Assignment 2: Molecular dynamics model of a collection of water molecules

Practical information

Deadline: Sunday 20/2 16.00

Resources:

- ERDA for file storage
- Jupyter for the Terminal to access DAG
- DAG for testing, visualization, and benchmarks

Introduction

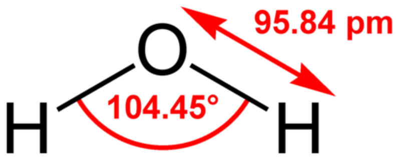
N-body simulations are common in physics and chemistry. The basic model has *O*(N^2) complexity (for N bodies the number of calculations needed is proportional to N^2), where each body is updated by applying the forces of all other bodies. In the case of molecular dynamics (MD) the goal is to obtain the physical movements of the interacting molecules. The atoms of the molecules interact by certain energy potentials, and the system evolution is obtained numerically by integrating Newton's equations of motion. This method is a powerful investigatory tool in physics, chemistry, materials science, and biophysics. We need to define certain intramolecular and intermolecular potentials to perform an MD simulation. The intermolecular forces should be calculated between every atom, and therefore to integrate one step, *O*(N^2) calculations will be performed. The intramolecular forces are calculated between the atoms in each molecule and therefore has *O*(N) complexity.

Modern MD simulation software such as GROMACS and NEMD use certain approximations to reduce this problem to an *O*(n) problem, and they are used for simulating systems of millions of particles for millions of time steps.

In this tutorial, we will make a simple MD program to simulate *N* water molecules. Three atoms represent each water molecule, and therefore the system contains 3 *N* particles. These particles interact with one another with a set of potentials.

For atoms belonging to the same molecule, two potentials exist. Harmonic and angle potentials. The Harmonic one is to model the covalent bond.

$$V_{bond}(r) = \frac{k_b}{2}(r - l_0)^2 \quad (1)$$



The angle potential is an interaction between three particles

$$V_{angle}(\phi) = \frac{k_a}{2}(\phi - \phi_0)^2 \quad (2)$$

Non-bonded potentials describe interactions between any pair of particles. It is very common that in MD algorithm non-bonded potentials is only applied among the particles that do not interact with one another through bonded potentials. This usually creates a numerically stable simulation. In this MD code, we use Lennard Jones and Coulomb potentials for the non-bonded potentials. The r^{-6} term in LJ potentials models the Van der Waals force.
What does r^{-12} model?

$$V_{LJ}(r) = \varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r}\right)^{12} - \left(\frac{\sigma_{ij}}{r}\right)^{6}\right]$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}$$
$$\sigma_{ij} = \frac{\sigma_i + \sigma_j}{2}$$

In many popular MD forcefields (CHARMM, AMBER), you often find that q1 and q2 are smaller than 1e. How can this be?

$$V_E(r) = k\frac{q_1 q_2}{r}$$

Using the potentials, we can obtain the total force acting on each particle and we can integrate the equation of motion by a means of some integrator algorithm; here we are using the leap-frog integrator.

$$v\left(t+\frac{1}{2}\Delta t\right) = v\left(t-\frac{1}{2}\Delta t\right) + \frac{\Delta t}{m}F(t)$$
$$r(t+\Delta t) = r(t) + \Delta t v\left(t+\frac{1}{2}\Delta t\right)$$

How to use the code

For this tutorial we need g++ and python, which is provided on ERDA. Spin up a Jupyter session on DAG. Important! Select the "HPC notebook" notebook image. This is the image we use for the course. In the launcher launch the Terminal.

