

# Hands-on 1: Download and installation

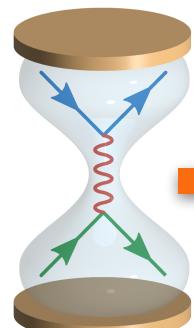
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Department of Applied Physics and Materials Science, Caltech, USA

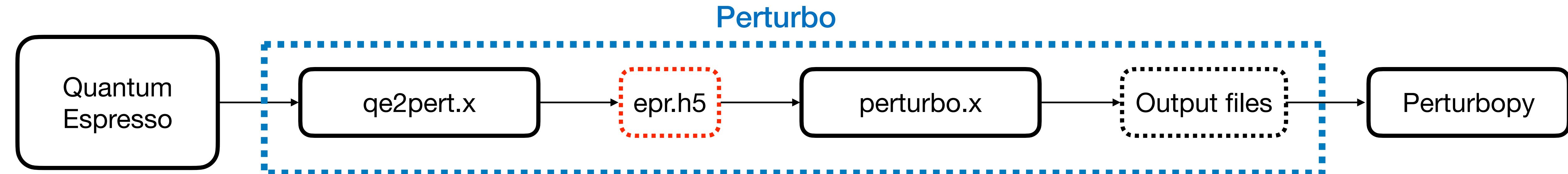
# Outline

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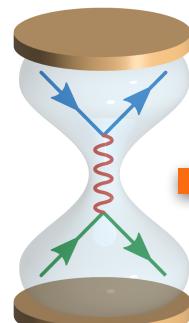
- Workflow
- Website
- Download and installation from scratch
- Brief Perturbopy introduction
- Docker containers



# Perturbo Workflow



- Quantum Espresso: provides all supplementary files
- qe2pert.x: compute electron-phonon matrix elements in the Wannier basis with this files
- epr.h5 file: HDF5 file containing results from qe2pert.x, **required for all perturbo.x calculations**
- perturbo.x: core executable of Perturbo, performs calculations for the different calculation modes
- Perturbopy: postprocessing Python package, which helps to analyze the results and test work of the Perturbo



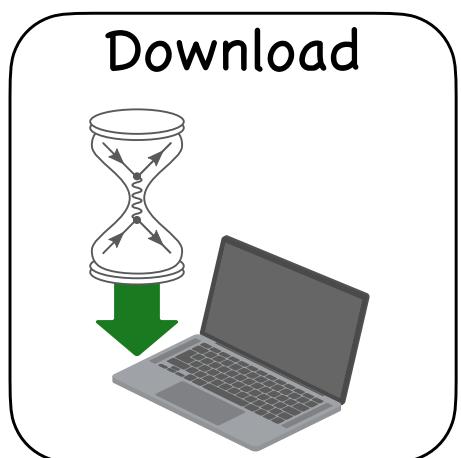
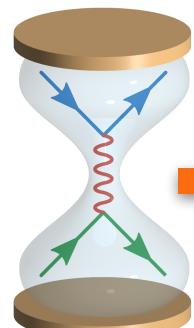
# Perturbo Website

The screenshot shows the Perturbo website homepage. At the top, there's a blue header bar with the Perturbo logo (hourglass icon) and the word "Perturbo". Below the header, there's a navigation bar with links for "Sidebar", "Forum", "News", and "Download". On the left, a sidebar titled "Getting started" is open, showing a list of links: Home, Capabilities, Download and installation, Publications, Tutorials, Other examples, Workshops, Platforms, Utilities, Releases, and Input parameters. The main content area includes sections for "News" (with a speaker icon), "Perturbo Workshop" (with a note about a workshop on September 18-19, 2025), "Perturbo 3.0.0 is released!" (with a note about the release of version 3.0.0 compatible with QE 7.3), and "Generating input files" (with a note about the transfer of the input generation script to the Perturbopy package). Below these sections is a row of six icons representing different features: Download, Tutorials, Workflow, Inputs, Forum, and Postprocessing.

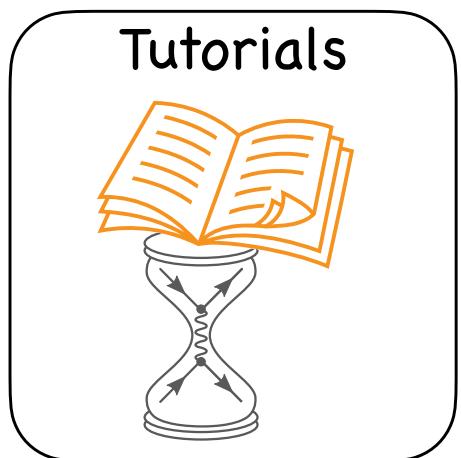
PERTURBO is open source software to compute from first principles the scattering processes between charge carriers (electrons and holes) and phonons, defects, and photons in solid state materials, including metals, semiconductors, oxides, and insulators.

