MM 55: Methods in Computational Materials Modelling III: Machine learning and statistics

Time: Thursday 11:45–13:00 Location: H53

MM 55.1 Thu 11:45 H53

Gaussian approximation potentials: the case of α-iron — •Daniele Dragoni[1], Tom Daff[2], Gábor Csányi[2], and Nicola Marzari[1] — [1]Theory and Simulation of Materials (THEOS), and National Center for Computational Design and Discovery of Novel Materials (MARVEL), École polytechnique fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Engineering Laboratory, University of Cambridge, Trumpington Street, Cambridge, CB2 1PZ, United Kingdom

Interatomic potentials are typically based on functional forms driven by physical intuition and fitted to experimental or computational data. The moderate flexibility of these functional forms limits their ability to be systematically improved by increasing the fitting datasets, although ensuring a modicum degree of transferability. Recently, a novel trend has emerged where potential-energy surfaces are represented by neural networks fitted on large numbers of first-principles calculations, thus maximizing flexibility but requiring extensive datasets to ensure transferability. Gaussian Approximation Potentials in particular are a novel class of potentials based on non-linear, non-parametric Gaussian-process regression. We apply this approach to the case of α-iron, training a GAP model from energies, stresses and forces taken from first-principles molecular dynamics simulations of pristine and defected bulk systems, and of surfaces with different crystallographic orientations, covering roughly 10^5 local atomic environments. Finally, we verify this GAP model by comparing its predicted structural, vibrational, and thermodynamic properties against those derived from first-principles.

MM 55.2 Thu 12:00 H53

Local Pattern Discovery for Uncovering Physically Interpretable Characterizations of Material Configurations — •Mario Boley, Bryan R. Goldsmith, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin.

Currently, machine learning applications to data from atomistic material simulations mostly focus on the inference of a global prediction model for some quantities of interest, such as (relative) energies. However, due to their global prediction-based objective, these models are usually not well suited for the discovery of physically interpretable characterizations of *local* groups of subsets of material, in particular when aiming at partitioning the configurational space of a system at finite temperature.

In contrast to predictive global modelling, local pattern discovery techniques directly aim to uncover specific local properties of the data. Moreover, they describe these properties through models that are built from discrete symbols corresponding to meaningful notions of the discovery domain. Therefore, they constitute an important complimentary part of the data mining toolbox for the automatic analysis of materials-science data repositories. As an exemplary application of local pattern discovery for materials science, we consider the automatic discovery of configurational basins of gold clusters and their characterization in terms of interpretable features such as their coordination histogram and their moments of inertia, or (non-linear) functions of those features.

MM 55.3 Thu 12:15 H53

Automated Convergence Checks with the Python Based Library PyIron — •Jan Janssen, Tilmann Hickel, and Joerg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Over the last years methodological and computational progress in atomistic simulations has substantially improved the predictive power in materials design. To guarantee the desired numerical precision, simulation tools that run the necessary complex simulation protocols and convergence checks automatically are critical but scarce. Based on our recently developed PyIron library which provides an efficient framework to implement such protocols we have developed an automatized tool for fitting the Birch-Murnaghan equation of states with prescribed accuracy targets. The tool includes an approach to handle the intrinsic energy fluctuation in DFT simulations. By making a Monte-Carlo based sensitivity analysis that includes the intrinsic model errors as well as the energy fluctuations we determine the numerically most efficient volume range for the approximation. The achievable accuracy as well as the performance gains of such an approach will be discussed.

MM 55.4 Thu 12:30 H53

Examination of electrolyte diffusion in dye-sensitized solar cells using virtual random walk — •Tomasz Blachowicz[1], Andrea Ehrmann[2], Hafed Zghidi[3], and Maksym Walczak[3] — [1]Silesian University of Technology, Institute of Physics, Gliwice, Poland — [2]Bielefeld University of Applied Sciences, Faculty of Engineering Sciences and Mathematics, Bielefeld (Germany) — [3]Silesian University of Technology, Faculty of Automatic Control, Electronics and Computer Science, Gliwice (Poland)

Statistical analysis of optically captured microphotographs revealing different physical phenomena is an important research tool, supporting other standard experimental and theoretical research efforts. The statistical analysis relies on performing a virtual random walk on positions where the matter exists. Thus, this is especially suited for spatial and structural analysis of different materials.

The method enables recognition, in a quantitative way, and characterization of difference spatial elements, their sizes and frequencies of occurence. A parameter describing these properties is so called Hurst exponent.

In the current work, results from analysis of different scenarios from liquid/solid state interaction at interfaces, e.g. dyestuff on TiO2 layers on glass or textile, are examined. Image sequences obtained enable identification of uniformity levels for the liquid phase spread on a solid substrate.

MM 55.5 Thu 12:45 H53

Quantitative analysis of the interface layers in textile-3D print composites by image processing — •Andrea Ehrmann[1], Tomasz Blachowicz[2], Hafed Zghidi[3], Maksym Walczak[3], and Nils Grimmelsmann[1] — [1]Bielefeld University of Applied Sciences, Faculty of Engineering Sciences and Mathematics, Bielefeld, Germany — [2]Silesian University of Technology, Institute of Physics, Gliwice, Poland — [3]Silesian University of Technology, Faculty of Automatic Control, Electronics and Computer Science, Gliwice (Poland)

Computational materials modeling is nowadays standard research technique as a counterpart to classical experimental and theoretical activity.

In this work we identify different solid-state phases derived from analysis of grey-scaled two-dimensional images captured optically. An original image was split into virtual sub-layers falling into different ranges at the grey-level level. Numerical analysis performed at the sub-images was carried out using a random walk approach. The method enables quantitative diagnosis of different material components and differentiation between samples prepared at different physical conditions.

We will depict results of cross section micrographs taken from FDM printing with different thermoplastics on textile substrates, allowing for giving a quantitative description of the interface layer structure.