CFDEM - マイクロスケールからメータースケールへの結合フローの例とその問題点

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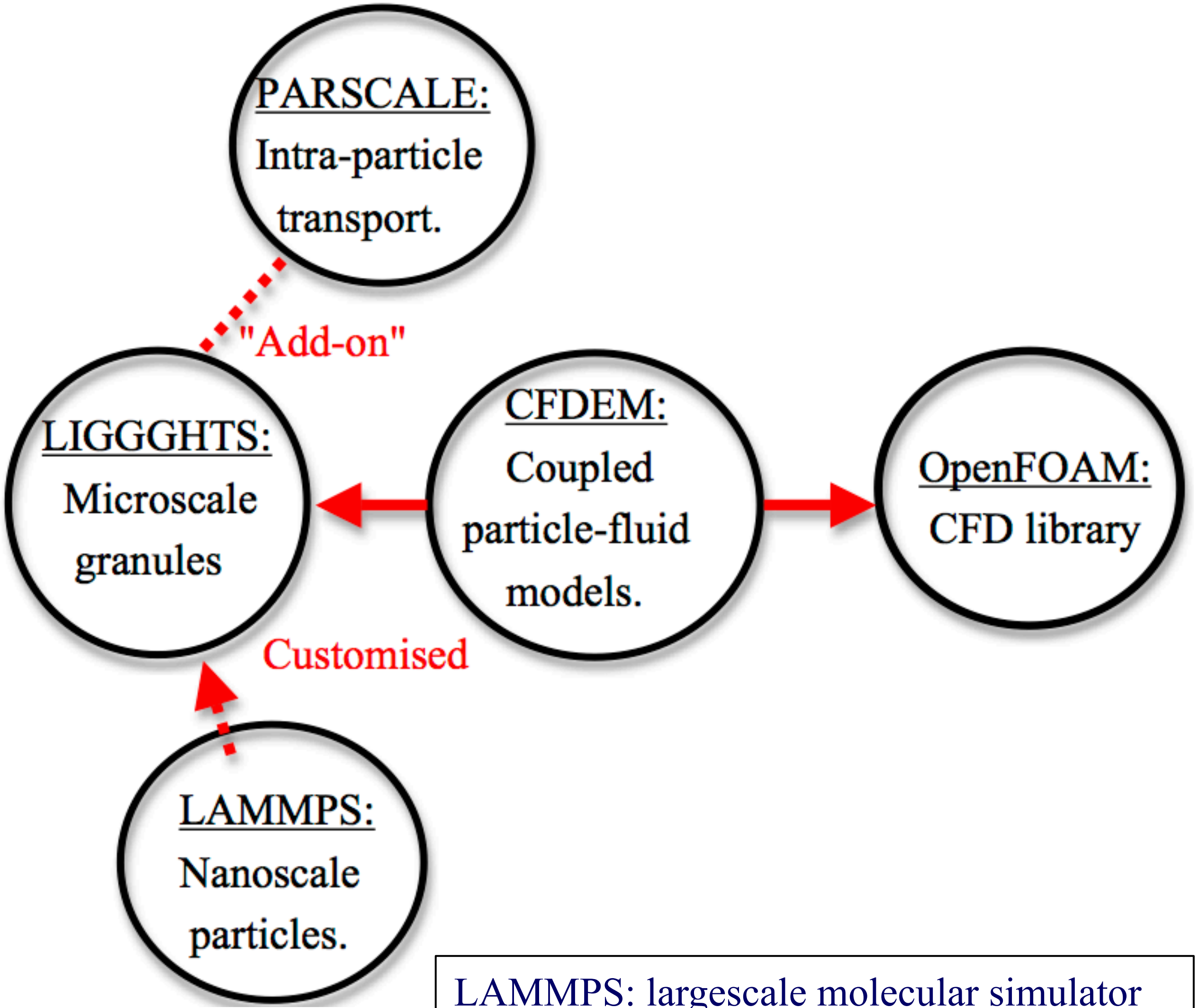
1. What is CFDEM?

CFDEM couples "CFD" with "Discrete Element Modelling".



LAMMPS: largescale molecular simulator

Opensource CFDEM

Project:

www.cfdem.com

Hosted by:

DCS Computing Gmbh

(who provide commercial support and additional add-ons to CFDEM)

Speed-up boosts from

a) LAMMPS parallel capability

b) CFDEM 'coarsened' representation

c) CFDEM load balancing

2.1 Basic Equations - Fluid

A VOF-style formulation in which both the fluid and particles occupy a certain volume fraction of space. (Particle VOF is a smoothed interpolation from discrete locations.)

$$\frac{\partial \alpha_f \rho_f}{\partial t} + \nabla \cdot \left(\alpha_f \rho_f \mathbf{u}_f\right) = 0$$

Fluid Continuity Equation

$$\frac{\partial \left(\alpha_f \rho_f \mathbf{u}_f\right)}{\partial t} + \nabla \cdot \left(\alpha_f \rho_f \mathbf{u}_f \mathbf{u}_f\right) = -\alpha_f \nabla p + \nabla \cdot \left(\alpha_f \tau\right) + \alpha_f \rho_f \mathbf{g} - \mathrm{K}_{sf}\left(\mathbf{u}_f - \mathbf{u}_s\right)$$

Fluid Momentum Equation. This representation is called "Model A" i.e. the pressure gradient is multiplied by fluid VOF. A sufficiently general description.

$$\left(\mathrm{K}_{sf}\right)_j = \frac{1}{V_j} \sum_{i=1}^{i=N} \frac{w_i \beta_i \left(\mathbf{f}_{s->f}\right)_i}{\left|\left(\mathbf{u}_f - \mathbf{u}_s\right)_i\right|}$$

Solid-Fluid Coupling Source Term

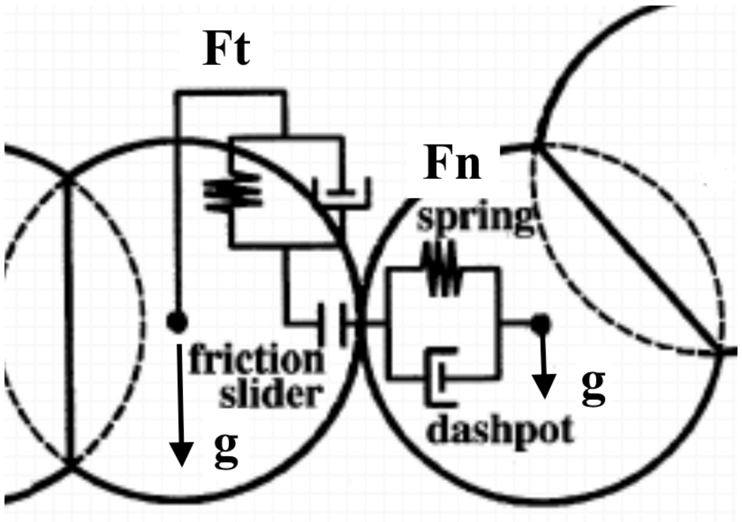
2.2 Basic Equations - Particle

Particle motion is described by a Lagrange equation in which the effects of fluid drag and pressure are included as source terms.

$$\frac{\partial^2 \mathbf{x}_p}{\partial t^2} = \frac{\mathbf{F}_n}{m_p} + \frac{\mathbf{F}_t}{m_p} + \mathbf{g} - \frac{\beta}{\rho_p \alpha_p}\left(\mathbf{u}_p - \mathbf{u}_f\right) - \frac{1}{\rho_p}\nabla p$$

Equation of motion for particle:

For granular flows the particles are modelled as soft spheres characterized with suitable elastic properties and experience normal and tangential contact forces during a collision with a neighbour



Spring and dashpot model for the normal **Fn** and tangential **Ft** contact forces present during a collision of two soft-sphere neighbours.

