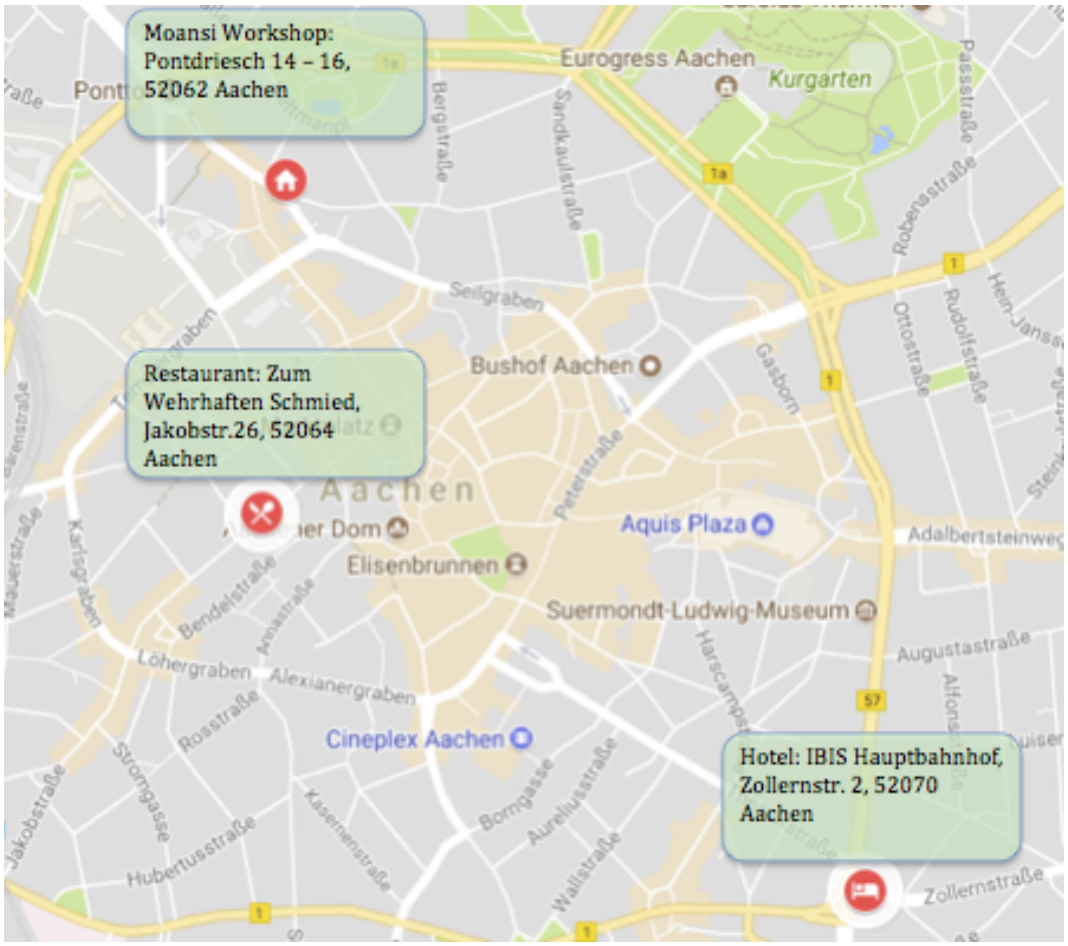
MOANSI Annual Meeting 2017

RWTH Aachen University

Mathematics Department and Center for Computational Engineering Science (MATHCCES)

October 12 and 13, 2017

Pontdriesch 14 - 16, 52080 Aachen, Room 008, SeMath



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Speakers

Speaker **Benedict Leimkuhler**

Stochastic Particle Models and Numerical Methods: From Atomistic Molecular Dynamics to Active Matter

Scheduling

10:30 – 11:15, Thursday, October 12, 2017

Abstract

“Molecular dynamics” describes a broad family of N-body models used for equilibrium and non-equilibrium simulation in chemistry, physics, engineering and biology. In its classical form, the standard MD model describes a conservative system of interacting point masses, but the method gains power as bells and whistles are added such as constraints and rigid bodies, stochastic perturbations, thermostats and barostats. Powerful codes like NAMD, Anton and Gromacs allow simulation of solvated proteins and drug-binding processes on increasingly relevant timescales. MD can be “scaled up” by coarse-graining, resulting in systems such as dissipative particle dynamics that are useful for mesoscale modelling of materials, polymers and multi-component fluid suspensions. Models of quite similar form occur in studies of active particles, including flocking birds, schooling fish, pedestrian dynamics–even the formation of political consensus–where MD-like techniques are intriguingly applicable. Surprisingly, all these models ultimately rest on a straightforward algorithmic core–the integrator–which is iterated millions or billions of times–the ”beating heart“ of every simulation.

