Readme

Parts 1 and 2 of this assignment are located in separate folders. Within each folder is a shell script, \_compile\_and\_run.sh, that will compile all relevant executables and run them with the inputs required for generating results as used in the report. If this shell script fails, this document contains more explicit instructions on compiling and running the files.

To generate the plots in the report, python scripts have been added to the pre-made results folders. If results have been generated correctly, these files should generate all plots of interest.

# Part 1

Part 1 contains only a single cpp runtime script, simulation.cpp, along with its dependencies:

* forces\_and\_integrators.cpp   
  Contains all functions relevant to the physical properties of the system and time-series integration (e.g. RK-4 Integration, planetary gravity etc)
* sysvec\_utils.cpp   
  Utility functions and overloads for system state vectors
* vector\_utils.cpp   
  Utility functions and overloads for vectors
* manybody\_example.hpp   
  Contains parameters for an example run (mode 4) of the simulation with many bodies

To compile, call:

g++ -o simulation simulation.cpp forces\_and\_integrators.cpp sysvec\_utils.cpp vector\_utils.cpp

Once compiled, the executable will generate and save results for questions 1-3 if called with the relevant command line flag. To produce results for all questions and save with the filename required for plotting, use:

./simulation 1 ./results/pt\_1a.dat 100

./simulation 2 ./results/pt\_1b.dat 100

./simulation 3 ./results/pt\_1c.dat 100

./simulation 4 ./results/pt\_1d.dat 2600 1 1 0.01 5

All of these files can be compiled automatically by using the shell script “\_compile.sh”.

# Part 2

Part 2 contains 3 compile-able cpp scripts:

* singlegrid.cpp  
  Runs a single MCMC chain for a grid of fixed size at fixed temperature and describes / prints the resultant end state
* temp\_sweep.cpp   
  Calculates performs progressive MCMC chains over a range of temperatures and saves the mean and variance of energy and spin for each temperature and each chain.
* singlegrid\_parallel.cpp  
  Runs several MCMC chains and prints their running times. For use in multi-thread benchmarking

Alongside the dependencies:

* vector\_utils.cpp   
  Utility functions and overloads for vectors. Re-used from assignment 1. In this instance only really used to generate temperature grids more easily
* monte\_carlo.cpp  
  Contains all functions related to the MCMC runs, including functions for calculating the mean and variance of vectors
* grid.hpp  
  Contains an object class for the grid along with all physically relevant functions, like energy calculations

As monte\_carlo.cpp contains openMP functions and is included in all executables, all files must be compiled using the -fopenmp flag:

g++ -o singlegrid singlegrid.cpp monte\_carlo.cpp rand\_utils.cpp vector\_utils.cpp -fopenmp

g++ -o temp\_sweep temp\_sweep.cpp monte\_carlo.cpp rand\_utils.cpp vector\_utils.cpp -fopenmp

g++ -o singlegrid\_parallel singlegrid\_parallel.cpp monte\_carlo.cpp rand\_utils.cpp vector\_utils.cpp -fopenmp

All results for plotting / answering questions are generated by temp\_sweep.cpp. To produce the results as used in the report, call with command line arguments like:

./temp\_sweep 8 0.0 5.0 32 ./results/temp\_sweep\_8.dat

./temp\_sweep 16 0.0 5.0 32 ./results/temp\_sweep\_16.dat

./temp\_sweep 32 0.0 5.0 32 ./results/temp\_sweep\_32.dat

./temp\_sweep 64 0.0 5.0 32 ./results/temp\_sweep\_64.dat

For parts a and b, and for part c:

./temp\_sweep 128 2.0 2.269 32 ./results/temp\_sweep\_128\_nearcrit.dat 100000 1000 1

## Running / Inputs

All compiled executables are set to take arguments from command line. Arguments must be given in order, and will defer to default values if not provided. E.g.

./simulation 1 ./results/pt\_1a.dat 100

Will run simulation with , save results to ./results/pt\_1a.dat, use a maximum simulation time of , and will use default values for and .

**Part 1: simulation**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Input** | **Type** | **Constraints** | | **Default** | **Desc** |
| mode | int | 1-4 | | 1 | Determines the type of simulation to run.:   1. Question 1a – no interaction 2. Question 1b – interaction with no orbital kick 3. Question 3b – interaction with kick to achieve moon orbit 4. Example of chaotic many body behaviour |
| output\_dir | str |  |  | results/sim\_results.dat | Filename to save outputs to |
| tmax | double | >0 | | 100 | Max sim time |
| v\_launch | double | >0 | | 1.1376 | Launch velocity for modes 1-3 |
| thet | double | >0 | | -1.08 | Starting angle of moon in orbit, rad |
| dt | double | >0, | <tmax | 0.01 | Timestep for RK4 integration |
| sparseness | int | >0, | <maxits | 1 | Number of int steps per output line. Increase if output files are becoming too large. |

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**Part 2: singlegrid**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Input** | **Type** | **Constraints** | **Default** | **Desc** |
| N | int | >0 | 8 | Side-length of NxN Grid |
| T | double | >=0 |  | Temperature for MCMC simulation |
| Nits | int | >0 | 10,000 | Number of full sweeps of the grid / samples to draw for the chain |
| Nburn | int | >=-0 | 1,000 | Number of burn-in iterations in MCMC |
| flips\_per | int | >0 | 0(NxN) | Number of bit flips per 'sample' If set to zero, will default to flips. |
| seed | int |  | 0 | Seed for random number generation |

**Part 2: singlegrid\_parallel**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Input** | **Type** | **Constraints** | **Default** | **Desc** |
| N | int | >0 | 64 | Side-length of NxN Grid |
| T | double | >=0 |  | Temperature for MCMC simulation |
| Nits | int | >0 | 10,000 | Number of full sweeps of the grid / samples to draw for the chain |
| Nburn | int | >=0 | 1,000 | Number of burn-in iterations in MCMC |

**Part 2: temp\_sweep**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Input** | **Type** | **Constraints** | **Default** | **Desc** |
| N | int | >0 | 16 | Side-length of NxN Grid |
| T\_min | double | >=0 | 0.0 | Minimum temp for sweep |
| T\_max | double | >=0 | 5.0 | Maximum temp for sweep |
| Ntemps | int | >0 | 32 | Number of temperatures in sweep |
| Output\_dir | str |  | ./results/temp\_sweep.dat | Filename to save outputs to |
| Nits | int | >0 | 10,000 | Number of full sweeps of the grid / samples to draw for the chain |
| Nburn | int | >=-0 | 1,000 | Number of burn-in iterations in MCMC |
| flips\_per | int | >0 | 0(NxN) | Number of bit flips per 'sample' If set to zero, will default to flips.  Increase if samples are too correlated. Can decrease for better performance at high T. |
| seed | int |  | 0 | Seed for random number generation |
| printgrid | bool |  | True | If true, will print the final state of the grid at each temperature for the last chain as it completes its sweep |