ONETEPConv Documentation

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1 What is ONETEPConv?

ONETEPConv a set of scripts, written in the Bash scripting language, aimed to make the calculation of Energy and Force convergence data more automated.

To have confidence in any DFT calculation it is important that the calculation is run with sufficient accuracy for the purpose required. At the most basic level, this can be done via comparing the convergence of properties such as the Total System Energy or Forces with respect to varying the resolution of the basis set.

By providing ONETEPConv with an example .dat file, ONETEPConv will generate duplicates of this input .dat file, each time varying one parameter of the basis set to form a 'convergence sweep'. ONETEPConv has the following features:

- .dat file generation:

  - Varying equivalent Kinetic Energy Cutoff (Parameter: 'CUTOFF_ENERGY')
  - Varying Radius of the NGWFs per species (Parameter in: %block_species section)
  - Varying Number of NGWFs per species (Parameter in: %block_species section)

- To speed up sweeps, ONETEPConv supports resuming calculations (reuse_calculations T) from the result of previous calculations (reading .dkn and .tighbox_ngwfs)

- Results analysis:

  - Collates the resulting data into sorted .csv files ready for analysis

2 Usage

1. Place a template .dat file into /input/

(a) Ensure the .dat contains a geometry which is not fully geometry optimised because non-zero forces are required to investigate force convergence

(b) Ensure the .dat file is a Single Point Energy calculation with 'WRITE_FORCES T'

(c) Ensure the .dat file has 'WRITE_DENSITY_PLOT F' as writing these files required unnecessary computation and space requirements.

(d) Do not use a high quality basis set in the template, as it will be used for all calculations. It is sufficient to use a low quality basis set and observe the effect of increasing each parameter (kinetic energy cutoff, ngwf radius, number of ngwfs) respectively.

2. Place the .recpots norm-conserving pseudopotentials that you would like to use into the /recpots/ folder

3. Configure ONETEPConv by editing ./input/settings.conv

4. Run ONETEPConv from the root directory:

```
./conv_generate.sh
```

(a) This will generate .dat files in the ./cutoff, ./num_ngwfs and ./ngwf_radius folders respectively

5. Within each subdirectory, run ONETEP manually. You may wish to use a script similar to the provided 'run_jobs.sh'.

6. Extract the results of ONETEPConv into sorted CSV files by running:

```
./extract_to_csv.sh
```

(a) This will generate .csv files in the ./cutoff, ./num_ngwfs and ./ngwf_radius folders respectively, containing both energies (Ha) and forces (Ha/bohr) for each result.

3 ONETEPConv Settings

These can be edited within ./input/settings.conv

- clean: T/F

  Remove all input files in subfolders generated from previous runs

- reuse_calculations: T/F

Reuse a density kernel and NGWFs found in ./input/. This will copy these files into the respective folders, and ensure they are read in by the .dat file. Speeds up the calculations in principle. Note that for this to be enabled, you must have already performed a Single Point Energy calculation and placed the .dkn and .tighbox_ngwfs into ./input. If this is set to T, ensure you set READ_TIGHTBOX_NGWFS T and READ_DENSKERN T in your initial .dat file. If this is set to, ensure that this is not the case.

Kinetic Energy Cutoff Sweep Settings

- min_cutoff: x .
  [float] [units=eV]

  For the Kinetic Energy Cutoff scan, this is the starting (minimum) value of the Kinetic Energy Cutoff

- cutoff_spacing: x .
  [float] [units=eV]

  This is the spacing between each Single Point Energy calculation for the Kinetic Energy Cutoff sweep.

- cutoff_number_of_SPE: x
  [integer]

  This is how many Single Point Energy calculations will be performed, starting from $min_cutoff defined above

  - i.e. max_cutoff=($min_cutoff)+ ($cutoff_spacing*$cutoff_number_of_SPE)

NGWF Radius Sweep Settings

- min_NGWF_radius: x .
  [float] [units=bohr]

  Starting NGWF radius for the sweep

- NGWF_radius_spacing: x .
  [float] [units=bohr]

  Spacing between each Single Point Energy calculation

- NGWF_radius_number_of_SPE: x
  [integer]

  This is how many Single Point Energy calculations will be performed, starting from $min_NGWF_radius defined above.

– i.e. max_NGWF_radius=($min_NGWF_radius)+
($NGWF_radius_spacing*$NGWF_radius_number_of_SPE)

NGWF Quantity Sweep Settings

- increased_ngwfs: x
  [integer]

  The NGWFs quantity sweep will begin with the number defined in the initial.dat file. Each additional Single Point Energy calculation will increase the number of NGWFs by 1.

- per_element: T/F

  Setting this to True will mean that the '%block_species' parameters (NGWF radius/quantity) will be varied on a per_species basis. This is the default behavior. Setting this to False will vary all species parameters simultaneously, which could be useful for quickly investigating what range of parameters may be required.

4   Tips for Settings up ONETEP Calculations

- See http://www2.tcm.phy.cam.ac.uk/onetep/Main/Utilities for a variety of useful scripts.

  – For example, 'dat2bounds' calculates the width of your system including NGWF radii, and based on this provides a suggestion as to what a sensible box size might be for either a periodic vacuum padded cell or an open boundary condition simulation (e.g. Implicit Solvent).

- Along with Cutoff Energy, and NGWF parameters, you must also ensure that the SCF convergence is small enough for the calculation accuracy required (NGWF_THRESHOLD_ORIG)

- For calculations involving a periodic slab (x,y direction) which is vacuum separated (z direction), it is important to test the convergence of the slab thickness with respect to your properties of interest.

- If SCF Convergence is taking many iterations, one option is to try a smaller kinetic energy preconditioning parameter 'K_ZERO' (e.g. setting it to 2.5 a_0^{-1}), however it is important to ensure that the accuracy of your calculations is still maintained.

- As a rule of thumb for new users of ONETEP, the following parameters usually fall in the below range, depending on the required accuracy of the calculation:

  – NGWF radius: 7 bohr to 10 bohr

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- Cutoff energy: 700 eV to 1200 eV

- Usually this would match the valence chemistry e.g. 1 for Hydrogen or 4 for Oxygen. You may need to increase this in some cases, e.g. Silicon crystal required 9 NGWFs for an accurate description (see doi:10.1063/1.2796168).