NITheCS

National Institute for
Theoretical and Computational Sciences

NITheCS Mini-school

Wednesday 11, 18 and 25 May 2022, 14h00 – 15h00

Dr Kingsley Obodo (North-West University) and Dr Cecil Ouma (Next-Einstein forum fellow)

‘Quantum ESPRESSO’

Action plan 11th May 2022

- Accessing Quantum espresso either via your own computer or the CHPC

- Structure files in CIF format obtained from either:
  a) Materialsproject{https://materialsproject.org/materials/mp-1094034/#}, Crystallography
  b) Open Database {https://www.iucr.org › resources› cif},
  c) http://rruff.geo.arizona.edu/AMS/minerals/Platinum,
  d) The Open Quantum Materials Database {https://oqmd.org/}, etc.

- Converting CIF to QE input file using either:
  a) BURAI works in windows,
  b) Materialscloud {https://www.materialscloud.org/work/tools/qeinputgenerator}, etc.

- Calculations intended:
  - Single point calculation (scf)
  - Lattice constant (relax)
  - Lattice constant and cell optimization (vc-relax)

Action plan 11th May 2022

- Require optimizations:
  a) Lattice constant optimization (a, b & c),
  b) KPOINT optimization,
  c) ECUT optimization, Cell optimization.

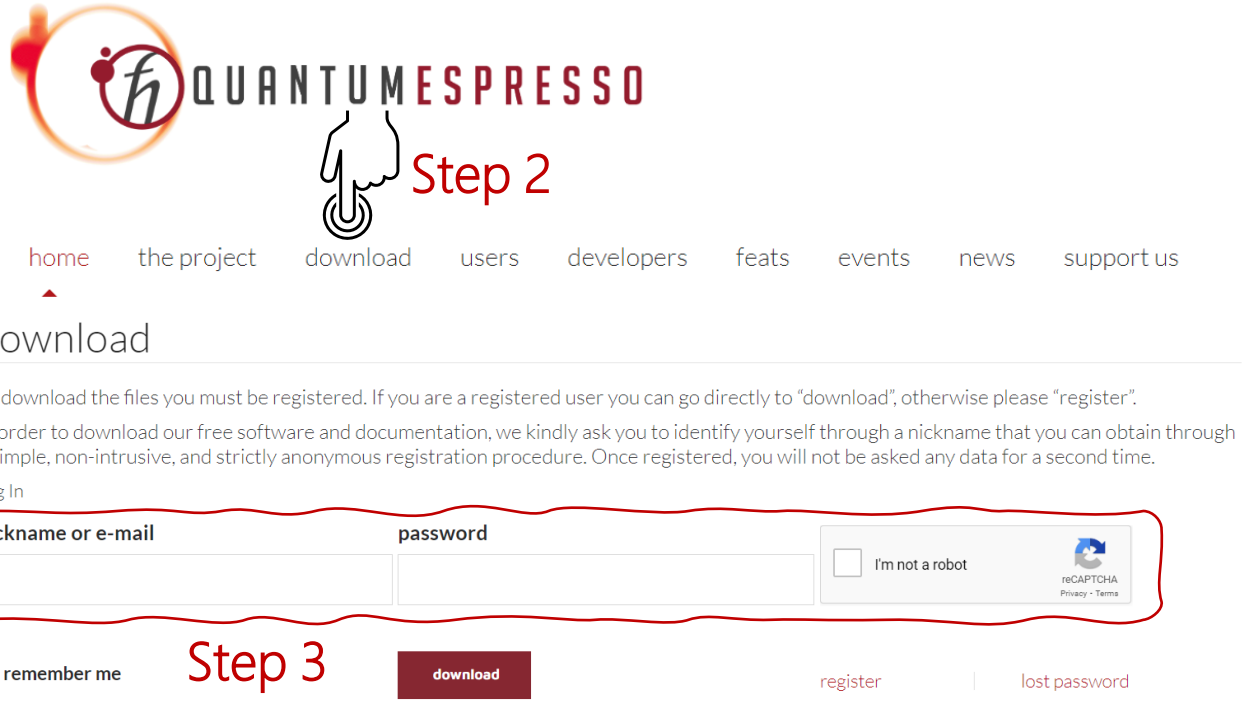
- Assignment: Perform the band structure and density of states calculation on pristine Ti3C2bulk and monolayer. If you have any queries do not hesitate to contact me.
  This we will work on in the next class.

