

MM 67: Methods in Computational Materials Modelling (methodological aspect, numerics)

Method development

Time: Thursday 17:30–19:00

Location: TC 006

MM 67.1 Thu 17:30 TC 006

Linear Scaling first-principles constant pressure molecular dynamics in Conquest — ●ZAMAAN RAZA¹, SHEREIF MUJAHED², DAVID BOWLER², and TSUYOSHI MIYAZAKI¹ — ¹National Institute for Materials Science (NIMS), Tsukuba, Japan — ²London Centre for Nanotechnology (LCN), University College London, United Kingdom

Density functional theory (DFT) calculations have become commonplace in the characterisation, design and prediction of materials, but conventional implementations scale poorly. Conquest (<http://ordern.github.io>) is a first principles electronic structure code that can perform DFT calculations that scale linearly with the number for atoms, and is capable of almost ideal parallel efficiency even when using more than 200,000 cores to deal with million-atom systems. Its capabilities include Born-Oppenheimer molecular dynamics (MD) in the micro-canonical and canonical ensembles, and extended-Lagrangian MD which includes electronic degrees of freedom in the equations of motion, solving fundamental problems involving time-reversibility.

Constant pressure MD provides a closer match to experimental and planetary interior conditions than constant volume, and facilitates the modeling of polymorphic phase transitions. Moreover, it is often difficult to choose the correct volume when modeling complex amorphous or biological systems. In this talk, we discuss the implementation of isobaric-isothermal (NPT) molecular dynamics in Conquest, and demonstrate that efficient and robust NPT simulations are now possible for systems containing 10,000+ atoms.

MM 67.2 Thu 17:45 TC 006

Treatments of disorder within electronic structure calculations — ●ALBERTO MARMODORO and HUBERT EBERT — Dept. Chemie, LMU, München

The coherent potential approximation (CPA) has proved to be a powerful tool to account for disorder in solid state systems. Among reasons for its success one can enumerate the ability to describe both diagonal [1] and off-diagonal [2] breakdown of long range order (LRO); suitability to account for an arbitrary concentration of defects, not constrained to the diluted limit; flexibility of the underlying alloy analogy model to also set up a first principles description of finite temperature effects in the magnetic [3] and positional [4] degrees of freedom. Additional aspects coming over the years under scrutiny have concerned the single-site nature of the theory, to also incorporate short-range order (SRO) effects [5]; and its effective medium construction in terms of a self-consistent arithmetic average procedure, as opposed to other statistics mainly proposed in the study of localization problems [6-7]. We look into this line of developments through examples spanning from model hamiltonians to multiple scattering adaptations.

- (1) P. Soven, Phys.Rev. **156**, 809, (1967) (2) G. Bouzerar et al. Phys.Rev.B **66**,1, (2002)
- (3) J. Staunton et al., JMMM, **45**, 15-22, (1984); (4) H. Ebert et al., Phys.Rev.B **91**, 165132, (2015)
- (5) D. Rowlands et al., Phys.Rev.B, **67**, 115109, (2003)
- (6) V.Dobrosavljevic et al., Phys.Rev.Let. **78**, 3943, (1997); (7) H.Terletska et al., Phys.Rev.B **95**, 134204, (2017)

MM 67.3 Thu 18:00 TC 006

Multilevel Adaptive Sparse Grids for parametric stochastic materials models — ●SANDRA DÖPKING¹, DANIEL STROBUSCH², CHRISTOPH SCHEURER², and SEBASTIAN MATERA¹ — ¹Freie Universität Berlin — ²Technische Universität München

Many material models require sampling to obtain the desired model output, e.g. molecular dynamics or Monte Carlo sampling. Most of these models depend on a number of parameters which show a high variability. This can be an effect of uncertainties due to the limited accuracy of the underlying method. Or, the model might represent a class of materials with different material parameters. We present a Multilevel Adaptive Sparse Grid approach to explore the parameter space and to construct a surrogate of the often expensive original model. In this approach, the points in the parameter space are adaptively chosen which reduces the total number of costly model evaluations. Moreover, the multi-level structure of the sparse grids allows us to reduce

the sampling accuracy and therefore the cpu-time spend for the model evaluation in each refinement step. We demonstrate the methodology for a first-principles kinetic Monte Carlo (1p-kMC) model for heterogeneous CO oxidation, where we address the impact of the uncertain reaction energetics derived from Density Functional Theory. We find that the multi-level approach reduces the computational cost significantly compared to non-adaptive, single level sparse grids – without compromising the accuracy of the results. For this model, we observe that DFT uncertainty can have a tremendous impact on the simulation output and that 1p-kMC predictions have to be interpreted carefully.

