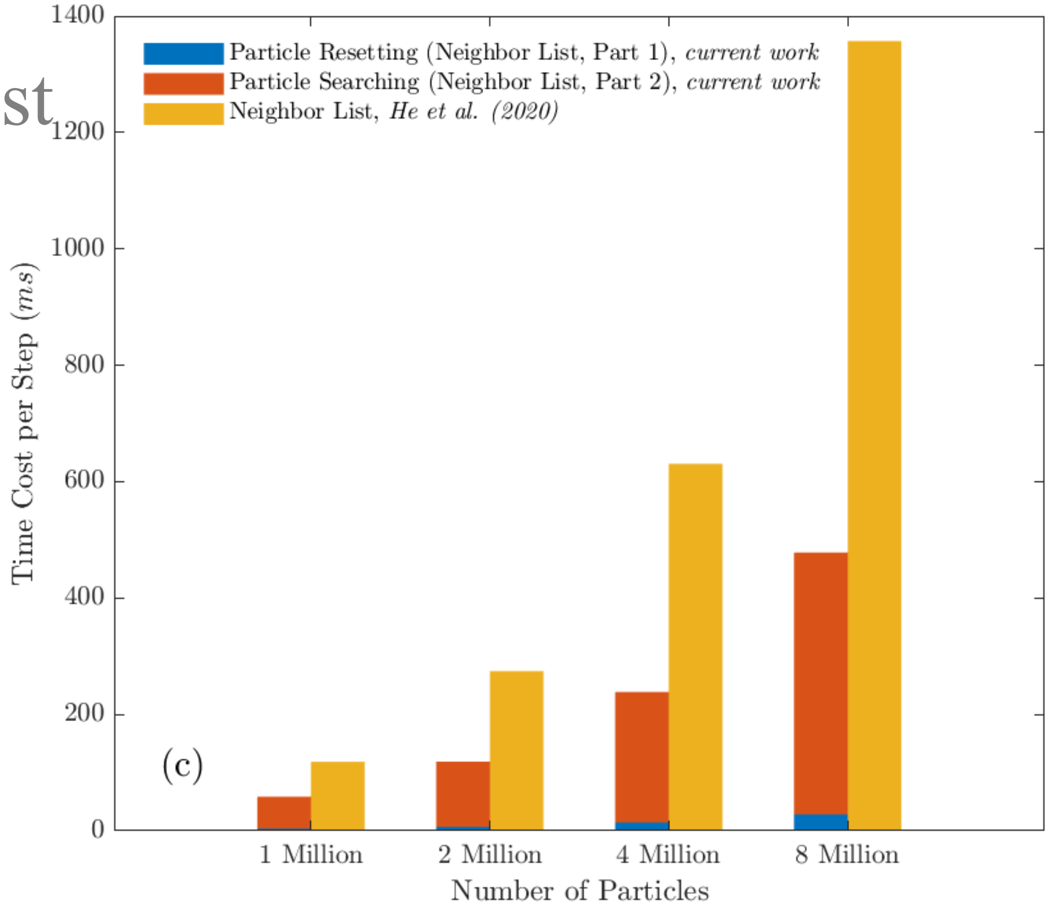
# Performance, Coupling

- The average time for the source terms calculation of the CFD cells and the coupling process with the CFD solver. Particle-fluid force calculation is presented in the phase coupling for the He et al.'s solver based on their architecture.

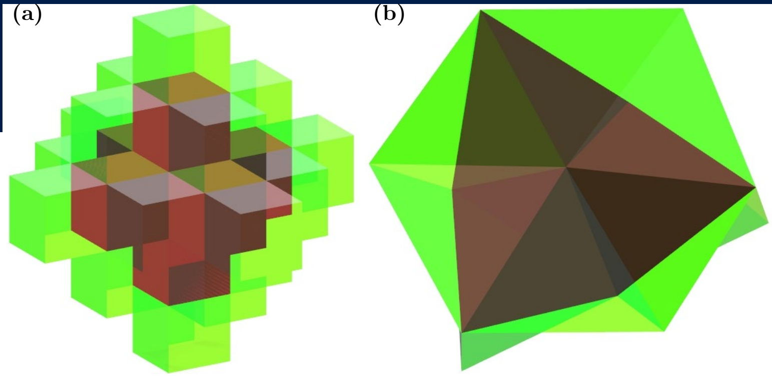


# Performance, Neigh. List

- ❑ The average time for neighbor list function for the current and He et al.'s solvers.



THE UNIVERSITY OF MAINE




# Gaussian Integral Method (GIM)

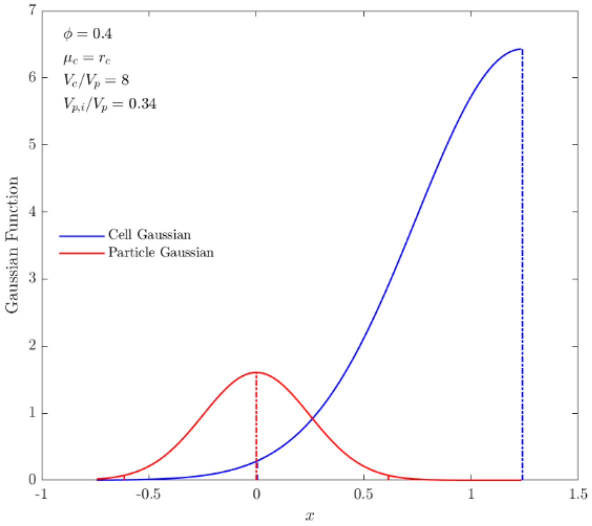
$$G_c(x) = \frac{V_c}{\sqrt{2\pi\sigma_c^2}} e^{\frac{-(x-\mu_c)^2}{2\sigma_c^2}}, \qquad \sigma_c = \phi\left(\frac{3}{4\pi}V_c\right)^{1/3}$$

