

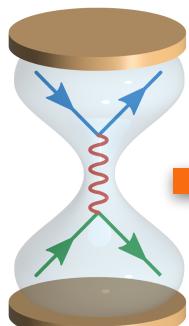
Hands-on 1: Download and installation

Sergei Kliavinek

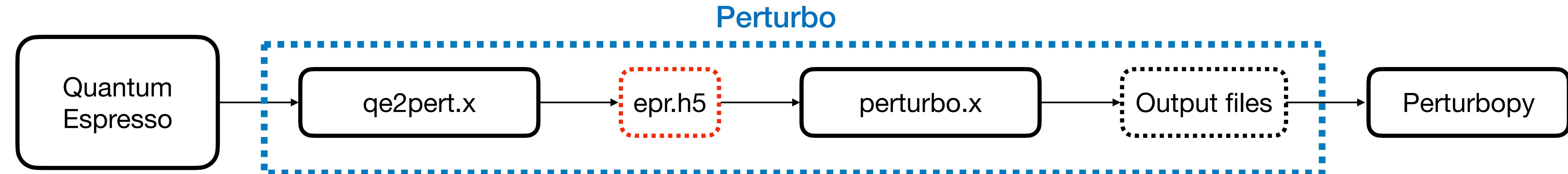
Prof. Marco Bernardi's Research Group
Department of Applied Physics and Materials Science, Caltech, USA

Outline

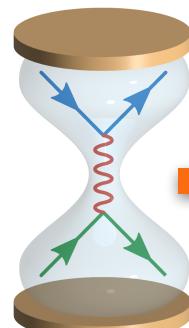
- Workflow
- Website
- Download and installation from scratch
- Brief Perturbopy introduction
- Docker containers



