# Overview

The Dispersion program was written to perform harmonic lattice dynamics (LD) calculations for an atomic lattice given ground state atomic positions and interatomic force constants. Information on the seven operations currently available in the program are given below, including their required input arguments and data files. Information on how to run this program from the command line is given in the [Runtime Instructions](#_Runtime_Instructions), and explanations of all input and data files are given in the [Input Files](#_Input_Files) and [Data Files](#_Data_Files) sections. The results of the calculations performed by this program can also be plotted using GNU plot. More information on this subject is given in the [Plotting](#_Plotting) section.

## Dispersion Operations

The general function of the Dispersion program is based on operations which the user chooses to carry out in a sequential order. There are seven implemented so far, each with a corresponding operation number used at runtime:

1. **dispersion**: calculates phonon dispersion along BZ paths
   * Inputs: None
   * Required Data
     1. lattice.txt
     2. dynMat.txt
2. **modeshapes**: calculate phonon modeshapes at individual k-points
   * Inputs: None
   * Required Data
     1. lattice.txt
     2. dynMat.txt
3. **dispMS**: calculate phonon dispersion and modeshapes along BZ paths
   * Inputs: None
   * Required Data
     1. lattice.txt
     2. dynMat.txt
4. **plotDisp**: plot phonon dispersion
   * Inputs
     1. Plot title (*string title*)
   * Required Data: None (see [Plotting](#_Plotting))
5. **plotComp**: plot phonon dispersion comparison
   * Inputs
     1. Plot title (*string title*)
     2. Path to comparison frequencies (*string compPath*)
     3. Label for computed dispersion curves (*string dispLabel*)
     4. Label for comparison dispersion curves (*string compLabel*)
   * Required Data: None (see [Plotting](#_Plotting))
6. **dat2lat**: reads lattice positions from a LAMMPS .dat file
   * Inputs
     1. Path to LAMMPS .dat file (*string datPath*)
   * Required Data
     1. Atomic positions in a LAMMPS .dat file
7. **dat2dyn**: reads interatomic force constants from a LAMMPS .dat file
   * Inputs
     1. Path to LAMMPS .dat file (*string datPath*)
   * Required Data
     1. Interatomic force constants in a LAMMPS .dat file

# Runtime Instructions

Before beginning your calculations, be sure to have a directory containing all of your input and data files. If following these instructions brings you to a runtime error, please make sure that you are able to run the example cases in which the directories and files are provided. To start the Dispersion program, simply run the executable from the command line with the desired command line options:

./path/to/Dispersion $(dir) $(nThread) $(iMode)

To run the example case for bulk Germanium from the directory containing Dispersion:

./Dispersion "examples/Ge\_2x2x2-CC/" 1 1

Explanations for each of the command line options are given below.

## Command Line Options

**dir**: path to input file directory (default is examples/Si\_2x2x2-CC/)

**nThread**: number of OpenMP threads used in parallel computations (default is 1)

**iMode**: a binary prescribing how to receive input instructions (default is 0)

0 – receive input instructions through the interactive menu

1 – receive input instructions from an existing input file

## Interactive Menu

The interactive menu is the default input option for the Dispersion program as it does not require a calculation input file (input.txt). Instead, the user chooses individual operations to perform from the menu using their operation numbers.

### Menu Display

\*\*\* DISPERSION OPERATIONS \*\*\*

COMPUTATION

1) dispersion: calculate phonon dispersion along BZ paths

2) modeshapes: calculate phonon modeshapes at individual k-points

3) dispMS: calculate phonon dispersion and modeshapes along BZ paths

PLOTTING

4) plotDisp: plot phonon dispersion

5) plotComp: plot phonon dispersion comparison

UTILITY

6) dat2lat: read positions from a LAMMPS file and write a lattice.txt file

7) dat2dyn: read force constants from a LAMMPS file and write a dynMat.txt file

0) EXIT PROGRAM

# Input Files

The format and naming conventions for each input file were chosen for simplicity and should be relatively easy to produce. The most complicated is the parameter file, which should be copied directly. Examples of each input file can be found in docs/, as well as the subdirectories of examples/, or copied from below.

## Calculation Input File

The calculation input file **input.txt** is a short and simple file which directs the Dispersion program to carry out a specified series of operations. The first line of the file begins with “ops:” followed by a comma-separated list of desired operation numbers. The second line contains the phrase “args:” only, and each following line should contain the arguments for the operations specified on the first line (in order).

### Example Calculation Parameter File

ops: 6, 7, 1, 4

args:

examples/Si\_2x2x2-CC/dat/Si\_2x2x2-CC\_Min.dat

examples/Si\_2x2x2-CC/dat/Si\_2x2x2-CC\_Dyn.dat

Phonon Dispersion, Bulk Silicon

This example file directs the Dispersion program to read minimized atomic positions and interatomic force constants for the example case of bulk Silicon and proceed to compute and plot the corresponding phonon dispersion diagram.

