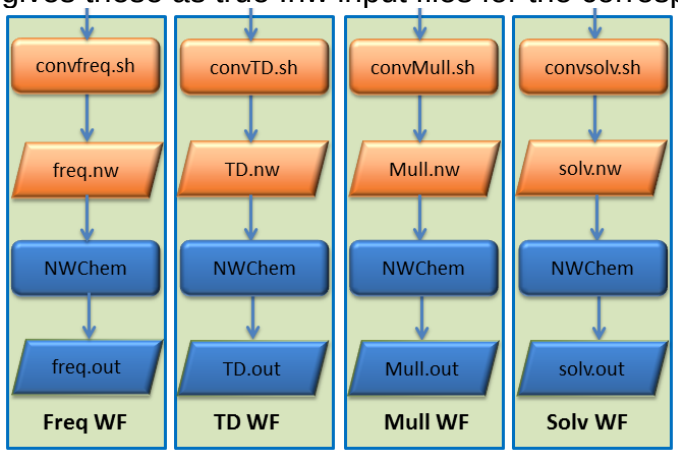
ER-flow Application Description Template

Application Name:
NWChem – Solvation

Application domain:
Quantum Chemistry

Brief description of application
In the Solvation workflow the input file format is OUT and the output file formats are OUT but also HESS, ZMAT, CUBE and many more if desired for printing out additional output. The input data sizes are between 1 and 10 KB, the output sizes are about 1-100 MB, the memory usage is between 8 and 32 GB, and the disk usage is low. The processing time is between minutes and weeks depending on the size of the molecule. Integrated into the workflow are “empty” .nw files which are combined with extracted geometry data to new .nw input files. The converter combines the extracted geometry with suited .nw files and gives these as true .nw input files for the corresponding jobs into the NWChem processing.



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.).

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