OCLIMAX User Manual

September 2020 (version 3.0)

Introduction

OCLIMAX is a free program to perform simulation of neutron scattering S(Q,E) for powders and single crystals from atomistic models. It is designed to calculate full S(Q,E) including contributions from all combinations of elastic, inelastic, coherent, and incoherent scattering. For the input, OCLIMAX can use either the phonon information from a lattice dynamics simulation or an atomic coordinate trajectory from a molecular dynamics (MD) simulation (the latter is only for powders with incoherent approximation). The output from OCLIMAX can be used to directly compare with experimental data collected at various neutron scattering instruments, or for additional analysis to extract information such as thermal neutron scattering cross-sections. The program is released as a Docker® container, and it comes with a python script that converts the atomistic simulation results from various codes (e.g., VASP, CASTEP, Phonopy, CP2K, etc.) to the input format needed by OCLIMAX, as well as other python scripts for visualization and analysis of the results. The output from OCLIMAX is in standard ASCII format (e.g., CSV, SPE) that can be easily loaded in other programs such as Origin, Excel, Mantidplot, or DAVE. A diagram summarizing the idea of OCLIMAX and a table listing the currently available features are given below.

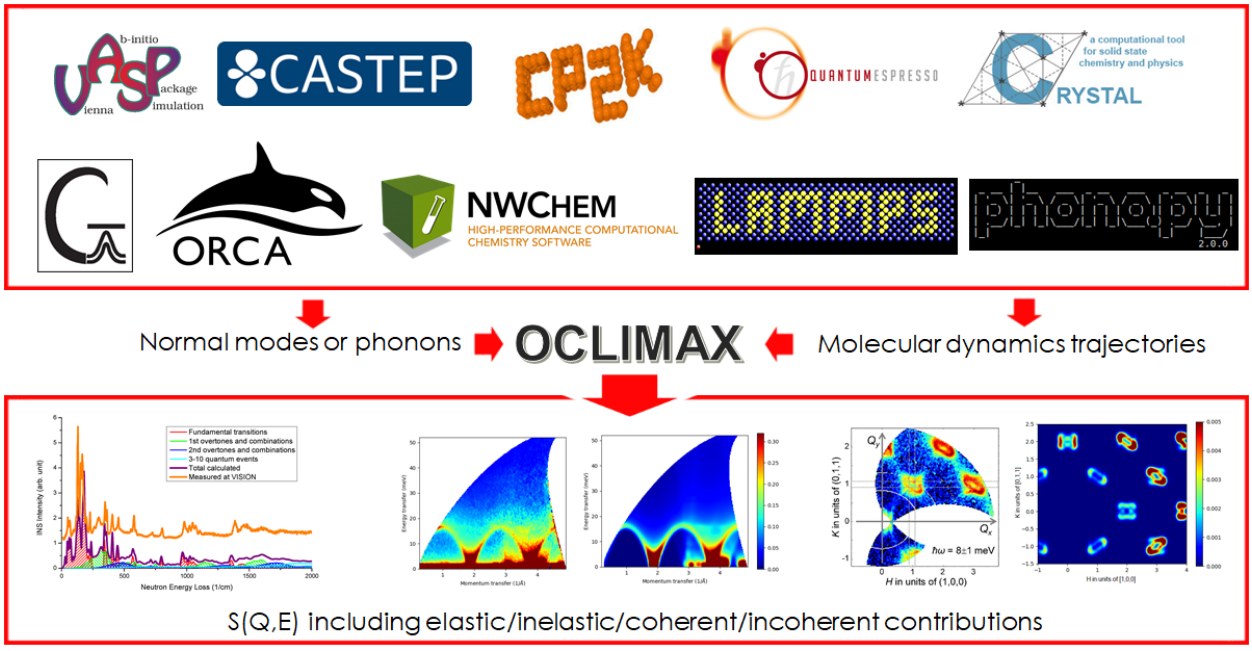

Figure 1. OCLIMAX connects atomistic models and neutron scattering experiments.

Main features of OCLIMAX:

- Powders (coherent, incoherent, elastic, inelastic) and single crystals (coherent, elastic, inelastic)
- Temperature effects (quantum treatment of Debye-Waller factor and phonon populations)
- Multiphonon excitations (powders)
- Arbitrary instrument geometry and resolution
- Arbitrary cuts in 4-dimensional Q-E space (single crystals)
- Interface with atomistic modeling tools (e.g. various DFT codes)
- Interface with neutron scattering data analysis tools (e.g. DAVE and Mantid)
- User-friendly (multiple platforms, easy to use, fast on PCs)
- S(Q,E) in absolute unit (barn/energy) (powders)
- Parameter-free calculation of thermal neutron scattering cross-sections
- MD trajectories to neutron scattering spectra (powders)

System requirement

As long you can install and run Docker (https://www.docker.com/), you can use OCLIMAX. Docker Community Edition (CE) is free, and supports all major operating systems (Linux, Mac, Windows).

Update March 2023:

It is now possible to run OCLIMAX without Docker on Linux and Windows computers. You may download the executable files at https://sites.google.com/site/ornliceman/download/executable

The way to run the executable version is similar to the Docker version, except that the Docker command of “oclimax run” should be replaced by “oclimax_run” (Linux) or “oclimax_run.exe” (Windows), and “oclimax convert” should be replaced by “oclimax_convert” or “oclimax_convert.exe”. The “oclimax pull” command will not work, and you will need to redownload the executable files to get the newest version. The optional “pclimax.py” script is replaced by “oclimax_plot” or “oclimax_plot.exe”.

