Discrete Element Method in STAR-CCM+

Material Presented at STAR Korean Conference 2012

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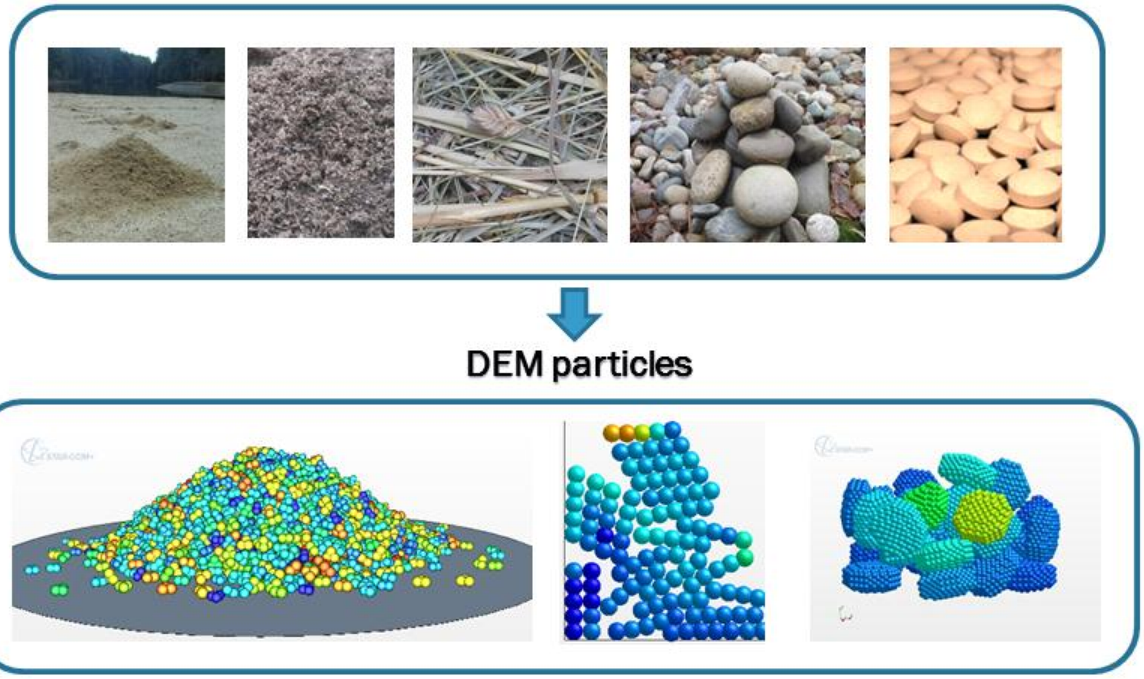
Introduction

Discrete Element Method (DEM) is used to simulate particle flow. Particles are everywhere around us: Dirt, sand, pebbles, grains, hay, minerals, ores, manufactured materials like tablets, powders, etc.

DEM is about modeling behavior of particles of different sizes and shapes. In this presentation the DEM capabilities in STAR-CCM+ software are discussed and illustrated by simulation examples. The presentation is structured as follows. First, the particle flow regimes that are most suitable for DEM are discussed, as well as advantages of DEM compared to other Multiphase methods for modeling solid flow. The properties and types of DEM particles defined in STAR-CCM+ are discussed next, followed by discussion of contact models. Finally, the details of integration of DEM in STAR-CCM+ are illustrated on the examples involving 1-way and 2-way coupling with CFD.