In the terminal (or the folder view on the right side) you can see two folders: `erda_mount` and `hpc_course`. `erda_mount` contains your own storage area. This is where you save files. In the folder `hpc_course` the exercises are stored. If you have not done so already, start by making a new folder in your storage area for the course. Then copy the exercise to the folder and enter in to the folder. You can write '`ls`' to get a file listing of the folder.

```
cd erda_mount
mkdir HPPC
cd HPPC
cp -a ~/hpc_course/module2 .
cd module2
ls
```

To be able to edit the files for the exercise navigate to the same folder in the file view. Here you can open four files:

- Makefile
- Water_sequential.cpp
- Water_vectorised.cpp
- Water_visualizer.ipynb

Before you can run the code, you need to compile it. This can be done with make. You should see something like this in the terminal:

```
$ make
g++ Water_sequential.cpp -O1 -Wall -march=znver1 -g -std=c++14 -o seq
g++ Water_vectorised.cpp -O1 -Wall -march=znver1 -g -std=c++14 -fopenmp-simd -o vec
$
```

Two binaries are produced: `seq` and `vec`. `seq` is the binary of the reference code, while `vec` is the binary of your code. To begin with the two C++ source code files are very similar.

You can use the `seq` binary file to run a simulation. In the command line you can change some default system configurations. Use `seq -h` to get a terse line with the command options:

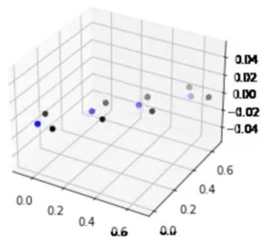
```
$ seq -h
MD -steps <number of steps> -no_mol <number of molecules> -fwrite <io frequency> -dt
<size of timestep> -ofile <filename>
```

Try run the command. It should be very quick and produce something like:

```
$ ./seq
Elapsed time:   0.1057
Accumulated forces Bonds    : 9.0655e+06
Accumulated forces Angles   : 7.2358e+06
Accumulated forces Non-bond: 6.7306e+07
```

The default values of the input parameters are defined in the "Sim_Configuration" class. Please read the source. The output tells us how long time it took to execute the main loop and three checksums. The checksums pertain to each part of the force update, and is a good cross check for errors. If the checksums are not the same for the `seq` and the `vec` binary, something has gone awry.

When the simulation is finished, you can use the python notebook to visualize the trajectory file "trajectory.txt" and check the system evolution. The movie will show frames like the one shown on the right with the 3D position of the molecules (and atoms):

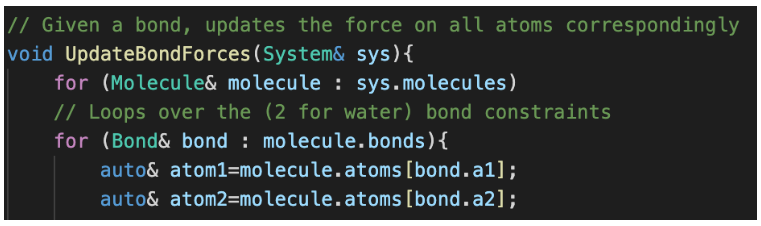


Code structure:

The main function reads all the common line options and pass them to a function on the `Sim_Configuration` class to update the input parameters. Then in the main function, a system containing a set of water particles is returned by the `MakeWater` function. The configuration of this system is evolved by `Evolve` function. Every `data_period` time steps, the position of the atoms is stored, they can later be read by notebook.

