



Laboratory Session

PHYS3061 INTRODUCTION TO COMPUTER SIMULATIONS OF
PHYSICAL SYSTEMS

LAB 0

SPRING 2022

Lab 0 outline

- ▶ Lab assessment information
- ▶ Useful tips for programming
- ▶ Guides for useful tools
- ▶ Two small tasks:
 - VMD .xyz file
 - Implement small functions on dot and cross product by code
- ▶ “submit” function to submit your labs

Assessment Scheme

Late submission policy for programming assignment

- -1% of that lab per day for first 7 days
- -2% of that lab per day 7 days afterwards
- Capped at 20%

Accepted Programming Language

Programming Language	Who to ask for language specific problems? E. g. How can I do ... in ... I cannot compile the code, it says
C/C++	WANG Shengyuan, ZHAO Wenjing, Reo SZE, XI Bin,
Python	Reo SZE, XI Bin
Julia (limited help)	ZHAO Wenjing

Making Correction

Feedback send to course email

- ▶ set email forward if you don't check frequently
- ▶ submit to labX_corrected (e.g. lab1_corrected)
 - ▶ Half of the grade will be returned if you correct your mistakes
 - ▶ Please include the amendment description
- ▶ Two tutorials: one after lab2 and one after lab4

*We strongly recommend you to **fix your code**. Broken code **WILL** affect program correctness of later Labs.*

Designing and Debugging

- ▶ **Design** carefully and preferably with flow charts.
- ▶ **Write short functions or methods** when programming. Specify the input, output and purpose of the function.
- ▶ **Test function** by function and **print** out important variables regularly.
- ▶ **Test with simple cases**, gradually add new functionalities and test sophisticated cases.



The Practical Aspect

How to edit your code?

It will definitely help you in finding bugs and save some typing.

Visual Studio for windows: <https://visualstudio.microsoft.com/zh-hans/>

Xcode for Mac: In Apple Store (find old versions: <https://xcodereleases.com/>)

For C/C++

Pycharm/Jupyter Notebook

- ▶ For Python

Simple editor: Nano/vim

- ▶ Provided on own server.

Useful Files

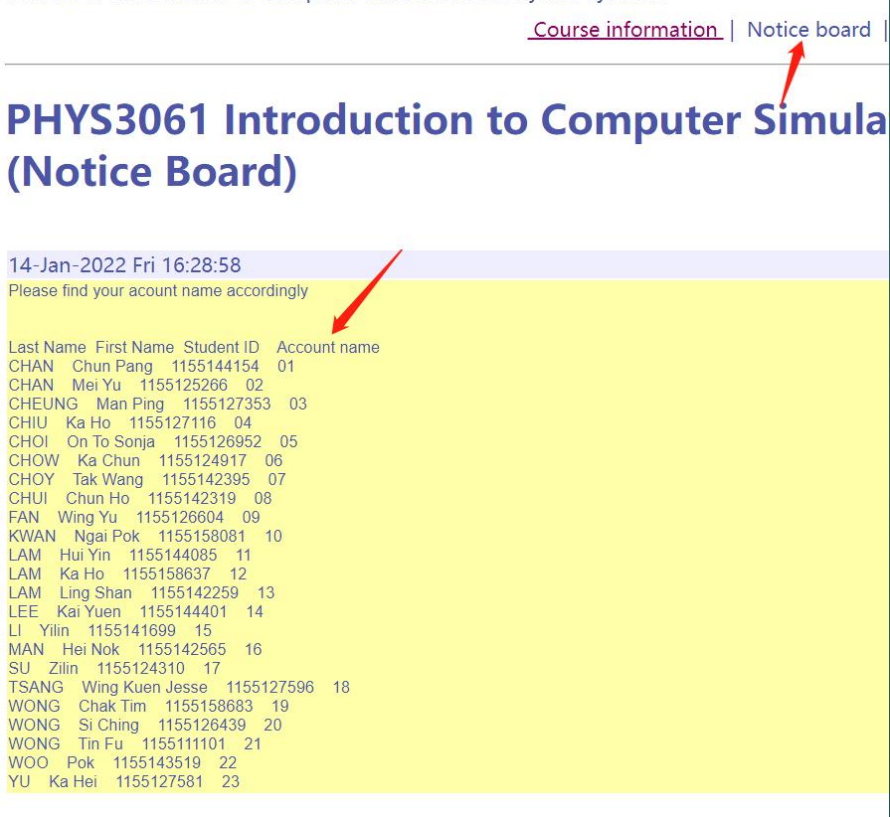
Login, submit your labs, change your password



Programming Tutorial and References	
• access_dept_srv_guide.pdf	
• C & C++ IDE	
• Unix command cheat sheet	
• Example for read and write files(C).	
• Sample code of passing and returning array_(C).	
• Sample code of passing array_(C++).	
• Animation Example for vmd	
• Example for read and write files(C++).	