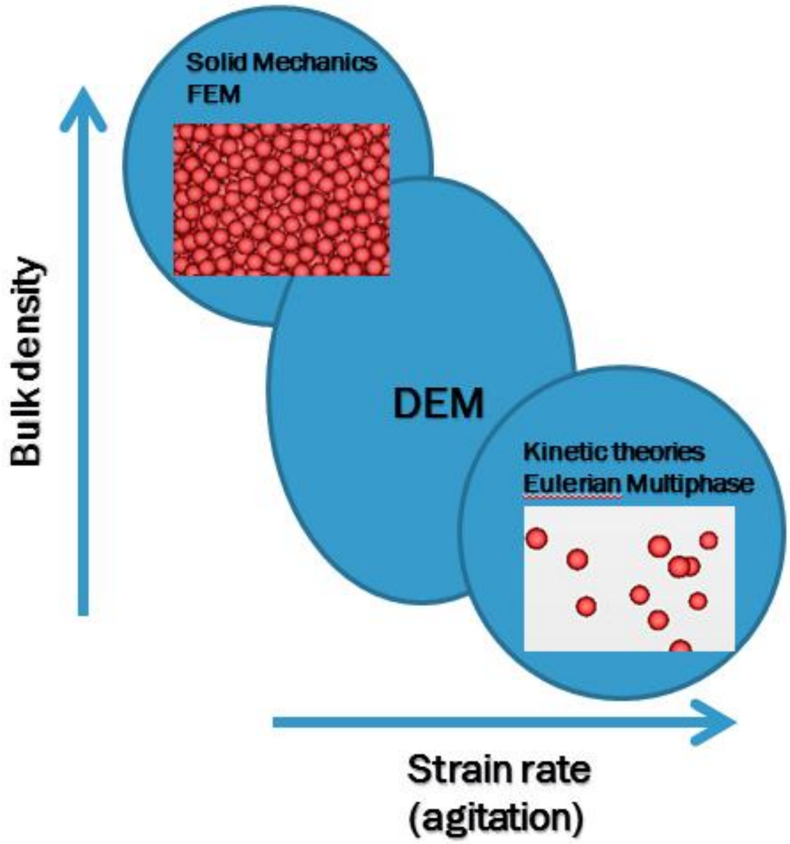


DEM overview

DEM was established in 1979 by P.A. Cundall, O.D.L. Strack as a method that can simulate motion of large number of discrete objects, particles. Within this method the state of each particle is calculated using classical mechanics. For particles, both translational and rotational degrees of freedom are resolved. Energy is dissipated during the collisions between particles.

DEM method requires small integration timesteps to properly resolve surface contacts between particles, so DEM calculations are CPU intensive. No mesh is required for DEM. In applications to granular flows DEM provides granular bulk state solution which results from particle interactions and detailed resolution other method cannot archive. No constitutive relations are used in DEM and the results can be interpreted over large range of length scales and time scales.

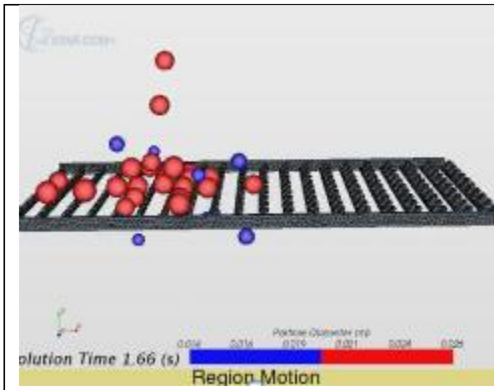
DEM range of applicability

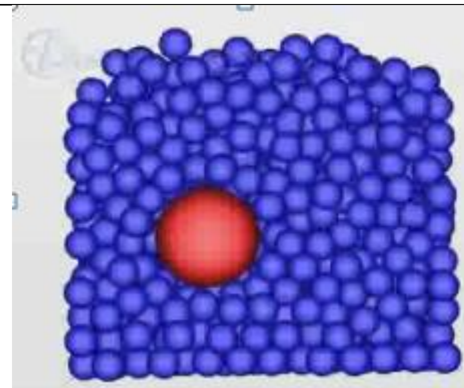


DEM is best method when simulated process has

- Densely packed particles
- Frequent collisions
- Dependence on
    - Particle shape
    - Particle size distribution
    - Particle contact physics: friction, cohesion, etc

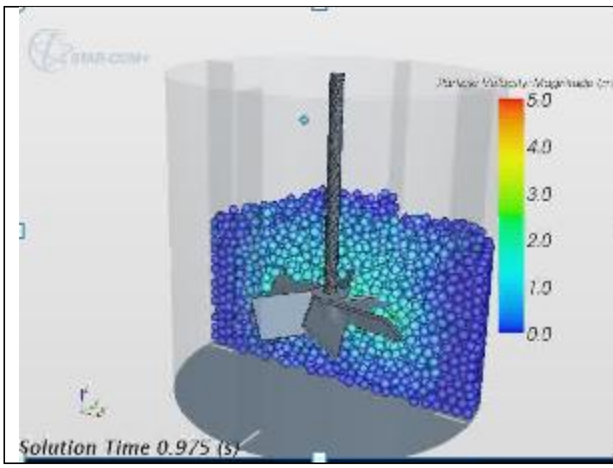
For example, for modeling the segregation of particles by size, DEM is likely the only possible method as in examples of vibratory sieving and 'Brazil nut effect', shown below.