## [Website](#)

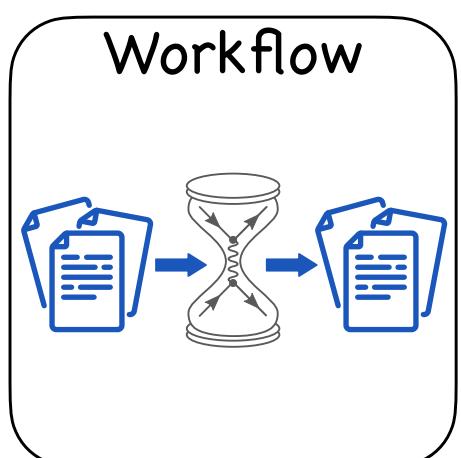
Contain guides to the installation, run of each calculation modes, workflow explanation, workshops materials etc.



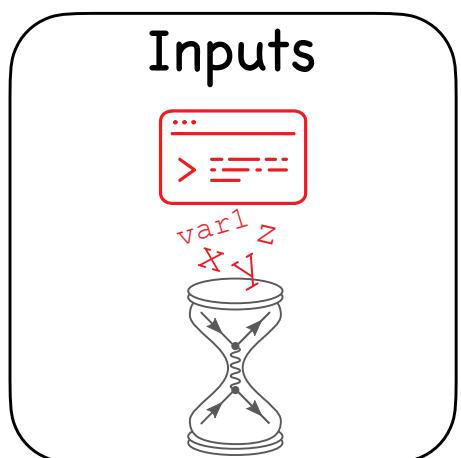
How to obtain Perturbo code, compile supplementary packages and Perturbo itself in different scenarios



Detailed tutorials for each calculation mode, input/output files description



Visualize order of calculations. Summary of input/output files, templates for input files, tutorials links



Explanation of input parameters, list of mandatory/optional parameters for each calculation mode

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# Supplementary packages

Perturbo requires Quantum Espresso, Wannier90 and HDF5 libraries



Download HDF5: <https://support.hdfgroup.org/downloads/>

Install HDF5:

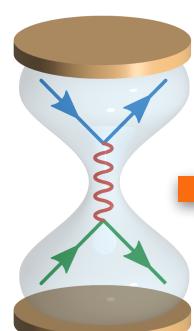
```
>> wget https://support.hdfgroup.org/ftp/HDF5/releases/hdf5-1.12/hdf5-1.12.0/src/hdf5-1.12.0.tar.gz  
>> tar -xzf hdf5-1.12.0.tar.gz  
>> cd hdf5-1.12.0  
>> ./configure --prefix=/opt/hdf5 --enable-fortran --enable-shared --enable-parallel  
>> make && make install
```

WANNIER90



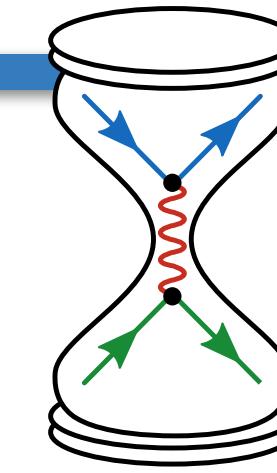
Download and Install Quantum Espresso:

```
>> wget https://gitlab.com/QEF/q-e/-/archive/qe-7.3/q-e-qe-7.3.tar.gz  
>> tar -xzf q-e-qe-7.3.tar.gz  
>> cd q-e-qe-7.3  
>> ./configure --with-hdf5="/opt/hdf5"  
>> make pw ph pp w90
```



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# Download and Install Perturbo



# Perturbo

## 1. Fill out download [form](#)

PERTURBO code download

Thank you for your interest in the PERTURBO code. In order to get access to the code, please fill out the form below. Once you fill out the form, the download link will be sent automatically to the email address that you specify.

## 2. Obtain code from Github [repository](#)

master 6 Branches 12 Tags

alex2shiyu Merge pull request #198 from perturbo-code/new-release

.github/workflows clean up the space

config add files and folder

docs Add one item regar

pert-src add files and folder

Local Codespaces

Clone

HTTPS SSH GitHub CLI

git@github.com:perturbo-code/perturbo.git

Use a password-protected SSH key.

