SOE 6: Focus Session: GPU Computing (with DY) - Contributed Talks

Time: Monday 15:00–15:45 Location: GÖR 226

SOE 6.1 Mon 15:00 GÖR 226

GPU-accelerated analysis of high frequency financial data — •Florian Dittrich[1], Simon Weisseno[1], Lucas Schabhüser[1], and Tobias Preis[2,3] — [1]Spline Consulting e.V., Johannes Gutenberg University Mainz, Staudinger Weg 9, 55099 Mainz, Germany — [2]Center for Polymer Studies, Department of Physics, 590 Commonwealth Avenue, Boston, MA 02215, USA — [3]Artemis Capital Asset Management GmbH, Gartenstr. 14, 65558 Holzheim, Germany

We apply the concept of general-purpose computing on graphics processing units (GPGPU) to the analysis of time series. We use the recently introduced pattern formation conformity [T. Preis et al., New Journal of Physics 11 (2009) 093024], which quantifies pattern-based complex short-time correlations in a time series, for analyzing high-frequency financial data sets. In addition, we evaluate the predictive power for time series using such pattern-based correlations.

SOE 6.2 Mon 15:15 GÖR 226

Interacting many-body simulations using graphics processing units — •Tobias Kramer — Institute for Theoretical Physics, Uni Regensburg

Already the solution of the interacting classical many-body problem is difficult to achieve, since the integration of the equations of motions couples all positions of the particles contained in the system. Transport calculations in nanodevices require to include the contacts within the simulation and to study the effect of interactions there.

Classical and quantum-mechanical equations of motions can be related by the time-dependent variational principle as we detail for Coulombic interacting electrons in a magnetic field (1). Interacting systems require to carefully consider the questions of self-consistency, since all particles must be linked together and it is not possible to run one particle trajectory after each other. The emergence of an mean-field potential out of a large (10000 electrons!) many-body calculation is shown in (2). The calculation is only possible due to our usage of graphics processing units, which are ideal tools to study interacting systems.

(1) T. Kramer, Two interacting electrons in a magnetic field: comparison of semiclassical, quantum, and variational solutions, arxiv:1009.6051 (2) T. Kramer, V. Krueckl, E. Heller, and R. Parrott Self-consistent calculation of electric potentials in Hall devices, Phys. Rev. B, 81, 205306 (2010)

SOE 6.3 Mon 15:30 GÖR 226

Lattice-Boltzmann Simulations on GPUs — •Dominic Roehm — Institute for Computational Physics Universität Stuttgart

In coarse-grained Molecular dynamics (MD) simulations of large macromolecules, the number of solvent molecules is normally so large that most of the computation time is spent on the solvent. For this reason one is interested in replacing the solvent by a lattice fluid using the Lattice-Boltzmann (LB) method. The LB method is well known and on large length and timescales it leads to a hydrodynamic flow field that satisfies the Navier-Stokes equation. If the lattice fluid should be coupled to a conventional MD simulation of the coarse-grained particles, it is necessary to thermalize the fluid. While the MD particles are easily coupled via friction terms to the fluid, the correct thermalization of the lattice fluid requires to switch into mode space, which makes thermalized LB more complex and computationally expensive.

However, the LB method is particularly well suited for the highly parallel architecture of graphics processors (GPUs). We present a fully thermalized GPU-LB implementation which is coupled to a MD that is running on a conventional CPU using the simulation package ESPResSo (http://www.espressomd.org). This implementation is on a single NVIDIA GTX480 about 50 times faster than on a recent AMD Athlon IIX4 quadcore, therefore replacing a full compute rack by a single desktop PC with a highend graphics card.