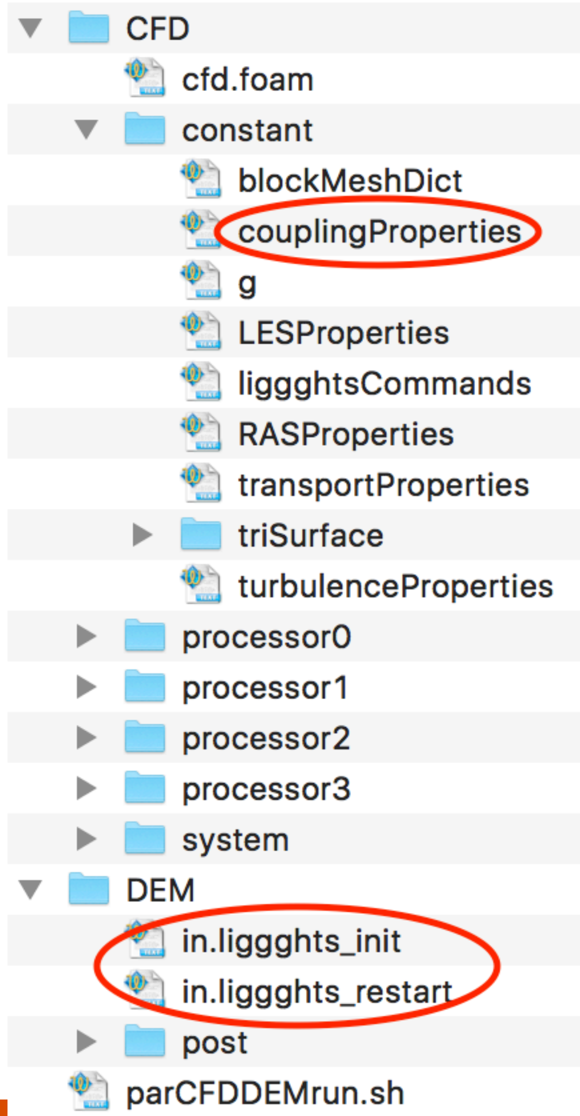
3. CFDEM Solvers

The following solvers are available in the default CFDEM distribution:

Solver	Description
cfdemSolverIB	Transient incompressible immersed boundary solver for resolved fluid-solid flows.
cfdemSolverPisoScalar	cfdemSolverPiso with a fluid temperature equation (granular heat source term)
cfdemSolverPisoSTM	cfdemSolverPiso with a solid temperature equation (fluid heating source term)
cfdemSolverPiso (considered in the demos)	**Transient, incompressible solver for 4-way (fluid-solid, solid-fluid, solid-neighbour, neighbour-solid) unresolved fluid-solid flows.**

4 Typical CFDEM Case

The following is a typical CFDEM case layout:



Typical couplingProperties settings:

```
modelType "A"; // A or B

couplingInterval 100;// Couple every 100 deltaT(solid) seconds

voidFractionModel bigParticle;//bigParticle;divided;centre;

dataExchangeModel twoWayMPI;

averagingModel dense;//dilute;dense

smoothingModel off;

        //localPSizeDiffSmoothing;constDiffSmoothing;

forceModels

(

  GidaspowDrag

  gradPForce

  viscForce

    ..

);
```

5 Typical DEM (LIGGGHTS) input script

The following is a typical CFDEM case layout:

- CFD
  - cfd.foam
  - constant
    - blockMeshDict
    - couplingProperties
    - g
    - LESProperties
    - liggghtsCommands
    - RASProperties
    - transportProperties
    - triSurface
    - turbulenceProperties
  - processor0
  - processor1
  - processor2
  - processor3
  - system
- DEM
  - in.liggghts_init
  - in.liggghts_restart
  - post
- parCFDDEMrun.sh

Typical LIGGGHTS script:

atom_style granular

Material properties of granules

fix m1 all property/global youngsModulus peratomtype 5.e6

pair style

pair_style gran model hertz tangential history # Hertzian without cohesion

Behaviour at walls

fix ywalls1 all wall/gran model hertz tangential history primitive type 1 yplane 0.0

cfd coupling

fix cfd all couple/cfd couple_every 100 mpi

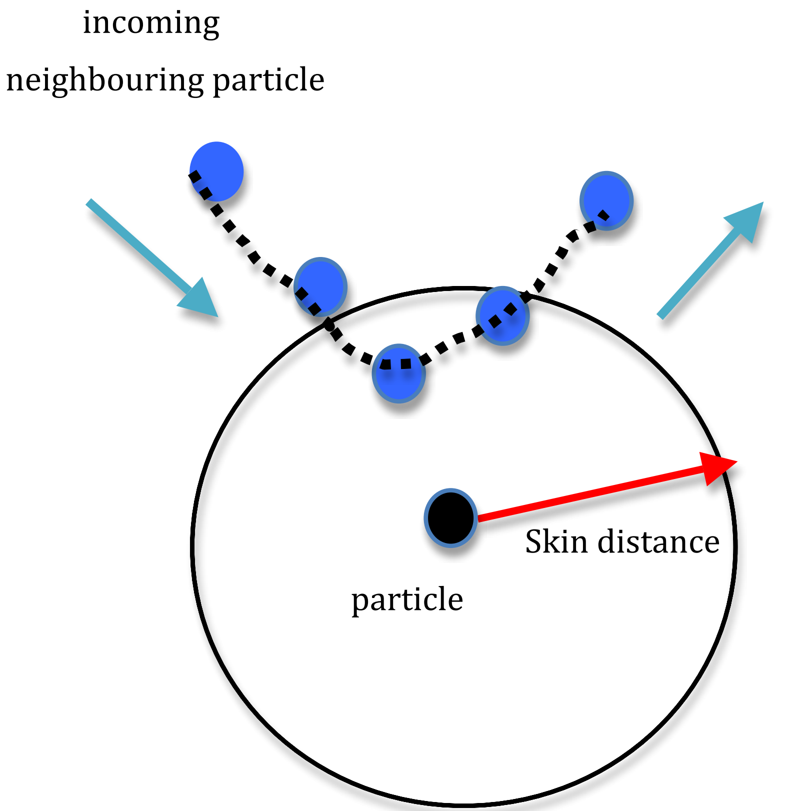
Post-processing: compute dragforce at walls

compute dragtotal all reduce sum f_dragforce[1] f_dragforce[2] f_dragforce[3]

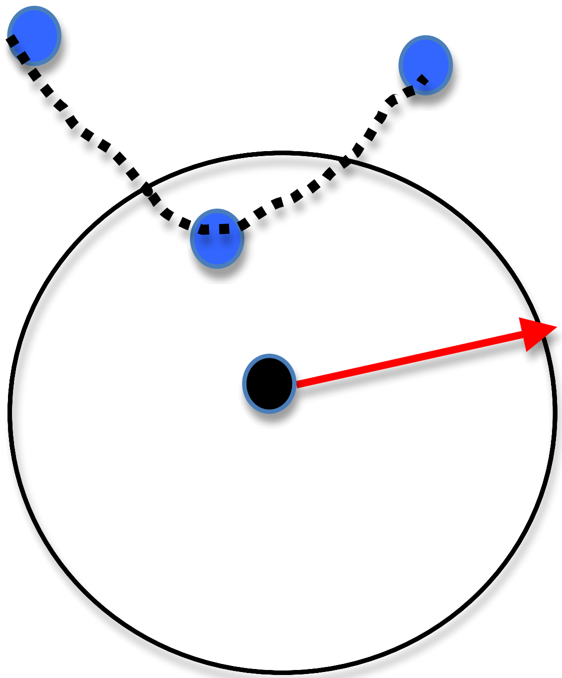
6. Particle-neighbour collisions

i) Particles interact with neighbours within a user-defined collision sphere.

ii) Choose a suitable 'skin radius' (usually the particle diameter) and time-step to allow for accurate collision modelling.