In this talk I will describe our efforts to establish a systematic framework for the design of integrators for stochastic particle simulation including their ergodic properties, accuracy, and their flexible application. I will then consider a few case studies to illustrate the amazing range of possibilities of these techniques.

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Speaker **Konstantin Fackeldey**
Set Free Markov State Models in Molecular Simulations

Scheduling
11:15 – 11:45, Thursday, October 12, 2017

Abstract
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Speaker **Sebastian Matera**

Distribution Based Global Sensitivity Analysis for Electronic Structure Based Kinetic Models

Scheduling

11:45 – 12:15, Thursday, October 12, 2017

Abstract

The last years have seen an increasing interest in (chemical) kinetic models which have been parametrized using first principles electronic structure calculations. While these allow to access material properties without fitting the model to experimental data, commonly employed electronic structure theories rely on some approximations and thereby the estimated parameters carry an usually sizeable error.

Using a first principles kinetic Monte Carlo model for the CO oxidation on the RuO2(110) surface as a example, I will address the propagation of these errors to the kinetic model's output. For this, I will employ a newly developed distribution based approach to global sensitivity analysis. This approach allows to estimate all sensitivity indices from a single set of sampling points of the parameter space and is also applicable to stochastic model outputs. Further, the resulting sensitivity indices might be interpreted as induced uncertainty by the respective uncertain parameter.

For the model at hand, we find sizeable uncertainties but also that only a subset of all errors control this. This information might be used to identify those parameters which are worth a determination with a more accurate electronic structure method."

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Speaker **Johannes Zimmer**

Canonical Structure of Irreversible Markov Chains and Applications

Scheduling

12:15 - 12:45, Thursday, October 12, 2017

Abstract

We consider dynamical fluctuations in systems described by Markov chains, and discuss a canonical structure that provides a unifying description of dynamical large deviations for irreversible Markov chains, Onsager theory, and macroscopic fluctuation theory. For Markov chains, this theory involves a non-linear relation between probability currents and their conjugate forces. We discuss the resulting 'geometric' structure, which is a generalised gradient flow. It is shown that various physically natural splittings can be introduced, which can help to derive applications such as an understanding of acceleration of convergence to equilibrium and dissipation bounds. This is joint work with Marcus Kaiser and Rob Jack.

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Speaker **Ralf Banisch**

Reaction Coordinate Identification for Metastable Dynamics

Scheduling

14:00 – 14:30, Thursday, October 12, 2017

Abstract

We consider complex dynamical systems showing metastable behavior but no local separation of fast and slow time scales. The talk raises the question of whether such systems exhibit a low-dimensional manifold supporting its effective dynamics. For answering this question, we aim at finding nonlinear coordinates, called reaction coordinates, such that the projection of the dynamics onto these coordinates preserves the dominant time scales of the dynamics. We show that, based on a specific reducibility property, the existence of good low-dimensional reaction coordinates preserving the dominant time scales is guaranteed. Based on this theoretical framework, we develop and test a novel numerical approach for computing good reaction coordinates. The proposed algorithmic approach is fully local and thus not prone to the curse of dimension with respect to the state space of the dynamics. Hence, it is a promising method for data-based model reduction of complex dynamical systems such as molecular dynamics.

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Speaker **Bernd Schmidt**

Existence and Convergence of Solutions of the Boundary Value Problem in Atomistic and Continuum Nonlinear Elasticity Theory

Scheduling

14:30 – 15:00, Thursday, October 12, 2017

Abstract

We show existence of solutions for the equations of static atomistic nonlinear elasticity theory on a bounded domain with prescribed boundary values. We also show their convergence to the solutions of continuum nonlinear elasticity theory, with energy density given by the Cauchy-Born rule, as the interatomic distances tend to zero. These results hold for small data close to a stable lattice for general finite range interaction potentials. We also discuss the notion of stability in detail.

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Speaker **Heinz-Jürgen Flad**

Singular Analysis of Coupled Cluster Equations and its Implication for Simulation

Scheduling

15:00 – 15:30, Thursday, October 12, 2017

Abstract

Coupled cluster theory is presently considered as the ultimate benchmark in quantum chemistry. The present work focuses on nonlinear coupled cluster models within the random phase approximation (RPA). We present a detailed asymptotic analysis of these models using techniques from singular analysis and discuss its computational consequences.

