CPP 34: Condensed Matter Simulations augmented by Advanced Statistical Methodologies II (joint session DY/CPP)

Time: Tuesday 14:00–15:15 Location: BH-N 128

CPP 34.1 Tue 14:00 BH-N 128

Nonlinear Network description for many-body quantum systems in continuous space — •Markus Holzmann[1], Michele Ruggeri[2], and Saverio Moroni[3] — [1]LPMMC, UMR 5493 of CNRS, Université Grenoble Alpes, F-38100 Grenoble France — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [3]DEMOCRITOS National Simulation Center, Istituto Officina dei Materiali del CNR and SISSA, Via Bonomea 265, I-34136 Trieste, Italy

We show that the recently introduced iterative backflow renormalization [1] can be interpreted as a general neural network in continuum space with non-linear functions in the hidden units [2]. We use this wave function within Variational Monte Carlo for fermionic and bosonic liquid helium in two and three dimensions, where we typically find a tenfold increase in accuracy over currently used wave functions. For two dimensional 4 He, we also show that the iterative backflow wave function can describe both the liquid and the solid phase with the same functional form - a feature shared with the Shadow Wave Function, but now joined by much higher accuracy.

[1] M. Taddei, M. Ruggeri, S. Moroni, and M. Holzmann, Phys. Rev. B 91, 115106 (2015).

[2] M. Ruggeri, S. Moroni, and M. Holzmann, cond-mat/1711.01993 (2017).

CPP 34.2 Tue 14:15 BH-N 128

Massively parallel multicanonical simulations — Jonathan Gross[1], •Johannes Zierenberg[2], Martin Weigel[3], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, D 04009 Leipzig, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany, — [3]Applied Mathematics Research Centre, Coventry University, Coventry CV1 5FB, England

Generalized-ensemble Monte Carlo simulations such as the multicanonical method and similar techniques are among the most efficient approaches for simulations of systems undergoing discontinuous phase transitions or with rugged free-energy landscapes. As Markov chain methods, they are inherently serial computationally. It was demonstrated recently, however, that a combination of independent simulations that communicate weight updates at variable intervals allows for the efficient utilization of parallel computational resources for multicanonical simulations. Implementing this approach for the many-thread architecture provided by current generations of graphics processing units (GPUs), we show how it can be efficiently employed with of the order of 10^4 parallel walkers and beyond, thus constituting a versatile tool for Monte Carlo simulations in the era of massively parallel computing. We provide the fully documented source code for the approach applied to the paradigmatic example of the two-dimensional Ising model as starting point and reference for practitioners in the field.

CPP 34.3 Tue 14:30 BH-N 128

Multiferroic properties of HoMn2O5 compounds: A Monte Carlo Study — •A.S ERCHIDI ELYACOUBI, R Masrour, and A Jabar — Cady Ayyed University, National School of Applied Sciences, PB 63 46000, Safi, Morocco.

The class of HoMn2O5 compounds offers multiferroic properties where the refined magnetic zig-zag order breaks the inversion symmetry. The polarization and magnetization are found. The ferroelectric transition temperature are determined. The polarization is induced solely by different exchange couplings of the two different Mn4+ and Mn3+ magnetic ions. The magnetic and ferroelectric cycle have been deduced. The variation of the polarization by an external magnetic field depends strongly on the direction of that field. HoMn2O5 compounds;

CPP 34.4 Tue 14:45 BH-N 128

Identifying the relevant degrees of freedom in mesoscale models of liquid water with Bayesian formalism — •Julija Zavadlav and Petros Koumoutsakos — Computational Science and Engineering Laboratory, ETH Zurich, Zurich, CH-8092, Switzerland

Coarse-graining (CG) has become an established methodology in molecular modeling to access time and length scales that are computationally beyond the reach of the conventional atomistic simulations. However, it often involves making several a priori assumptions, which are rarely systematically addressed. Typically, these assumptions pertain to the level of coarse-graining and the model complexity. We address this issue for mesoscale models of liquid water by investigating on an equal footing a number of CG models that differ in the level of coarse-graining and in the model complexity. To this end, we deploy the classical as well as a novel Hierarchical Bayesian methods [1,2] to quantify and calibrate the uncertainty of the models and to perform the model selection using the experimental data. Furthermore, we assess the efficiency-accuracy trade-off of developed models and provide guidelines for future water model design at the mesoscopic scale.

[1] S.Wu, P. Angelikopoulos, G. Tauriello, C. Papadimitriou, and P. Koumoutsakos, J. Chem. Phys. 145, 244112, 2016.

[2] L. Kulakova, G. Arampatzis, P. Angelikopoulos, P. Hadjidoukas, C. Papadimitriou, and P. Koumoutsakos, Sci. Rep., 7, 16576, 2017

CPP 34.5 Tue 15:00 BH-N 128

Data driven inference for the repulsive exponent of the Lennard-Jones potential in molecular dynamics simulations — •Georgios Arampatzis and Petros Koumoutsakos — Computational Science and Engineering Laboratory, Clausiusstrasse 33, ETH Zürich, CH-8092, Switzerland

The Lennard-Jones (LJ) potential is a cornerstone of Molecular Dynamics (MD) simulations and among the most widely used computational kernels in science. The LJ potential models atomistic attraction and repulsion with century old prescribed parameters ($q = 6$, $p = 12$, respectively), originally related by a factor of two for simplicity of calculations. We propose the inference of the repulsion exponent through Hierarchical Bayesian uncertainty quantification We use experimental data of the radial distribution function and dimer interaction energies from quantum mechanics simulations. We find that the repulsion exponent $p \approx 6.5$ provides an excellent fit for the experimental data of liquid argon, for a range of thermodynamic conditions, as well as for saturated argon vapour. Calibration using the quantum simulation data did not provide a good fit in these cases. However, values $p \approx 12.7$ obtained by dimer quantum simulations are preferred for the argon gas while lower values are promoted by experimental data. These results show that the proposed LJ 6-p potential applies to a wider range of thermodynamic conditions, than the classical LJ 6-12 potential. We suggest that calibration of the repulsive exponent in the LJ potential widens the range of applicability and accuracy of MD simulations.