Assignment 1: Molecular dynamics model of a collection of water molecules

Practical information

Deadline: Saturday 29/9 23.59

Resources:

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

Hand-in:

- A report of up to 3 pages in length (excluding the code)
- Your vectorized (Struct-of-Array) code both as source file as well as in pdf
- Use the template on Absalon to include your code in the report

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 biology. We need to define certain intramolecular and intermolecular potentials to perform a MD simulation.

While mathematically the intermolecular forces affecting each atom depends on every other atom, the vast majority of the force is caused by the few nearest molecules. For this reason, we will use the approximation of only considering the *n_closest* (set to 8) molecules, the “neighbours”. Since this changes very slowly compared to e.g. the oscillations on bonds, we update the list of neighbours only once every 100 steps

Modern MD simulation software such as GROMACS and NEMD use certain approximations to reduce this problem to an $O(n)$ problem using a much more sophisticated technique than our “neighbours” method, and they are used for simulating systems of millions of particles for millions of time steps.

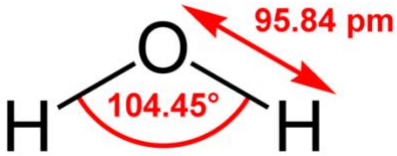
In this tutorial, we will make a simple MD program to simulate *N* water molecules. Three atoms represent each water molecule, and therefore the system contains 3 *N* particles. These particles interact with one another with a set of potentials.

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

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



where k_a, k_b are force constants, $l_0 = 95.48$ pm the bond length, and $\phi_0 = 104.45°$ the bond angle.

Non-bonded potentials describe interactions between any pair of particles. Non-bonded potentials are only applied among the particles that do not interact with one another through bonded potentials, because they are already included in the bonded forces. 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?

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

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

For the Coulomb potential, in many popular MD forcefields (e.g. CHARMM, AMBER) q1 and q2 are often smaller than one elementary charge. *How can the charges be less than an elementary charge?*

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

Using the potentials, we can obtain the total force acting on each particle and we can integrate the equation of motion by 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++, gfortran or python for either the C++, Fortran or Python version of the exercise. They are all provided on ERDA. Spin up a Jupyter session on DAG. In the launcher, launch the Terminal.

In the terminal (or the folder view on the right side) you can see `work` that contains your own storage area. This is where you save files. If you have not done so already, start by making a git checkout of the course repository. In the terminal this can be done as follows:

```
mkdir AHPC
cd AHPC
git clone https://github.com/haugboel/ahpc.git
```

Alternatively, if you are used to git, you may go to github, fork the `ahpc` repository, and clone your own version. This way you can commit and track changes yourself. If you do not do this, it is maybe good to create a second copy for reference, where you do not have any files changed:

```
git clone https://github.com/haugboel/ahpc.git ahpc_reference
```

You can get an overview of the week1 exercise by using the file browser on the left. In each of the "cpp", "fortran" and "python" subfolders there are the following files:

```
ahpc/week1/6water.avi                    : Example of the water molecule dynamics
ahpc/week1/Water_visualizer.ipynb        : Python script to visualize output data

ahpc/week1/cpp:                          : C++ files
Makefile                                 : Makefile with rules for compilation
Water_sequential.cpp                     : Reference sequential version
Water_vectorised.cpp                     : Starting point for the exercise

ahpc/week1/fortran:                      : Fortran files
Makefile
Water_sequential.f90
Water_vectorised.f90

ahpc/week1/python:                       : Python files
Water_sequential_lists.py                : Example of an implementation with lists
Water_sequential.py                      : Reference sequential version with Numpy
Water_vectorised.py
```

To be able to edit the files for the exercise navigate to the same folder in the file view. Here you can open files such as (for C++):

- 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=native -g -std=c++17 -o seq
g++ Water_vectorised.cpp -O1 -Wall -march=native -g -std=c++17 -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 identical except two new classes.

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:

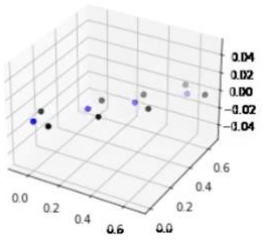
```
$ seq -h
MD -steps <number of steps> -no_mol <number of molecules> -fwrite <io frequency> -dt
<size of timestep> -ofile <filename>
```

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

```
./seq
Accumulated forces Bonds   : 3.4061e+08
Accumulated forces Angles  : 2.6864e+08
Accumulated forces Non-bond: 5.7982e+09
Elapsed total time:          1.7036
```

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 total and three checksums. The checksums pertain to each part of the force update, and are good cross checks for errors. If the checksums are not the same for the `seq` and the `vec` binary, probably 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. Please set the “datadir” variable correctly in the notebook.
The movie will show frames like the one shown on the right with the 3D position of the molecules (and atoms): Initial system is a bunch of water on a sphere which will fall in together, almost like a collapsing air bubble, and some small droplets will then be slung off.