GOOD: LIGGGHTS/DEM time step is small enough to correctly model particle (black) and neighbour (blue) collision.



BAD: LIGGGHTS/DEM time step is too large. Neighbours appear and disappear too quickly for accurate collision modelling.

7. Demo - Filter Flow (40 mm scale)

i) Particles are inserted at the top and descend (percolate) through the filter.

ii) The filter itself is composed of a randomly packed box of spheres (conveniently constructed in spaceClaim)

CFD mesh size: 1M cells

Finest mesh resolution: 0.0625mm

Average mesh resolution: 1mm

Total Particle Count: 1K

Particle radius: 0.1mm

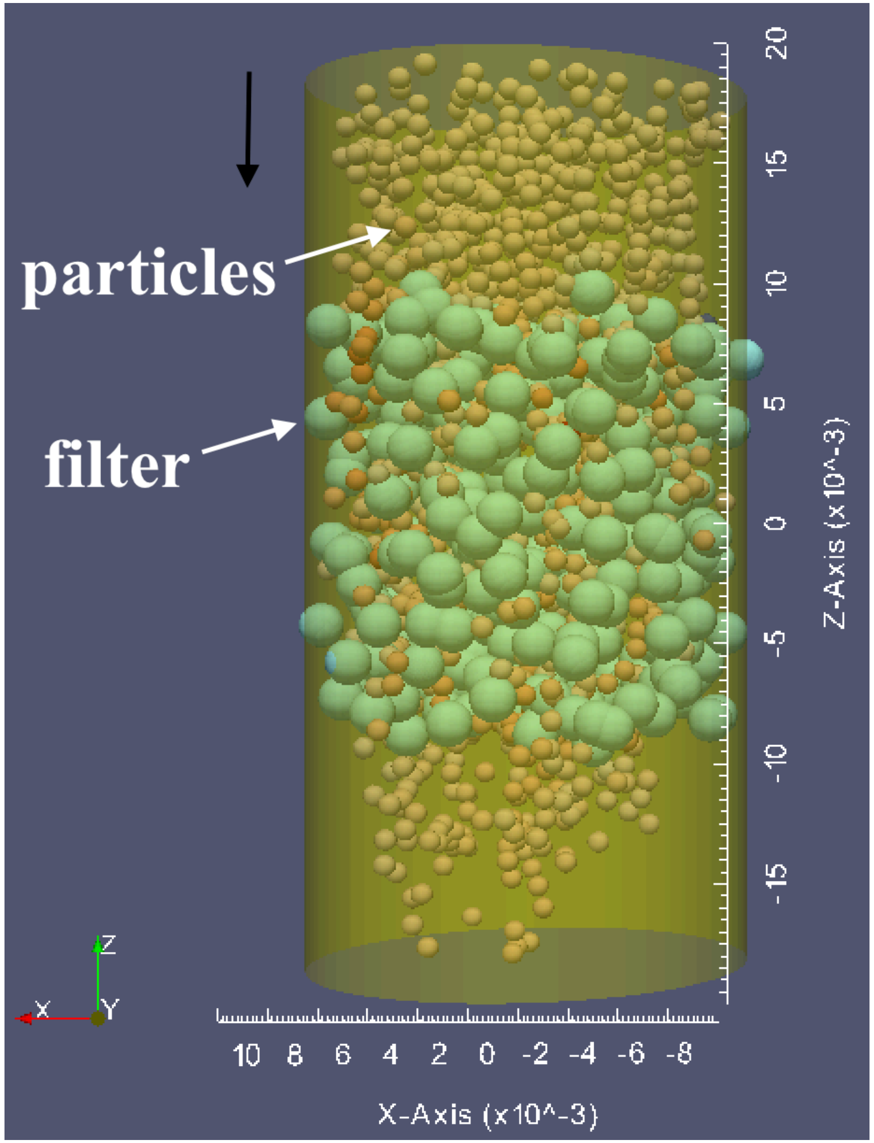
Liquid density 10 Kg/m^3

Inlet liquid flow speed: 0.1m/s

Particle Injection Rate: 5K particles/sec

Number of processors: 16

Execution time:1.1 hrs (simulating 5ms)



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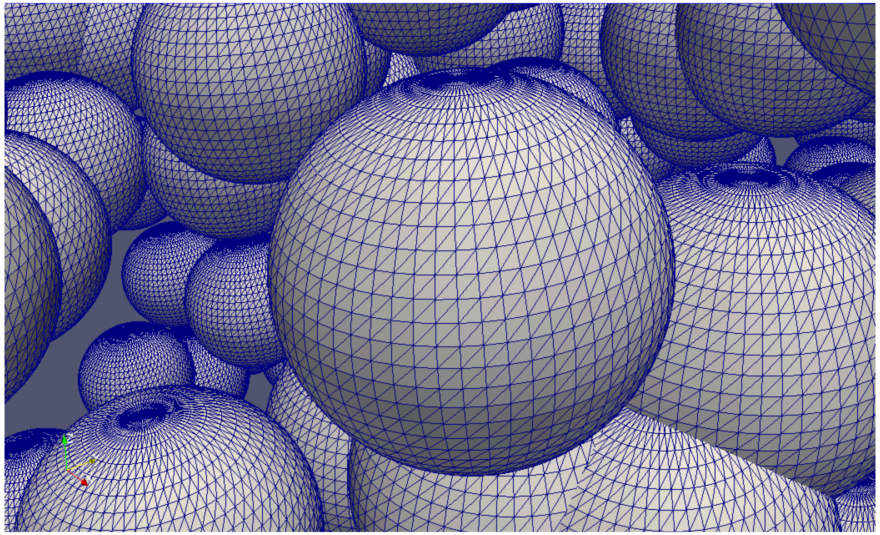
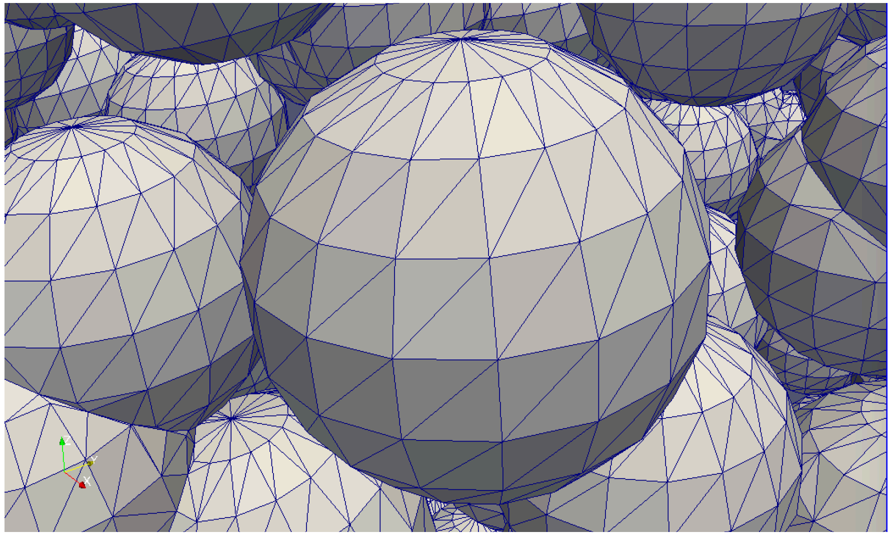
7.1 Filter Flow – STL files for surface meshes

STL files are imported into CFDEM and employed in impact detection. Each STL is decomposed amongst the various processors.