$$G_p(x) = \frac{V_p}{\sqrt{2\pi\sigma_p^2}} e^{\frac{-x^2}{2\sigma_p^2}}, \qquad \sigma_p = \phi r_p$$

$$\chi_{Max}, \chi_{min} = \frac{-\sigma_p^2\mu_c \pm \sqrt{\sigma_p^4\mu_c^2 + \sigma_p^2\left[\mu_c^2 + 2\sigma_c^2 \ln\left(\frac{\sigma_c V_p}{\sigma_p V_c}\right)\right](\sigma_c^2 - \sigma_p^2)}}{\sigma_c^2 - \sigma_p^2}$$

$$\xi_p = \frac{V_p}{\sum_{i=1}^{N_c} V_{p,i}}$$

$$\alpha_{s,i} = \frac{\sum_{p=1}^{N_p} \xi_p V_{p,i}}{V_{c,i}}$$

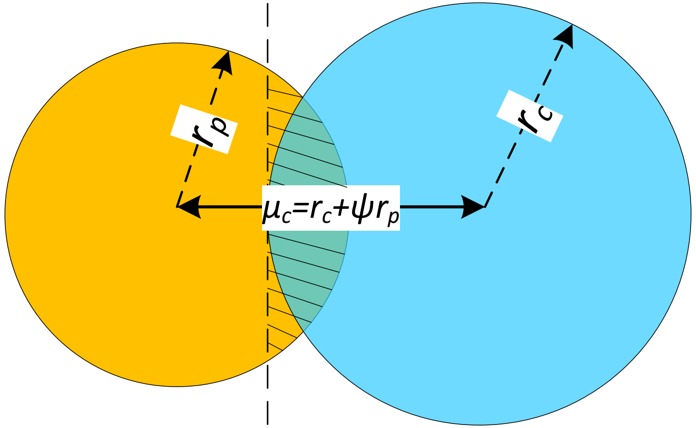


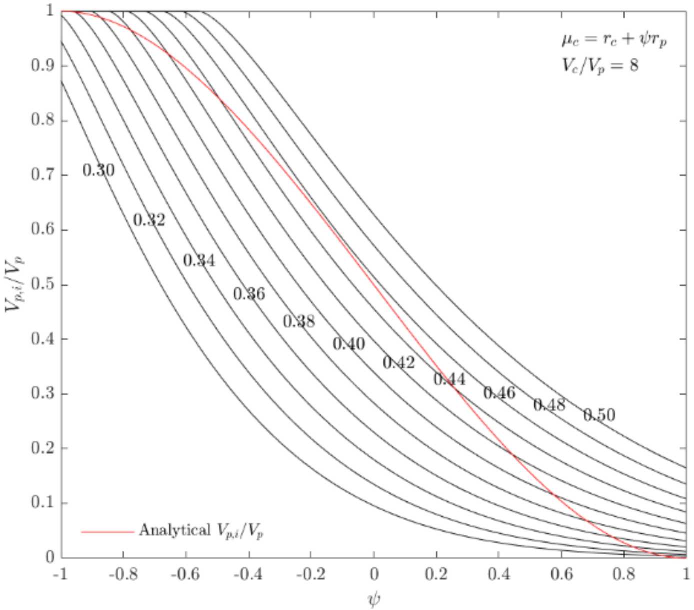

$$V_{p,i} = \int_{-\infty}^{\chi_{min}} G_p(x)dx \int_{\chi_{min}}^{\chi_{Max}} G_c(x)dx + \int_{\chi_{Max}}^{+\infty} G_p(x)dx = \frac{V_p}{2}\left[2 + \text{erf}\left(\frac{\chi_{min}}{\sqrt{2\sigma_p^2}}\right) - \text{erf}\left(\frac{\chi_{Max}}{\sqrt{2\sigma_p^2}}\right)\right] + \frac{V_c}{2}\left[\text{erf}\left(\frac{\chi_{Max}-\mu_c}{\sqrt{2\sigma_c^2}}\right) - \text{erf}\left(\frac{\chi_{min}-\mu_c}{\sqrt{2\sigma_c^2}}\right)\right]$$

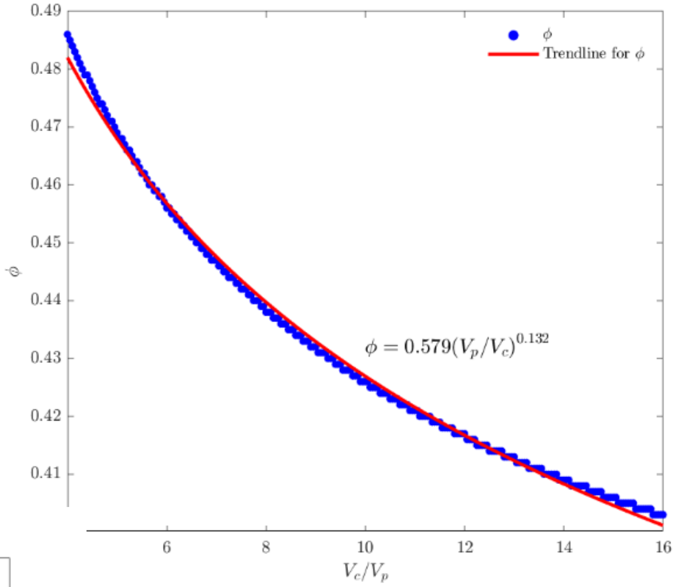
# Tuning of GIM

$$\frac{V_{p,i}}{V_p} = \frac{\pi {r_p}^3 (1+\psi)^2 \left(1 - \frac{1+\psi}{3}\right)}{\frac{4}{3}\pi {r_p}^3}$$

