

# AFLOW V 3.1.137

```
*****
*
*          aflow - STEFANO CURTAROLO Duke University 2003-2017          *
*          High-Throughput ab-initio Computing Project                  *
*
*****
LATEST VERSION OF THE FILE:          materials.duke.edu/AFLOW/aflow_apl.pdf
*****
```

Phonon calculations with deformations written by Michal Jahnatek, Pinku Nath, Jose J. Plata, Corey Uses and Ste

The current version of APL can calculate the phonon dispersion curves (output file PDIS), phonon density of state (file PDOS), and thermal properties (file THERMO). All are calculated in harmonic approximation. Two methods of calculation can be selected: direct (supercell) method (DM) or linear response method (LR). The resulted file can be transformed by next tool apl2agr into agr, ps, eps, or png form (located in SOURCES/APL2AGR).

APL expects the well relaxed structure on input. There is no additional relaxation inside the APL. So, you have to prepare a such structure by separate aflow run with relaxation mode for forces. For phonon calculation, generally, you have to setup 3 things: 1) Tell to aflow you want a phonon calculation. 2) Which method of calculation to use. 3) What to calculate.

1) To perform a phonon calculation this line has to be present in aflow.in:

```
[AFLOW_APL]CALC
```

The APL is checking its existence in aflow.in. If it does not exist, the job is not supposed to be for phonon calculation and no other phonon settings are read.

2) The user has possibility to switch between two methods of calculation by keyword ENGINE. For direct method (DM), also known as supercell method, one has to write:

```
[AFLOW_APL]ENGINE=DM
```

This is also a default setting. For linear response method it is:

```
[AFLOW_APL]ENGINE=LR
```

Since this parameter has its own default settings, you do not need to specify it if you are fine with DM. Each method has its own, but also common parameters, which can be used to tune the whole calculation.

2.1) Common parameters used by both methods

The most important setting is the supercell dimension (the supercell is required by both methods). Supercell can be set in three ways:

```
[AFLOW_APL]SUPERCELL=numberXnumberXnumber
[AFLOW_APL]MINSHELL=number
[AFLOW_APL]MINATOMS=number
```

EXAMPLES:

Direct specification, like  
[AFLOW\_APL]SUPERCELL=4x4x4

Minimal nearest neighbor shell, specification like:

```
[AFLOW_APL]MINSHELL=6
```

The default settings is MINSHELL=6 and APL will construct the appropriate supercell. HOWEVER, THIS IS NOT THE RECOMMENDED WAY, BECAUSE INCLUSION OF 6 SHELL IS ENOUGH ONLY FOR VERY SIMPLE MATERIALS. There is no way or rule how to find the number of enough shells included into calculation. FOR BEST RESULTS YOU HAVE TO SPECIFY THE SUPERCELL DIMENSION DIRECTLY. We found the 4x4x4 is usually enough for all fcc systems; 3x3x2 for hcp; bcc are complicated, but generally it should be more that 3x3x3. Typically, the supercell with about 100 atoms should

be fine for 90% systems. You might find the MINATOMS option useful for large unit cells.

Minimal number of atoms, like:

```
[AFLOW_APL]MINATOMS=number
```

The code will homogeneously increase the volume of the supercells, until it finds a SUPERCELL(i,j,k) containing at least "number" atoms.

```
[AFLOW_APL]KPPRA=number
```

By default, AFLOW takes the number of KPOINTS (KPPRA) from the "[VASP\_KPOINTS\_FILE]KPPRA=number" entry. You can override the number with "[AFLOW\_APL]KPPRA=number". Look at README\_AFLOW.TXT for KPPRA.

```
[AFLOW_APL]KSCHEME=scheme
```

By default, AFLOW takes the KPOINTS scheme from the "[VASP\_KPOINTS\_FILE]KSCHEME=scheme" entry. You can override the scheme with "[AFLOW\_APL]KSCHEME=scheme". Look at README\_AFLOW.TXT for KSCHEME.

```
[AFLOW_APL]KPOINTS=EVEN | ODD
```

By default, AFLOW takes the KPOINTS parity from the "[VASP\_FORCE\_OPTION]KPOINTS=EVEN | ODD" entries, if available. You can override the entries with "[AFLOW\_APL]KPOINTS=EVEN | ODD". Look at README\_AFLOW.TXT for KPOINTS. This is useful for a small number of KPOINTS.

## 2.2) Direct method parameters

The supercell (direct) method can be modified by this parameters:

```
[AFLOW_APL]DXYZONLY=n
```

```
[AFLOW_APL]DMAG=0.015
```

```
[AFLOW_APL]DPM=y
```

```
[AFLOW_APL]ZEROSTATE=n
```

The DPM, DXYZONLY, and DMAG parameters control how the distortion vectors will be generated. Generally, APL will try atom distortions along the [100],[010],[001],[110],[101],[011],[111] direction. It will apply all site symmetry operations, and that direction which produces the highest number of new independent vectors will be used in next calculation. For each unique atom of the primitive cell we need to know the forces acting along three independent directions. Hence, if one distortion direction can produce by the symmetry three linear independent vectors, this atom needs to be distorted in only one direction and the rest two are calculated by the symmetry. This is the case of fcc lattice.

if you specify DXYZONLY=y, only the three trial directions ([100],[010],[001]) will be tried. This is important for cases when one primitive cell vector is much longer than others. All founded directions of distortion are of unit length. The real distortion is applied by some specified magnitude. This magnitude should be small enough. It can be set by keyword DMAG. The default value is 0.015 Angs., what is generally accepted value also by other software packages and works well for all systems.