DEM practical CPU time limits

- Less than few million particles
- Less than one minute of Physical Time



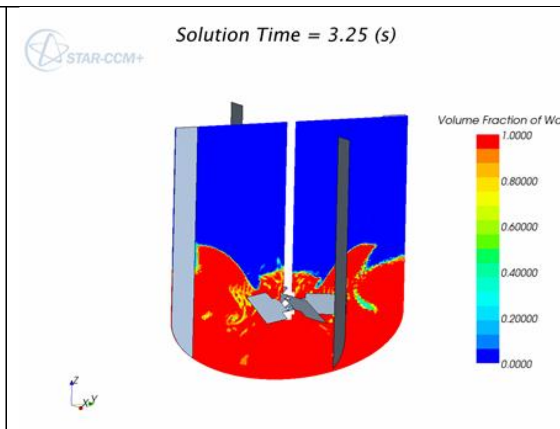
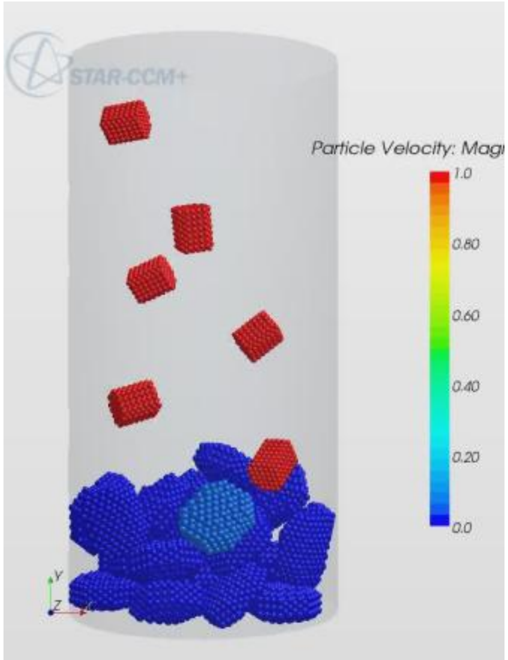


Figure above, left, shows the mixing of dry particles using DEM in the regime were collision determine the bulk flow pattern. In this regime the bulk stress field cannot be predicted by continuum approach. In the same figure on the right the Eulerian multiphase method is used to mix the solid and fluid phase in the same geometry. Eulerian methods are more appropriate for the regimes were particle-particle contacts do not affect the flow significantly.

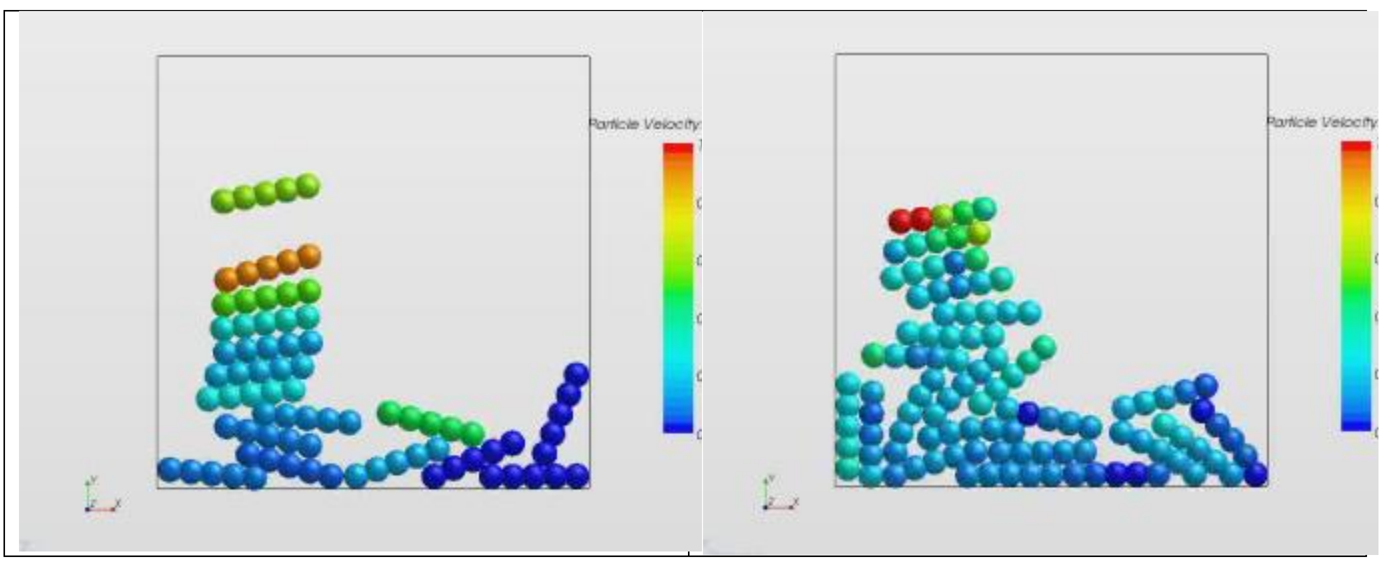
DEM particles

In STAR-CMM+ the DEM particle primitive is sphere. It is ideal for contact detection. Particles are elastic: No permanent deformation happens due to collisions. It is possible, however, modeling the particles of different shapes by creating the particle from gluing spheres together. There are two types of non-spherical particles in STAR-CCM+

- Composite particles
    - Many spheres ‘glued together’ form target shape
    - Particle is rigid and unbreakable, no bending resistance
    - 