MM 67.4 Thu 18:15 TC 006

How to simulate nuclear quantum effects accurately at the cost of molecular dynamics — ●VENKAT KAPIL¹, JÖRG BEHLER², JOOST VANDEVONDELE³, and MICHELE CERIOTTI¹ — ¹EPFL, Lausanne, Switzerland — ²Universität Göttingen, Göttingen, Germany — ³CSCS, ETH Zurich, Zurich, Switzerland

The precise description of quantum nuclear fluctuations in atomistic modelling is possible by employing path integral techniques, which involve a considerable computational overhead due to the need of simulating multiple replicas of the system. Consequently, the cost is still prohibitive when combined with advanced electronic structure methods. An elegant way of reducing the number of replicas is by applying a correction based on a high order factorization of the Boltzmann operator. However, the high cost of computing the correction has prevented the use of this technique to condense phase systems. In this work, we present a molecular dynamics scheme which alleviates the cost of explicitly computing the expensive correction, that allows us to utilize the improved efficiency of the high order scheme. Furthermore, we demonstrate how to synergically use multiple time step integration in real and imaginary time to reduce down to zero, the cost of modelling quantum effects while describing inter atomic interactions at high levels of electronic structure theory.

MM 67.5 Thu 18:30 TC 006

Workflows and provenance tracking for high-throughput computational materials discovery — ●MARTIN UHRIN, SEBASTIAAN HUBER, GIOVANNI PIZZI, and NICOLA MARZARI — EPFL STI IMX THEOS, Lausanne, Switzerland

The last decade has seen a push in computational materials science towards cementing high-throughput approaches as a cornerstone of materials discovery and understanding. This in turn requires the development of new tools to enable researchers to shift from running individual calculations to manage thousands, if not millions of these, in a reliable, intuitive and reproducible way. In order to answer these needs, we have developed AiiDA, a python platform, to enable domain experts to encode their scientific expertise in highly customisable workflows that are easy to write, document, debug and share ensuring that such expertise is retained and can be built upon. Meanwhile, a database backend is used to automatically store the full provenance as a graph of inputs, calculations and corresponding outputs, allowing the user to see exactly where any result came from, or continue to work from any intermediate step. I will show how one can write and run AiiDA workflows in ipython notebooks and highlight the many advantages over the more traditional, ‘throwaway script’, approach and highlight some published high-throughput computational materials modelling projects that have been performed using AiiDA.

MM 67.6 Thu 18:45 TC 006

Effective treatment of formation energies for automated high-throughput computational materials design — ●RICO FRIEDRICH¹, CORMAC TOHER^{1,2}, ANDREW SUPKA^{3,4}, MARCO FORNARI^{1,3,4}, MARCO BUONGIORNO NARDELLI^{1,5}, and STEFANO CURTAROLO^{1,2} — ¹Center for Materials Genomics, Duke Univ. — ²Mat. Sci., Elec. Eng., Phys. and Chem., Duke Univ. — ³Dept. of Phys., Central Michigan Univ. — ⁴Science of Advanced Materials Program, Central Michigan Univ. — ⁵Dept. of Phys. and Dept. of Chem., Univ. of North Texas

Automated high-throughput computational materials design, as implemented in the AFLOW framework [1], aims at the systematic pre-

diction and optimization of materials properties for technological applications. The approach requires an accurate and efficient description of formation energies to assess the thermodynamic stability of new compounds. This presents a major challenge to standard computational materials science approaches such as density functional theory (DFT). Significant errors arise when calculating total energy differences between chemically dissimilar materials due to incomplete error

cancellation [2]. This is particularly the case for oxides (and other chalcogenides), where the chemical natures of diatomic (O_2) molecules, elemental metals and solid oxides are very different. We discuss various approaches to compute the formation energies of materials and compare their accuracy with respect to experimental reference data.

[1] S. Curtarolo *et al.*, Comput. Mater. Sci. **58**, 218 (2012).

[2] V. Stevanović *et al.*, Phys. Rev. B **85**, 115104 (2012).