

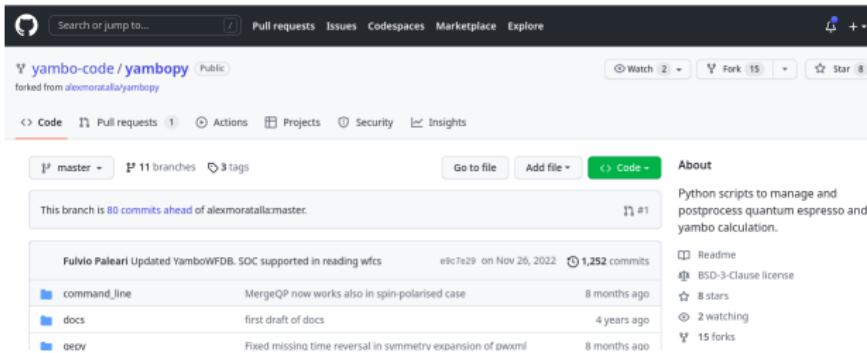
Introduction to YamboPy

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Yambopy

- ▶ This project provides python scripts to manage and postprocess quantum espresso and yambo calculation.
- ▶ Can automate your calculations,
- ▶ provide post-processing capabilities
- ▶ Visualization
- ▶ Input file manipulation, etc.
- ▶ Its FOSS! <https://github.com/yambo-code/yambopy>



Why?

- ▶ Automation reduces **mistakes**.
- ▶ Increase the **pace** of your work.
- ▶ **High Throughput** studies.
- ▶ Key: **reproducibility**, can we achieve this?

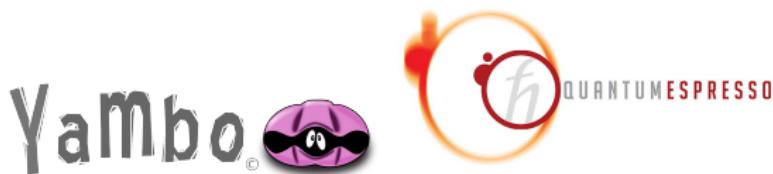
The screenshot shows a GitHub repository page for 'yambo-code/yambopy'. The repository is public and forked from 'alexmoratalla/yambopy'. The main navigation bar includes links for Pull requests, Issues, Codespaces, Marketplace, and Explore. The repository name 'yambo-code / yambopy' is displayed along with its status as 'Public' and the number of forks (15) and stars (8). Below the header, there are tabs for Code, Pull requests (1), Actions, Projects, Security, and Insights. The 'Code' tab is selected. A dropdown menu shows the current branch is 'master'. Other branches listed are '11 branches' and '3 tags'. A commit message indicates 'This branch is 80 commits ahead of alexmoratalla/master'. The commit list shows three recent commits by Fulvio Paleari:

Author	Commit Message	Date	Commits
Fulvio Paleari	Updated YamboWFDB: SOC supported in reading wfc	on Nov 20, 2022	1,252 commits
	MergeQP now works also in spin-polarised case	8 months ago	
	first draft of docs	4 years ago	
	Fixed missing time reversal in symmetry expansion of pwxml	8 months ago	

On the right side of the page, there is an 'About' section with a detailed description of the repository: 'Python scripts to manage and postprocess quantum espresso and yambo calculation.' It also lists the Readme, BSD-3-Clause license, 8 stars, 2 watching, and 15 forks.

Requirements

- ▶ These python scripts require **python3**
- ▶ We will need:
 1. **yambopy**, Already Installed
 2. **yambo**, Installed
 3. **Quantum Espresso**, installed



Aims of this Exercise:

- ▶ We will work on the Convergences and Approximations tutorial: [click here](#)
- ▶ And the database tutorial: [click here](#)
- ▶ Finally the BSE exercise: [Click here](#)



Retreving the files:

- ▶ Copy the files to your home directory and work from there:

```
1 ~$ cp -r /media/ictpuser/smr3694/ictptutor/yambopy/tutorial ~/  
     tutorial  
2 ~$ cd ~/tutorial
```



Getting started

- ▶ You have to use spack to get the environment that provides yambopy:

```
1 ~$ spack load quantum-espresso
2 ~$ spack load yambo
3 ~$ spack load anaconda3
```



Running yambopy:

- ▶ First exercise,

```
1 ~$ cd tutorial/run_calculations  
2 ~$ python gs_bn.py -sn  
3 ...
```

- ▶ Follow the steps here: [click this](#)
- ▶ You will run QE followed by GW convergence



Analysis:

- ▶ Yambopy provides the capability to read and analyze the yambo NetCDF databases, for this exercise, start from this directory:

```
1 ~$ cd ~tutorial/databases_yambopy  
2 ~$ yambopy save -nscf BSE_saves/QE_saves/hBN.save  
3 ...
```

- ▶ Continue with the tutorial: [click here](#)



BSE with Yambopy

- ▶ This requires the first exercise to have been done
- ▶ We continue from the first exercise's directory:

```
1 ~$ cd ~tutorial/run_calculations  
2 ~$  
3 ...
```

- ▶ Continue with the instructions here: [click this](#)



Thanks

- ▶ Thank you for your attention.
- ▶ questions?

