

INSTALLING QUANTUM ESPRESSO

MacOS Terminal

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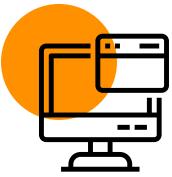
MacOS Terminal

Background

How is it different from other operating systems



Quantum Espresso



Installation

Packages

Steps

Errors



Sample Calculations

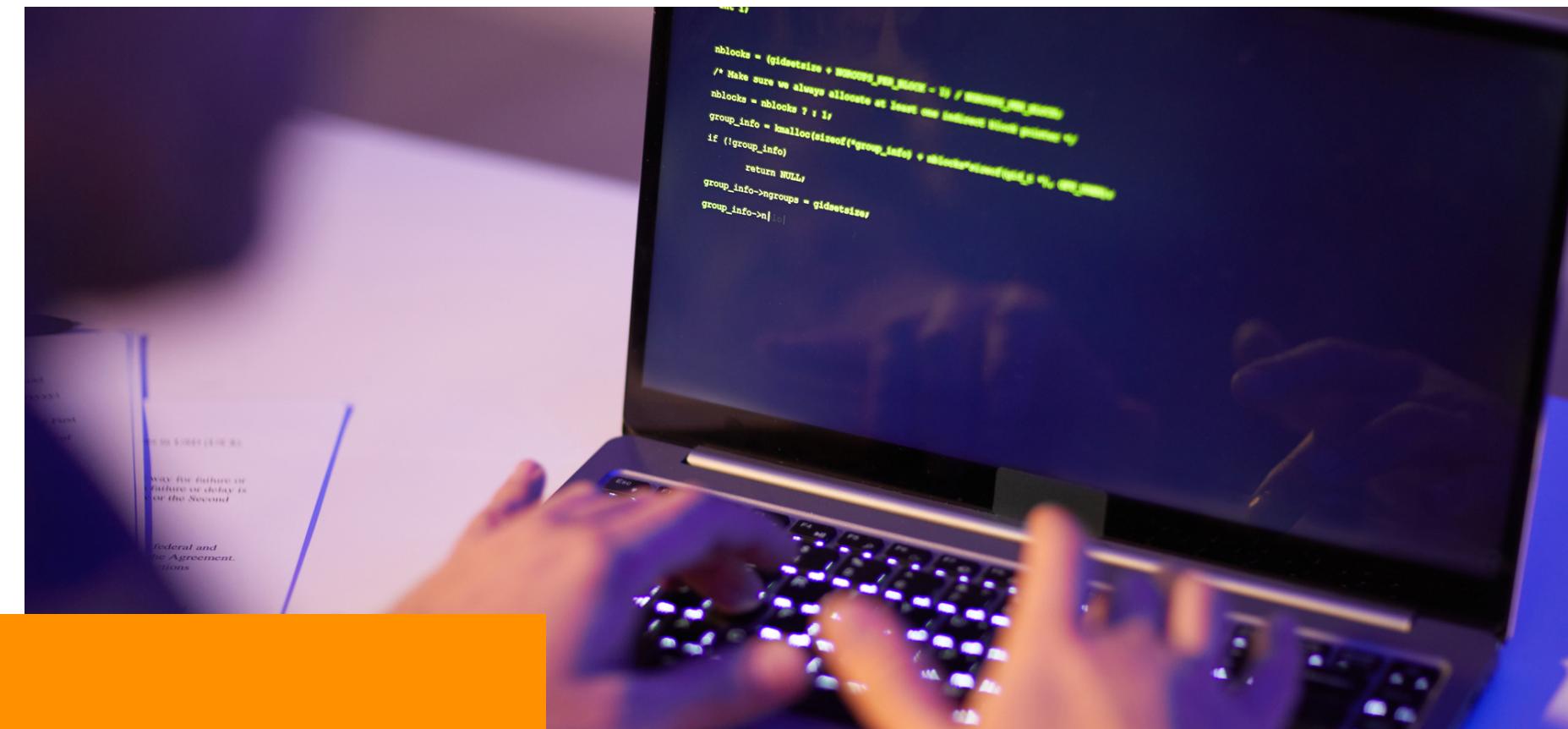


Table of Contents

About the MacOS Terminal

- Unix-based operating system
 - Web and database servers are Unix as well
 - MacOS X (2001): Darwin operating system (public source code)
- Usage of Z shell (zsh) as the command line interface
 - Bourne-again shell for older versions, same with Linux
 - Better configuration and features



*Direct installation of
Quantum Espresso*

Made for Unix systems (Linux and
MacOS)



Windows Counterpart

Usage of PowerShell, with the
Command Prompt as the
command line interface



More about **QUANTUM ESPRESSO**



A suite of open-source codes for electronic-structure calculations and materials modeling

- Density Functional Theory (DFT)
- Electronic structures and properties
- Molecular dynamics
- Stress and strain modeling
- Structure optimization



