

Evaluation of coarse graining strategy and degree in DEM-CFD simulations of cyclone flow

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Detailed modelling of cyclones

Requirements for cyclone modelling

- Capture gas-solid complex swirling flow
- Model particle-wall and particle-particle collisions to obtain solids accumulation and descent
- Consider particle pickup by the upflowing vortex (inefficiency)
- Take polydispersion into account

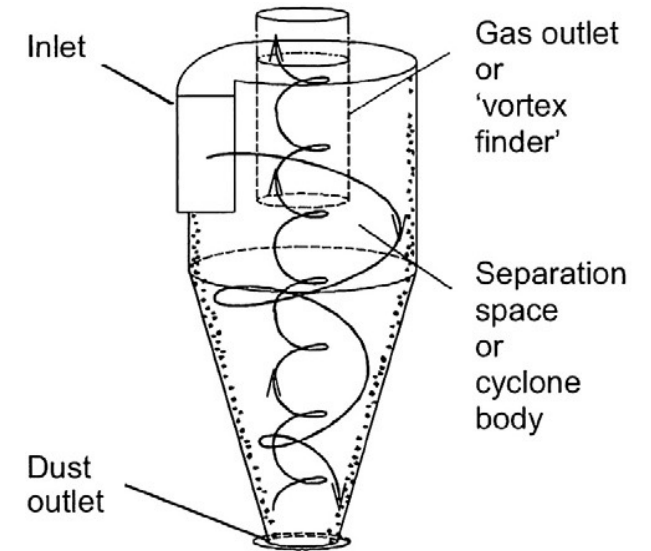
DEM is attractive for its ability to provide detailed and good collision representation. DEM-CFD applied to large particle DMC (Chu et al., 2016)

For the industrial scale, e.g. 1 m barrel diameter, 15 m/s inlet velocity, 0.2%vol loading of 100 μm particles:

No. of particles/sec $\sim 10^9 \div 10^{10}$ (UNFEASIBLE)

- **AIM: Explore whether *coarse-grain* DEM can be a solution**

Chu K., Chen J., Yu A.B., *Min. Eng.* (2016)



Modelling fluid-particle flow using DEM-CFD

Lagrangian discrete elements (**DEM**)

$$m_i \frac{d\mathbf{v}_i}{dt} = \sum_{j=1}^{N_c} \mathbf{f}_{c,ij} + \mathbf{f}_{d,i} + \mathbf{f}_{b,i} + \mathbf{f}_{g,i}$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_{j=1}^{N_c} \mathbf{T}_{c,ij}$$

Hertz-Mindlin contact

Di Felice drag model

Eulerian local-average Navier-Stokes (**CFD**)

$$\frac{\partial \varepsilon \rho_f}{\partial t} + \nabla \cdot (\varepsilon \rho_f \mathbf{u}) = 0$$

$$\frac{D \varepsilon \rho_f \mathbf{u}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \mathbf{F}_{fp} + \varepsilon \rho_f \mathbf{g}$$

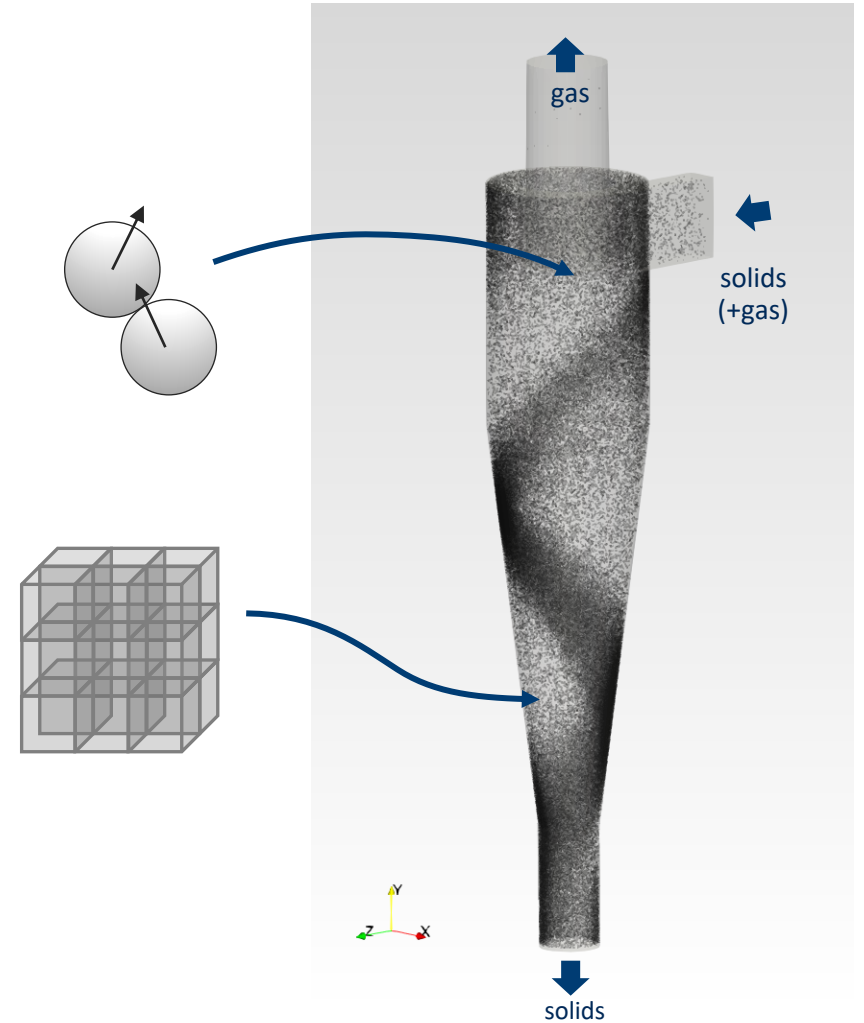
$$\mathbf{F}_{fp} = -\frac{1}{\Omega} \sum_i (\mathbf{f}_{d,i} + \mathbf{f}_{b,i})$$

MFiX DEM

v. 18.1.5

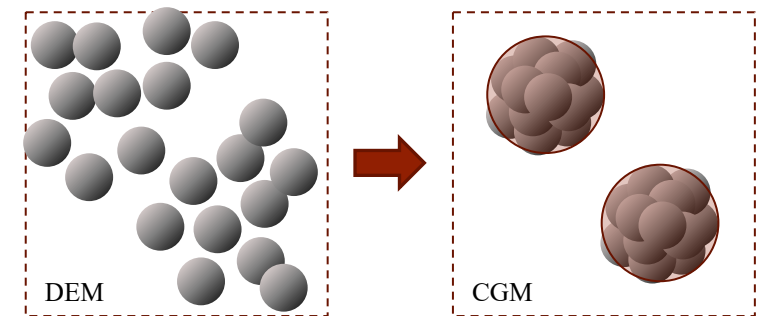
<http://mfix.netl.doe.gov/mfix/>

+ own implementations



Coarse-grain methodology

- Principle of CG-DEM:
DEM particles lumped into f times bigger, representative computational grains (*parcels*)
- Concept: still discrete entities with scaled, *equivalent* properties.
- Preservation of total gravitational and fluid-particle force, of translational and rotational kinetic energy before/after collisions, including dissipation.
- Original derivations (but many subsequent users)



