ER-flow Application Description Template

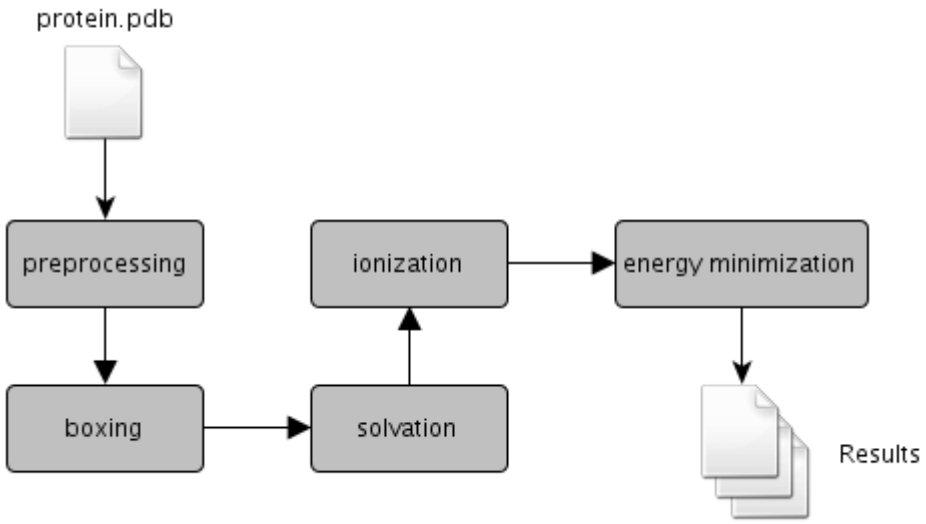
Application Name:
GROMACS – Energy Minimisation (EM)

Application domain:
Molecular Dynamics

Brief description of application

The workflow is intended for the new and inexperienced GROMACS user. The user has to provide a plain .pdb file containing the coordinates of a protein. After molecule selection, a force field and water model can be selected, followed by the number of energy minimization steps. Furthermore resource settings can be adjusted. Usally the default settings give reasonable results, producing a solvated and minimized simulation system within a couple of minutes (depending on cluster availability). Such a system can be used for long time simulation with GROMACS or may be processed further with other tools.

Force field based simulation tools like GROMACS work with so called topologies, describing the interactions within a protein with specific energy functions. Therefore only biomolecules that are described by the available forcefields can be simulated. Pure proteins allways work well, but if you want to simulate some fancy liquid crystals with strangly conjugated PI-systems you may run out of topology parameters.



data:
input data format: PDB input data value range
output data format: XTC, TRR, PDB, GRO, XVG output data value range
sample data: https://mosgrid.de/help/molecular-dynamics
application: http://www.gromacs.org/
documentation: http://manual.gromacs.org/
publication: http://pubs.acs.org/doi/abs/10.1021/ct700301q

Execution environment
DCI: UNICORE, MoSGrid VO
middleware: gUSE/UNICORE workflow system: ws-pgrade

Execution characteristics
data size (per unit, typical number of units):
input 1-50 MB temporary output 0.05-10 GB
processing time (per unit): 5 min up to multiple weeks

memory usage: 1-32 GB disk usage: low
Target users Community, projects: MoSGrid (mosgrid.de), SCI-BUS (sci-bus.eu) number of users: 10 user type: end-user:
Usage scenario for workflow in the ER-FLOW (how workflow will be reused, metaworkflow, how expected to contribute to project indicators, etc.).
Contact information (author) name: Sonja Herres-Pawlis, Jens Krüger e-mail: Sonja.herres-pawlis@cup.uni-muenchen.de