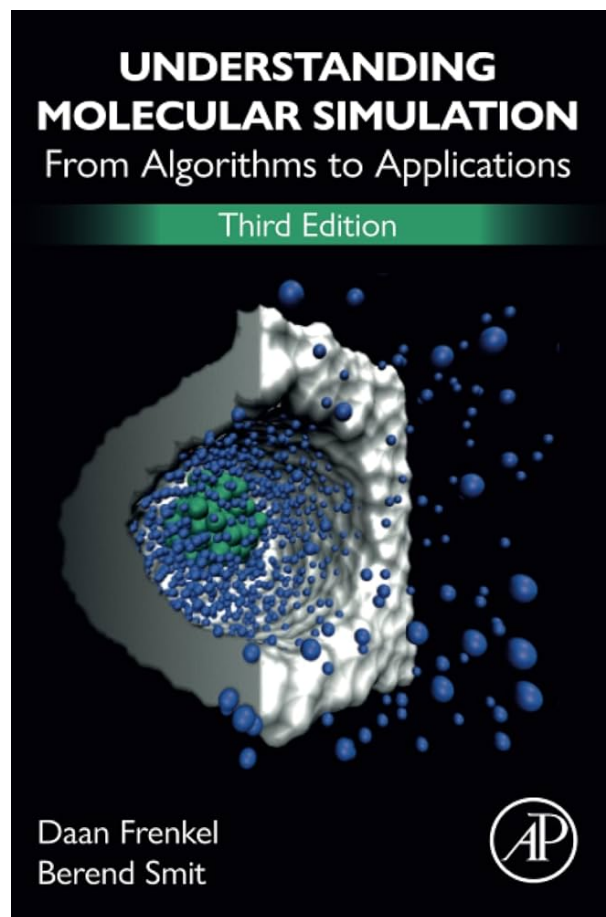




CH-420

UNDERSTANDING ADVANCED  
MOLECULAR SIMULATION



BLOCK 0 - SOLUTION  
COMPUTATIONAL CARPENTRY

# 1 The Terminal

1. Download the directory "Block\_0" on Moodle
2. `$ mv Block_0 Block_0_EM`
3. `$ cp -r Block_0_EM`
4. `$ rm -r Block_0_EM`
5. `$ cd Block_0_EM` then `$ ls`
6. `$ mkdir Exercise_1`
7. `$ cd Exercise_1` then `$ pwd`
8. `$ vi Exercise_1.sh` then `$ shift wq!` to save it
9. `$ vi Exercise_1.sh` then write the following lines:  

```
#!/bin/bash  
echo "Elias Moubarak"
```

then give permission for running `$ chmod u+x Exercise_1.sh` Finally, run it `$ ./Exercise_1.sh`

# 2 Plot with Matplotlib

The data file is "exercise\_2.dat" and the code is in "plot\_script.ipynb"

# 3 Programming in C

1. Create a .c file then write/modify the code
2. Create the executable "run" by compiling the code: `$ gcc -o run filename.c`
3. In the third part, including math.h brings in the declaration of the various functions and not their definition. The definition is present in the math library libm.a. You need to link your program with this library so that the calls to functions like pow() are resolved: `$ gcc -o run filename.c -lm`
4. Run the executable: `$ ./run`

The solutions are in the codes: part1.c, part2.c and part3.c. "numbers.dat" is the accompanying data file and "plotscript.ipynb" is the plotting script.