



Institut für Theoretische und Angewandte Physik
(künftig Institut für Funktionelle Materie und Quantentechnologien)
Universität Stuttgart

Seminar zur Physik der kondensierten Materie

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hält

**am Dienstag, den 10. Dezember 2013, 15:30 Uhr
im Seminarraum 6.331, Pfaffenwaldring 57**

einen Vortrag mit dem Titel

Adaptive Load-Balancing in Particle Simulations with Short-Range Interaction

Particle simulations with short-range interaction like Molecular Dynamics are nowadays executed on thousands of processors in parallel. The typical parallelization strategies are domain-decomposition schemes, where the simulation volume is subdivided into equally sized domains, each handled by one processor.

In case the particles, and thus the computational load, are inhomogeneously distributed, this simple scheme may cause a serious performance bottleneck. Because processors need to exchange information regularly, the wall-time to compute one time-step is bounded by the processor taking the longest time to complete, while other processors are waiting idle. In such a situation, adaptive load-balancing can improve performance significantly. The task in load-balancing is to assign an approximately equal amount of work to each processor.

In this talk, we will present a new approach for load-balancing based on three dimensional domains with non-orthogonal shapes. This algorithm is able to balance highly inhomogeneous and constantly changing particle distributions. For example it has been used to simulate the impact of molten droplets at velocities of 1000m/s on a solid surface. Using adaptive load-balancing has reduced the runtime for such a simulation by a factor of about 3.

This algorithm that been recently implemented into the IMD-code. It is build on top of its existing data-structures and the communication scheme, thus requiring only limited modifications within the existing code and introduces only a very small overhead. However, alternative communication routines have been tested as well and are found to be beneficial in certain cases.

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