Particles in a CFD cell

Grains (*parcels*) in the same cell

Paper	Concepts	Application
Kuwagi et al. (2004)	“Similar particle assembly” (SPA)	Fixed and fluidized beds of free and cohesive particles
Sakai and Koshizuka (2009)	Coarse-graining based on energy preservation	Pneumatic conveying – linear contact model
Bierwisch et al. (2009)	Coarse-graining based on stress and energy preservation	Cohesive powder flow in cavity filling – Hertz with cohesion (JKR-like) model
Hilton and Cleary (2012)	Similar to SPA with rotation by Sakai	Bubbling fluidized beds

Kuwagi, Takeda & Horio, *Fluidization XI* (2004)
 Sakai & Koshizuka *Chem. Eng. Sci.* (2009)
 Bierwisch et al. *J. Mech. Phys. Sol.* (2009)
 Hilton & Cleary, *9th Int. Conf. CFD in Min. Proc. Ind.* (2012)

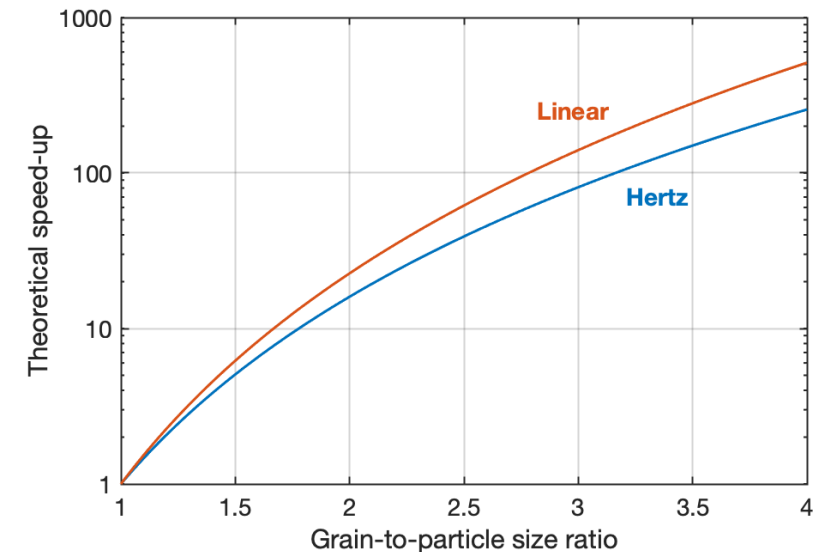
Modelling using *coarse-grain* DEM-CFD

Advantages

- Highly reduced computational cost
 - The total number of particles depends on the cubic power of the grain-to-particle size ratio
 - Also, the contact time (limiting the integration time step) scales positively
 - Reported overall speed-up of $O\left(\frac{d_G^{4.5}}{d_P}\right)$ for the linear contact model and $O\left(\frac{d_G^4}{d_P}\right)$ for Hertz-based model.
- Still detailed results

Disadvantages

- Loss of fidelity (to be quantified)
- Need for sub-grain corrections?

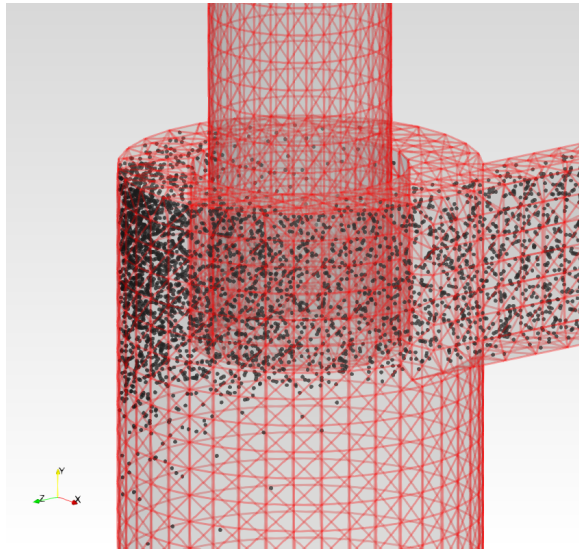


Modelling cyclones flow using DEM-CFD

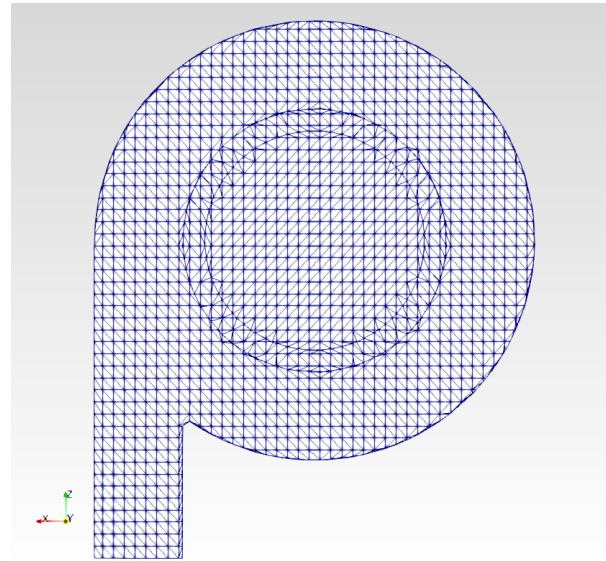
Fluid flow limited by grid resolution:

Compressible, *no turbulence* (but *gas-particle interaction accounts for high-Re flows*)

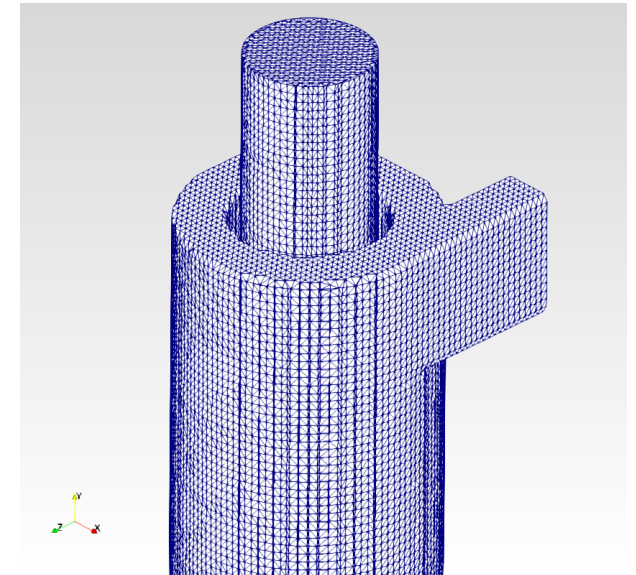
Complex geometry:



Particle contacts with triangulated surface (STL)



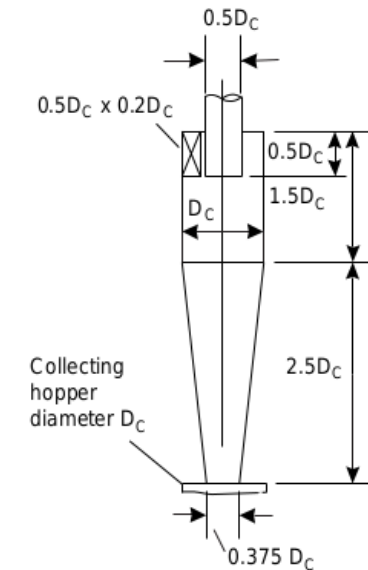
Cartesian cut-cell technique (113k cells)
for the gas phase flow



Testing the *coarse-grain* DEM-CFD on cyclone

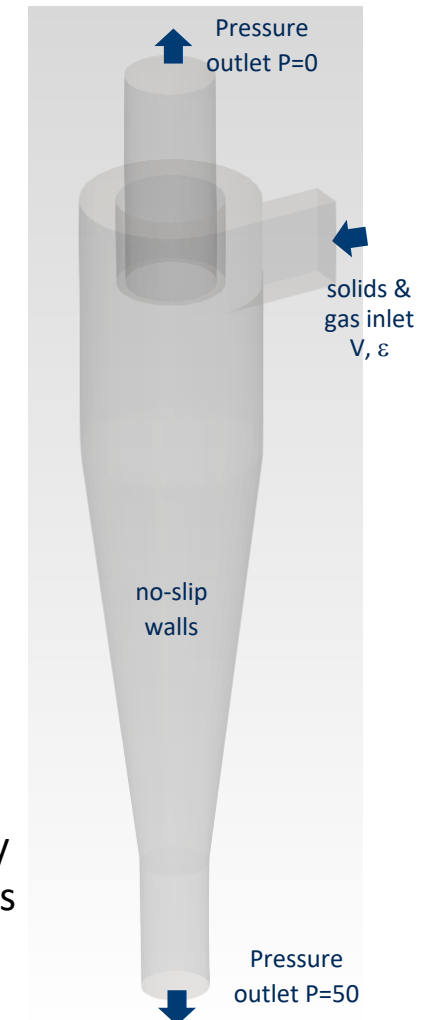
Simulated lab-scale tangential (Stairmand HE) design

Cyclone type/size	Stairmand high efficiency/ $D_{\text{barrel}}=90$ mm			
Tangential inlet (width × height)	18 × 45 mm (0.2D × 0.5D)			
Grid size (diameter × height)	2.5 × 3 mm			
Particle properties	$D = 500 \mu\text{m}$, $\rho = 2500 \text{ kg m}^{-3}$			
Contact model	Hertz, $E = 5 \cdot 10^7 \text{ Pa}$, $e_n = 0.9$			
Solids loading (%vol)	0.1%, 0.2%, 0.5%, 1%			
Inlet velocities	10, 14, 20 m/s			
Particle or grain size, d [μm]	500	1000	1500	2000
Particles per grain, NPG [-]	1 (DEM)	8	27	64
Grain-to-particle size ratio	1	2	3	4
Holdup in number of grains, [-]	136k–717k	11k–94k	6k–25k	2.8k–10.6k
Solid-phase time-step, Δt_s [10^{-6} s]	0.6	1.9	3.1	4.1
Fluid-phase (typical) time-step	$5 \cdot 10^{-4}$ s			