Quantum ESPRESSO: The basics & download

- An integrated suite of Open-Source computer codes for electronic-structure calculations and materials modelling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.
- An open-source project
- Also referred to as PWSCF or QE
- What can QE do:
  - Ground-state calculations
  - Structural Optimization, molecular dynamics, potential energy surfaces
  - Electrochemistry and special boundary conditions
  - Response properties (DFPT)
  - Spectroscopic properties
  - Quantum Transport
  - Platforms

How to obtain QE

Step 1 https://www.quantum-espresso.org/



Quantum ESPRESSO: The basics & download

register

Would you mind telling something about yourself?

In order to keep providing the best open-source quantum simulation software available, to meet user expectations and the requests of our funding agencies, *we need to know a little bit about you for our files.*

The Quantum ESPRESSO Foundation is committed to your privacy. We do not request your name and the anonymous data that we collect will only be used to draft statistics about the number of (unique) downloads and the geographical, gender, and professional distribution of our users. This statistics may be published on this web site or used to write the reports that our public funding agencies request and to stir the future policies of the Quantum ESPRESSO Foundation and Project.

nickname *

nickname

email *

email

country *

--Select Country--

privacy policy *

☐ **accept our privacy policy**

click to see our privacy policy

Register

Step 3

register

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be used to draft statistics about the number of (unique) downloads and
statistics may be published on this web site or used to write the reports
the Quantum ESPRESSO Foundation and Project.

Thank you for registering. Click HERE to log in and download the files.

Step 4

download

To download the files you must be registered. If you are a registered user you can go directly to "download", otherwise please "register".

In order to download our free software and documentation, we kindly ask you to identify yourself through a nickname that you can obtain through a simple, non-intrusive, and strictly anonymous registration procedure. Once registered, you will not be asked any data for a second time.

Log In

nickname or e-mail Cecil

password ••••••••••••••

I'm not a robot reCAPTCHA Privacy - Terms

☑ **remember me**

download

register | lost password

Step 5

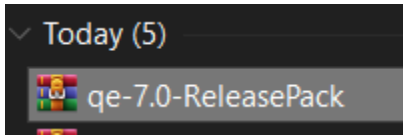
Quantum ESPRESSO: The basics & download

download

logout

SOFTWARE	DOCUMENTATION	OTHER
Full source code of Quantum ESPRESSO v7.0. Ready for compilation in all supported platforms. For more details and instructions see the release notes contained in the archive.	The full documentation bundle of Quantum ESPRESSO v7.0. Here you can find all the information on the features and capabilities of Quantum ESPRESSO.	This archive contains the XSD schemas used by Quantum ESPRESSO applications in version 7.0. To download the package, press the button below.
Quantum ESPRESSO V.7.0	Quantum ESPRESSO V.7.0 Docs	Quantum ESPRESSO V.7.0 Schemas