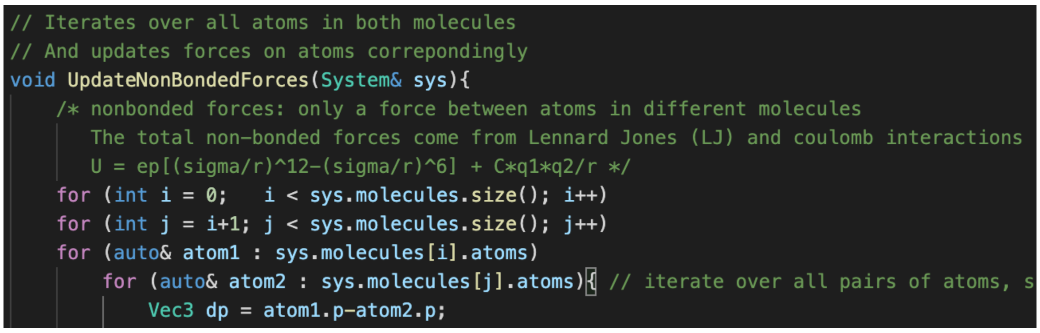
Objects in the system

The code is built with a class oriented Array-of-Structures layout corresponding to the different physical entities that are relavant for the problem. The **System** class contains a vector of molecules and the global time. Then **Molecule** class contains vectors of atoms, bonds and angles. The **Bonds** and **Angles** classes contain the constants relevant for the bonds and angles with respect to the atoms in the molecules. Finally, the **Atoms** object contains positions, velocities, forces, name, charge and LJ potential coefficients. To evolve the atoms forward in time we implement the leap-frog integrator in the **Evolve** function. To calculate the forces we use three functions: **UpdateBondForces**, **UpdateAngleForces**, and **UpdateNonBondedForces**. Notice how we loop over the molecules and the atoms using simple iterators in the two first cases:



```
// Given a bond, updates the force on all atoms correspondingly
void UpdateBondForces(System& sys){
    for (Molecule& molecule : sys.molecules)
    // Loops over the (2 for water) bond constraints
    for (Bond& bond : molecule.bonds){
        auto& atom1=molecule.atoms[bond.a1];
        auto& atom2=molecule.atoms[bond.a2];
```

While in the last case we need to loop over all combinations of different molecules, and therefore use a traditional loop, but over an "upper triangle" in the indices:
To make the code simpler and closer to the math we have created a Vec3 class that define 3D vectors and vector operations, such as dot and cross products, and the norm of a vector.



```
// Iterates over all atoms in both molecules
// And updates forces on atoms correpondingly
void UpdateNonBondedForces(System& sys){
    /* nonbonded forces: only a force between atoms in different molecules
       The total non-bonded forces come from Lennard Jones (LJ) and coulomb interactions
       U = ep[(sigma/r)^12-(sigma/r)^6] + C*q1*q2/r */
    for (int i = 0;   i < sys.molecules.size(); i++)
    for (int j = i+1; j < sys.molecules.size(); j++)
    for (auto& atom1 : sys.molecules[i].atoms)
        for (auto& atom2 : sys.molecules[j].atoms){ // iterate over all pairs of atoms, s
            Vec3 dp = atom1.p-atom2.p;
```

Task 1: Create a Struct-of-Arrays version of the program (amenable to vectorization) [Points: 5]

The sequential version of the program uses a data layout with the data for each atom collected in to a structure. This has two advantages: i) the code is simple, compact, and expressive. ii) different data describing a single body are close to each other in memory, resulting in optimal cache usage. This layout is called "array-of-structs" or AoS. The drawback is that when looping over elements of different atoms memory access is scattered, prohibiting efficient vectorisation of the loops. To vectorise the code, and make it amenable for execution with SIMD units (or on a GPU or other data parallel accelerators), the data has instead to be laid out in an orthogonal format, called "struct-of-arrays" or SoA.
In the vector version of the code, `Water_vectorised.cpp`, that is ready for OpenMP SIMD parallelisation, the `Atom` class has been changed in to an `Atoms` class containing multiple atoms / vectors to follow the SoA data layout, and the `Molecule` class has become a `Molecules` class containing `no_mol` identical molecules.

Bonus: You can take it even further and rewrite it as an array-of-structs-of-arrays (AoSoA) to gain both the advantage of vectorisation and memory bandwith; feel free to explore this for the very most optimal performance.

