openLOWDIN

Release 0.1

openLOWDIN

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CHAPTER

ONE

ABOUT

openLOWDIN is a computational program that implements the Any Particle Molecular Orbital (APMO) method to study systems containing any type and number of quantum species, such as electrons, positrons, quantum nuclei, muons, or drude oscillators.

What can we do in Lowdin? The current version of the code encompasses the following quantum chemistry methods:

- HF
- DFT
- MP2
- CI (CIS, CISD, CIST, CISDTQ, FCI, CIPSI)
- PT (PT2, PT3, PP3, RENPP3, OVGF)
- NOCI

Check more details in the *Theory* and *Tutorials*

At present, openLOWDIN code is publicly available at https://github.com/efposadac/openLOWDIN And the openLOWDIN manual at https://github.com/openLOWDIN/openLOWDIN_manual

Check the following papers for further information

10.1002/qua.24500 10.1002/qua.25705

CHAPTER

TWO

DEVELOPERS

2.1 Active developers (alphabetical order)

- Andrés Reyes
- Edwin Posada
- Jorge Charry
- Félix Moncada

2.2 Contributors (alphabetic order)

- Jhonathan Romero (APMO/Propagators)
- Sergio Gonzalez (APMO: Older versions)
- Nestor Aguirre (APMO: Older versions)
- Danilo González Forero (APMO/COSMO)
- Jose Mauricio Rodas Rodriguez (APMO/(QM/MM))
- Carlos Ortiz-Mahecha (APMO/CC)
- Alejandro Peña Torres (APMO/CC)
- Laura Pedraza-González (APMO/core)
- Manuel Diaz (APMO/Propagators)
- Teresa Tamayo-Mendoza (Development of higher order propagator methods)
- Roberto Flores-Moreno (ADFT/ADPT/Propagators)

CHAPTER

THREE

INSTALLATION

Compile: (see below for a step-by-step example)

- run *./configure* in LOWDIN root directory. Be sure that you have permissions to write in the installation directory and have properly exported the *$PATH* environment.
- run *make*

Install:

- run *make install*

Uninstall

- run *make uninstall*

Documentation

- run *make doc*

The *make doc* command produces both latex and html documentation using doxygen program. Be sure you have installed doxygen, for instance in a debian-based distribution run:

 # apt-get install doxygen graphviz

To use latex documentation in doc/latex folder, run command:

pdflatex refman.tex

To visualize the html documentation use:

<web browser> doc/html/index.html

Clean the project

- run *make clean* and then *make distclean*

—

Step-by-step installation example: (replace apt-get with your preferred package manager)

sudo apt-get update sudo apt-get -y install wget git build-essential liblapack-dev libblas-dev libgsl0-dev autotools-dev automake libtool gfortran python3 gawk libeigen3-dev libgmp-dev libboost-all-dev # Define ENV Variables export WORKDIR=$PWD/dependencies export PATH=$PATH:$WORKDIR/bin export C_INCLUDE_PATH=$C_INCLUDE_PATH:$WORKDIR/include:$WORKDIR/include/libint2:/usr/include/eigen3 export CPLUS_INCLUDE_PATH=$CPLUS_INCLUDE_PATH:$WORKDIR/include:$WORKDIR/include/libint2:/usr/include/e export LIBRARY_PATH=$LIBRARY_PATH:$WORKDIR/lib export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$WORKDIR/lib # Create work directories mkdir $WORKDIR mkdir $WORKDIR/bin mkdir $WORKDIR/lib cd $WORKDIR

Libint2 # If you have Ubuntu, you can get this precompiled Libint2 library wget https://www.dropbox.com/s/d3d44j238lkfwcr/libint-master-SEP052019.tgz tar xzvf libint-master-SEP052019.tgz