STL-handing in CFDEM is fairly basic.



High resolution STL employed for **CFD mesh generation**.



Coarse STLs employed for **impact estimation in CFDEM** (reduces memory overhead considerably).

..small errors from mismatch...

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8. Micro-filter – 2 particle types

CALCULATION CONDITIONS:

Particle Properties:

Particle Type 1: radius 100 microns

Particle Type 2: radius 260 microns

Particle Type 1&2: density 2000Kg/m^3

Particle Injection Rate: 0.1M particles/sec

Particle Phase time-step (estimated from

Rayleigh contact time): 1e-07s

Fluid Properties:

Similar to Water

Laminar Simulation

Inlet flow speed: 1m/s

CFD time-step (max Courant ~ 4): 1e-06s

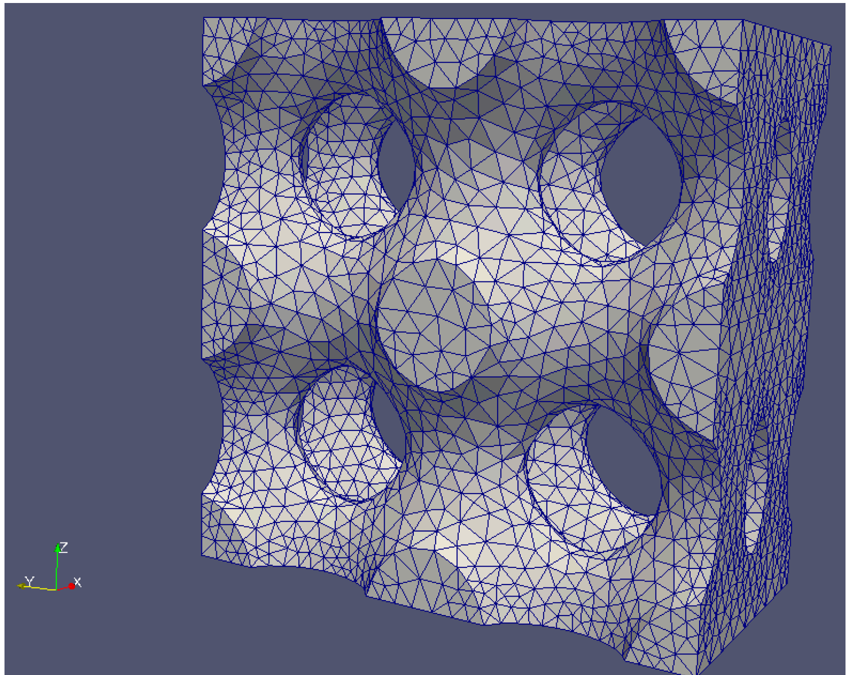
Output interval: 5e-05s

i) This type of flow tests the lower limit of CFDEM applicability i.e. drag models may no longer be suitable.

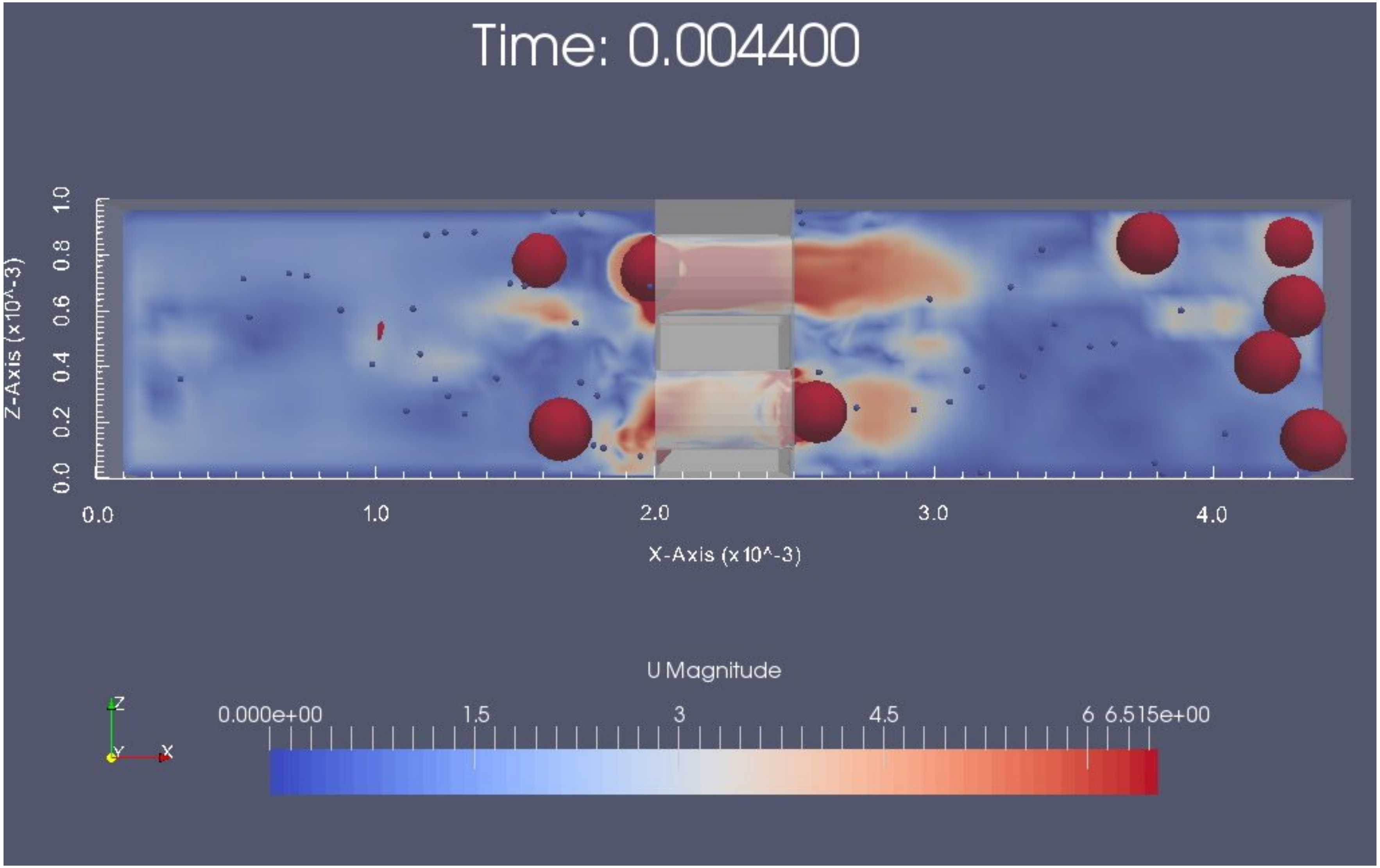
ii) Wall and charge effects become signifcant e.g.. zeta potential.

iii) For sub-microscale modelling use the fluctuating Navier Stokes Equations (e.g. https://ccse.lbl.gov/index.html)

The STL surface file consists of a well-conditioned triangulation.