If you have access to analysis.sns.gov, the Linux version is also available there under /SNS/VIS/shared/YQ/oclimax/. You may use it directly on the analysis cluster to perform your simulations.

Docker installation

Find the right version of Docker CE for your computer following the link:

https://hub.docker.com/search/?type=edition&offering=community

Install Docker following the corresponding instructions for your system. For common issues related to Docker installation, please see the FAQ section of this manual. You may also google the error message and most likely you will find a working solution online.

OCLIMAX installation/update

With Docker successfully installed and running, OCLIMAX can be easily installed by following these steps:

- *Linux or Mac (Note added March 2023: due to a change in google site, the following way to install OCLIMAX is no longer available. Please refer to the new installation procedures for Linux and Mac computers)*

  ~~curl -sL https://sites.google.com/site/ornliceman/getoclimax | bash~~
  ~~oclimax pull~~

- *Linux or Mac (after March 2023)*

Go to https://sites.google.com/site/ornliceman/download

Download the file "oclimax" to a directory in your $PATH (e.g., /usr/bin or $HOME/bin). Run

```
chmod a+rx oclimax
oclimax pull
```

- *Windows 10*

Go to https://sites.google.com/site/ornliceman/download

Download oclimax.win to your working directory. Change the file extension from "win" to "bat". Open "Command Prompt" or "Windows PowerShell", go to the working directory, run

```
oclimax.bat pull (in Command Prompt)   OR
.\oclimax.bat pull (in Windows PowerShell)
```

In the rest part of the manual, all examples will be given in Linux/Mac format. If you are running Windows 10, please change the command from "oclimax" to "oclimax.bat" (in Command Prompt) or ".\oclimax.bat" (in Windows PowerShell). Also note that in Windows PowerShell, although ".\" is needed at the beginning of the line, the input file names should NOT contain ".\". If you use Tab to automatically complete the file names, ".\" is also

automatically added. Please remove the ".\" before the file names. For example, a working command line in Windows PowerShell should be like:

.\oclimax.bat run aluminum.oclimax aluminum.params

File format and conversion

OCLIMAX requires an input data file in any of the three formats: *.aclimax (non-periodic and periodic systems, incoherent approximation only), *.oclimax (periodic systems, any simulation), or *.tclimax (MD trajectory, incoherent approximation only). One exception is single crystal simulation, for which two *.oclimax files are needed. For calculations with non-default setting, a parameter file *.params is also required. The *.aclimax/*.oclimax file contains information on the atomic structure and phonons, and the *.params file contains parameters defining the simulation. The *.aclimax/*.oclimax/*.tclimax file can be obtained by running a conversion script on the output file(s) from your atomistic simulation software (e.g., VASP, Phonopy). When running OCLIMAX through Docker, the command line for file conversion should be:

oclimax convert -input_tag input_file1 [input_file2 ... -output_tag output_file]

Please note that to obtain an *.aclimax/*.oclimax file, your input file(s) must contain not only the frequencies, but also the polarization vectors (eigenmodes). As an example, if you are using Phonopy, please make sure this tag is in your *.conf file "EIGENVECTORS = .TRUE."

If you are converting a file that does not contain cell information (e.g., xyz file) into a file that requires cell information (e.g., oclimax file), you will need to provide such information by adding "-cell lattice_file" after the input files. An example:

oclimax convert -input_tag input_file -cell lattice_file -o

If the conversion is taking longer than a few minutes, your original data file could be tool large, which means your phonon sampling could be too/unnecessarily dense. As a rule of thumb, your data file containing the phonon frequencies and polarization vectors should be much smaller than 1Gb. For most cases, a data file 100Mb or smaller is sufficient and only in very rare cases the file needs to be larger than that. If you are not sure, you may start with lower sampling density and increase until you have converged result.

A list of supported input/output format is given below:

