ON-DEM Handbook Slide Deck

COST Action CA22132: Open Network on DEM Simulations

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Open Network on Discrete Element Method Simulations

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Part I

CFD-DEM Coupling

Overview of Coupling Methodologies

Fluid-particle interactions govern many critical processes. The choice of methodology depends heavily on the required resolution, scale, and available computational resources.

Primary Methods Discussed:

- Under-Resolved (Unresolved) CFD-DEM
- Fully Resolved CFD-DEM
- Pore Model (Pore-Scale)
- Lattice Boltzmann Method (LBM-DEM)
- Smoothed Particle Hydrodynamics (SPH-DEM)
- Immersed Boundary Method (IBM-DEM)
- Volume of Fluids (VOF-DEM)

1. Under-Resolved CFD-DEM

Concept: Fluid mesh cells are significantly larger than individual particles. Fluid properties are locally averaged, and interactions are based on empirical drag models.

Pros

- Highly computationally efficient.
- Suitable for large-scale, industrial simulations (millions of particles).
- Robust empirical drag models are well-established.

Cons

- Lacks detailed flow resolution around individual particles.
- Heavily reliant on empirical correlations.
- Struggles with highly dense beds or complex particle shapes.

2. Fully Resolved CFD-DEM

Concept: The CFD mesh is significantly smaller than the particles, capturing the exact flow field and boundary layer around every single particle directly.

Pros

- Provides fundamental insights into local hydrodynamics.
- No need for empirical drag models.
- Excellent for studying non-spherical and complex particle shapes.

Cons

- Extremely computationally expensive.
- Limited to small domains (thousands, not millions of particles).
- Mesh generation and dynamic updating are highly complex.

3. Pore Model (Pore Network)

Concept: Represents the void space between particles as a network of interconnected pores and throats, solving for network conductivity rather than full Navier-Stokes equations.

Pros

- Computationally faster than fully resolved CFD for porous media.
- Excellent for multi-phase flow and capillary effects.
- Directly links macroscopic permeability to microscopic structure.

Cons

- Extracting an accurate pore network from dynamic DEM packing is difficult.
- Typically assumes creeping (low Reynolds number) flow.
- Dynamic coupling (constantly moving particles) is challenging.

4. Lattice Boltzmann Method (LBM-DEM)

Concept: Tracks the probability distribution of fictitious fluid particles colliding and streaming over a discrete lattice grid, rather than solving macroscopic Navier-Stokes.

Pros

- Highly parallelizable; highly efficient on modern GPUs.
- Handles complex/moving boundaries naturally without complex meshing.
- Accurate for transient and aeroacoustic phenomena.

Cons

- Higher memory requirements than traditional finite volume methods.
- Can suffer from stability issues at high Reynolds numbers.
- Uniform grid can be inefficient for localized high-resolution needs.

5. Smoothed Particle Hydrodynamics (SPH-DEM)

Concept: A fully meshfree, Lagrangian approach where the fluid is discretised into interacting 'particles'. Both fluid (SPH) and solids (DEM) share a particle-based framework.

Pros

- No mesh generation or grid entanglement issues.
- Suited for highly dynamic flows, large deformations, and free surfaces.
- Natural tracking of fluid-solid interfaces.

Cons

- Enforcing rigorous boundary conditions (like no-slip walls) is complex.
- Prone to numerical over-dissipation or artificial viscosity.
- Generally more computationally expensive per fluid volume than Eulerian methods.

6. Immersed Boundary Method (IBM-DEM)

Concept: A fully resolved approach using a fixed, stationary background fluid grid. Solid boundaries are represented by adding mathematical forcing terms to the Navier-Stokes equations, rather than fitting the mesh to the particle.

Pros

- Completely avoids computationally expensive dynamic remeshing.
- Highly efficient for simulating moving and interacting boundaries.
- Scales well on parallel computing architectures.

Cons

- The solid-fluid interface is 'smeared,' reducing boundary layer accuracy compared to body-fitted meshes.
- High grid resolution is still required to capture the interface forcing accurately.

7. Coarse-Grained / Parcel CFD-DEM

Concept: Groups multiple physical particles into a single computational ‘parcel’ or macroscopic particle to drastically reduce the number of entities tracked in the DEM solver.

Pros

- The only viable discrete way to model industrial-scale systems (billions of particles).
- Massive reduction in computational time and memory usage.

Cons

- Exact microscopic physics (like specific particle-particle collision dynamics) are lost or averaged.
- Requires careful tuning of scaling factors (e.g., spring stiffness) to maintain bulk behaviour.

8. Volume of Fluid with DEM (VOF-DEM)

Concept: Combines standard CFD-DEM with an interface tracking method (VOF) to model systems with interacting particles and two distinct fluid phases (e.g., air and liquid).

