Optimized Communication

Scheme for Massively Parallel Simulations of Polydisperse Particle

Systems with Large Size Ratios

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ABSTRACT

The standard method to parallelize particle based simulations with a hard contact interaction model and impulsive contact reactions[1] is to subdivide the simulation domain into subdomains. Each subdomain is handled by a different process and particle related information is communicated to neighbouring domains. This next neighbour communication shows perfect scalability even for a very large number of processes[2]. However it imposes an upper limit for the particle size as information can not propagate to the subdomain after the next one. Making the subdomains larger is not an option as it limits the usage of supercomputers which require thousands of processes to run efficiently.

One way to overcome this problem is to introduce global particles which are known on every process. This however requires all to all communication to keep the particles in sync which impedes good scaling performance on large systems.

Here we propose a new communication scheme which can handle polydisperse particles of arbitrary size ratios. The largest particles are allowed to overlap more than one subdomain and are not restricted in size. The communication scheme is based on point to point communication and completely avoids expensive collective operations. Only processes which really have to know about a particle will participate in the communication corresponding to this particle. Aggressive message aggregation is used to reduce the amount of messages sent. Also an information caching system is applied to further reduce the number of messages.

We implemented the communication scheme into our rigid body physics engine module *pe* of the waLBerla framework[3] and investigated the scaling behaviour on the Juqueen supercomputer in Jülich. We achieved perfect weak scalability up to the full machine. For the strong scaling the communication protocol converges to an all to all communication as large particles overlap more and more subdomains. Therefore as soon as this process starts the parallel efficiency deteriorates.

REFERENCES

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