****
To convert a lattice dynamics simulation, -input_tag and the corresponding input file(s) can be:
-c: CASTEP input file(s): *.phonon
-vp: VASP+Phonopy input file(s): POSCAR-unitcell mesh.yaml
-vpd: VASP+Phonopy input file(s): POSCAR-unitcell band.yaml

```
-vo: VASP                    input file(s): POSCAR OUTCAR
-yaml: Phonopy          input file(s): mesh.yaml (new format containing atomic coordinates)
-yamld: Phonopy       input file(s): band.yaml (new format containing atomic coordinates)
-cp2k: CP2K                  input file(s): *.mol
-crystal: Crystal            input file(s): *.out
-nwchem: NWChem             input file(s): *-freq.out
-gaus: Gaussian              input file(s): *.log
-orca: ORCA                  input file(s): *.out
-dmol: DMol                  input file(s): *.outmol
-xyz: DFTB+                  input file(s): *.xyz (with vibrational modes)
-climax: aclimax/oclimax     input file(s): *.aclimax or *.oclimax file
**************************************************************************
To provide the missing lattice constants, add -cell lattice_file in the following format
-cell:          input file(s): a lattice_file containing lattice parameters
                a b c                          ax ay az
                alpha beta gamma     or        bx by bz
                                               cx cy cz
**************************************************************************
-output_tag can be the following, and -a is the default
-a: the old aclimax format for incoherent calculation only.
-o: the new oclimax format which can be used for both incoherent and coherent calculations.
-pm: mass-weighted and normalized phonon file at gamma point only.
-p: phonon file including the denormalized gamma point modes for visualization with JMol.
-x: xyz file including the denormalized gamma point modes for visualization with JMol.
-cif: cif file including the structure only.
Note -o, -p/-pm, and -cif are only available for periodic systems.
**************************************************************************
The name of the output file (excluding the suffix) can be specified after the -output_tag.
The default output is out.*
**************************************************************************
To convert a molecular dynamics trajectory, -input_tag and the corresponding input file can be:
-ct: CASTEP MD               input file: *.md
-vt: VASP MD                 input file: XDATCAR
-xt: xyz traj (e.g.CP2K)     input file: *.xyz
-lt: LAMMPS MD               input file: dump (format: id,element,x,y,z [Angstrom])
Note that after the input file, the time step in the unit of fs must be provided
For example: oclimax convert -vt XDATCAR 0.5
The name of the output file (excluding the suffix) can be specified after the time step
The default output is out.tclimax
**************************************************************************
```

Running OCLIMAX

After obtaining the *.aclimax/*.oclimax/*.tclimax file, you may run the simulation by:

oclimax run file.aclimax (or file.oclimax or file.tclimax) [file.params]

The parameter file contains the parameters defining the simulation. If no parameter file is provided, a calculation using the default parameters will be performed. If you don't have a starting parameter file, you may run

oclimax run

to generate a default parameter file (default.params) for you to edit. Details on the parameters can be found in the next section.

Note that for single crystal simulations, three input files are needed. See detailed explanation for keyword TASK.

Description of the parameters

The default parameters as listed in the default.params file are:

```
*******************************************************************************
## General parameters
TASK   =       0       # 0:inc approx. 1:coh+inc. 2:s-xtal Q-E. 3:s-xtal Q-Q
INSTR  =       0       # 0:VISION 1:indirect 2:direct 3:S(Q,E) or S(Qx,Qy) map
TEMP   =       0.00    # Temperature [K]
E_UNIT  =      0       # Energy unit (0:cm-1,1:meV,2:THz)
OUTPUT =       0       # 0:standard,1:restart,2:SPE,3:full,4:DOS,5:modes,6:S(Q),7:MSD

## Additional general parameters
MAXO =         10              # Maximum order of excitation
CONV  =        2               # Start convolution from order=CONV (2 or 3)
PHASE =        0               # Phase factor of polarization vector (0 or 1)
MASK  =        0               # Set 1 to apply mask on S(Q,E)/S(Qx,Qy) map (INSTR=3)
NORM =         1               # Set 1 to normalize intensity
ELASTIC =  -0.10E+01 -0.10E+01        # e1>0:add el in S(Q,E),e2>0:apply S(Q) res

## E parameters
MINE   =       8.00            # Energy range (minimum) to calculate [eu]
MAXE   =       5000.00         # Energy range (maximum) to calculate [eu]
dE     =       1.000           # Energy bin size [eu]
ECUT   =       1.000           # Exclude modes below this cutoff energy [eu]
ERES   =   0.25E+01  0.50E-02  0.10E-06    # E resolution coeff [eu,1,eu^-1,…]

## Q parameters
MINQ  =        0.50            # Q range (minimum) to calculate
```

```
MAXQ =      20.00          # Q range (maximum) to calculate
dQ   =      0.50           # Q bin size
QRES =      -0.10E+01      # Q resolution coeff

## Instrument parameters
THETA =     135.0  45.0    # List of scattering angles [degree]
Ef   =      32.00          # Final energy [eu] (INSTR=1)
Ei   =      5000.00        # Incident energy [eu] (INSTR=2)
L1   =      11.60          # L1 [m] for DGS (INSTR=2 or 3, ERES=0)
L2   =      2.00           # L2 [m] for DGS (INSTR=2 or 3, ERES=0)
L3   =      3.00           # L3 [m] for DGS (INSTR=2 or 3, ERES=0)
dt_m =      3.91           # dt_m [us] for DGS (INSTR=2 or 3, ERES=0)
dt_ch =     5.95           # dt_ch [us] for DGS (INSTR=2 or 3, ERES=0)
dL3  =      3.50           # dL3 [cm] for DGS (INSTR=2 or 3, ERES=0)

## Single crystal parameters
HKL  =      0.0  0.0  0.0  # HKL (TASK=2 or 3)
Q_vec =     0.0  0.0  1.0  # Q vector dir (TASK=2 or 3)
Q_vec_y =   1.0  0.0  0.0  # Q vector dir y-axis (TASK=3)
MINQ_y =    1.00           # Q range (minimum) y-axis (TASK=3)
MAXQ_y =    2.00           # Q range (maximum) y-axis (TASK=3)
dQ_y =      0.02           # Q bin size y-axis (TASK=3)

## Wing parameters
WING =      0              # Wing calculation (0:no wing,1:isotropic,2:ST tensor)
A_ISO =     0.0350         # Isotropic A_external for wing calculation
W_WIDTH =   150.0          # Energy width [eu] of initial wing
**********************************************************************
```

Detailed descriptions for each parameter:

Keyword: TASK

Values: 0, 1, 2, 3 (default: 0)

Description: TASK defines the type of calculation. Set TASK to 0 for powder calculation with incoherent approximation. For hydrogenous materials, amorphous materials, or materials with complex crystal structure (large unit cells), the coherent effect is usually negligible and the incoherent approximation is sufficient. Set TASK to 1 will perform full powder calculation including the coherent effect. The calculation usually takes much longer but it is necessary for coherent scatterers with a simple crystal structure of high symmetry.