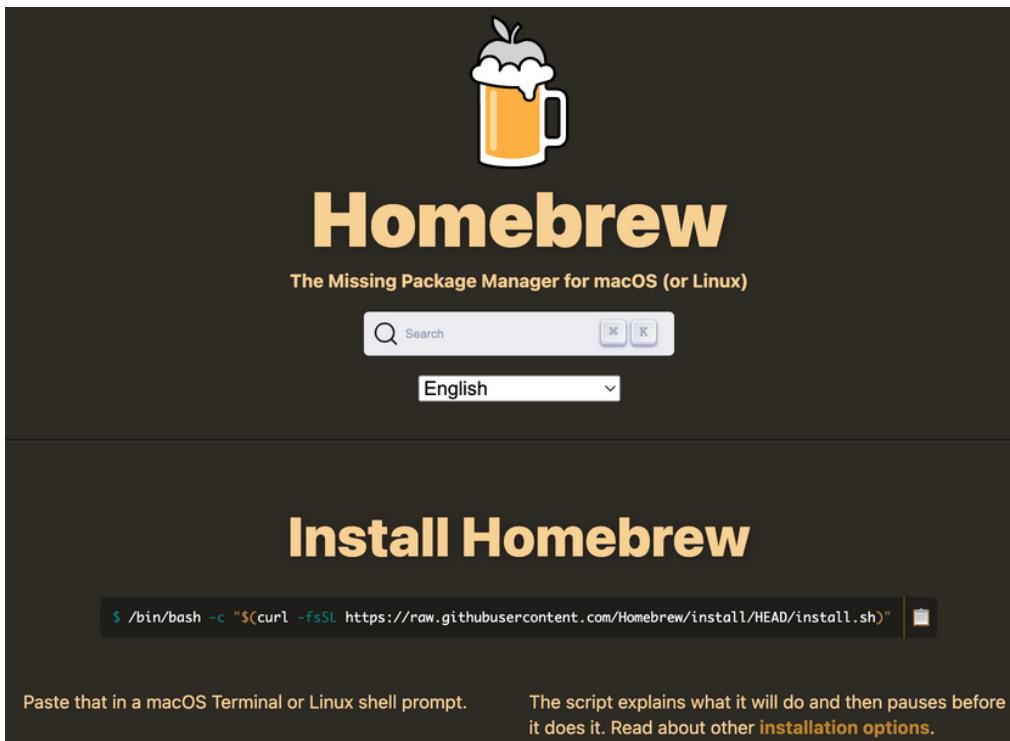
Written in Fortran, works in Unix environments
(bash, zsh)

A GUIDE FOR INSTALLATION (V7.2)

STEPS

PACKAGES

Installing the Homebrew package manager (brew.sh)



```
Clarissas-Air-2:~ clarissa$ /bin/bash -c "$(curl -fsSL https://raw.githubusercontent.com/Homebrew/install/HEAD/install.sh)"  
==> Checking for `sudo` access (which may request your password)...]  
Password:  
==> This script will install:  
/opt/homebrew/bin/brew  
/opt/homebrew/share/doc/homebrew  
/opt/homebrew/share/man/man1/brew.1  
/opt/homebrew/share/zsh/site-functions/_brew  
/opt/homebrew/etc/bash_completion.d/brew  
/opt/homebrew
```



brew commands

for installing compilers (brew install), updating packages (brew update), update all packages (brew upgrade)

Packages you need



GCC

- GNU Compiler Collection
- support for Fortran
- source code -> bytes

brew install gcc



OPEN-MPI

- Open Message Passing Interface
- for parallel computing

brew install open-mpi



FFTW3

- Fast Fourier Transform in the West
- basis sets, structures and properties calculations

brew install fftw



VECLIBFORT

- Fortran compatible version of VecLib
- Vector computations

brew install veclibfort

```
Clarissas-Air-2:~ clarissa$ brew install gcc open-mpi fftw3 veclibfort
Warning: No available formula with the name "fftw3". Did you mean fftw?
==> Searching for similarly named formulae and casks...
==> Formulae
fftw ✓

To install fftw ✓, run:
  brew install fftw ✓
Clarissas-Air-2:~ clarissa$ brew install gcc open-mpi fftw veclibfort
```

SOFTWARE

Full source code of QUANTUM ESPRESSO v7.2. Ready for compilation in all supported platforms. For more details and instructions see the release notes contained in the archive.