Usually, in effort to filter out the anharmonic effects from the forces, it is important to calculate forces in both directions of distortion, i.e., DMAG is applied by positive and also negative sign. This is controlled by keyword DPM. If you specify DPM=y (default), twice more distortion vectors will be generated, and the final force acting on each atom is calculated as  $0.5 * ( f(+) - f(-) )$ .

Sometimes, it can happen the calculating structure is not well relaxed or can not be in a given precision. In this case, even the unstrained state has some non-zero forces. In this case is good to subtract these forces from all states. This can be done by ZEROSTATE=y, what means the APL will generate the calculation of this unstrained state and the obtained forces for this state will be subtracted from all other strained calculations. (!not well tested part)

## 2.3) Linear response parameters

The use of the linear response method as is implemented in VASP is more complicated. Every time you specify this method (ENGINE=LR), APL will check you binary file of VASP for version. If it is not 5.2 or higher it will refuse to continue. Moreover, vasp52 binary has to be run with special settings in you .bashrc, otherwise the calculation will crash after the first completely converged electronic loop. Hence, check you have these lines in you .bashrc:

```
ulimit -s unlimited
```

In case of LR method, APL is not responsible for finding the appropriate set of distortion vectors and all stuff for generation and creation of supercells. All is done by VASP. Hence, expect quite long run. Please note, the VASP is using the mode XYZONLY, hence finally more distortions are generated as are needed. As result, the VASP will generate file DYNMAT, where all forces acting on atoms after each distortion are located. This is the main input file for APL for the next calculation.

#### 2.4) Linear response parameters

If you know the studied system is polar, the phonon properties have to be calculated specially, where the dipole-dipole interaction is taking into account. This can be specified by keyword POLAR.

```
[AFLOW_APL]POLAR=y
```

In this case, APL will prepare also next run by VASP52, where Born effective charges and dielectric constant matrix will be calculated with Linear Response (DFTP).

These both quantities will be used later in correction of dynamic matrices for correct TO-LO splittings. The default setting is POLAR=n.

Note that TO-LO splitting is calculated only with >VASP52.

Epsilon and the Born charges are calculated in two ways: with LEPSILON or LCALCEPS. Default is the latter. You can switch the code by changing the lines of aflow\_apl.h

```
#undef AFLOW_APL_VASP_USE_LEPSILON
#define AFLOW_APL_VASP_USE_LCALCEPS
```

#### 3) Generally, you can specify what to calculate by these keyword:

```
[AFLOW_APL]DC=y
[AFLOW_APL]DPM=y
[AFLOW_APL]ZEROSTATE=y
[AFLOW_APL]DOS=y
[AFLOW_APL]TP=y
```

The default setup is no for all. Each calculation mode has its own set of parameters.

#### 3.1) Phonon dispersion curves calculation (DC=y)

The most important setting for this module is the path in the reciprocal space for which the frequencies should be calculated. The APL can do it automatically, via AFLOW-SYM, The procedure is: AFLOW-SYM is called to obtain the spacegroup number of primitive cell. Then, this number is used to get the path from the settings used for the calculation of the electronic structure in aflow. If you wish to skip this calculation, the space group has to be specified in aflow.in, like:

```
[AFLOW_APL]DCINITPATH = RHL
```

where you can specify the lattice variation as introduced in [\[doi=10.1016/j.commat.2010.05.010\]](https://doi.org/10.1016/j.commat.2010.05.010)

or

```
[AFLOW_APL]DCINITSG = 166
```

If everything is OK, the APL will calculate the dispersion curves along the same path as is used for electronic structure. If you need to calculate it by an another path, you can specified it as:

```
[AFLOW_APL]DCUSERPATH = G-X|X-U|K-G|G-L
```

where G,X,U,L points are the same points as are defined inside the aflow (for electronic structure). The number of points in which each sub-path (G-X,X-U,...) will be calculated can be set as:

```
[AFLOW_APL]DCPOINTS=100
```

what is also a default setting. The calculated dispersion curves are saved in file PDIS, where the 1st column is ID of points in sub-path, the 2nd is the position in the whole path, ... the next

column correspond to one phonon branch. There is  $3 * \text{natoms\_in\_primitive\_cell}$  branches. The frequencies are in units specified by (default)

```
[AFLOW_APL]FREQFORMAT = "THZ | ALLOW_NEGATIVE"
```

which means the frequency is returned in THz and also negative values are allowed to return. The OR operator is important for use. If ALLOW\_NEGATIVE is not added, only the positive values are returned (negative values are returned as zero).