Set TASK to 2 for single crystal Q-ω calculations. For single crystal calculations, two *.oclimax files will be needed as input: one with a uniform sampling in the Brillouin zone and the other one sampling alone the trajectory of interest. The command line should be:

oclimax run uniform.oclimax file.params trajectory.oclimax

Set TASK to 3 for single crystal Q-Q calculations. In this case, the second *.oclimax file should contain a mesh sampling along the plane of interest. The command line should be:

oclimax run uniform.oclimax file.params plane.oclimax

Note that in all the oclimax files, only the q points within the first Brillouin zone are needed.

Keyword: INSTR

Values: 0, 1, 2, 3 (default: 0)

Description: INSTR specify the instrument geometry (i.e., sampling in the Q-E space) for the calculation. Set INSTR to 0 to simulate INS spectra for VISION@SNS. Set INSTR to 1 for a generic indirect geometry instrument (parameters such as final energy and scattering angles can be specified). Set INSTR to 2 to simulate the spectra on certain detectors (specified by scattering angles) on a direct geometry instrument. Set INSTR to 3 to generate the 2D Q-E or Q-Q map.

Applicability: If TASK=2 or 3, then INSTR is taken as 3 by default, and all parameters for INSTR=3 will be applied.

Keyword: TEMP (default: 0.0)

Values: a non-negative real number

Description: TEMP specifies the temperature for the INS calculation. The Bose-Einstein population and Debye-Waller factor will be included in the calculation.

Keyword: E_UNIT

Values: 0, 1, 2 (default: 0)

Description: Energy unit in both input (*.params) and output files: 0 for wavenumber, 1 for meV, and 2 to THz. Note that when changing this setup, please make sure that all energy-related values in the parameter file are given in the newly specified unit. This includes all parameters containing [eu] in the comment line.

Keyword: OUTPUT

Values: a list of any value in [0, 1, 2, 3, 4, 5, 6, 7] (default: 0)

Description: Type of output files. By default, the calculation will generate a standard csv file containing the calculated spectra (or map). Only the total intensity will be given for the convenience of visualization, except for the VISION calculation in which the order-specific spectra are also listed. Add 3 to OUTPUT for full output containing spectrum for each individual order. If you would like to adjust the resolution without recalculating from scratch, you may save a restart file by adding 1 to OUTPUT, and then re-run the calculation from the restart file, with a new resolution. For the 2D Q-E calculation, if you would like to generate a SPE file that can be loaded and analyzed with DAVE, add 2 to OUTPUT. Adding 4 to OUTPUT will generate the total and partial phonon density of states, as well as the neutron-weighted total and partial phonon density of states. Adding 5 will output mode-specific intensities (fundamentals for powders only). Adding 6 will generate the structure factor S(Q), and adding 7 will output the mean square displacement and root mean square displacement for each atom.

Keyword: MAXO

Values: a positive integer (default: 10)

Description: Maximum order for multi-phonon calculations. Normally 10 is sufficient, but a test of convergence is encouraged when calculating very high energy excitations.

Applicability: Currently not supported for single crystal calculations

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Keyword: CONV

Values: 2 or 3 (default: 2)

Description: Starting order to use convolution. OCLIMAX can calculate the 2^{nd} order excitation either by a more rigorous expansion or by simple convolution of the fundamentals. Usually the former is more accurate but the latter is a lot faster. Using 2 is almost always sufficient, and 3 should only be used for very small systems.

Applicability: Currently not supported for single crystal calculations

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Keyword: PHASE

Values: 0 or 1 (default: 0)

Description: There are two different ways to include the phase factor in the polarization vectors, and different programs may follow different conventions. The correct setting of this keyword depends on the program you used for phonon calculation. For example, with Phonopy it should be 0, whereas with CASTEP it should be 1. If you are not sure, you may try both and see which one returns more reasonable results. For phonon calculations performed at Γ point only, or incoherent calculations, this keyword is irrelevant.

Applicability: Only relevant for coherent calculation (TASK>0)

Keyword: MASK

Values: 0 or 1 (default: 0)

Description: Set MASK to 1 to apply the envelope to the data in the Q-E map according to the detector coverage and calculated kinematics.

Applicability: Only used when INSTR=3

Keyword: NORM

Values: 0 or 1 (default: 1)

Description: Set NORM to 1 to normalize the intensity to its absolute unit (barn/eV divided by the total scattering cross-section of all atoms in the cell). Note that earlier versions of OCLIMAX do not perform this normalization. Therefore, to reproduce the absolute intensity from a previous OCLIMAX calculation, set NORM=0.

