NTZ
Naturwissenschaftlich
Theoretisches Zentrum

Universität Leipzig
Fakultät für Physik und
Geowissenschaften
Institut für Theoretische Physik

Joint NTZ-SFB/TRR 102 Colloquium

within Workshop CompPhys15

Am Donnerstag, dem 26.11.2015 um 17:00 Uhr spricht

Prof. Dr. Dennis C. Rapaport

(Bar-Ilan University, Ramat-Gan, Israel)

über

Simulating emergent phenomena (with GPU-based molecular dynamics)

Abstract:

Emergent phenomena are especially fascinating because they are not obvious consequences of the design of the systems in which they appear, a characteristic equally relevant when attempting to simulate them. Several systems that exhibit surprisingly rich emergent behavior will be described, each studied by MD (molecular dynamics) simulation. (a) In the case of fluids studied at the atomistic level, not only can complex hydrodynamic phenomena in convecting and rotating fluids - the Rayleigh-Benard and Taylor-Couette instabilities - be reproduced within the limited engths and time scales accessible to MD, but there is even quantitative agreement. (b) Modeling self-assembly processes associated with virus capsid growth reveals the ability to achieve complete, error-free shells, where paradoxically, high yields are due to reversible bond formation. (c) Studies of granular mixtures show behavior that, in the case of a rotating drum, reproduces known but counterintuitive axial and radial segregation, and in the case of a vertically vibrated layer, predicts a novel form of horizontal segregation. These simulations tend to be comparatively large and lengthy, and in some cases multiple runs are needed because the outcomes are unpredictable, so the use of GPU-based parallel computing is beneficial; the methodology involved will be outlined. While MD is subject to limitations, both conceptual and computational, the results offer exciting indications of what can be accomplished.

Ort: Kleiner Hörsaal, Linnéstraße 5

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