Pros

- Ideal for wet granulation, capillary bridging, and droplet-particle impacts.
- Captures complex free-surface fluid dynamics around moving solids.

Cons

- Extremely computationally demanding (requires very fine mesh for the VOF interface).
- Managing surface tension, contact angles, and dynamic contact lines on moving particles is highly complex.

Active Codes in the Network

Current CFD-DEM Software Implementations:

a) Hybrid
b) LIGGGHTS-PreCICE-OpenFOAM
c) Mercury-PreCICE-OpenFOAM
d) MercurySPH-DEM
e) Moomph
f) OpenFOAM with internal DEM
g) PhasicFlowPlus
h) Yade-OpenFOAM
i) Yade-PoreFlow

Methodology to Code Mapping

Overview of capabilities within the network:

Code / Software	Unresolved	Resolved	Pore Model	LBM	SPH	IBM	Parcel	VOF
Hybrid				✓				
LIGGGHTS-PreCICE-OpenFOAM	✓							
Mercury-PreCICE-OpenFOAM	✓	(✓)						
MercurySPH-DEM					✓			
Moomph	✓							
OpenFOAM with internal DEM	✓							
PhasicFlowPlus	✓	✓						
Yade-OpenFOAM	✓	✓						
Yade-PoreFlow			✓					

Fully Resolved CFD-DEM: Mathematical Framework

Governing Principles

In fully-resolved simulations, the equations of motion for the fluid and the particles are solved completely separately.

- The fluid is resolved on a scale significantly smaller than the particles (typically 8π times smaller than the smallest particle diameter).
- The fluid strictly follows the incompressible Navier-Stokes equations (continuity and momentum).
- Instead of using empirical drag models, all interaction information is passed exactly at the particle-fluid interface (Γ_{pf}).
- To minimise the number of fluid elements in these very dilute systems, mesh-adaptivity can be applied.

Fully Resolved CFD-DEM: Governing Equations

Incompressible Navier-Stokes

The fluid domain is strictly governed by the conservation of mass (continuity) and momentum.

Continuity Equation:

$$\nabla \cdot \vec{u}_f = 0$$

Momentum Equation:

$$\rho_f \left(\frac{\partial \vec{u}_f}{\partial t} + \vec{u}_f \cdot \nabla \vec{u}_f \right) = -\nabla p + \mu \nabla^2 \vec{u}_f + \rho_f \vec{g}$$

Where $\vec{u}_f$ is fluid velocity, ρ_f is fluid density, p is pressure, μ is dynamic viscosity, and $\vec{g}$ is gravitational acceleration.

Connectivity Conditions at the Boundary

The coupling relies on two primary boundary conditions at the particle-fluid interface (Γ_{pf}), which prescribe velocities and provide the particle with all fluid forces acting on its surface.

1. Kinematic Boundary Condition (No-Slip):

$$\vec{u}_f = \vec{u}_{\Gamma_{pf}} \quad \text{on} \quad \Gamma_{pf}$$

2. Dynamic Boundary Condition (Stress Matching):

$$\sigma_f \cdot \vec{n} = t_{\Gamma_{pf}} \quad \text{on} \quad \Gamma_{pf}$$

Where $\vec{u}_f$ is the fluid velocity, σ_f is the fluid stress tensor, $\vec{n}$ is the normal vector, and $t_{\Gamma_{pf}}$ represents the interface traction

Fully Resolved CFD-DEM: Force Computation

Integrating the Fluid Stress Tensor

Forces like buoyancy, virtual mass, and drag do not need to be modelled empirically; they are implicitly captured by integrating the fluid stress tensor (σ_f) over the particle's surface.
The stress tensor consists of two primary components:

- **Hydrostatic Pressure:** Because the direction of this force passes directly through the particle's centre-of-mass, it primarily dictates the translational movement of the particle.
- **Deviatoric Stress:** This component determines the particle's rotation. The resulting rotational velocity is calculated after integrating this stress over the entire particle surface.

Fully Resolved CFD-DEM: Stress Tensor & Torque

Mathematical Formulation of Interfacial Forces

The fluid stress tensor σ_f explicitly defines both the pressure and viscous shear forces acting on the particle surface.