For your account

► Please check the list here



[Course information](#) | [Notice board](#)

PHYS3061 Introduction to Computer Simula (Notice Board)

14-Jan-2022 Fri 16:28:58

Please find your account name accordingly

Last Name	First Name	Student ID	Account name
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CHAN	Mei Yu	1155125266	02
CHEUNG	Man Ping	1155127353	03
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CHOW	Ka Chun	1155124917	06
CHOY	Tak Wang	1155142395	07
CHUI	Chun Ho	1155142319	08
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KWAN	Ngai Pok	1155158081	10
LAM	Hui Yin	1155144085	11
LAM	Ka Ho	1155158637	12
LAM	Ling Shan	1155142259	13
LEE	Kai Yuen	1155144401	14
LI	Yilin	1155141699	15
MAN	Hei Nok	1155142565	16
SU	Zilin	1155124310	17
TSANG	Wing Kuen Jesse	1155127596	18
WONG	Chak Tim	1155158683	19
WONG	Si Ching	1155126439	20
WONG	Tin Fu	1155111101	21
WOO	Pok	1155143519	22
YU	Ka Hei	1155127581	23

Log in your account

- ▶ To login your account: (See *access_dept_srv_guide.pdf* Sec. 1 for more detail)
 - ▶ Follow the instruction on the guide
 - ▶ ID: 3061-YY@intelXX.phy.cuhk.edu.hk (YY=01~60, please find your account name, XX=17~50, but some are broken, try another)
 - ▶ Password: **compsim2022**
- ▶ Windows can use the mobaXterm
<https://mobaxterm.mobatek.net/download.html>
- ▶ Mac can use the Terminal.
- ▶ Command: ssh



```
Last login: Sat Jan 16 13:05:10 on ttys000
iksbaddeMacBook-Pro:~ iksbad$ ssh 3061-01@intel17.phy.cuhk.edu.hk
```

For your account

- **Change your password via this instruction.** (See *access_dept_srv_guide.pdf* Sec. 4 for more detail)

WELCOME TO UNIX NETWORK OF PHYSICS DEPARTMENT

Welcome! This is the first time you login this account. We suggest you to change your password before you use this account. You can change password via our webmail system :

1. Goto <http://webmail.phy.cuhk.edu.hk/>
2. Login your account
3. Click the [Change Password] Icon

UNIX Enquiry : Mr.Jason Chan (Rm348, mwchan@phy.cuhk.edu.hk, Ext6308)

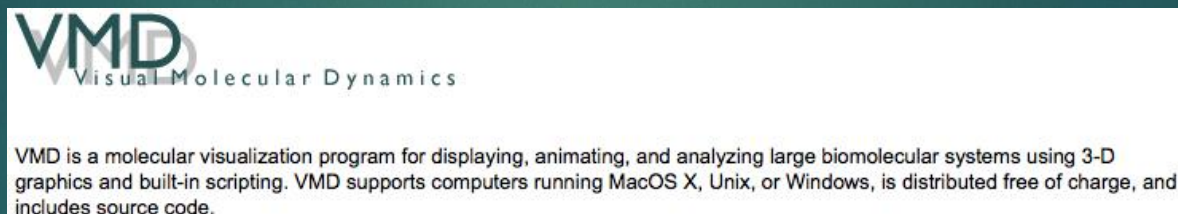
How to compile

- ▶ C: `gcc -o compiledfile targetfile`
- ▶ C++: `g++ -o compiledfile targetfile`
- ▶ Python: `python targetfile.py`

Visualization Tool: VMD



We require using VMD to display your results



Download:

<http://www.ks.uiuc.edu/Research/vmd/>

Verified for both Windows and Mac, but choose the version according to your own computer.