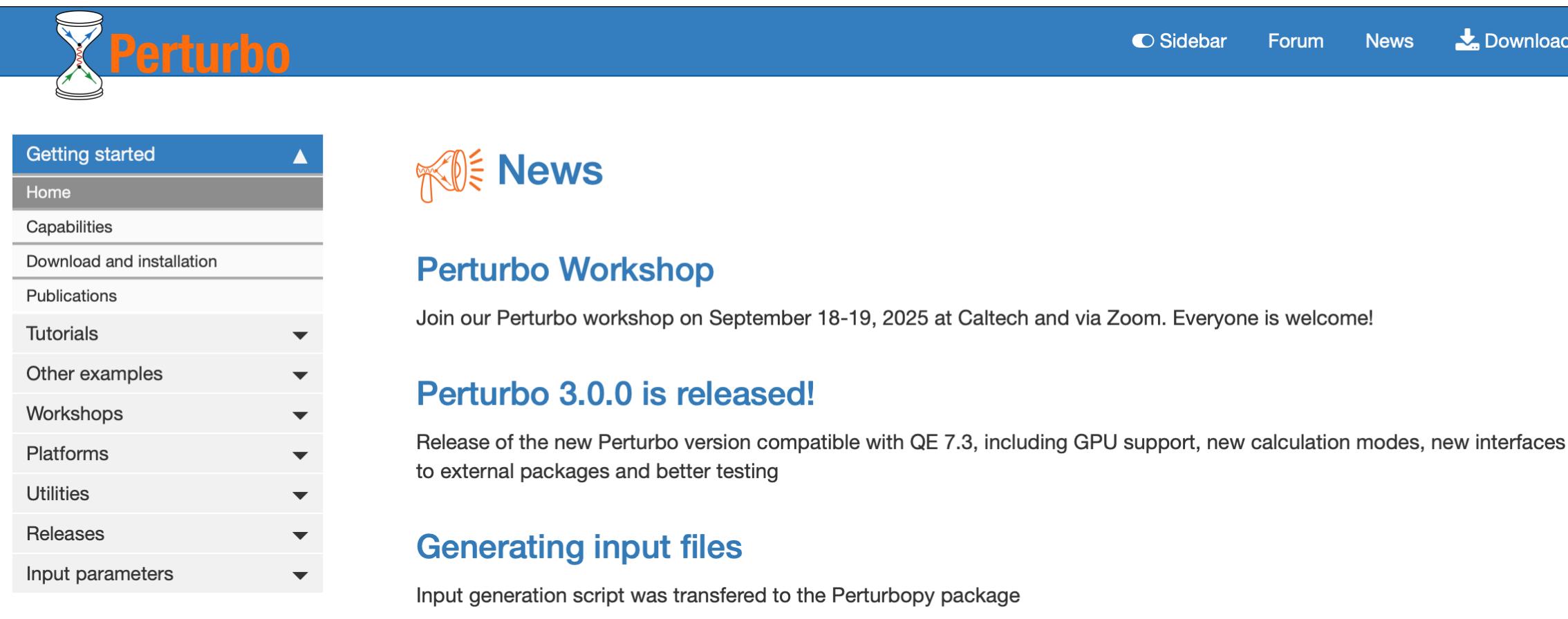
Perturbo Workflow



- 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



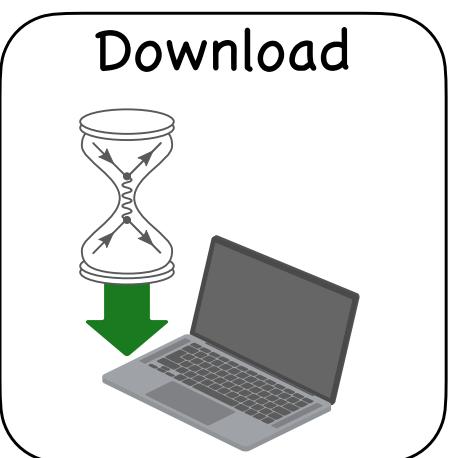
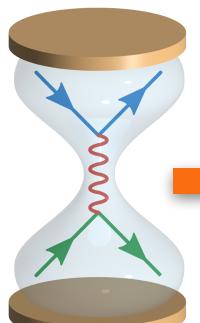
Perturbo Website



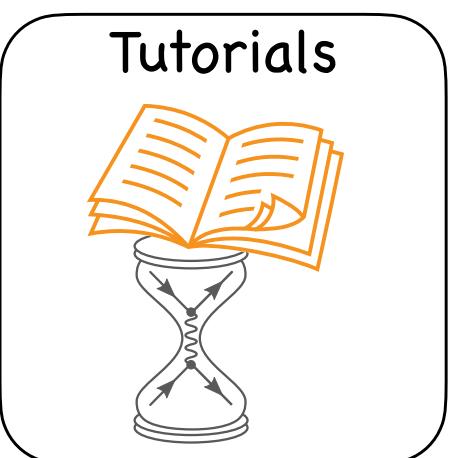
The screenshot shows the Perturbo website homepage. At the top, there's a blue header bar with the Perturbo logo (hourglass icon) and the word "Perturbo". Below the header, there's a navigation bar with links for "Sidebar", "Forum", "News", and "Download". On the left, a sidebar titled "Getting started" 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 has 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 being compatible with QE 7.3), and "Generating input files" (with a note about the input generation script being transferred to the Perturbopy package). There are also six small icons representing "Download", "Tutorials", "Workflow", "Inputs", "Forum", and "Postprocessing".

Website

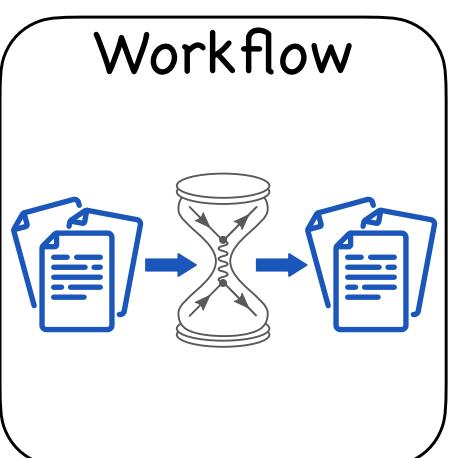
Contain guides to the installation, run of each calculation modes, workflow explanation, workshops materials etc.