Cyclone design

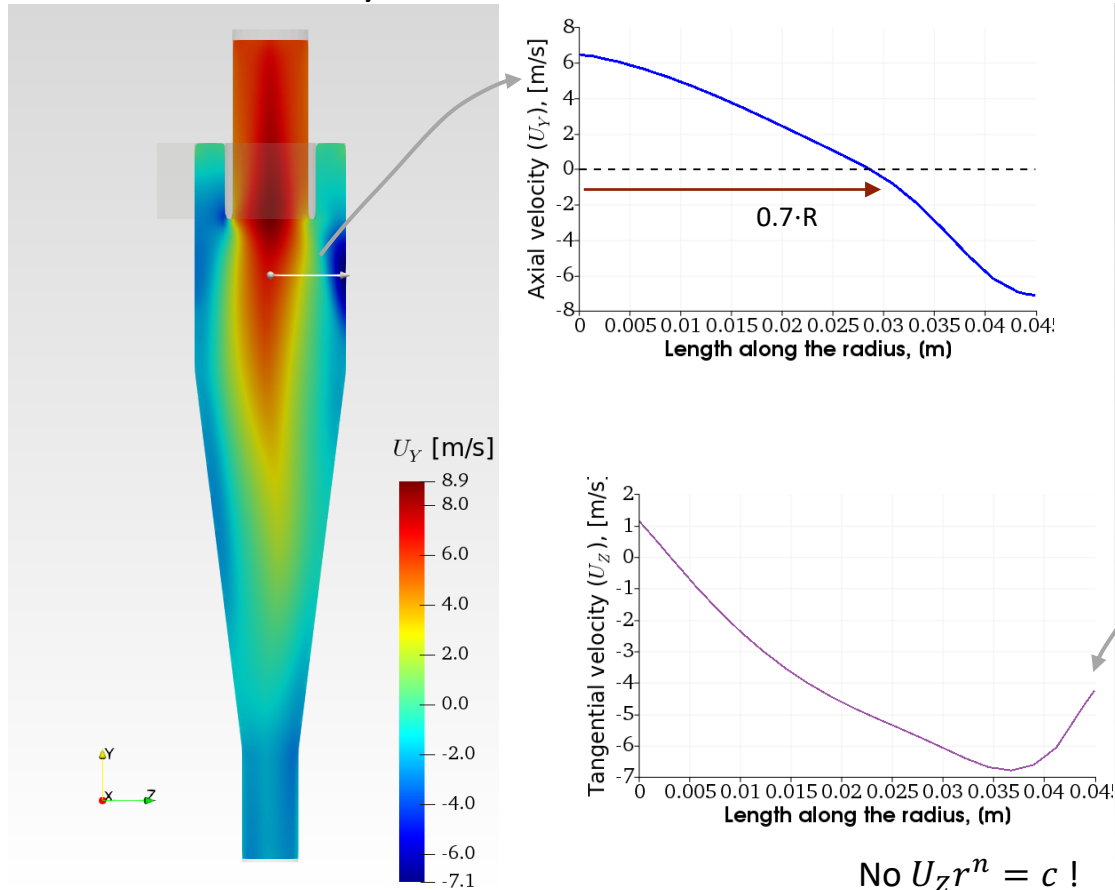
Boundary conditions



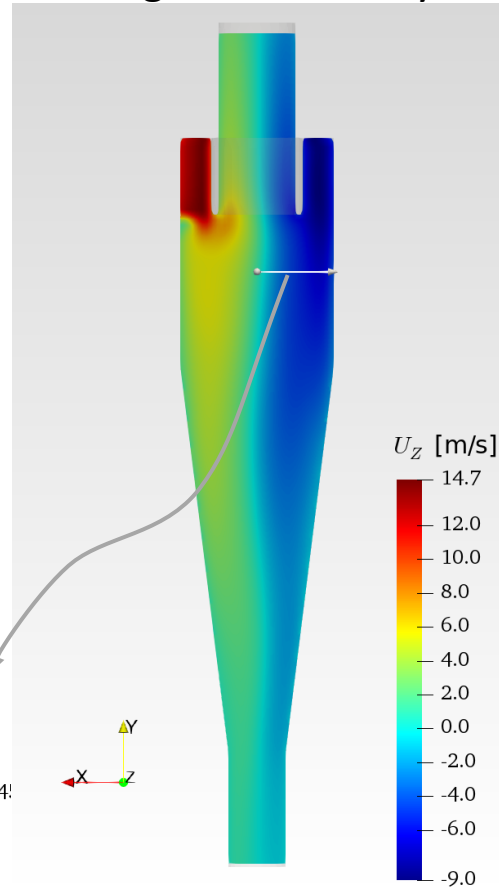
CFD of single-phase fluid flow inside the cyclone

Flow properties at $u_{inlet} = 14$ m/s

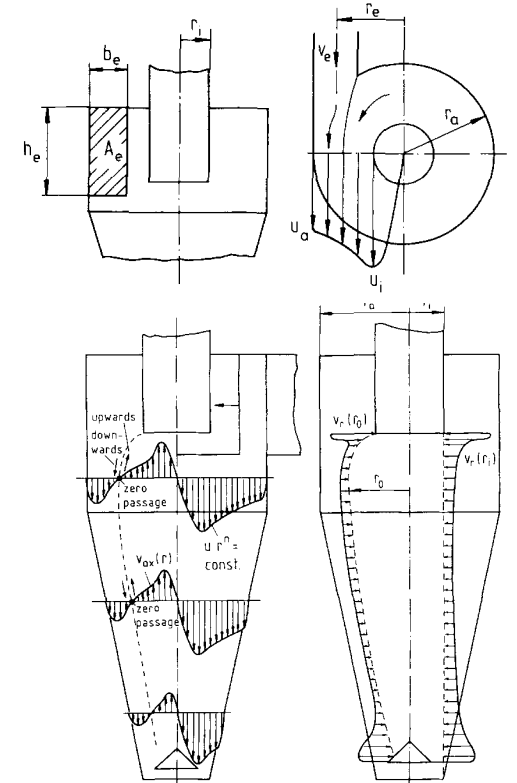
Axial velocity



Tangential velocity



No $U_z r^n = c$!

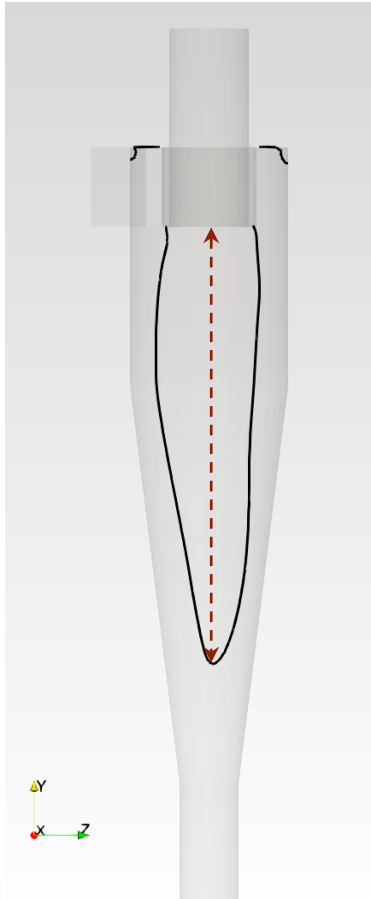


Cyclone theory

Trefz & Muschelknautz, *CET*, 1993

Analysis of the physical features of the flow

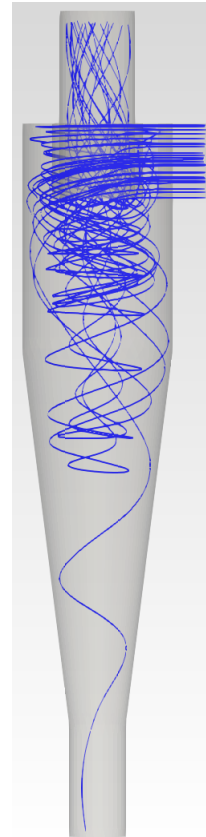
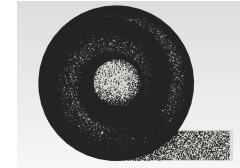
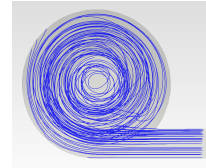
Vortex shape and length