Export Static Results



In .XYZ format

<number of atoms>

comment line

atom_symbol11 x₁ y₁ z₁

atom_symbol12 x₂ y₂ z₂

...

atom_symbol1n x_n y_n z_n

An example:

3

Example for Argon (in angstrom)

Ar 0.00000 0.00000 3.33333

Ar 1.11111 0.00000 0.00000

Ar 0.00000 -2.22222 0.00000

Description on Wiki is useful:

https://en.wikipedia.org/wiki/XYZ_file_format

Export Animation

Repeat the static block
for animation

- Atom number, atom type do not need to be conserved

3

Example for Argon (in angstrom) frame 1

Ar 0.00000 0.00000 3.33333

Ar 1.11111 0.00000 0.00000

Ar 0.00000 -2.22222 0.00000

3

Here are coordinates for frame 2

Ar 2.22222 0.00000 0.00000

Ar 0.00000 0.00000 0.00000

Ar 0.00000 0.00000 1.00000

3

Here are coordinates for frame 3

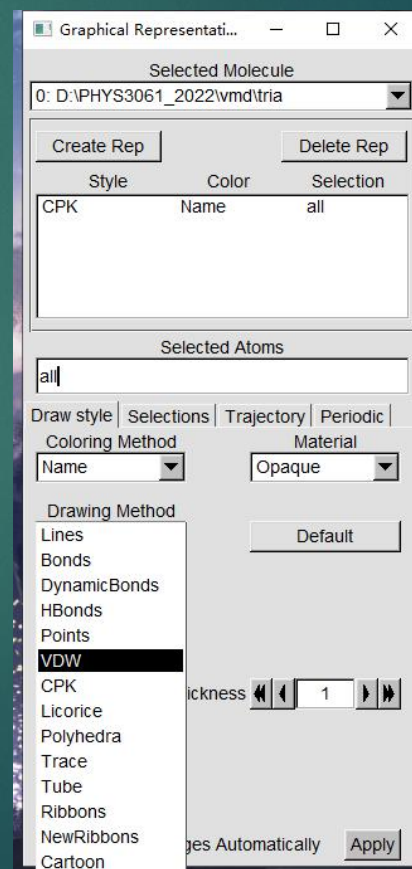
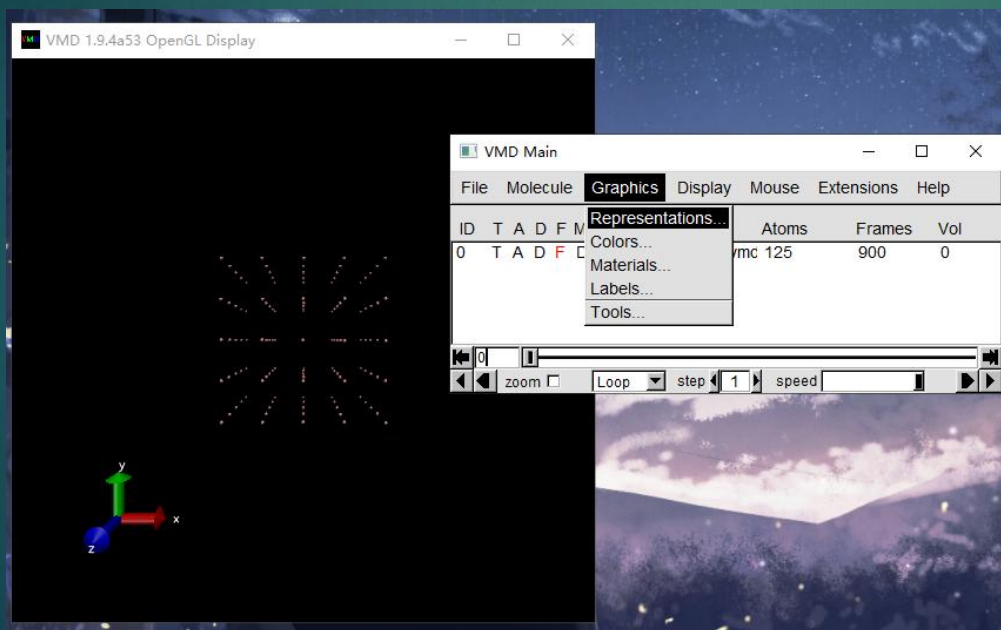
...

