

ER-flow Application Description Template

Application Name: GROMACS – Single TPR												
Application domain: Molecular Dynamics												
Brief description of application <p>This is a very basic workflow for experienced users, who mainly want to take advantage of the computational resources available through MoSGrid. It is assumed that the user is familiar with GROMACS and that a .tpr containing all information needed for a simulation has been prepared elsewhere. The user has to upload that file and specify the resource settings. In general all jobs are queued in the underlying grid system. The smaller the resource requirements are, the faster the job is started. It is strongly recommended to do a pilot run, setting the maximal runtime (corresponds to -maxh option of mdrun, i.e. the computational core of GROMACS) to a couple of minutes, in order to get an idea of the performance.</p> <div style="text-align: center; margin: 10px 0;"> <pre> graph LR A[topol.tpr] --> B[GROMACS (mdrun)] B --> C[Results] </pre> </div> <p>data:</p> <table style="width: 100%; border: none;"> <tr> <td style="padding-left: 20px;">input data format: TPR</td> <td style="padding-left: 200px;">input data value range</td> </tr> <tr> <td style="padding-left: 20px;">output data format: XTC, TRR, PDB, GRO, XVG</td> <td style="padding-left: 200px;">output data value range</td> </tr> <tr> <td colspan="2" style="padding-left: 20px;">sample data: https://mosgrid.de/help/molecular-dynamics</td> </tr> <tr> <td colspan="2" style="padding-left: 20px;">application: http://www.gromacs.org/</td> </tr> <tr> <td colspan="2" style="padding-left: 20px;">documentation: http://manual.gromacs.org/</td> </tr> <tr> <td colspan="2" style="padding-left: 20px;">publication: http://pubs.acs.org/doi/abs/10.1021/ct700301q</td> </tr> </table>	input data format: TPR	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	
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Execution environment DCI: UNICORE, MoSGrid VO middleware: gUSE/UNICORE workflow system: ws-pgrade												
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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												