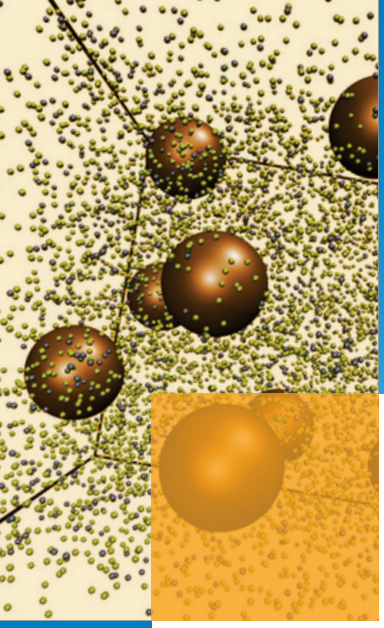


University of Stuttgart
SFB 716

www.sfb716.uni-stuttgart.de

Colloquium of the SFB 716

June 1st, 2017 | 4 pm

University of Stuttgart
Campus Vaihingen
Allmandring 3
Room 1.079

The Collaborative Research Center (SFB) 716 invites colleagues and interested persons to the upcoming colloquium. In this lecture series renowned researchers and members of our subprojects talk about their research findings regarding dynamic simulation of systems with large particle numbers.

TALK

Julian Heinrich

Universität Tübingen, Applied Bioinformatics Group

Aquaria and the Dark Proteome

In this talk, I will cover the Aquaria-resource and our survey of the "dark" proteome — regions of proteins where molecular conformation is completely unknown. We found that nearly half of the proteome in eukaryotes is dark and that, surprisingly, most of the darkness cannot be accounted for. We also found that the dark proteome has unexpected features, including an association with secretory tissues, disulfide bonding, low evolutionary conservation, and very few known interactions with other proteins.

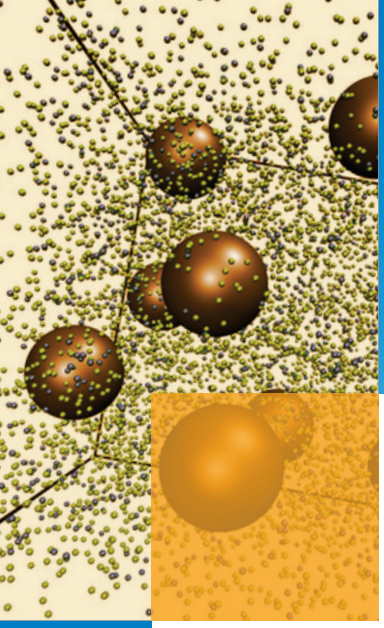
TALK

Michael Lahnert

Institut für Parallele und Verteilte Systeme (IPVS), Subproject D.8

Towards Dynamically-Adaptive Simulations With Large Particle Numbers

In modern day simulations researchers have a particular interest in modeling physical, chemical, or biological processes on multiple time and length scales and combine them in a single simulation. One particular example for such an approach are (coarse grained) molecular ensembles embedded in a liquid or gas. This approach may be used to simulate e.g. transportation of biomolecules through a nano pore or the filtration of dust particles. To model those phenomena different subsystems are required, each of which is described by different sets of equations.



Colloquium of the SFB 716

To tackle these problems we want to use ESPResSo, which is a very versatile and feature rich molecular dynamics (MD) simulation tool which is developed in the SFB 716. It uses a thermalized D3Q19 implementation of the lattice-Boltzmann method (LBM) on a regular grid to simulate a background flow. This simple spatial discretization prevents the transition to physically more relevant time and length scales.

To overcome this problem we want to use adaptive mesh refinement (AMR) to reduce the number of degrees of freedom in the system. As not all regions in the simulation domain have the same relevance to the solution, AMR allows focusing on regions of high interest while reducing computational load in regions where that level of detail is not required.

While there are various different approaches to AMR we want to focus on two important aspects:

1) We want to focus on a minimally-invasive integration to preserve as much of the expert knowledge as possible that is already contained in the application.

2) We want the AMR library to be as lightweight and scalable as possible to avoid introducing additional costs.

To this end, we choose the forest-of-octrees approach and p4est, an efficient and well scaling grid library.

Our contribution consists of two important aspects:

First, we extended p4est to be better suited in terms of a minimally-invasive integration into an existing application.

Second, we replaced the regular linked-cell and LBM grids in ESPResSo to reduce the number of degrees of freedom in the system.

We will show first results for an adaptive LBM simulation and our coupling between LBM and MD as well as upscaling tests of our implementations.