- An animation example has been provided for you to visualize in VMD
open *AnimationExample.xyz* in VMD and play with it

Set Representation of your animation

Graphics->Representation->Drawing Method->VDW or CPK

- ▶ **VDW (van der Waals)**: Each atom is now represented by a sphere
- ▶ **CPK**: a combination of both 'Bonds' and 'VDW' in that it draws the atoms as spheres and the bonds as cylinders, smaller spheres than **VDW**



Assignment submission

1. Source code, data file, description

- ▶ Data file must be in proper, readable format, usually in .txt and .xyz
- ▶ Group files and submit through unix “submit” (See [access_dept_srv_guide.pdf](#) Sec. 3 for more detail)
- ▶ Size of E-mail <10 MB. You may use cloud or website to show the cartoon or data files.
- ▶ A brief description of the simulation results **is required** for each lab.
- ▶ Write sufficient comments and clear variable and function names.
- ▶ If you submit files with the same name more than once, only the last one is kept

2. Report (only for lab1 and term-long project)

- ▶ In .pdf, .docx or .doc format
- ▶ Submit on the system.

Pass Array

```
#include<iostream>
#include<string>

using namespace std;

// pass by pointer
void myPrint01(int arr[], int lenArray) {
    cout << "Method 1 " << endl;

    for (int i = 0; i < lenArray; i++) {
        cout << arr[i] << endl; // print out each array element
    }
}

// pass by pointer
void myPrint02(int* arr, int lenArray) {
    cout << "Method 2 " << endl;

    for (int i = 0; i < lenArray; i++) {
        cout << *(arr++) << endl; // print out each array element by pointer
    }
}

void test01() {
    int arr01[5] = { 1,2,3,4,5 };
    int lenArray = 5;

    int* p;
    p = arr01;
    myPrint01(p, lenArray);
    myPrint02(p, lenArray);
}

void main() {
    test01();
}
```

arr01 is the address of the array as well as the address of the first element of the array

Global variables and constants define

```
#include<iostream>
#include<string>

#define PI 3.1415926 // define a constant before compile, can be visited everywhere in this script

using namespace std;

// Two global variables that will be visited everywhere in this script
int para_A = 100;
int Array[3] = { 1,2,3 };

void test() {
    cout << "para_A is " << para_A << endl;

    cout << "Array has elements: " << endl;
    for (int i = 0; i < 3; i++) {
        cout << Array[i] << endl;
    }

    cout << "2PI is " << 2 * PI << endl;
}

void main(){
    test();
}
```


How to read or write a file in C

```
#include <stdio.h>

int main()
{
    FILE *fp = NULL;

    // "w" means write at the beginning of the code, "a" means write at the end of the code
    fp = fopen("/tmp/test.txt", "w");
    fprintf(fp, "This is testing for fprintf...\n");
    fputs("This is testing for fputs...\n", fp);
    fclose(fp);
}
```

Write

```
#include <stdio.h>

int main()
{
    FILE *fp = NULL;
    char buff[255];

    fp = fopen("/tmp/test.txt", "r"); // "r" means read the file
    fscanf(fp, "%s", buff);          // will stop when meet "space bar"
    printf("1: %s\n", buff);

    fgets(buff, 255, (FILE*)fp);     // will read a message with length of 255, till \n
    printf("2: %s\n", buff);

    fgets(buff, 255, (FILE*)fp);     // will read a message with length of 255, till \n
    printf("3: %s\n", buff);
    fclose(fp);
}

/*
(The result should be)
1: This
2: is testing for fprintf...
3: This is testing for fputs...
*/
```

Read

How to read or write a file in C++

```
#include<iostream>
#include<string>
#include<fstream>

using namespace std;

int main()
{
    // *****write*****

    //ofstream OutFile;          //choose a file

    //OutFile.open("Test1.xlsx");    //creat and open

    ofstream OutFile("Test.txt"); // creat and open, and set this file name OutFile in code

    OutFile << "Welcome to PHYS3061 Lab session!"; //write content

    OutFile.close();              //close Test.txt

    // *****read*****

    ifstream readFile("Test.txt");

    char temp[1024] = { 0 };

    //readFile >> temp;           //will stop when meet "space bar"

    readFile.getline(temp,1024); //will read a message with length of 1024, till \n

    cout << temp << endl;        // ouput the content

    readFile.close();            // close Test.txt

    system("PAUSE");
    return 0;
}
```

D:\PHYS3061_2022\3061test\testArray\x64\Debug\testArray.exe

Welcome to PHYS3061 Lab session!
请按任意键继续. . .

