DY 17: Modeling and Data Analysis

Time: Wednesday 9:30–11:45 Location: ZEU 146

DY 17.1 Wed 9:30 ZEU 146

Analytical solutions for a model of tow-phase-flow in porous media — •Christoph Wolber and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart, Allmandring 3, 70569 Stuttgart

Modeling immiscible two-phase flow in porous media on a macroscopic scale has proven difficult due to hysteresis and residual saturation. The traditional Buckley-Leverett- theory has to resolve these difficulties by explicitly introducing hysteresis into core concepts like capillary pressure and relative permeability. A new approach distinguishes between percolating and non percolating components of the fluid phases (2006b Phys. Rev. E 73 016307). The hysteresis is reproduced and can be linked to the entrapped fluids that are the physical cause of it. Analytical solutions for a hyperbolic limit have been studied with the method of characteristics. They show shocks and rarefaction waves as expected of hyperbolic partial differential equations. In addition to reproducing the results of the traditional theory where they are valid, the new theory can model processes where imbibition and drainage take place at the same time at different sites as well as flow-reversal problems.

DY 17.2 Wed 9:45 ZEU 146

Generation of drainage or imbibition waves from nonconstant initial saturations of trapped disconnected fluid parts during two-phase immiscible displacement — •Rouven Steinle and Rudolf Hilfer — Institut für Computerphysik, Universität Stuttgart, 70569 Stuttgart, Deutschland

For two-phase immiscible displacement in a homogeneous porous medium with spatially constant initial saturation the traditional Darcy theory predicts no changes of the saturations during drainage or imbibition when the boundary saturations are kept constant. The physical content of a recent generalization of the traditional Darcy theory is tested by studying a similar initial and boundary value problem. The generalized theory distinguishes between percolating and nonpercolating (trapped, disconnected) fluid phases [1]. The initial value problem now requires to specify initial profiles separately for the percolating and nonpercolating phases. When the initial nonpercolating profiles are position dependent drainage or imbibition waves may be generated depending on the initial profiles [2]. These results allow to test the generalized theory by comparing its predictions to experiment.

[1] R. Hilfer, *Macroscopic capillarity without a constitutive capillary pressure function*, Physica A, vol. 371, pp. 209, (2006)

[2] A. Monge Sánchez, *Numerical Solutions of Macroscopic Equations for Multiphase Flows in Porous Media*, Master Thesis, (2013)

DY 17.3 Wed 10:00 ZEU 146

Iterative Modellierung elektronischer Verteilungsfunktionen – Auf dem Weg zur Lumineszenz — •Juri Romazanov, Mourad el Kharrazi, Orkhan Osmani und Marika Schleberger — Fakultät für Physik, Universität Duisburg-Essen, Duisburg

Bis heute gibt es keine einheitliche Beschreibung der Dynamik des Elektronengases im Festkörper nach einer Anregung durch schwere, schnelle Ionen ($E > 1$ MeV/u). Ein häufig verwendeter Ansatz ist es, die Dynamik der Elektronen durch eine effektive Temperatur zu modellieren, oder eine Beschreibung im Rahmen kinetischer Methoden. Für die Überpüfung dieser Theorien wurde bisher häufig die modellierte ioneninduzierte Strukturveränderung mit experimentell beobachteten Strukturveränderungen verglichen. Diese "post-mortem" Analysen erlauben es jedoch nicht, Rückschlüsse auf die Kurzzeitdynamik der Elektronen zu ziehen. Um das ioneninduzierte Nichtgleichgewicht der elektronischen Verteilungsfunktion besser zu verstehen, stellen wir im Rahmen dieses Vortrags eine neue Methode vor, welche an die Photolumineszenz-Spektroskopie angelehnt ist. Aus experimentell gemessenen, zeitabhängigen Lumineszenz-Spektren kann die zeitliche Entwicklung der elektronischen Verteilungsfunktion berechnet werden. Umgekehrt lassen sich Lumineszenz-Spektren modellieren, um durch den Vergleich von Experiment und Theorie Rückschlüsse über das ioneninduzierte Nichtgleichgewicht zu ziehen. Diese Modellierung lässt sich mit dem von Rees eingeführten Formalismus [1] effizient durchführen, wie in diesem Vortrag gezeigt wird.

