CPP 28: Condensed Matter Simulations augmented by Advanced Statistical Methodologies I (joint session DY/CPP)

Time: Tuesday 11:00–12:30 Location: BH-N 334

CPP 28.1 Tue 11:00 BH-N 334

Markov State Modeling of Sliding Friction — •Martina Teruzzi — SISSA (International School for Advanced Studies), Trieste

Friction, despite being a well-known and studied phenomenon, still lacks a general theory or approach, mainly due to the presence of many degrees of freedom and the difficulty in identifying few relevant collective variables. We propose a method based on Markov State Modeling, a technique aimed at reducing the dimensionality of the system, by singling out the relevant slow timescales and the observables that best describe them. After successful application to a small toy model (1D Frenkel-Kontorova) we now apply this approach to more complicated systems, identifying few significant states that best characterize them through a rather general and automatic algorithm. This approach can provide insight into the main mechanisms of new frictional systems and, in perspective, could be enhanced by biased sampling to achieve a proper description of rare events, difficult to be sampled by standard dynamics.

CPP 28.2 Tue 11:15 BH-N 334

Loss of Memory in Dense Sheared Particulate Systems — •Lou Kondic[1], Lenka Kovalcinova[1], Miro Kramar[2], and Konstantin Mischaikow[3] — [1]NJIT, Newark, NJ, USA — [2]INRIA Saclay, Paris, France — [3]Rutgers, Piscataway, NJ, USA

We carry out discrete element/MD simulations of dense sheared particulate systems, with the focus on understanding and characterizing dynamical properties of force networks that develop on the mesoscale. These force networks are known to play a crucial role in connecting microscale dynamics of the particles and macroscopic properties of the whole system. The results of the simulations are analysed using topological tools, that allow to fully quantify and even compare the states of the system. These tools identify in an objective and precise manner the time interval needed for the system to loose its memory, or in other words, the time interval after which any information about system state is lost. We will show that the process of memory loss may differ even if the inertial number, measuring the ratio of inertial to imposed forces, is kept constant.

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CPP 28.3 Tue 11:30 BH-N 334

Adaptive population Monte Carlo simulations — •Martin Weigel[1], Lev Yu. Barash[2,3], Lev N. Shchur[2,3,4], and Wolfhard Janke[5] — [1]Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England — [2]Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia — [3]Science Center in Chenogolovka,142432 Chernogolovka, Russia — [4]National Research University Higher School of Economics, 101000 Moscow, Russia — [5]Institut für Theoretische Physik, Universität Leipzig, Postfach 100920 04009, Leipzig, Germany

Population annealing is a sequential Monte Carlo scheme that is potentially able to make use of highly parallel computational resources. Additionally, it promises to allow for the accelerated simulation of systems with complex free-energy landscapes, much alike to the much more well known replica-exchange or parallel tempering approach. We equip this method with self-adaptive schemes for choosing the algorithmic parameters, including the temperature and sweep protocols as well as the population size. The resulting method is significantly more efficient for simulations of systems with complex free-energy landscapes than some more traditional approaches, and it is particularly well suited for massively parallel computing environments such as (clusters of) GPUs.

CPP 28.4 Tue 11:45 BH-N 334

Diagnostics of neural networks for machine learning phases and phase transitions — •Philippe L. Suchsland and Stefan Wessel — RWTH Aachen University, Aachen, Germany

Machine learning schemes based on neural networks have recently been proposed as new tools for classifying phases of matter as well as detecting phase transitions. One motivation behind such proposals is the ability of appropriately designed and trained neural networks to identify patterns from a large set of data without having to explicitly describe them. We apply both supervised and unsupervised machine learning schemes to basic models of statistical physics. In particular, we consider the 2D Ising model in the presence of extended domain-wall configurations as well as the 2D XY model that exhibits a Kosterlitz-Thouless transition. In both cases, we identify the physical properties of the models that are relevant for the classification task. This reveals how reliable these schemes are with respect to minimizing the amount of preprocessing of bare sample configurations before feeding them into the learning process.

CPP 28.5 Tue 12:00 BH-N 334

Hyperdynamics approach to the non-equilibrium states coupled to the thermal bath — •Yuri S. Nagornov and Ryosuke Akashi — University of Tokyo, Department of Physics, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

Efficient numerical simulation method for rare events driven by thermal fluctuation has long been a hot topic in a wide range of fields in condensed-matter physics. The target phenomena in this context, such as crystal nucleation, atomic diffusion etc., occur in time scales of microseconds or even longer and are intractable by atomistic molecular dynamics simulation. Solutions to this problem have long been attempted by introducing collective variables to seek for escape paths and/or efficiently sampling the phase space to represent the canonical ensemble. However, an ideal approach is rather desired (i) not to respect the prior knowledge of appropriate collective variables and (ii) not to require the system to reach the thermal equilibrium since many of the above mentioned phenomena can occur under non-equilibrium situations. Along the line of the Langer*s theory, we formulate a differential equation for the distribution of the variables that evolve on an elevated potential surface under thermal fluctuation, from which its real probability of realization can be retrieved. This formalism enables us non-empirical exploration of rare events and evaluation of its probability to occur simultaneously. An algorithm with a modified form of the Langevin molecular dynamics is thereby constructed, which is in spirit an extension of the hyperdynamics approach. Applications to simple model systems will be presented.

CPP 28.6 Tue 12:15 BH-N 334

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