Quantum ESPRESSO V.7.2

<https://www.quantum-espresso.org>



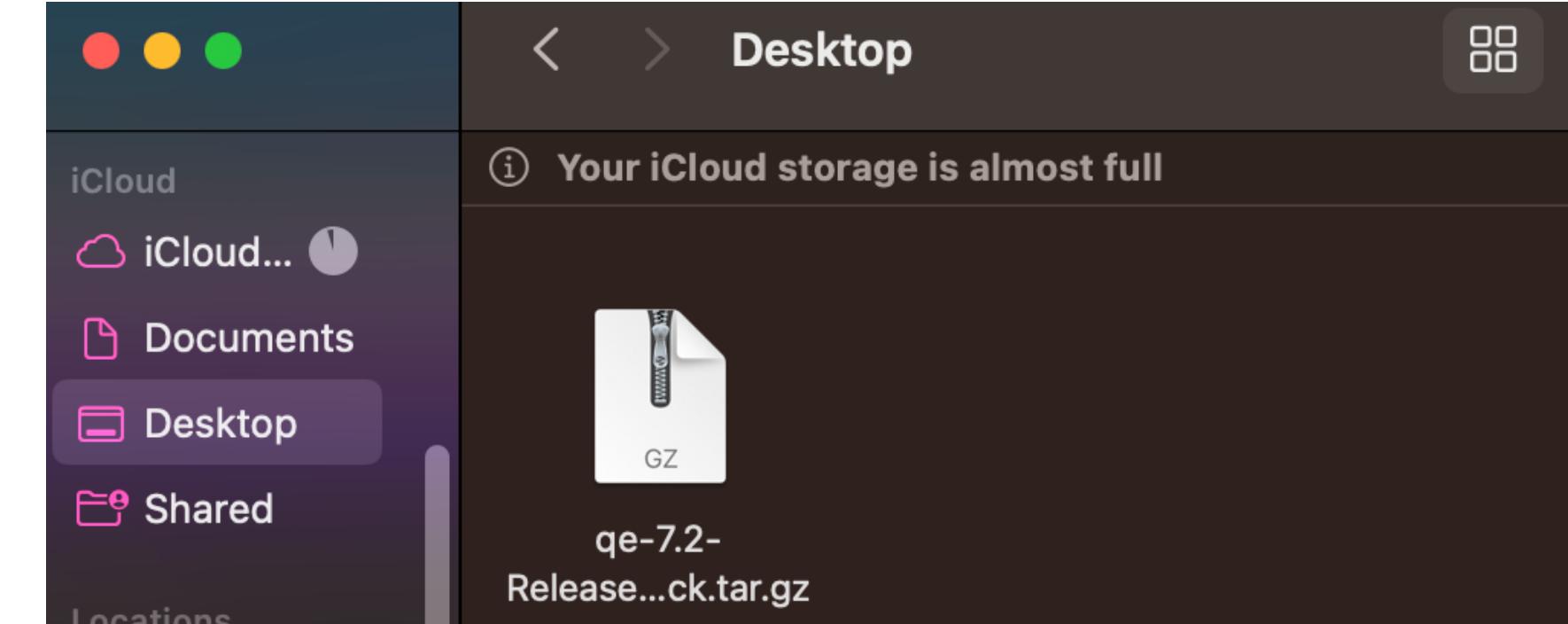
1. Access [quantum-espresso.org](https://www.quantum-espresso.org)
2. Under *Downloads*, register an account
3. Upon logging in, you can access the *Downloads* with a list of versions
4. After choosing a version, click the *Quantum ESPRESSO V.X.Y* button to download the tar.gz file