Keyword: ELASTIC

Values: two real numbers (default: -1.0 -1.0)

Description: If you would like to include elastic scattering in the calculated S(Q,E), set the first number positive and make MINE<0<MAX. The resolution will be calculated according to ERES and QRES. If you would like to apply Q resolution (as defined by QRES) to the calculated S(Q) in the output file (when OUTPUT includes 6), set the second number positive. These numbers are set to be real numbers for potential future usage.

Keyword: MINE

Values: a real number (default: 8.0)

Description: Minimum energy for the INS calculation. For neutron energy gain calculation, set MINE to a negative number. For MINE<0, you have the choice to include the elastic line (diffraction) in the calculation, see keyword ELASTIC for more details.

Keyword: MAXE (default: 5000.0)

Values: a real number

Description: Maximum energy for the INS calculation. It is important to note that OCLIMAX will only calculate the spectrum within the [MINE,MAXE] range. Therefore, if you are running a finite temperature simulation where the intensity on the neutron energy gain side is not negligible, AND you want to include higher order excitations in the calculation, you may have to include the neutron energy gain part in your calculation to obtain full and accurate convolution results for the higher order intensities. In this case, you must set MINE<0 and test the [MINE,MAXE] range to make sure the final spectrum in the energy range of your interest is converged.

Keyword: dE (default: 1.0)

Values: a positive real number

Description: Energy bin size for the calculation. The number of energy bins will be (MAXE-MINE)/dE+1. You may set this to be compatible with your experimental bin size. If you are not sure, a reasonable starting point is to have a few thousand energy bins with a proper combination of MAXE, MINE, and dE.

Keyword: ECUT

Values: a positive real number (default: 1.0)

Description: In a phonon calculation one may have negative frequencies due to convergence issues or intrinsic instability. The translation modes will have (near) zero frequencies at gamma point. These modes should not be included in the INS calculation. ECUT will be the cutoff set to exclude these unwanted modes (i.e., any mode with its frequency below ECUT will not be used for INS calculation).

Keyword: ERES

Values: a list of real numbers c0, c1, c2, … (default: 2.5 0.005 0.0000001)

Description: Coefficients that specify the energy resolution as a function of energy transfer. The standard deviation of the Gaussian resolution function at energy transfer E will be calculated as $c0+c1*E+c2*E^2+\ldots$ If ERES is a single negative number, no resolution function will be applied. If ERES is a single zero number, the resolution will be calculated according to the instrument geometry (parameters specified later). Note that for Gaussian function, the full-width-half-maximum (FWHM) is about 2.3548 times of the standard deviation. The units for these numbers are [eu,1,eu^-1,…] and they should be consistent with the UNIT setting.

Keyword: MINQ

Values: a positive real number (default: 0.5)

Description: Minimum momentum transfer for the INS calculation. Unit is $Å^{-1}$ for TASK = 0 or 1, for TASK = 2 or 3 the unit is in r.l.u.

Applicability: Only used when INSTR=3

Keyword: MAXQ

Values: a positive real number (default: 20.0)

Description: Maximum momentum transfer for the INS calculation. Unit is $Å^{-1}$ for TASK = 0 or 1; for TASK = 2 or 3 the unit is in r.l.u.

Applicability: Only used when INSTR=3

Keyword: dQ

Values: a positive real number (default: 0.5)

Description: Bin size for momentum transfer. The number of Q bins will be (MAXQ-MINQ)/dQ+1. You may set this to be compatible with your experimental bin size. If you are not sure, a reasonable starting point is to have about 50~100 Q bins with a proper combination of MAXQ, MINQ, and dQ.

Applicability: Only used when INSTR=3

Keyword: QRES

Values: a list of real numbers c0, c1, c2, … (default: 0.1)

Description: Coefficients that specify the Q resolution as a function of momentum transfer. The standard deviation of the Gaussian resolution function at momentum transfer Q will be calculated as $c0+c1*Q+c2*Q^2+\ldots$ If QRES is a single negative number, no resolution function will be applied. If ERES is a single zero number, the resolution will be calculated according to the instrument geometry (not implemented yet). Note that for Gaussian function, the full-width-half-maximum (FWHM) is about 2.3548 times of the standard deviation. The units of these coefficients should be consistent with the unit of MAXQ/MINQ/dQ.

Applicability: Only used when INSTR=3

Keyword: THETA

Values: a list of positive real numbers in the range of [0,180], separated by space (default: 135 45)

Description: For INSTR=1 or 2, these numbers specify the scattering angles at which you would like to calculate the INS spectra. For INSTR=3 and MASK=1, two numbers are expected and they should specify the minimum and maximum scattering angles for the instrument, which will be used to generate the envelope in the 2D Q-E map.

Applicability: Only used when INSTR=1 or 2, and for a different purpose when INSTR=3 and MASK=1

Keyword: Ef

Values: a positive real number (default: 32.0)

Description: Final energy for a generic indirect geometry instrument.

Applicability: Only used when INSTR=1

Keyword: Ei

Values: a positive real number (default: 5000.0)

Description: Incident energy for a direct geometry instrument.

