Modern Approaches to Coupling Scales in Materials Simulation

Hotel Jäger von Fall, Lenggries, Bavaria, Germany
Organizers: Harald Oberhofer, Johannes Margraf
Webpage: http://macsims.ch.tum.de

Our workshop was held at Hotel Jäger von Fall which sits on a peninsula on the Sylvensteinsee, an artificial lake in the Bavarian foothills of the Alps near the Austrian border, a very remote location chosen deliberately to allow participants to concentrate fully on the scientific program. Transportation from and to the nearest train station was accomplished with a shuttle-bus courtesy of the Technical University of Munich (TUM), driven by some of the participating TUM members. For the most part the weather was very inviting, inspiring a small number of participants to take a refreshing swim during the breaks, it turns out that the water was very clear but also very, very cold.

The two evenings of the workshop where filled with a poster-session on Monday, held outdoors due to the lovely weather, and a conference dinner, again outdoors, on Tuesday.

The event was supported by **Psi-k**, the **German science foundation (DFG)**, the **international graduate school of science and engineering (IGSSE)**, as well as the **Technical University of Munich**.

1 Scientific Objectives

Multi-scale simulation approaches rely on a hierarchy of increasingly accurate and highly resolved methods to capture the different time- and length-scales relevant to a process of interest. Traditionally, this might involve coupling classical molecular dynamics with electronic structure calculations (QM/MM), or embedding a quantum mechanical system in a point charge or continuum environment. In this context, the models comprising the individual layers of the multi-scale hierarchy are often unrelated. For instance, the empirical potential and DFT method in a QM/MM simulation are independently defined at the beginning of the simulation. Enormous advances in electronic structure algorithms and hardware now allow first principles calculations to be carried out on a truly massive scale. This leads to a novel perspective of multi-scale models: electronic structure data can be generated with high enough quality and quantity to allow the application of coarse graining and machine learning techniques. Instead of defining separate physical models at different scales, the electronic structure method directly informs the next layer of the multi-scale hierarchy. The goal of this workshop was to bridge the gap between traditional, layered multi-scale techniques and the more direct coarse graining and machine learning approaches to the simulation of extended systems, thereby bringing together researchers working on QM/MM or other embedding techniques with those who apply coarse graining and interpolation to electronic structure data in different contexts (e.g. potential energy

surfaces, electronic properties, charge transport, rate constants in catalysis) and with different methods (neural networks, Gaussian process regression, kernel ridge regression, splining, etc).

2 Realisation of the scientific program

In order to achieve this goal we invited experts with backgrounds in three different methodological fields, (1) Deriving empirical potentials from first-principles calculations, (2) going from electronic structure calculations to macroscopic observables, and (3) contrasting these novel methods to state-of-the-art embedding techniques. The **20 invited** participants headlined with their presentations the scientific program over the three days of the workshop, which was roughly subdivided according to the three big thematic blocks. The program was complemented by **19 non-invited** participants who participated through oral presentations or posters. Thereby, talks were allocated on a first-come first-serve basis. In total, there were **25 talks**, which were 25 minutes in length with 5 minutes of discussion time right after the presentation. Additional, general discussion time was provided at the end of each day. Discussions thereby ranged from detail questions on the presented methods, their applicability or the results to general deliberations on possible future collaborations. The poster session on the evening of the first day further inspired intensive discussions e.g. on the possibilities of using machine learning techniques to try to predict charge transport properties of organic crystals, or reactivities of heterogeneous catalysts as well as shapes of semiconductor clusters used in a solid-state embedding scheme. In total **9 posters** were presented, touching all three of the intended fields of the workshop.

After arrival, registration and a light lunch, the scientific program kicked off with a session on charge transport and organic semi-conductors. Jochen Blumberger (UC London, UK), Denis Andrienko (MPI Mainz, DE), and Sibylle Gemming (Helmholtz Zentrum Dresden, DE) presented their coarse grained efforts to study charge transport in organic systems, while Noa Marom (Carnegie Mellon University, USA) discussed machine learning-based crystal structure prediction techniques. In the second session of the first day, Karsten Reuter (TUM, DE) presented a number of solid-state and liquid embedding techniques, geared towards high accuracy studies of surface reactions. Sebastian Matera (Freie Universität Berlin, DE) showed the efficacy of modern interpolation techniques for kinetic studies, while Volker Deringer (University of Cambridge, UK) discussed applying machine learned potentials to sample disordered carbon structures. The following discussion session saw mixed questions to all the speakers of the day in front of the full panel. The scientific program of the second day kicked of with a session on modern embedding approaches, with talks given by Thomas Miller (Caltech, USA) on QM/QM embedding, Andrew Logsdail (University of Cardiff, UK) on solid state QM/MM, and Nicolas Hörmann (EPFL, CH) on implicit solvation and its effects. The rest of the day, the focus then lay on machine learning and coarse graining to either generate advanced potentials or derive structure/function relationships. Talks were given by Matthias Rupp (Fritz Haber Institute, DE), Milica Todorovic (Aalto University, FI), Pavlo Dral (MPI Mülheim, DE), and Tristan Bereau (MPI Mainz, DE). This was followed by a session of contributed talks, following the same topics. The final day of the workshop started with a session on tight binding and semi-empirics, parametrised from first principles with presentations by Thomas Hammerschmidt (Ruhr Universität Bochum, DE), Tim Clark (FAU Erlangen, DE), and Bernd Meyer (FAU Erlangen, DE).