Downloading and extracting Quantum ESPRESSO from quantum-espresso.org

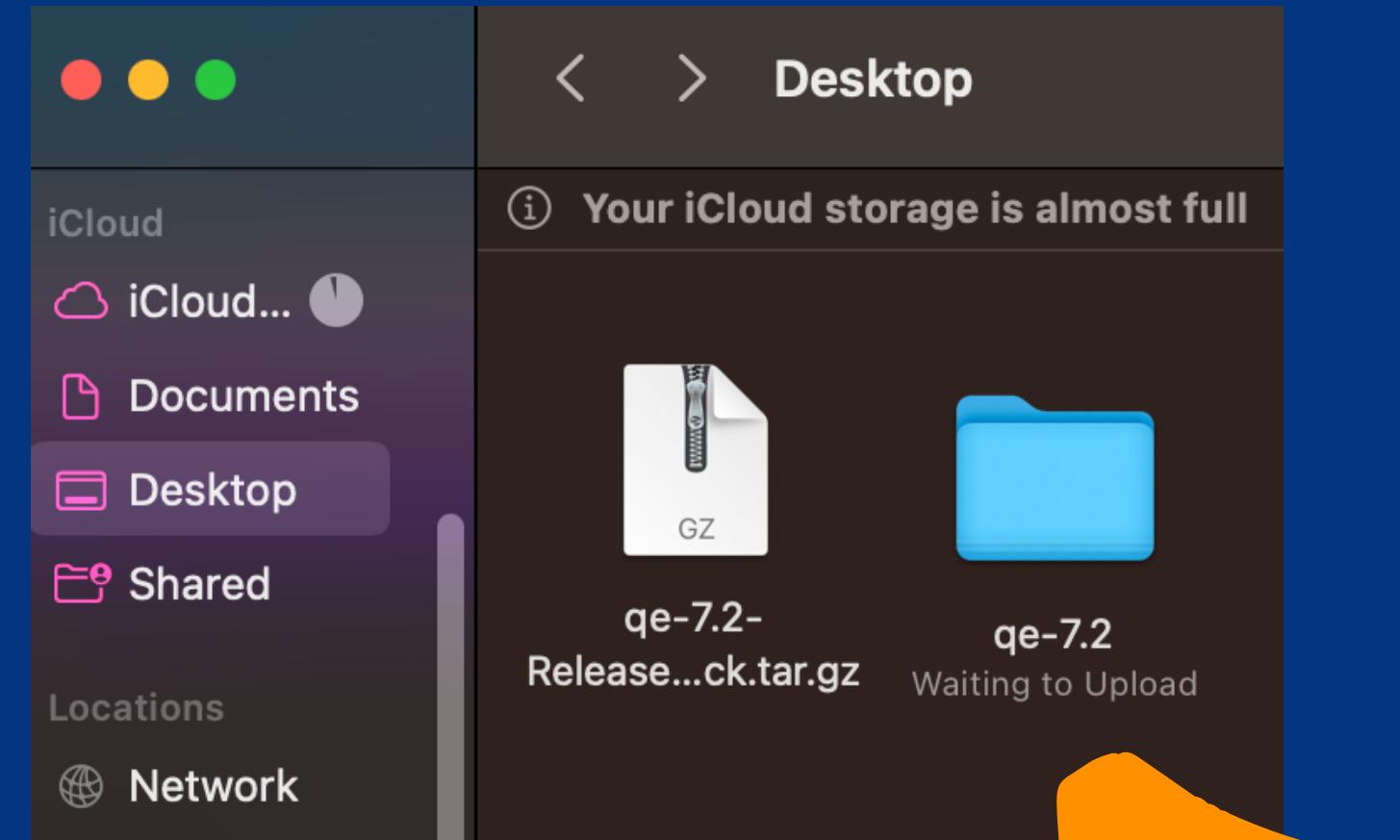


`tar -zxvf qe-7.2-ReleasePack.tar.gz`

tar.gz is a zipped file containing all the source code of Quantum ESPRESSO version 7.2. This would be extracted using tar -zxvf



```
[Clarissas-Air-2:~ clarissa$ cd Desktop  
[Clarissas-Air-2:Desktop clarissa$ tar -zxvf qe-7.2-ReleasePack.tar.gz
```



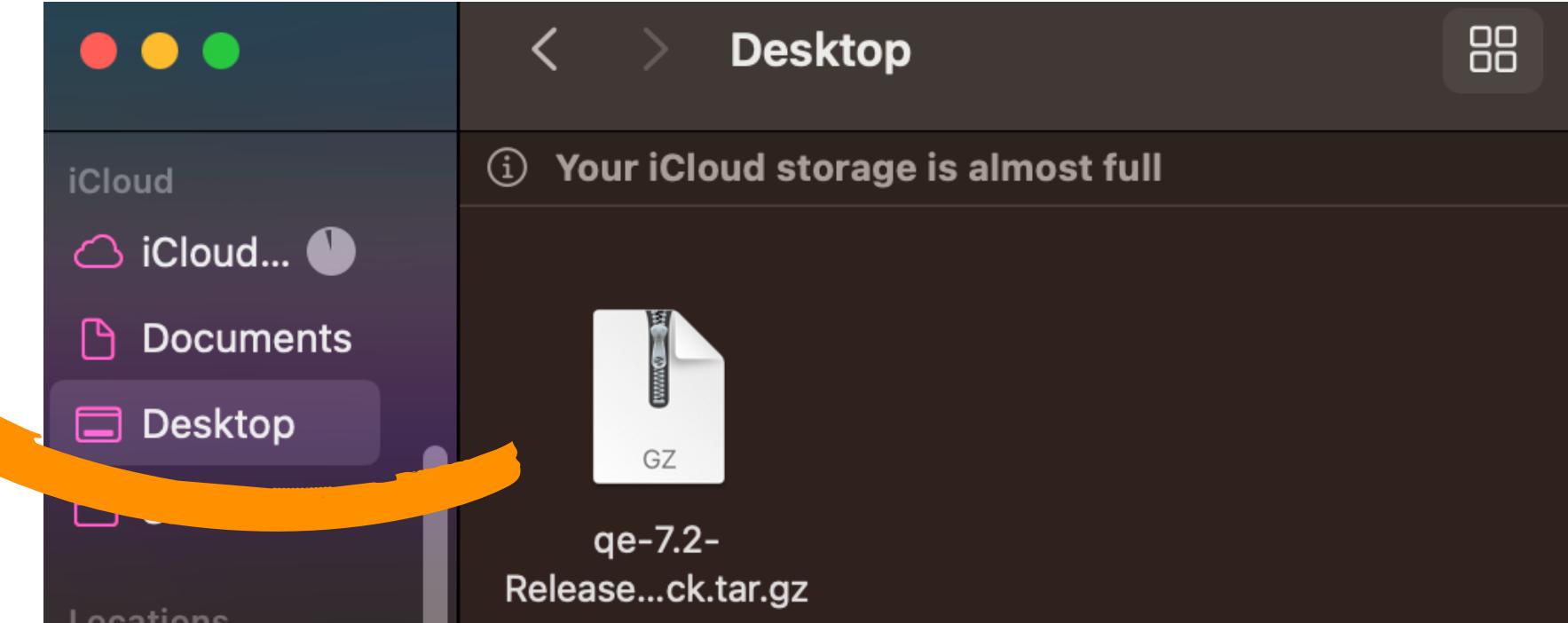
Success!

