

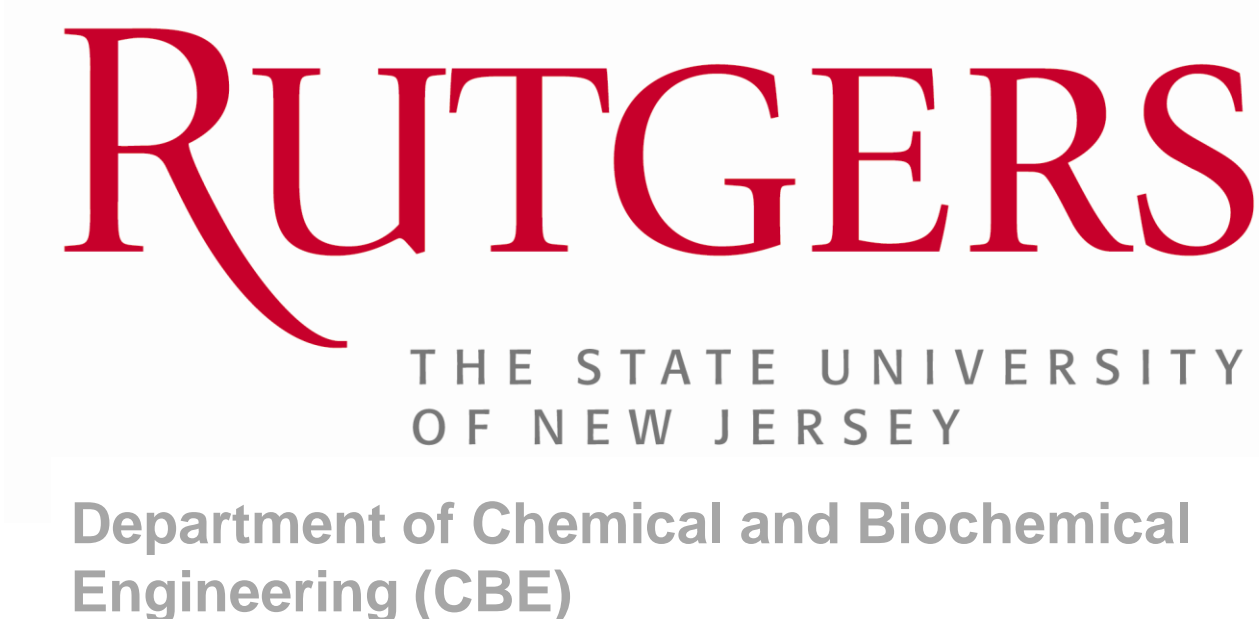
Large-scale GPU simulations of Granular Flows and Fluidized Beds, an LBM-DEM Coupling Approach

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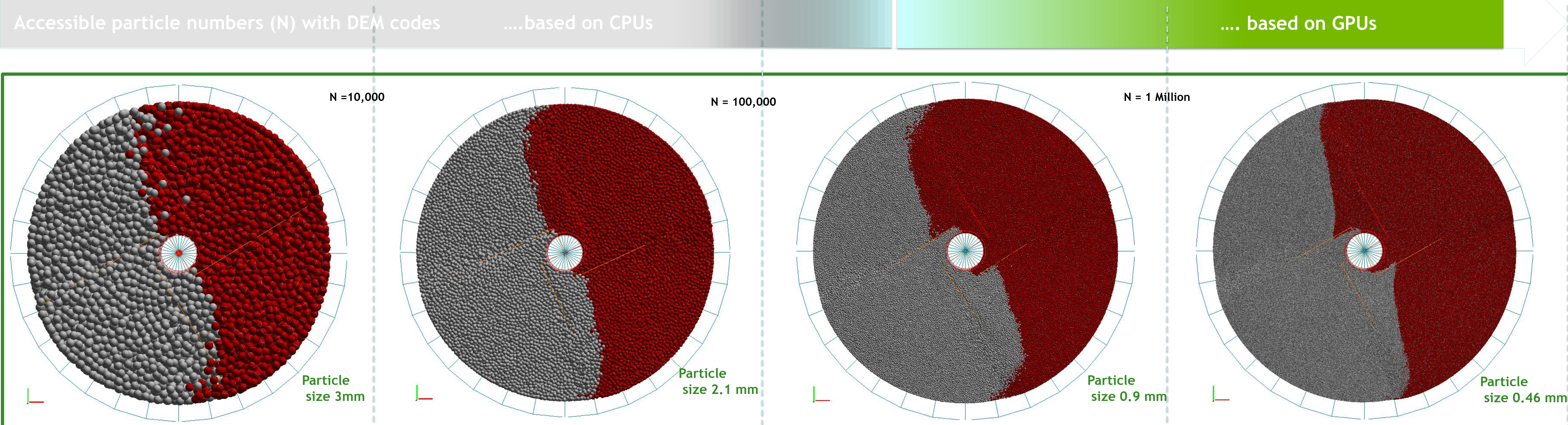
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Introduction

