Usage Report for Fiscal Year 2015

Project Title:

Molecular dynamics simulation of virus in water in atomistic resolution

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1. The project goal is to study molecular properties of a virus in water at all atom resolution including explicit water molecules. The study is based on molecular dynamics models of the virus shell (the capsid). We need the Supercomputer for our calculation because full system with the capsid and the water molecules contains few millions atoms and other machines do not allow to perform so heavy simulations.
2. Molecular dynamics simulation using GROMACS.
3. No results
4. No conclusion
5. Molecular dynamics simulation of the whole virus with DNA inside.
6. No job was executed, because GROMACS was not tuned for Massively Parallel Computer (MPC). It calculated very slowly (12000 water molecules on 32 cores progressed 22ps during 1 hour).