

CSE 498/598k: Homework #2 Update

Due: 11/05/04

1 Compiling ProtoMol

1.1 In general

You will find a tarball of the PROTOMOL2 source code at

```
/afs/nd.edu/coursefa.04/cse/cse598k.01/www/hw/hw2/protomol2.tar.gz
```

Copy the source code into your directory. Unzip and untar the source with the command:

```
gzip -dc protomol2.tar.gz | tar -xf -
```

You may now remove the file `protomol2.tar.gz`. Enter the `protomol2` directory. In order to compile PROTOMOL2, you will need to run the following commands:

```
aclocal; autoheader; autoconf; automake -a;
```

```
./configure --with-gcc
```

```
make clean; make depend; make
```

This will take about 30 minutes to compile on a relatively new processor. You can ignore the warnings from the `make depend` command. Once compiled, the executable can be found in `protomol2/applications/protomol-app/protomol`.

1.2 Fitz/Chem labs

Unfortunately, OIT does not believe in using recent versions of software packages. PROTOMOL requires `gcc` version 3.0.1 or higher and `autoconf` version 2.58 or higher. Currently, the lab machines only contain `autoconf` version 2.56 which was released 2002-11-15. For reference, version 2.59 was released 2003-12-16.

The solution is to log into one of the sun machines in the clusters to run the `autoconf` commands:

```
aclocal; autoheader; autoconf; automake -a;
```

Recall that the Sun machines are the “authors”:

```
shakespeare moliere milton dickens austen bronte goethe schiller tolstoy chekov  
tagore twain faulkner steinbeck tolkien cslewis thomas breathed larson trudeau
```

2 Deliverables

2.1 Problem #1

Please change your program to output 3 files during the run:

solar.energies - Contains 4 columns: Time, Total En, Kinetic En, Potential En

solar.positions - Contains 3 columns: Time, X, Y

solar.velocities - Contains 3 columns: Time, X, Y

Where Time = timestep * step #

Ideally, I would like to be able to specify the timestep and the cutoff on the command line, but if not there then please define them near the top of your program so that I can quickly change them.

2.2 Problem #2

I forgot to give you the masses of the atoms in the config files. So that I don't totally mess up your config file readers, you may hard code these values into your program:

Atom Mass

CH3 15.035

CH2 14.027

Please change your program to output 2 file during the run:

butane.energies - Contains 7 columns: Time, Total En, Kinetic En, Potential En, Bond En, Angle En, Dihedral En

butane.forces - Contains 4 columns: Time, Bond forces, angle forces, dihedral forces

The equations for the forces are actually somewhat hard to derive. Fortunately, some people smarter than I have already done this. The equations for the angle force can be found at:

<http://www.nd.edu/~lcls/download/alpha107/doc/programmerguide/node5.html#SECTION00522000000000000000>

The equations for the dihedral force can be found at:

<http://www.nd.edu/~lcls/download/alpha107/doc/programmerguide/node5.html#SECTION00523000000000000000>

2.3 Problem #3

Read the tutorial [protomol2/doc/tutorial/tutorial2_0.pdf](#). Also, for reference, I have placed a presentation on the website called [mattheySolar.pdf](#). In the directory [protomol2/framework/forces](#) you will find a skeleton file called `GravitationForce.h`. Finish the code to make PROTOMOL correctly compute the gravitation forces and energies. On the web page, you will find a set of input files for PROTOMOL. These are similar to the input files already given, but there is a configuration file designed for use with PROTOMOL. To run PROTOMOL, simply call the executable with the configuration file:

```
protomol input-file.conf
```

2.4 What to turn in

For problems #1 and #2, please place your code into your dropbox under the directory of “hw2”. If you know how to write a “makefile” then place that there as well. Otherwise, describe in your writeup exactly how I should compile your programs.

For your writeup, please describe how each of your programs work. Describe any assumptions that you made. Describe any parameters that I may need to change to run your programs. Be sure to include your partners name if you worked with someone else.

For problem #3, place the output files from your PROTOMOL2 run into your dropbox as well as your modified copy of `GravitationForce.h`.

Finally, please include your answers to the reading questions.