Trendline: $\phi = 0.579 \left(\frac{V_p}{V_c}\right)^{0.132}$

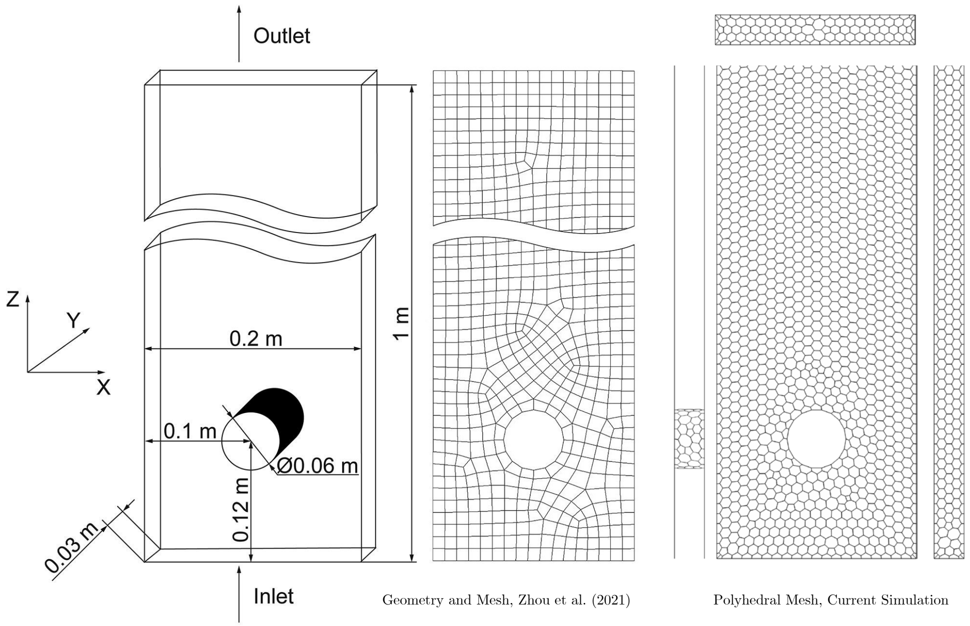


Immersed Tube Simulation

- The geometry and hexahedral mesh of Zhou et al. (2021) simulation (left) and polyhedral mesh of current simulation (right).



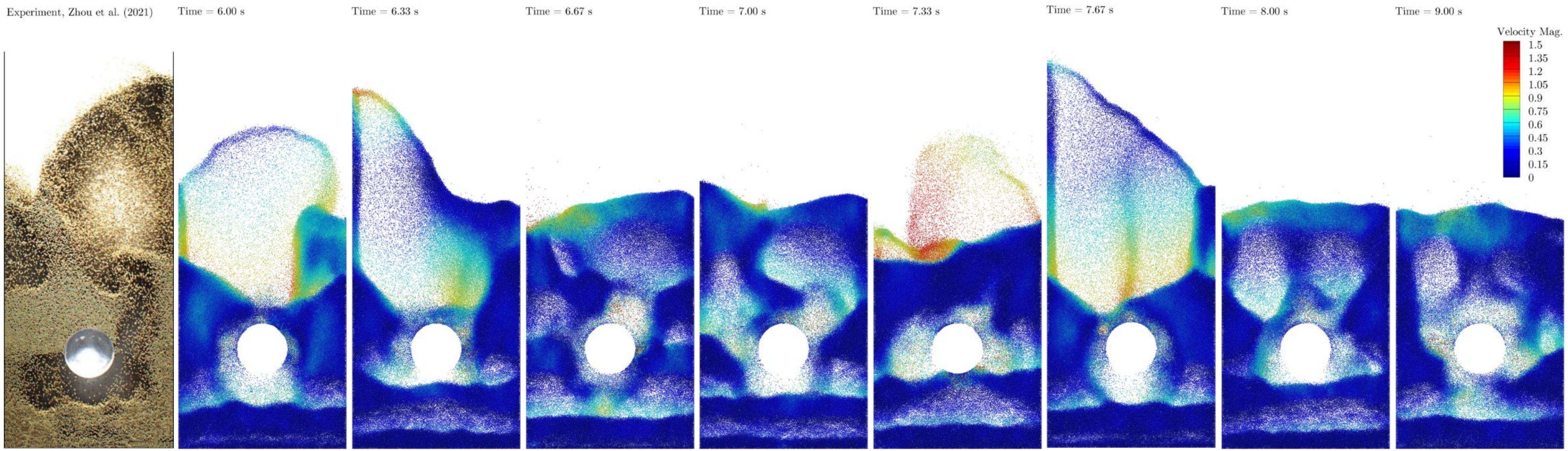

Geometry and Mesh, Zhou et al. (2021)

