Workshop on Force-Field Development (Forces 2014)

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Many processes in nature and technology can be rationalized with computer simulations of a few thousands to a few hundred millions of atoms. Examples range from protein folding via plastic deformation to the dynamics of explosions. Simulating such processes in a meaningful fashion is outside the scope of electronic-structure based techniques and will remain so for the next few decades, even if computers and algorithms keep improving at the current rate. Gaining useful insight into the various processes then often requires one to use low-cost force fields that still properly reflect the intricate quantum mechanics responsible for interatomic bonding and repulsion. For instance, the failure mechanism of a specific material can only be unraveled in simulations that accurately account for defect energetics. This cannot be achieved with generic two-body potentials. To advance the field, a workshop on the development of force fields was held in Jülich from November 3–5, 2014.

Seventy participants from four continents attended the workshop, in which eleven invited talks, seven contributed talks, as well as twenty posters were presented. Topics included, amongst others, the systematic and fitting-free bottom-up design of force fields from first principles, machine-learning strategies, force fields for non-equilibrium (excited electronic states) to potential repositories and force-field standardization. The IOP journal Modeling and Simulation in Materials Science and Engineering (MSMSE) will dedicate a special issue Force Fields: From Atoms to Materials to this very successful workshop. Ten invited contributions to the proceedings volume are currently under review and expected to be published within the next six months. More details on the workshop, including a link to the special MSMSE link in the near future, can be found at http://www.fz-juelich.de/ias/jsc/ForceFields2014

Figure 1: Participants of the NIC workshop Force Fields: From Atoms to Materials in front of the Jülich Supercomputing Centre.