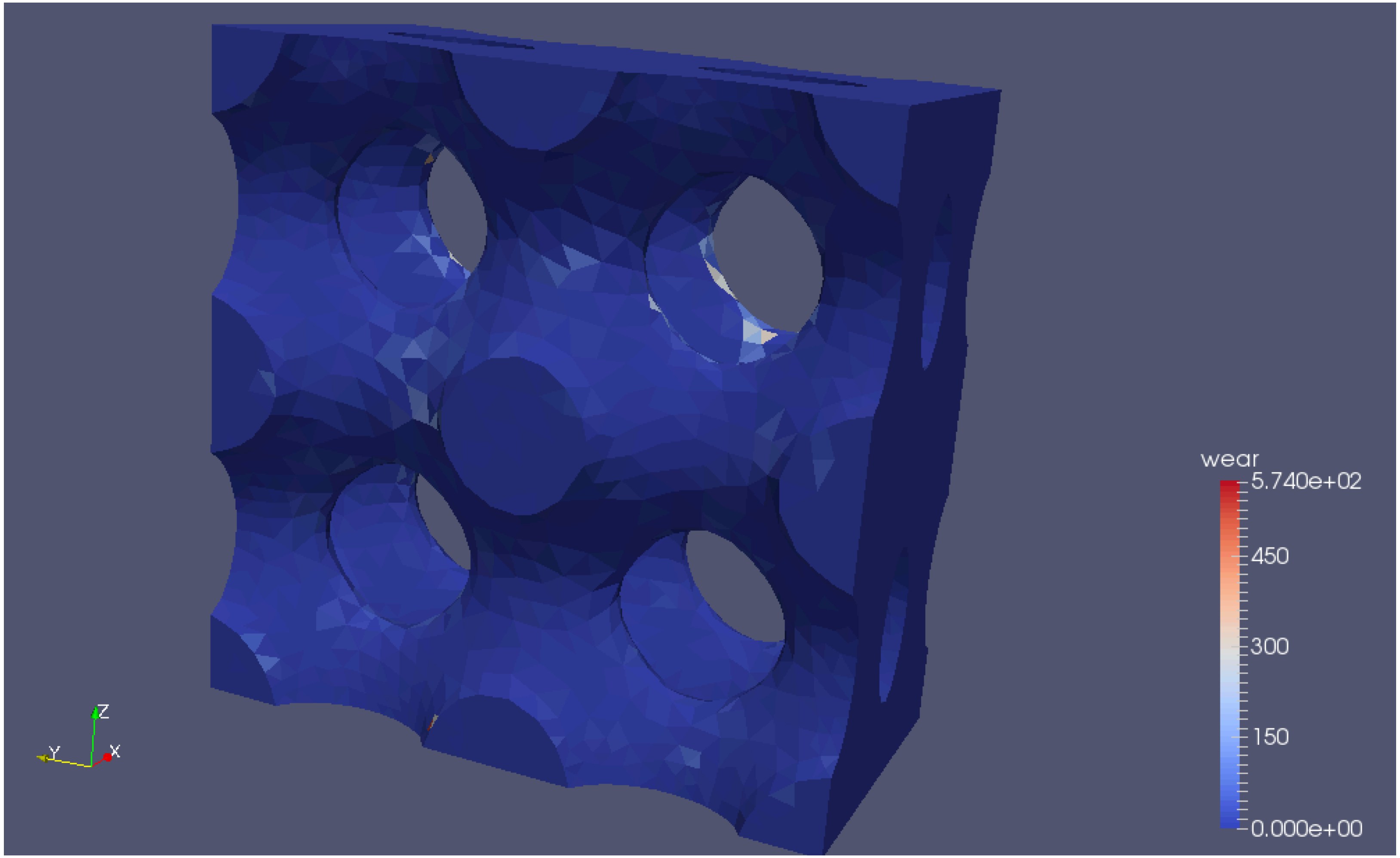


8.1. Micro-filter – image



8.2. Micro-filter – post processing

CFDEM's "Finnie Wear Model" implementation will predict the rate of mass loss [kg/m^2] from a target surface.



9. Dusty Tornado (lenghscale ~ 1m)

Finest mesh resolution: ~1mm

Mesh size: ~2M cells

Number of processors:16

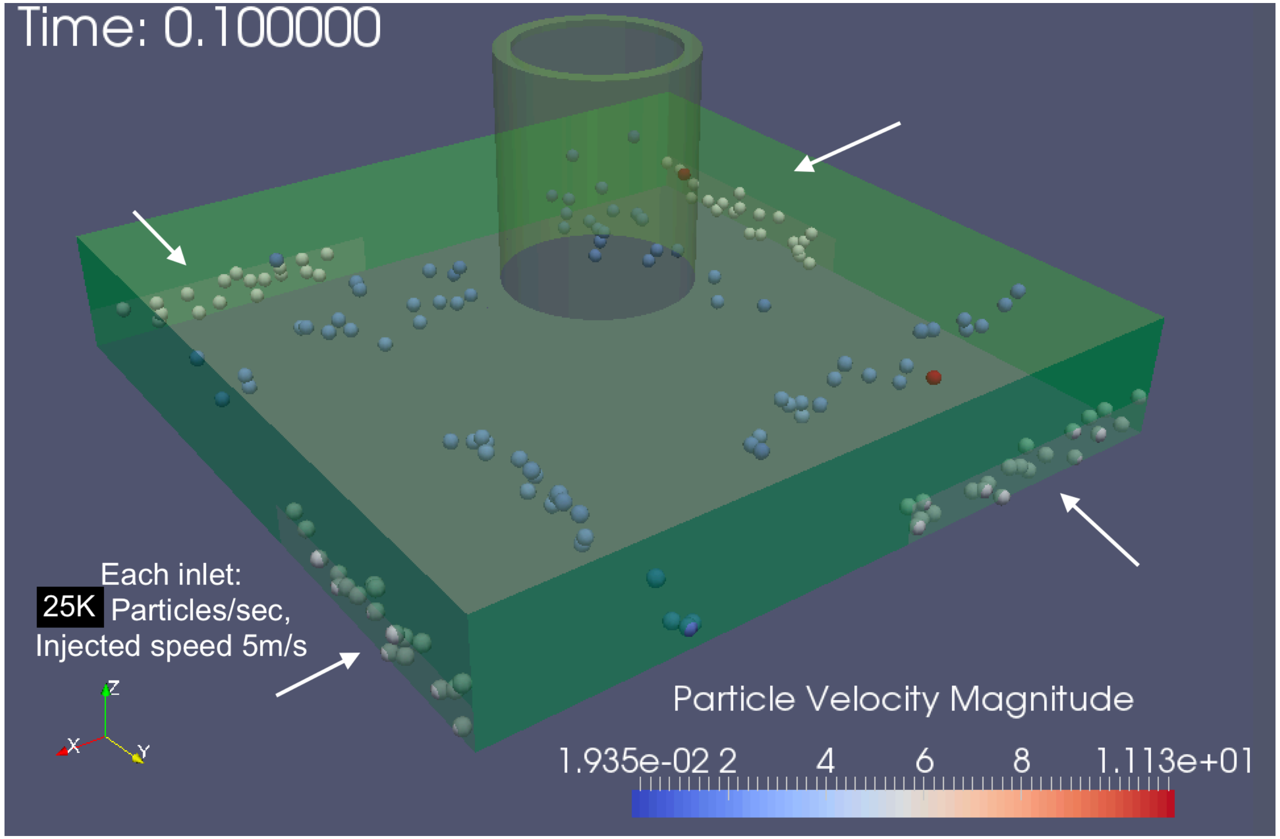
Particles: 125K

Particle radius: 0.25mm

Inlet Air Speed: 5m/s

Execution time 12hrs

(simulating t=1s)