Granular flows are extremely important for the pharmaceutical and chemical industry, as well as for other scientific branches dealing with granular media. Thus, the understanding of the impact of particle size and related effects on the mean as well as on the fluctuating flow field in granular flows is critical for design and optimization of powder processing. We use a specialized simulation tool written in C and CUDA, a massive parallelization technique which runs on the Graphics Processing Unit (GPU). It was chosen to be able to simulate significantly higher amounts of particles in acceptable runtime. We focus on flow fields and wet-mixing properties obtained in the lower million particle range. In our talk, we present simulation results of a pitched blade mixer on a laboratory scale. Particles with a medium particle size of 365 micrometers are blended at 30-60 rpm for several turns (> 10 revolutions). The GPU implementation enable the DEM simulation of quartz powders in the real geometric resolution.

In order to investigate the mixing process during the continuous spraying of a liquid, the DEM code was extended. Liquid films and bridges determine the spread of the fluid in the aggregates. Depending on the wetness level on the particle surfaces, capillary forces account for cohesion and agglomeration. The simulations will shed light on the optimum location and the type of fluid entry, and allow predictions of the time until a homogeneous moisture distribution in a blended bulk can be achieved. In an extension of this project, highly resolved two-phase flows of one million particles will be investigated, which are important, e.g., in fluid bed drying. Here we focus on both, a gas-phase simulated using the Lattice Boltzmann Method (LBM) and a coupled solid-phase of discrete particles, simulated by using Discrete Element method (DEM).



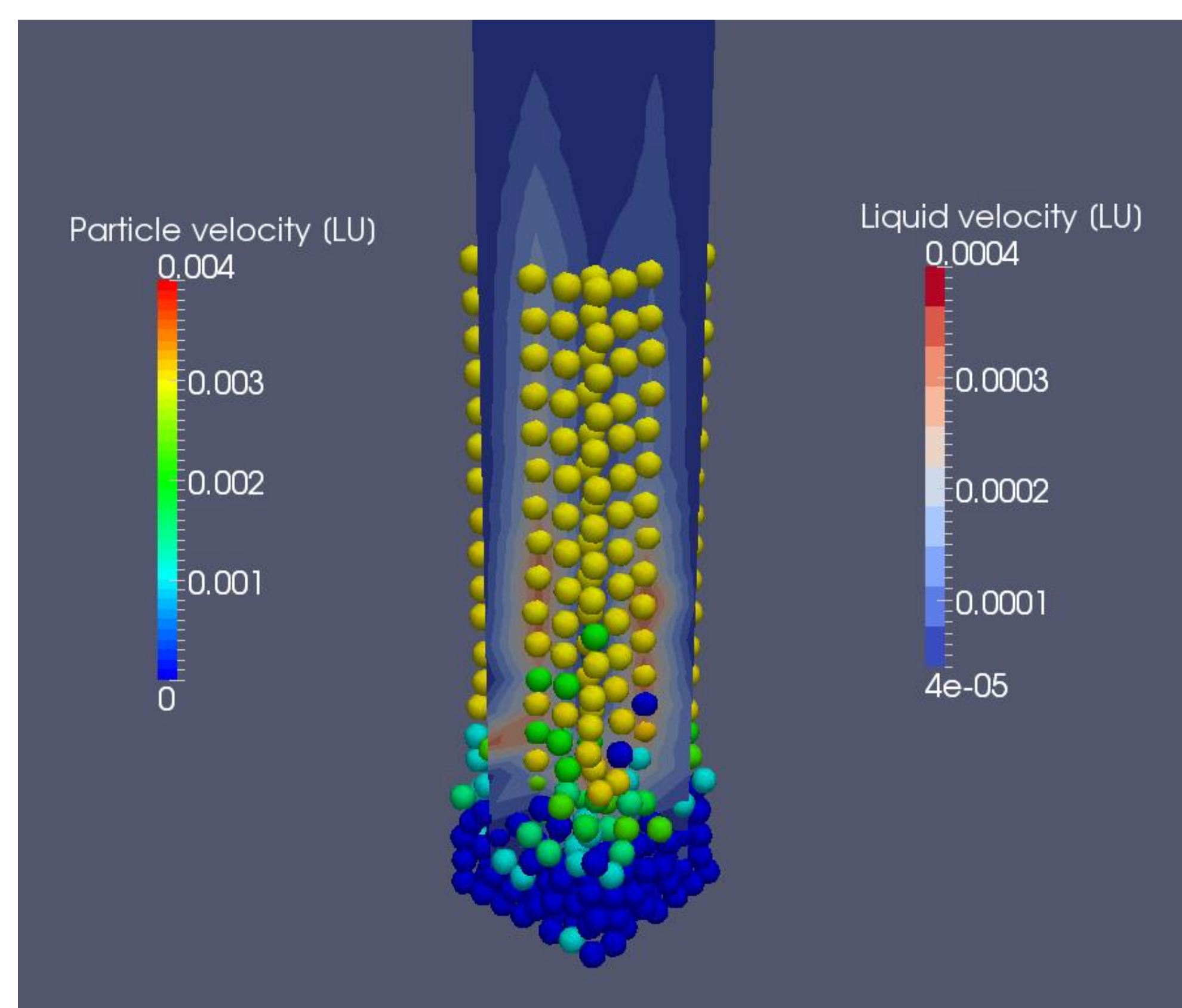
Large number of particles allows for realistic flow simulation of powdery material, consisting of small grains ($\varnothing < 1\text{mm}$).