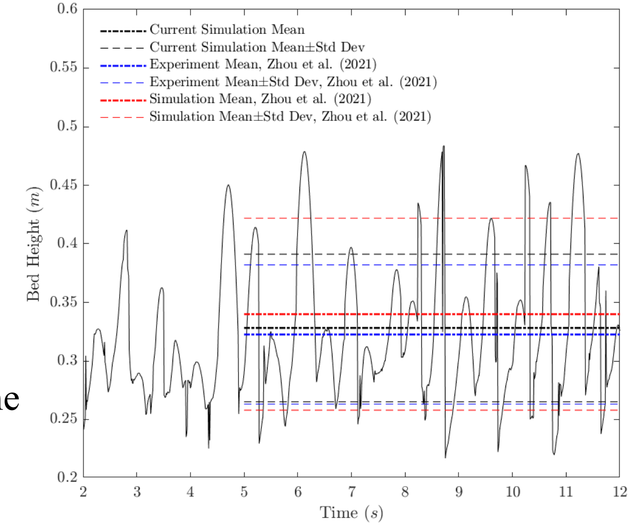
Polyhedral Mesh, Current Simulation

| Simulation parameters | Notation | Value |
|---|---|---|
| **Bed** | | |
| **Width** $(m)$ | $W$ | 0.2 |
| **Transverse thickness** $(m)$ | $T$ | 0.03 |
| **Height** $(m)$ | $H$ | 1.0 |
| **Number of Cells (Polyhedral)** | | 9640 |
| | | |
| **Particles (glass beads)** | | |
| **Number** | $N_p$ | 310000 |
| **Diameter** $(mm)$ | $d_p$ | 1.5 |
| **Density** $(kg/m^3)$ | $\rho_s$ | 2576 |
| **Young's modulus** $(Pa)$ | $Y$ | $2.0 \times 10^7$ |
| **Poisson's ratio** | $\upsilon$ | 0.25 |
| **Coefficient of normal restitution** | $e$ | 0.9 |
| **Coefficient of sliding friction** | $\mu_s$ | 0.3 |
| **Coefficient of rolling friction** | $\mu_r$ | 0.01 |
| | | |
| **Fluid (air)** | | |
| **Gas density** $(kg/m^3)$ | $\rho_f$ | 1.225 |
| **Gas inlet superficial velocity** $(m/s)$ | $\bar{v}_f$ | 1.8 |
| **Gas viscosity** $(Pa.s)$ | $\mu_f$ | $1.8 \times 10^{-5}$ |

# Immersed Tube Simulation, DEM

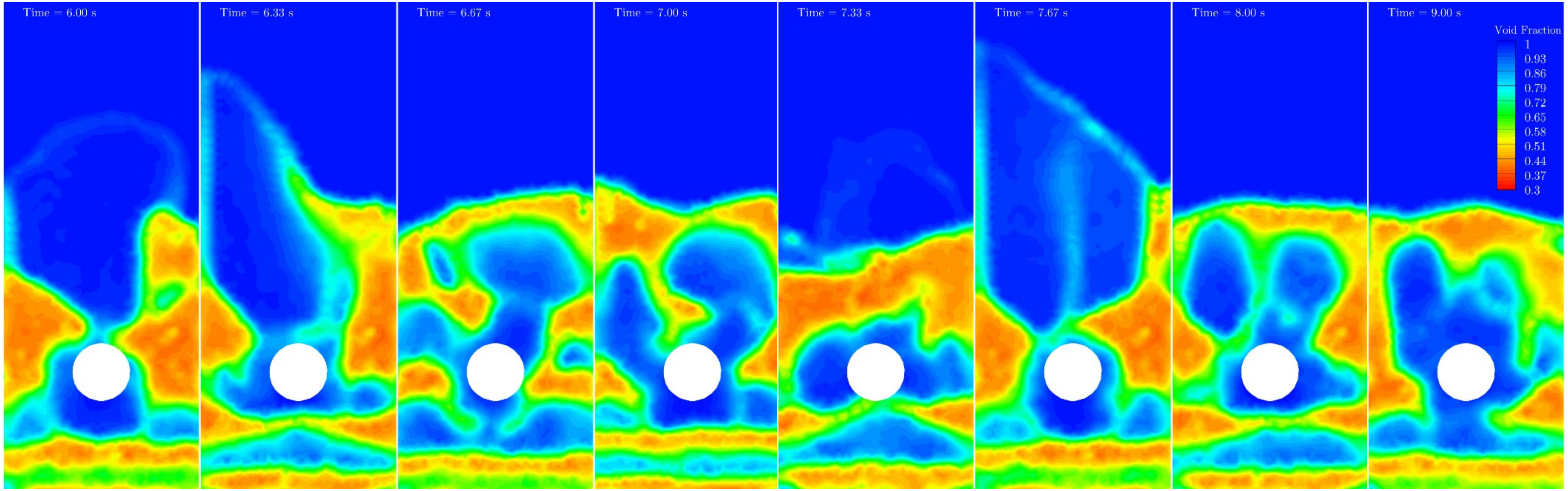
- The snapshot of the particles' position for the 6 *s* to 9 *s* time of the simulation. The right-hand side is the snapshots of the Zhou et al. experiment and simulation.



