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Title: Multiscale Modeling of Materials

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Summary

This symposium is dedicated to multiscale materials modelling aiming to describe complex phenomena in which several mechanisms with disparately different characteristic time- and space-scales come to the fore. Such systems include crack propagation, epitaxial growth, and multiphase fluid including flows with moving contact lines. We invite contributions implementing different multiscale modeling methods such as atomistic modeling with molecular dynamics (classical and ab-initio) or Monte Carlo, coarse grained methods such as dissipative particle dynamics, iterative Boltzmann inversion, hybrid multiscale methods, hierarchical multiscale modeling, continuum methods (based e.g. on finite elements) and atomistic-based continuum methods.

Scope

Multiscale (fluid-solid) materials modelling combines synergistically existing and emerging methods from different scientific disciplines in order to bridge the wide range of time- and length-scales that are present in various phenomena and processes in materials science such as epitaxial growth, multiphase fluid flows in complex environments (such as fractured and porous media) and associated wetting effects, fluid-solid interaction including interaction between solids and complex fluids and failure of multifunctional materials and nanocomposites. The appropriate modeling of the complex behavior of fluid-solid materials represents a significant technological and financial interest. The appropriate description of various phenomena necessitates the atomistic modeling using ab-initio or classical molecular dynamics, however such methods are computationally prohibitive despite drastic improvement in computational power and necessarily restrict the analysis to small scales. Thus, mesoscopic methods based on coarse graining techniques such as dissipative particle dynamics and other particle methods have been developed in recent years. The

combination of such methods with classical continuum methods based e.g. on finite-element discretization, is particularly attractive as it leads to models with high computational efficiency and allows bridging the nano- with the macro-scale.

In particular, there are two main multiscale modelling strategies that are been pursued. The hierarchical/parameter passing framework where parameters extracted at smaller scales are used as input at modelling at larger scales and the concurrent approach tries to solve all scales concurrently.

Today multiscale modelling is a truly cross disciplinary area which involves physicists and applied mathematicians, as well as engineers, chemists and biologists on the academic front, and industrial scientists and engineers on the applied front. The proposed symposium aims to address recent advances in this rapidly growing field by bringing together leading experts from different communities.

Topics

- Multiscale modeling
- Coarse grained methods
- Molecular dynamics (classical and ab-initio)
- Dissipative particle dynamics
- Dynamic force mapping
- Iterative Boltzmann inversion
- Concurrent multiscale schemes
- Hybrid multiscale schemes
- Hierarchical multiscale schemes
- Smoothed particle hydrodynamics
- Fluid-particle models
- Continuum methods (e.g. finite elements)
- Atomistic-based continuum methods
- Fluid-solid interactions
- Solid-fluid systems
- Complex flow modeling

Tentative list of invited speakers *(to be updated)*

- **Prof. Ingo Steinbach,** Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany
- **Prof. Markus Schmuck**, School of Mathematical & Computer Sciences, Heriot-Watt University, Edinburgh, United Kingdom

Special Issues publications

The symposium organizers are planning to arrange special issues for selected papers of the conference in international journals such as

Molecular Simulation,
Materials Science and Technology,
Computational Materials Science.
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