## 2. Compile Perturbo

### 1) Clone Perturbo in the QE folder:

```
>> git clone git@github.com:perturbo-code/perturbo.git  
>> cd perturbo
```

### 2) Choose and copy right make.sys file:

```
>> cp config/make_ifort_parallel.sys make.sys
```

### 3) Add HDF5 paths, if you've compiled QE without it:

```
>> IFLAGS += -I/path/to/hdf5/include  
>> HDF5_LIBS = -L/path/to/hdf5/lib -lhdf5 -lhdf5_fortran
```

### 4) Compile

```
>> make
```

# Pertubo output files

## YAML

```
bands:

  number of bands: 8

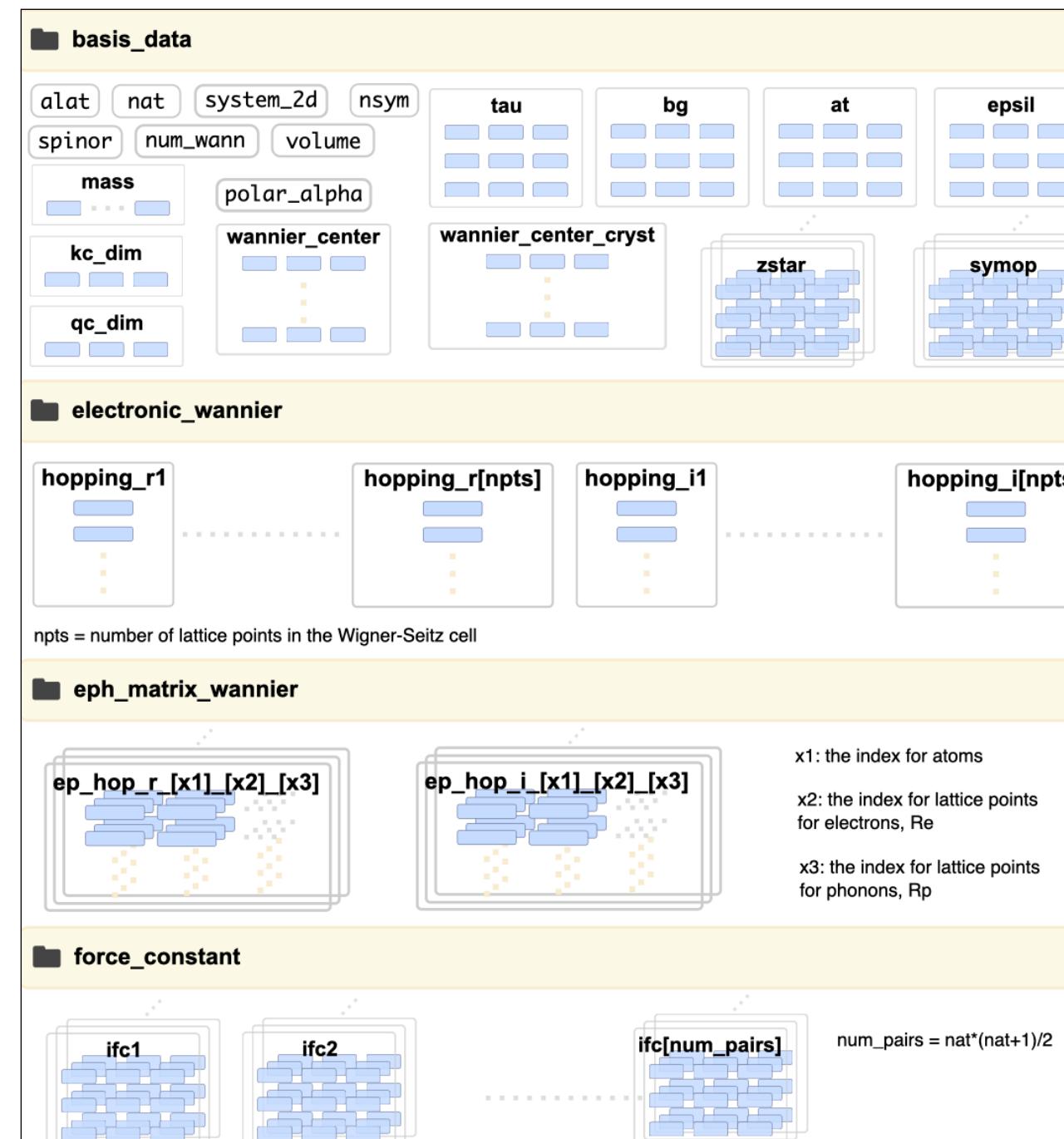
  k-path coordinate units: arbitrary
  k-path coordinates:
    - 0.000000
    .....
    - 3.7802390

  k-point coordinate units: crystal
  k-point coordinates:
    - [ 0.50000, 0.50000, 0.50000, ]
    .....
    - [ 0.00000, 0.00000, 0.00000, ]

  band units: eV
  band index:

    1:
      - -3.4658249872
      .....
      - -5.8116812661
      .....
    8:
      - 13.6984850767
      .....
      - 9.4608102223
```