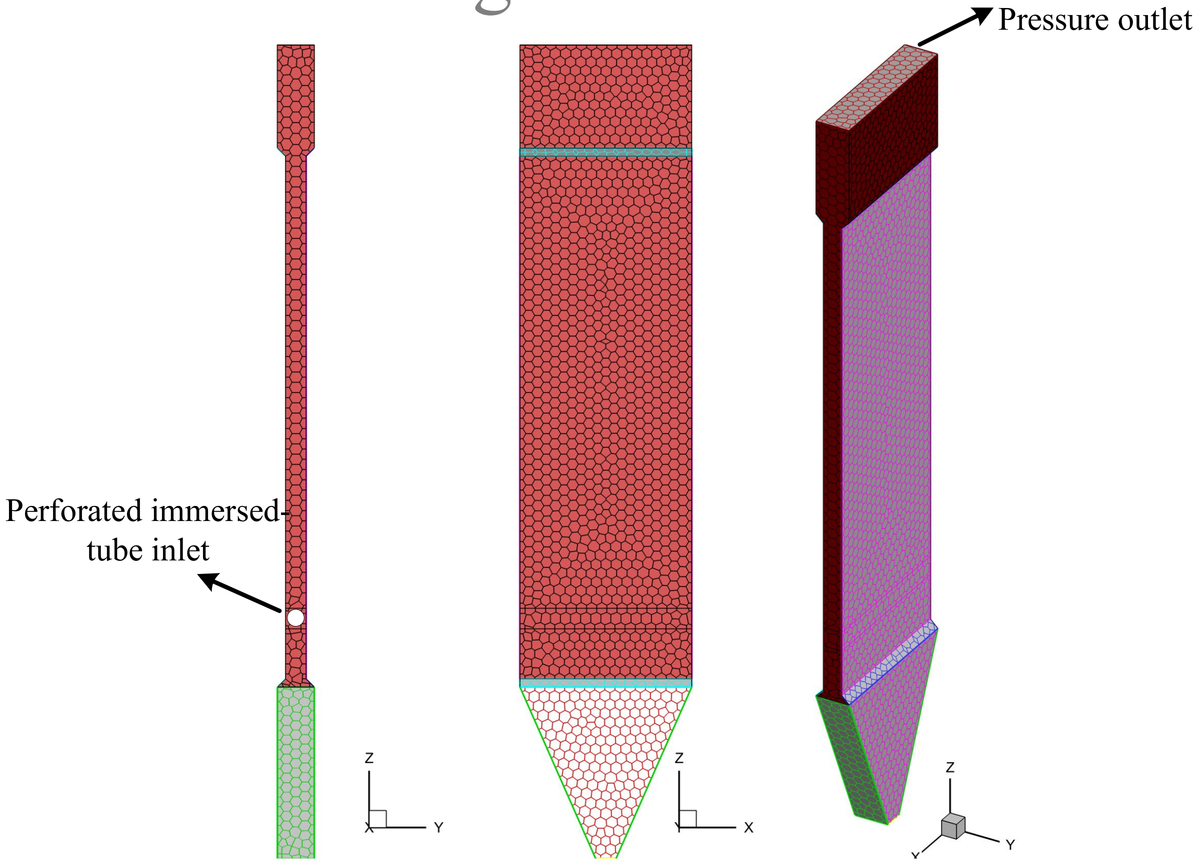



# Immersed Tube Simulation, CFD

- The contours of the cells void fraction for the 6 $s$ to 9 $s$ time of the simulation on the middle plane on the domain.