Otherwise, download and compile with minimal (default am), G12, fPIC options (libint2 commit 668b10c4bdca5876984058742d4212675eb93f3f) # git clone https://github.com/evaleev/libint.git # cd libint # git checkout 668b10c4bdca5876984058742d4212675eb93f3f # ./autogen.sh # mkdir ../build # cd ../build # ../libint/configure –prefix=$WORKDIR –with-max-am=6 –enable-g12=4 –with-g12-max-am=4 –with-cxxgen-optflags # make -j 4 # make install # ../libint/configure –prefix=$WORKDIR

cd -

Libint1 git clone https://github.com/evaleev/libint.git cd libint git checkout v1 aclocal -I lib/autoconf autoconf ./configure –prefix=$WORKDIR make -j 4 make install make clean make distclean cd -

Libxc cd $WORKDIR # If you have Ubuntu, you can get this precompiled Libxc library wget https://www.dropbox.com/s/6cja3zzhl1cq46i/libxc-master-MAY242023.tgz tar xzvf libxc-master-MAY242023.tgz # Otherwise, download and compile with default options (libxc commit 4bd0e1e36347c6d0a4e378a2c8d891ae43f8c951) # git clone https://gitlab.com/libxc/libxc.git # cd libxc # git checkout 4bd0e1e36347c6d0a4e378a2c8d891ae43f8c951 # autoreconf -i # ./configure –enable-shared –prefix=$WORKDIR # make -j 4 # make install

cd ..

Configure Lowdin ./configure -p $WORKDIR/bin -s /tmp -l “-lblas -llapack” # Build Lowdin make -j 4 # Install Lowdin make install # Run Tests make test

CHAPTER

FOUR

GETTING STARTED

CHAPTER

FIVE

THEORY

Since Pythagoras, we know that $a^2 + b^2 = c^2$.

$$(a + b)^2 = a^2 + 2ab + b^2$$
$$(a - b)^2 = a^2 - 2ab + b^2$$

CHAPTER

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CONFIGURATION INTERACTION

The APMO/CI wave function is written as a linear combination of CI configurations between all quantum species

$$|\Phi_0\rangle = c_0|\Psi_0\rangle + \sum_{\alpha}\sum_{ia\in\alpha} c_i^a|\Psi_i^a\rangle + \sum_{\alpha,\beta}\sum_{\substack{ia\in\alpha\\ jb\in\beta}} c_{ij}^{ab}|\Psi_{ij}^{ab}\rangle + \sum_{\alpha,\beta}\sum_{\substack{ia\in\alpha\\ jb\in\alpha\\ kc\in\beta}} c_{ijk}^{abc}|\Psi_{ijk}^{abc}\rangle + \cdots \tag{6.1}$$

CHAPTER

SEVEN

TUTORIALS

In this section you can find multiples examples for openLOWDIN

CHAPTER

EIGHT

POSITRONIC SYSTEMS

This is an example on how to run a *Configuration Interaction* calculations for PsH

```
GEOMETRY
        e-(H)   SHARON-E-6S2P         0.00        0.00         0.00 addParticles=1
        H        dirac                        0.00        0.00         0.00
        e+        SHARON-E+6S2P        0.00        0.00        0.00
END GEOMETRY

TASKS
        method = "UHF"
        configurationInteractionLevel ="FCI"
        !configurationInteractionLevel ="CISD"
END TASKS

CONTROL
readCoefficients=F
numberOfCIstates=3
CINaturalOrbitals=T
        CIStatesToPrint = 1
        !CIdiagonalizationMethod = "DSYEVX"
        CIdiagonalizationMethod = "JADAMILU"
        !CIPrintEigenVectorsFormat = "NONE"
        CIPrintEigenVectorsFormat = "OCCUPIED"
        !CIPrintEigenVectorsFormat = "ORBITALS"
        CIPrintThreshold = 5e-2
        buildTwoParticlesMatrixForOneParticle=T
END CONTROL

INPUT_CI
        species="E-ALPHA" core=0 active=0
        species="E-BETA" core=0 active=0
        species="E+" core=0 active=0
END INPUT_CI
```

CHAPTER

NINE

INDICES AND TABLES

- genindex
- modindex
- search