DY 17: Modeling and Data Analysis

Time: Tuesday 9:30–12:00 Location: BH-N 333

DY 17.1 Tue 9:30 BH-N 333

Structure, equation of state and transport properties of molten calcium carbonate (CaCO_3) from atomistic simulations — Rodolphe Vuilleumier[1], •Ari Paavo Seitsonen[1,2], Nicolas Sator[3], and Bertrand Guillot[3] — [1]Département de Chimie, École Normale Supérieure Paris, France — [2]Institut für Chemie, Universität Zürich, Switzerland — [3]Sorbonne Universités, Université Paris 6 et CNRS, UMR 7600, LPTMC, Paris, France

We have performed first-principle molecular dynamics (FPMD) simulations to evaluate the physical properties (liquid structure, density, atomic vibrational motion, diffusion coefficients and electrical conductivity) of liquid calcium carbonate (CaCO_3), which are up to now poorly known. As compared with silicate melts, molten CaCO_3 is characterized by a low density, a viscosity almost as low as that of water and a high conductivity. An empirical force field has been developed for predicting the properties of molten CaCO_3 at any state point in the liquid stability field and used in classical MD simulations, from which the equation of state and the phase diagram of the liquid phase have been obtained. The self diffusion coefficients, viscosity, and the electrical conductivity with pressure and temperature have been investigated and the results fitted to analytical forms. It is shown that the Stokes-Einstein equation, expressing the viscosity as a function of diffusion motion, is followed and that the Nernst-Einstein equation relating the electrical conductivity to the diffusion coefficients of charge carriers leads to an accurate prediction of the conductivity when a constant correcting factor is applied.

DY 17.2 Tue 9:45 BH-N 333

Optical detection of infrared and Raman modes in $NdFeO_3$ under pressure * theory and experiment — •K. M. Lebecki[4], D. Legut[5], M. Mihalik jr.[1], M. Míšek[2,6], M. Vávra[1,3], M. Mihalik[1], K. V. Kamenev[2], and M. Zentková[1] — [1]Institute of Experimental Physics, Slovak Academy of Sciences, Košice, Slovak Republic — [2]Centre for Science at Extreme Conditions, University of Edinburgh, Edinburgh, United Kingdom — [3]Institute of Chemistry, Faculty of Science, P. J. Šafarik University, Košice, Slovak Republic — [4]Nanotechnology Centre, VSB Technical University of Ostrava, Ostrava-Poruba, Czech Republic — [5]IT4Innovations Centre, VSB Technical University of Ostrava, Ostrava-Poruba, Czech Republic — [6]Faculty of Mathematics and Physics, Charles University in Prague, Czech Republic

We determine lattice vibrations in $NdFeO_3$ crystal using first-principles calculations. We assign them to Raman- and infrared active modes according to the group theory. The direct method is used to obtain the Hellman-Feynman forces. The supercell approach with the finite displacement method is used to calculate phonon properties. Lattice vibrations, phonon density of states, dispersion curves, etc. are obtained by the Phonopy program within harmonic approximation. Finally, our results are compared with other calculations using interatomic force constants and with our Raman experimental data for pressures up to 110 kbar.

DY 17.3 Tue 10:00 BH-N 333

Optimizing Large-Scale ODE Simulations — •Mario Mulansky — Institute for Complex Systems (ISC), CNR, Sesto Fiorentino, Firenze, Italy

Efficient computational methods are crucial in many parts of science. Here, we present a strategy to speed up Runge-Kutta-based ODE simulations of large systems with nearest-neighbor coupling. By introducing granularity we are able to transform the algorithm from bandwidth bound to CPU bound. By additionally employing SIMD instructions we are able to boost the efficiency even further. In total, a performance increase of up to a factor three is reached when using cache optimization and SIMD instructions compared to a standard implementation.

DY 17.4 Tue 10:15 BH-N 333

A Bayesian method for the analysis of deterministic and stochastic time series — •Coryn Bailer-Jones — Max Planck Institute for Astronomy, Heidelberg, Germany

I introduce a general, Bayesian method for modelling univariate time series data assumed to be drawn from a continuous, stochastic process. The method accommodates arbitrary temporal sampling, and takes into account measurement uncertainties for arbitrary error models (not just Gaussian) on both the time and signal variables. Any model for the deterministic component of the variation of the signal with time is supported, as is any model of the stochastic component of the signal and time variables. The posterior probability distribution over model parameters is determined via Markov Chain Monte Carlo sampling. Models are then compared using the "cross-validation likelihood", a version of the Bayesian evidence which is less sensitive to the prior. I illustrate the method on astronomical time series data using both deterministic models and a purely stochastic model, the Ornstein-Uhlenbeck process. This latter process appears to be a good description of several astronomical phenomena, including the flux variability of objects as different as brown dwarfs and active galactic nuclei.