Reference: "A Trial of Generating a Tornado-like Vortex by Large Eddy Simulation", Annals of Disas. Prev. Res. Inst. Kyoto Univ. No. 51B, 2008. Maruyama, T.

Single-phase turbulence models for dense dusty flows becomes uncertain with CFDEM. Experimental validation required.

10. Dusty flow over a car in a wind tunnel (lengthscale ~ 5m).

Mesh size: ~10M cells

Number of processors:16

Particles: 2.5K

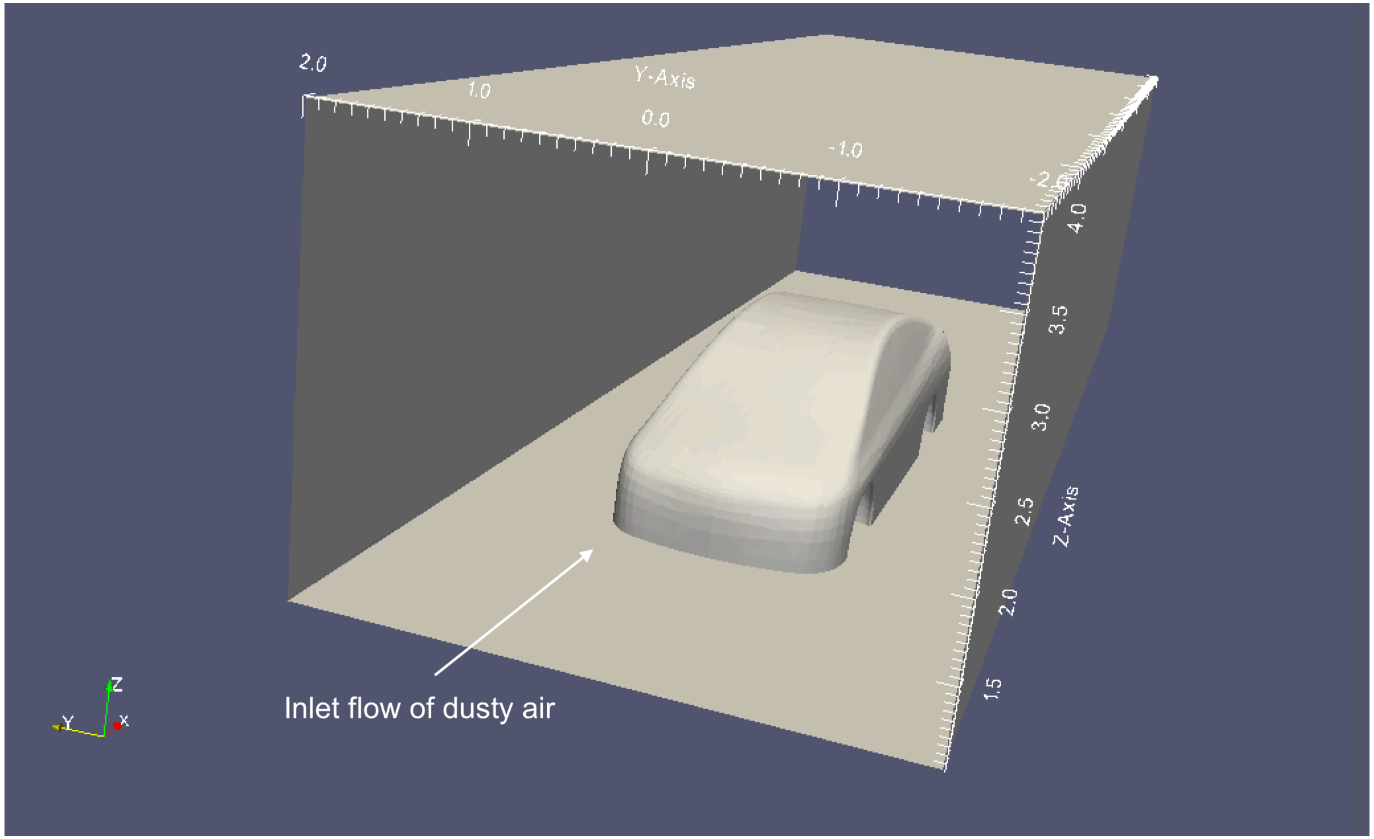
Particle radius: 0.5cm

Particle inlet flow speed: 5 m/s

Air inlet flow speed: 30 m/s

Execution time 12hrs

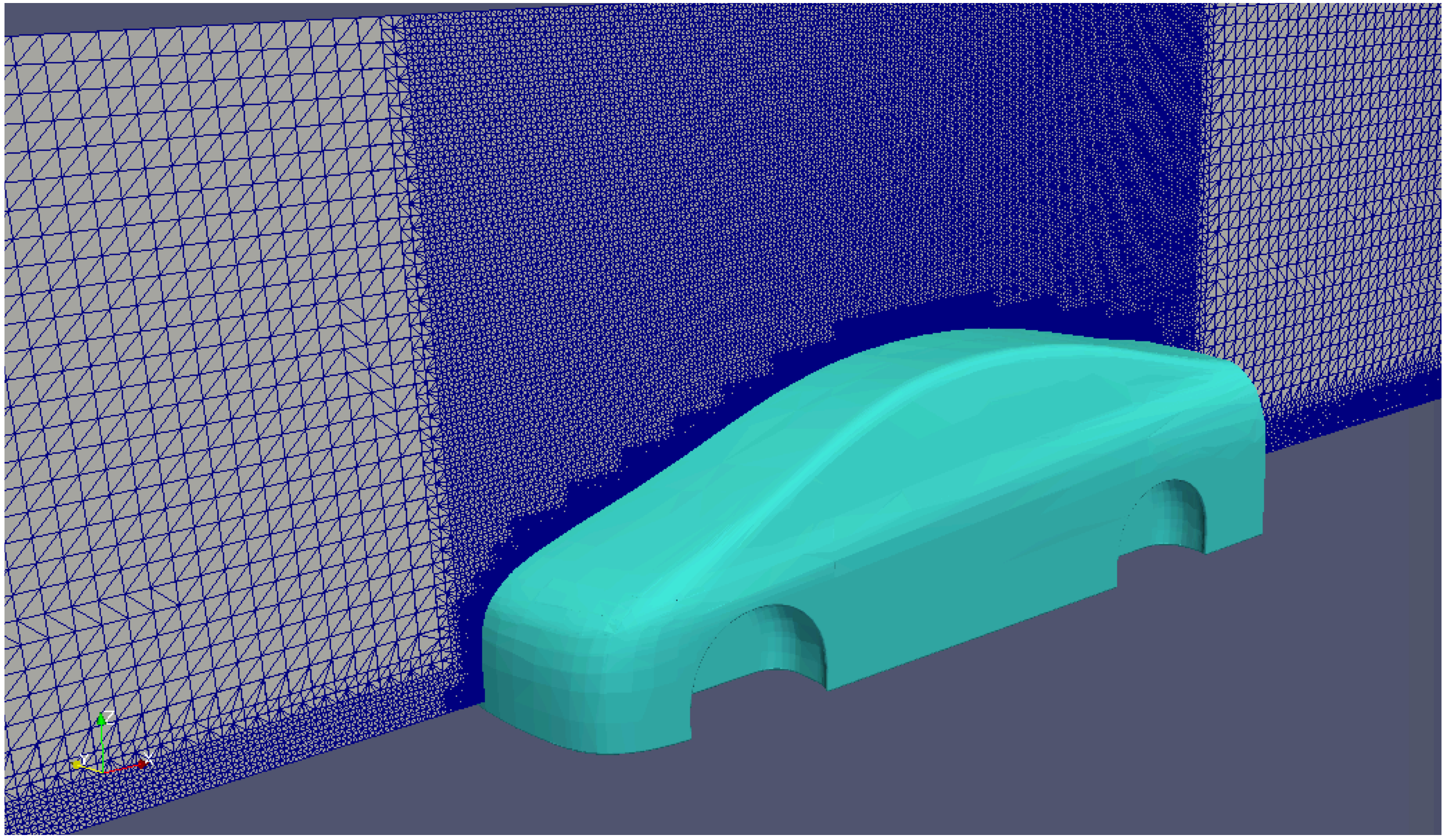
(simulating t=0.5s)