Other options are

```
[AFLOW_APL]FREQFORMAT = "RECIPROCAL_CM" or "CM-1"  
[AFLOW_APL]FREQFORMAT = "MEV"  
[AFLOW_APL]FREQFORMAT = "OMEGA"  
[AFLOW_APL]FREQFORMAT = "HERTZ"
```

### 3.2) Phonon density of states calculation (DOS=y)

There are implemented two method for integration in Brillouin zone - Linear Tetrahedron method (LT) and root sampling method (RS). As default is selected LT. User can switch between them by as:

```
[AFLOW_APL]DOSMETHOD=LT
```

or

```
[AFLOW_APL]DOSMETHOD=RS
```

The mesh of qpoints used for numerical integration should be set as:

```
[AFLOW_APL]DOSMESH=21x21x21
```

The setting 21x21x21 is also the default setting. The APL will automatically find the irreducible part of BZ (the list of irreducible qpoints with appropriate summation weights). Only for these qpoints a dynamic matrix is constructed and diagonalized. In case of linear tetrahedron method, the list of irreducible tetrahedrons with their weights is constructed and used in summation. The function of density of states will be evaluated in finite number of points, which can be set as:

```
[AFLOW_APL]DOSPOINTS=2000
```

The density of 2000 points is the default setting. The resulted DOS function can be smeared by gaussian of specific width. This is quite important for RS method to have a nice looking pictures. The default setting of smearing for RS method is 0.05, but can be changed as:

```
[AFLOW_APL]DOSSMEAR=0.05
```

For LT method the default setting is 0.0, so no smearing.

### 3.3) Thermal properties calculation (TP=y)

Generally, APL is calculating the zero point vibrational energy (U0), the internal energy (U), the vibrational free energy (Fv), the vibrational entropy (Sv), and isochoric specific heat (cv) for a given range of temperature. This range can be set as

```
[AFLOW_APL]TPT=0:2000:10
```

what means it will calculate all upper mentioned properties from 0 to 2000 K by step of 10 K. This is also a default setting.

### 4) The APL has integrated hibernate system, which is switched on by default. To turn it down:

```
[AFLOW_APL]HIBERNATE=n
```

This system means the calculated force constant matrices are stored in external file called apl.xml.bz2. Once this file exists and you will run aflow for phonon calculation again, it

will automatically use this data (awake from it) and speed up calculation.

5) Inputs and inheritance.

The minimal input is:

```
[AFLOW_APL]CALC
[AFLOW_APL]MINATOMS=100
#[AFLOW_APL]SUPERCELL=4x4x4
[AFLOW_APL]DC=y
[AFLOW_APL]DPM=y
[AFLOW_APL]ZEROSTATE=y
[AFLOW_APL]DOS=y
[AFLOW_APL]TP=y
```

5.1) Inheritance

The generated ARUN.APL\*\*\*/aflow.in input files inherit some options from the master aflow.in

If present, the following options are passed to the local aflow.in

```
[VASP_FORCE_OPTION]AUTO_PSEUDOPOTENTIALS=...
[VASP_FORCE_OPTION]SPIN=...
[VASP_FORCE_OPTION]TYPE=...
[VASP_FORCE_OPTION]AUTO_MAGMOM=...
[VASP_FORCE_OPTION]BADER=...
[VASP_FORCE_OPTION]ELF=...
[VASP_FORCE_OPTION]ABMIX=...
[VASP_FORCE_OPTION]KPOINTS=...
[VASP_FORCE_OPTION]IGNORE_AFIX=...
```

Other options are added by default, they are:

```
[VASP_FORCE_OPTION]WAVECAR=OFF
[VASP_FORCE_OPTION]CHGCAR=OFF
[VASP_FORCE_OPTION]PREC=ACCURATE
[VASP_FORCE_OPTION]ALGO=NORMAL
```

To avoid intercepting NPAR warnings introduced in vasp52+, the extra option is added

```
[VASP_FORCE_OPTION]IGNORE_AFIX=NPARG
```

6) EXAMPLE: PbS with Linear Response use the following:

For Deformation engine, put [AFLOW\_APL]ENGINE=DM and uncomment #[AFLOW\_APL]DMAG=0.015

```
[AFLOW] *****
[AFLOW] SYSTEM=PbS
[AFLOW] *****
[AFLOW_MODE=VASP]
[AFLOW_MODE_ZIP=bzip2]
[AFLOW_MODE_BINARY=vasp53s]
[AFLOW] *****
#[AFLOW_MODE_MPI]
[AFLOW_MODE_MPI_MODE]NCPUS=MAX
[AFLOW_MODE_MPI_MODE]COMMAND="mpirun -np"
[AFLOW_MODE_MPI_MODE]AUTOTUNE
[AFLOW_MODE_MPI_MODE]BINARY="mpivas53s"
[AFLOW] *****
[AFLOW_APL]CALC
[AFLOW_APL]ENGINE=LR
#[AFLOW_APL]DMAG=0.015
[AFLOW_APL]POLAR=Y
[AFLOW_APL]SUPERCELL=4x4x4
[AFLOW_APL]DC=Y
#[AFLOW_APL]DCINITSG=227
#[AFLOW_APL]DCUSERPATH=Gamma-X|X-U|K-Gamma|Gamma-L
[AFLOW_APL]DCINITPATH=FCC
[AFLOW_APL]DOS=Y
[AFLOW_APL]TP=Y
[AFLOW_APL]TPT=0:2000:10
[AFLOW_APL]KPPRA=1024
```

```

[AFLOW_APL] KSCHEME=G
[AFLOW_APL] KPOINTS=EVEN
[AFLOW_APL] DOSMESH=30x30x30
[AFLOW] *****
[VASP_RUN] RELAX=2
#[VASP_FORCE_OPTION] KPOINTS=KEEPK,EVEN,KSHIFT_GAMMA_EVEN,KSCHEME_GAMMA,GAMMA,IBZKPT
[VASP_FORCE_OPTION] SYM=ON
[VASP_FORCE_OPTION] AUTO_PSEUDOPOTENTIALS=potpaw_PBE
[VASP_FORCE_OPTION] NBANDS
[VASP_FORCE_OPTION] SPIN=OFF
[VASP_FORCE_OPTION] RELAX_MODE=FORCES
[VASP_FORCE_OPTION] PREC=PHONONS
[VASP_FORCE_OPTION] ALGO=FAST
[VASP_FORCE_OPTION] RELAX
[VASP_FORCE_OPTION] TYPE=DEFAULT
[VASP_FORCE_OPTION] CONVERT_UNIT_CELL=SPRIM,MINK
[AFLOW] *****
[VASP_INCAR_MODE_EXPLICIT] START
SYSTEM=PbS
[VASP_INCAR_MODE_EXPLICIT] STOP
[AFLOW] *****
[VASP_KPOINTS_MODE_IMPLICIT]
[VASP_KPOINTS_FILE] KSCHEME=G
[VASP_KPOINTS_FILE] KPPRA=400
[AFLOW] *****
[VASP_POTCAR_MODE_IMPLICIT]
[VASP_POTCAR_FILE] Pb
[VASP_POTCAR_FILE] S
[AFLOW] *****
[VASP_POSCAR_MODE_EXPLICIT] START
PbS [FCC,FCC,cF8]
1.224745
  0.00000000000000  2.45291416610433  2.45291416610433
  2.45291416610433  0.00000000000000  2.45291416610433
  2.45291416610433  2.45291416610433  0.00000000000000
1 1
Direct(2) [A1B1]
  0.00000000000000  0.00000000000000  0.00000000000000  Pb
  0.50000000000000  0.50000000000000  0.50000000000000  S
[VASP_POSCAR_MODE_EXPLICIT] STOP
[AFLOW] *****

```

#CO - START 170601

\*\*\*\*\*  
NB:

Any shared tags between APL/QHA/AAPPL can be equivalently specified with [AFLOW\_APL], [AFLOW\_QHA], [AFLOW\_AAPL] in the afLOW.in.

This allows users the flexibility to first run an APL calculation, then proceed with a subsequent analysis (QHA) without the need to change the tags.

\*\*\*\*\*  
#CO - END 170601

#### 7) Quasi-harmonic approximation (Gruneisen parameter and Equation of state calculations)

Thermal properties calculated using a quasi-harmonic(QH) model.

This implementation in AFLOW written by Pinku Nath and Stefano Curtarolo,

and is described in the paper "Computational Materials Science Volume 125, December 2016, Pages 8291".

Following properties can be calculated..

Gruneisen parameter along high-symmetry path

Mode Gruneisen in q-mesh

Average Gruneisen parameter

Mean-square displacement

Projected mean-square displacement

Equation of states (Cp, thermal-expansion, Bulk Modulus etc.)

The current version of AFLOW-QH can calculate the Gruneisen parameter, heat capacity, vibrational free energy and other thermal properties, as a function of temperature. The results are written in a variety of formats. The following keywords can be used to calculate AFLOW-QH properties.

```
[AFLOW_QHA]CALC // Gruneisen parameter option
[AFLOW_QHA]DISPLACEMENTS=y // Phonon mean square displacements option
[AFLOW_QHA]PROJECTION_DIR=h:k:l // Phonon mean square displacements option along a particular direction (hkl)
[AFLOW_QHA]EOS=y // Equation of state calculation
```

#### 7.1) Gruneisen Parameter calculation ([AFLOW\_QHA]CALC)

Calculate Gruneisen Parameters using the quasi-harmonic approximation.

```
[AFLOW_QHA]CALC
[AFLOW_QHA]GP_VOL_DISTORTION_PERCENTAGE=0.03 [percentage of volume distortion magnitude w.r.t equilibrium]
[AFLOW_QHA]CUTOFF_FREQ=0.001 [in AMU unit] [default value is 1e-5] frequency cutoff
```

During the first [AFLOW] execution two directories are going to be created with positive and negative distortion. For example with "GP\_VOL\_DISTORTION\_PERCENTAGE=0.03" will create ARUN.APL\_PHONON\_P0.03 and ARUN.APL\_PHONON\_MO.03. Data can be extracted from the second run by performing the following two steps

(1) REMOVE/RENAME LOCK files from current directory and ARUN.APL\_PHONON\_\* directories e.g. [rm -rf LOCK\* APL\_\*]   
 [\*\*WARNING DO NOT REMOVE LOCK from any other directories except current and ARUN.APL\_PHONON\_\* directories]

(2) aflow -run=multi -rsort -D ./ > out &   
 During run a directory "[ARUN.APL.QH.TMP]" is going to be created which stores some necessary files

(3) If you are using a differently named aflow.in and LOCK files (e.g. apl\_ahow.in and apl\_LOCK) then use the following   
 (a) rm \*.bz2 apl\_LOCK ARUN.APL\_PHONON\_\*/apl\_LOCK\*   
 (b) aflow --use\_ahow.in=apl\_ahow.in --use\_LOCK=apl\_LOCK -run=multi -rsort -D ./ > out &

OUTPUT file names:

```
[ahow.apl.qh.out] file storing the average and acoustic Gruneisen parameter for user defined temperature range
[ahow.apl.gp.pdis.out] file storing the calculated Gruneisen parameter along high-symmetry k-points, for GP calculations
[ahow.apl.gp.mesh.out] file storing the calculated Gruneisen parameter in Monkhorst-Pack k-points and frequencies
[ahow.apl.gp.freq.mesh.out] file storing Gruneisen parameter and frequencies for each phonon mode in uniform grid
[ahow.apl.branch.index.out] file storing phonon mode indices that has generated iafter unfolding phonon branches
```

If the phonon frequencies are negative there will be no GP calculations.