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Speaker **Giulia Rossetti**
Computational Methods for Drug Design

Scheduling
16:15 – 16:45, Thursday, October 12, 2017

Abstract
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Speaker **Paolo Gatto**

The Polarizable Continuum Model within the Domain-Decomposition Paradigm

Scheduling

16:45 – 17:15, Thursday, October 12, 2017

Abstract

Within implicit solvation models, we recently proposed a Schwarz's domain-decomposition strategy for the computation of the electrostatic energy due to the solvent, based on the Polarizable Continuum Model (PCM). The methodological development started with the so-called ddCOSMO method, and was recently generalized to the PCM equation, resulting in the ddPCM method. The ddPCM method is an extension of ddCOMO in the sense that the discretization reduces to ddCOSMO for large dielectric constants. In this talk, I review the ddPCM approach, and present our latest results on the derivation of analytical forces resulting from the ddPCM discretization.

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Speaker **Gabriele Ciaramella**

Analysis of the Parallel Schwarz Method for Growing Chains of Fixed-Sized Subdomains

Scheduling

17:15 – 17:45, Thursday, October 12, 2017

Abstract

A new class of Schwarz methods was recently presented in the literature for the solution of solvation models, where the electrostatic energy contribution to the solvation energy can be computed by solving a system of elliptic partial differential equations [1,2]. Numerical simulations have shown an unusual convergence behaviour of Schwarz methods for the solution of this problem, where each atom corresponds to a subdomain: the convergence of the Schwarz methods is independent of the number of atoms [1], even though there is no coarse grid correction. Despite the successful implementation of Schwarz methods for this solvation model, a rigorous analysis for this unusual convergence behaviour is required, since no theoretical results are given in the corresponding literature. In this talk, we analyze the behaviour of the Schwarz method for the solution of a chain of atoms and show that its convergence does not depend on the number of atoms (subdomains). We use two different techniques to prove this result. The first technique is based on a Fourier expansion of the error and the analysis of transfer matrices constructed for an approximate model. The second one consists in an application of the maximum-principle and allows us to analyze very general geometries.

[1] Cances et al., Domain decomposition for implicit solvation models, J. of Chem. P. (2013).

[2] Lipparini et al., Fast Domain Decomposition Algorithm for Continuum Solvation Models, J. Chem. Theory Comput. (2013)."

Institution

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Speaker **Eric Cancès**

A Priori and a Posteriori Error Estimators for First-Principle Molecular Simulation

Scheduling

08:30 – 09:15, Friday, October 13, 2017

Abstract

First-principle molecular simulation based on electronic structure calculation has become an essential tool in chemistry, condensed matter physics, molecular biology, materials science, and nanosciences. In this talk, I will focus on Density Functional Theory and the Kohn-Sham model, which is to date the most widely used approach in electronic structure calculation, since it provides the best compromise between accuracy and computational efficiency. The Kohn-Sham model is a constrained optimization problem, whose Euler-Lagrange equations have the form of a coupled system of nonlinear elliptic eigenvalue problems. I will present some recent advances on the numerical analysis of this model, which paves the road to high-fidelity numerical simulations (with a posteriori error bounds) of the electronic structure of large molecular systems.

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Speaker **Caroline Lasser**
Time-Correlation Functions

Scheduling
09:15 – 09:45, Thursday, October 13, 2017

Abstract
TBA

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Speaker **Felix Henneke**

Frequency-sparse optimal quantum control

Scheduling

09:45 – 10:15, Friday, October 13, 2017

Abstract

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Speaker **Christian Lubich**

Dynamical Low-Rank Approximation

Scheduling

10:45 – 11:15, Friday, October 13, 2017

Abstract

The fundamental technique of obtaining reduced models of quantum dynamics is the Dirac-Frenkel time-dependent variational principle, where the time derivative of the wave-function, as given by the Schrödinger equation, is projected onto the tangent space of an approximation manifold at the current approximation. A particularly interesting case arises when the approximation manifold is chosen as a manifold of low-rank tensors or tensor tree networks. Such approximations are widely used in quantum physics and chemistry. We present a technique for time integration of the resulting equations of motion, which in contrast to standard methods is robust with respect to the unavoidable appearance of small singular values in the approximation.

Institution

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Speaker **Jan Hamaekers**

An Adaptive Multiscale Approach for Electronic Structure Methods

Scheduling

11:15 – 11:45, Friday, October 13, 2017

Abstract

In this talk, we introduce a new scheme for the efficient numerical treatment of the electronic Schrödinger equation for molecules. It is based on the combination of a many-body expansion, which corresponds to the so-called bond order dissection Anova approach, with a hierarchy of basis sets of increasing order. Here, the energy is represented as a finite sum of contributions associated to subsets of nuclei and basis sets in a telescoping sum like fashion. Under the assumption of data locality of the electronic density (nearsightedness of electronic matter), the terms of this expansion decay rapidly and higher terms may be neglected. We further extend the approach in a dimension-adaptive fashion to generate quasi-optimal approximations, i.e. a specific truncation of the hierarchical series such that the total benefit is maximized for a fixed amount of costs. This way, we are able to achieve substantial speed up factors compared to conventional first principles methods depending on the molecular system under consideration. In particular, the method can deal efficiently with molecular systems which include only a small active part that needs to be described by accurate but expensive models. Finally, we discuss to apply such a multi-level many-body decomposition in the context of machine learning for many-body systems.

