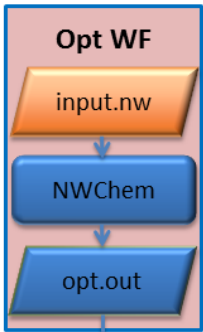


ER-flow Application Description Template

Application Name: NWChem – Basic
Application domain: Quantum Chemistry
Brief description of application The basic workflow is to submit a NWChem file for a geometry optimization and to obtain an output file.  <pre>graph TD; A[input.nw] --> B[NWChem]; B --> C[opt.out]; subgraph Opt_WF [Opt WF]; A; B; C; end</pre>
data: input data format: nwchem input file input data value range output data format: out.file output data value range sample data: http://www.nwchem-sw.org/index.php/Release61:Sample application: www.nwchem-sw.org documentation: http://www.nwchem-w.org/index.php/Release61:NWChem_Documentation publication: http://144.206.159.178/ft/216/12505/254919.pdf
Execution environment DCI: UNICORE, MoSGrid VO (computing, data, VO, etc) middleware: gUSE/UNICORE workflow system: ws-pgrade
Execution characteristics data size (per unit, typical number of units): input 1 MB temporary output 1-100 MB processing time (per unit): 5 min up to 3 weeks memory usage: 1-32 GB disk usage: medium
Target users Community, projects: MoSGrid (mosgrid.de) number of users: 15 user type: end-user, student
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) Sonja Herres-Pawlis, sonja.herres-pawlis@cup.uni-muenchen.de Richard Grunzke, richard.grunzke@tu-dresden.de