Applicability: Only used when INSTR=2, or when INSTR=3 and MASK=1

Keyword: L1

Values: a positive real number (default: 11.6)

Description: Length of primary flight path (from moderator to Fermi chopper) of a direct geometry instrument (in meter). The resolution of a direct geometry instrument is calculated as

$$\frac{d\omega}{E_i} = 2\sqrt{\left(1+\frac{L_2}{L_3}\left(\frac{v_f}{v_i}\right)^3\right)^2\left(\frac{dt_m}{t_1}\right)^2+\left(1+\frac{L_1+L_2}{L_3}\left(\frac{v_f}{v_i}\right)^3\right)^2\left(\frac{dt_c}{t_1}\right)^2+\left(\frac{v_f}{v_i}\right)^4\left(\frac{dL_3}{L_3}\right)^2}.$$

The resolution at each energy transfer can be calculated knowing Ei, L1, L2, L3, dt_m, dt_ch, and dL3 (Ref. [1]). These parameters vary by instrument and specific setting for the data collection (e.g., incident energy, chopper frequency). The default values are for ACRS at 300 meV incident energy, and they are only for reference.

Applicability: Only used when INSTR=2 or 3, and RES=0

Keyword: L2

Values: a positive real number (default: 2.0)

Description: Length of secondary flight path (from Fermi chopper to sample) of a direct geometry instrument (in meter).

Applicability: Only used when INSTR=2 or 3, and RES=0

Keyword: L3

Values: a positive real number (default: 3.0)

Description: Length of third flight path (from sample to detector) of a direct geometry instrument (in meter).

Applicability: Only used when INSTR=2 or 3, and RES=0

Keyword: dt_m

Values: a positive real number (default: 2.66)

Description: Time spread of the moderator (in microsecond).

Applicability: Only used when INSTR=2 or 3, and RES=0

Keyword: dt_ch

Values: a positive real number (default: 5.83)

Description: Time pulse width through the Fermi chopper (in microsecond).

Applicability: Only used when INSTR=2 or 3, and RES=0

Keyword: dL3

Values: a positive real number (default: 3.0)

Description: Path length uncertainty determined by sample and detector sizes (in centimeter).

Applicability: Only used when INSTR=2 or 3, and RES=0

Keyword: HKL

Values: three integers separated by space (default: 0 0 0)

Description: Shift of the beam center.

Applicability: Only used when TASK=2 or 3

Keyword: Q_vec

Values: three integers separated by space (default: 0 0 1)

Description: Vector pointing to the direction of dispersion.

Applicability: Only used when TASK=2 or 3

Keyword: Q_vec_y

Values: three integers separated by space (default: 1 0 0)

Description: Vector pointing to the direction of dispersion (y-axis).

Applicability: Only used when TASK=3

Keyword: MINQ_y

Values: a positive real number (default: 1.0)

Description: Minimum for the y-axis (in r.l.u.) in single crystal Q-Q calculation.

Applicability: Only used when TASK=3

Keyword: MAXQ_y

Values: a positive real number (default: 2.0)

Description: Maximum for the y-axis (in r.l.u.) in single crystal Q-Q calculation.

Applicability: Only used when TASK=3

Keyword: dQ_y

Values: a positive real number (default: 0.02)

Description: Bin size for y-axis (in r.l.u.) in single crystal Q-Q calculation.

Applicability: Only used when TASK=3

Keyword: WING

Values: 0, 1, 2 (default: 0)

Description: Set WING to 1 or 2 to perform phonon wing calculation. The purpose of wing calculation is to mimic the intermolecular/translational modes when you only have the vibrational frequencies and vectors calculated on an isolated molecular. If your phonon calculation was performed on a 3D periodic system (i.e., full solid calculation), then wing calculation is not meaningful and should always be turned off. This is also why it is only useful for TASK=0. For WING=1, the calculation will use an isotropic A_external, whereas for WING=2, A_external will be calculated from the ST tensor.

Applicability: Only used when TASK=0

Keyword: A_ISO

Values: a positive real number (default: 0.035)

Description: Isotropic A for wing calculation.

Applicability: Only used when TASK=0 and WING=1

Keyword: W_WIDTH

Values: a positive real number (default: 150.0)

Description: Width of the wing.

Applicability: Only used when TASK=0 and WING>0

Analyzing/visualizing the results

A python script is provided to quickly visualize the calculated results. To obtain the script, go to https://sites.google.com/site/ornliceman/download

Download pclimax.py. Note that although the script is compatible with python2, it is still recommended to use python3.

To plot a .csv data file with default settings, run

```
python pclimax.py file.csv
```

You may also run the script with additional options, as explained below:

```
**********************************************************************
** Usage: pclimax.py {-m} *.csv {-s [1,2] -q [2:8] -x [0:100] -y [0:100] -z [0:2.5] -f}   **
**     -m : meV,  -w : wavenumber (cm-1),  -t : THz   (default: unit in csv)              **
**     -s : spectrum index,  -x/y/z : range to plot                                      **
**     -q : integrate Q-range to extract GPDOS, data saved in Q-cut.dat [2D S(Q,E) only] **
**     -e : integrate E-range to extract S(Q), data saved in E-cut.dat  [2D S(Q,E) only] **
**     -f : save plot to a png file (optional filename follows)                          **
** Note that -m/w/t must be the first tag (if there is one) and -f must be the last      **
**********************************************************************
```

The ASCII data files can also be easily imported into third-party software (such as Origin, Excel, Mantidplot, and DAVE) for more sophisticated visualization and data analysis.