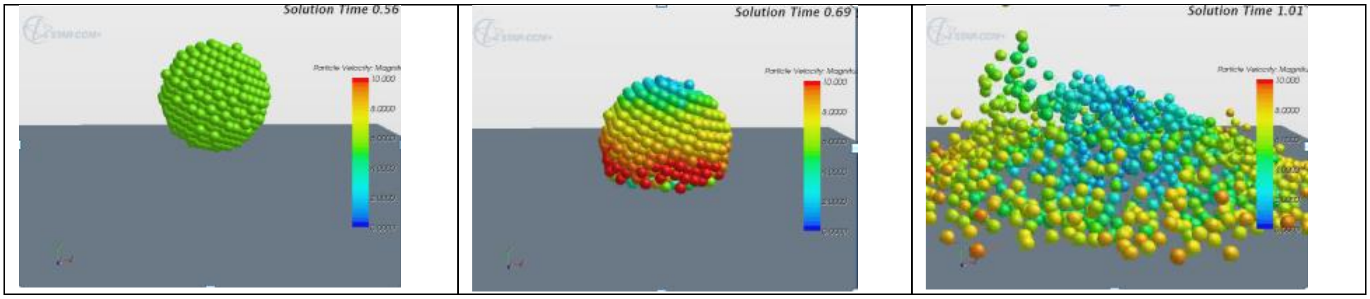
- Clumped partilces
    - Can be elastically deformed
    - Can be broken

Figure below illustrates the difference between composite (left) and clumped (right) particles.



In particular, several clumped particles in the right picture are clearly bended. Unlike in Composite particle, the Bonded Particle model is used to calculate the forces between spheres in Clumped particle.

Clumped particles are breakable. Their user-set properties include: maximum tensile and shear stress, friction, rolling friction, and restitution parameters. The bond breaks when the stress on the bond exceeds maximum, either for tensile or for shear. After breaking, each sphere or ‘chip’ is essentially a new particle.



DEM in STAR-CCM+ details

DEM in STAR-CCM+ is implemented within Lagrangian framework. It reuses the following known concepts

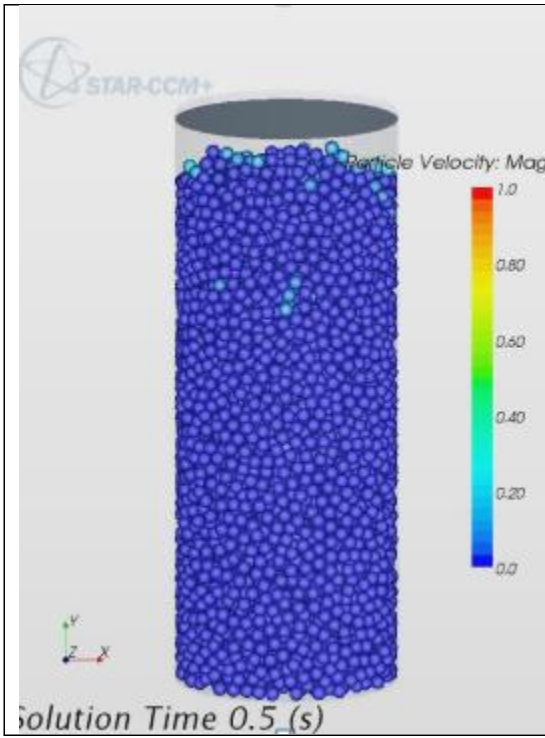
- Lagrangian phase
- Injectors
- Boundary interactions
- Sub stepping of the solution

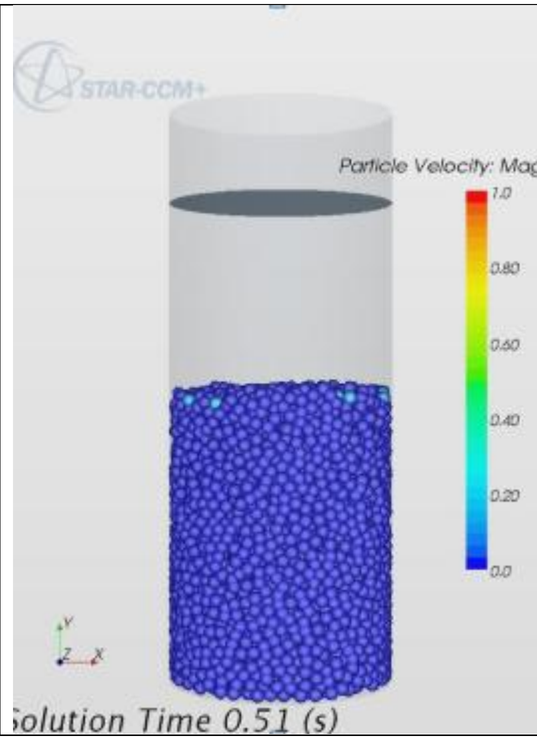
And it extends the concept of Material particle by additional tracking of Orientation, Angular motion, Inter-particle collisions. Soft particle model is used to in resolving collisions: the force is the function of overlap between particles in contact.