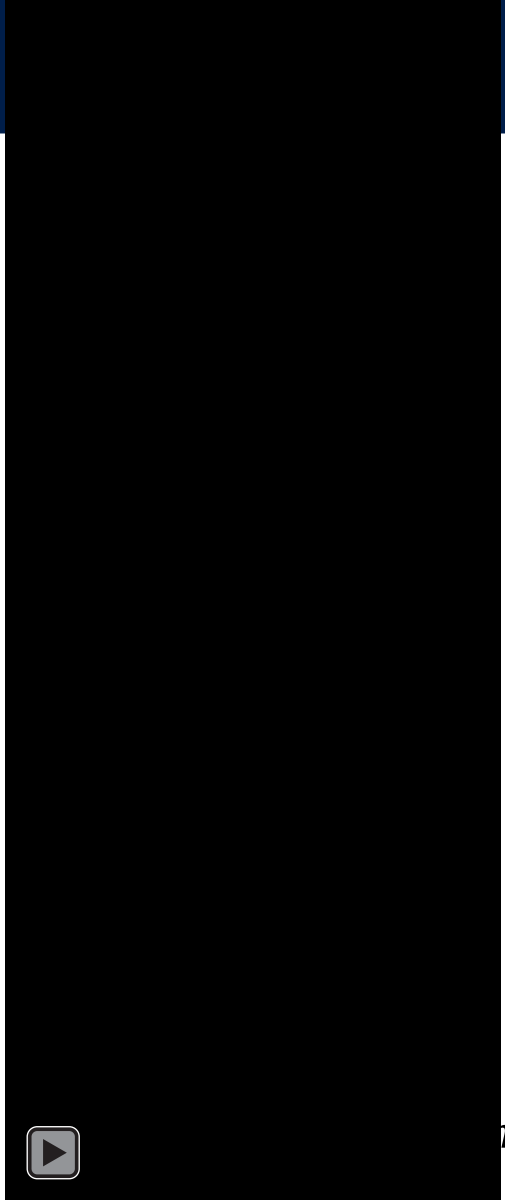


# Bubbling Fluidized Bed

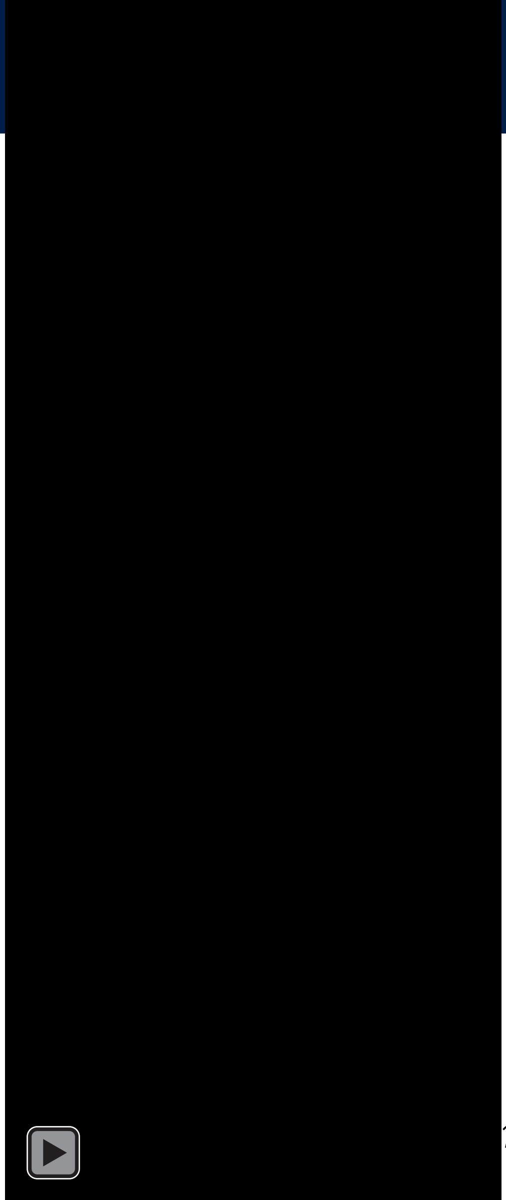



| Simulation parameters | Notation | Value |
| --- | --- | --- |
| ***Bed*** | | |
| **Width** $(m)$ | $W$ | 0.1 |
| **Transverse thickness** $(m)$ | $T$ | 0.021, 0.012 |
| **Height** $(m)$ | $H$ | 0.553 |
| **Number of Cells (Polyhedral)** | | 5792 |
| | | |
| ***Particles (glass beads)*** | | |
| **Number** | $N_p$ | 600000 |
| **Diameter** $(mm)$ | $d_p$ | 1.0 |
| **Density** $(kg/m^3)$ | $\rho_s$ | 1000 |
| **Young's modulus** $(Pa)$ | $Y$ | $1.0 \times 10^6$ |
| **Poisson's ratio** | $\upsilon$ | 0.25 |
| **Coefficient of normal restitution** | $e$ | 0.77 |
| **Coefficient of sliding friction** | $\mu_s$ | 0.3 |
| **Coefficient of rolling friction** | $\mu_r$ | 0.01 |
| | | |
| ***Fluid (air)*** | | |
| **Gas density** $(kg/m^3)$ | $\rho_f$ | 1.225 |
| **Gas inlet superficial velocity** $(m/s)$ | $\overline{v}_f$ | 0.4, 0.6 |
| **Gas viscosity** $(Pa.s)$ | $\mu_f$ | $1.8 \times 10^{-5}$ |

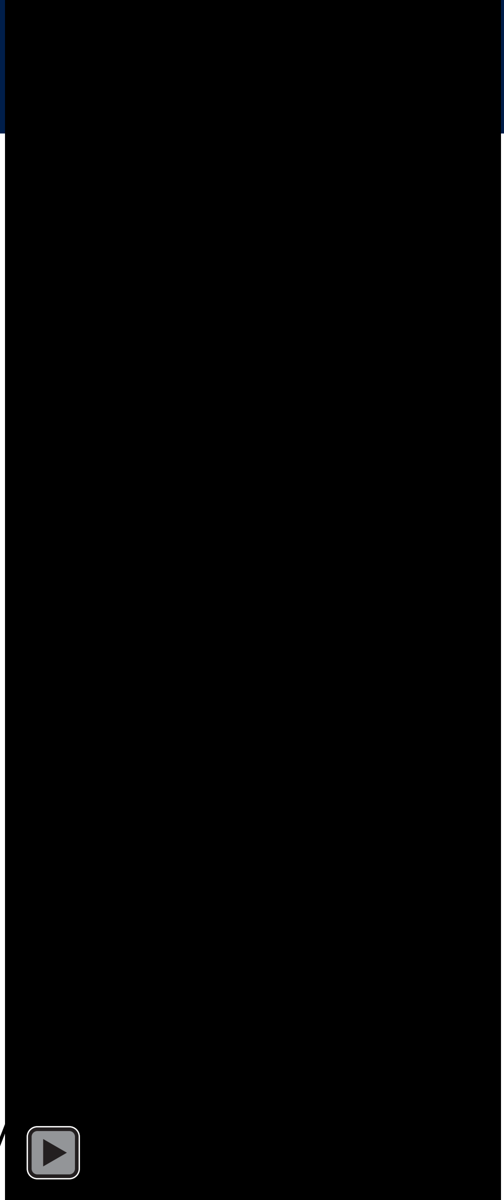
1865 THE UNIVERSITY OF MAINE



$n/s$



$m/$



THE UNIVERSITY OF MAINE

# Publications

- Kianimoqadam, A., Lapp, J., 2024. **Asynchronous GPU-based DEM solver embedded in commercial CFD software with polyhedral mesh support**. *Powder Technology*, p.120040.

- Kianimoqadam, A., Lapp, J., 2024. **Gaussian integral method for void fraction**. *in progress*. arXiv:2408.00909

THE UNIVERSITY OF MAINE

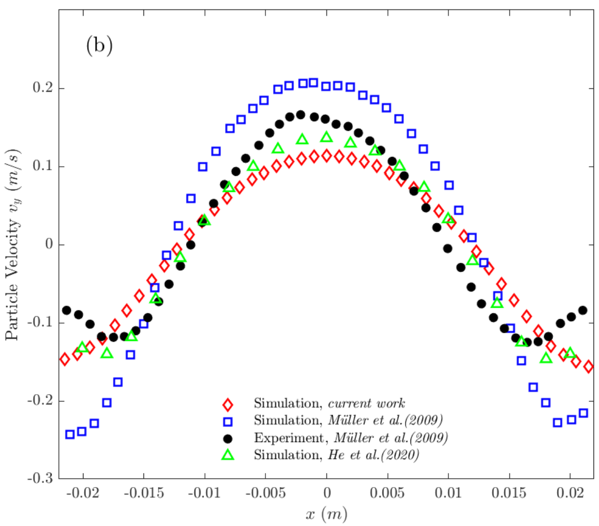
# Thank you!

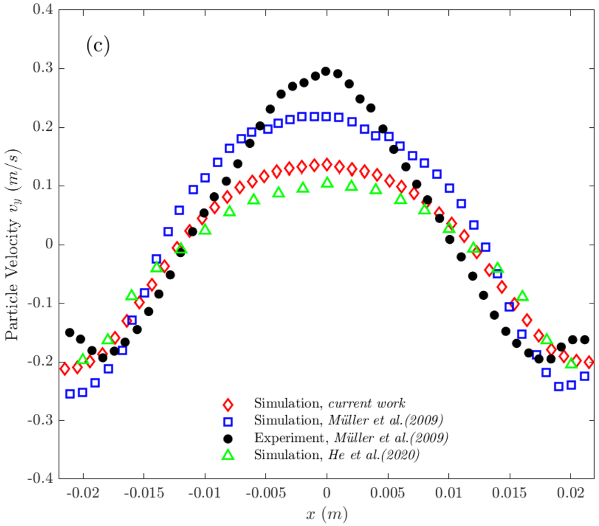
Open to thoughts and questions.