Examples

Three examples are provided which can be downloaded at https://sites.google.com/site/ornliceman/download

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The first example is a ZIF-8 VISION spectra simulation. Since the spectra will be dominated by hydrogen incoherent scattering, we only perform simulation under incoherent approximation (i.e., TASK = 0). The default instrument is VISION:

```
oclimax run ZIF-8.aclimax
```

After the simulation is done, you may plot all the spectra:

python pclimax.py ZIF-8_vis_inc_0K.csv

Or to look at only the total spectrum and fundamentals in the backscattering banks:

python pclimax.py ZIF-8_vis_inc_0K.csv -s [1,3] -x [0:3500] -y [0:15]

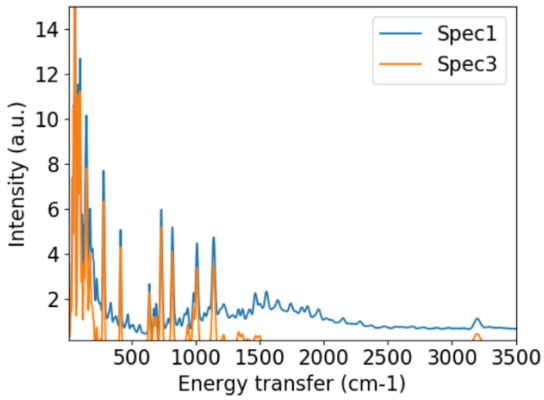

Figure 2. Calculated VISION spectra for ZIF-8, fundamental only (orange) and total (blue). The results can be compared with the experimental data published in Ref [2].

The second example is a Q-E map calculation for aluminum. Since the coherent effect is strong in this case, we will need to perform full calculation (i.e., TASK = 1):

oclimax run aluminum.oclimax aluminum.params

Note that the simulation may take a few minutes. After the simulation is done, you may plot the Q-E map:

python pclimax.py aluminum_2Dmesh_coh_10K.csv -z [0:8]

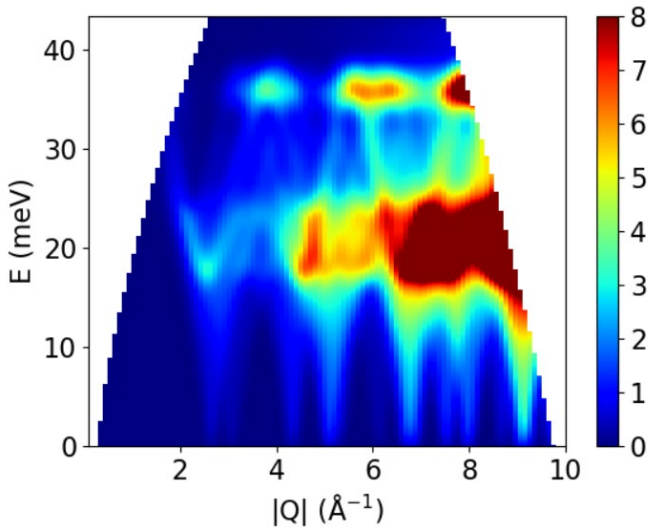

Figure 3. Calculated S(Q,E) for polycrystalline aluminum at 10K. The results can be compared with the experimental data published in Ref [3].

The last example is for calculation of Q-E and Q-Q maps on single crystal copper. The Q-E calculation will be performed with TASK=2:

```
oclimax run Cu_dos.oclimax Cu_disp_H11.params Cu_disp_H11.oclimax
```

The result (left figure below) can be visualized as:

```
python pclimax.py Cu_disp_H11_2Dmesh_scqw_300K.csv -z [0:0.01]
```

The Q-Q calculation (for energy in 8±1 meV) will be performed with TASK=3:

```
oclimax run Cu_dos.oclimax Cu_qq.params Cu_qq.oclimax
```

The result (corresponds to the right figure below) can be visualized as:

```
python pclimax.py Cu_qq_2Dmesh_scqq_300K.csv -z [0:0.0005]
```