7.2) [AFLOW\_QHA]DISPLACEMENTS=y   
 Mean square displacements [Angstrom unit] in the user defined temperature range. While calculating displacements   
 [OUTPUT FILE NAME] aflow.apl.displacements.out

7.3) [AFLOW\_QHA]PROJECTION\_DIR=h:k:l   
 Projected mean square displacements [Angstrom units] along Cartesian axes [h k l] direction in the user defined temperature range   
 [OUTPUT FILE NAME] aflow.apl.projected\_displacements.out

#### 7.4) Equation of state calculations (EOS=y)

Quasi-harmonic equation of states can be calculated using EOS keywords. While calculating EOS, GRUNEISEN parameter and other thermal properties. The following additional keywords are necessary to calculate EOS:

```
[AFLOW_QHA]EOS_VOLRANGE_DIST:=-2:4:0.5 // Percentage of distortion magnitude w.r.t equilibrium configuration
// Format is start_volume:end_volume:increment. For example, -2:4:0.5 represents -2% to 4% with increment of 0.5%
```

```
[AFLOW_QHA]EOS_KPOINTS_MODE:=8000:10000:20:50000 // Default values are KPPRA=8000, STATIC_KPPRA=10000, KPOINTS_INCREMENT=20
```

During first [AFLOW] execution, two sets of directories with prefixes "ARUN.APL\_PHONON\_" and "ARUN.APL\_STATIC\_" are going to be created. For example, "ARUN.APL\_PHONON\_P1.5" represents phonon directory with positive 1.5% distortion, and "ARUN.APL\_STATIC\_S3.5" represents static directory with positive 3.5% distortion respectively.

Data can be extracted in the second run by using following steps:

(1) REMOVE LOCK files from current directory and ARUN.APL\_PHONON\_ directories e.g. `rm -rf LOCK* ARUN.APL_PHONON_*`  
[\*\*WARNING DO NOT REMOVE LOCK from anyother directories except current and ARUN.APL\_PHONON\_ directories

(2) `aflow -run=multi -rsort -D ./ > out &`

(3) If you are using a differently named aflow.in and LOCK files (e.g. `apl_aflow.in` and `apl_LOCK`) then use the following:

(a) `rm *.bz2 apl_LOCK ARUN.APL_PHONON_*/apl_LOCK*`

(b) `aflow --use_aflow.in=apl_aflow.in --use_LOCK=apl_LOCK -run=multi -rsort -D ./ > out &`

Output file names:

[`aflow.apl.FVT.out`] => free energies, volume, data for user defined temperatures

[`aflow.apl.eos.out`] => EOS for all user defined temperatures

[`aflow.apl.err_fit.out`] => errors associated with fitting methods.

7.5) Data fitting can be performed either using `lmsder` [this is a robust and efficient version of the Levenberg-Marquardt algorithm] or `lmdcr` [this is an unscaled version of the Levenberg-Marquardt algorithm]. There are 3 fitting functions available

[`AFLOW_QHA`]`FITTING_TYPE=BM1` // Murnaghan EOS (Murnaghan F D, Am. J. Math. 49, p235 (1937))

[`AFLOW_QHA`]`FITTING_TYPE=BM2` // Birch-Murnaghan 3rd-order EOS (Birch F, Phys. Rev. 71, p809 (1947))

[`AFLOW_QHA`]`FITTING_TYPE=BM3` // Birch-Murnaghan 4th-order EOS, (Journal of Computational Chemistry 2001)

default option is BM1

7.6) Example qsub file file

```
#!/bin/bash
#
# These commands set up the Grid Environment for your job:
#PBS -q debug
#PBS -l nodes=1:ppn=32
#PBS -l walltime=2:00:00
#PBS -N Si_test2
#PBS -o out.$PBS_JOBID
#PBS -e err.$PBS_JOBID

AFLOW="AFLOW_PATH/"
source /opt/intel/bin/compilervars.sh intel64
export PATH=$PATH:/MAIN/bin/VASP:$AFLOW

cd $PBS_O_WORKDIR

# choose random directory
touch log.$PBS_JOBID
$AFLOW/aflow --monitor >> log.$PBS_JOBID &
$AFLOW/aflow --force -multi --machine=qrats -D ./ >> log.$PBS_JOBID

#post processing
# remove all bz2 files except qsub1.sh
if [ -f qsub1.sh.bz2 ]; then bzip2 -d qsub1.sh.bz2; fi
if [ -f aflow.fgroup.out.bz2 ]; then rm *.bz2; fi

#(1) rename all phonon LOCK to LOCK.old
for i in $( ls LOCK* ARUN.APL_PHONON_*/LOCK* ); do mv $i $i.old; done

#(2) run aflow-multi with rsort option
$AFLOW/aflow --force -multi -rsort --machine=qrats -D ./ >> log.$PBS_JOBID
```