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Speaker **Venera Khoromskaia**

Highlights of Tensor Methods in Grid-Based Electronic Structure Calculations

Scheduling

11:45 – 12:15, Friday, October 13, 2017

Abstract

"Novel tensor numerical methods are based on representation of d-variate functions and operators on large $n^{\otimes d}$ grids in the rank-structured tensor formats which provide $O(dn)$ complexity of numerical calculations instead of $O(n^d)$ by conventional methods. A starting point was our tensor-structured Hartree-Fock solver based on the tensor-structured calculation of the electron repulsion integrals (ERI), and the Laplace and nuclear potential operators, using a general basis, discretized on $n \times n \times n$ 3D Cartesian grids [3,4]. The low-rank representation of the Newton kernel and of the electron density enable a 3D grid-based tensor convolution in $O(n \log n)$ complexity [1,2]. Two-electron integrals tensor is computed in a form of Cholesky factorization by "1D density fitting" [3]. Efficient rank reduction algorithms are developed for reducing the ranks of canonical tensors at necessary steps. In calculation of all 3D operators in the Hartree-Fock equation the 3D analytical integration is completely avoided, since it is substituted by the grid-based tensor algorithms of 1D complexity. This enables usage of 3D grids of size of the order of 10^{15} in Matlab calculations on a laptop, high accuracy is controlled by tensor ranks.

Tensor factorization of two-electron integrals is used for efficient calculation of excitation energies for molecules by the Bethe-Salpeter equation. Further developments concern crystalline systems, where one of the challenges is the summation of electrostatic potentials on large 3D lattices in a non-periodic case [5]. Our tensor method for summation of the long-range potentials on $L \times L \times L$ 3D lattices provides computational complexity of the order of $O(L)$ which is much less as compared with $O(L^3)$ in traditional approaches, like Ewald-type summation. Matlab simulations for fast tensor-based summation of millions of Newton kernels in a box will be demonstrated. Recently introduced Range-Separated (RS) tensor format [6] applies to arbitrarily located potentials.

1. B. N. Khoromskij and V. Khoromskaia. Multigrid Tensor Approximation of Function Related Arrays. SIAM J Sci. Comp., **31**(4) 3002-3026 (2009).

2. B.N. Khoromskij, V. Khoromskaia, and H.-J. Flad. Numerical Solution of the Hartree-Fock Equation in Multilevel Tensor-structured Format. SIAM J. Sci. Comp., **33**(1), 45-65 (2011).

3. V. Khoromskaia, B.N. Khoromskij and R. Schneider. Tensor-structured Calculation of the Two-electron Integrals in a general Basis. SIAM J. Sci. Comp., **35** (2), A987-A1010, 2013.

4. V. Khoromskaia. Black-box Hartree-Fock solver by tensor numerical methods. CMAM, vol. 14 (2014) No.1, pp. 89-111.

5. V. Khoromskaia and B. N. Khoromskij. Fast tensor method for grid-based summation of long-range potentials on 3D lattices with defects. Numer. Lin. Algebra Appl., 23, 2016, pp. 249-271.

6. P. Benner, V. Khoromskaia and B. N. Khoromskij. Tensor Summation of Many-particle Potentials. Preprint arXiv:1606.09218, 2016.

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Speaker **Max Pfeffer**

Tensor methods in Quantum Chemistry

Scheduling

12:15 – 12:45, Friday, October 13, 2017

Abstract

Tensor decompositions are a hot topic in high-dimensional Numerics. In Quantum Chemistry, the electronic Schrödinger equation predicts the wave functions of electrons in atoms and molecules. Typical discretisations result in high-dimensional eigenvalue problems. These can be treated efficiently using the Density Matrix Renormalisation Group (DMRG) algorithm. This is a tensor based method that approximates the ground state energy by successively optimising on small subspaces. The algorithm is rank adaptive, a feature that is thought to model the Von Neumann entropy. A generalisation of the DMRG has been proposed that allows for the computation of several excited states as well as the ground state. In this talk, we will present basic theory of tensor decompositions and give an insight into the workings of the DMRG algorithm.

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Participants

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