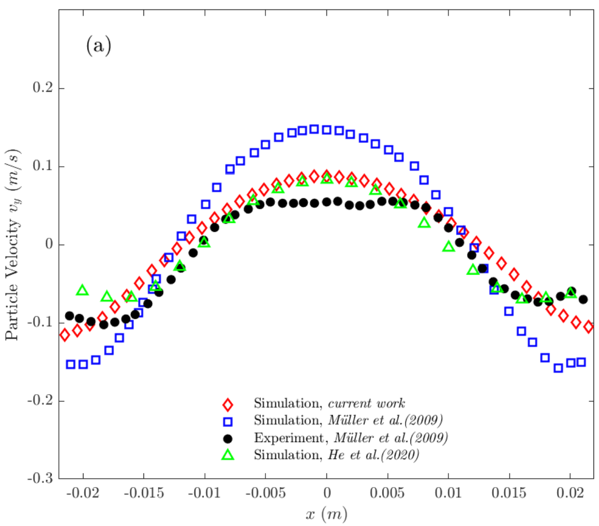
Alireza.Kianimoqadam@maine.edu

# Validation

- Validation against Müller et al. (2008) experimental and simulation results:
  - Time-averaged particle velocity profile at heights 0.015 m (a), 0.025 m (b), and 0.035 m (c) of the bed.

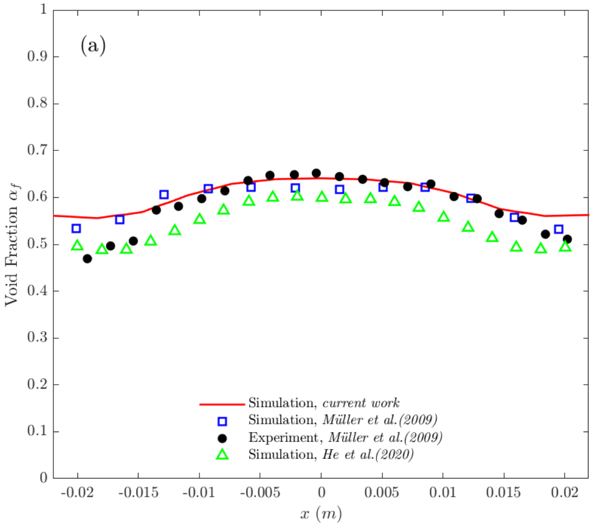


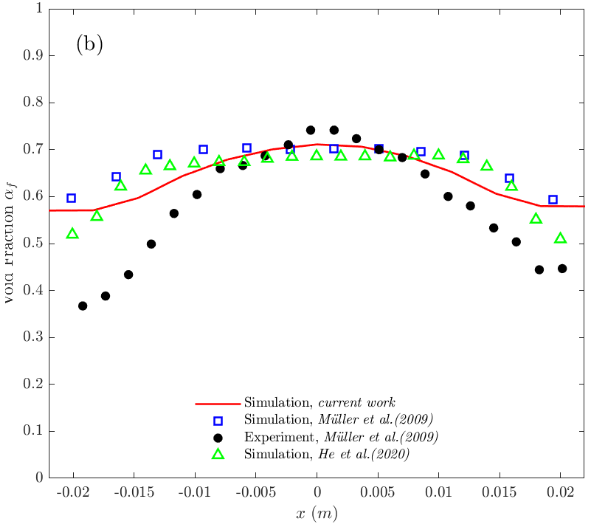



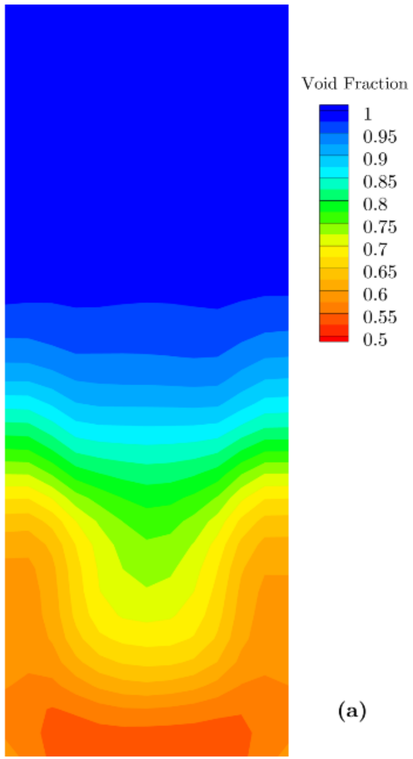



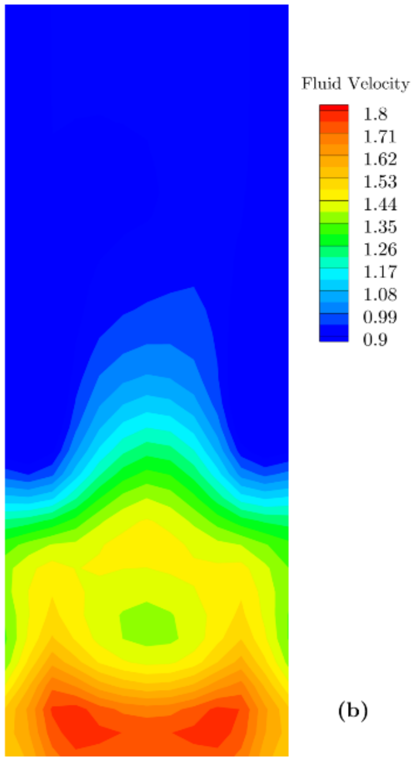
# Validation

- Validation against Müller et al. (2009) experimental and simulation
    - The time-averaged void fraction at heights 16.4 mm (a) and 31.2 mm (b) of the bed