Step 5

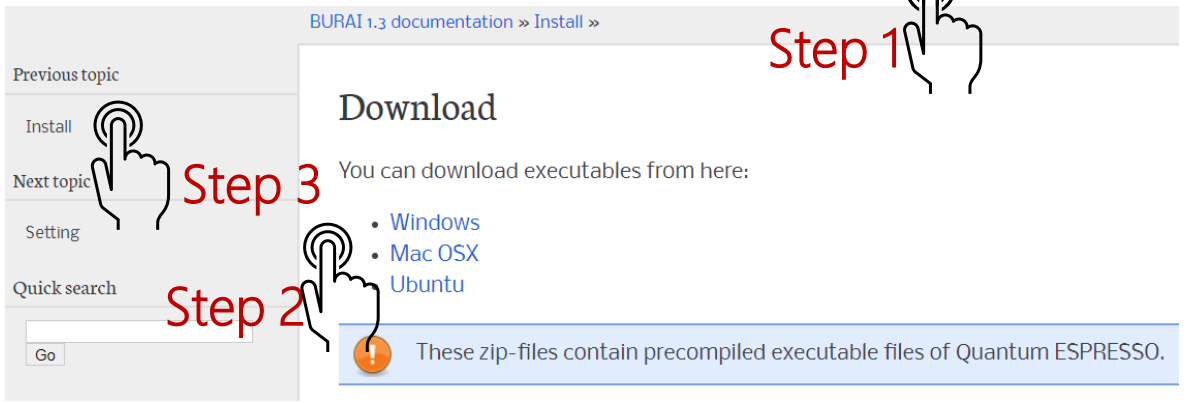


Instructions for the impatient:

```
cd qe-X.Y.Z/
./configure
 make all
```

Other installations (Windows)

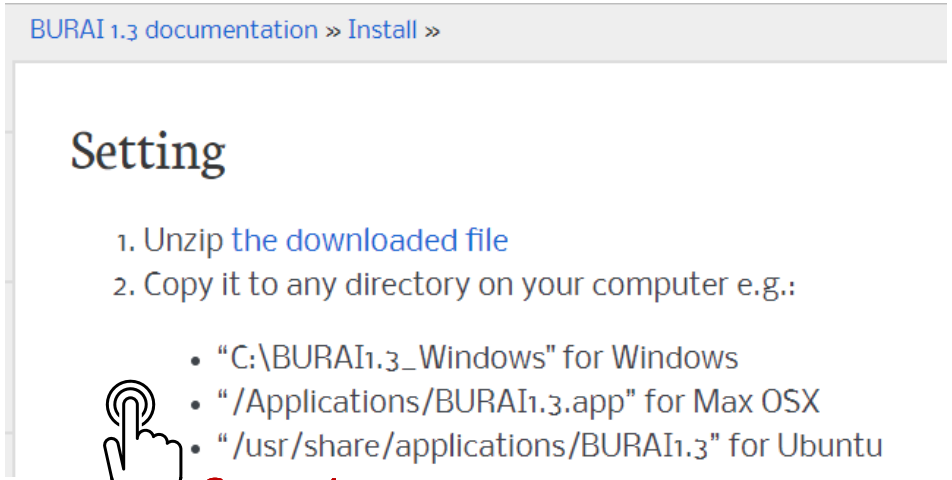
https://burai.readthedocs.io/en/latest/install/download.html



