Documentation for DiSPy

Introduction

DiSPy is a utility for applying the *distortion symmetry method* (DSM) to the calculation of minimum energy pathways using the nudged elastic band (NEB) algorithm. The following document contains information on how to run DiSPy, including all relevant necessary input parameters. Details on the DSM can be found in Ref. [1, 3]. Example calculations can be found in the "examples" folder.

Running DiSPy

For prerequisites to running, please see the "README" file in the main DiSPy folder. The program is run by typing: `dispy INPUT_FILE_NAME`. Note that the "PIR_data.txt" file is required to also be in the same folder as the input file. This contains the listing of the irreducible representations of the space groups by Stokes and coworkers [2].

Input File and Path

Parameters for a calculation are inputted via a plain-text input file formatted as follows:

```
#---Sample DiSPy input file

PERTURB=FALSE
INTERPOLATE=FALSE
IMAGES=9
SYMPREC=0.1
ANGLE_TOLERANCE=-1.0
VECTOR_TOLERANCE(A)=0.1,0.1,0.1
GENERAL_TOLERANCE=0.05
IMAGE_DIR=/input/dir
INPUT_FORMAT=VASP
OUTPUT_FORMAT=VASP

TRANS_NUM=0
TRANS_MAT=0
OSHIFT=0,0,0

MIN_MOVE=0.1
```

```
IRR_NUM=7601
IRR_DIM=1
MODE_TYPES=1
MODE_COEFF=1
RANDOM=FALSE

PERTURB_MAG=0.1
```

Here, we have the name of the parameter, followed by an '=' sign, followed by the setting. Parameters are separated by line, with order being inconsequential. Any comments should be on a separate line and can be in any format.

Paths are inputted via a set of images in any format supported by the Atomic Simulation Environment (ASE). See "Image Directory" in the parameters section for more details. It is strongly recommended that all inputted images come from a path that has been relaxed using the NEB algorithm.

Parameters

- **Image Directory**
  - Name in input file: image_dir
  - Format: String
  - Explanation: This directory should include files specifying the images to be analyzed with filenames in alphanumeric ascending order. Each file should specify exactly one image, and the directory should contain no other files (the app automatically removes the .DS_Store file on MacOS). Images should be in a format readable by the Atomic Simulation Environment (ASE).
  - Default: None, must always specify.
- **Interpolation**
  - Name in input file: interpolate
  - Format: T/F (enter either true/false or t/f)
  - Explanation: If true, the program performs linear interpolation between the first and last images in the image directory to create intermediate images. If false, the program takes the image files inside the image directory as a series of images.
  - Default: False
- **Number of Images**
  - Name in input file: images
  - Format: Odd positive integer

  - Explanation: The total number of image files in the image directory folder, or the total number desired after interpolation including the initial and final images.
  - Default: None, must always specify.

- **Perturb**
  - Name in input file: perturb
  - Format: T/F (enter either true/false or t/f)
  - Explanation: If true, the program will generate and apply path perturbations using information from other relevant input parameters. If false, it will only identify the distortion group elements, isomorphic space group, and present possible irreducible representations to construct perturbations with.
  - Default: False

- **Symmetry Tolerance**
  - Name in input file: symprec
  - Format: Positive integer
  - Explanation: This is the 'symprec' parameter used as a tolerance for determining symmetry in `SPGLIB`.
  - Default: 0.001

- **Angle Tolerance**
  - Name in input file: angle_tolerance
  - Format: Positive or negative float
  - Explanation: This is the 'angle_tolerance' parameter used as an angle tolerance for determining symmetry in `SPGLIB`.
  - Default: -1.0

- **General Tolerance**
  - Name in input file: general_tolerance
  - Format: Positive float
  - Explanation: This is a general tolerance used for identifying and matching matrix representations of symmetry elements.
  - Default: 0.001

- **Vector Tolerance**
  - Name in input file: vector_tolerance(f) or vector_tolerance(a)
  - Format: Positive three-element vector consisting of three floats separated by commas. Units are specified in parentheses as (f/a).

- Explanation: This is the tolerance for matching vectors of atomic positions. One can either specify this in fractional units or angstroms: in the input file, the user specifies the units with 'vector_tolerance(f)' (fractional) or 'vector_tolerance(a)' (angstrom).
- Default: fractional, 0.001,0.001,0.001

- **Vector Tolerance**
  - Name in input file: vector_tolerance(f) or vector_tolerance(a)
  - Format: Positive three-element vector consisting of three floats separated by commas. Units are specified in parentheses as (f/a).
  - Explanation: This is the tolerance for matching vectors of atomic positions. One can either specify this in fractional units or angstroms: in the input file, the user specifies the units with 'vector_tolerance(f)' (fractional) or 'vector_tolerance(a)' (angstrom).
  - Default: fractional, 0.001,0.001,0.001

- **Translation Tolerance**
  - Name in input file: translation_tolerance(f) or translation_tolerance(a)
  - Format: See 'Vector Tolerance'
  - Explanation: This is a special tolerance for matching translations in symmetry operations, which can differ more than atomic positions.
  - Default: Equivalent to vector tolerance value.