Lattice-Boltzmann Scheme

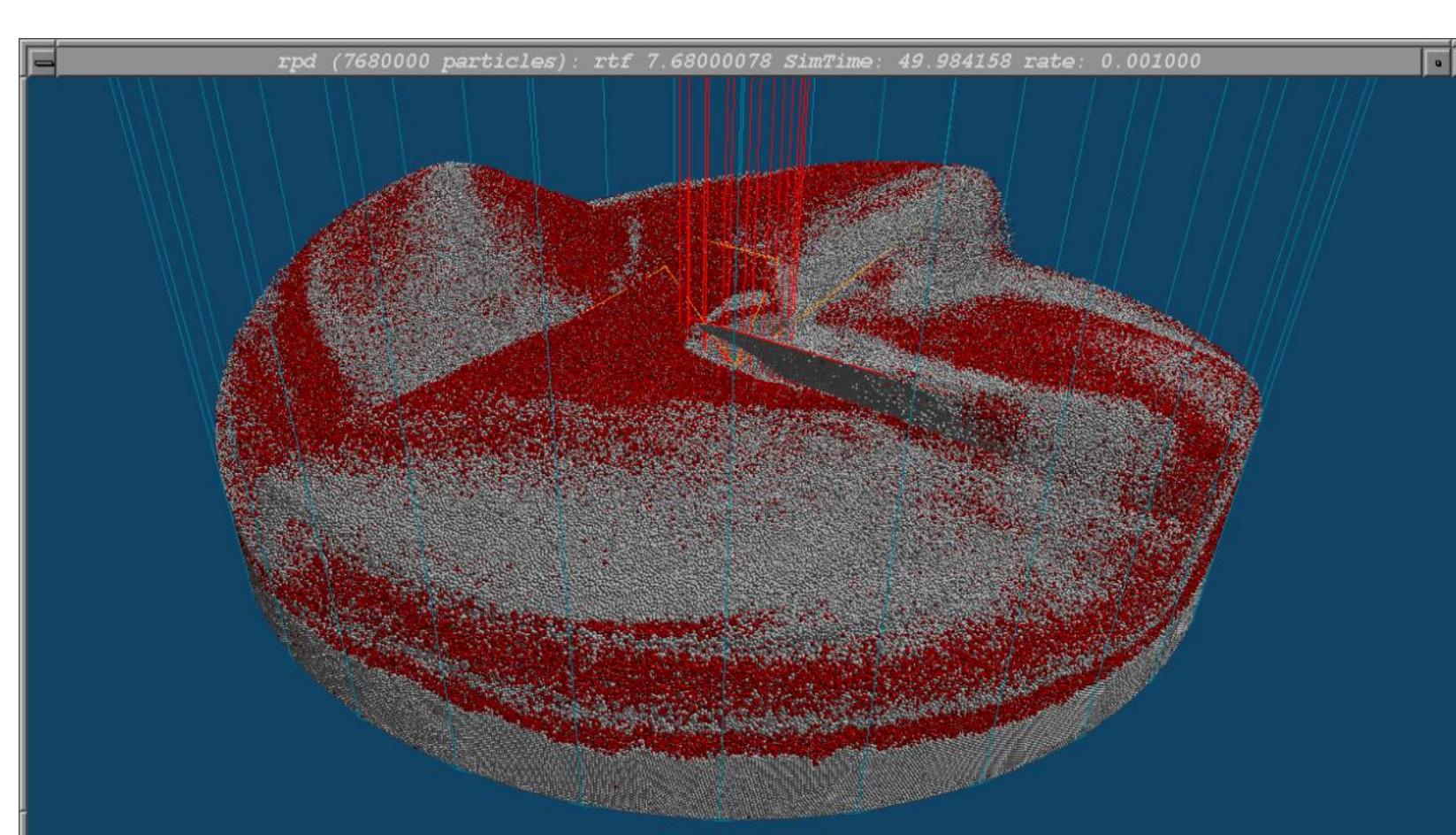
A variation of LB scheme due to Eggels & Somers is used to solve for the large-scale motions of the turbulent flow. The scheme is based on the Boltzmann kinetic equation which can be used to recover the macroscopic hydrodynamic behavior of fluids.