Basic contact models

In STAR-CCM+ the basic contact models are Hertz-Mindling and Walton-Braun. Hertz-Mindlin is the default basic contact model most widely used in DEM simulations. It is non-linear model: Force is proportional to the overlap to the power of 3/2. It is based on the classical Hertz theory of contact.

Walton-Braun (WB) contact model is used for modeling particles that can 'plastically' deform. Within WB model each particle can have residual overlap, depending on the history of the contact. The figure below shows two results for simulating filling the container with the same amount of same-size particles. In the first case, shown in left side, the Hert-Mindlin contact models was used, while in the second case, shown in right side, the Walton-Braun model was used.

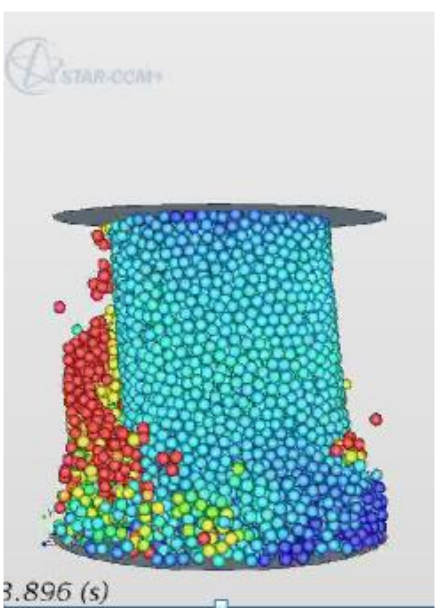




Optional contact models

In addition to basic either Hertz-Mindlin or Walton-Braun model STAR-CCM+ offers the models that allow to simulate consolidated particles. In particular, linear cohesion model can be used for 'sticky' particles. Cohesion model is useful when modeling the cohesive effect of moisture for particle of sizes bigger than 1e-4 m. It also can be used to model the effect of attractive Van-der-Waals forces for powder particles.

Another optional contact model, a bonded particle model, can be used to simulate particles 'cemented together', as in rock. In this model, bond can be broken if the stress on bond exceeds the threshold values. Snapshot from simulation of compression test of the bonded material is shown in figure below.

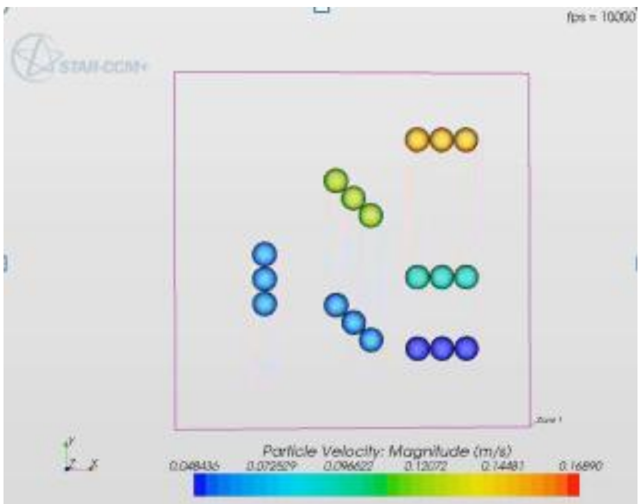


One way coupling with CFD

In STAR-CCM+ the following fluid drag models for DEM particles are available

- Di Felice
- Gidaspow
- Haider Levenspiel
- User defined

Drag model accounts for projected length and area for composite and clumped particles. In figure below the fluid inlet is located at the bottom boundary and the pressure outlet at the top. Particle's velocity depends on the orientation of the particle relative to the fluid field: Particles that are aligned with the fluid flow are moving with the lowest velocity.



In one-way coupling, buoyancy force and pressure gradient force are properly accounted.

