

Scientific Computing

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CBC Talk on Mathematics Meets Chemistry, a New Paradigm for Implicit Solvation Models - June 6, 2014

Dr. Benjamin Stamm from University of Pierre et Marie Curie (Paris) and CNRS, will visit CBC and give a talk.

Total number of participants: 9
 Total number of guests outside of CBC: 1
 Number of different nationalities represented: 4
 Total number of speakers: 1
 Total number of talks: 1

Mathematics meets chemistry: a new paradigm for implicit solvation models

Computational chemistry has attracted much attention since last years choice of the Nobel prize winners in chemistry for their contributions to multi-scale models such as the QM/MM method. The large majority of chemically interesting phenomena take place in liquid phase, where the environment (*e.g.*, solvent) can play a crucial role in determining the structure, the properties and the dynamics of the system to be studied. In a practical context, accounting for all solvent molecules in a either Molecular Dynamics (MD) or even Quantum Mechanical (QM) computation is infeasible due to the complexity of the underlying equations. A particular choice of a multi-scale model is to model the solvent environment by a conducting continuum medium (COSMO-model) and the resulting electrostatic energy contribution to the solvation energy can be computed by solving a Poisson equation in the Van der Waals cavity of the solute molecule.

The mathematical problem is therefore set (and well-posed) and we illustrate, after an introduction to the subject, how to approximate the solution using Schwarz's domain decomposition method adapted to integral equations. In this manner, the problem can be solved iteratively and the coupling of the local problems is determined by the connectivity of the molecule (in contrast to fast multipole-based boundary element solvers). The resulting numerical scheme is extremely fast and a linear scaling of the computing resources with respect to the number of atoms of the solute molecule can be achieved. In numerical examples we show how this approach outperforms existing methods such as the fast multipole method by several orders of magnitude.

What	
When	Jun 06, 2014 from 10:00 AM to 11:00 AM
Where	Bakrommet @ simula
Contact Name	August Johansson
Attendees	Andre Massing August Johansson Benjamin Stamm Kent-Andre Mardal Magne Nordaar Marie Rognes Martin Alnæs Simon Funke Timo Koch
Add event to calendar	 vCal  iCal