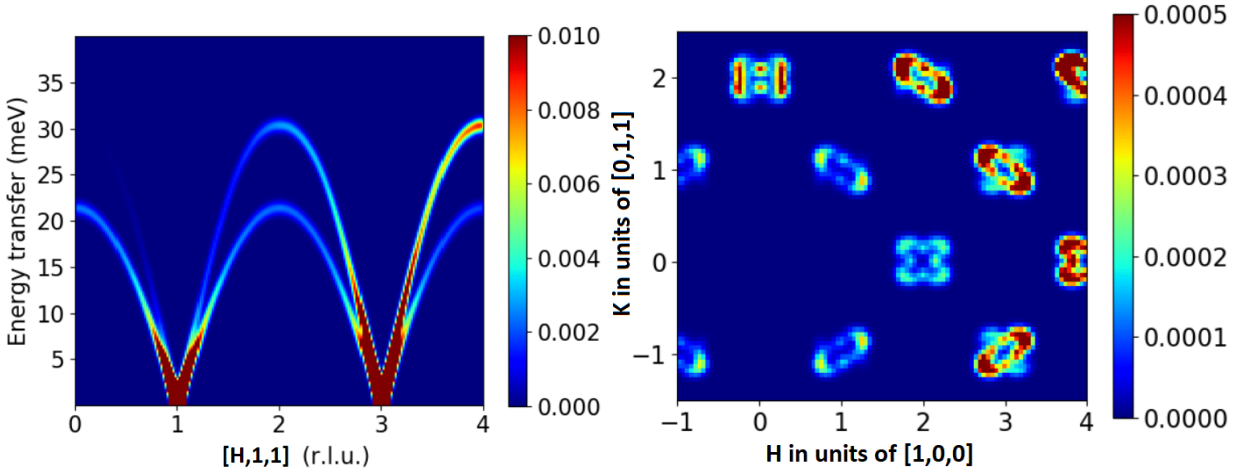

Figure 4. Calculated single crystal INS spectra for copper. The results can be compared with the experimental data published in Ref [4].

Note that the above calculations can be improved with a denser sampling in the phonon calculation and smaller bin sizes for INS simulation. To reduce the file size and computing time, these examples are provided for demonstration purposes only.

Citation

OCLIMAX is free. Please cite the following paper is you used OCLIMAX for your research.

Cheng, Y. Q.; Daemen, L. L.; Kolesnikov, A. I.; Ramirez-Cuesta, A. J., Simulation of Inelastic Neutron Scattering Spectra Using OCLIMAX. Journal of Chemical Theory and Computation 2019, 15 (3), 1974-1982.

https://pubs.acs.org/doi/10.1021/acs.jctc.8b01250

If you used OCLIMAX to calculate neutron scattering cross-sections, please also cite:

Cheng, Y. Q.; Kolesnikov, A. I.; Ramirez-Cuesta, A. J., Calculation of the Thermal Neutron Scattering Cross-Section of Solids Using OCLIMAX. Journal of Chemical Theory and Computation 2020, 16 (8), 5212-5217.

https://pubs.acs.org/doi/10.1021/acs.jctc.0c00569

If you used MD trajectories for your INS calculations, please also cite:

Cheng, Y. Q.; Kolesnikov, A. I.; Ramirez-Cuesta, A. J., Simulation of Inelastic Neutron Scattering Spectra Directly from Molecular Dynamics Trajectories. Journal of Chemical Theory and Computation 2020.

https://pubs.acs.org/doi/full/10.1021/acs.jctc.0c00937

Contact

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FAQs

1. Docker on Windows does not start properly.

In general, you may find the solutions for issues with Docker installation/execution online by googling the error message. For your convenience, a few links are provided for some common issues.

An issue related to virtualization and its solution can be found here:

https://docs.docker.com/docker-for-windows/troubleshoot/#virtualization-must-be-enabled

If you need instructions to enable virtualization, see here:

https://blogs.technet.microsoft.com/canitpro/2015/09/08/step-by-step-enabling-hyper-v-for-use-on-windows-10/

https://support.bluestacks.com/hc/en-us/articles/115003910391-How-can-I-enable-virtualization-VT-on-my-PC-

If the above links didn't solve your problem, see the following:

https://stackoverflow.com/questions/39684974/docker-for-windows-error-hardware-assisted-virtualization-and-data-execution-p

If you cannot run docker because you are not in the user group, see below:

https://icij.gitbook.io/datashare/faq-errors/you-are-not-allowed-to-use-docker-you-must-be-in-the-docker-users-group-.-what-should-i-do

2. My "oclimax convert" command failed.

Please note that your input file(s) must contain not only the frequencies, but also the polarization vectors (eigenmodes). If you are using Phonopy, please make sure this tag is in your conf file "EIGENVECTORS = .TRUE."

It is also possible that the conversion script didn't recognize the specific file format you have (e.g., the format from the DFT program may have changed). If you are unable to solve the issue, please contact the author for assistance.

3. My "oclimax run" command failed on "end of file" error.

Please make sure the input files are complete and provided in the right order (oclimax file first and then params file). In the case of single crystal, the first oclimax file is the uniform sampling, followed by the params file; the last file is the trajectory sampling (1D for Q-E map or 2D for Q-Q map).

If you are using Windows PowerShell, please make sure the input file names do not start with and do not contain ".\". Sometimes this is automatically added if you use Tab to complete the file names.

4. The pclimax.py script doesn't work.

If the issue is caused by the python version or missing libraries on your computer, the easiest solution is to install Anaconda Python.

https://www.anaconda.com/products/individual

On a Windows computer you can run the script in Anaconda Prompt. On a Linux/Mac computer make sure you are using the Anaconda Python by checking "which python".

References

[1] D. L. Abernathy et al. Design and operation of the wide angular-range chopper spectrometer ARCS at the Spallation Neutron Source. Rev. Sci. Instrum. **83**, 015114 (2012).

[2] M. E. Casco et al. Gate-opening effect in ZIF-8: First experimental proof using inelastic neutron scattering. Chemical Communications, **2**, 3639-3642 (2016).

[3] D. L. Roach et al. The interpretation of polycrystalline coherent inelastic neutron scattering from aluminium. J. Appl. Cryst. **46**, 1755-1770 (2013).

[4] H. Seto et al. Inelastic and quasi-elastic neutron scattering spectrometers in J-PARC. Biochimica et Biophysica Acta, **1861**, 3651-3660 (2017).