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 evolves in a `for loop`. 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 relevant for the problem. In Fortran this is implemented with Types, but otherwise it is identical. The **System** class (type in Fortran) contains a vector (array in fortran) of molecules and the global time. The **Molecule** class contains vectors of atoms, bonds, angles and the neighbour lists for each molecule. The **Bonds** and **Angles** classes contain the constants relevant for the bonds and angles with respect to the atoms in the molecules. The **Atom** class contains positions, velocities, forces, name, charge and LJ potential coefficients. Finally, **neighbours** are a list of the indexes of up to nClosest neighbors with which we will calculate intermolecular forces. To evolve the atoms forward in time we implement the leap-frog integrator in the **UpdateKDK** function. To calculate the forces and update the neighbours, we use four functions **UpdateBondForces**, **UpdateAngleForces**, **UpdateNonBondedForces** and every 100 timesteps, **BuildNeighborList**. They have slightly different namings in the Fortran code using underscores instead of CamelCase. This is usually done in Fortran because Fortran is case insensitive.

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

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 when handling one “object” at a time. This layout is called “array-of-structs” or AoS. The drawback is that when looping over elements of different atoms (as in intermolecular forces) the data of interest is interleaved on the cache lines of the other info, wasting precious memory space and throughput. In a language like python this is much worse, since each element is allocated separately scattered around memory, and we update the state of each atom one by one using loops. To optimize 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`, a part from the `Atom` class there is also an `Atoms` class containing multiple atoms / vectors to follow the SoA data layout, and the `Molecule` class has been mirrored in to a `Molecules` class containing `no_mol` identical molecules.

Bonus: You can take it even further and store each component of the Vec3’s describing position, velocities and forces separately to further ease vectorization; feel free to explore this for the very most

optimal performance. This is a natural (necessary!) option to do in Python creating numpy arrays of shape (3, no_mol).

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.

Taking the C++ code as an example, 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!

In the rapport you should:

- **Show that your code gives a correct checksum**
- **Write a small (≈1-3 lines per function modified) description of your changes**

Task 2: Investigate the performance of the code with a profiler

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 by looking at the main routine of the C++/Fortran/Python code. It is easy to add more timers, if you would like to get individual timings of different parts of the code. An alternative is to use a profiler.

C++ and Fortran

In this exercise for the Fortran and/or C++ codes 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 and 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=native -g -std=c++17 -o seq
g++ Water_vectorised.cpp -O1 -pg -Wall -march=native -g -std=c++17 -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/AHPC/ahpc/week1/cpp$ ./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/ AHPC/ahpc/week1/cpp $ 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&)
  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. 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 100 molecules, which functions (and with which percentage) contributes most to the runtime**
- **How does it change if modelling 10 molecules, 100 molecules, 1000 and 50000 molecules. Explain why the percentages change. Think about your choice of number of timesteps to balance good statistics and reasonable runtime.**
- **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 for each of the system sizes? Discuss the observations; both vectorization, reuse of data in cache (L1, L2, and L3), and overall memory usage affect your results.**

Python

In this exercise for the Python code you will use the builtin *cProfile* tool and the packaged *line_profiler* tool. The first makes it possible to get an idea of how much each function takes to run, while the latter makes it possible to get line level profiling for individual python routines. You can read a short introduction to line_profiler here:

https://researchcomputing.princeton.edu/python-profiling

If you run the exercise on ERDA the fastest way to get access to the package is with pip install like this:

```
jovyan@...$ pip install line_profiler
```

This has to be done every time you start a new session, but it only takes a few seconds. You can add decorators to profile specific functions, and you can also profile the full program and get a line-by-line printout of the cost of each line by calling this one-liner:

```
jovyan@...$ python -m kernprof -lv -p Water_sequential.py Water_sequential.py
```

The line profiler has detailed documentation here

https://kernprof.readthedocs.io/en/latest/index.html

Notice that there is a significant overhead in calling the line profiler but it allows you to pinpoint what lines / statements / function calls in your program takes time. This can be very valuable in Python since the overhead of the Python interpreter sometimes gives non-obvious results. You my even use it to improve your solution!

Timing on the function level can be extracted with cProfile. Simply enable it when executing with python:

```
jovyan@...$ python -m cProfile Water_sequential.py > out.prof
```

