Quick User Manual

Large Scale Ab Initio and Density Functional Theory Calculations
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1 Introduction

Quick is a linear scaling ab initio and density functional theory program for calculation of energies, charges and geometries of systems up to ~3,000 atoms. Available features include:

- Linear scaling Divide and Conquer (D&C) calculations [1-3].
- Single point ab initio and density functional theory calculations.
- Geometry Optimization(steepest decent, conjugate gradient, BFGS, and LBFGS available)
- Implicit solvation and Self Consistent Reaction Field(SCRF) calculations[4]
- Mulliken,[5] CM1[6] and CM2[7] charge analysis

The program was originally developed by Ed Brothers. His work includes the development of the standard Hartree-Fock and density functional theory energy and gradient calculations, geometry optimization routines, Mulliken charge analysis, strategy and front end of the program. Ken Ayers and Xiao He optimized the code.

2 Installation of Quick

The Binary Distribution requires some knowledge of the Linux/Unix environment. The following steps will show you the types of commands you will need to execute in order to properly install Quick.

The distribution is founed with a tar.gz file. This file must be uncompressed in order to install the application. To begin, put the tar.gz file in a place where you like it. Anywhere will do, but a good place for it may be /usr/local. Once you put the file in /usr/local you will need to type the following:

% tar xzvf quick-<platform>-<version>.tar.gz

Next, cd into the directory in order to view its contents. You should familiarize yourself with the directories found within the distribution.

% cd /usr/local/quick-<platform>-<version>

The set of test cases found in this directory should provide the user with a sample of the inputs required by Quick. Please enter each directory and run through the tests in order to familiarize yourself with the workings of Quick.

% cd Quick_Tests

In order to finally run Quick, you will need a license file. This file will ....

3 Keywords

3.1 Hamiltonians

HF Hartree-Fock Hamiltonian to be used.

UHF Unrestrictecd Hartree-Fock Hamiltonian to be used.

DFT Density Functional Theory to be used.

UDFT Unrestricted Density Functional Theory to be used.

NOTE: One Hamiltonian must be selected. There is no default.

3.2 Geometry Optimization

OPTIMIZE=Integer
do a maximum of Integer cycles of optimization. Default: 3 x Number of atoms.

DIIS-OPTIMIZE
use DIIS for geomety optimization.

RESTART
read in restart file from previous run.

GRADIENT
calculate analytical gradient.

HESSIAN calculate analytical hessian.

FREQUENCY
calculate frequencies.

3.3 SCF Convergence

SCF=Integer
user defined maximum self-consistent field cycles = Integer. Default: 200

DIIS-SCF use Pulay's DIIS method[8] for SCF convergence acceleration.

DENSERMS=FLOAT
user defined density matrix maximum RMS for convergence. Default : 1.0D-8.

MATRIXZERO=FLOAT
user defined matrix elements less than Float considered zero. Default : 1.0D-12.

3.4 Output

GAP print HOMO-LUMO gap.

IP calculate ionization potential

3.5 General

MULT=Integer
a multiplicity Integer is to be placed on system.

GEOM=PDB
allows input file to be PDB formatted data. If the PDB file is provided, the name of the file should be "<BASE_NAME>.pdb".

3.6 Atomic Charges

CHARGE=INT
a net charge is to be placed on system.

MULLIKEN
use Mulliken[8] charges for PME and/or SCRF, write Mulliken charges to charge output file of MC-run.

CM1 use CM1[9] charges for PME and/or SCRF, write CM1 charges to charge output file of MC-run.

CM2 use CM2[10] charges for PME and/or SCRF, write CM2 charges to charge output file of MC- run.

3.7 Self Consistent Reaction Field (SCRF)

QuickPB use in addition to SCRF keyword to use internal code. Note: this code is still being validated and is subject to change in future Quick releases.

INDI=INT
used to set the internal dielectric constant to the value specified. The default value for this keyword is 1.

EXDI=INT
used to set the external dielectric constant to the value specified. The default values for this keyword is 80.

SCALE=DOUBLE
allows the user to set the grid space (per angstrom). The default value for this keyword is 1.8.

PERFILL=INT
sets percentage of the box that is filled by the system being studied (ie. PERFILL=80 means the protein will take up 80% of the total box), thus controlling the size of the surrounding water box. A smaller value will give more accurate results but take longer to calculate. The default value for this keyword is 60% which is good for small molecules, but the user may want to increase to 80% for large calculations.

ION=DOUBLE
sets the ionic strengh of the solvent surrounding the system of interest. The default value for this keyword is 0 (ie. water).

PROBRAD=DOUBLE

allows the user to set the radius of the probe for the interior surface charges. The default values of this keyword is 1.4.

FINESURF

turns on non-uniform grid (aka Fine Surface) algorithm in DivPB. This algorithm applys the grid density specified by SCALE (See [SCALE], page 4.) only around the solute surface, but cuts the grid density elsewhere to 0.5*SCALE saving time during DivPB calculations. Due to the nature of the algorithm and implementation, non-uniform grid is not suitable for small molecules. The recommended SCALE value when using FINESURF is 2 or more.

4 Test Runs and Examples

The quick directory contains some test runs and examples. These can be found in the directory examples. The actual tests can be found in the following subdirectories:

Info on the tests and how to set them up can be found in the README files.

4.1 SCF

This directory contains files necessary to do SCF single point calculation.

```
HF BASIS=3-21G*

C    1.0582    0.9353    0.8103
H    1.4145    1.5662    0.0000
H    1.2065    1.4452    1.7588
H    0.0000    0.7294    0.6710
H    1.6121    0.0000    0.8114
```

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