The scheme solves the following set of coupled partial differential equation:

$$\partial_t \mathbf{f} + \mathbf{e} \nabla \mathbf{f} = \Omega(\mathbf{f})$$



Coupled fluid flow and discrete particles. Combined numerical simulation of LBM and DEM.



Large-scale DEM simulation of mixing in a pitched-blade mixer. Particles initially colored. Simulation after 1.5 revolutions. 7.68 million particles.

Particle Dynamics

Trajectories of the individual particles are computed in the Lagrangian manner taking into account the drag force, the gravity, the slip-shear lift forces, and the lift force resulting from particle rotation. The following set of equations are solved for the new particle position, the new linear velocity components, and the angular velocity:

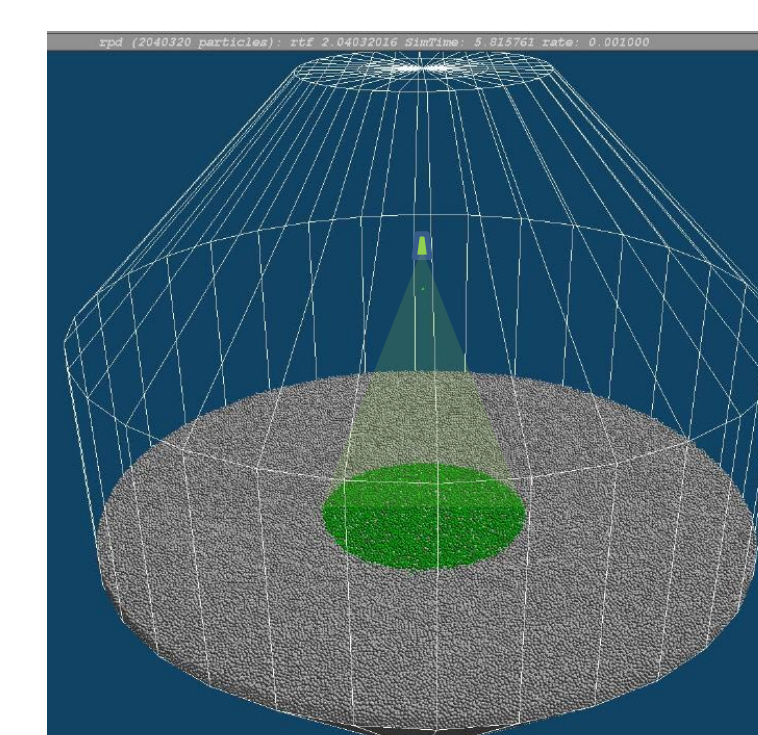
$$\begin{aligned} d_t \mathbf{x}_p &= \mathbf{u}_p \\ m_p d_t \mathbf{u}_p &= \mathbf{F}_p \\ I_p d_t \boldsymbol{\omega}_p &= \mathbf{T} \end{aligned}$$

The force coupling between phases, i.e., the two-way coupling is achieved by the clipped fourth-order polynomial mapping function. Collisions of particles are modeled using the contact dynamics following the work of S. Luding.

Ongoing Research

The coupling of DEM, LBM and the incorporation of wetting is necessary for the simulation of much more complex processes, such as top-spray coating and granulation in fluid bed reactors.

Here, the challenge in numerical modeling is the interplay of air, liquid, particles and heat.



DEM extended for dry impregnation process in a double cone blender. Spray nozzle and resulting spray zone (green area). 2million particles.



Schematic of the top-spray coating process. (Device Glatt220)

Progress & Results

- Our results show significant increase of possible simulation problem size using CUDA parallelization.
- Coupled LBM/DEM allows for application on complex pharmaceutical engineering processes like fluidized beds.
- Coupled large-scale simulations are under development.