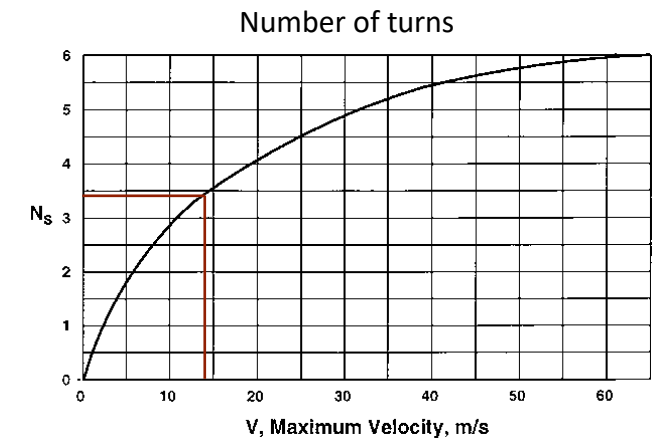
Gas-solid flow



DEM (NPG = 1)
 $\varepsilon_s = 0.5\%$
 $u_{in} = 14 \text{ m/s}$



Strand formation at $\sim 15^\circ$



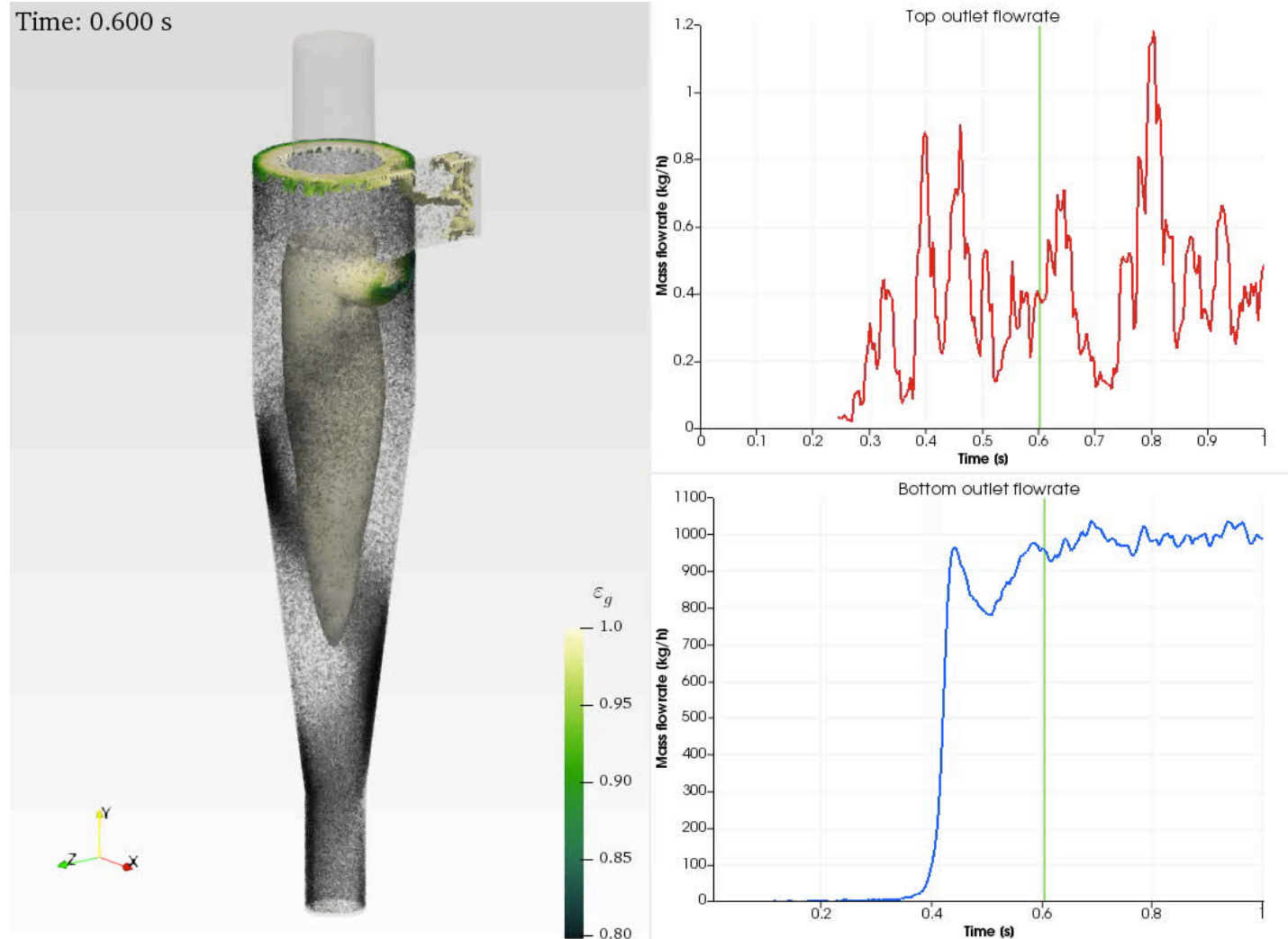
Knowlton, Chap. 22, *Handbook Fl. & F-P systems* (2003)

Two-phase flow dynamics

In the simulations, fluid and particle motions are tracked, with special attention to solids separation

DEM (NPG = 1)
 $\varepsilon_s = 1\%$
 $u_{in} = 14 \text{ m/s}$

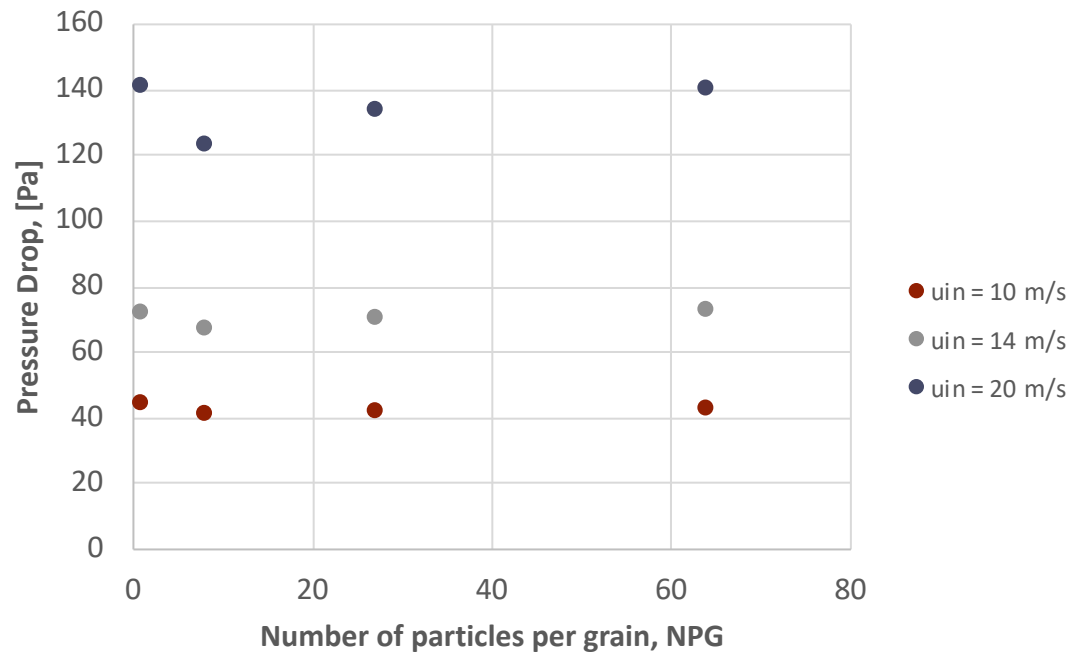
Starting from approximately 0.6 s the cyclone operates steadily