The final session of the workshop was dedicated to presentations by Bernd Hartke (Universität Kiel, DE), Jörg Behler (Göttingen University, DE), and Patrick Rinke (Aalto University, FI)

In summary, the workshop succeeded in bringing together experts in embedding, machine learning and coarse graining for a lively exchange of ideas. This exchange is intended to help foster future collaborations for a synthesis of methods otherwise not easily reachable. The workshop also had a high percentage of participants currently working to obtain their PhD degrees, helping them to gain a more complete overview of the theoretical methods available and to place their own research into an international context. The workshop had a strong international participation, with **20 foreign participants**, further helping to connect the German research community to its international counterparts. Feedback taken afterwards showed a very high degree of satisfaction among all of the participants. We therefore consider our workshop very successful in attaining the stated goals.

3 Detailed Scientific Program

3.1 List of Participants

Prof. Bernd Meyer (I)	Dr. Denis Andrienko (I)	Dr. Peter Brommer
Prof. Jochen Blumberger (I)	Dr. Tristan Bereau (I)	Dr. Simon Rittmeyer
Prof. Jörg Behler (I)	Dr. Andrew Logsdail (I)	Dr. Petr Grigorev
Prof. Noa Marom (I)	Dr. Milica Todorovic (I)	Dr. Chiara Panosetti
Prof. Tim Clark (I)	Dr. Sebastian Matera (I)	MSc. Riccardo Alessandri
Prof. Karsten Reuter (I)	Dr. Thomas Hammerschmitt (I)	MSc. Selim Sami
Prof. Bernd Hartke (I)	Dr. Volker Deringer (I)	MChem. Harry Jenkins
Prof. Patrick Rinke (I)	Dr. Harald Oberhofer	MSc. Jakob Filser
Prof. Sibylle Gemming (I)	Dr. Mie Andersen	MSc. Sina Stocker
Prof. Florian Libisch	Dr. Johannes Margraf	MSc. Christian Kunkel
Dr. Pavlo Dral (I)	Dr. Gautam Anand	MSc. Christoph Muschielok
Dr. Matthias Rupp (I)	Dr. Berk Onat	MSc. Matthias Kick
Dr. Thomas Miller (I)	Dr. Peng Chen	MSc. Annika Stuke
Dr. Nicolas Hörmann (I)	Dr. Joaquin Miranda	

(I) indicates invited speakers (20 in total). In total, the workshop had 41 participants, 32 of which had a doctoral degree or higher. 9 PhD students actively participated in the workshop, either giving talks or presenting posters. Half of the participants came from foreign institutions, mostly within the EU, but also two colleagues from the USA participated. 15% of the participants were female (invited speakers + non-invited participants).

3.2 Workshop Program

	Monday	Tuesday	Wednesday
09:00		Thomas Miller	Thomas Hammerschmidt
09:30	Arrival	Andrew Logsdail	Tim Clark
10:00		Nico Hörmann	Bernd Meyer
10:30		Refreshment Break	Refreshment Break
11:00	Registration	Petr Grigorev	Bernd Hartke
11:30		Matthias Rupp	Jörg Behler
12:00		Workshop Picture	Patrick Rinke
12:30	Lunch		
13:00		Lunch	Lunch
13:30	Jochen Blumberger		
14:00	Denis Andrienko	Milica Todorovic	Discussions Day 3
14:30	Sibylle Gemming	Pavlo Dral	
15:00	Noa Marom	Tristan Bereau	Wrap-up & Farewell
15:30	Refreshment Break	Refreshment Break	
16:00	Karsten Reuter	Florian Libisch	Departure
16:30	Sebastian Matera	Berk Onat	
17:00	Selim Sami	Peter Brommer	
17:30	Volker Deringer	Discussions Day 2	
18:00	Discussions Day 1		
18:30			
19:00			
19:30	Dinner & Poster Session	Conference Dinner	
20:00			
20:30			
21:00			