## Calculation Parameter File

Calculation parameters must be stored in a file named **params.txt** formatted as indicated below. Due to the varied nature of the information in this file, its format is somewhat complicated, so it is advised that you copy the parameter file format below or from one of the examples cases to avoid improper formatting. Note that the q-points provided in this file should be normalized to for the appropriate lattice constant . In the event that dispersion curves or modeshapes aren't requested, "Brillouin zone path critical q-points" or "Modeshape q-points" will be ignored.

### Example Calculation Parameter File

Number of basis atoms: 8

Unit cell basis vectors:

5.4320 0.0000 0.0000

0.0000 5.4320 0.0000

0.0000 0.0000 5.4320

Supercell box vectors:

10.8640 0.0000 0.0000

0.0000 10.8640 0.0000

0.0000 0.0000 10.8640

Number of Brillouin zone paths: 5

Brillouin zone path critical q-points:

0.0 0.0 0.0 0.0 1.0 0.0 100

0.0 1.0 0.0 1.0 1.0 0.0 100

1.0 1.0 0.0 0.0 0.0 0.0 100

0.0 0.0 0.0 1.0 0.0 0.0 100

1.0 0.0 0.0 1.0 1.0 0.0 100

Number of modeshape q-points: 1

Modeshape q-points:

0.0 0.0 0.0

## Configuration File

In addition to the input files listed above, the user can optionally provide a configuration file **config.txt** that modifies some of the options during calculations, including the maximum number of eigenvalue/eigenmode pairs to compute. If no configuration file is provided, the default values in the example below will be used.

asDyn 1 // Acoustic sum rule flag (0-don't apply, 1-apply)

maxEVs 1000 // Maximum number of eigenvalues/vectors (sparsification limit)

wIm 1920 // Width of plot images in pixels

hIm 1080 // Height of plot images in pixels

compInt 5 // Plotting interval for comparison data

# Data Files

## Atomic Position File

If no operation is used to read atomic positions directly from a LAMMPS .dat file, they must be stored in a file named **lattice.txt** formatted so that the space-separated Cartesian positions of each atom are written to a single line:

r1x r1y r1z

r2x r2y r2z

...

rNx rNy rNz

where N is the total number of atoms. The positions provided should be for a relaxed lattice at 0 K and must be in order of the lattice basis. That is, each group of nbasis atoms beginning with 1- nbasis must belong to one unit cell.

## Interatomic Force Constant File

If no operation is used to read interatomic force constants directly from a LAMMPS .dat file, they must be stored in a file named **dynMat.txt** formatted as a dynamical matrix. That is, the file should contain 3N lines each with 3N space-separated columns corresponding to the elements of the dynamical matrix (often referred to as Phi in the literature, referred to here as D for legibility):

D11xx D11xy D11xz ... D1Nxx D1Nxy D1Nxz

D11yx D11yy D11yz ... D1Nyx D1Nyy D1Nyz

D11zx D11zy D11zz ... D1Nzx D1Nzy D1Nzz

...

DN1xx DN1xy DN1xz ... DNNxx DNNxy DNNxz

DN1yx DN1yy DN1yz ... DNNyx DNNyy DNNyz

DN1zx DN1zy DN1zz ... DNNzx DNNzy DNNzz

where N is the total number of atoms. Mathematically, each of the dynamical matrix elements should be given by:

where is the potential energy of the lattice and is the cartesian component of the displacement of the atom. A LAMMPS .dat file containing these interatomic force constants can be produced by using the *dynamical\_matrix* command from the PHONONS package of LAMMPS (note: this is **not** installed with LAMMPS by default).

# Output Files

## Frequencies

## Modeshapes

## k Points

In addition to the primary output files listed above, the Dispersion program provides a file containing the k points used in dispersion calculations, **kpoints.txt**. These are given in physical (**not** normalized) units

k1a k1b k1c

k2a k2b k2c

...

kNa kNb kNc

where N is the total number of k points across the Brillouin zone and a, b, and c refer to the basis vector direction (typically a, b, c -> x, y, z).

# Plotting

The plotDisp and plotComp operations are capable of producing GNU plot scripts for plotting phonon dispersion curves, but they will not produce the plots themselves. Furthermore, since these functions simply write the GNU plot scripts, they do not require any output files from LD calculations to run. However, running *gnuplot* on these scripts in the event that the provided paths to frequency files don’t actually exist will result in a *gnuplot* error. The plot scripts produced by these operations can be edited directly by the user to customize the plots (e.g. to set a maximum frequency).