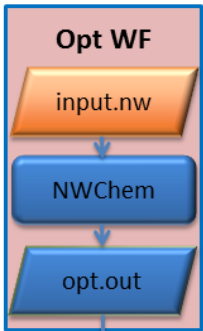


# ER-flow Application Description Template

<b>Application Name:</b> NWChem – Transition State Search
<b>Application domain:</b> Quantum Chemistry
<b>Brief description of application</b> The search for transition states is a complicated process, but crucial in the theoretical description of chemical reaction mechanisms. Here, the computational challenge lies in the fact that the simulation code does not have to search for an energetic minimum, but for a saddle point (a higher-order minimum). This is time-consuming and often fails. If the user has really found such a saddle-point, it can only be verified by a following frequency calculation. This indicates by zero negative frequencies a normal minimum and by one negative frequency a saddle-point. We have developed a rather simple workflow using NWChem which performs a transition state search. It is useful for more advanced users who want to combine it with some of the above-described sub-workflows to a more complex workflows (meta-workflows, vide infra). The input file is a pre-prepared TS.nw file.
 <pre>graph TD; subgraph Opt_WF [Opt WF]; direction TB; A[input.nw] --&gt; B[NWChem]; B --&gt; C[opt.out]; end</pre>
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: <a href="http://www.nwchem-sw.org/index.php/Release61:Sample">http://www.nwchem-sw.org/index.php/Release61:Sample</a> application: <a href="http://www.nwchem-sw.org">www.nwchem-sw.org</a> documentation: <a href="http://www.nwchem-w.org/index.php/Release61:NWChem_Documentation">http://www.nwchem-w.org/index.php/Release61:NWChem_Documentation</a> publication: <a href="http://144.206.159.178/ft/216/12505/254919.pdf">http://144.206.159.178/ft/216/12505/254919.pdf</a>
<b>Execution environment</b> DCI: UNICORE, MoSGrid VO (computing, data, VO, etc) middleware: gUSE/UNICORE workflow system: ws-pgrade
<b>Execution characteristics</b> 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
<b>Target users</b> Community, projects: MoSGrid ( <a href="http://mosgrid.de">mosgrid.de</a> ) number of users: 15  user type: end-user
<b>Usage scenario for workflow in the ER-FLOW</b> (how workflow will be reused, metaworkflow, how expected to contribute to project indicators, etc.).

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