# Users' guide of MakePES

Kiyoshi Yagi
kiyoshi.yagi@riken.jp

Theoretical Molecular Science Laboratory
RIKEN Cluster for Pioneering Research

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# Contents of Sample Files

Sample files are found in sindo-4.0/doc/MakePES/sample_MakePES

1.basic/
    VSCF, VCI[3]-(8), VMP2-(4), VQDPT2-(4)

2.h2co/
    VCI[3]-(6), VMP2-(4), VQDPT2-(4)

3.water-hexamer/
    nc-VCI[3]-(6), nc-VQDPT2-(4)

NOTE

MakePES is a command line based program. This manual assumes that you are familiar with the commands in UNIX, and that you are working on Bourne Shell (bash).

# 1. Basic example

Proceed to 1.basic and find input files,

```
> cd 1.basic
> ls
GaussianTemplate   h2co-b3lyp-dz.minfo   makePES.xml   ref/   resources.info
```

- h2co-b3lyp-dz.minfo

  Includes the equilibrium geometry, harmonic frequencies, and vibrational displacement vectors. They can be visualized by JSindo.

java -cp "/Users/kyagi/tmp/jar/*" Fchk2Minfo h2co-b3lyp-dz

<key value="value" />

key and value are case insensitive unless noted.

<makePES>

<qchem>

id: ID of this qchem (default = the number it appears in the file)

<template>

xml: yes or no (default no)

<xyzfile>

xml: yes or no (default no)

<qff>

# 1. Basic Usage

## 1.1. Preparing an input file

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.

# List of all keys

## General keys

- runtype: QFF/GRID/HYBRID
  The type of run. One of the following must be specified.

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

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

- activemode: string of mode index
  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.

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

- interdomain: true / false
  Calculates inter-domain coupling terms, when true. (default = false)

  QFF計算では、実行された量子化学計算の情報から、Gradientで数値微分の場合はtiij, uiiij、Hessianで数値微分の場合は3MRまでドメイン間カップリングが計算可能だが、interdomain = falseではこれらは出力されない。出力したい場合は、interdomain=trueで再計算する。

  Hessianの場合、minfo.filesからデータを読み込めば、追加の量子化学計算なく3MRまで計算できため、実は計算負荷の軽減にはならない。4MRは追加計算が必要となる。

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

- dryrun: true/false
  Generates the input files for the quantum chemistry program and exits without execution, when true. (default = false)

- xyzfile: filename
  Name of a xyz file, where the coordinates are written. (default = makeQFF for QFF and makeGrid for GRID)

- qchem: command lines (see below)
  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 : Gaussian03/09/16
  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.

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 .xyz), 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 qchem = generic to create a xyz file.
2. Get the grid ID and xyz coordinates from the xyz 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.

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

# QFF keys

- stepsize: real number

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

- ndifftype: grad/hess

  The type of numerical differentiations.

  grad : Numerical 3rd-order diff. of gradient.

  hess (default) : Numerical 2nd-order diff. of hessian.

- mopfile: file name

  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.

- gradient and hessian: input/current

  Specifies where the gradient and Hessian are retrieved.

  input (default) : From the input minfo file.

  current : From the current calculation. (mkqff-eq.minfo)

  "input" is useful for combining accurate geometry, gradient, and Hessian, read from the input minfo file, with lower-level cubic and quartic terms, which are calculated by MakePES module.

  On the other hand, one might think of another strategy, where the geometry and 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.

- interdomain_hc: true/false
  Prints the harmonic coupling, when true. (default = true)

- genhs: true/false
  Generate the 001.hs file, when true. (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.

# GRID keys

- ngrid: integer number
  The number of grid points along each coordinates. (default = 11)

- fullmc: true/false
  All the mode coupling up to the MR-th order is generated, when true. (default = false)

- mc1, mc2, mc3: string of mode index
  The 1, 2, or 3MR terms separated by camma or space. For example,

  mc1:

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

  or

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

  generates grid points for Q1,Q2,Q3, and Q5.

  mc2:

```
<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 (Q2, Q1),(Q4, Q1),(Q4, Q2), and (Q4, Q3).

  mc3:

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

  generates the grid points for (Q3, Q2, Q1) and (Q4, Q2, Q1).

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

# HYBRID keys

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

- mopfile: file name
  The name of mop file, in which the QFF coefficients are written. (default = prop_no_1.mop)

- ngrid: integer number
  The number of grid points along each coordinates. (default = 11)

- mcsstrength: real number
  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.

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.