research center pharmaceutical engineering

eXtended Particle System

GPU Based Particle Simulation Framework With Fluid Coupling Ability

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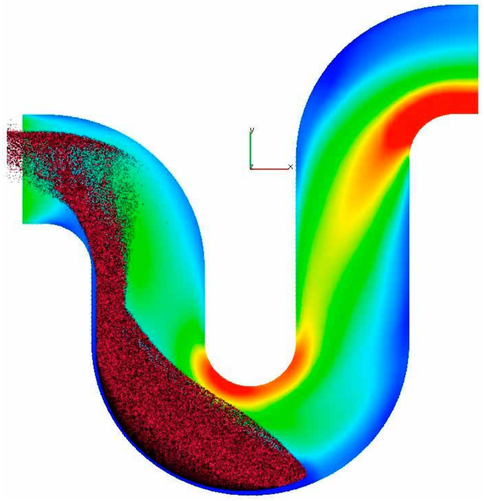
Introduction

Understanding of granular flow is extremely important for the pharmaceutical industry. We use the Discrete Element Method (DEM) to compute granular flows based on particle-particle pair interactions. This method is computational expensive for large amounts of particles. In order to simulate realistic systems in reasonable time we use the massive parallel computational abilities of modern GPUs. To deal with fluidized processes, like wet coaters or fluidized bed applications, we use a coupling interface with the industrial simulation software AVL FIRE® to add support for Computational Fluid Dynamics (CFD). The biggest challenge is to keep the computation time per time step and the memory consumption as low as possible.

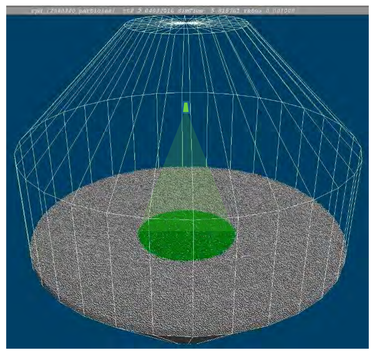
Examples of Coupled Real-World Simulations

The particles are fluidized by the air flow simulated by AVL FIRE®. While they travel through the device they can get coated by multiple pre-defined spray cones using a ray-tracing method. Various spray properties can be defined depending on the simulation goal, including material density, spray rate and temperature. Coated particles can grow due to applied spray mass. Even more particles can be heated or cooled by air, spray liquid or particle-particle contact.



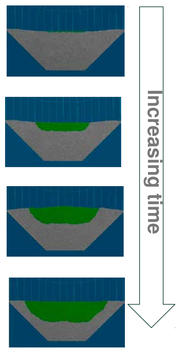
Fine granular in an inhaler device.

Showing air velocity and particle movement through the device.

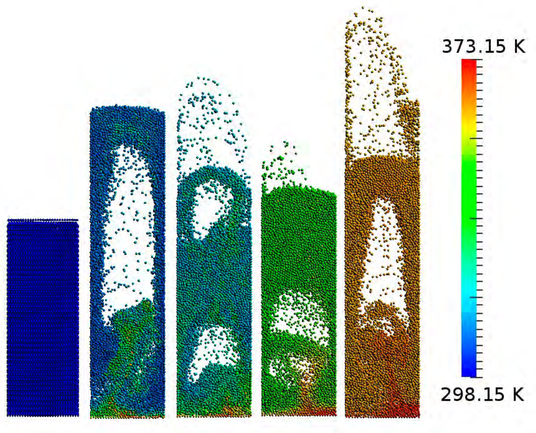


DEM extended for dry impregnation process in a double cone blender.

Spray nozzle and resulting spray zone (green area). 2million particles.

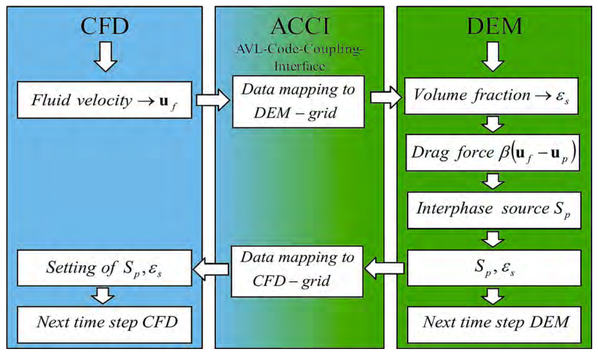


Fluid transfer: Spreading of liquid inside the particle bed, sectional view



Fluidized-bed

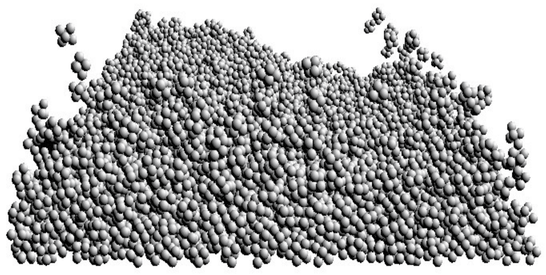
Particles are heated due to hot air flow.



The two simulation processes exchange their simulation data directly.

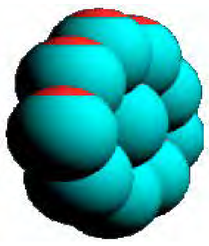
Implementation of Multi-Sphere Approach

As spherical particles are used in rare cases only, an approximation of real shapes can be done by sticking several spheres together forming new particle shapes. In this case the collision detection keeps being as simple as with spherical particles, with similar computational effort. In our implementation arbitrary shapes can be predefined giving the possibility of simulating a whole range of different granulars.



Multisphere example

Particles falling into a box



Multisphere shape example

A tablet consisting of eleven spheres

Overview and Outlook

Feature List:

- Up to 8 • 10^6 particles/GB GPU memory
- Only 1 sec Wall clock time per time step for 20 • 10^6 Particles (Kepler)
- Supports Real-World boundaries via STL input files
- Particle coating via ray-tracing method
- Simulation of heat flow
  - Between particles, air and liquid
- Modular software design
  - Highly extend- and configurable
- Single or interactive mode
  - Supports a detachable GUI as well
- Optional coupling with a CFD solver
  - via the AVL FIRE® coupling interface (ACCI)

Outlook:

- Implementation of
  - Convex polyhedral shaped particles
  - More realistic tablet shaped particle
    - Intersection of 3 spheres
  - History dependent implementation of tangential force
- Multi-GPU support
- Dynamic cell space adaption
- More sophisticated user interface