

HOMEWORK 9 ADDITIONAL INFORMATION

Compiling Quantum Espresso and Phon in Windows

1. Cygwin

- Download Cygwin, a unix-like environment for windows: www.cygwin.com
- Run the setup.exe for Cygwin
- Click install from internet, and make the root directory c:\cygwin
- Select any directory to store packages
- Select a server to download the package list
- Go to Devel and make sure not to skip the gcc C compiler, and the gcc fortran compiler (you might also want to include the c++ compiler for future use)
- Also in Devel, make sure to include gdb: the GNU Debugger and make
- Go into Math, and include **LAPACK (this is very important, do not forget it)**
- Click next to install cygwin with all the selected packages mentioned
- When installation is complete, there will be a folder c:\cygwin which is the root directory for cygwin.

2. G95 compiler

- Download the g95 compiler for Cygwin here: <http://ftp.g95.org/g95-x86-cygwin.tgz> and install to the root cygwin directory
- In cygwin, go to the directory with the g95 compiler and install it by typing: -
xvzf g95-x86-cygwin.tgz

3. Quantum Espresso

- Now, download the quantum espresso package from <http://www.pwscf.org/downloads/PWversion/4.0.4/espresso-4.0.4.tar.gz> and put it into its own folder (I put it in C:\Cygwin\home\Shai\espresso\)
- Unarchive the files by going into cygwin, navigating to the espresso directory, and typing:

```
tar -xvf espresso-4.0.1.tar.gz
```

- Now type:

```
cd espresso-4.0.1
```

in order to change directories to where the code for quantum espresso is

- Type this to make sure you have all the compilers set up:

```
configure
```

- If you are ready with all the compilers (you should be) than you will see it says successful.
- To compile the package type

```
make all
```

- After some time, if there are no errors, you will have all of the executables in the the folder called /bin/

4. Phon program

- Download the Phon package from <http://chianti.geol.ucl.ac.uk/~dario/phon.1.19.tar.Z> and save it in its own folder (I put it in C:\Cygwin\home\Shai\PHON\)
- Unarchive Phon

- c. In the /src/ folder, you will see a file called makefile.g95. Open this file to edit it.
- d. Delete the line that starts with LIB= (it is only needed for MAC OS)
- e. Where that line was put in this line to link to the BLAS and LAPACK libraries:

```
LIB = $LC:/cygwin/lib/lapack/cygblas.dll  
LC:/cygwin/lib/lapack/cyglapack.dll
```
- f. Save makefile.g95
- g. In cygwin, go to the /src/ folder. Type this to change the name of the file:
- h. `mv makefile.g95 makefile`
- i. type this to compile

```
make
```
- j. if everything was done right, there will be a file called phon which is the executable for the linear displacement method