Step 1

Step 3

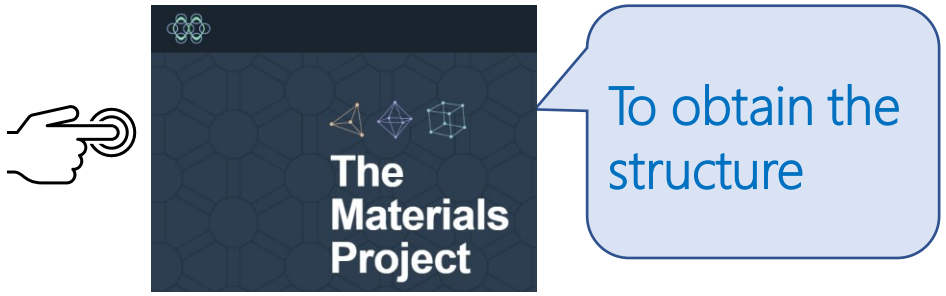
Step 2



Step 4

Input file generation & Running on CHPC

NB: This tutorial will use Ti_3C_2 Mxene for all examples given



To obtain the structure

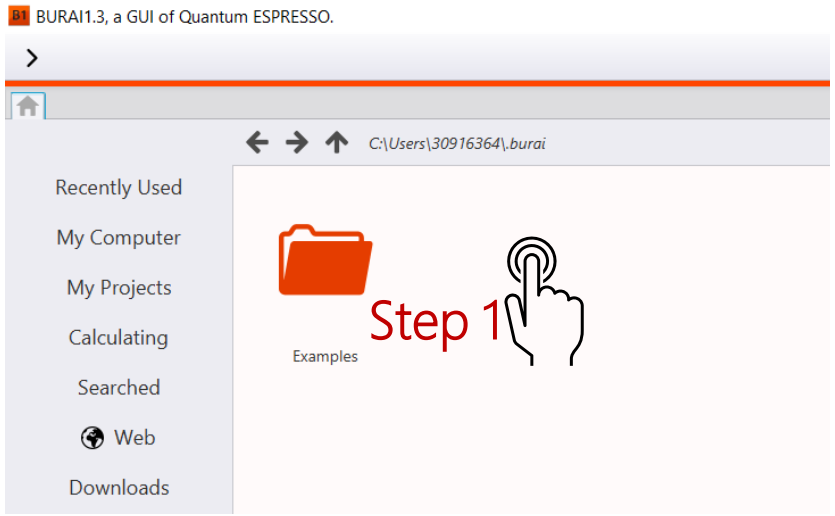
Generate the input files necessary for running on CHPC or a Linux system

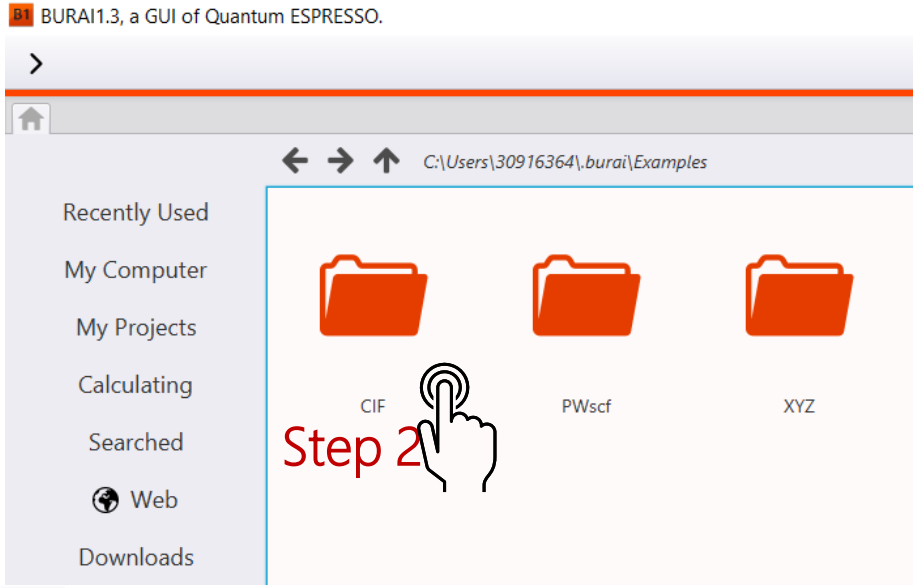
Run on CHPC

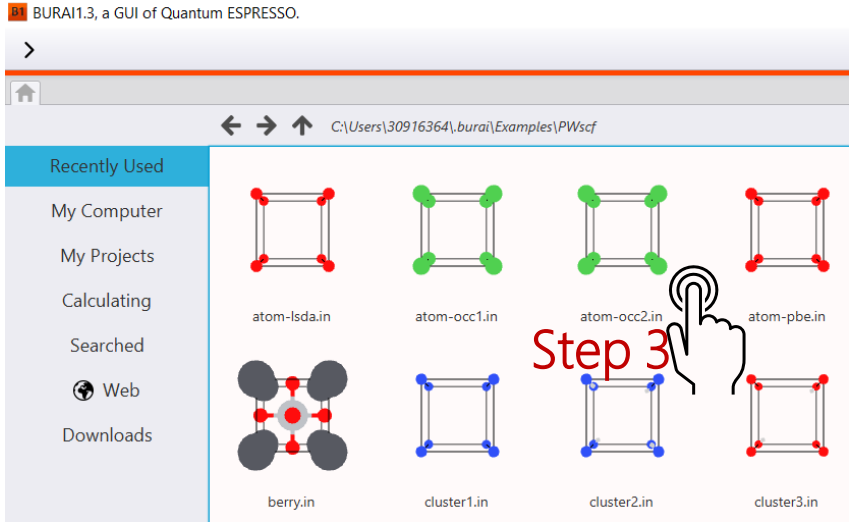
- ssh {username}@lengau.chpc.ac.za; where {username = studentXX, where XX = ass… number}
- cd to the /mnt/lustre/users/studen… …ns must be ran on /mnt/lustre
- To copy files from local com… …pc: scp–r
- We need a PBS submiss… …n this calculation, generate…
- Enter qesp_6.7 (ta… … autocomplete}. NOTE QE inpu… …d with {NAME}.in
- The project… …PC
- Numbe… …all time 04:00
- Ente…
- C… … PW
- …bmit and n to review file before s… …on
- Sub…itting job "qsub{filename}.pbs"
- Checking status of job "qstat–u $USER"
- Cancelling job "qdelJob ID number"