# Wachem et al. (2001) fluidized bed (Validation)

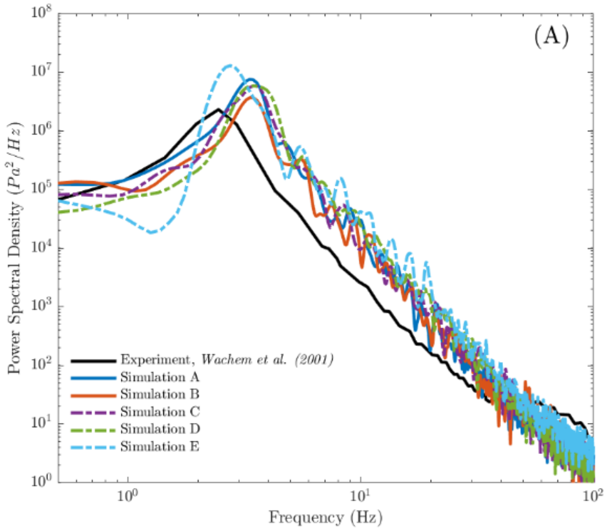
- parameters of Wachem et al. (2001) fluidized bed experiment (left) and grid information of simulation cases (right)

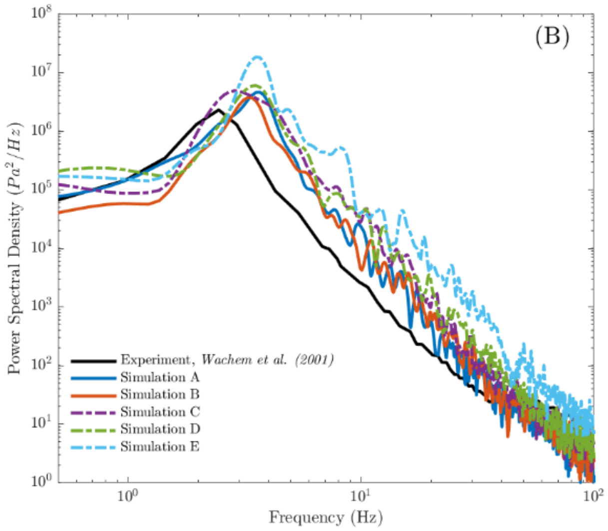
| Grid Name | Grid Type | $N_W \times N_T \times N_H$ | $N_{cells}$ | $\sqrt[3]{V_{cell}}/d_p$ |
|---|---|---|---|---|
| Grid A | structured | 33 × 3 × 181 | 17919 | 1.76 |
| Grid B | structured | 26 × 2 × 140 | 7280 | 2.38 |
| Grid D | Polyhedral | – | 25605 | 1.56 |
| Grid E | Polyhedral | – | 17840 | 1.76 |
| Grid F | Polyhedral | – | 7302 | 2.37 |

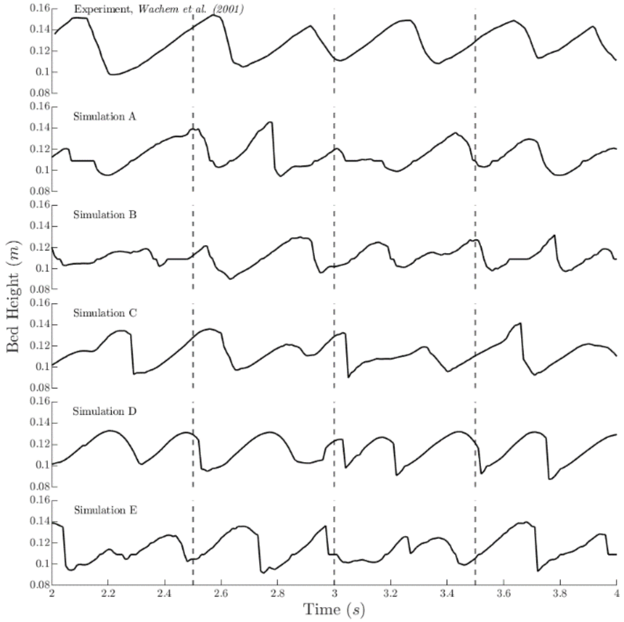
| Simulation parameters | Notation | Value |
|---|---|---|
| **Bed** | | |
| Width ($m$) | $W$ | 0.09 |
| Transverse thickness ($m$) | $T$ | 0.008 |
| Height ($m$) | $H$ | 0.5 |
| **Particles** | | |
| Total mass ($kg$) | $\sum m_p$ | 0.039 |
| Diameter ($mm$) | $d_p$ | 1.545 |
| Density ($kg/m^3$) | $\rho_s$ | 1150 |
| Young's modulus ($Pa$) | $Y$ | $1.2 \times 10^5$ |
| Poisson's ratio | $\upsilon$ | 0.33 |
| Coefficient of normal restitution | $e$ | 0.9 |
| Coefficient of sliding friction | $\mu_s$ | 0.3 |
| **Fluid (air)** | | |
| Gas density ($kg/m^3$) | $\rho_f$ | 1.28 |
| Gas inlet superficial velocity ($m/s$) | $\bar{v}_f$ | 0.9 |
| Gas viscosity ($Pa.s$) | $\mu_f$ | $1.7 \times 10^{-5}$ |

# Wachem et al. (2001) fluidized bed (Validation)

- The Power Spectral density of the relative pressure fluctuations as a function of frequency for the cases with optimization (A) and without optimization (B) and Wachem et al.'s experiment
- Bed height fluctuation at the height of 45 mm, comparing five different simulation strategies with the experimental data from Wachem et al.



- End of Supporting slides.