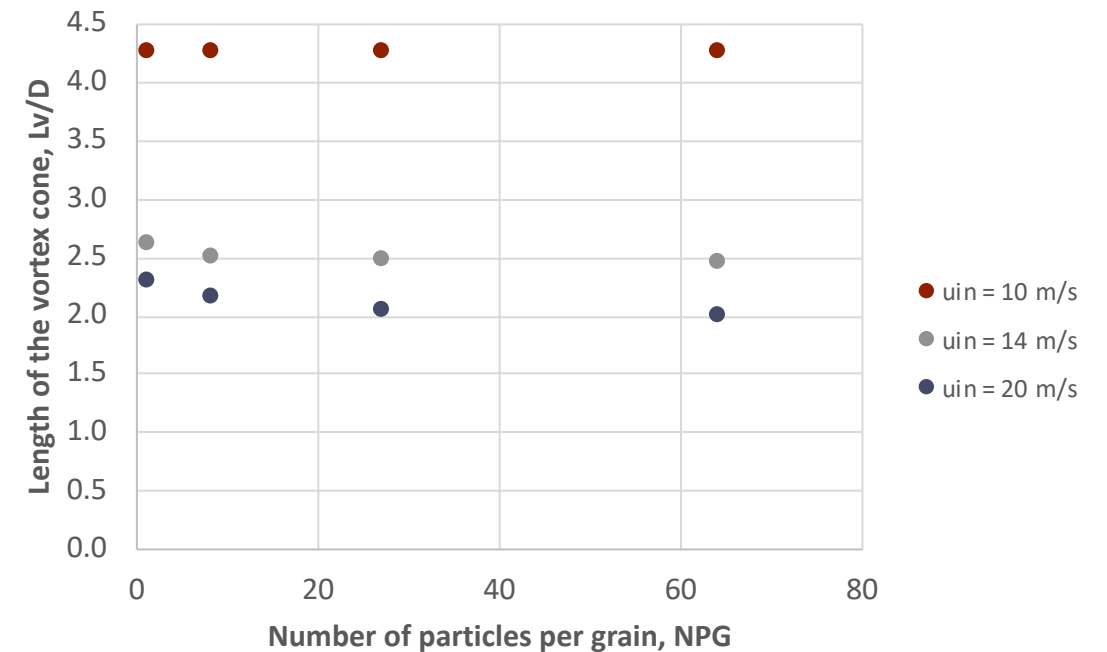
Effect of the coarse graining degree: macro-scale

Loading $\varepsilon_s = 0.5\%$

Pressure drop



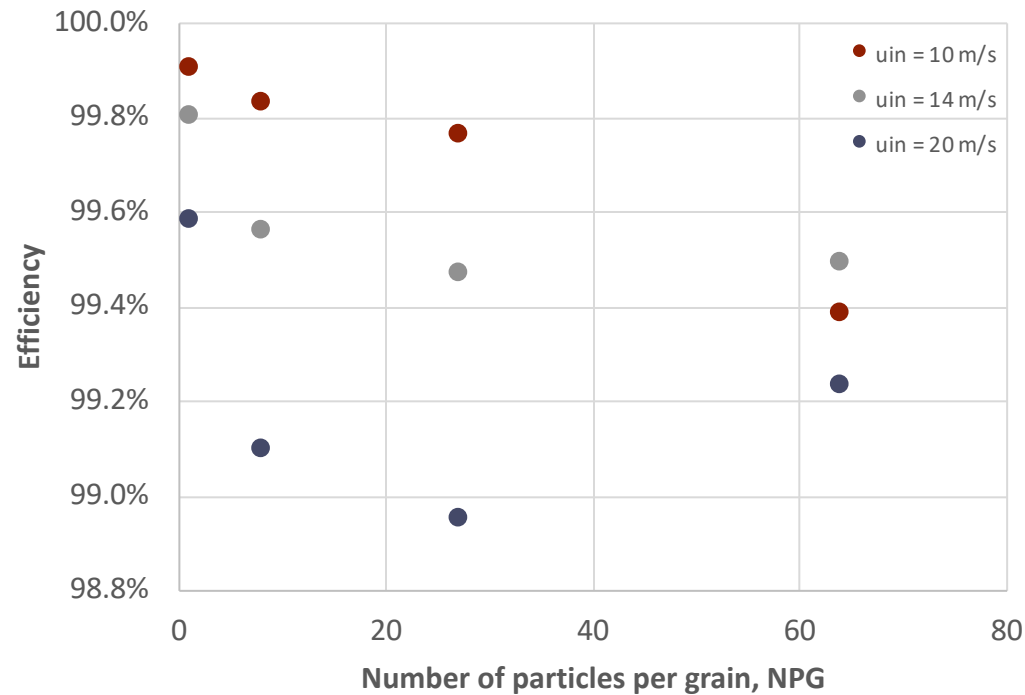
Vortex length



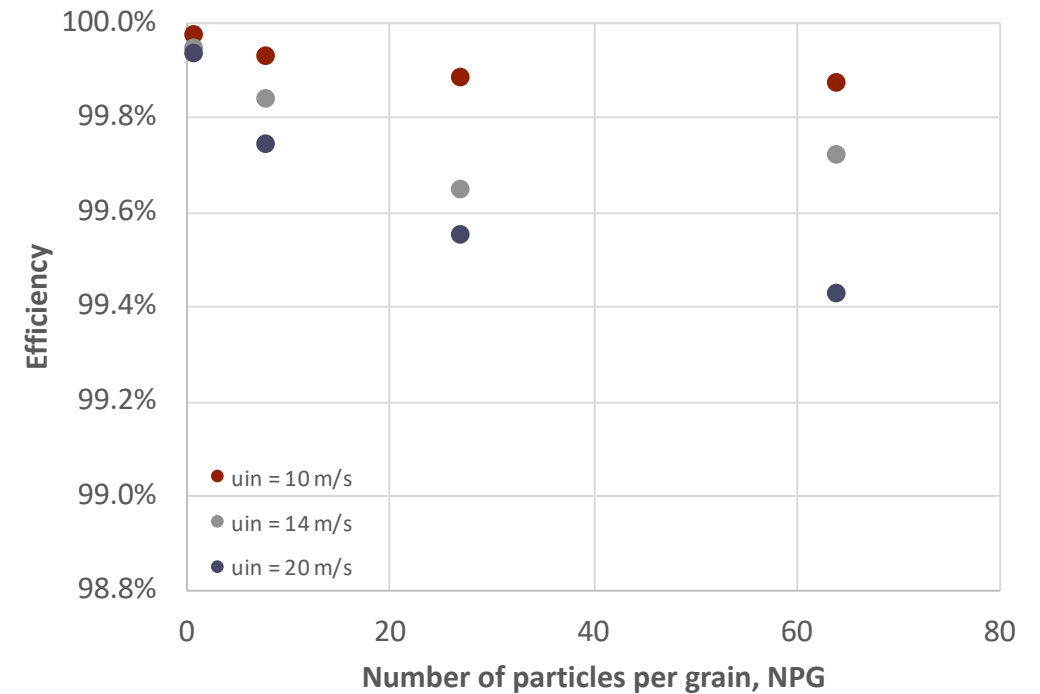
Effect of the coarse graining degree: macro-scale

