iGVPT2

version 1.0.0

by

Loïc Barnes & Abdul-Rahman Allouche

Institut Lumière Matière – UMR5306 Université Claude Bernard Lyon 1

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1)What is iGVPT2?

iGVPT2 is an interface for quantum chemistry softwares to compute anharmonic corrections to vibrational frequencies. iGVPT2 can generate files for Quartic Force Field (QFF) calculations, recuperate the results and calculate the anharmonic frequencies with several schemes of VPT2 (GVPT2, DCPT2, HDCPT2). At the moment, calculations with OpenMopac, Gaussian, Orca are implemented and DFTB+ is also possible via a plug-in and Gamess, Firefly and Molpro via a script shell.
The reading of harmonic frequencies, masses, normal modes is implemented for Gaussian, OpenMopac, Orca, Molpro, Gamess and Firefly.
iGVPT2 can also perform a numerical frequencies analysis using the softwares evoked before. For the calculation of the harmonic frequencies, it generates all the files needed.

2) Platforms

iGVPT2 has been tested on Linux (Debian) and MacOSX for the moment.
It is written in C/C++ and uses the OpenBabel library.

3) Availability

iGVPT2 is free only for education and research purposes. The sources files are not available.

4) Citation

5) Licence

Agreement between The TheoChem team, Institut Lumière Matière, UMR5306 CNRS, Université Claude Bernard Lyon 1, Campus LyonTech- La Doua, Bâtiment Kastler, 10 rue Ada Byron, 69622 Villeurbanne CEDEX, France (TheoChem/iLM) and the downloader (Licencee in the sequel)

a) The Licencee acquires a non-exclusive, non-transferrable, revocable licence for using the iGVPT2 code intended to anharmonic frequencies based on GVPT2 approach. This licence is provided free of charge, contingent upon the agreement that iGVPT2 is used for non-profit research exclusively; any commercial use whatsoever is prohibited. The software is provided "as is", without warranty of any kind, express or implied, including but not limited to the warranties of merchantability, fitness for a particular purpose and noninfringement. in no event shall the authors or copyright holders be liable for any claim, damages or other liability, whether in an action of contract, tort or otherwise, arising from, out of or in connection with the software or the use or other dealings in the software.

b) The Licencee guarantees that the software or any part thereof shall not be made accessible to

third parties without the explicit written consent of TheoChem/iLM.

c) In future publications of work performed using iGVPT2, its use will be properly acknowledged with the following references:

> 1)Fast and Accurate Hybrid QM//MM Approach for Computing, Anharmonic Corrections to Vibrational Frequencies, Loïc Barnes, Baptiste Schindler, Isabelle Compagnon and Abdul-Rahman Allouche, Journal of Molecular Modeling (submitted)

6) Installation

You only need to unpack to use the binary:
cd $HOME
tar -zxvf iGVPT2.tar.gz

7) Possibilities of iGVPT2

7-1 Theory

If you want to know more about the theory, please read the article REF(iGVPT2).

7-2 Details

Once you have the optimized geometry and the harmonic frequencies using any quantum chemistry software (Gaussian, Orca, OpenMopac, OpenBabel, Molpro, Fireply, Gamess), you can compute the anharmonic frequencies with the VPT2 method with any software (Gaussian, Orca, OpenMopac, OpenBabel, Molpro, Fireply, Gamess, DFTB+). If a method is not implemented in the softwares cited before, you can always add a new software via a plug-in like we did with DFTB+ or via a script shell (Molpro, Gamess, Firefly).
To treat the resonances, you can use several schemes, GVPT2, DCPT2, VPT2, HDCPT2 via the keyword VPT2Model for the energies and via PropModel for the intensities.
So to perform a GVPT2 calculation for the energies and a DCPT2 one for the intensities, you need to write down in the input file:
VPT2Model=GVPT2
PropModel=DCPT2