Will be tacked later

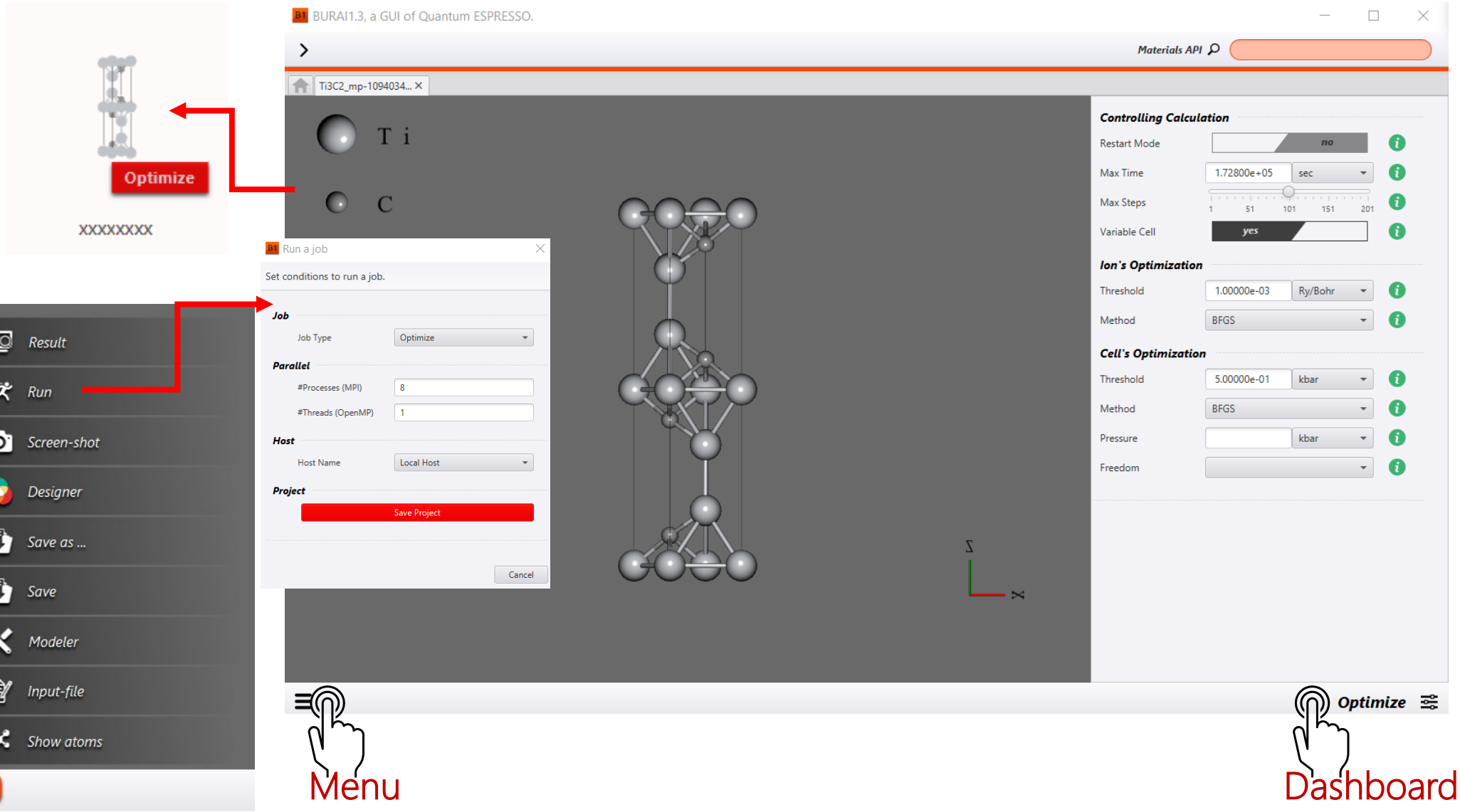
Quantum ESPRESSO: Input file generation & visualization (BURAI)