Downloading and extracting Quantum ESPRESSO from quantum-espresso.org



`tar -zxvf qe-7.2-ReleasePack.tar.gz`

tar.gz is a zipped file containing all the source code of Quantum ESPRESSO version 7.2. This would be extracted using `tar -zxvf`



```
[Clarissas-Air-2:~ clarissa$ cd Desktop  
[Clarissas-Air-2:Desktop clarissa$ tar -zxvf qe-7.2-ReleasePack.tar.gz
```

Configuring the QE directory

```
1 warning generated.  
clang: error: no input files  
make[1]: *** [laxlib.fh] Error 1  
make: *** [libla] Error 1
```

continuing without editing the make.inc file first will result to an error in the next step



`cd qe-7.2`

Go to the qe-7.2 directory



`./configure`

Configure (yields make.inc file)



`CPP = gcc -E`

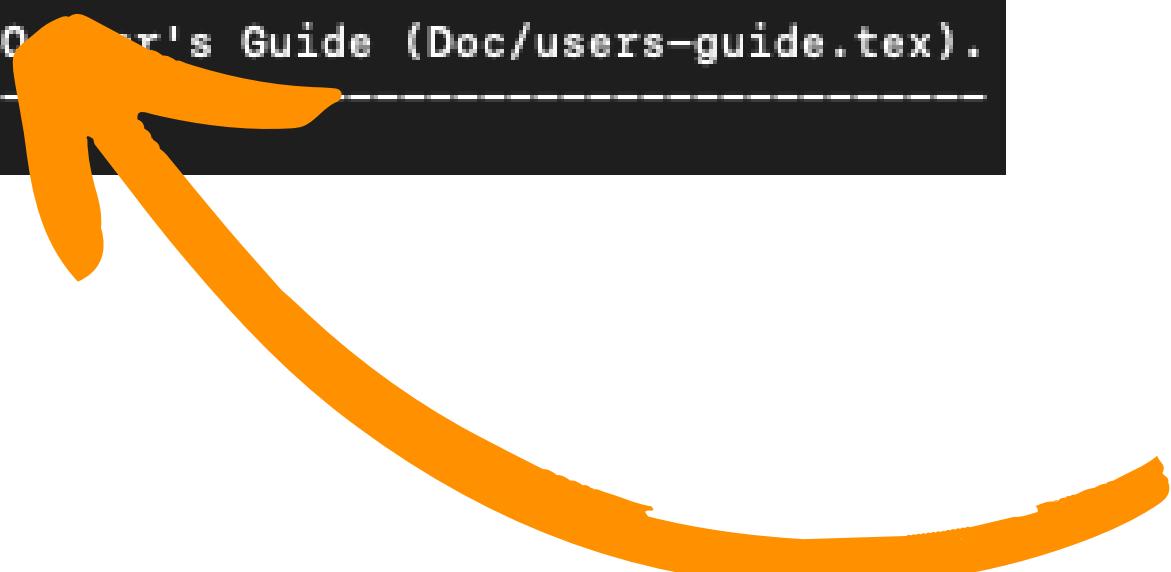
Resolve error: redefine CPP in make.inc as

```
CPP = gcc -E  
CPPFLAGS = -P -traditional -Uvector $(DFLAGS) $(IFLAGS)
```

Configuring the QE directory

```
Please check if this is what you expect.  
  
If any libraries are missing, you may specify a list of directories  
to search and retry, as follows:  
./configure LIBDIRS="list of directories, separated by spaces"  
  
Parallel environment detected successfully.\  
Configured for compilation of parallel executables.  
  
For more info, read the ESPRESSO User's Guide (Doc/users-guide.tex).  
--  
configure: success
```

Success!



cd qe-7.2

Go to the qe-7.2 directory



./configure

Configure (yields make.inc file)