Fluid Stress Tensor:

$$\sigma_f = -p\mathbf{I} + \mu\left(\nabla\vec{u}_f + (\nabla\vec{u}_f)^T\right)$$

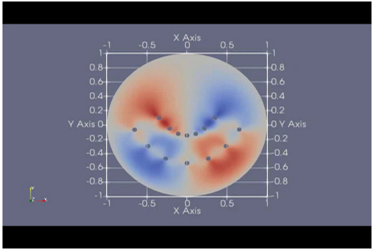
Hydrodynamic Torque Calculation:

$$\vec{T}_f = \oint_{\Gamma_{pf}} (\vec{r} - \vec{r}_c) \times (\sigma_f \cdot \vec{n})\, dA$$

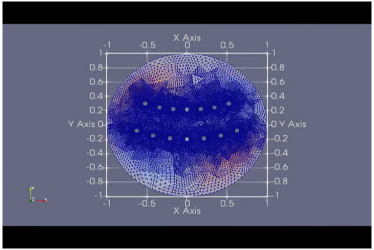
Where $\mathbf{I}$ is the identity tensor, $\vec{r}_c$ is the particle center of mass, and $\vec{n}$ is the outward surface normal.

Fully Resolved CFD-DEM: Adaptive Remeshing

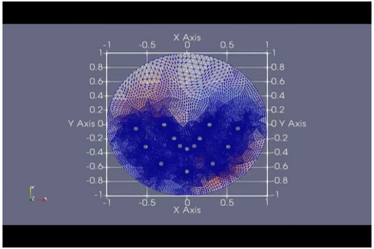
1. Flow Field



2. Initial Mesh



3. Adapted Mesh



Chronological Breakdown:

- **Stage 1:** The solver calculates the high-resolution pressure and velocity fields around the particles.
- **Stage 2:** The body-fitted mesh explicitly conforms to the solid particle perimeters.
- **Stage 3 (Adaptive Refinement):** At every time step, the solver evaluates spatial errors and generates a new, refined mesh topology to meet strict error tolerances, particularly in the narrowing gaps.

Acknowledgments: Fully Resolved Implementation

oomph-lib Framework

The fully resolved fluid-particle coupling examples and adaptive remeshing demonstrations shown in this section are built using **oomph-lib**.

- **Developer:** The core implementation and underlying adaptive meshing routines were developed by Andrew Hazel.
- **Framework:** oomph-lib is an object-oriented, open-source finite-element library explicitly designed for complex multi-physics and fluid-structure interaction problems.

Fully Resolved CFD-DEM: Handling Moving Particles

Why ALE is More Than Just Remeshing

Because the mesh is physically fitted to the particle surfaces, the fluid grid must continuously adapt. Doing this efficiently requires moving beyond basic remeshing.

- **The Problem with Simple Remeshing:** Generating a brand-new mesh at every single time step is computationally crushing and introduces severe interpolation errors (numerical diffusion) into the flow field.
- **The ALE Solution (The 'Rubber Band'):** Arbitrary Lagrangian-Eulerian (ALE) methods stretch the existing grid instead. Boundary nodes move exactly with the particle, while internal nodes deform smoothly to absorb the motion.
- **Convective Flux Correction:** Crucially, ALE mathematically modifies the Navier-Stokes equations to subtract the mesh's own velocity, ensuring fluid fluxes remain perfectly accurate across a moving grid.
- **Topological Remeshing (The Fallback):** Only when elements become critically skewed (the rubber band is about to snap) does the solver finally halt, generate a fresh grid, and project the fields.

Fully Resolved CFD-DEM: Particle Contact

The Lubrication Singularity & The Roughness Layer

Handling physical particle-particle (and particle-wall) contact is one of the most significant numerical challenges in fully resolved methods.

The Problem: Lubrication Singularity

- As two smooth spheres approach, the fluid pressure approaches infinity.
- In a continuum fluid model, the spheres would never touch.
- Furthermore, can lead to infinite mesh refinement .

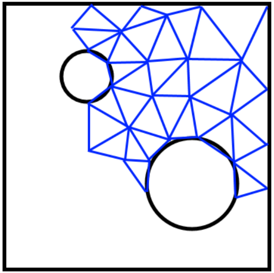
The Solution: Roughness Layer

- A microscopic roughness layer is defined.
- below this threshold, the CFD lubrication forces are capped.
- The DEM soft-sphere model then takes over.

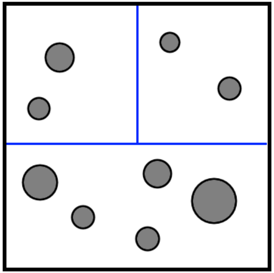
Multiresolution

Particle-Fluid Coupling: Scale Separation

Fully-Resolved



Under-Resolved

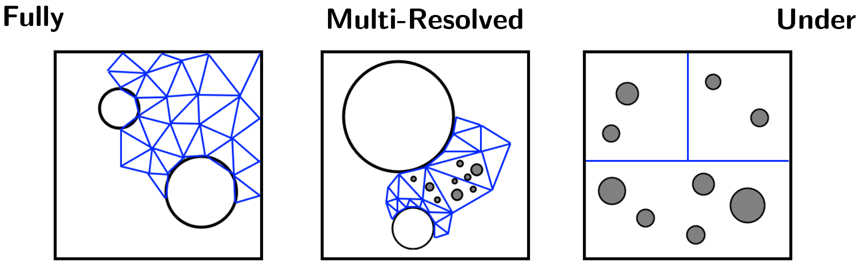


Key Characteristics:

- **Fully:** Highly resolved fluid field, but computationally slow. No empirical models needed. Mesh size $h < \frac{1}{8\pi} d_{\text{min}}$.
- **Under:** Low fluid resolution, but fast. Heavily reliant on closure relations (drag models). Mesh size $h > 3d_{\text{max}}$.

Challenge: Neither method works efficiently for highly polydisperse particle size distributions.

Particle-Fluid Coupling: The Multi-Resolved Approach



Key Characteristics:

- **Fully:** Highly resolved fluid field, but computationally slow. Mesh size $h < \frac{1}{8\pi} d_{\text{min}}$.
- **Under:** Low fluid resolution, but fast. Mesh size $h > 3d_{\text{max}}$.
- **Multi:** Bridges the gap by applying fully- and under-resolved simultaneously. It explicitly handles large size ratios and speeds up computation time for complex, realistic processes.

Part II

Benchmarks

CFD-DEM

Granular Rayleigh-Taylor Instability Benchmark

Status: On Hold

Benchmark Objective

- The primary aim is to recover the results from section 7 of [**?**].
- It is treated as a pure benchmark against the Robinson data rather than a validation case, as it is unclear why the system should strictly follow the Rayleigh-Taylor instability.

Physical Setup & Methodology

- The simulation involves a set of granular materials arranged on a grid falling into a fluid.
- A perturbation is applied to the initial particle positions.
- The growth on this interface is then analysed as a function of the perturbation's wave number.

Problem: The accuracy of the original data cannot be verified.

Sedimentation of a Constant Porosity Block Benchmark

Status: On Hold

Benchmark Objective

- The primary target is to recover the analytical solution presented in equation (36) from section 5 of [**?**].
- This case is strictly classified as a verification benchmark.

Physical Setup & Methodology

- The simulation models a porous block of granular materials falling within a container.
- It serves as a natural extension of a single spherical particle falling in a fluid under a gravitational field, but importantly includes fluid back flow.
- There is a known theoretical, analytic solution for the terminal velocity of the particle for a given applied drag model.

Segregation in a Fluid-Saturated Rotating Drum Benchmark

Status: On Hold

Benchmark Objective

- The target is to validate the numerical codes against experimental data of segregation profiles.
- Unlike the previous cases, this is strictly classified as a validation benchmark.

Physical Setup & Methodology

- The setup considers two different sizes of glass beads inside a rotating drum filled with a viscous liquid.
- The goal is to analyse the segregation profile as a function of drum RPM, fluid density, and fluid viscosity.

Problem: The original experimental paper was never published and the data is missing, though the experimental setup still exists to recreate it.

Industrial Challenge: Powder Dosing (Double Screw Feeder)

Status: Active

Challenge Objective

- This is an active challenge aimed at evaluating 'blind' DEM simulations against experimental results of the dosing process.
- The overarching goal is to enhance precise material delivery while optimising consistency and reducing errors.
- Key comparison parameters include achieved mixing indices (e.g., coefficient of blending performance), segregation amounts, and the effects of agitator and screw rotational speeds.

Industrial Partnership & Data

- The industrial partner, Bayer, is providing two materials alongside relevant material characterisation and laboratory-scale data.
- The provided lab data includes starting mass, filling level, rotational screw and agitator speeds, and dosing time.

Powder Dosing Challenge: Setup & Implementation

Status: Active

Simulation Setup & Flexibility

- Participants must calibrate their chosen contact models using the provided material data.
- Because the process involves fine and cohesive particles, participants have the flexibility to choose appropriate contact laws (e.g., Hertzian/Linear elastic with JKR or DMT for adhesion).

Material Properties & Availability

- The measured probability density functions (PDFs) of the materials are provided, alongside literature data for paracetamol (e.g., density of 1200 kg/m^3) for guidance.
- Full descriptions of the experiments, equipment geometry, and datasets are hosted on Zenodo Record 18588605.

Participating Codes & Leads

- **MercuryDPM:** Holger Götz.
- Note: Every benchmark requires at least two different DEM codes, so additional collaborators are needed.

References I

Martin Robinson, Stefan Luding, and Marco Ramaioli.
Fluid–particle flow and validation using two-way-coupled mesoscale sph-dem.
International Journal of Multiphase Flow, 59:121–134, 2014.