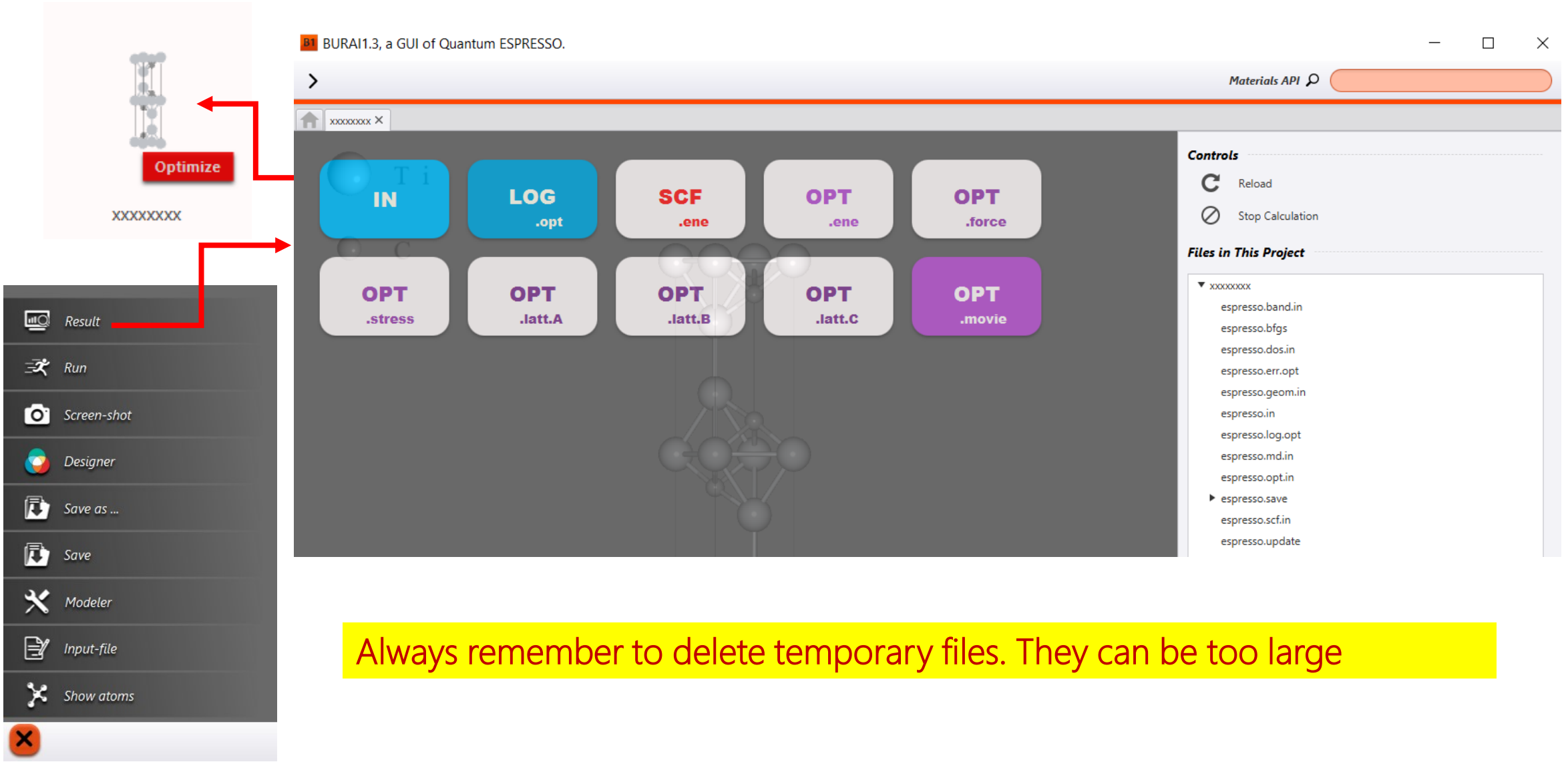




Quantum ESPRESSO: Input file generation & visualization (BURAI)