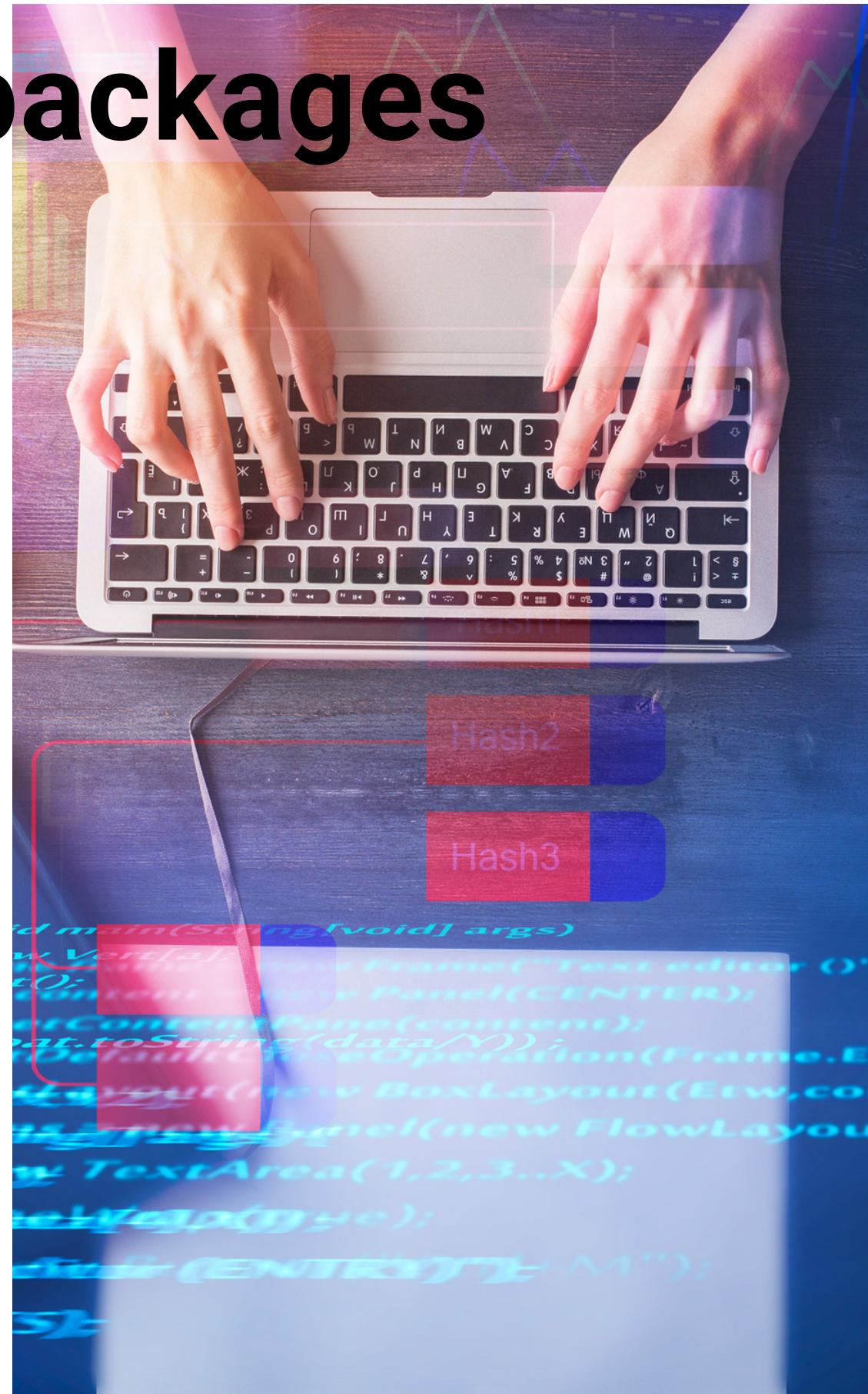
CPP = gcc -E

Resolve error: redefine CPP in make.inc as

```
qe-7.1 — vi make.inc — 99x60  
  
CPP = gcc -E  
CPPFLAGS = -P -traditional -Uvector $(DFLAGS) $(IFLAGS)
```

Compiling packages

- Compiling and creating executables needed to run calculations
- *cmake* instead of *make* could be used depending on the installed package
- to check if the compilation is successful, the *bin* folder should have executable file contents



make [-j N] pw

For compiling only the PWscf package



make [-j N] all

For compiling ALL packages. [-j N] executes the compilation in parallel for N processors. No need to add for series compilation

Compiling packages

- Compiling and creating executables needed to run calculations
- *cmake* instead of *make* could be used depending on the installed package
- to check if the compilation is successful, the *bin* folder should have executable file contents

```
[Clarissa-Air-2:qe-7.2 clarissa$ ls bin
alpha2f.x          gww_fit.x          ph.x           q2qstar.x
average.x          head.x            phcg.x         q2r.x
band_interpolation.x hp.x             plan_avg.x    rism1d.x
bands.x            ibrav2cell.x       plotband.x   scan_ibrav.x
bse_main.x          initial_state.x  plotproj.x   simple.x
cell2ibrav.x        kcw.x            plotrho.x   simple_bse.x
cp.x               kcwp_pp_interp.x pmw.x          simple_ip.x
cppp.x             kcwp_pp_sh.x    postahc.x   spectra_correction.x
d3hess.x           kpoints.x        pp.x          sumpdos.x
dist.x              lambda.x        ppacf.x      turbo_davidson.x
dos.x               ld1.x            pprism.x     turbo_eels.x
dvscf_q2r.x        manycp.x        projwfc.x   turbo_lanczos.x
dynmat.x            manypw.x        pw.x          turbo_magnon.x
epa.x               matdyn.x        pw2bgw.x    turbo_spectrum.x
epsilon.x           molecularnexafs.x pw2critic.x wannier90.x
ev.x                molecularpdos.x pw2gw.x     wannier_ham.x
fermi_proj..        neb.x            pw2wannier90.x wannier_plot.x
fermi_velocity.x    open_grid.x      pw4gww.x    wfck2r.x
fqha.x              oscdft_et.x    pwcond.x    wfdd.x
fs.x                oscdft_pp.x    pwgui        xspectra.x
gww.x              path_interpolation.x pwii2xsf.x
```