Similarly to the tornado cases, the eddies of traditional single phase turbulence models are likely to be damped at high particle concentrations (see end). If we accept this limitation we might hope to estimate the effect of dust impacts on a car, for example.

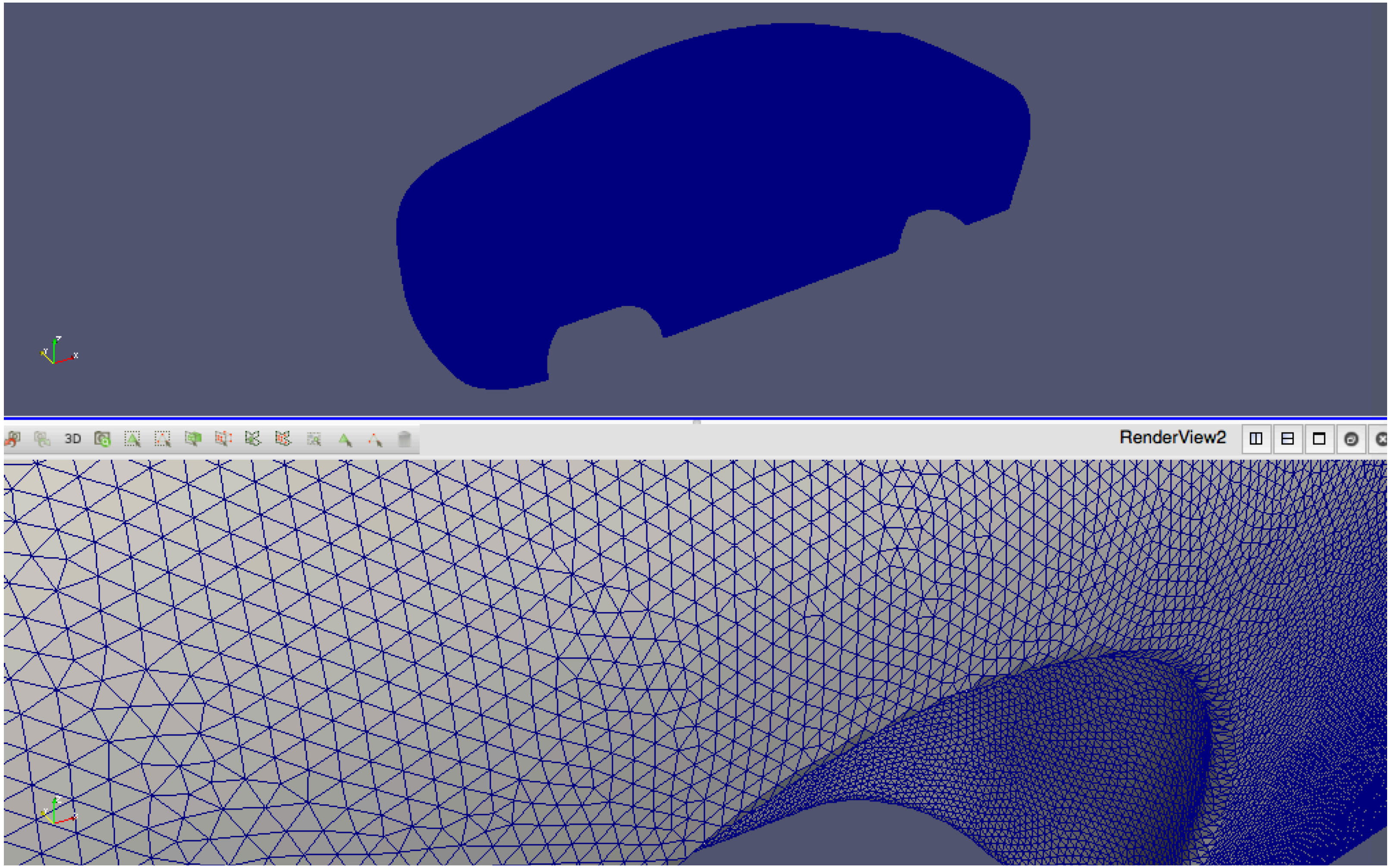
10.1 Dusty flow over a car (lengthscale ~ 5m)

A simple mesh is employed using a reasonable resolution for the car STL.