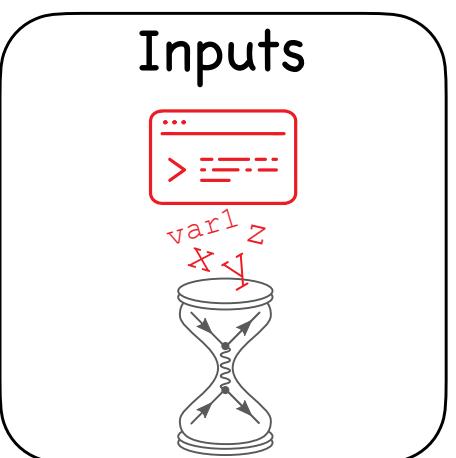
How to obtain Perturbo code, compile supplementary packages and Perturbo itself in different scenarios



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

Pertubo requires Quantum Espresso, Wannier90 and HDF5 libraries



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

Install HDF5:

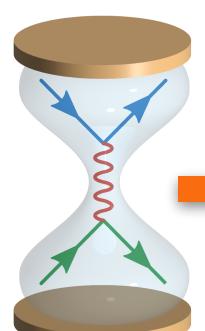
```
wget https://support.hdfgroup.org/ftp/HDF5/releases/hdf5-1.12/hdf5-1.12.0/src/hdf5-1.12.0.tar.gz  
tar -xzf hdf5-1.12.0.tar.gz  
cd hdf5-1.12.0  
.configure --prefix=/opt/hdf5 --enable-fortran --enable-shared --enable-parallel  
make && make install
```

WANNIER90



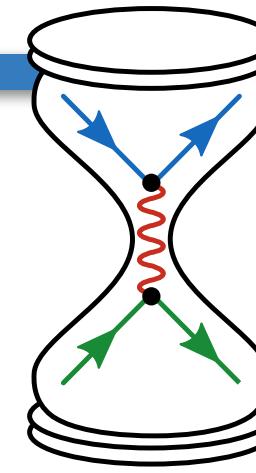
Download and Install Quantum Espresso:

```
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
```



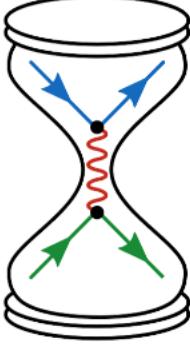
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Download and Install Perturbo



