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Improving Algorithms for Particle Simulation on Modern GPUs

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Understanding of granular flow is important in many fields. Especially in the pharmaceutical industry simulation is a crucial tool to gain process understanding. We use the Discrete Element Method (DEM) to compute granular flows based on particle-particle pair interactions.

Typically, huge amounts of particles are needed to accurately model real-world problems, in conjunction with small time steps. Therefore, massively parallel algorithms designed for modern Graphics Processing Units (GPUs) were developed to make computation times acceptable.

This work focuses on important aspects to be considered when designing GPU algorithms for particle simulation. The main objective is to improve overall performance, especially for dynamic systems, when the number of interactions per particle varies greatly, or the calculation complexity of interaction pairs (contacts) is high. This is often the case when the particles are being mixed during the simulated process, heavily vary in size, or the simulation contains particles of non-spherical shape (e.g. bi-convex tablets, polyhedral shapes).

Examples will be presented, showing the huge improvement in performance, mainly due to increased data locality and execution convergence, while the register usage is lowered. As a side effect, contact tracking is made possible, which enables contact history, usually needed by tangential force models. Also, applications like analysis of stress or force chains are feasible, to just name a few.

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