7.7) Example aflow.in for quasi-harmonic calculations:

[`AFLOW`]`SYSTEM=Si2`

#[`AFLOW`] single element calculation

[`AFLOW`] \*\*\*\*\*



```

[AFLOW] input file for aflow
[AFLOW_MODE=VASP]
[AFLOW] *****
[AFLOW_MODE_ZIP=bzip2]
[AFLOW_MODE_BINARY=vasp53s]
[AFLOW] *****
[AFLOW] *****
#[AFLOW_MODE_MPI]
[AFLOW_MODE_MPI_MODE]NCPUS=MAX
[AFLOW_MODE_MPI_MODE]COMMAND ="mpirun -np"
[AFLOW_MODE_MPI_MODE]AUTOTUNE
[AFLOW_MODE_MPI_MODE]BINARY="mpivasp53s"
[AFLOW] *****
[AFLOW_SYMMETRY]CALC
#[AFLOW_SYMMETRY]SGROUP_WRITE
#[AFLOW_SYMMETRY]SGROUP_RADIUS=7.77
[AFLOW] *****
#[AFLOW_NEIGHBOURS]CALC
[AFLOW_NEIGHBOURS]RADIUS=7.7
[AFLOW_NEIGHBOURS]DRADIUS=0.1
[AFLOW] *****
[AFLOW_QHA]CALC
[AFLOW_QHA]ENGINE=DM
[AFLOW_QHA]DMAG=0.015
[AFLOW_QHA]MINATOMS=100
#[AFLOW_QHA]SUPERCELL=2x2x2
[AFLOW_QHA]POLAR=y
[AFLOW_QHA]DISPLACEMENTS=y
[AFLOW_QHA]PROJECTION_DIR=1:1:1
[AFLOW_QHA]GP_VOL_DISTORTION_PERCENTAGE=0.03
[AFLOW_QHA]EOS=n
[AFLOW_QHA]EOS_VOLRANGE_DIST=-2:4:0.5
[AFLOW_QHA]EOS_KPOINTS_MODE=32768:10000:20:100000
[AFLOW_QHA]DC=y
[AFLOW_QHA]DPM=y
[AFLOW_QHA]ZEROSTATE=y
#[AFLOW_QHA]DCINITSG=227
#[AFLOW_QHA]DCUSERPATH=Gamma-X|X-U|K-Gamma|Gamma-L
[AFLOW_QHA]DOS=y
[AFLOW_QHA]TP=y
[AFLOW_QHA]TPT=0:2000:10
[AFLOW] *****
[VASP_FORCE_OPTION]CHGCAR=OFF // ON | OFF (default ON)
[VASP_FORCE_OPTION]SYM=ON // ON | OFF (default ON)
[VASP_FORCE_OPTION]PREC=PHONONS
[VASP_FORCE_OPTION]AUTO_PSEUDOPOTENTIALS=potpaw_PBE // pot_LDA | pot_GGA | potpaw_LDA | potpaw_GGA | potpaw_P
[VASP_FORCE_OPTION]ALGO=NORMAL // (NORMAL | VERYFAST | FAST | ALL | DAMPED), PRESERVED (
[VASP_FORCE_OPTION]TYPE=DEFAULT // METAL | INSULATOR | SEMICONDUCTOR | DEFAULT (default D
[VASP_FORCE_OPTION]CONVERT_UNIT_CELL=SPRIM // SPRIM, SCONV, NIGGLI, MINK, INCELL, COMPACT, WS, CART,
[AFLOW] *****
[VASP_INCAR_MODE_EXPLICIT]START
[AFLOW]SYSTEM=Si2
NELM = 120
NELMIN=2
LPLANE=.TRUE.
LREAL=.FALSE.
LSCALU=.FALSE.
#NBANDS=XX # for hand modification
#IALGO=48 # for hand modification
[VASP_INCAR_MODE_EXPLICIT]STOP
[AFLOW] *****
[VASP_KPOINTS_MODE_IMPLICIT]
[VASP_KPOINTS_FILE]KScheme=M
[VASP_KPOINTS_FILE]KPPRA=400
[VASP_KPOINTS_FILE]STATIC_KScheme=M

```

```

[VASP_KPOINTS_FILE]STATIC_KPPRA=400
[VASP_KPOINTS_FILE]BANDS_LATTICE=FCC
[VASP_KPOINTS_FILE]BANDS_GRID=20
[AFLOW] *****
[VASP_POTCAR_MODE_IMPLICIT]
[VASP_POTCAR_FILE]Si
[AFLOW] potpaw_PBE: Si
[AFLOW] COMPOSITION_PP=|Si2|
[AFLOW] COMPOSITION=|Si2|
[AFLOW] VOLUME(A^3)=|0|
[AFLOW] MASS(amu)=|28.0855|
[AFLOW] *****
[AFLOW] Aflow automatically generated (aflow_avasp.cpp)
[AFLOW] *****
[AFLOW] aflow/aconvasp/aeq/apennsy in
[AFLOW] *****
[VASP_POSCAR_MODE_EXPLICIT]START
Si1 [FCC,FCC,cF8] (STD_PRIM doi:10.101
  1.224745000000000
    0.0000000000000000  2.2320315365242354  2.2320315365242354
  2.2320315365242354  0.0000000000000000  2.2320315365242354
  2.2320315365242354  2.2320315365242354  0.0000000000000000
Si
2
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.7500000000000000  0.7500000000000000  0.7500000000000000
[VASP_POSCAR_MODE_EXPLICIT]STOP
[AFLOW] *****

```

8) AAPL Automatic Anharmonic Phonon Library (Lattice thermal conductivity calculations).  
 AAPL predicts lattice thermal conductivity computing the anharmonic force constants and solving the Boltzmann equation.  
 This implementation in AFLOW was developed by Jose J. Plata  
 and is described in "XX".

