

ER-flow Application Description Template

<p>Application Name: NWChem – Mulliken</p>
<p>Application domain: Quantum Chemistry</p> <p>Brief description of application In the Mulliken 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.</p>
<pre> graph TD subgraph Freq_WF [Freq WF] C1[convfreq.sh] --> I1[/freq.nw/] I1 --> P1[NWChem] P1 --> O1[/freq.out/] end subgraph TD_WF [TD WF] C2[convTD.sh] --> I2[/TD.nw/] I2 --> P2[NWChem] P2 --> O2[/TD.out/] end subgraph Mull_WF [Mull WF] C3[convMull.sh] --> I3[/Mull.nw/] I3 --> P3[NWChem] P3 --> O3[/Mull.out/] end subgraph Solv_WF [Solv WF] C4[convsol.sh] --> I4[/solv.nw/] I4 --> P4[NWChem] P4 --> O4[/solv.out/] end </pre>
<p>data:</p> <p>input data format: nwchem input file or xyz data input data value range</p> <p>output data format: out.file output data value range</p> <p>sample data: http://www.nwchem-sw.org/index.php/Release61:Sample</p> <p>application: www.nwchem-sw.org</p> <p>documentation: http://www.nwchem-w.org/index.php/Release61:NWChem_Documentation</p> <p>publication: http://144.206.159.178/ft/216/12505/254919.pdf</p>
<p>Execution environment</p> <p>DCI: UNICORE, MoSGrid VO (computing, data, VO, etc)</p> <p>middleware: gUSE/UNICORE workflow system: ws-pgrade</p>
<p>Execution characteristics</p> <p>data size (per unit, typical number of units):</p> <p>input 1 MB temporary output 1-100 MB</p> <p>processing time (per unit): 5 min up to 3 weeks</p> <p>memory usage: 1-32 GB disk usage: medium</p>
<p>Target users</p> <p>Community, projects: MoSGrid (mosgrid.de) number of users: 15</p> <p>user type: end-user</p>
<p>Usage scenario for workflow in the ER-FLOW (how workflow will be reused, metaworkflow, how expected to contribute to project indicators, etc.).</p>

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