1 Manual

1.1 Introduction

This code collection is capable of determining lattice oscillations in different forms. The lattice oscillations can be computed from the dynamic structure factor (DSF), a velocity autocorrelation function (VACF), and projected velocity autocorrelations in **k**-space. The projected velocity autocorrelation (PVACF) can be projected onto a set of eigenvectors as for example eigenvectors obtained from the harmonic approximation.

1.2 Installation in UNIX

To install the PC in UNIX unpack the tarball tar -xvzf PC.1.tar.gz. Then go to the main folder cd PC. Then export the desired gnu compiler export FC=gfortran. Then type cmake -DCMAKE_BUILD_TYPE=Release CMakeLists.txt. Then type make and the executable should be found in ./bin/PC

Table 1: General MD spec flags

flag type	meaning default value
Step 1	tar-xvzf PC.tar.gz
Step 2	cd PC
Step 3	cmake -DCMAKE_BUILD_TYPE=Release CMakeLists.txt
Step 4	export FC=gfortran
Step 5	make
Step 6	find executable in ./bin folder

1.3 General settings

There is a set of general settings for the phonon computation. These flags will specify the MD conditions which is analyzed. The flags shown in table are specified in the Phonon.in file

Specifing one of the methods with DSTC,DYNSTRUC,PVACF,PVACFKO or PROJFAC needs also needs different input files. The different methods and their usage will be described in the following sections. The code also supports openmp parallelization. If you do not want the program to use all your cores do export OMP_NUM_THREADS=# of cores before execution.

Table 2: General MD spec flags

flag	meaning	type	default value
NSTART	structure in file to start sampling	integer	1
NEND	total number of structures in XDATCAR file	integer	-
DSTEP	analyze every $DTSEP^{th}$ structure	integer	1
TSTEP	time step in what unit ever	float	1.0
NX	number of periodic images in x	integer	-
NY	number of periodic images in y	integer	-
NZ	number of periodic images in z	integer	-
DSTC	time window for average correaltion functions	integer	NEND
DYNSTRUC	True/False switch on/off Dynamic structure factor	bool	False
PVACF	on/off projected VACF on eigenvectors and **k**-space	bool	False
PVACFKO	on/off projected VACF **k**-space only	bool	False
PROJFAC	on/off projected DSF on eigenvectors	bool	False

1.4 Dynamic Structure factor

To compute the DSF switch on the flag DYNSTRUC=True. And set the other remaining parameters defined in the Phonon.in file. To compute the DSF you have to specify a **k**-grid. This can be done by supplying a QPOINTS file called "QVectors.in" containing on the first line an integer with the number of **k**-points. Then the **k**-points are listed in a 3 column format. If no "QVectors.in" file is supplied the default **k**-points of the commensurate **k**-grid are used. As output you will obtain a file called DynamicStructureFactor.out containing the DSF. The first column is the frequency axis. Then in the following columns the Signals for the different **k**-points are listed. The File StructureFactor.out contains the static structure factor. The first column is the Qpath. And last the file StructureFactor_vs_t.out contains the structure factor in the time domain.

1.5 The projected velocity autocorrelation function in k space

To compute the **k** space projection of the velocity autocorrelation function set the flag PVACFKO=True. This method additionally needs a masses.in file described in section **??**. Also the atoms have to be assigned to the unitcells in which they are located. This can be done with the BoxList.in file described in section **??**. As output you are going to obtain numberd PVACF_KO.out{II} files where II is an index from 1 up to the number of atoms per unit cell. The first column of this file contains the frequency grid and the following

columns contain the signals for the used q-vectors. So a kspace projected velocity autocorrelation is computed for every atom in the unitcell. In the files PVACF_KO_vs_t.out{II} you will find the time signals.

1.6 projected velocity autocorrelation PVACF

To compute the projected velocity autocorrelation function set the flag PVACF=True. This computes a PVACF projected onto a set of basis vectors and onto a set of **k**-vectors. The routine needs the input files BoxList.in, masses.in and BasisVector.in files. If no BasisVector.in file is supplied the code will try to find a QVectors.in file. If this file is found the **k**-vectors from this file are used and a diagonal basis. If no QVectors.in file is supplied the default **k**-vectors will be used in combination with the diagonal basis. As output you will obtain PVACF.out{II} files. These files will contain the frequency axis on the first column and the signals for every **k**-vector on the following columns. Such a file will be written for every phonon branch. The files PVACF_vs_t.out{II} will contain the corresponding time signals with the time axis on the first column.

1.7 Projected Dynamic Structure factor

To compute the projected dynamic structure factor set the flag PROJFAC=True. This computes a DSF projected onto a set of basis vectors and onto a set of **k**-vectors. The routine needs the input files BoxList.in, masses.in and BasisVector.in files. If no BasisVector.in file is supplied the code will try to find a QVectors.in file. If this file is found the **k**-vectors from this file are used and a diagonal basis. If no QVectors.in file is supplied the default **k**-vectors will be used in combination with the diagonal basis. As output you will obtain ProjectedDSF.out{II} files. These files will contain the frequency axis on the first column and the signals for every **k**-vector on the following columns. Such a file will be written for every phonon branch. The files StructureFactorProj_vs_t.out{II} will contain the corresponding time signals with the time axis on the first column.

1.8 Input file BoxList.in

The BoxList.in file contains a connection table assigning every atom to a unit cell building up the super cell. The file contains a table where the number of lines are the number of unitcells building up the table. Every line contains N integer numbers, where N defines the number of atoms per

unitcell. The numbers represent the atom number in the XDATCAR file. This file is needed for PVACF and PVACKO.

1.9 Input file masses.in

The masses.in contains the number of atoms in the unit cell on the first line. The following lines contain a single number describing the mass of the atoms in the unit cell. The order has to be the same as in the XDATCAR file. This file is needed for PVACF and PVACKO.

1.10 The BasisVector.in file

This file is needed when computing PVACF or PROJFAC. The projected velocity autocorrelation function in **k**-space and onto a set of basis vectors. The PROJFAC is a projection of the dynamic structure factor onto the same set of eigenvectors. The file contains 4 integer numbers on the first line. The first number is the number of different **k**-points. The second number is the number of branches per **k**-point. The third number defines the number of atoms in the unit cell. And the last number defines the dimensionality of the underlying space. Which is 3. The file is then structured as follows. The next line contains the first **k**-vector. Then without an empty line in-between the first phonon branch of **k**-vector one follows. Then an empty line and the next phonon branch follows. The number of lines per branch is the number of atoms per unit cell. Like this all branches for the first **k** point are listed. Then 2 empty lines follow and the next **k**-vector is defined. Followed by the first phonon branch. Then followed by the eigenvectors of the other branches separated by single empty line.