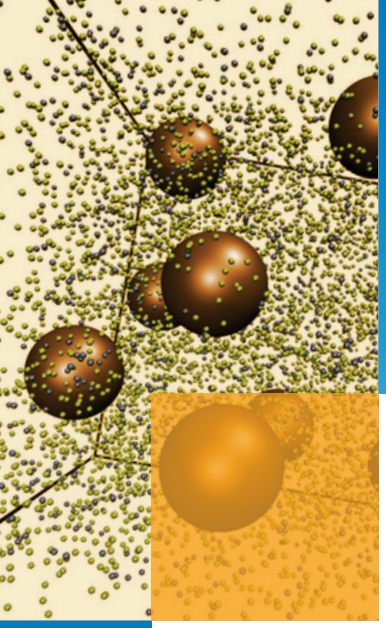

SFB 716

University of Stuttgart
Germany

Colloquium of the SFB 716

October 27, 2016 | 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

Prof. Ivo Nezbeda

Faculty of Science, J. E. Purkinje University, Usti nad Labem, and Institute of Chemical Process Fundamentals, Czech Academy of Sciences, Prague

Polarizable versus non-polarizable interaction models in simulations of fluids

Any molecular simulation is associated with two choices: (i) force field, i.e., an intermolecular interaction model with specified parameters and (ii) simulation methodology. The former choice depends on the goals of simulations and the latter with the former choice and also with the goals of the simulation study. Whereas in theoretical studies even very simplified model can be used, in studies of real systems aiming at prediction of their properties the best available models should be used. However, this has not been always the case for a number of reasons.

After decades of using rigid pairwise additive models, with advances of quantum chemistry and computer technology, along with sufficient amount of gathered experimental evidence, it is time that pairwise non-additive interactions be incorporated into interaction models used in simulations.

Incorporation of polarizability represent the most natural first step beyond pairwise additivity. However, it also brings a number of problems which seem to be the main obstacle for a wider application of polarizable models.

In the first part of the talk several examples will be given demonstrating incapability of pairwise additive models to capture, not even qualitatively, behavior of certain fluid systems and and then a recently developed new Monte Carlo method, the Multi-Particle-Move MC, will be discussed in detail along with its different implementations for specific goals. At the end of the talk ethic of publishing simulation data will be briefly mentioned.

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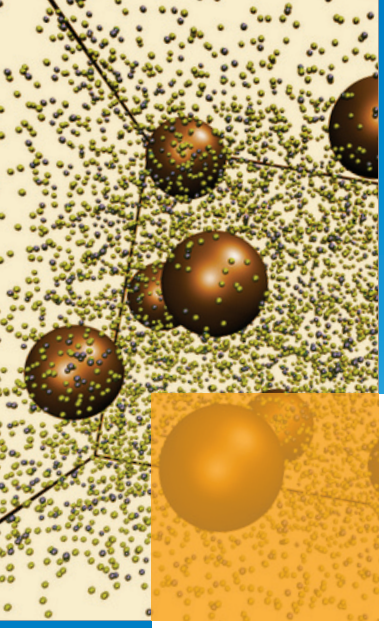

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TALK

Stephen Copplestone

Institute of Aerodynamics and Gas Dynamics (IAG), Subproject B.8

PICLas: A Highly Flexible Particle Code for the Simulation of Reactive Plasma Flows

PICLas[1] is 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. Application areas include the simulation of electric propulsion systems, atmospheric entry manoeuvres and laser ablation. As other state-of-the-art simulation codes, PICLas couples methods that consider charged particles as well as particle collisions with chemical reactions, which are handeled in a stochastic manner. Possible chemical reactions that occur at different stages within a plasma, are modeled on a microscopic level by employing the recently developed Q-K model[2].

The talk will focus on the combined concepts realised in PICLas for the simulation of reactive plasma flows. Additional emphasis will be directed towards the laser ablation of metals, where the impacting laser generates a plasma plume in front of a surface that expands into vacuum or a background medium. Different effects within the expanding plume are responsible for charge separation and particle acceleration[3], which fundamentally affect the expansion characteristics that are important for subsequent laser-plasma interactions.

[1] 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". *Comptes Rendus Mécanique* 342.10-11 (2014), 662–670.

[2] G. A. Bird, "The QK model for gas-phase chemical reaction rates", *Physics of Fluids*, Vol. 23, Issue 10, 2011, p. 106101.

[3] T. Nedelea and H. Urbassek, "Particle-in-cell-study of charge-state segregation in expanding plasmas due to three-body recombination", *Journal of Physics D: Applied Physics*, Vol. 37, Issue 21, 2004, pp. 2981-2986.