ER-flow Application Description Template

Name:
Population UNI

Type: workflow

Application domain:
Computational chemistry, quantum chemistry

Brief description of application
Besides the standard natural bond orbital analysis implemented in many quantum chemical codes, the state of the art is represented by the NBO6.0 analysis. This is a standalone programme which needs special input. Hence, after the basic optimisation with NWChem a special input file for the subsequent single point job has to be generated by a script. This input file then goes into the single point calculation using NWChem (sp files). The output files of these calculations are then the input files for NBO6, AOMix and AIM. AOMix and AIM are small but commercial programmes where a working group licence is needed. They provide with different kinds of population analyses which allow for different orbital dissections, electronic analyses, calculation of bonding parameters and so on.

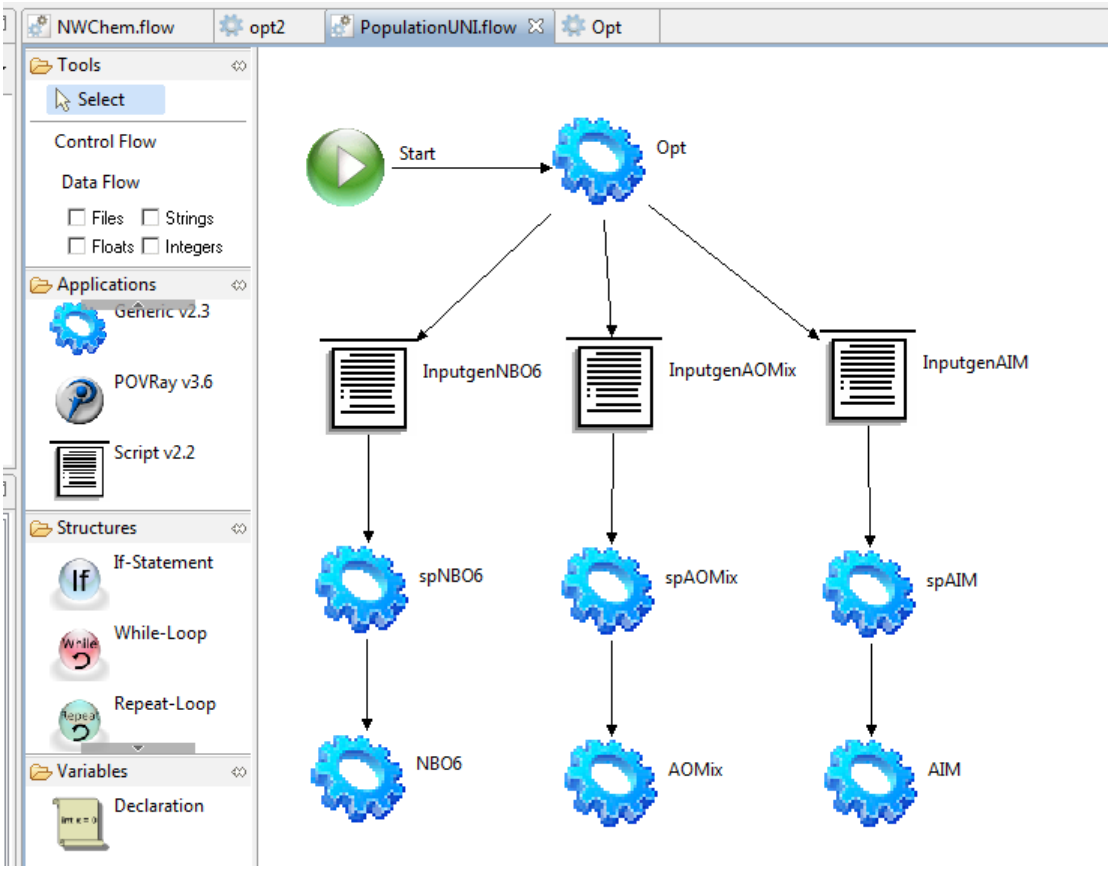
NBO6.0: http://nbo6.chem.wisc.edu/
Through their close association with elementary Lewis structure diagrams, NBOs provide a *direct link to familiar valency and bonding concepts*. Unlike delocalized MOs (whose sprawling forms vary bewilderingly even between closely related systems), NBOs are *highly conserved and transferable* from one molecular environment to another. NBO provides *mutually consistent and comprehensive* analysis tools, ensuring harmonious chemical interpretations from one property to another. The program is *uniformly implemented* in leading electronic structure packages, providing an *authoritative framework for state-of-the-art professional discourse*. Widespread acceptance of the NBO paradigm is reflected in the burgeoning number of published applications (currently, ~1300 per year).

AOMix: http://www.sg-chem.net/aomix/
AOMix is a user-friendly software for the molecular orbital (MO) analysis. It calculates the MO compositions in terms of the constituent chemical fragments (you can specify them as atoms, groups of atoms, atomic orbitals, fragment molecular orbitals, groups of atomic orbitals, etc.) in the molecule or atom. AOMix automatically processes output files of multiple quantum-chemical packages (see the list below). AOMix also allows you to analyze chemical structure (bonding/antibonding nature of molecular orbitals) using overlap populations (total and per molecular orbital), valence indices, 2-center (Mayer, Lowdin, Wiberg, and bond-order symmetry components) and 3-, 4-, 5- and 6-center bond orders.

AIM: http://www.aim2000.de/
The Quantum Theory of Atoms in Molecules (QTAIM) is a model of molecular and condensed matter electronic systems (such as crystals) in which the principal objects of molecular structure - atoms and bonds - are natural expressions of a system's observable electron density distribution function. An electron density distribution of a molecule is a probability distribution that describes the average manner in which the electronic charge is distributed throughout real space in the attractive field exerted by the nuclei. According to

QTAIM, molecular structure is revealed by the stationary points of the electron density together with the gradient paths of the electron density that originate and terminate at these points.

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 hours 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 which generates the input files for NWChem jobs which generate the input files for the population analyses of the other codes.



Data

input data format: .nw
output data format: .out
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.

input data value range 1-100 kb
output data value range 0.1 - 10 mb

NBO6.0: http://nbo6.chem.wisc.edu/
AOMix: http://www.sg-chem.net/aomix/
AIM: http://www.aim2000.de/

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: 50

user type: end-user

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