For lattice thermal conductivity calculation, generally, you have to setup  
 3 things: 1) Tell to aflow you want a lattice thermal conductivity calculation. 2) Define the parameters for conduction.  
 3) Choose how to solve the BTE.

NOTE: Lattice thermal conductivity prediction requires accurate forces (harmonic and anharmonic force constants) and must be very well converged. A new accuracy flag has been included for this purpose:

```
[VASP_FORCE_OPTION]PREC=PHONONS
```

8.1) Lattice thermal conductivity calculation ([AFLOW\_AAPL]CALC).  
 Calculate lattice thermal conductivity solving the BTE. Harmonic force constants are also required.

```
[AFLOW_AAPL]CALC
```

8.2) Anharmonic force constants calculations.  
 Different parameters should be include to setup the anharmonic force constants calculations

8.2.1) Supercell. The most important setting is the supercell dimension.

Supercell can be set in three ways as it was explained previously.

EXAMPLES:

```
[AFLOW_AAPL]SUPERCELL=4x4x4
```

8.2.2) Distorsion magnitude. It controls de magnitude of the distorsion of the atoms with respect to their equilibrium positions [Angstrom units].

EXAMPLES:

```
[AFLOW_AAPL]TDMAG=0.015 //Default: 0.015
```

8.2.3) Cutoff. A cutoff for the anharmonic force constant should be applied because of the high computational cost. This radius can be define as a distance, CUT\_RAD [Angstrom], or as coordination shells, CUT\_SHELL [number of neighbor shells].

EXAMPLES:  
 [AFLOW\_AAPL]CUT\_RAD=5.3 //Default: 5.0  
 [AFLOW\_AAPL]CUT\_SHELL=3 //Default: 3

8.2.4) Sumrule. Sumrules are critical to obtain accurate lattice thermal conductivity values. The variable SUMRULE defines the threshold [ev/Angstrom/Angstrom/Angstrom].

EXAMPLES:  
 [AFLOW\_AAPL]SUMRULE=1E-7 //Default: 1E-5

### 8.3) Solving the BTE

8.3.1) Solver. There are two possible options: the relaxation time approximation (RTA) and the full solution using a self consistent field (FULL) using as initial iteration the RTA solution.

EXAMPLES:  
 [AFLOW\_AAPL]BTE=FULL //Default: RTA

8.3.2) Grid. Phonon scattering is evaluated in a discrete mesh of q-points. The higher the density the more accurate the final values will be. However, a very dense mesh can create memory issues.

EXAMPLES:  
 [AFLOW\_AAPL]THERMALGRID=21x21x21 // Default: 16x16x16

8.3.3) Elastic/isotopic effects. Elastic scattering is produced by the abundance of the isotopes of each element. The kind of scattering can be included in the calculation of the relaxation time using the ISOTOPE flag

EXAMPLES:  
 [AFLOW\_AAPL]ISOTOPE=y //Default: no

8.3.4) Scattering at boundaries. Two different methods are implemented to predict the lattice thermal conductivity for polycrystalline samples with an average size of the crystals. Both methods cannot be used at the same time. Computing the cumulative kappa, (CUMULATIVE) aflow compute the lattice thermal conductivity for different size based on the RTA solution. Using the BOUNDARY flag you will include an extra term for the scattering time. However, a specific average size [nm] must be specified.

EXAMPLES:  
 [AFLOW\_AAPL]CUMULATIVE=y //Default: no  
 OR  
 [AFLOW\_AAPL]BOUNDARY=y //Default: no  
 [AFLOW\_AAPL]NANO\_SIZE=y //Default: no

8.3.5) Temperature range Generally, AAPL is calculating the lattice thermal conductivity for a given range of temperature. This range can be set as

[AFLOW\_AAPL]TCT=0:2000:10 // Default 100:700:100

what means it will calculate lattice thermal conductivity from 0 to 2000 K by step of 10 K. This is also a default setting.

