Particle Simulations Using Discrete Element Method (DEM), A Massively-Parallel Implementation On GPUs

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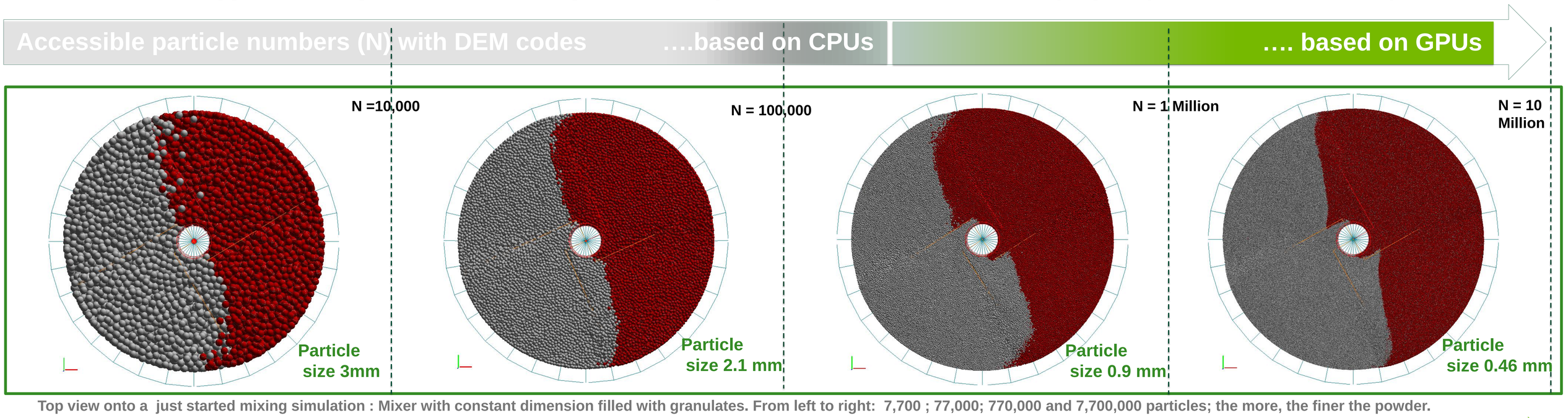
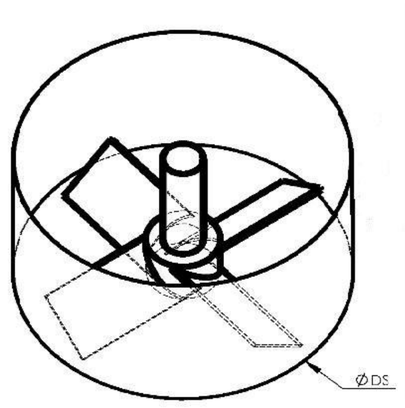
Introduction

Understanding of granular flow is extremely important for the pharmaceutical industry. We apply Discrete Element Method (DEM) to simulate complex powder flow problems on the computer. In order to account for mixing, impregnation or coating processes, DEM algorithms must be extended. The biggest challenge is to include a large number of particles in a simulation and keeping the job run time at an acceptable level*.



Top view onto a just started mixing simulation : Mixer with constant dimension filled with granulates. From left to right: 7,700 ; 77,000; 770,000 and 7,700,000 particles; the more, the finer the powder.

Large number of particles allows for realistic flow simulation of powdery material, consisting of tiny grains (Ø < 1mm).



Mixing device and raw material; Analysis and optimization of process parameters is expensive and time consuming in product development stages.

Numerical Methods and Modeling

Adapted to HPC Tesla GPU Compute Device

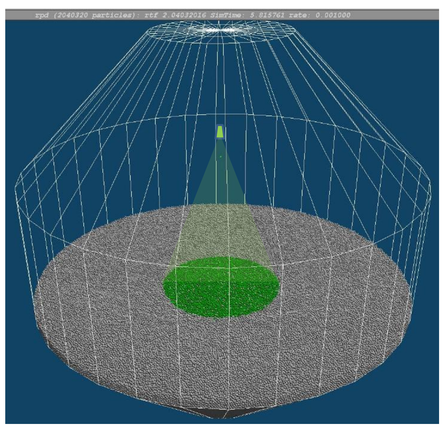
- **DEM simulation of the particle flow with massively parallel CUDA approach and fluid spread extension.**

  (speedup of 50 compared to CPU)
- **Flexible spray nozzles by implementation of ray threading projection algorithm using CUDA threads for fast and realistic spray zone detection.**

  (speedup of 600 compared to CPU implementation)

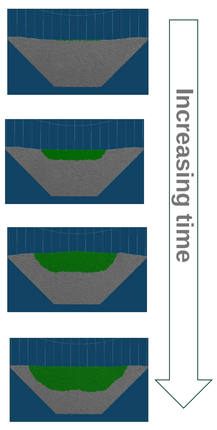
***DEM simulations of 100,000 particles run for one week wall clock time on a CPU to simulate one minute process time. The same problem finishes in a few hours using our GPU implementation.**

Application and Results

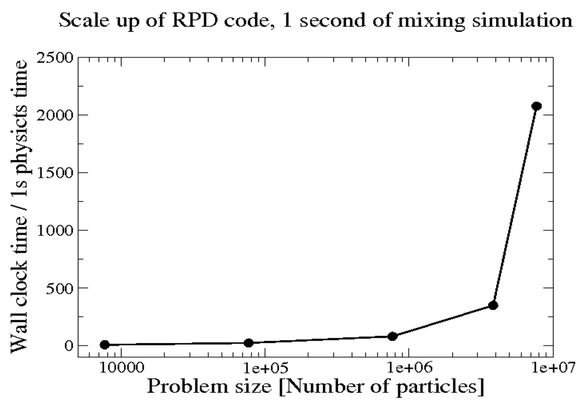


DEM extended for dry impregnation process in a double cone blender.