Overall separation efficiency

Loading $\varepsilon_s = 0.2\%$



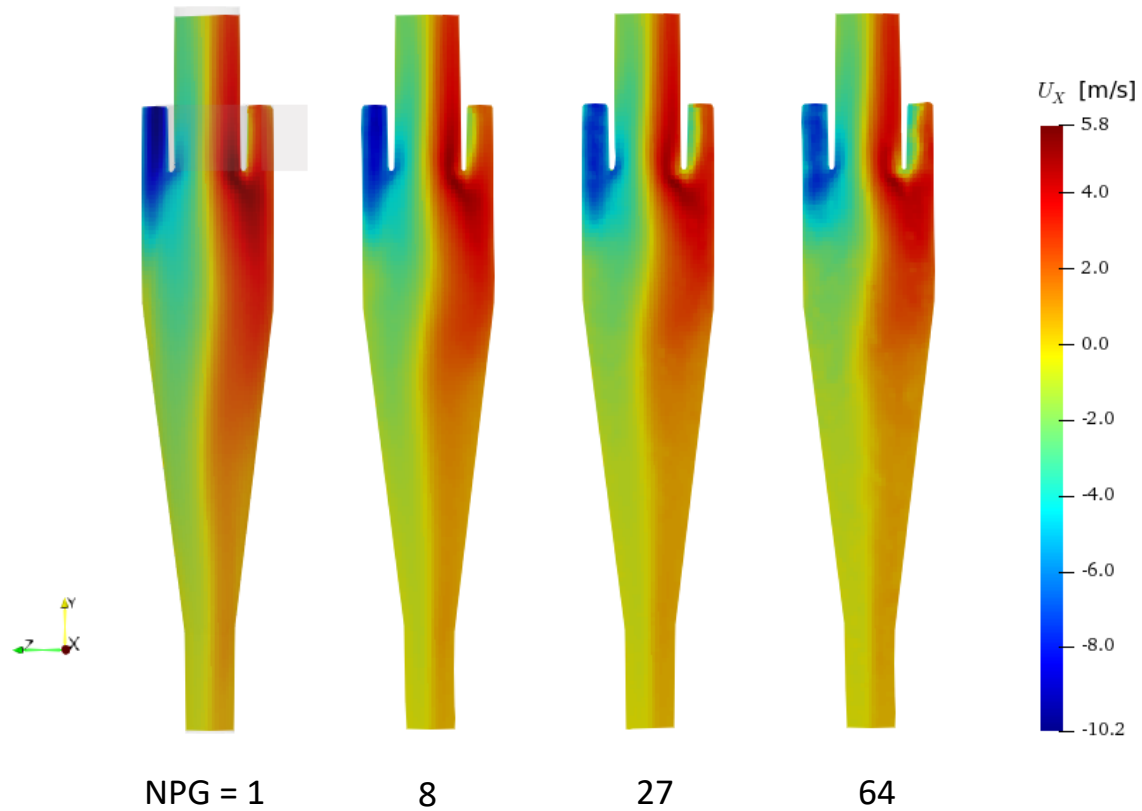
Loading $\varepsilon_s = 0.5\%$



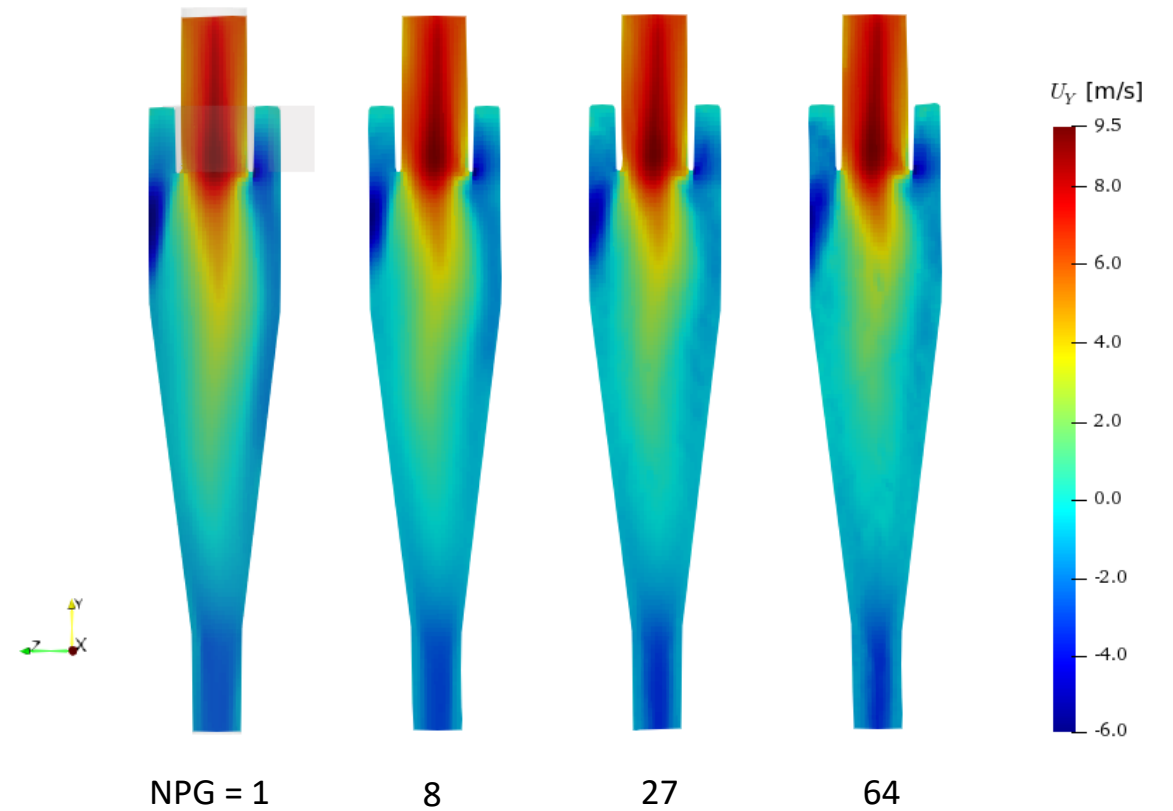
Effect of the coarse graining degree: gas flow