Task 1: Generating XYZ File

- ▶ Write a program to generate an XYZ file
- ▶ Requirement
 - ▶ Animated
 - ▶ .xyz file is properly formatted
- ▶ The atoms and coordinates are not important
- ▶ Use loop to write files.

How to upload the files to server

- ▶ Use `scp` command.
 - ▶ *Secure copy protocol*
 - ▶ Suppose you want to upload *files_to_be_uploaded* from your own PC to department server:
 - ▶ command: `scp files_to_be_uploaded 3061-01@intel17.phy.cuhk.edu.hk:~/test/`

```
(base)
binxi@LAPTOP-PGG84KRK MINGW64 ~/demo_scp
$ ls
files_to_be_uploaded
(base)
binxi@LAPTOP-PGG84KRK MINGW64 ~/demo_scp
$ pwd
/c/Users/binxi/demo_scp
(base)
binxi@LAPTOP-PGG84KRK MINGW64 ~/demo_scp
$ scp files_to_be_uploaded 3061-01@intel17.phy.cuhk.edu.hk:~/test/
3061-01@intel17.phy.cuhk.edu.hk's password: 
```

Annotations:

- user**: points to `binxi`
- machine**: points to `LAPTOP-PGG84KRK`
- path**: points to `~/demo_scp`
- file name**: points to `files_to_be_uploaded`
- file**: points to `files_to_be_uploaded` in the `scp` command
- username**: points to `3061-01` in the `scp` command
- hostname**: points to `intel17.phy.cuhk.edu.hk` in the `scp` command
- target position**: points to `~/test/` in the `scp` command

How to download files from server

► Use scp command. (Cont'd)

- Suppose you want to download *file_to_be_downloaded* from department sever to your own PC:
- command: `scp 3061-01@intel17.phy.cuhk.edu.hk:~/test/file_to_be_downloaded .`

```
binxi@LAPTOP-PGG84KRRK MINGW64 ~/demo_scp
$ ls
files_to_be_uploaded
(base)
binxi@LAPTOP-PGG84KRRK MINGW64 ~/demo_scp
$ scp 3061-01@intel17.phy.cuhk.edu.hk:~/test/file_to_be_downloaded .
3061-01@intel17.phy.cuhk.edu.hk's password:
file_to_be_downloaded 100% 25 0.3KB/s 00:00
(base)
binxi@LAPTOP-PGG84KRRK MINGW64 ~/demo_scp
$ ls
file_to_be_downloaded files_to_be_uploaded
```