[1] H. D. Rees, J. Phys. Chem. Solids 30, 643 (1969)

DY 17.4 Wed 10:15 ZEU 146

Spin crossover in liquid (Mg,Fe)O from first-principles simulations — •Eero Holmstrom and Lars Stixrude — Department of Earth Sciences, University College London, Gower Street, London WC1E 6BT, UK

When a planet is formed through accretion, it is likely that substantial or complete melting of the body occurs. Understanding the molten state of planetary materials is important, because their solidification sets the initial conditions for the creation and evolution of the lithosphere and atmosphere of planets like the Earth. Using density-functional theory molecular dynamics simulations in conjunction with thermodynamic integration, we model liquid (Mg,Fe)O, the molten phase of the abundant Earth material ferropericlase, at high pressures and temperatures. Firstly, we present a phase diagram of the spin crossover of the Fe ions from a high-spin to a low-spin state with increasing pressure, and predict the equation of state of the melt. Secondly, we compute the electrical conductivity of the liquid. Finally, we assess the implications of our results for the early Earth and other planets.

15 min break

DY 17.5 Wed 10:45 ZEU 146

The fluctuation function of the detrended fluctuation analysis - Investigation of the AR(1) process — •Marc Höll and Holger Kantz — Max-Planck-Institut für Physik komplexer Systeme, Dresden

We derive an analytical expression for the fluctuation function of the first order autoregressive process AR(1) by means of the detrended fluctuation analysis (DFA). This process is short-range correlated and therefore the fluctuation exponent should be $\alpha = \frac{1}{2}$. However the fluctuation function exhibits a crossover between a region with $\alpha > \frac{1}{2}$ and the expected $\frac{1}{2}$. We calculate the crossover point and compare it with the characteristic correlation time of the process.

DY 17.6 Wed 11:00 ZEU 146

Kriging-supported Adaptive Sampling for Non-Oscillatory Central Schemes — •D. G. Roehm[1], R. S. Pavel[2], T. C. Germann[3], and A. L. McPherson[4] — [1]ICP, Universität Stuttgart, Stuttgart, Germany — [2]ECE, University of Delaware, Newark, USA — [3]T1, LANL, Los Alamos, USA — [4]CCS, LANL, Los Alamos, USA

We propose an enhanced adaptive sampling method for heterogeneous multi-scale simulations with stochastic data, based on a non-oscillatory high-resolution scheme for 2D hyperbolic conservation laws. This general framework is used to compute the evolution of a mechanical shock-wave in a perfect copper crystal on the macro-scale by evaluating stress and energy fluxes on the micro-scale. A finite-volume method was used as the macro-scale solver, which launches for every volume element a light-weighted MD simulation (called CoMD) to incorporate details from the micro scale. Since the execution of an MD simulation is rather costly, we reduced the number of actual MD simulations through the use of an adaptive sampling scheme. Our adaptive scheme utilizes a key-value database for ordinary Kriging and a gradient analysis to reduce the number of finer-scale response functions. Kriging estimates an unknown value at a certain location by using weighted averages of the neighboring points. It also provides an error estimate, which we use as trigger for our adaptive scheme. In this contribution we will focus on how the accuracy of the physical values is affected by several thresholds in our adaptive scheme and their connection to the overall performance. The presented adaptive scheme allows for the future inclusion of details present in real materials. (LA-UR-13-29087)

DY 17.7 Wed 11:15 ZEU 146

Optimal model-free prediction of multivariate time series — •Jakob Runge — Potsdam Institute for Climate Impact Research, Potsdam, Germany, and Humboldt University Berlin

We address the problem of predicting a single time series from a set of multivariate predictors in an information theoretic framework. We investigate in how far this can be done optimally given the available information and develop a practical prediction algorithm. The performance and challenges are demonstrated on multivariate nonlinear stochastic delay processes as well as on real data.

DY 17.8 Wed 11:30 ZEU 146

Reconstruction of correlates and construction of surrogates in networked systems — •Annette Witt[1] and Jan Nagler[2] — [1]Max-Planck Institute for Dynamics and Self-Organization and BCCN, Göttingen, Germany — [2]ETH Zürich, Switzerland

Networks with N nodes are considered, each node is associated either to a time series (on the data level) or to its generating stochastic process (on the model level). A link between nodes is represented by a cross correlation functions (ccf), self-loops stand for autocorrelation functions (acf). For the data level we establish conditions for the reconstruction of the complete network from a subnetwork and show that subnetworks which are minimal for reconstruction must connect all N nodes and belong to one of the two network types, namely (i) single-self-loop-trees, where the subnetwork is a tree (i.e. loop-free) with N-1 ccfs and a single acf, and (ii) single-odd-loop-networks, where the given subnetwork consists of N ccfs of which an odd number forms a single loop. For the first time, a parameter-free exact method for the construction of networks on the realization level from networked stochastic processes is given which is employed for generating multi-variate series time with a prescribed cross-spectral matrix. Consequently, the framework is applicable to short- and long-range correlated time series.