CHL Lab

11/01/17: Building Gromacs and SolEFP on Stampede2

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Gromacs:

Added /opt/apps/intel17/impi17_0/gromacs/5.1.2/share/gromacs/bin to $PATH
Exported GMXLIB=$HOME/gmx/forcefields

To run gmx features: type gmx
To run mdrun with parallelization: type ibrun mdrun_mpi

SolEFP:

1. Added module load intel to ~/.bashrc

2. Installed python2.7.12 in $HOME/programs/python2.7.

```
./configure --prefix=$HOME/programs/python2.7
make
make test
make install
```

Added $HOME/programs/python2.7/bin to $PATH (to overwrite the existing python, add to before the existing paths!)

3. Installed pp:

```
python setup.py install
```

4. Installed numpy linked with mkl libraries following globulion's instructions.
    1. Note1: Add lapack_libs = to site.cfg, because the lapack libraries are deprecated in the newer version of intel. So your site.cfg should look like:

```
[mkl]
library_dirs = /opt/intel/mkl/lib/intel64
include_dirs = /opt/intel/mkl/include
mkl_libs = mkl_rt
lapack_libs =
```

    2. Note2: No need for the —prefix=$HOME option in install; leave it out
    3. Note3: The MKL library paths (LD_LIBRARY_PATH) are already set in stampede2

5. Installed scipy linked with mkl libraries following globulion's instructions.
    1. Note1: No need for the —prefix=$HOME option in install; leave it out

6. Installed matplotlib:
python setup.py install

7. MDAnalysis:
python setup.py install

8. Installed scitools:
python setup.py install

9. Installed PyQuante:
    1. Added basis for Ca in PyQuante/Basis/p6311pp_1d_1p.py
    2. python setup.py install

10. Installed libbbg
    1. Modified the install script:
        1. Change prefix to $HOME/programs/python2.7
        2. Change *export LIBBBG_LIB=$PREFIX/lib/python2.7/dist-packages/* to *export LIBBBG_LIB=$PREFIX/lib/python2.7/site-packages/*
    2. Modified utilities.py:
        1. Change *import_matplotlib = int(os.environ['LIBBBG_IMPORT_MATPLOTLIB'])* to *import_matplotlib=1*
    3. bash install

11. Installed coulomb
python setup.py install

12. Installed solvshift
    1. Added fragments for ca++ ad indole to slv-master/frg
    2. Modified solvshift/slvpar.py:
        1. Added 'ca++', 'indole' to solveshift.slvpar.params
        2. Added 20:'Ca' to solveshift.slvpar.__atomic_symbols
    3. Modified solvshift/setup.py:
        1. Added 'ca++', 'indole' to molecules
    4. Modified the install_slv script:
        1. Change prefix to $HOME/programs/python2.7
        2. Change *export LIBBBG_LIB=$PREFIX/lib/python2.7/dist-packages/* to *export LIBBBG_LIB=$PREFIX/lib/python2.7/site-packages/*
    5. bash install_slv
    6. Exported SLV_DATA=$HOME/programs/python2.7/lib/python2.7/site-packages/solvshift-dat
    7. Copied util as $HOME/programs/slv_util
    8. Added $HOME/programs/slv_util to path

9. uploaded solefp.files (with modified gmx.tc) to $HOME/solefp

Success!