Perturbo

1. Fill out download [form](#)

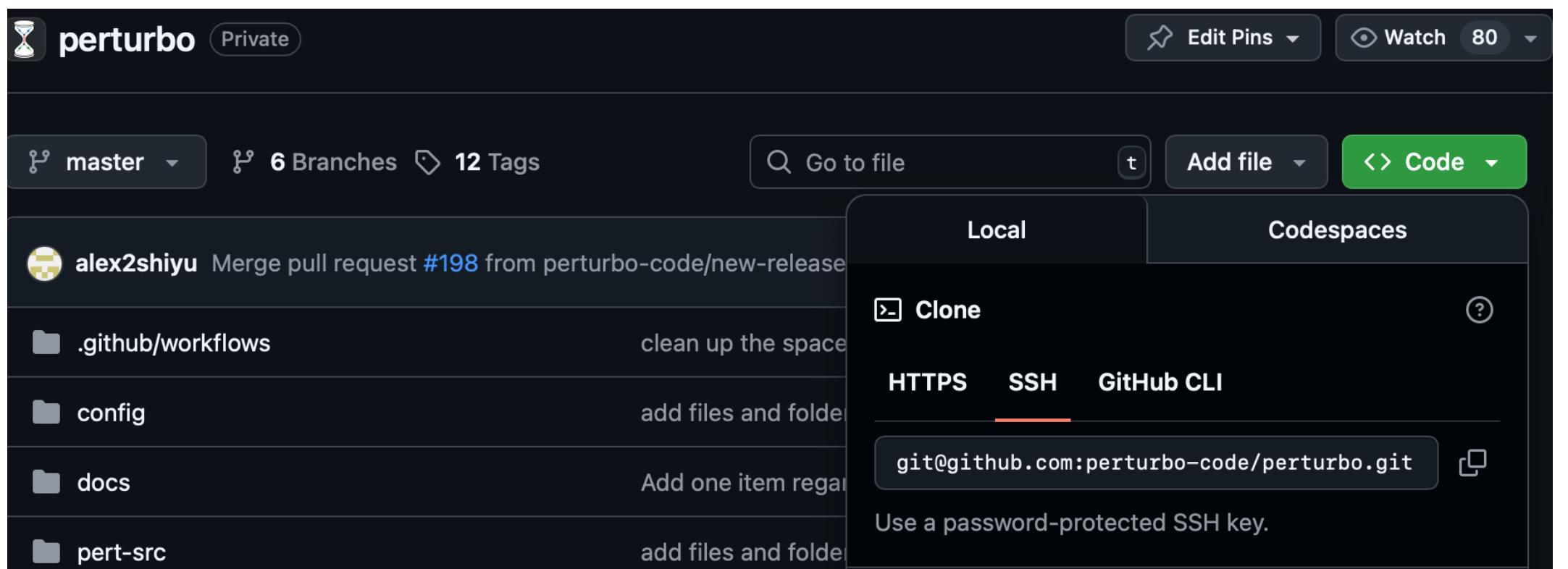


PERTURBO

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](#)



The screenshot shows the GitHub repository page for 'perturbo'. It has 6 branches and 12 tags. The 'master' branch is selected. A 'Clone' button for HTTPS is highlighted, showing the URL: `git@github.com:perturbo-code/perturbo.git`.

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

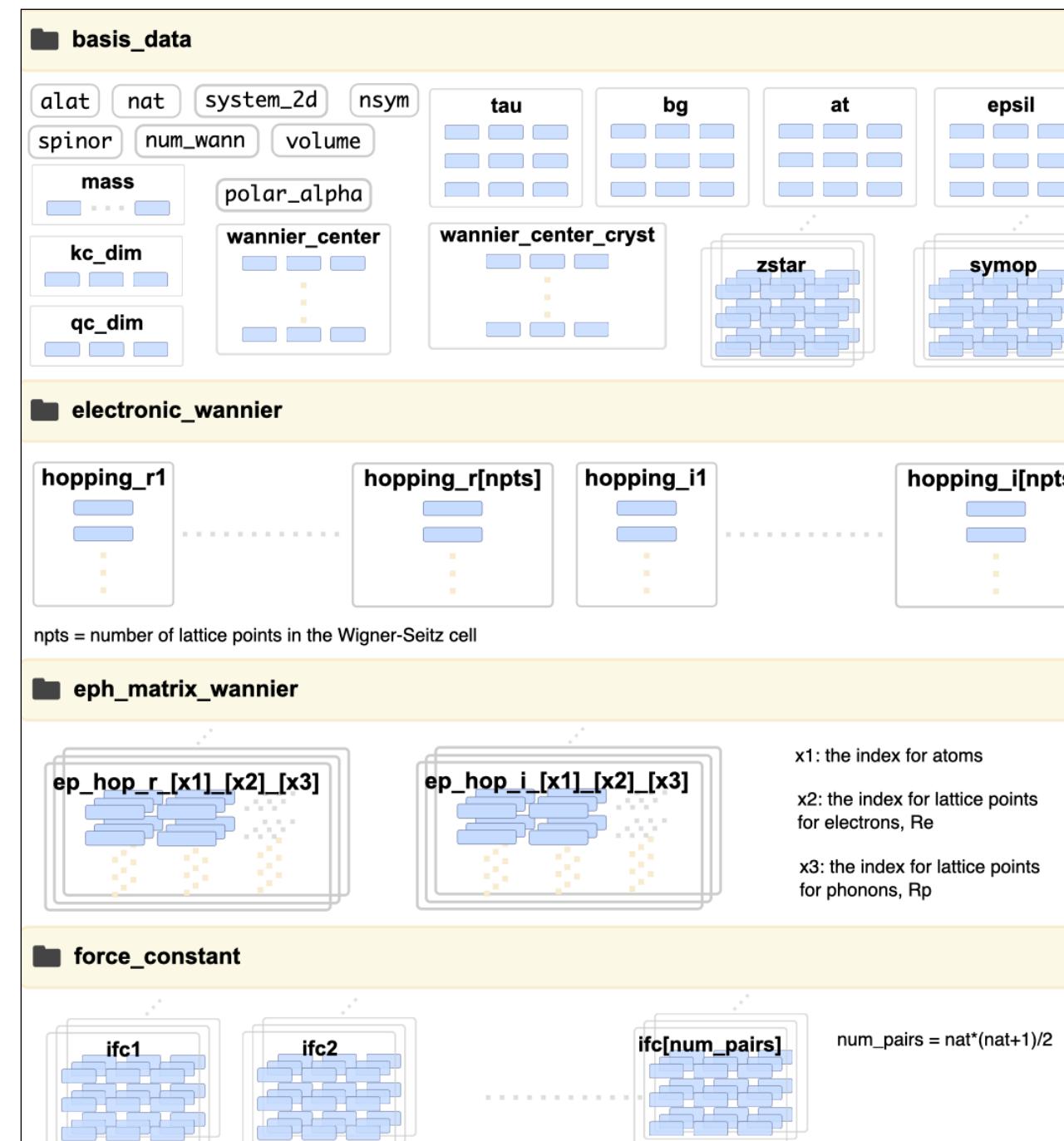
  k-path coordinate units: arbitrary
  k-path coordinates:
    - 0.000000
    .....
    - 3.7802390