DY 17.5 Tue 10:30 BH-N 333

Learning equations of motion from sparse observations — •Andreas Ruttor, Philipp Batz, and Manfred Opper — Technische Universität Berlin

Equations of motion describe the dynamics of a system in terms of differential equations. These can be derived from theory if all the relevant properties are exactly known. But for real devices, e.g. robots, this is usually not the case. Instead one can drive the system applying a noisy control force and learn the equations of motion by observing its behavior. For that purpose we use a non-parametric approach based on Gaussian process regression, which does not require a detailed model of the dynamics, but still allows to include prior knowledge. As our method is based on estimating the probability distribution in phase space, it works with sparse observations, where the time intervals between data points are large.

DY 17.6 Tue 10:45 BH-N 333

State estimation and observability analysis employing delay coordinates — •Ulrich Parlitz[1,2], Jan Schumann-Bischoff[1,2], and Stefan Luther[1,2] — [1]Max Planck Institute for Dynamics and Selforganization, Göttingen, Germany — [2]Institute for Nonlinear Dynamics, Georg-August-Universität Göttingen, Germany

For many dynamical processes in physics and other fields of science a model is known, but some of its variables and parameter values are difficult to observe or measure directly. In this case one may try to estimate the unknown quantities by adapting the model to time series generated by the process of interest. We shall revisit this problem by addressing the question whether the estimation problem is solvable in principle (observability) [1,2] and how synchronization based estimation methods can be improved to achieve good estimates based on few observables, only [3]. For both tasks delay coordinates will be employed and the main concepts will be illustrated using examples including the Lorenz-96 model and other chaotic systems.

[1] U. Parlitz, J. Schumann-Bischoff, and S. Luther, Phys. Rev. E 89, 050902(R) (2014).

[2] U. Parlitz, J. Schumann-Bischoff, and S. Luther, Chaos 24, 024411 (2014).

[3] D. Rey, M. Eldridge, M. Kostuk, H.D.I. Abarbanel, J. Schumann-Bischoff, U. Parlitz, Physics Letters A 378, 869-873 (2014).

15 min. break

DY 17.7 Tue 11:15 BH-N 333

A new typology of El Niño and La Niña phases based on evolving climate networks — •Marc Wiedermann[1,2], Alexander Radebach[2,3], Reik V. Donner[1], Jonathan F. Donges[1,4], and Jürgen Kurths[1,2] — [1]Potsdam Insitute for Climate Impact Research, Germany — [2]Humboldt University, Berlin, Germany — [3]Mercator Research Institute on Global Commons and Climate Change, Berlin, Germany — [4]Stockholm Resilience Centre, Stockholm University, Sweden

The El Niño Southern Oscillation (ENSO) has a large impact on the global climate system. Its variability can roughly be categorized into El Niño (anomalously warm), La Niña (anomalously cold) and normal periods. Recently, it has been suggested that El Niño and La Niña can be further discriminated into two different types. However, no formal criterion for this distinction has been introduced so far. Here, we use evolving climate networks from daily surface air temperature

fields and investigate the time-evolution of their structural properties. During certain El Niño and La Niña periods global network measures show distinct peaks indicating an induced reorganization of the global climate system. For ENSO events without such reorganization, we find substantially different spatial patterns of degree and other local measures than for the other events. This observation can be attributed to the general signature of normal vs. anomalous ENSO events. In this spirit, characteristics involved in the assessment of evolving climate networks allow to detect structural similarities between different ENSO periods and systematically categorize these different stages.

DY 17.8 Tue 11:30 BH-N 333

Eigenvalue Density of the Doubly Correlated Wishart Model: Exact Results — •Daniel Waltner, Tim Wirtz, and Thomas Guhr — Fakultät für Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

Data sets collected at different times and different observing points can possess correlations at different times *and* at different positions. The doubly correlated Wishart model takes both into account. We calculate the eigenvalue density of the Wishart correlation matrices using supersymmetry. In the complex case we obtain a new closed form expression which we compare to previous results in the literature. In the much more complicated real case we derive an expression for the density in terms of a fourfold integral. Finally, we calculate the density in the limit of large correlation matrices.

DY 17.9 Tue 11:45 BH-N 333

Entropy maps of complex excitable dynamics in cardiac cell cultures — •Alexander Schlemmer[1,2], T.K. Shajahan[1], Sebastian Berg[1,2], Stefan Luther[1,2], and Ulrich Parlitz[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, 37077 Göttingen, Germany — [2]Institute for Nonlinear Dynamics, Georg-August-Universität Göttingen, Am Fassberg 17, 37077 Göttingen, Germany

The characterization of spatiotemporal complexity remains a challenging task. This holds in particular for the analysis of data from fluorescence imaging (optical mapping), which allows for the measurement of membrane potential and intracellular calcium at high spatial and temporal resolution. Hitherto methods include dominant frequency maps and the analysis of phase singularities. While these methods address some important aspects of cardiac dynamics, however they only consider very specific properties of excitable media.

We implemented several information-theoretical quantities derived from symbolic chains and wavelet-spectra. Using optical mapping from embryonic chicken cell culture experiments the methods have been validated and benchmarked. We discuss our findings with respect to dominant frequency maps and analysis of phase singularities. In this context we present a workflow to preprocess, filter and analyse large amounts of video data using the above techniques.