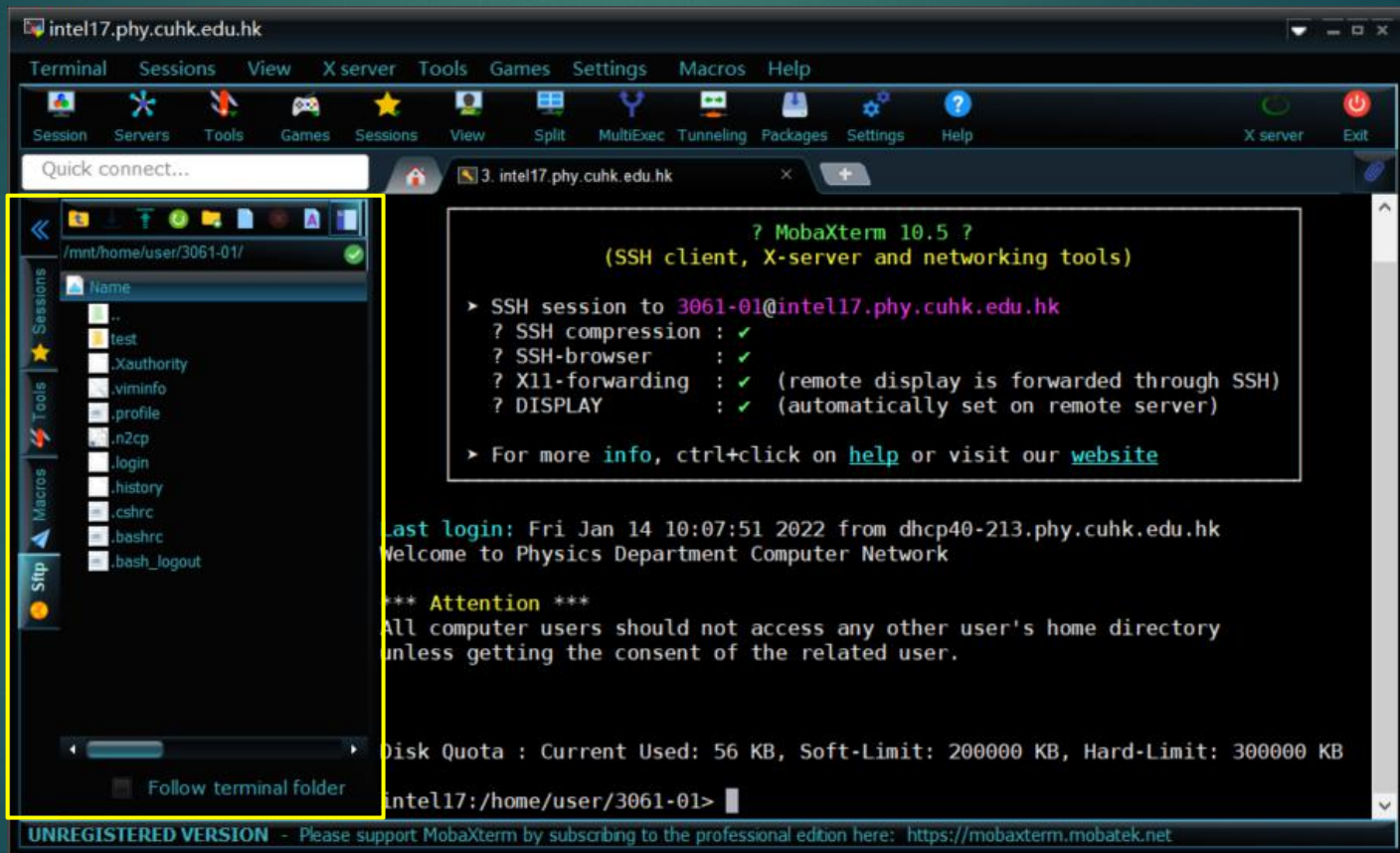
target file path

position on your PC, . means current position

- NOTE: if you want to upload a directory, add tag `-r` after `scp`
`scp -r <directory_name> 3061-01@intel17.phy.cuhk.edu.hk:~/test/`
`scp -r 3061-01@intel17.phy.cuhk.edu.hk:~/test/<directory_name>/ .`

How to upload the files to server

- Drag and drop on MobaXterm (See *access_dept_srv_guide.pdf* Sec. 2 for more detail)



How to submit

```
intel17:/home/user/3061-01> ls
test
intel17:/home/user/3061-01> submit
Submitting homework.... (Press Ctrl-C to quit)
Student : 3061-01
Tutor   : phys3061

Which set of homework submitting (e.g. hw1, lab3 ...etc) : lab0
Your enter is lab0 , correct? [y] y
Enter the file(s) to submit (use space to separate files) : test/
total 4
-rw----- 1 3061-01 games 25 Jan 14 10:09 file_to_be_downloaded
Do you want to submit the above file(s) to phys3061? [y] y
The files are successfully delivered, you shall receive a confirmation
email within a few minutes, if not, please contact your course tutor or
Mr.Jason Chan (mwchan@phy.cuhk.edu.hk) to check.
```

Type "submit"

Type "lab X"

Type "y"

Type your file's name

Type "y"

Compress your files before submit them

- ▶ If submitting multiple file
 - ▶ Put all files in a directory
 - ▶ Group all files using "*tar zcf files.tar.gz dir*"

Task 2: Write a few small functions on dot product and cross product

Tips:

- ▶ 3D (x,y,z) Input two vectors from keyboards
- ▶ Dot product gives a scalar, and cross product gives a vector

After you finish the two tasks:

- ▶ Group them into a folder, and compress it
- ▶ Submit it into lab0

Thanks !