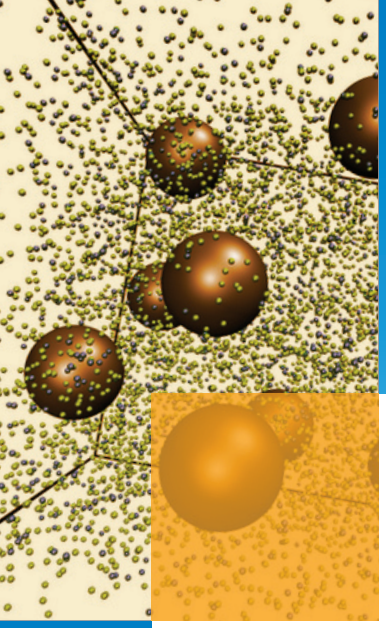


University of Stuttgart
SFB 716

Colloquium of the SFB 716

April 27th, 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.

www.sfb716.uni-stuttgart.de

TALK

Enrico Napoli

Università di Palermo Viale delle Scienze

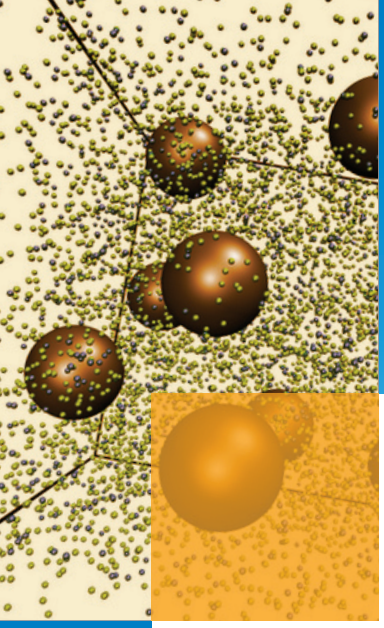
Coupling Smoothed Particle Hydrodynamics and Finite Volume methods for incompressible flow simulations

Finite Volumes (FV) and Smoothed Particle Hydrodynamics (SPH) are well-established numerical methods for the simulation of compressible and incompressible fluid flows, widely used in several different engineering and scientific applications.

Although grid-based methods like FV have achieved large robustness and efficiency in the Computational Fluid Dynamics, several difficulties still remain when dealing with highly complex geometries, solid-fluid moving interfaces or rapidly evolving free-surface flows (e.g. wave breaking). In the last decade thus a growing interest has developed in the use of mesh-less methods, among which SPH is probably one of the most used.

Since SPH is still less computationally efficient than FV, a coupled approach can be used in order to make use of the specific advantages of both methods.

The approach presented in the talk is based on the partitioning of the computational domain into a portion discretized with a structured grid of hexahedral elements (the FV-domain) and a portion filled with Lagrangian particles (the SPH-domain), separated by an interface made of triangular elements. A smooth transition between the solutions in the FV and SPH regions is guaranteed by the introduction of a layer of grid cells in the SPH-domain and of a band of virtual particles in the FV one, on which the hydrodynamic variables are obtained through suitable interpolation procedures from the local solutions. Several test cases are used in order to test the efficiency and accuracy of the coupled approach, showing that a significant reduction in the computational efforts can be achieved with respect to the standard SPH method.



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TALK

Jörg Baz

Institute of Thermodynamics and Thermal Process Engineering (ITT), Subproject A.9

Atomistic Simulations of Supramolecular Complexes in Aqueous Solution

Functional organic materials composed of dye-based molecules that stack into various structures by non-covalent intermolecular forces have fascinating optical and mechanical properties. These novel materials are of increasing importance for many high-technology applications. Here is a need for a rational design of such materials based on the engineering of dye-dye interactions and the prediction of how these interactions impact the properties of nano- or bulk state materials. The required insight into the underlying physical processes can be derived from investigations on dye assemblies that constitute the intermediate state of matter between monomeric dyes and supramolecular materials. Perylene di-imide derivatives (PDIs) emerged as a prototype class of molecules for the elucidation of the transition from monomeric to bulk materials via the supramolecular state. Their self-assembly into complex structures is determined by size and shape of the monomeric unit, system composition and thermodynamic boundary conditions. Given this diversity of factors, a molecular-level understanding of the various driving forces is essential for the rational material design.

In this project the free energy for the formation of dimers and higher aggregates are calculated for prototypical molecular building blocks carrying different functional groups in different solvent environments using molecular dynamics free-energy simulations based on force fields inherited from the area of biomolecular simulations.