Testing for executables for verification



cd test suite

the test suite is a directory containing validation tests to check which packages are erroneous or missing



make run-tests

execute/run test suite

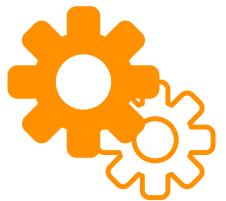
```
pw_workflow_vc-relax_dos - vc-relax-dos-1.in (arg(s): 1): Passed.  
pw_workflow_vc-relax_dos - vc-relax-dos-2.in (arg(s): 2): Passed.  
  
pw_workflow_vc-relax_scf - vc-relax-scf-1.in (arg(s): 1): Passed.  
pw_workflow_vc-relax_scf - vc-relax-scf-2.in (arg(s): 2): Passed.  
  
All done. ERROR: only 239 out of 244 tests passed (4 unknown).  
Failed test in:  
    /Users/clarissa/Desktop/qe-7.2/test-suite/pw_metaGGA/  
make: *** [run-tests-pw] Error 1  
  
pw_metaGGA - metaGGA-spin.in: **FAILED**.  
Different sets of data extracted from benchmark and test.  
    Data only in benchmark: n1, ef1, e1.
```



The expected output should yield "Passed" in the packages or executables being tested

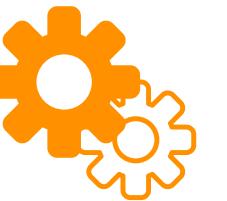
In cases that the packages yield error, the error message specifies missing dependencies or any incompatibilities

Some reminders...



ENVIRONMENT CONFLICTS

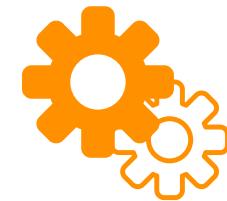
- Interfering with Anaconda environment
- QE installation may lead to errors



SETTING PATH

- Add QE to the PATH
- Allows QE to be executable from whichever directory

```
echo 'export PATH="/root/qe-7.2/bin:$PATH"' >> ~/.bashrc
```



COMPILERS

- You may select a parallel compiler (mpif90)
- Disable parallel and enable serial

```
./configure --disable-parallel  
./configure --enable-openmp
```

RUNNING SAMPLE CALCULATIONS

TROUBLESHOOTING

SCF



vi si.in

opening the text file named si.in that will then become the input file for the SCF calculation



Adding the contents of the input file

setting the type of calculation, material specifications, and other parameters

```
&control
    calculation = 'scf',
    prefix = 'si',
    pseudo_dir = '/Users/clarissa/Desktop/qe-7.2/pseudo/'
/
&system
    ibrav = 2,
    celldm(1) = 10.20,
    nat = 2,
    ntyp = 1,
    ecutwfc = 20.0,
/
&electrons
/
ATOMIC_SPECIES
Si 28.086 Si.pz-vbc.UPF
ATOMIC_POSITIONS (alat)
Si 0.00 0.00 0.00
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 0 0 0
```



Self consistent field calculation (SCF) for silicon



vi si.in

opening the text file named *si.in* that will then become the input file for the SCF calculation



Adding the contents of the input file

setting the type of calculation, material specifications, and other parameters

```
&control
    calculation = 'scf',
    prefix = 'si',
    pseudo_dir = '/Users/clarissa/Desktop/qe-7.2/pseudo/'
/
&system
    ibrav = 2,
    celldm(1) = 10.20,
    nat = 2,
    ntyp = 1,
    ecutwfc = 20.0,
/
&electrons
/
ATOMIC_SPECIES
Si 28.086 Si.pz-vbc.UPF
ATOMIC_POSITIONS (alat)
Si 0.00 0.00 0.00
Si 0.25 0.25 0.25
K_POINTS (automatic)
6 6 6 0 0 0
```



&control: type of calculation and location of the pseudopotential file
(also used to set the output file location through *outdir* and filename through *prefix*)

&system: lattice and structure parameters

&electrons: adjust iterations, factors, and thresholds involving electron calculations

ATOMIC_SPECIES: material or atomic species involved, addition of pseudopotential file