If it is difficult to obtain the harmonic frequencies because of the large computational time, iGVPT2 can perform a numerical frequency analysis. The program generates all the single-point files needed to do it.
You can ask for a one step or two steps job meaning that every cartesian coordinate will be displaced of +delta for a one step job and +delta and -delta for a two steps job. The keywords corresponding are:
GenerateFilesOneStepForFreq or GenerateFilesForFreq

You can specify if you want to compute the gradient to reduce the number of points :

GenerateGradFilesOneStepForFreq or GenerateGradFilesForFreq

For a two steps job with gradient 6N files, with N the number of atoms, will be generated. You can calculate the energy and/or gradient with any software (Gaussian, Orca, OpenMopac, OpenBabel, DFTB+, Molpro, Gamess, Firefly).

Then to compute the harmonic frequencies, use the keywords :

ComputeFrequenciesOneStepFromFiles
ComputeFrequenciesOneStepFromGradFiles
ComputeFrequenciesFromFiles
ComputeFrequenciesFromGradFiles

according to the way you generated the files.

Once you have the harmonic frequencies, you can calculate the anharmonic frequencies.
If you want to perform a QFF-2MR calculation, you have to use the keyword GenerateQFFnMRFiles and the keyword QFFnModes, the former must be set to 2. 1MR to 4MR are implemented in iGVPT2.
IGVPT2 will read the optimized geometry and the normal modes. The geometry will be displaced along the normal modes and iGVPT2 will generate the QFF files according to the order of the QFFnMR.
When the creation of every file is done, you can run the calculations either in serial or in parallel.
After all the calculations are done, you need to retrieve every energy and dipole. To do that, you need to change the keyword. You have to use the keyword ComputeQFFnMRFromFiles instead of GenerateQFFnMRFiles.
You can ask a calculation from just one file containing all the energies, dipoles, effective masses, frequencies, see below for the format of that kind of file.
To run the anharmonic calculation from that file, the keyword is ComputeQFFnMRFromEnerg.

Format file:

Frequencies [cm^-1]
freq 1
freq 2
freq 3
Mass [uma]
mass 1
mass 2
mass 3
Delta [Bohr]
delta 1
delta 2
delta 3
Energies [Hartree]
e1
e2
⋮
Dipoles [AU]

x1 y1 z1
x2 y2 z2
⋮ ⋮ ⋮

The units for each quantity is indicated in [ ].
Specify the model for the treatment of the resonances for the energies and the intensities :
VPT2Model = VPT2, GVPT2, DCPT2 et HDCPT2
PropModel

7-3 Description of important keywords

RunType : this keyword control what job will be done, a single-point, a gradient calculation, a VPT2 calculation, etc. With this keyword you can ask a hybrid DFT//MM calculation to compute anharmonic spectra, see REF(hybridMM) for more informations.

Model : Specify the software used (Gaussian, Orca, Mopac, Generic)

QMKeys : Specify all the options for the calculation for the software designated in Model
(for instance for Gaussian : B3LYP/6-31G SCF(Tight) Opt Freq)

GaussianCommand : the script/binary used to run the calculation with Gaussian. Model must be equal to Gaussian.

GenericCommand : the command that allows calculation with new softwares, like a plug-in or script shell. Model must be equal to Generic.

OrcaCommand : the script/binary used to run the calculation with Orca. Model must be equal to Orca.

MopacCommand : the script/binary used to run the calculation with Mopac. Model must be equal to Mopac.

