ER-flow Application Description Template

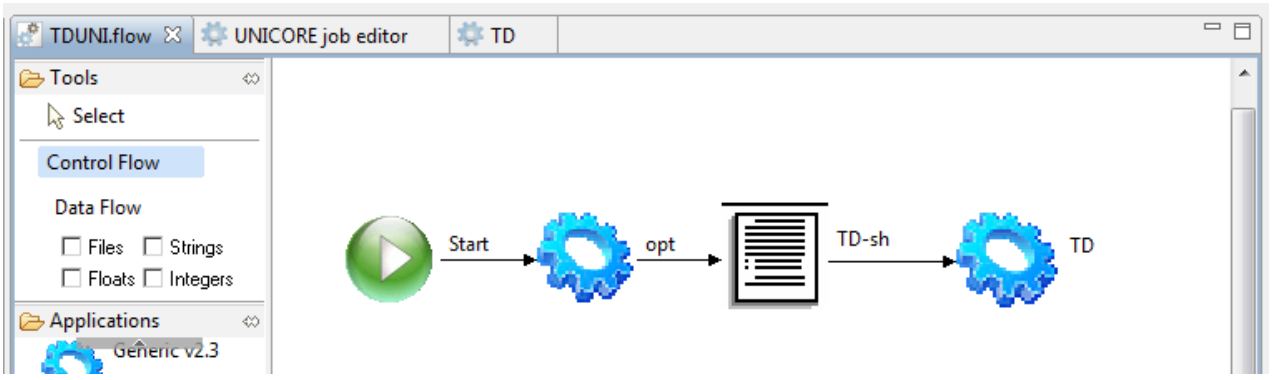
Name:
TD UNI

Type: workflow

Application domain:
Computational chemistry, quantum chemistry

Brief description of application
Time-dependent DFT serves for the calculation of optical transitions by ground state DFT. It replaces the complicated many-body time-dependent Schrödinger equation by a set of time-dependent single-particle equations whose orbitals yield the same time-dependent density. This is possible because the Runge-Gross theorem proves that, for a given initial wavefunction, particle statistics and interaction, a given time-dependent density can arise from at most one time-dependent external potential. This means that the time-dependent potential (and all other properties) is a functional of the time-dependent density.
After the fundamental geometry optimisation, the TD-DFT step is performed in this workflow.
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 NW 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. 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 script. This script combines this geometry data with prepared nw-input-files for the subsequent TD jobs. As final output, the TD-DFT output file TD.out is 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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