## HDF5



## ASCII text (legacy)



Click to close legacy-format ASCII text outputs of the bands calculation

We also obtain an output file called 'prefix'.bands (in this case, si.bands) which contains a copy of the interpolated band structure in the following legacy-format:

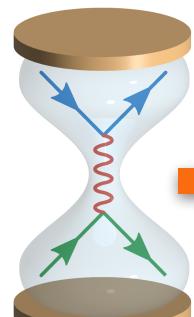
0.0000000	0.50000	0.50000	0.50000	-3.4658249872
.....	.....	.....	.....	.....
3.7802390	0.00000	0.00000	0.00000	-5.8116812661
.....	.....	.....	.....	.....
0.0000000	0.50000	0.50000	0.50000	13.6984850767
.....	.....	.....	.....	.....
3.7802390	0.00000	0.00000	0.00000	9.4608102223

Note that there are 8 blocks in this example, one for each of the 8 bands. The 1<sup>st</sup> column is an irrelevant coordinate used to plot the band structure. The 2<sup>nd</sup> to 4<sup>th</sup> columns are the x, y, and z coordinates of the crystal momenta in **crystal coordinates**. The 5<sup>th</sup> column is the energy, in eV units, of each electronic state.

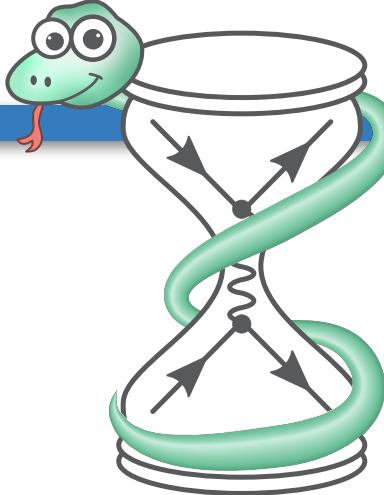
- Stores inputs and outputs from Pertubo calculation
- Can be easily read by high level programming languages

- Stores too large/complex data for YAML
- Specialized scientific format
- Can be easily read by high level programming languages

- Same data as other format
- **Exist solely for legacy, not recommended**



# Perturbopy (brief intro)



# PerturboPy

Python package for postprocessing and testing  
Perturbo

Functionality:

**Postprocessing:**

- Exports data from Perturbo output files to Python
- Contains built-in methods for generating plots and performing calculations

**Test suite for Perturbo:**

- Use Python methods to test calculations in Perturbo test folder
- Check correct compilation and installation of the Perturbo
- Help during code development

[Website](#)

**Installation:**

Option 1 - use [PyPI](#) (recommended)

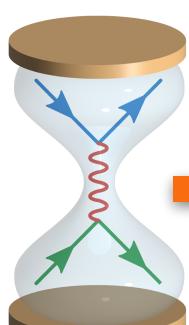
>> pip install perturbopy

The screenshot shows the PyPI project page for 'perturbopy 0.7.1'. At the top, there's a search bar with 'Type '/' to search projects' and navigation links for 'Help', 'Docs', 'Sponsors', 'Log in', and 'Register'. Below the search bar, the project name 'perturbopy 0.7.1' is displayed with a green checkmark next to 'Latest version'. A 'pip install perturbopy' button is shown. To the right, there's a 'Released: Mar 7, 2025' timestamp. The main content area describes the project as 'Suite of Python scripts for Perturbo testing and postprocessing'.

Option 2 - download from the [GitHub](#):

The screenshot shows the GitHub repository page for 'perturbopy'. It displays the repository structure with branches 'main' and '4 Branches', and tags '5 Tags'. A pull request 'hurricane642 Update version to 0.7.1 (#105)' is visible. The repository contains files like '.github/workflows', 'docs', 'src/perturbopy', 'tests', '.gitignore', and '.readthedocs.yaml'. On the right, there's a 'Clone' section with options for 'HTTPS', 'SSH', and 'GitHub CLI', and a link to 'git@github.com:perturbo-code/perturbopy.git'. A note says 'Use a password-protected SSH key.' Below that are links for 'Open with GitHub Desktop' and 'Download ZIP'.

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# Docker usage



Build a 'micro-OS', called **image**, light-weight and containing solely packages, interesting for us. In our case, it would be HDF5, QE, W90 and Pertubo.

More on the Docker usage for the Pertubo you can find on the [GitHub](#)