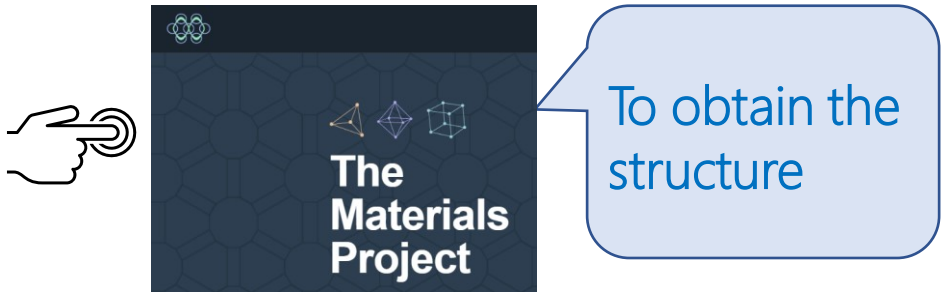
Quantum ESPRESSO: Input file generation & visualization (BURAI)



Always remember to delete temporary files. They can be too large

Input file generation & Running on CHPC

NB: This tutorial will use Ti3C2 Mxene for all examples given

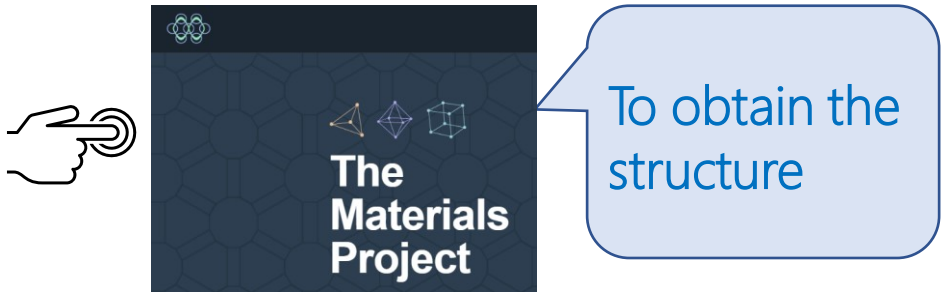


Run on own computer

- Then for scf, relax, vc-relax use the pw.x command.
- Open the input file using your favourite text editor, change calculation = 'scf' to 'relax' or 'vc-relax'.
- 'scf' does a single point calculation; 'relax' does atomic position relaxation, 'vc-relax' does full optimization.
- There are other type of calculations such as 'nscf', 'bands', etc.
- To run in serial, use pw.x< {inputfilename} > {outputfilename} &; with & calculation runs in the background
- To run in parallel use mpirun–np 2 pw.x< {inputfilename} > {outputfilename}; -np "Number of process" and the number can vary based on your computer.
- ps–a shows jobs running in the background.
- From the output file, the total energy can be read. The total energy is important to ensure structural minimization and calculation of other properties (to be discussed later).

Input file generation & Running on CHPC

NB: This tutorial will use Ti3C2 Mxene for all examples given



Running on CHPC

- ssh {username}@lengau.chpc.ac.za; where {username = studentXX, where XX = assigned number}
- cd to the /mnt/lustre/users/studentXX; calculations must be ran on /mnt/lustre
- To copy files from local computer to the chpc: scp–r
- We need a PBS submission script to run this calculation, generate one as follows
- Enter qesp_6.7 (tab key helps to autocomplete}. NOTE QE input file should end with {NAME}.in
- The project name is WCHPC
- Number of nodes 1, wall time 04:00
- Enter email address
- Calculation type PW
- Click y to submit and n to review file before submission
- Submitting job "qsub{filename}.pbs"
- Checking status of job "qstat–u $USER"
- Cancelling job "qdelJob ID number"