  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:

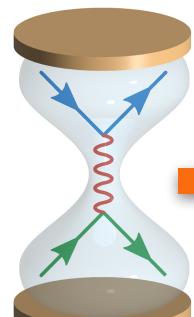
0.000000	0.50000	0.50000	0.50000	-3.4658249872
.....
3.7802390	0.00000	0.00000	0.00000	-5.8116812661
.....
0.000000	0.50000	0.50000	0.50000	13.6984850767
.....
3.7802390	0.00000	0.00000	0.00000	9.4608102223

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

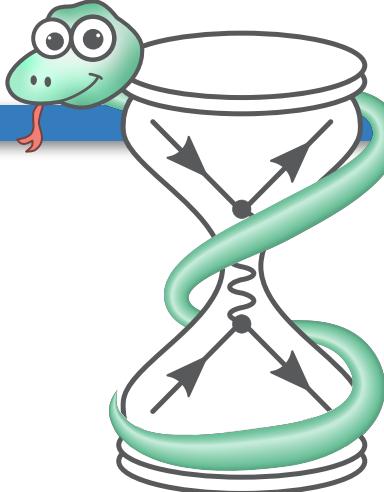
- Stores inputs and outputs from Pertubo calculation
- Can be easily read by high level programming languages

- 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

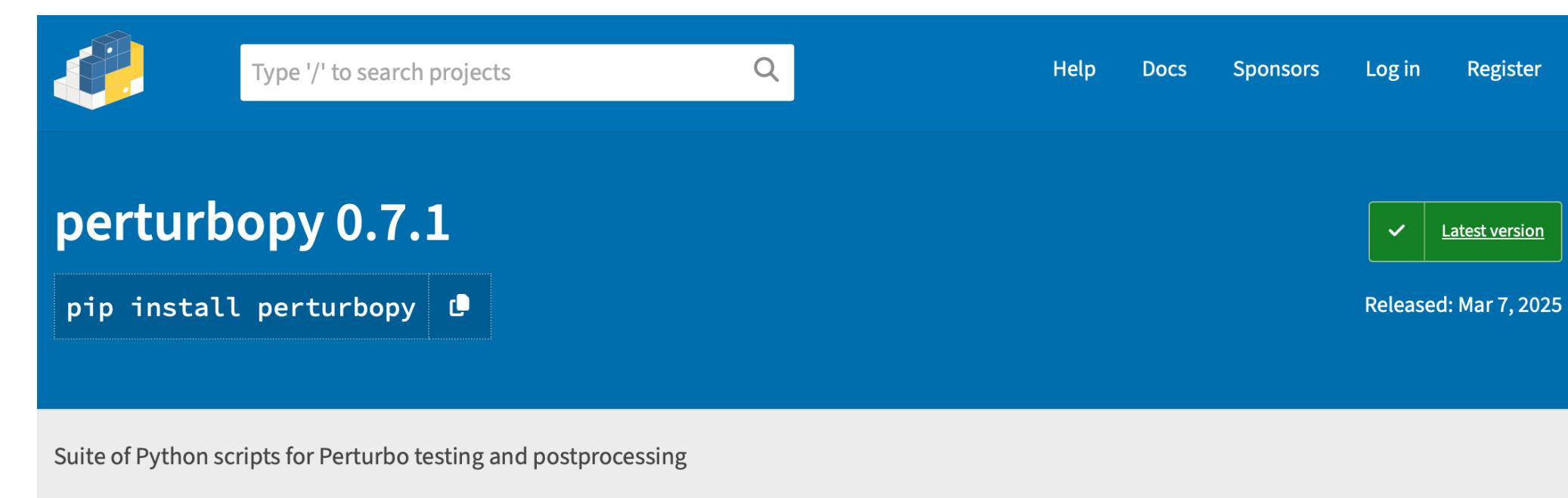
Test suite for Perturbo:

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

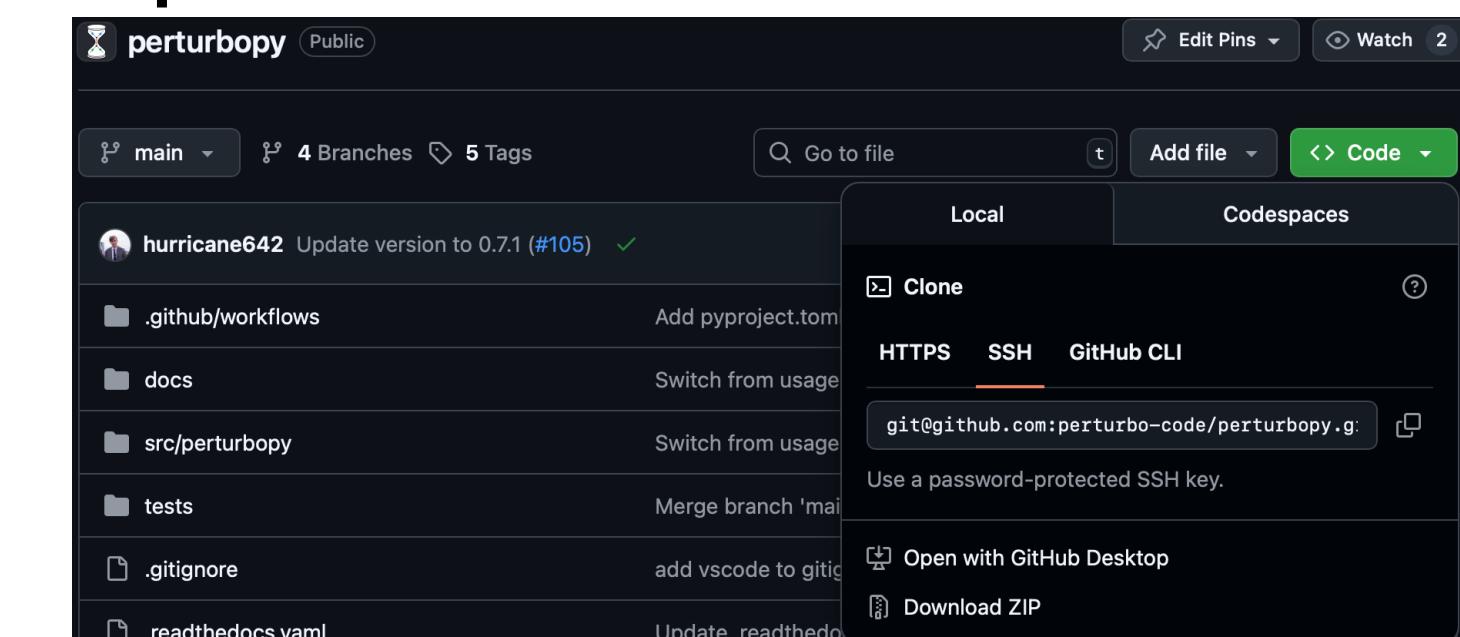
[Website](#)

Installation:

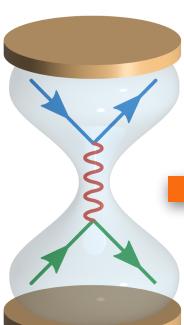
Option 1 - use [PyPI](#) (recommended)
pip install perturbopy



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



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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](#)

