

ER-flow Application Description Template

Name:

SpecWSUNI

Type: workflow

Application domain:

Computational chemistry, quantum chemistry

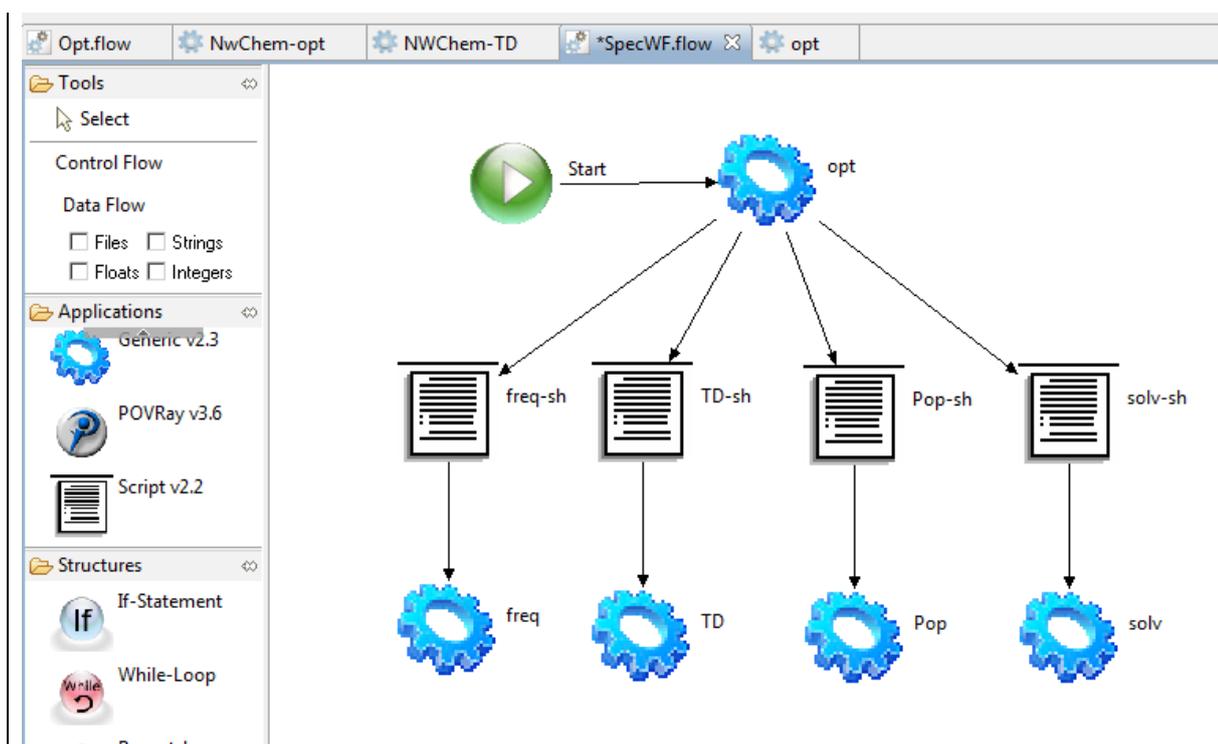
Brief description of application

We have developed a series of workflows using NWChem. They are highly useful for beginners who just want to perform a spectroscopic analysis. Spectroscopic analyses are widely used in organic and especially inorganic chemistry in order to simulate the UV/Vis absorption of a regarded molecule (TD job), its infra-red and/or Raman vibrations (frequency job), its relaxation in a solvent of choice (solvation job) and its population analysis (Mulliken job).

This analysis comprises a basic WF as optimisation followed by freq WF, TD WF, Mull WF and solv WF. A frequency workflow (freq WF) performs a frequency calculation, a step which is always needed to characterise a minimum as stable minimum. A time-dependent DFT workflow (TD WF) performs a TD-DFT calculation in order to obtain the optical properties of a molecule. The Mulliken workflow (Mull WF) calculates the Mulliken charges of every atom of a molecule. The solvent workflow (solv WF) arranges a solvent sheath around a molecule and performs a further optimisation step.

In this particular case, we have implemented it in UNICORE since this is directly running on several clusters without time delay. For larger calculations the UNICORE Rich Client offers good steering properties.

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 processing time is between minutes and weeks depending on the size of the molecule. The first input file is a opt.nw file for a basic optimisation simulation. The output of the first basic WF is a opt.out file which is parsed for the geometry by the subsequent workflows. They combine this geometry data with prepared nw-input-files for the subsequent freq, TD, Mull and solv jobs. As final output, the four output files freq.out, TD.out, Mull.out and solv.out are obtained.



Data

input data format: .nw

input data value range 1-100 kb

output data format: .out

output data value range 0.1 - 10 mb

sample data: (link)

application NWChem, www.nwchem-sw.org/index.php/Download.

documentation http://www.nwchem-sw.org/index.php/Release62:NWChem_Documentation

publication <http://www.sciencedirect.com/science/article/pii/S0010465510001438>.

Execution environment

DCI: UNICORE Rich Client (MoSGrid resources)

middleware: UNICORE

workflow system: UNICORE

Execution characteristics

data size (per unit, typical number of units):

input 1-100 kb temporary 1-100 mb output 0.1 - 10 mb

processing time (per unit): n.d.

memory usage: 20000 mb

disk usage: 100 mb

Target users

Community, projects: Chemists

number of users: 100

user type: end-user

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