To accomplish the task you will have to restructure the loops calculating the forces such that the innermost loop is iterating over all the identical atoms in the system (compared to the original version where the outer loop was iterating over all the molecules). You also have to make small changes to the initialization of the water molecules, to the output routine and to the leap-frog integrator loop. Finally, in the System class instead of using a vector of Molecule:

```
    std::vector<Molecule> molecules;          // all the molecules in the system
```

You can now use a single copy of the new Molecules class:

```
    Molecules molecules;          // all the molecules in the system
```

Typically a loop that before looked like (from the leap-frog update):

```
    for (Molecule& molecule : sys.molecules)
    for (auto& atom : molecule.atoms){
```

will now become

```
    Molecules& molecule = sys.molecules;
    for (auto& atom : molecule.atoms)
    for (int i = 0;   i < molecule.no_mol; i++){
```

Notice how we used a reference to sys.molecules to keep the variable names the same.

When your code is complete, you should be able to remove the Atom and Molecule classes and obtain the same results and checksums with the "`seq`" and "`vec`" executables. Verify!

Task 2: Investigate the performance of the code with a profiler [Points: 3]

Optimising a code too early can result in a lot of lost time. A powerful tool for investigating how well a code performs is a profiler. The alternative to a profiler is to include timings in the code. You can already see how to do this with the chronos library in the main routine.
In this exercise you will use the simple text based profiler *gprof* that is available on ERDA, and indeed on most Linux machines. gprof requires the code to be compiled with a certain flag "-pg".
Open the Makefile in a text editor you can see that there already are three suggested combinations of compile flags specified with the variable `OPT`. make will always use the last definition in the Makefile. Edit the Makefile to select the flag combination for profiling, remove the binaries and recompile. This should result in a terminal output like this:

```
jovyan@...$ make clean
rm -fr seq vec
jovyan@...$ make
g++ Water_sequential.cpp -O1 -pg -Wall -march=znver1 -g -std=c++14 -o seq
g++ Water_vectorised.cpp -O1 -pg -Wall -march=znver1 -g -std=c++14 -fopenmp-simd -o
vec
jovyan@...$
```