- **Transformation Matrix Number**
  - Name in input file: trans_num
  - Format: Positive integer or '-1'
  - Explanation: Image from which to take the transformation matrix and origin shift that puts the distortion group in the standard/default setting (starts at 1). This is an optional parameter: the default value of '0' will tell the program to determine the transformation matrix and origin shift manually. Alternatively, if the value is set to '-1' a matrix and vector can be manually entered (see Transformation Matrix and Origin Shift).
  - Default: 0

- **Transformation Matrix**
  - Name in input file: trans_mat
  - Format: Nine-element vector consisting of nine floats separated by commas. This is converted to a matrix through the reshape function in numpy.

- Explanation: This is a direct way to specify a transformation matrix. If no form of the transformation matrix is provided, the program will attempt to manually determine it.
- Default: 1,0,0,0,1,0,0,0,1

- **Origin Shift**
  - Name in input file: oshift
  - Format: Three-element vector consisting of three floats separated by commas.
  - Explanation: This is a direct way to specify an origin shift. If no form of the origin shift is provided, the program will attempt to manually determine it.
  - Default: 0,0,0

- **Input Format**
  - Name in input file: input_format
  - Format: String
  - Explanation: This is the format of the input image files to be read by the program. All types listed in the Atomic Simulation Environment (ASE) documentation are supported. If left blank, the program will attempt to detect the format.
  - Default: Detect format.

- **Output Format**
  - Name in input file: output_format
  - Format: String
  - Explanation: This is the format of the input image files to be output by the program. All types listed in the Atomic Simulation Environment (ASE) documentation are supported.
  - Default: VASP

- **Irrep Number**
  - Name in input file: irr_num
  - Format: Positive integer
  - Explanation: This is the identifying number in the listing by Stokes *et al.* of the irreducible representation (irrep) that one wishes to use to construct the path perturbation. The number can be taken from one of the possible ones output by the program after determining the isomorphic space group. Kernel groups of the irrep can be looked by using the `ISOSUBGROUP` program by Stokes *et al.*
  - Default: none

- **Irrep Dimension**
  - Name in input file: irr_dim
  - Format: Positive integer
  - Explanation: This is the dimension of the irreducible representation (irrep).
  - Default: 1
- **Mode Coefficients**
  - Name in input file: mode_coeff
  - Format: N-element vector consisting of positive and negative floats separated by commas, where 'N' is the dimension of the irreducible representation chosen (irrep).
  - Explanation: These are the coefficients of the individual modes in multidimensional irreducible representation to use when taking a linear combination. In other words, these are the entries in the order parameter vector.
  - Default: 1
- **Minimum Movement**
  - Name in input file: min_move
  - Format: Positive float.
  - Explanation: This is the cutoff displacement (in angstroms) in any lattice vector direction to have an atom included in the basis for perturbation. Atoms which are displaced below this number will not be considered for perturbation.
  - Default: 0
- **Random Coefficients**
  - Name in input file: random
  - Format: T/F (enter either true/false or t/f)
  - Explanation: If true, this turns on random coefficients if multiple instances of modes that transform as the same one-dimensional perturbation are found. If false, the linear combination of the multiple modes will be taken directly.
  - Default: False
- **Perturbation Magnitude**
  - Name in input file: perturb_mag
  - Format: Positive float
  - Explanation: This is the maximum magnitude of perturbation for any one atom in any lattice vector direction (in angstroms).
  - Default: 0.1

File Output

All outputted files will be contained in the folder labeled "results". If this folder already exists, it will be copied and renamed "results_old_v#" before the new folder is created.

The standard output from the program is written to the "results/output.out" file. All of the perturbed images in the format specified in the input file (with the default being VASP-POSCAR formatted) are contained in "results/output_structures/". Two XYZ-formatted movie files for the pathway before and after perturbation are also outputted in the 'results' folder.

References

[1] J. M. Munro, H. Akamatsu, H. Padmanabhan, V. S. Liu, Y. Shi, L.-Q. Chen, B. K. VanLeeuwen, I. Dabo, and V. Gopalan. Discovering minimum energy pathways via distortion symmetry groups. *Physical Review B*, 2018.

[2] H. T. Stokes, B. J. Campbell, and R. Cordes. Tabulation of irreducible representations of the crystallographic space groups and their superspace extensions. *Acta Crystallographica Section A Foundations of Crystallography*, 69(4):388–395, July 2013.

[3] B. K. VanLeeuwen and V. Gopalan. The antisymmetry of distortions. *Nature Communications*, 6:8818, 2015.