HOWTO run A-TDEP

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The TDEP method has been developped by Olle Hellman *et al.* [1, 2, 3] in 2011 and the A-TDEP implementation in ABINIT has been performed and used for the first time in 2015 by Johann Bouchet and François Bottin [4, 5].

1 Prerequisite and theory

The approach used in this code is detailed in a publication dedicated to the development of all formula. We strongly encourage all the users to carefully read this paper before beginning. All the vibrational, elastic and thermodynamic quantities computed by A-TDEP are presented with the same writing conventions as the ones used in the output files of A-TDEP. In the same manner, a comprehensive understanding of some ABINIT basic variables is also required in order to fill the input file and read the output file of A-TDEP.

In addition, the paper explaining the theory and implementation of A-TDEP is also useful to understand the limitations and convergences which are inherent to the present method. These particular points are sometimes discussed in the article, with some references and illustrating examples.

2 The ABINIT computation

To run A-TDEP, a preliminary ABINIT simulation is needed. This one could be a molecular dynamic trajectory or a set of "ground state" calculations on specific configurations (representative of a given thermodynamic state). After that, all the configurations have to be merged : (*i*) in a single NetCDF file `HIST.nc` or (*ii*) in three separated ASCII files `fcart.dat`, `xred.dat` and `etot.dat` corresponding to the forces in cartesian coordinates, the positions in reduced coordinates and total energies (in Ha), respectively, as they are written in the output file of ABINIT. In the later case, the three files can be built easily by concatenating in each one all the time steps or configurations (using a `grep` shell instruction, for example).

3 The a-TDEP computation

In a same manner as performed for ABINIT, the use of A-TDEP is quite simple. One has just to execute TDEP as follows :

```
tdep < input.files > log
```

with the `input.files` file containing three lines. The first one defines the input file, the second one is the NETCDF file (if present, see above) and the third one defines the root of all the output files :

```
input.in
HIST.nc
output
```

The detection of the `HIST.nc` file is performed at the beginning so, if this one is absent, the code will automatically search the three ASCII `.dat` files.

4 The input files

An example of an A-TDEP calculation (in the special case where the NETCDF file `HIST.nc` is employed) is the test `t37` of the `v8` suite. The two input files are given in the `Input` directory: `t37.in` and `t37_HIST.nc`. Let us describe briefly the `t37.in` file.

```
      NormalMode
# Unit cell definition
           brav   7   0
  natom_unitcell            5
   xred_unitcell   0.0 0.0 0.0  0.5 0.5 0.5  0.0 0.5 0.5  0.5 0.0 0.5  0.5 0.5 0.0
  typat_unitcell   3   2   1   1   1
# Supercell definition
    multiplicity   2.00   0.00   0.00   0.00   2.00   0.00   0.00   0.00   2.00
     temperature    495.05
# Computation details
       nstep_max       101
       nstep_min         1
            Rcut     7.426
# Optional inputs
         Ngqpt2 2 2 2
         TheEnd
```

The input file format is fixed. So :

1. this file begins with a "`NormalMode`" or "`DebugMode`" keyword and finishes with "`TheEnd`" (all the lines after are not read).
2. all the lines between "`# Unit cell definition`" and "`# Optional inputs`" are fixed.

3. Between "`# Optional inputs`" and "`TheEnd`", the format is free.

Even if all the input variables are defined elsewhere (see the `variables_tdep.py` file), we will briefly explain the present input file thereafter.

1. The section "`# Unit cell definition`" defines the bravais lattice `brav` (here, it is a simple cubic), the number of atoms in the unitcell `natom_unitcell` (here, there are 5 atoms), their reduced coordinates in the unitcell `xred_unitcell` (here, it is a perovskite) and the type of atoms in the unitcell `typat_unitcell` (here, there are one atom A, one atom B and 3 atoms C).

2. The section "`# Supercell definition`" defines the multiplicity of the supercell with respect to the unitcell `multiplicity` (here, it is a simple 2×2×2 multiplication of the unitcell) and the temperature of the system `temperature` (here, it is 495.05 K).

3. The section"`# Computation details`" defines the range [`nstep_max` ; `nstep_min`] of time steps or configurations (here, there are 100 time steps) and the cutoff radius for the pair interactions `Rcut` (here, all the interaction pairs with a bond length larger than 7.426 bohr will not be considered).

4. The section "`# Optional inputs`" can define a large number of optional keywords (here, `Ngqpt2` defining the **q**-point grid for the vDOS integration is set to 2 2 2 in order to have a test sufficiently fast, which means that all the thermodynamic quantities have no sense.)

Note that some input variables, not defined in the `input.in` file, are obtained from the `HIST.nc` file. In particular, the features of the supercell.

`TODO : Explain the extra input variables when the 3 ASCII files are employed.`

5 The output files

A large number of output files are obtained after an execution of A-TDEP. Three output files are given in the `Refs` directory:

1. `t37.out` is the main output file. It includes an echo of the input variables, some intermediary results, the definition of the various shells of interaction, the second order IFCs for all the atoms in each shell, the elastic constants and moduli, the energy of the model...

2. `t37omega.dat` contains the dispersion of phonon frequencies (in meV) along a path in the Brillouin Zone,

3. `t37thermo.dat` lists all the thermodynamic quantities obtained by considering the system as a quantum harmonic crystal : specific heat, vibrational energy, entropy and free energy. It also gives all these contributions as a function of temperature in the harmonic approximation.

Other files, not given in the `Refs` directory, are also obtained :

4. `sym.dat` details all the symmetry operations of the bravais lattice,
5. `qpt.dat` defines the **q**-point grid used to compute the phonon frequencies contained in the `omega.dat` file,
6. `xred_average.xyz` includes the ideal and average positions in the supercell,
7. `Indym*.dat` contain all the symmetry relations between one or two atoms in the unitcell or the supercell,
8. `vdos.dat` displays the vibrational density of states (in meV),
9. `dij.dat` lists the dynamical matrices for a particular set of **q**-points,
10. `etotMDvsTDEP2.dat` compares the MD trajectory with the one computed using the second order IFCs (these ones must be superimposed, as much as possible) ,
11. `fcartMDvsTDEP2.dat` plots the MD forces wrt the forces computed using the the second order IFCs (the cloud of points must be closer to the first bisector),
12. `eigenvectors.dat` lists all the eigenvectors for a particular set of **q**-points,
13. `nbcoeff-phij.dat` shows how the number of IFC coefficients are reduced (for each shell and each symmetry),
14. ...

References

[1] O. Hellman, I.A. Abrikosov and S.I. Simak, *Lattice dynamics of anharmonic solids from first principles*, Phys. Rev. B **84**, 180301(R) (2011).

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[3] O. Hellman and I.A. Abrikosov, *Temperature-dependent effective third-order interatomic force constants from first principles*, Phys. Rev. B **88**, 144301 (2013).

[4] J. Bouchet and F. Bottin, *Thermal evolution of vibrational properties of α-U*, Phys. Rev. B **92**, 174108 (2015)

[5] J. Bouchet and F. Bottin, *High-temperature and high-pressure phase transitions in uranium*, Phys. Rev. B **95** 054113 (2017).