It will trace all functions, also functions that are builtin to python or part of imported packages. It is therefore good practice to send the output to a text file that can then be investigated. By default the functions are sorted according to their cumulative time, e.g. how much time is spent executing the function including function calls inside the function. The first lines could look like this

```
(python3) jovyan@9b607bd691d7:~/work/ahpc/week1/python$ head -30 outprof
Accumulated forces Bonds   : 22356.58434
Accumulated forces Angles  : 102124.06249
Accumulated forces Non-bond: 6340811.85366
Elapsed total time:          1.6656
         323876 function calls (321772 primitive calls) in 1.892 seconds

   Ordered by: cumulative time

   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
     94/1    0.001    0.000    1.892    1.892 {built-in method builtins.exec}
        1    0.000    0.000    1.892    1.892 Water_sequential.py:1(<module>)
       20    0.984    0.049    1.407    0.070 Water_sequential.py:214(UpdateNonBondedForces)
        8    0.001    0.000    0.717    0.090 __init__.py:1(<module>)
   101180    0.361    0.000    0.361    0.000 Water_sequential.py:30(mag)
    104/1    0.001    0.000    0.215    0.215 <frozen importlib._bootstrap>:1349(_find_and_load)
    104/1    0.001    0.000    0.215    0.215 <frozen importlib._bootstrap>:1304(_find_and_load_unlocked)
    101/1    0.000    0.000    0.215    0.215 <frozen importlib._bootstrap>:911(_load_unlocked)
     93/1    0.001    0.000    0.215    0.215 <frozen importlib._bootstrap_external>:993(exec_module)
    255/2    0.000    0.000    0.214    0.107 <frozen importlib._bootstrap>:480(_call_with_frames_removed)
    354/4    0.000    0.000    0.206    0.051 {built-in method builtins.__import__}
   204/31    0.001    0.000    0.203    0.007 <frozen importlib._bootstrap>:1390(_handle_fromlist)
    91180    0.148    0.000    0.148    0.000 Water_sequential.py:33(mag2)
       20    0.044    0.002    0.119    0.006 Water_sequential.py:170(UpdateAngleForces)
        1    0.000    0.000    0.099    0.099 _index_tricks_impl.py:1(<module>)
        1    0.000    0.000    0.093    0.093 defmatrix.py:1(<module>)
        1    0.000    0.000    0.090    0.090 _linalg.py:1(<module>)
```

We may concentrate on the functions in our code by using e.g. `grep` on the commandline

```
(python3) jovyan@9b607bd691d7:~/work/ahpc/week1/python$ grep Water_sequential outprof
        1    0.000    0.000    1.892    1.892 Water_sequential.py:1(<module>)
       20    0.984    0.049    1.407    0.070 Water_sequential.py:214(UpdateNonBondedForces)
   101180    0.361    0.000    0.361    0.000 Water_sequential.py:30(mag)
    91180    0.148    0.000    0.148    0.000 Water_sequential.py:33(mag2)
       20    0.044    0.002    0.119    0.006 Water_sequential.py:170(UpdateAngleForces)
       20    0.027    0.001    0.055    0.003 Water_sequential.py:154(UpdateBondForces)
       20    0.036    0.002    0.045    0.002 Water_sequential.py:249(UpdateKDK)
        1    0.019    0.019    0.036    0.036 Water_sequential.py:128(BuildNeighborList)
     6000    0.019    0.000    0.029    0.000 Water_sequential.py:36(cross)
    13300    0.007    0.000    0.021    0.000 Water_sequential.py:27(Vec3)
        1    0.003    0.003    0.006    0.006 Water_sequential.py:260(MakeWater)
     2000    0.003    0.000    0.003    0.000 Water_sequential.py:41(dot)
        2    0.002    0.001    0.003    0.001 Water_sequential.py:310(WriteOutput)
      300    0.001    0.000    0.002    0.000 Water_sequential.py:46(__init__)
        1    0.000    0.000    0.000    0.000 Water_sequential.py:75(Molecule)
        1    0.000    0.000    0.000    0.000 Water_sequential.py:88(Sim_Configuration)
      100    0.000    0.000    0.000    0.000 Water_sequential.py:76(__init__)
        1    0.000    0.000    0.000    0.000 Water_sequential.py:66(Angle)
        1    0.000    0.000    0.000    0.000 Water_sequential.py:89(__init__)
        2    0.000    0.000    0.000    0.000 Water_sequential.py:59(__init__)
        1    0.000    0.000    0.000    0.000 Water_sequential.py:45(Atom)
        1    0.000    0.000    0.000    0.000 Water_sequential.py:67(__init__)
        1    0.000    0.000    0.000    0.000 Water_sequential.py:58(Bond)
        1    0.000    0.000    0.000    0.000 Water_sequential.py:83(System)
        1    0.000    0.000    0.000    0.000 Water_sequential.py:84(__init__)
```

It is clear that the bulk of the time is used by the forcing functions and the vector operators. 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, how the original version compares to your solution, and to investigate how the performance changes please try to profile runs with different parameters.

Questions:

- **Using 100 molecules, which functions (and with which percentage) contributes most to the runtime**
- **How does it change if modelling 10 molecules, 100 molecules, and 1000 molecules. Explain why the percentages change. Think about your choice of number of timesteps to balance good statistics and reasonable runtime.**
- **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 for each of the system sizes? Discuss the observations; both vectorization, reuse of data in cache (L1, L2, and L3), overall memory usage, and number of python statements to be executed affect your results.**