Two-way coupling with CFD

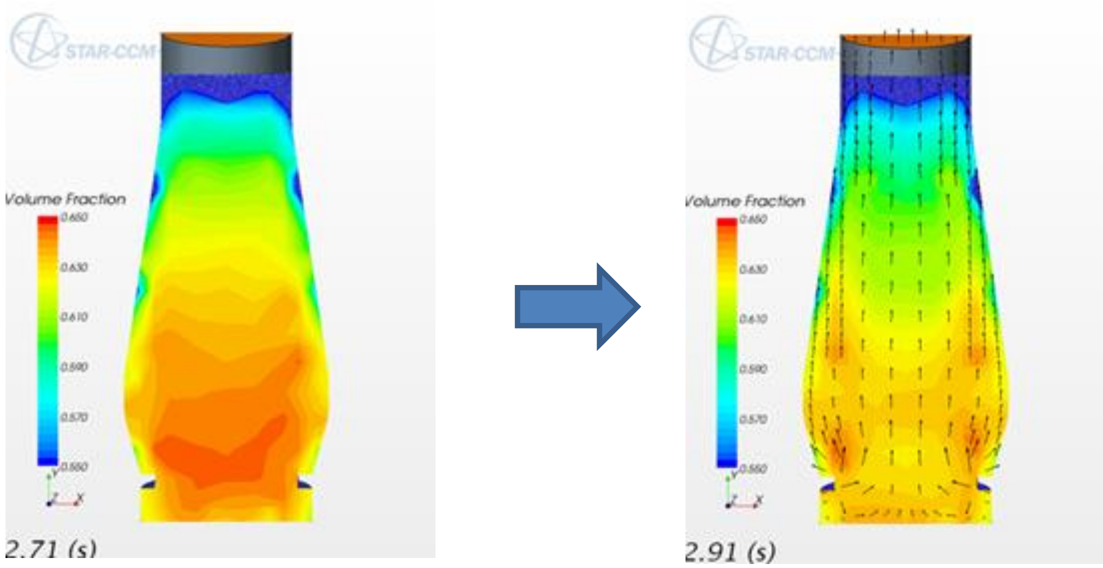
STAR-CCM+ also offers a two-way coupling with CFD. When activated, particle phase exchange mass, momentum and energy with fluid phase

- Lagrangian source terms appear in fluid phase equations (flow through porous media)
- Local void fraction value is evaluated periodically

Two-way coupling simulations are CPU very intensive. In 'particles in chemical reactor' example shown in figure below

- Million particles
- 96 core simulation
- Physical time 0.2 s
- DEM timestep 5E-6 s

Simulation time was ~48 h



Other features of DEM in STAR-CCM+

DEM in STAR-CCM+ is fully integrated into STAR-CCM+ and benefits from

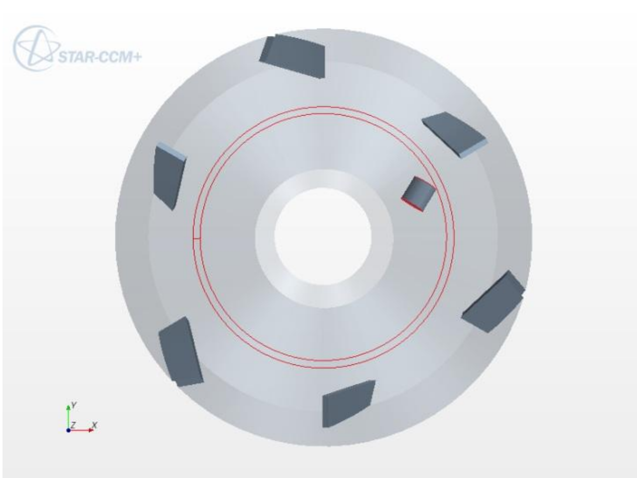
- Familiar and easy to use interface
- Client server paradigm
- Parallel computation
- CAD Import
- Powerful STAR-CCM+ post processing
- STAR-CCM+ Java Macro System
- Reporting, user defined field functions
- Seamless and flexible integration with STAR-CCM+ boundary condition definitions
    - Independent behavior for particles and flow. Example: Porous baffle permeable for flow, impermeable for particles

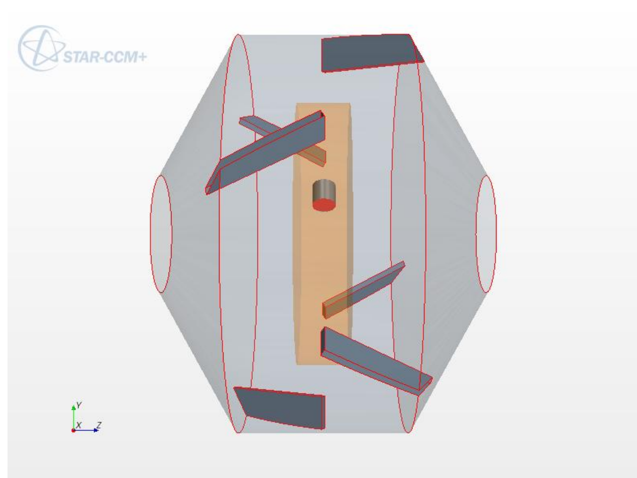
Particle flow in mixing or coating equipment

The example discussed next will illustrate the DEM capabilities

- In using macros for running the simulation and analyzing result
- In application for complex systems: Particle and fluid flow, complex geometry, moving geometry parts, multiple regions

