SINDO 4.0 User's Manual: MakePES

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February 20, 2018

Contents

Acknowledgment

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- Grant-in-aid:
  2007-2012 Scientific Research (KAKENHI) on Priority Areas (477) "Molecular Science for Supra Functional Systems" supported by MEXT, Japan.

1 MakePES

This section lists the keys and values used in RunMakePES program. They appear in makePES.xml in the form of,

```
<entry key=‘‘key’’> key value </entry>
```

The keys in red indicate that they are mandatory. The values are case insensitive except when it is noted.

In the following, the keys are divided into four sections. General Keys (Sec. 1.1) are common input for all types of run, while those in QFF Keys (Sec. 1.2), Grid Keys (Sec. 1.3), and Hybrid Keys (Sec. 1.4) are relevant input parameters for generating the QFF, grid potential, and hybrid potential, respectively.

1.1 General Keys

- runtype
  The type of run. One of the following must be specified.

  QFF : Generate the quartic force field.
  GRID : Generate the grid potential.
  HYBRID : Generate the hybrid potential.

- molecule
  The name of minfo file containing the vibrational data. The value is case sensitive.

- MR
  The order of mode coupling expansion. Can take 1, 2, or 3. (default = 3)

- activemode
  Specifies active modes for PES generation. All modes are active by default. The mode numbers should be separated by camma or space. A hyphen can be used for a sequence of mode number. For example,

  ```
  <entry key="activemode"> 1,2,3,5 </entry>
  ```

  is equivalnet to,

  ```
  <entry key="activemode"> 1-3 5 </entry>
  ```

  which means Q_1,Q_2,Q_3, and Q_5 are active, and Q_4 isn't.

- removefiles
  Removes the input/output files of the quantum chemistry program, when true. (default = false)

- dipole
  Generates the dipole moment surface in addition to the PES, when true. (default = false)

- dryrun
  Generates the input files for the quantum chemistry program and exit without execution (default = false)

- qchem
  In each line after the entry tag of this key follows the type of the quantum chemistry program, a template file to generate input files for the program, and a label. The three components may be separated by space or camma. For example, the input looks like,

```
<entry key="qchem">
Gaussian GaussianInput.xml MP2/aug-cc-pVTZ (11)
</entry>
```

  The first value (Gaussian) specifies the quantum chemistry program, which may take one of the following:

Gaussian	: Gaussian03 or 09
Molpro	: Molpro2012
ACESII	: ACESII
QChem	: Q-Chem4.3
Generic	: Generic (see below)

  The second value (GaussianInput.xml) is the name of the XML file, which contains the information to generate the input files for the program. This value is case sensitive. For more information on how to prepare the XML file for each program, see Appendix 3.

  The third value (MP2/aug-cc-pVTZ (11)) is a label that is tagged to the PES data files. This name will be printed in the output of SINDO, so it is recommended to give a name, for example, the level of the electronic structure calculation, the number of grid points, etc.

  This key extends to two lines when the hybrid PES is specified for the runtyp. The first and the second lines specify the quantum chemistry calculations for the QFF and Grid PES generation, respectively. In this case, the input would look like,

```
<entry key="qchem">
  Gaussian, MP2Input.xml, MP2/cc-pVDZ
  Gaussian, CCInput.xml, CCSD(T)/aug-cc-pVTZ (11)
</entry>
```

  When the first value is specified as "generic", MakePES creates a file (ending with .grdxyz), which contains the xyz coordinates of all grid points. This option is intended for users who want to create input files in their own way for the electronic structure calculation. In this case, the work flow is the following,

  1. Execute RunMakePES with dryrun = true and qchem = generic to create a grdxyz file.

2. Get the grid ID and xyz coordinates from the grdxyz file, and create **by yourself** input files for the electronic structure program.
3. Run the electronic structure calculations.
4. Convert **by yourself** the output information to a minfo format, and save as (grid ID).minfo. Note that only the [Electronic Data] section is needed.
5. Place the minfo files to minfo.files folder.
6. Re-run RunMakePES with dryrun = false.

Then, one should obtain the mop file or pot files for QFF and Grid, respectively.

1.2 QFF Keys

- stepsize
  The step size for numerical differentiations in dimensionless unit ($\sqrt{w/\ \hbar} * Q$). (default = 0.5)

- ndifftype
  The type of numerical differentiations. (default = hess)

  grad : Numerical 3rd-order diff. of gradient.
  hess : Numerical 2nd-order diff. of hessian.

- mopfile
  The name of mop file, in which the QFF coefficients are written. (default = prop_no_1.mop)
  This format is compatible with the MIDAS software developed by Christiansen and coworkers.

- genhs
  Generate the 001.hs file. (default = false)
  001.hs is a file which contains the QFF coefficients in the old format; however, this format is deprecated and not recommended to use unless for a debugging purpose to compare the result with the previous version of SINDO.

- gradient_and_hessian
  Specifies where the gradient and Hessian should be retrieved. (default = "input")

  input : From the input minfo file.
  current : From the current calculation. (mkqff-0.minfo)

  This option set to "input" (which is the default) is intended for combining accurate geometry, gradient, and Hessian, which are read from the input minfo file, with lower-level cubic and quartic terms, which are calculated here. On the other hand, one might think of another strategy, where the geometry and normal/optimized coordinates are derived from a low-level of theory, and the QFF at a higher-level of theory. In that case, this option should be set to "current", which incorporates the gradient and Hessian obtained from the current calculation.

1.3 Grid Keys

- ngrid
  The number of grid points along each coordinates. (default = 11)
- fullmc
  All the mode coupling up to the MR-th order is generated, when true. (default = false)
- mc1
  The 1MR terms separated by camma or space. For example,

  ```
  <entry key="mc1"> 1,2,3,5 </entry>
  ```

  or

  ```
  <entry key="mc1"> 1-3 5 </entry>
  ```

  generates the grid points for Q_1,Q_2,Q_3, and Q_5.
- mc2
  The 2MR terms separated by camma or space. For example,

  ```
  <entry key="mc2"> 1,2, 1,4, 2,4, 3,4 </entry>
  ```

  or

  ```
  <entry key="mc2"> 1,2, 1-3,4 </entry>
  ```

  generates the grid points for (Q_2, Q_1),(Q_4, Q_1),(Q_4, Q_2), and (Q_4, Q_3).
- mc3
  The 3MR terms separated by camma or space. For example,

  ```
  <entry key="mc3"> 1,2,3, 1,2,4 </entry>
  ```

  generates the grid points for (Q_3, Q_2, Q_1) and (Q_4, Q_2, Q_1).

NOTE: One of fullmc, mc1, mc2, or mc3 must be present in the input file.

1.4 Hybrid Keys

- ngrid
  The number of grid points along each coordinates. (default = 11)
- mcstrength
  The threshold value (in cm^{-1}) to select the mode coupling term for generating the grid potential. The coupling terms with MCS larger than this value are generated.
- mopfile
  The name of mop file, in which the QFF coefficients are written. (default = prop_no_1.mop)

NOTE: Hybrid PES requires two lines in qchem entry, where the first and second line specifies the quantum chemistry jobs for QFF and Grid, respectively.

2 Miscellaneous Java Tools

3 Interface with Quantum Chemistry Programs

3.1 Gaussian

3.2 Molpro

3.3 ACESII

3.4 QChem

4 Files

References