ATOMIC_POSITIONS: coordinates of elements and atoms

K_POINTS: grid and shift for sampling (through Monkhorst–Pack method)



pw.x -inp si.in > si.out

running the executable file (pw.x)

```
Clarissas-Air-2:Sample clarissa$ pw.x -inp si.in> si.out
Note: The following floating-point exceptions are signalling: IEEE_INVALID_FLAG IEEE
_DIVIDE_BY_ZERO IEEE_OVERFLOW_FLAG IEEE_UNDERFLOW_FLAG
```



cat si.in

viewing the contents of the output file

```
Clarissas-Air-2:Sample clarissa$ cat si.out

Program PWSCF v.7.2 starts on 5Jun2023 at 2:38: 4

This program is part of the open-source Quantum ESPRESSO suite
for quantum simulation of materials; please cite
  "P. Giannozzi et al., J. Phys.:Condens. Matter 21 395502 (2009);"
  "P. Giannozzi et al., J. Phys.:Condens. Matter 29 465901 (2017);"
  "P. Giannozzi et al., J. Chem. Phys. 152 154105 (2020);"
  URL http://www.quantum-espresso.org",
in publications or presentations arising from this work. More details at
http://www.quantum-espresso.org/quote

Parallel version (MPI), running on 1 processors

MPI processes distributed on 1 nodes
0 MiB available memory on the printing compute node when the environment starts

Reading input from si.in

Current dimensions of program PWSCF are:
Max number of different atomic species (ntypx) = 10
Max number of k-points (nkp) = 40000
Max angular momentum in pseudopotentials (lmaxx) = 4
```



Self consistent field calculation (SCF) for silicon



Errors encountered

In this case, the input text file had erroneous contents (curly quotation marks should be replaced with normal quotation marks, ‘ vs. ’)

MPI_ABORT was invoked on rank 0 in communicator **MPI_COMM_WORLD** with errorcode 1.

NOTE: invoking **MPI_ABORT** causes Open MPI to kill all MPI processes. You may or may not see output from other processes, depending on exactly when Open MPI kills them.



Resources for checking errors

Aside from Stack Overflow and mail-archive.com, one could also use ChatGPT (responsibly) for checking errors. Here is a sample prompt:

A what is wrong with these lines from my input file
&control

```
calculation = 'scf',
prefix = 'si',
pseudo_dir = '/Users/clarissa/Desktop/qe-7.2/pseudo/'
```

The issue with the lines you provided from your input file is the incorrect quotation marks used in the `pseudo_dir` parameter. In the original lines you shared:

```
bash Copy code
&control
  calculation = 'scf',
  prefix = 'si',
  pseudo_dir = '/Users/clarissa/Desktop/qe-7.2/pseudo/'
```



Self consistent field calculation (SCF) for silicon



grep -e 'total energy' -e estimate si.out

finding lines within the output file that satisfies "total energy," or "estimate." This can be used to find how convergence is reached



grep -e level si.out

It is expected to find the highest occupied level and lowest unoccupied level, then use the results to find the band gap (difference)

```
Clarissas-Air-2:Sample clarissa$ grep -e level si.out
      highest occupied level (ev):      6.2545
```

```
Clarissas-Air-2:Sample clarissa$ grep -e 'total energy' -e estimate si.out
      total energy          =      -15.84226998 Ry
      estimated scf accuracy <       0.06188135 Ry
      total energy          =      -15.84543004 Ry
      estimated scf accuracy <       0.00224652 Ry
      total energy          =      -15.84586291 Ry
      estimated scf accuracy <       0.00006963 Ry
      total energy          =      -15.84588489 Ry
      estimated scf accuracy <       0.00000159 Ry
      total energy          =      -15.84588635 Ry
      estimated scf accuracy <       0.00000018 Ry
The total energy is the sum of the following terms:
```



Self consistent field calculation (SCF) for silicon

References

- Behery, A. (2022, December 13). Linux Shells Explained. FreeCodeCamp. <https://www.freecodecamp.org/news/linux-shells-explained/>
- Andrade, F. (2022, August 29). Is a Mac or Windows PC Better for Programming? GeekCulture. <https://medium.com/geekculture/is-a-mac-or-windows-pc-better-for-programming-d5556bf06f1>
- Trent, M., & McCormack, D. (2005). Beginning Mac OS® X Programming. Wrox
- Giannozzi, P., et al. (2009). Quantum ESPRESSO: a modular and open-source software project for quantum simulations of materials. *Journal of Physics: Condensed Matter*, 21(39), 395502. DOI: 10.1088/0953-8984/21/39/395502
- Quantum ESPRESSO. (2022). Quantum ESPRESSO User Guide (v.7.0.). Quantum ESPRESSO. https://www.quantum-espresso.org/wp-content/uploads/2022/03/user_guide.pdf
- Homebrew. (n.d.). Homebrew Formulae. <https://formulae.brew.sh/>
- Quantum ESPRESSO. (n.d.). Pseudopotentials. Quantum ESPRESSO. <https://www.quantum-espresso.org/pseudopotentials/>
- QuantumNerd. (2019, June 23). Quantum Espresso Tutorial 2019: 5. How to run / input file [Video]. YouTube. <https://www.youtube.com/watch?v=mQ1D3tXWqD4>
- Materials Square. (2019, January 1). Convergence Test: K-Points Optimization for Silicon Bulk. Materials Square. <https://www.materialssquare.com/blog/2-convergence-test-k-points-optimization-for-silicon-bulk-2#:~:text=In%20Quantum%20Espresso%2C%20selecting%20the,point%20mesh%20of%20each%20axis>
- Das, P. (n.d.). Self consistent field calculation for silicon. GitHub Pages. <https://pranabdias.github.io/espresso/hands-on/scf>