CPP 14: Condensed-Matter Simulations augmented by Advanced Statistical Methodologies (joint session DY/CPP)

Time: Friday 10:00–11:00 Location: H2

CPP 14.1 Fri 10:00 H2

Simple model to describe stability of thin domains — •Ruben Khachaturyan[1], Arne J. Klomp[2], Karsten Albe[2], and Anna Anna Grünebohm[1] — [1]Interdisciplinary Center for Advanced Materials Simulation, Ruhr-University Bochum — [2]Department of Materials Science, Technical University of Darmstadt, Darmstadt, Germany

Ferro domains are important for contemporary electronics, particularly decreasing domain size allowing for denser information storage per unit area. Thermal fluctuations limit domain stability, which is the key property for ferroic data storage. Therefore the ability to estimate the expected lifetime of a domain is of crucial importance. In this work, we simulate 180° domains in BaTiO3 with different widths at various temperatures using ab initio based molecular dynamics simulation employing LAMMPS and feram codes. We then derived a model to analyze the lifetime of the domains depending on their width and temperature. The model treats domain walls as fluctuating strings. String stiffness reflects the information about energy for domain wall roughening and thermal fluctuations are considered as a field of random forces. Our findings allowed us to interpret the stochastic nature of thin domain collapses and identify associated energies. With further development of the model, we are planning to consider the behavior of ferroelastic and ferromagnetic domain walls.

CPP 14.2 Fri 10:15 H2

Population Annealing Monte Carlo Using the Rejection-Free n-Fold Way Update Applied to a Frustrated Ising Model on the Honeycomb Lattice — •Denis Gessert[1,2] and Martin Weigel[1,3] — [1]Centre for Fluid and Complex Systems, Coventry University, Coventry, CV1 5FB, United Kingdom — [2]Institut für Theoretische Physik, Leipzig University, Postfach 100920, D-04009 Leipzig, Germany — [3]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

Population annealing (PA) is a MC method well suited for the study of systems with a rough free energy landscape, e.g. glassy systems. PA is similar to an equilibrium version of parallel simulated annealing runs with the addition of a resampling step at each temperature. While a large population may improve imperfect equilibration, it is evident PA will fail when almost no spins are flipped in the equilibration routine.

This is the case in systems with a low temperature phase transition where high Metropolis rejection rates make sampling phase space near infeasible. To overcome this slowdown we propose a combination of the PA framework with the rejection-free "n-fold way" update and achieve an exponential speed-up at low temperatures compared to Metropolis.

To test our method we study the Ising model with competing ferromagnetic nearest and antiferromagnetic next-to-nearest neighbor interactions of strengths $J_1 > 0$ and $J_2 < 0$, resp., on the honeycomb lattice. As T_c becomes arbitrarily small, when approaching the special point $J_2 = -J_1/4$ with $T_c = 0$, we consider this a good choice to test the efficacy of our method.

CPP 14.3 Fri 10:30 H2

Noncontact friction: The role of viscous friction and its non-universality — •Miru Lee[1], Niklas Weber[2], Richard Vink[2], Cynthia Volkert[2], and Matthias Krüger[1] — [1]Institut für Theoretische Physik, Friedrich- Hund-Platz 1, 37077 Göttingen — [2]Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

Obtaining theoretical predictions for friction during sliding motion is challenging due to the complex nature of the problem. In the so-called noncontact regime, the friction tensor is given by the leading order of the pairwise interactions between the probe and the surface atoms [1]. In such a regime, one can thus find an analytic expression of the friction tensor [2]. Starting from a stochastic viscoelastic solid model, we identify the two paradigmatic dissipation mechanisms [3]: phonon radiation, prevailing even in a purely elastic solid, and phonon damping, e.g., caused by viscous motion of crystal atoms. At small probe-surface separations, phonon damping dominates over phonon radiation, and vice versa at large separations. Phonon radiation is furthermore universal; there exists a general one-to-one mapping between the mean probe-surface force and the resulting friction. In contrast, phonon damping is non-universal, and no such general relation exists; it is subject to the details of the underlying pairwise interaction, e.g., the interaction range. For certain cases, the friction can even *decrease* with increasing surface area the probe interacts with.

[1] M. Lee, R. Vink, M. Krüger, Phys. Rev. B **101**, 235426 (2020)
[2] A. I. Volokitin, et. al., Phys. Rev. B **73**, 165423 (2006)
[3] M. Lee, R. Vink, C. Volkert, M. Krüger, In preparation.

CPP 14.4 Fri 10:45 H2

Investigation of transferability in LDOS based DFT surrogate models for multiscale simulations — •Lenz Fiedler[1,2] and Attila Cangi[1,2] — [1]Center for Advanced Systems Understanding (CASUS) — [2]Helmholtz-Zentrum Dresden-Rossendorf

Density Functional Theory (DFT) is one of the most important computational tools for materials science, as it combines high accuracy with general computational feasibility. However, applications important to scientific progress can pose problems to even the most advanced and efficient DFT codes due to size and/or complexity of the underlying simulations. Namely the modeling of materials across multiple length and time scales at ambient or extreme conditions, necessary for the understanding of important physical phenomena such as radiation damages in fusion reactor walls, evade traditional ab-initio treatment. DFT surrogate models are a useful tool in achieving this goal by reproducing DFT results at drastically reduced computational cost by using machine learning methods. Yet, a lack of transferability of many approaches lead to repeated and costly training data generation procedures. Here, we present results of an investigation to transfer such machine learning DFT surrogate models between different simulation cell sizes, with the goal of reducing the overall amount of computational time for training data generation. The models are based upon the Materials Learning Algorithms (MALA) package [1] and the therein implemented LDOS based machine learning workflow [2].

[1]: https://github.com/mala-project
[2]: J. A. Ellis et al., Phys. Rev. B 104, 035120, 2021