NTZ
Naturwissenschaftlich
Theoretisches Zentrum

Universität Leipzig
Fakultät für Physik und
Geowissenschaften
Institut für Theoretische Physik

Joint NTZ-SFB/TRR 102 Colloquium

within Workshop CompPhys17

Am Donnerstag, dem 30.11.2017 um 17:00 Uhr spricht

Prof. Dr. David P. Landau

(Center for Simulational Physics, The University of Georgia, Athens, GA, USA)

über

Complexity and optimization: Physical science meets biological science via computer simulations

Abstract:

Complexity is everywhere in nature, and it often manifests itself in the existence of a rough free energy landscape that is extraordinarily difficult to investigate. Other problems have no free energy but can be mapped onto complex free energy landscapes. Ground state searches correspond to optimization problems, but often knowledge of the thermodynamic behavior at different temperatures is also desired. Computer simulations have become the method of choice for studying a wide variety of systems, but traditional algorithms fail when the free energy has multiple minima and maxima that are widely separated in phase space. We will introduce a generic, parallel Replica Exchange Wang-Landau (REWL) Monte Carlo sampling method that is naturally suited for implementation on massively parallel, petaflop supercomputers. The approach introduces a replica-exchange framework involving densities of states that are determined iteratively for overlapping windows in energy space, each via traditional Wang-Landau sampling. The framework is valid for models of soft and hard condensed matter, including systems of biological interest. The significant scalability, performance advantages, and general applicability of the method are demonstrated using thousands of computing cores for several quite different models of interacting particles. Systems studied may have discrete or continuous degrees of freedom, and include those with both complex free energy landscapes and topological constraints.

Ort: Hörsaal für Theoretische Physik, Linnéstraße 5

Alle Teilnehmer sind ab 16:30 Uhr zu Kaffee und Gebäck in die Aula eingeladen.

gez. Prof. W. Janke