7-4 Example 1

In this example, we will calculate the GVPT2 frequencies for H2O in an hybrid way.
The harmonic frequencies are obtained with B3LYP/def2-TZVPP and the anharmonic corrections are obtained with PM6. The software Gaussian is used for every calculation.
In the directory, a script shell is included that allows to automatically do every step of the calculation, xMakeAll.
The first step is to compute the harmonic frequencies. It is a simple Opt Freq job with Gaussian. The file is h2oB3LYP.com and the output h2oB3LYP.log.
In the file h2oV.ici, in the line below « Geometry », you can specify the name in which you can find the geometry, the frequencies and the normal modes. So write h2oB3LYP.log below « Geometry ».
The second step is the generation of every QFF files. So you need to write
RunType=GenerateQFFnMRFiles in the file h2oV.ici. You can choose the order of the QFF-nMR.
Here we took QFFnModes=2.
In Model, you write the name of the software with which all the QFF files will be computed.
In QMKeys, you write all the options for all the QFF files. Be careful here, you need to add Symmetry=None, in QMKeys, because Gaussian will turn the geometry and that could lead to nonphysical intensities.

Then write the name of the script that will perform the calculation, here it is runG09.
You can run the file : igvpt2 h2oV.ici
All files are now generated. You can either run them in serial or in parallel. Both ways are in the script xMakeAll. Once every calculation is done, you can compute the anharmonic frequencies. All the derivatives will be calculated numerically with PM6 but iGVPT2 will use the second derivatives of the energy found in h2oB3LYP.log. If you want to calculate the intensities from the first derivatives of the dipole calculated with B3LYP/def2-TZVPP, you need to add them in the file like we do in the script.
To compute the derivatives, the keyword RunType must be equal to ComputeQFFnMRFromFiles.
A new file will be created : h2oVQFF.txt with all the derivatives.
The last thing to do is to create the file for the VPT2 calculation, h2oVQFF.ici. RunType must be equal to VPT2 now. Add the first derivatives calculated with B3LYP/def2-TZVPP, if you want. Then add the file h2oVQFF.txt in h2oVQFF.ici. Finally, run that file.
As mentionned before, a script doing all that is provided in the folder.

7-5 Example 2: Orca/DFTB

In this example, we will also calculate the GVPT2 frequencies for H2O in a hybrid way.
The harmonic frequencies are obtained with RI-B2PLYP/def2-TZVPP and the anharmonic corrections are obtained with DFTB3. The software Orca is used to compute the harmonic frequencies and the dftb+ software is used for the anharmonic corrections.
As DFTB+ calculation are not implemented in the iGVPT2 code, we did a plug-in, an external program to run a calculation with DFTB+.
To run that kind of calculation you need to write Generic in Model, and write the command in GenericCommand.
The program is called xCCRun and it is provided in the shell folder.
This program needs an options file named Options.txt. In this file you can choose if you want SCC corrections, third order corrections, dispersion, etc.
iGVPT2 creates a file containing an integer, corresponding to the type of calculation : 0 for an energy calculations, 1 for gradient, 2 for frequencies calculations, The string « Geometry » then the the geometry with a specific format, see section ? for further details.
The program xCCRun then will read all that and create an input file for dftb+ with all the options from Options.txt. Then xCCRun runs the calculation. Finally it retrieves any relevant piece of information and put it in a file read by iGVPT2 in which there are the energy, the dipole, the geometry, the forces if calculated.
In the example folder, there is a script xHybridOrcaDFTB+ to help you run the calculations.
All the steps are the same as in the precedent example. The only things to change have already been discussed and are the options : Model, GenericCommand.

7-6 Example 3: Orca/MMFF94

We will now see a final example to compute anharmonic frequencies. In this example we use a hybrid method : RI-B2PLYP to calculate harmonic frequencies and MMFF94, an empirical force field for the anharmonic part. In the article REF, we show that kind of method is fast and also quite precise compared to the experimental spectra.
The calculation with MMFF94 is directly implemented in iGVPT2 via the OpenBabel library.
The procedure is different compared to the previous examples.
You only one file to calculate the anharmonic spectra.
You have to write HybridMM in RunType to ask such a calculation. Write down QFFnModes, VPT2Model and the different options for VPT2. There is no file generate for QFF calculations, all

is done via the memory.
You just have to run the file : iGVPT2 3MR.ici > 3MR.out

Nevertheless it will generate a file 3MRQFF.txt with all the derivatives in it, in case you want to change the VPT2 parameters (Martin's cutoff, energy difference).