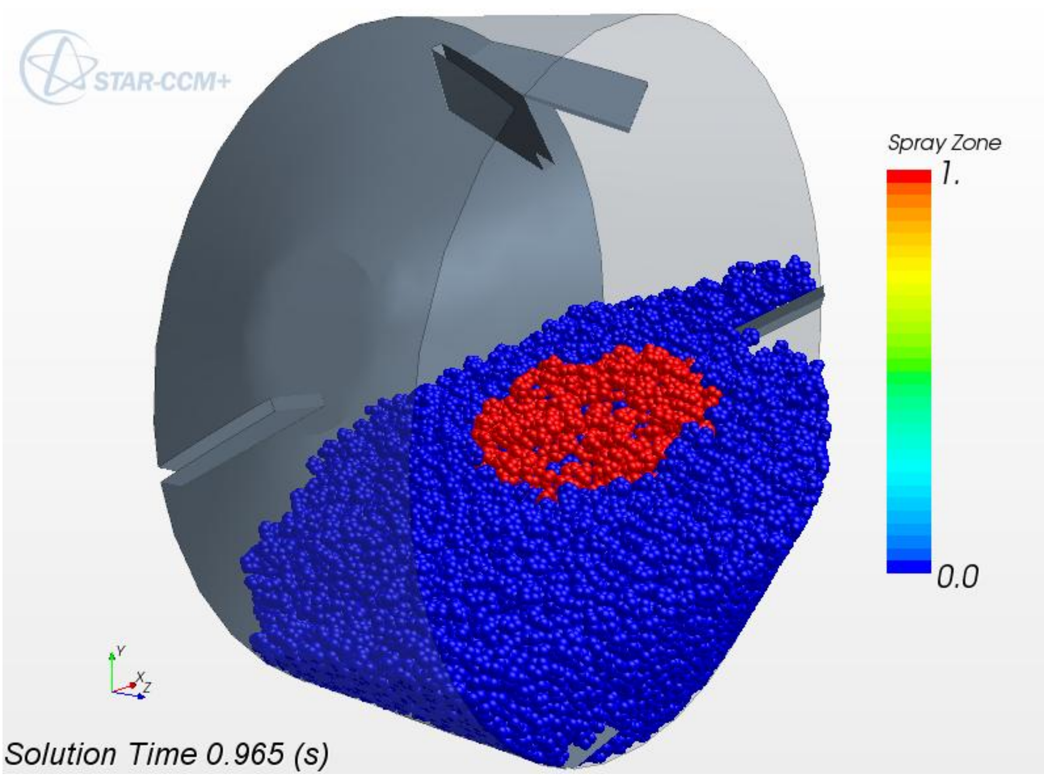
Geometry details are described in Reference: A. Dubey, et. al. "Effect of speed, loading and spray pattern on coating variability in a pan coater", Chemical Engineering Science Science 66 (2011) 5107-5115.





Geometry includes the rotating drum with mixing buffles rotating at set rpm and spray-nozzle positioned stationary inside the coater.

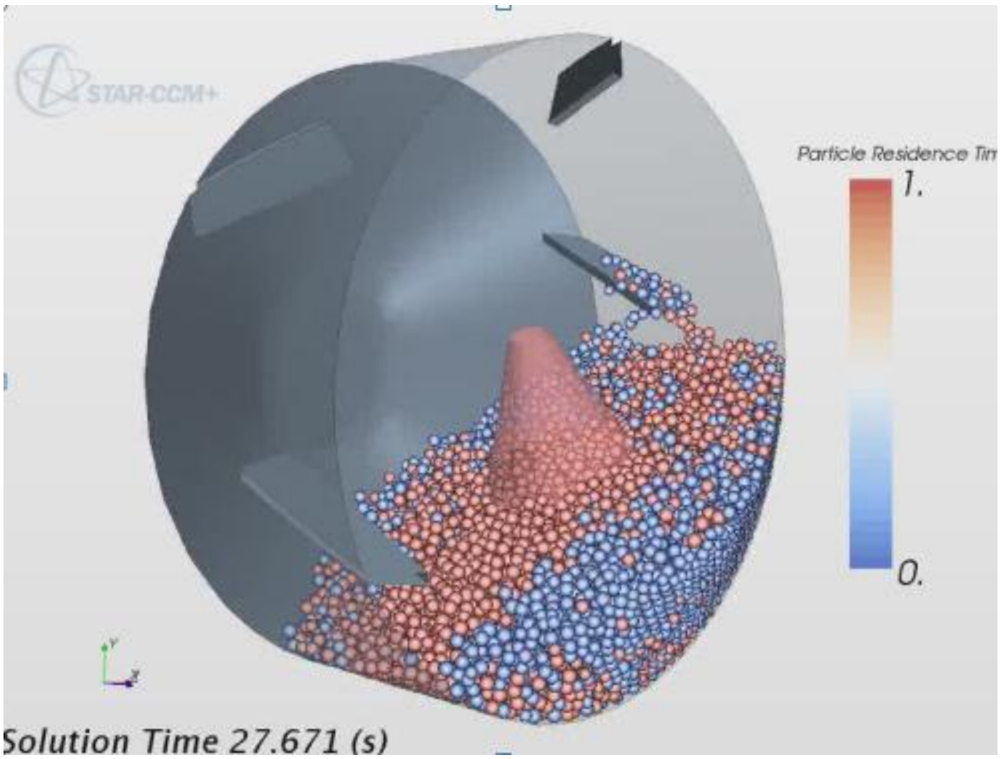
In this example, spray zone property of particles is defined using user set Filed Functions.