$$\varepsilon_s = 0.5\%, U_{in} = 14 \text{ m/s}$$

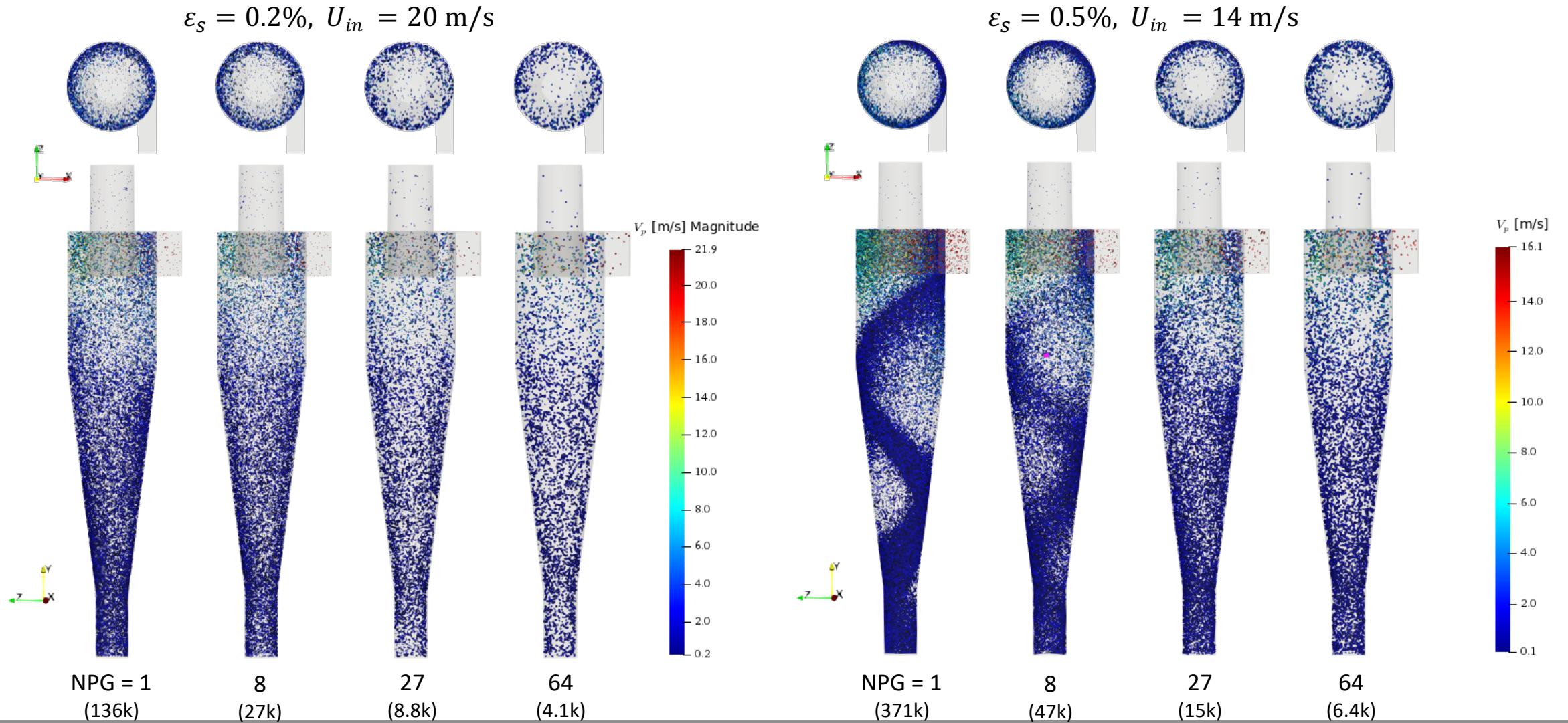
Tangential velocity



Axial velocity



Effect of the coarse graining degree: solids flow



Expected possible applications

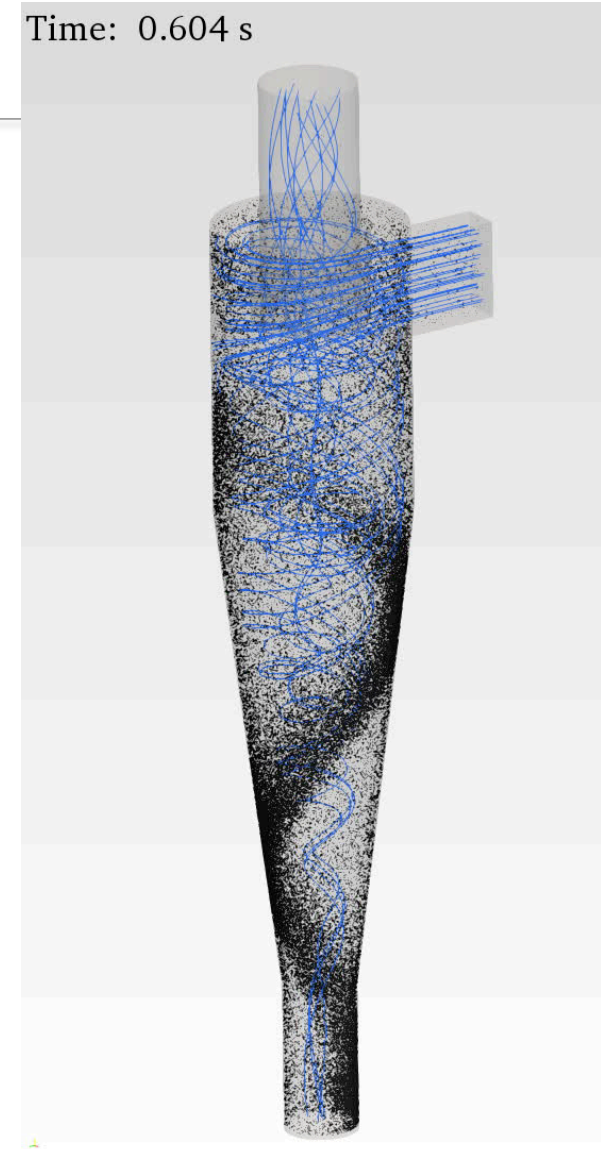
Running test on 9-cm dia. cyclone flow of 125 μm diameter particles with CG factor $f = 4$ ($NPG = 64$).

$$\varepsilon_s = 0.1\%$$

$$u_{in} = 14 \text{ m/s}$$

Steady-state solids holdup of **78600** grains corresponding to **>5M particles**.

Simulation time was **9 h / simulated s** on 32 cores of our cluster.



Conclusions

- Cyclones on the large scale or treating very fine particles is **prohibitive for reasonable DEM-CFD simulations** due to the number of particles and the small time-step.
- Coarse graining DEM particles provides **speedup** with the grain-to-particle size ratio to the **power of 4 or 4.5**, thereby appearing highly attractive.
- Our simulations showed that the physics into the coarse graining method (scaling parameters) is sufficient to guarantee preservation of macroscopic variables – compared to pure DEM – up to CG factor $f = 3$ (NPG=27). However, in one case **the solids flow field appeared deeply modified** (no strands) **already at $f = 3$** , denoting profound differences in the microdynamics of the particles/grains.
- Overall: in DEM-CFD models of cyclones there is a huge potential in CPU-time savings but reasonable accuracy is obtained below $f = 3$, further development and testing at $f = 3$ and beyond is required.

Perspectives

Most important challenges and open problems in CG:

- Fully characterize grain-grain collision and grain-wall collisions
- Develop and test CG parameter rules for rolling friction
- Further test the coarse graining degree to identify limits of applicability and assess how well quantities of interest are preserved
- Develop and test a reliable CG method for polydisperse solids, possibly with reaction and heat/mass transfer