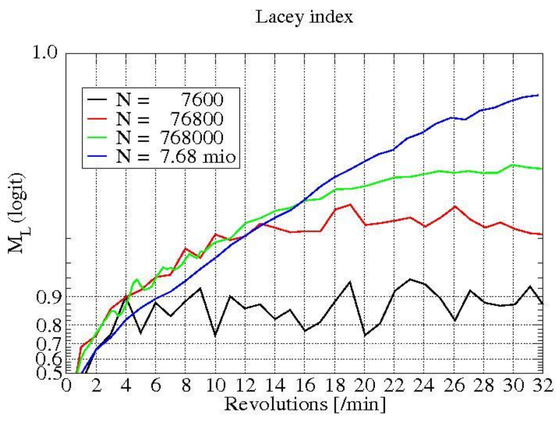
Spray nozzle and resulting spray zone (green area). 2million particles.



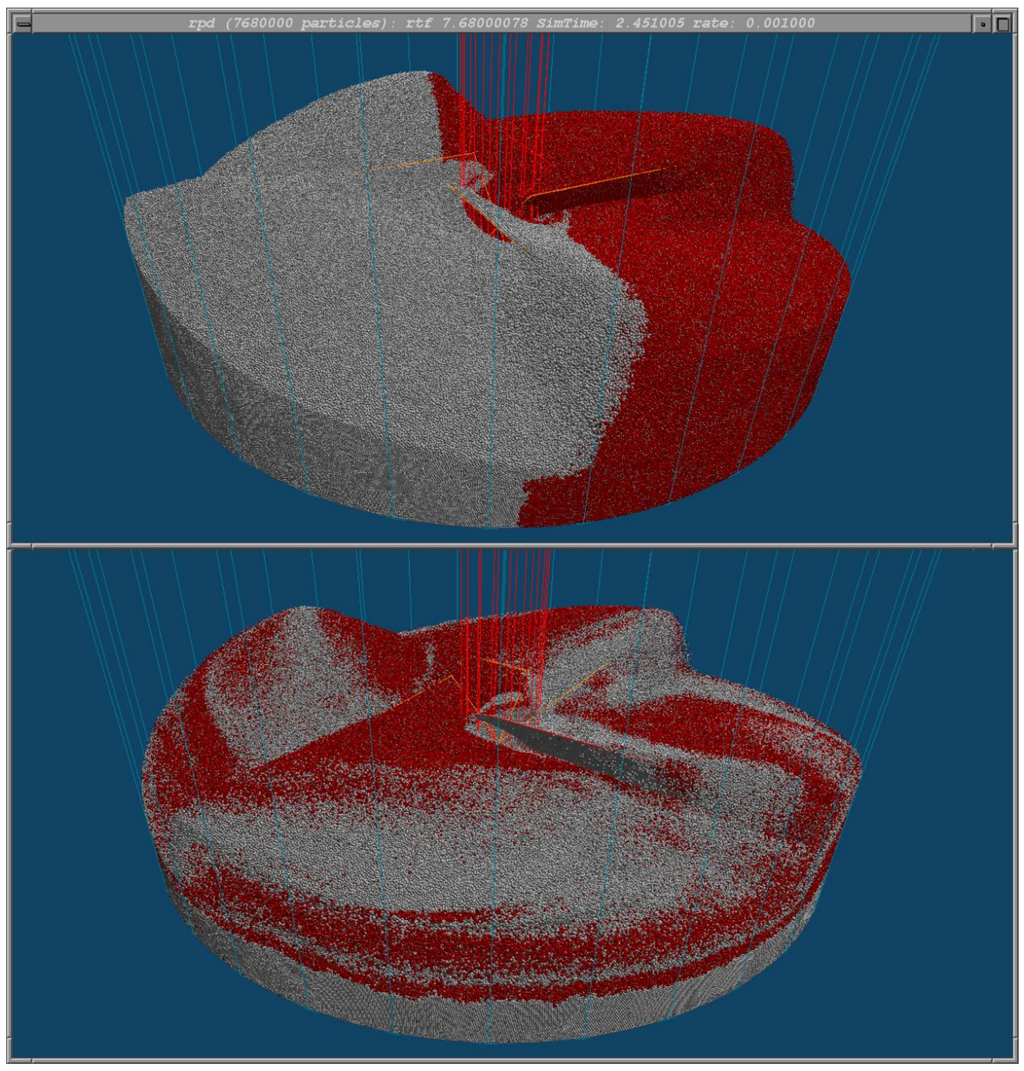
Fluid transfer: Spreading of liquid inside the particle bed, sectional view



Performance measurement on a **single Tesla C1060** compute device. Up to 4 million particles the scaling is almost linear in time.



Statistical analysis: Lacey index as a common measure of mixedness of powder blends. Only **large systems** result in smooth curves and **clear predictions** (green and blue).



DEM simulation of mixing in a pitched-blade mixer. Particles initially colored. Simulation short after beginning (top) and after 1.5 revolutions (bottom). 7.68 million particles.

Conclusions

- **Our results show significant increase of possible problem size using CUDA parallelization.**
- **Extended DEM allows for uniquely detailed application on pharmaceutical engineering processes.**
- **CUDA implementation enables 40 times more particles at shorter job run times compared to a CPU workstation.**