To get an idea of the basics of profiling spend 5 minutes reading through:
https://www.thegeekstuff.com/2012/08/gprof-tutorial/
After reading, try executing the new binary doing a simulation with four molecules for a large enough number of steps that the full execution takes around a second, and then try get a table of the most demanding functions using the command "`gprof -p -b ./seq gmon.out`". This should result in an output similar this:

```
jovyan@2f2b00cb86e1:~/erda_mount/Teaching/2022 HPPC/hpc_course/module2$ ./seq -steps 100000 -no_mol 4 -fwrite 1000000
Elapsed time:   0.8439
Accumulated forces Bonds   : 1.2924e+08
Accumulated forces Angles  : 1.7177e+08
Accumulated forces Non-bond: 8.5669e+08
jovyan@2f2b00cb86e1:~/erda_mount/Teaching/2022 HPPC/hpc_course/module2$ gprof -p -b  ./seq gmon.out
Flat profile:

Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls  us/call  us/call  name
 68.36      0.28     0.28   100000     2.80     3.27  UpdateNonBondedForces(System&)
 14.65      0.34     0.06 14000000     0.00     0.00  operator*(double, Vec3 const&)
  7.32      0.37     0.03   100000     0.30     0.33  UpdateBondForces(System&)
  4.88      0.39     0.02   100000     0.20     0.30  UpdateAngleForces(System&)
  2.44      0.40     0.01  1200000     0.01     0.01  cross(Vec3 const&, Vec3 const&)
  2.44      0.41     0.01   100000     0.10     4.10  Evolve(System&, Sim_Configuration&)
  0.00      0.41     0.00   400000     0.00     0.00  dot(Vec3 const&, Vec3 const&)
  0.00      0.41     0.00       42     0.00     0.00  void std::__cxx11::basic_string<char, std::char_traits<char>,
std::allocator<char> >::_M_construct<char*>(char*, char*, std::forward_iterator_tag)
  0.00      0.41     0.00       11     0.00     0.00  void std::__cxx11::basic_string<char, std::char_traits<char>,
std::allocator<char> >::_M_construct<char const*>(char const*, char const*, std::forward_iterator_tag)
  0.00       0.41      0.00          3      0.00      0.00  int __gnu_cxx::__stoa<long, int, char, int>(long (*)(char
const*, char**, int), char const*, char const*, unsigned long*, int)
  0.00        0.41       0.00           3       0.00        0.00  void std::vector<Molecule, std::allocator<Molecule>
>::_M_realloc_insert<Molecule>(__gnu_cxx::__normal_iterator<Molecule*,              std::vector<Molecule,
std::allocator<Molecule> > >, Molecule&&)
  0.00     0.41    0.00       2    0.00     0.00  WriteOutput(System&, std::basic_ofstream<char, std::char_traits<char>
>&)
  0.00      0.41     0.00        1     0.00     0.00  _GLOBAL__sub_I_accumulated_forces_bond
  0.00      0.41     0.00        1     0.00     0.00  MakeWater(int)
  0.00                   0.41                0.00                          1              0.00                 0.00
Sim_Configuration::Sim_Configuration(std::vector<std::__cxx11::basic_string<char,           std::char_traits<char>,
std::allocator<char> >, std::allocator<std::__cxx11::basic_string<char, std::char_traits<char>, std::allocator<char>
> > >)
  0.00      0.41     0.00        1     0.00     0.00  std::vector<Molecule, std::allocator<Molecule> >::~vector()
  0.00     0.41    0.00       1    0.00     0.00 std::vector<std::__cxx11::basic_string<char, std::char_traits<char>,
std::allocator<char> >, std::allocator<std::__cxx11::basic_string<char, std::char_traits<char>, std::allocator<char>
> > >::vector<char**, void>(char**, char**, std::allocator<std::__cxx11::basic_string<char, std::char_traits<char>,
std::allocator<char> > > const&)
  0.00     0.41    0.00       1    0.00     0.00 std::vector<std::__cxx11::basic_string<char, std::char_traits<char>,
std::allocator<char> >, std::allocator<std::__cxx11::basic_string<char, std::char_traits<char>, std::allocator<char>
> > >::~vector()
```

It is clear that the bulk of the time is used by the forcing functions and the vector operators. Evolve also takes some time because it does the leap-frog integration loop. The exact amount of time each function takes of course depends on the implementation, but also on the chosen parameters.

To get a better idea of the real performance of the code, please select the optimal compilation options "OPT=-O3 -ffast-math", but add the "-pg" flag. This will dramatically improve the runtime (by x10), because "-O3" tries to inline (reimplement directly in the body of functions) the vector operations and because "-ffast-math" removes a lot of checks for e.g. sqrt of negative numbers, divide by zero etc. Now use this to investigate how the performance changes.

Questions: (all using the optimal settings OPT==-O3 -ffast-math -pg)

- Using 4 molecules, which functions (and with which percentage) contributes most to the runtime
- How does it change if modelling 2 molecules, 16 molecules, and 128 molecules. Please explain why the percentages changes.
- Based on the above results, which function(s) are most important to get good performance.
- How does the vectorised (SoA) version perform compared to the original sequential (AoS) version running with 2 molecules and with 128 molecules. If there is a adifference in the relative performance, please discuss why this could be the case.

Task 3: Adding OpenMP SIMD pragmas to the code [Points: 2]

During the exercise you have developed a good idea about which are the main loops, in terms of performance, *in your vectorized code*. Add OpenMP SIMD pragmas to them. In the current code the performance should not change (though this will depend on the exact implementation), but it is still good practice to add them. There are four loop blocks where it is relevant to add pragmas. Verify that you still get the right checksums when recompiling with "`OPT=-O3 -ffast-math`". The highest impact should be seen in runs with more than 16 molecules.

Write a few lines in the report about where you have placed the pragmas, the benchmark results (using 16 molecules) and why you chose your pragmas as you did.