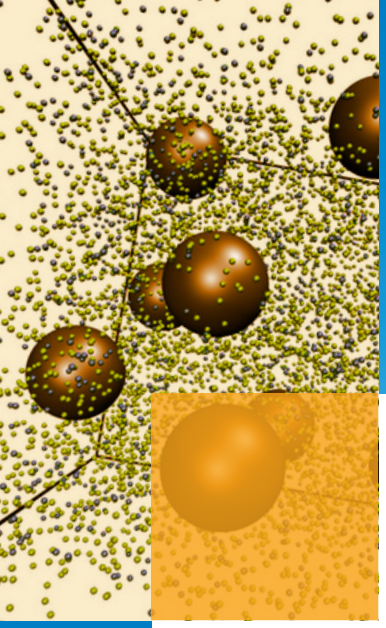


University of Stuttgart
SFB 716

www.sfb716.uni-stuttgart.de

Colloquium of the SFB 716

April 26th, 2018 | 4 pm

University of Stuttgart
Campus Vaihingen
Allmandring 3
Room 1.079

The Collaborative Research Center (SFB) 716 invites to the upcoming colloquium. In this lecture series guest speakers and members of our subprojects inform about their results regarding dynamic simulation of systems with large particle numbers.

TALK

Prof. Dr. Gerhard Hummer

Department of Theoretical Biophysics

Max Planck Institute of Biophysics, Frankfurt/Main

and

Department of Physics

Goethe University Frankfurt

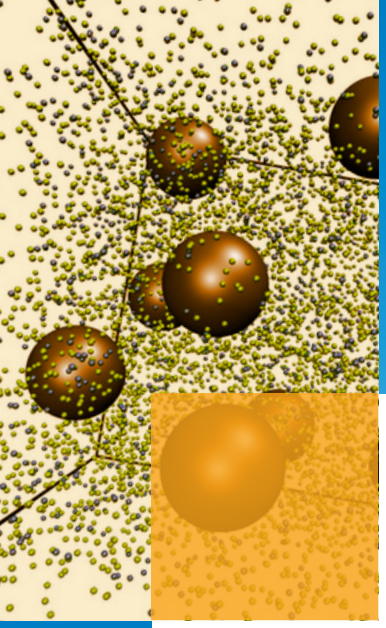
Dealing with Divergent Diffusion Coefficients in Large-Scale Lipid Membrane Simulations

We used molecular dynamics simulations to study the diffusive motions of lipids, membrane-spanning nanopores, and integral membrane proteins within lipid membranes. We found that their apparent diffusion coefficients diverge logarithmically as the width of the simulation box is increased, seemingly without bound. This divergence would appear to preclude the calculation of proper size-independent diffusion coefficients that can be compared to experiment.

However, in simulations with systems of more than 100 million particles, we show that a hydrodynamic model not only explains the divergence, but can also be used to obtain both proper diffusion coefficients and difficult-to-calculate membrane properties.

Hydrodynamics also accounts for the box-size dependence of the rotational diffusion of macromolecules. We show that the rotational diffusion tensors of proteins and nucleic acids can be determined directly from the time-dependent covariances of the quaternion describing their orientations in space. However, in molecular dynamics simulations the rotational dynamics is slowed as a result of the imposition of periodic boundary conditions. A simple hydrodynamic correction accounts quantitatively for this finite-size effect and makes it possible to estimate proper infinite-system rotational diffusion coefficients from simulations using small boxes.

Overall, the analysis of long simulation trajectories of large membrane, protein, and nucleic acid systems demonstrates that both translational and rotational diffusion coefficients suffer from significant finite-size effects. Hydrodynamics allows us to correct for the system-size dependences, giving us diffusion coefficients that can be compared to experiment.



Colloquium of the SFB 716

TALK

Stephen Copplestone

Subproject B.8

Institute of Aerodynamics and Gas Dynamics (IAG)

University of Stuttgart

Coupling MD Simulations of Laser Ablation with PIC-DSMC Simulations of Plasma Plume Expansions and subsequent Laser-Plasma Interactions

Plasmas created by laser light interacting with metals are of great interest regarding numerous fields, e.g., medical laser applications, spacecraft propulsion or material processing. The process of laser-solid interaction is examined by atomistic Molecular Dynamics (MD) simulations for a detailed description of the creation of lattice ions and their removal from the target surface[1].

In order to investigate the expansion of the plasma plume for larger spatial and temporal dimensions, the MD results are used as initial conditions for Particle-In-Cell (PIC) simulations, where particle collisions are incorporated using the Direct Simulation Monte Carlo (DSMC) method, which considers chemical reactions, e.g., impact ionization and recombination processes.

These combined methods[2] offer an elaborate simulation of the expansion characteristics, which are crucial for subsequent laser pulses interacting with the expanding plasma plume. The simulations are performed using PICLas[3], a parallel high-order three-dimensional PIC-DSMC solver developed cooperatively by the Institute of Space Systems and Institute of Aerodynamics and Gas Dynamics at the University of Stuttgart.

Authors:

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Marcel Pfeiffer and Stefanos Fasoulas, Institute of Space Systems, University of Stuttgart, Pfaffenwaldring 29, 70569 Stuttgart, Germany

Read more:

(1) J. Roth, C. Trichet, H.-R. Trebin, and S. Sonntag, Laser Ablation of Metals. Pages 159–168. Springer Berlin Heidelberg, Berlin, Heidelberg, 2011.

(2) V. V. Serikov, S. Kawamoto and K. Nanbu, Particle-in-cell plus direct simulation Monte Carlo (PIC-DSMC) approach for self-consistent plasma-gas simulations. In: IEEE Transactions on Plasma Science, vol. 27, no. 5, pp. 1389-1398, Oct 1999.

(3) C.-D. Munz, M. Auweter-Kurtz, S. Fasoulas, A. Mirza, P. Ortwein, M. Pfeiffer, and T. Stindl, Coupled Particle-In-Cell and Direct Simulation Monte Carlo method for simulating reactive plasma flows. In: Comptes Rendus Mécanique 342.10-11 (2014), 662–670.