8) The « CCheml »Format

extension .ici

All the keywords first, then the geometry is written after geometry either you put the name of the file you want iGVPT2 to read the geometry or you simply write the geometry with the following format :

Geometry
number of atoms | total charge of the molecule | total spin of the molecule
atomic symbol | MM symbol | PDB symbol | residue name | option | atomic charge | layer autre chose | x coordinate | y coordinate | z coordinate | number of connections | number of the atom connected with it | type of bond (1=single, 2=double, 3=triple, etc) | « GRADIENT » | xgrad | ygrad | zgrad

example: NH_3 molecule

Geometry
4 0 1
N NT N1 GAMA 0 -0.4 2 1 0.0 -0.000008 -0.252142 3 2 1 3 1 4 1 GRADIENT 0.0 0.0 0.0
H H H1 GAMA 0 0.1 2 1 0.0 0.912411 0.084011 1 1 1 GRADIENT 0.0 0.0 0.0
H H H2 GAMA 0 0.1 2 1 0.824806 -0.476201 0.084065 1 1 1 GRADIENT 0.0 0.0 0.0
H H H3 GAMA 0 0.1 2 1 -0.824806 -0.476201 0.084065 1 1 1 GRADIENT 0.0 0.0 0.0

Note that the GRADIENT part is not mandatory and you need the atomic connections only if you want to do a MM calculation so you can write 0 for the number of connections if you don't intend to use a MM potential.

9) List of all keywords

RunType: keyword to specify the type of calculation (energy, gradient, VPT2, HybridMM, ...)

Model: to specify the software for the calculation

QMKeys: to add the options to a QM calculations

HybridMM: to run MMFF94 for a QFF calculation

AlphaHDCPT2: set the parameter value alpha in the HDCPT2 model (default =)

BetaHDCPT2: set the parameter value beta in the HDCPT2 model (default =)

MartinCutOff1: set the value of the first Martin test parameter K1 (default =1 cm-1)

MartinCutOff2: set the value of the second Martin test parameter K2 (default =1 cm-1)

maxFrequencyDifferenceFermi: set the difference value between two frequencies to search for resonances.

GenerateFilesOneStepForFreq: generate energy files for numerical frequencies by a one step job, ie

GenerateFilesForFreq: generate energy files for numerical frequencies by a two steps job, ie

GenerateGradFilesOneStepForFreq: generate gradient files for numerical frequencies by a one step job, ie

GenerateGradFilesForFreq: generate gradient files for numerical frequencies by a two steps job, ie

ComputeFrequenciesOneStepFromFiles: compute the numerical frequencies from the energy files obtained by a one step job

ComputeFrequenciesOneStepFromGradFiles: compute the numerical frequencies from the gradient files obtained by a one step job

ComputeFrequenciesFromFiles: compute the numerical frequencies from the energy files obtained by a two steps job

ComputeFrequenciesFromGradFiles: compute the numerical frequencies from the gradient files obtained by a two steps job

VPT2Model: specify the scheme to treat the Fermi resonances for energies

PropModel: specify the scheme to treat the Fermi resonances for intensities

GaussianCommand: script or binary to run a Gaussian file

GenericCommand: script or binary to run any other software (DFTB+, Molpro, Gamess, Firefly) not implemented directly in iGVPT2.

OrcaCommand: script or binary to run an Orca file

QFFnModes: specify the number of quanta for the QFF calculation.

ComputeQFFnMRFromFiles: Compute the anharmonic derivatives once all the QFF files have been run.

GenerateQFFnMRFiles: generate all the QFF files for

ComputeQFFnMRFromEnerg: Calculate all the derivatives from a certain file see section 7-2 for more informations.