### 8.4) Example aflow.in for lattice thermal conductivity calculation:

```
[AFLOW]SYSTEM=Si2
#[AFLOW] single element calculation
[AFLOW] *****
[AFLOW] input file for aflow
[AFLOW_MODE=VASP]
[AFLOW] *****
[AFLOW_MODE_ZIP=bzip2]
[AFLOW_MODE_BINARY=vasp53s]
[AFLOW] *****
[AFLOW] *****
#[AFLOW_MODE_MPI]
[AFLOW_MODE_MPI_MODE]NCPUS=MAX
```

```

[AFLOW_MODE_MPI_MODE]COMMAND ="mpirun -np"
[AFLOW_MODE_MPI_MODE]AUTOTUNE
[AFLOW_MODE_MPI_MODE]BINARY="mpivasp53s"
[AFLOW] *****
[AFLOW_SYMMETRY]CALC
#[AFLOW_SYMMETRY]SGROUP_WRITE
#[AFLOW_SYMMETRY]SGROUP_RADIUS=7.77
[AFLOW] *****
#[AFLOW_NEIGHBOURS]CALC
[AFLOW_NEIGHBOURS]RADIUS=7.7
[AFLOW_NEIGHBOURS]DRADIUS=0.1
[AFLOW] *****
[AFLOW_AAPL]CALC
#[AFLOW_AAPL] HARMONIC
[AFLOW_AAPL]ENGINE=DM
[AFLOW_AAPL]DMAG=0.015
[AFLOW_AAPL]MINATOMS=100
#[AFLOW_AAPL]SUPERCELL=4x4x4
[AFLOW_AAPL]POLAR=y
[AFLOW_AAPL]DC=y
[AFLOW_AAPL]DPM=y
[AFLOW_AAPL]ZEROSTATE=y
[AFLOW_AAPL]DOS=y
[AFLOW_AAPL]TP=y
[AFLOW_AAPL]TPT=400:2000:10
#[AFLOW_AAPL] ANHARMONIC
[AFLOW_AAPL]TDMAG=0.015
[AFLOW_AAPL]CUT_SHELL=4
#[AFLOW_AAPL]CUT_RAD=4.5
[AFLOW_AAPL]SUMRULE=1E-5
[AFLOW_AAPL]BTE=FULL
[AFLOW_AAPL]THERMALGRID=21x21x21
[AFLOW_AAPL]ISOTOPE=y
#[AFLOW_AAPL]CUMULATIVEK=y
#[AFLOW_AAPL]BOUNDARY=n
#[AFLOW_AAPL]NANO_SIZE=100
[AFLOW_AAPL]TCT=200:700:20
[AFLOW] *****
[VASP_FORCE_OPTION]CHGCAR=OFF // ON | OFF (default ON)
[VASP_FORCE_OPTION]SYM=ON // ON | OFF (default ON)
[VASP_FORCE_OPTION]PREC=PHONONS
[VASP_FORCE_OPTION]AUTO_PSEUDOPOTENTIALS=potpaw_PBE // pot_LDA | pot_GGA | potpaw_LDA | potpaw_GGA | potpaw_P
[VASP_FORCE_OPTION]ALGO=NORMAL // (NORMAL | VERYFAST | FAST | ALL | DAMPED), PRESERVED (
[VASP_FORCE_OPTION]TYPE=DEFAULT // METAL | INSULATOR | SEMICONDUCTOR | DEFAULT (default D
[VASP_FORCE_OPTION]CONVERT_UNIT_CELL=SPRIM // SPRIM, SCONV, NIGGLI, MINK, INCELL, COMPACT, WS, CART,
[AFLOW] *****
[VASP_INCAR_MODE_EXPLICIT]START
[AFLOW]SYSTEM=Si2
NELM = 120
NELMIN=2
LPLANE=.TRUE.
LREAL=.FALSE.
LSCALU=.FALSE.
#NBANDS=XX # for hand modification
#IALGO=48 # for hand modification
[VASP_INCAR_MODE_EXPLICIT]STOP
[AFLOW] *****
[VASP_KPOINTS_MODE_IMPLICIT]
[VASP_KPOINTS_FILE]KSCHEME=M
[VASP_KPOINTS_FILE]KPPRA=400
[VASP_KPOINTS_FILE]STATIC_KSCHEME=M
[VASP_KPOINTS_FILE]STATIC_KPPRA=400
[VASP_KPOINTS_FILE]BANDS_LATTICE=FCC
[VASP_KPOINTS_FILE]BANDS_GRID=20
[AFLOW] *****

```

```

[VASP_POTCAR_MODE_IMPLICIT]
[VASP_POTCAR_FILE]Si
[AFLOW] potpaw_PBE: Si
[AFLOW] COMPOSITION_PP=|Si2|
[AFLOW] COMPOSITION=|Si2|
[AFLOW] VOLUME(A^3)=|0|
[AFLOW] MASS(amu)=|28.0855|
[AFLOW] *****
[AFLOW] Aflow automatically generated (aflow_avaxp.cpp)
[AFLOW] *****
[AFLOW] aflow/aconvasp/aqe/apennsy in
[AFLOW] *****
[VASP_POSCAR_MODE_EXPLICIT]START
Si1 [FCC,FCC,cF8] (STD_PRIM doi:10.101
  1.224745000000000
    0.0000000000000000    2.2320315365242354    2.2320315365242354
    2.2320315365242354    0.0000000000000000    2.2320315365242354
    2.2320315365242354    2.2320315365242354    0.0000000000000000
  Si
  2
Direct
  0.0000000000000000  0.0000000000000000  0.0000000000000000
  0.7500000000000000  0.7500000000000000  0.7500000000000000
[VASP_POSCAR_MODE_EXPLICIT]STOP
[AFLOW] *****

*****
*
*           aflow - STEFANO CURTAROLO Duke University 2003-2017           *
*           High-Throughput ab-initio Computing Project                   *
*
*****

```