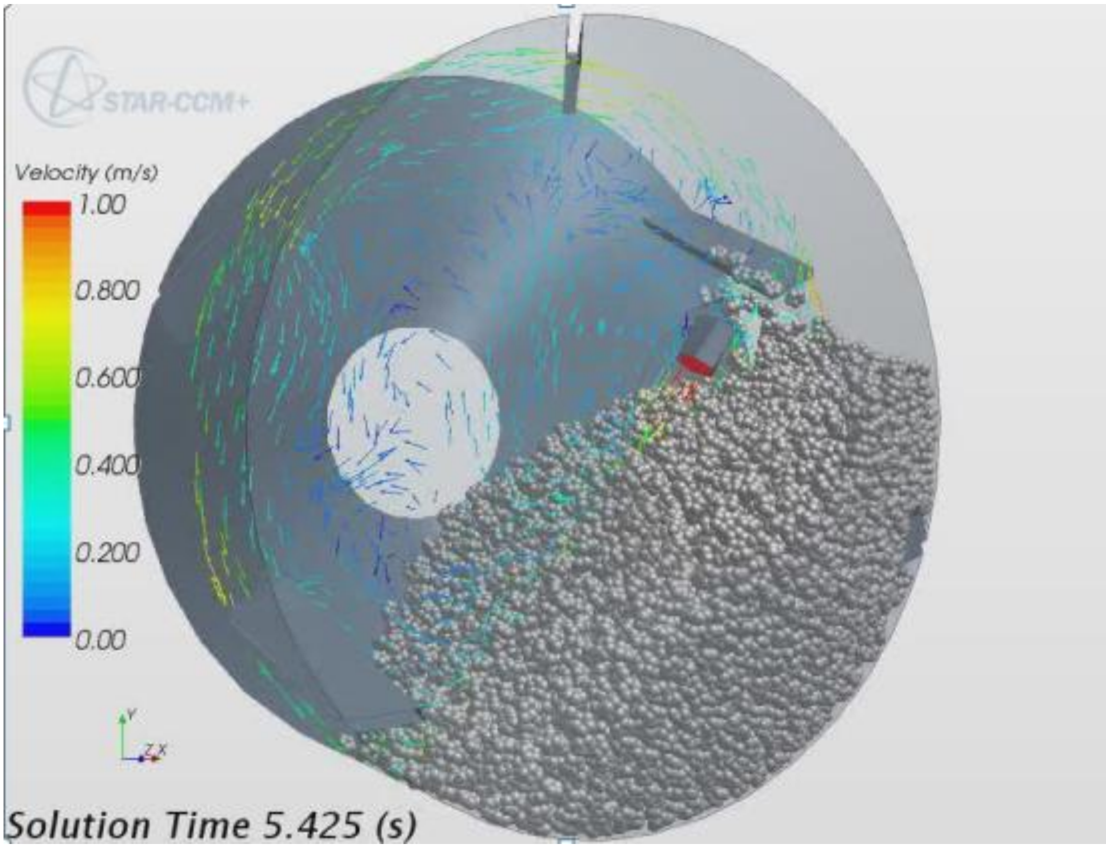
Example of calculating the residence time of particles in spray zone involves the following capabilities

- Outputting particle info
  - Using 'XYZ Internal table' capability. Columns: ID, Spray.Zone, X,Y,Z. Set 'Save to file' with trigger beingtimestep
- Setting input residence data
  - Using 'File Table' capability, Colums: ID, 0

- Setting Residence Time Filed Function by using interpolateTable capability
- Setting external data-analysis script which
    - Reads in list of XYZ tables
    - Sorts by ID, adds Spray Zone column to ‘File Table’ file
- Using macro to run model
    - Using ‘while’ loop to repeat cycle
        - Run Δt , set of table generated
        - Call external script, to update File table
        - Re-extract data in Residence Field Function



Finally, the composite particles of ‘tablet’ shape were simulated in this geometry with two-way coupling with CFD, see figure below



Summary

DEM, being fully integrated into STAR-CCM+, can use

- Powerful STAR-CCM+ post processing
- Reporting, user defined field functions
- STAR-CCM+ Java Macro
- One-way or two-way coupling with CFD

To set and analyze particle flow in mixing or coating equipment, estimate

- Mixing efficiency
- Coating efficiency
- Stress distribution in bulk, etc