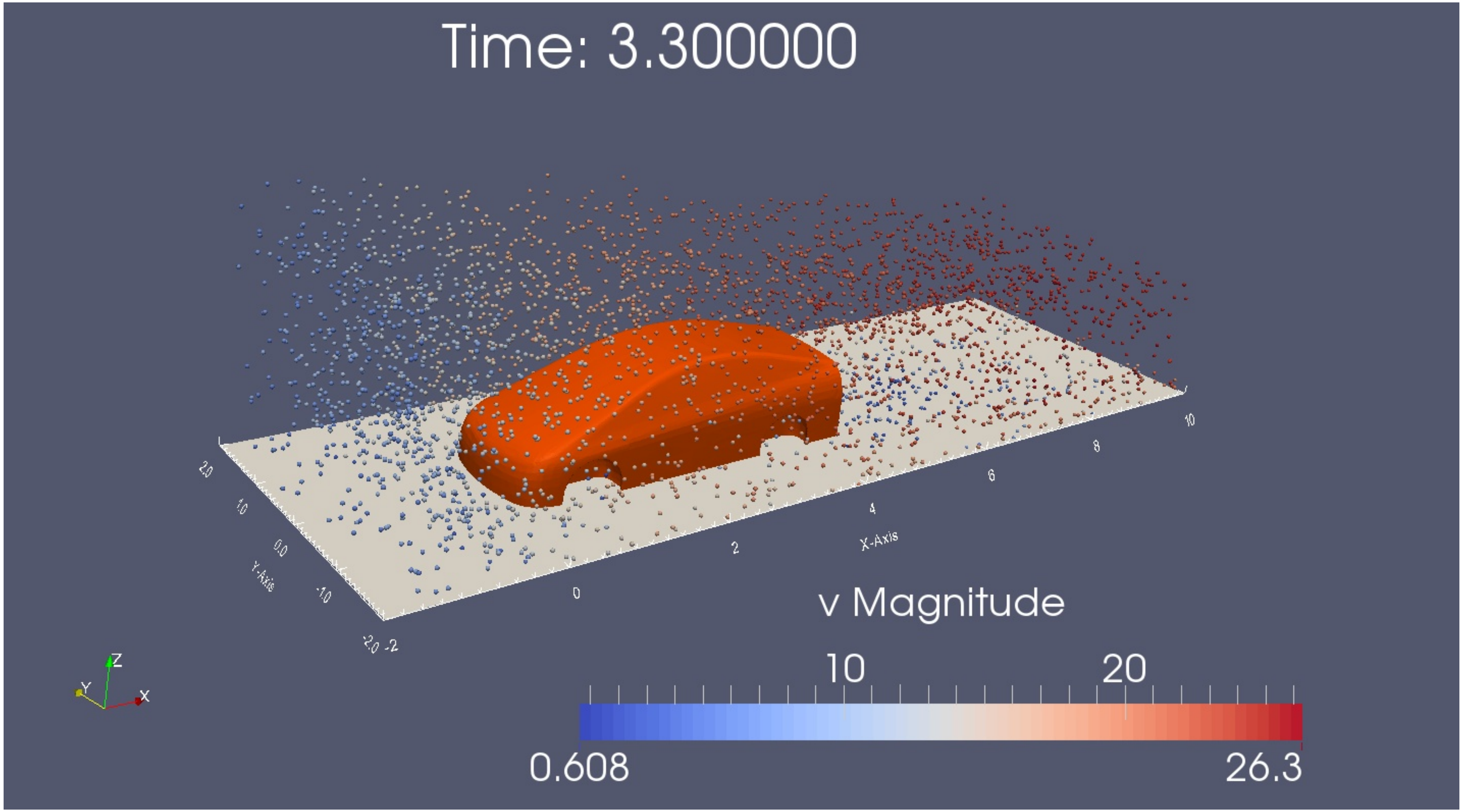


10.2 Dusty flow over a car (lengthscale ~ 5m)

CFDEM requires a well-conditioned STL (triangulation consists of triangles of aspect ratio close to unity). (You can use "foamToSurface -tri" to do this if necessary)



10.3 Dusty flow over a car – image (1)



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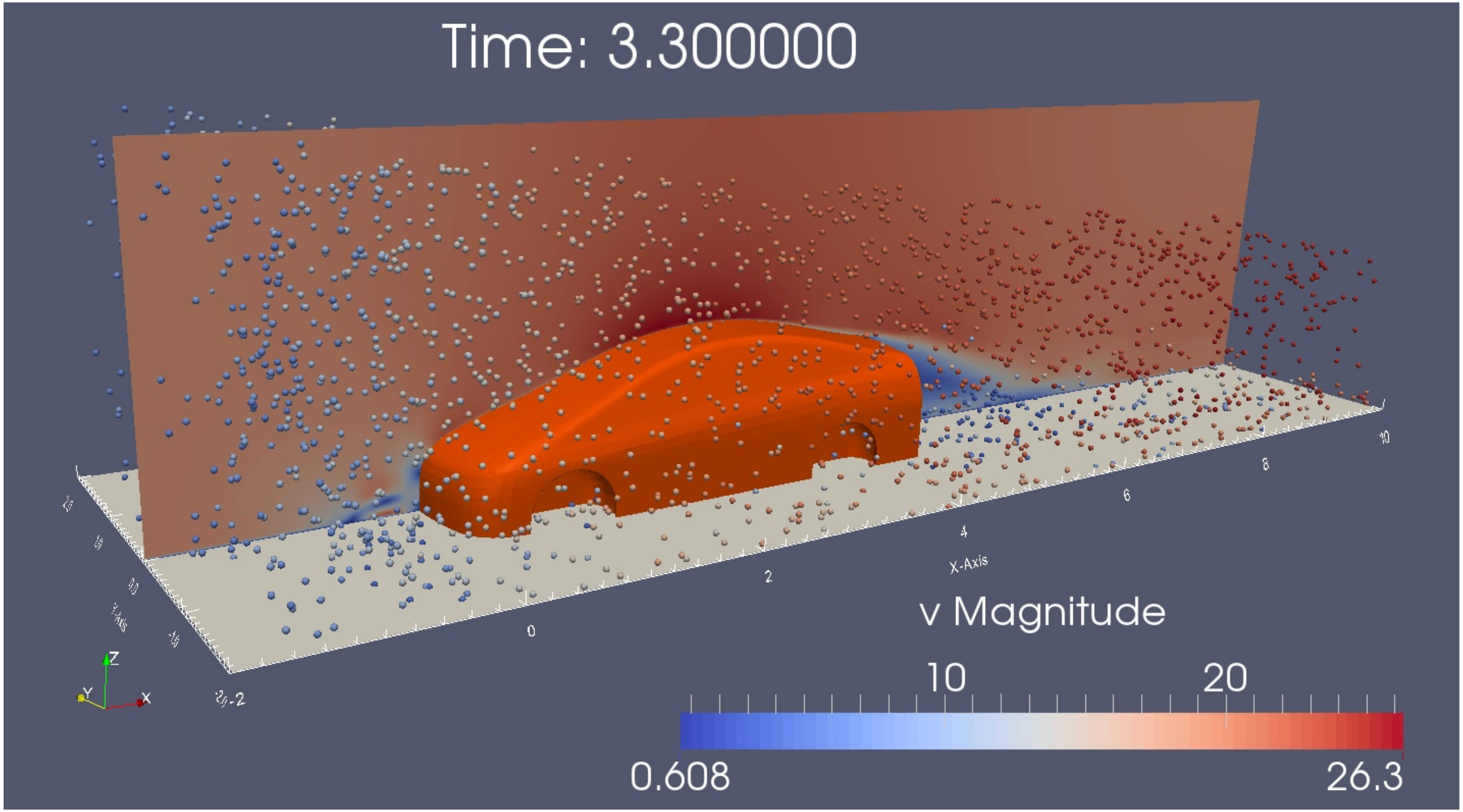
10.4 Dusty flow over a car – image (2)



Final Remarks:

1) Key Points for successful CFDEM computations:

a) Employ well-conditioned STL surface mesh for impact assessment.

b) Ensure the DEM timescale is small enough to allow for accurate collision modelling.

c) Activate CFDEM's "Big Particle" model when particle sizes might be larger than some mesh cells (e.g. in boundary layers).

2) CFDEM Issues:

a) At large particle speeds and densities the single-phase fluid turbulence models are no longer sufficient. Extending these to mixed flows is an active area of research.

An OpenSource (and OpenFOAM compatible) project to study such flows can be found at:

www.openqbmm.org

"An opensource implementation of Quadrature-Based Moment Methods".

OpenFOAM®実用化をサポート

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お問合せは下記までお願い致します。

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