ЛАБОРАТОРИЯ ИНФОРМАЦИОННЫХ ТЕХНОЛОГИЙ

СЕМИНАР ПО ГЕТЕРОГЕННЫМ ВЫЧИСЛЕНИЯМ

Wednesday, 7 September 2016, at 10.00

room 407

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Tutorial

LAMMPS and VMD – simulation and visualization of molecular dynamics

LAMMPS is a classical molecular dynamics code, and an acronym for Large-scale Atomic/Molecular Massively Parallel Simulator. It can be used to model atoms or, more generically, as a parallel particle simulator at the atomic, meso, or continuum scale. We will walk through some examples of simulation using this powerful packages that we will visualize with the help of VMD. Visual Molecular Dynamics (VMD) is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and build-in scripting.

The course will be held on the heterogeneous cluster HybriLIT (http://hybrilit.jinr.ru/) of LIT JINR.