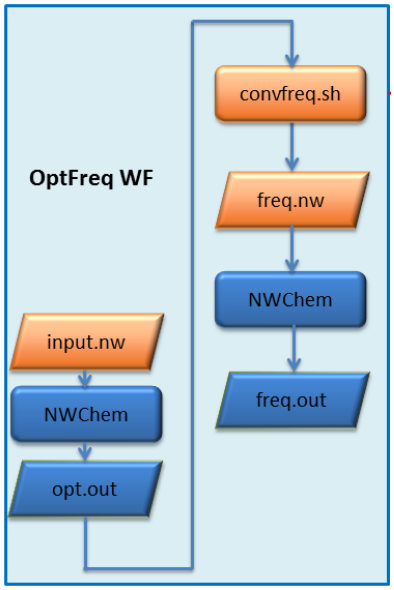
ER-flow Application Description Template

Application Name:
NWChem – Optimisation plus frequency calculation

Application domain:
Quantum Chemistry

Brief description of application
This is a useful workflow because it combines two fundamental steps in quantum chemistry: a geometry optimisation and a frequency calculation which is needed to confirm the stability of the minimum.
The input file is a pre-prepared .nw file of a desired molecule. The geometry is parsed by a converter (bash shell script), combined with an “empty” .nw frequency file which is then submitted again. After this step, standard output of NWChem can be obtained.



data:
input data format: nwchem input file or xyz data 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

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