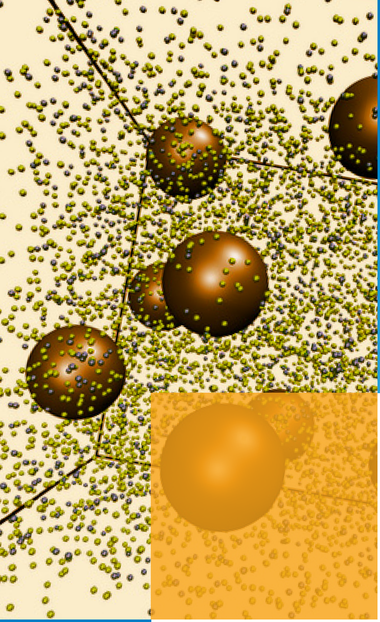


SFB 716 University of Stuttgart

38th SFB 716 Colloquium

www.sfb716.uni-stuttgart.de

January 10, 2013 | 4 pm

University of Stuttgart
Campus Vaihingen
Allmandring 3
Room 1.079

The Collaborative Research Center (SFB) 716 invites colleagues and interested person 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 1

Prof. Dr. Nico van der Vegt

Center of Smart Interfaces, Technische Universität Darmstadt

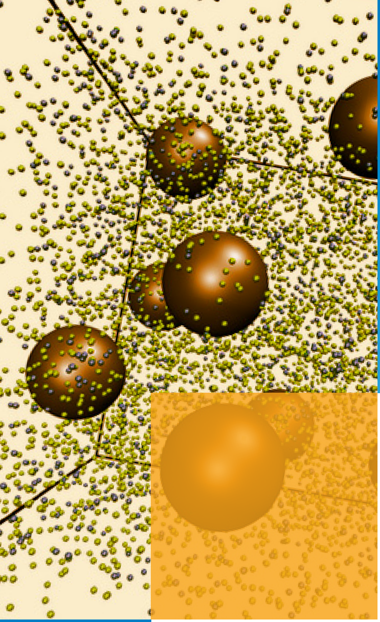
Free energy based potentials for multi-scale simulations of soft matter

I will discuss two recently introduced systematic coarse-graining methods that provide transferable coarse-grained potentials for scale-bridging simulations of soft matter systems.

The first method is based on direct calculation of pair potentials in the gas or liquid phase with thermodynamic integration or free energy perturbation methods. These so-called Conditional Reversible Work (CRW) potentials have been calculated for aliphatic groups, which serve as coarse-grained building blocks in macromolecular systems. It will be show that CRW models are chemically transferable to coarse-grained linear alkanes and thermodynamically transferable in the liquid phase branch of the phase diagram (1 atm.) between the melting and boiling points.

The second method is an extension of iterative Boltzmann inversion (IBI) and reproduces the density fluctuations at small scales which determine the thermodynamic solvation properties of multicomponent solutions. This socalled Kirkwood-Buff-IBI (KB-IBI) method has been applied to develop singlesite solvent models for aqueous solutions of urea and methanol and was used to study salting-in of hydrophobic solutes and the peptide group by urea.

CRW and KB-IBI models exhibit promising chemical and thermodynamic transferability and may potentially be applied to study phenomena away from equilibrium on mesoscopic time and length scales.



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TALK 2

M.Sc.
Martin
Obermayr

Fraunhofer
Institute for
Industrial
Mathematics,
Kaiserslautern

Application of the discrete element method for the prediction of draft forces in different types of soil

The prediction of reaction forces in soil-tool interaction is an important task for the design of machinery used in construction and agriculture. Especially for earth-moving machinery, it enables the assessment of fatigue life at an early stage of the product development, enhancing the reliability of the machines.

Soil can roughly be classified into cohesionless, cohesive, and cemented materials. In this talk, discrete element models for the different soil types are presented. They are based on spherical particles and feature normal repulsive and frictional contacts, rolling resistance with an elastic limit, as well as models for cohesive and cemented contacts.

In contrast to some applications in process engineering, it is almost impossible to describe soil particles individually by their micro-properties, i.e., their size, size distribution, and shape. Thus, in this research, only macroscopic properties, i.e., the shear strength, bulk density, and void ratio of the soil are used to parameterize the model.

The discrete element model is shown to be scale invariant in the quasi-static regime, i.e., if all length scales of the model are scaled by a constant factor, the results remain unaffected by the scaling. Dimensionless numbers together with some laboratory tests are used to identify appropriate model parameters.

The model is applied to small scale laboratory tests and large scale field tests and results of the simulations are compared to experimental results.