New NIC Research Group at Jülich Supercomputing Centre

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The partners in the John von Neumann-Institute for Computing (NIC), Jülich Research Centre among them, promote supercomputer-aided research in science and engineering by supporting research groups in selected fields. In April 2011 the NIC research group "Computational Materials Physics" started to work at the Jülich Supercomputing Centre. Its research activities involve atomistic and multiscale simulations of materials in non-equilibrium, in particular in the field of tribology, the analysis of materials under high pressures, and the development of classical force fields, in which the electrostatics of molecular systems is properly described. The group depends heavily on large-scale computational resources and contributes to the development of massively parallel simulation packages. It is lead by Prof. Martin Müser from Saarland University.

It is the main objective of the tribological section of the new NIC research group to develop and to parameterize new constitutive equations that describe interfacial dynamics of solids on macroscopic scales. This goal is achieved, in parts, by unraveling the molecular or meso-scale mechanisms that lead to friction between two rubbing bodies. One example is the study of dissipative forces in externally driven elastic manifolds that wrinkle in response to the presence of a counterbody (see figure). The NIC research group also investigates, if it is possible to alter materials used in optoelectronic memory applications so that they can be switched reversibly between their conducting, crystalline and insulating, amorphous phases through the application of stress. This question is addressed by density functional simulations of materials under compressive pressure and tensile load. A positive result could contribute to the development of fast and energy efficient memory. Lastly, our main objective of accurately describing the electrostatics of molecular systems is to make possible the simulation of redox reactions in terms of semi-empirical force fields. Goals in this line of research are the simulation of the atomistic dynamics in Galvanic elements with and without electrical load as well as the analysis of the molecular mechanisms leading to rubbing-induced electricity.