3D N-Body Simulation with CUDA and ThreeJS

Mohammad A.Raji, Alok Hota

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1 Introduction

N-body simulation is a simulation of the effects of physical forces between particles in a dynamical system, and is used in many areas such as astronomy, physics, and chemistry. The simulation is very time consuming due to the large number of particles and the need to calculate the force between all pairs.

In this work, we implement a serial and a parallel version of the simulation to show the effectiveness of GPU parallelization for the problem and also provide an interactive web interface for viewing the simulation results. Our simulation is tested with a maximum number of 1024 particles for 10,000 time steps.

2 Method

Our parallel implementation was designed with two general guidelines:

1:1 Ratio — Each thread or GPU core is assigned a single body or particle in the simulation for which it will calculate forces against all other pairs.

Tiling — Utilize memory tiling so that threads in a block can coordinate memory accesses. This increases performance by making coalescing read operations.

Thread block size is determined at runtime based on the number of bodies. Each thread in these blocks will coordinate to read one memory location from the next `TILE_SIZE` section of the global position array. By synchronizing along these reads, we coalesce the memory access, allowing for high burst speeds.

An additional improvement made was the use of a softening value, ε. This is done to prevent divergence in the kernel. Since each GPU core operates in lock-step with each other core in its warp, the highest performance is achieved when all threads follow the same execution path. However, conditional statements, such as an `if` block, cause divergence in the kernel. Some threads may follow the `true` execution path, while others follow the `false` path. To make sure all threads execute the correct code, both paths are executed in a warp. This can severely hinder performance, and presents an issue when calculating force between all pairs of bodies.

The formula for calculating gravitational force between two bodies is shown below:

$$F_g = G\frac{m_1 m_2}{r^2} \tag{1}$$

where G is the universal gravitational constant, m_1 and m_2 are the masses of two bodies, and r is the distance between their centers. Since we are comparing all pairs of bodies, this includes the calculation of force between a body and itself. This leads to a division by 0, since $r = 0$. In a serial implementation, this can be avoided with a simple `if` statement. However in parallel, to avoid divergence caused by a similar `if` statement, we use a modified formula using our ε softening value:

$$F_g = G\frac{m_1 m_2}{r^2 + \varepsilon^2} \tag{2}$$

where $0 < \varepsilon \ll 1$. This makes the calculation an approximation, however with sufficiently low values of ε, this approximation is acceptable.

3 User Interface

To view the simulation results, we created a web interface that receives the simulation results as a **csv** file and renders it as a simulation in a 3D environment using ThreeJS - the WebGL based library.

The presented web interface provides the following the features:

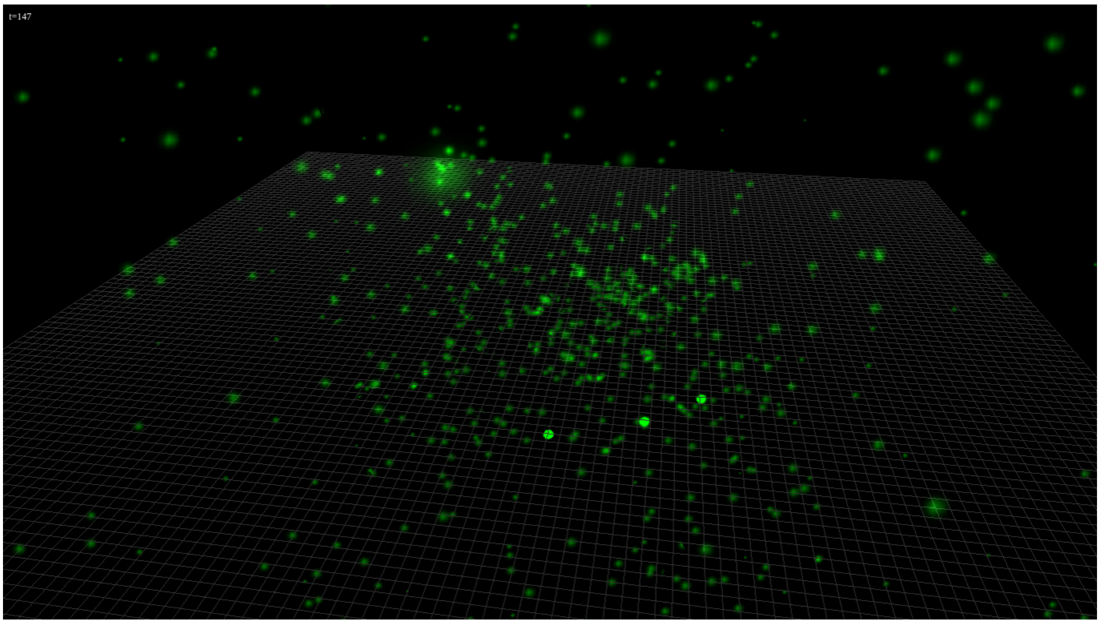
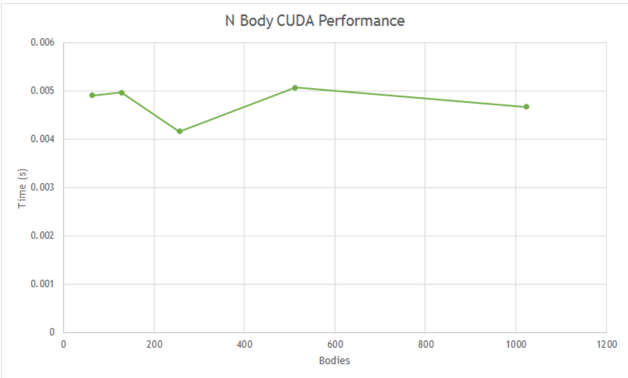
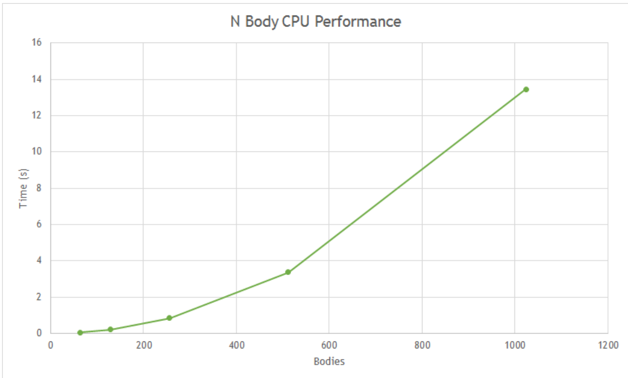


Figure 1: Web interface for our 3D n-body simulation



(a) Performance results for our parallel CUDA implementation



(b) Performance results for our parallel CUDA implementation

Figure 2: Performance comparison between our serial and parallel implementations

- Panning and zooming in a 3D environment
- Pausing and playing the simulation
- Manual and automatic rotation option

A screenshot of our web interface is shown in Figure 1.

4 Evaluation

We tested our implementations on a machine with four Xeon CPUs and an Nvidia Quadro FX3800 GPU with 192 cores.

For evaluation, the runtime of the serial and parallel implementations are compared. The values used for the number of particles in this comparison were 64, 128, 256, 512 and 1024. The implementations created a simulation file for 10000 timesteps. The large number of timesteps simulated, provides a flexible way to increase or decrease the speed of the visualization if needed. The results are shown in Figure 2.

5 Appendix A: Installation

The code for our work is available at http://github.com/ahota/nobody and can be downloaded using Git by running: `git clone http://github.com/ahota/nobody`.

5.1 Dependencies

For running the simulation, the only dependency is a machine with an Nvidia GPU that supports CUDA. For running the web interface, Python's Flask micro-framework needs to be installed to be able to serve the simulation interface as a web server. You can install Flask by running `sudo pip install flask`.

5.2 Compiling

The serial and the parallel implementations can be compiled by running `./src/simulator/compile.sh`.

5.3 Running the simulation

For the serial version, run `./src/simulator/nbody_cpu`. The parallel version can be executed by running `./src/simulator/nbody_cuda`. The parallel version's usage is as follows:

./nbody_cuda -b [NUMBER OF BODIES] -s [NUMBER OF TIMESTEPS] -t [DELTA T]

The parallel version provides an `nbd` file that can be fed into a script as input to make it ready for visualization. This can be done by running `python scale_for_vis.py <filename>`, where filename is the name of the file made by running the simulation. This script creates a simulation.csv file that has to be copied to `./ui/data/` for the web server to pick up. The python web server starts and serves at `localhost:5000` by running `python run.py` in `./src/ui/`. From now on, any web browser can view the simulation on http://localhost:5000.

6 Appendix B: Header file

```
#include<stdio.h>
#include<stdlib.h>
#include<string.h>
#include<unistd.h>
#include<math.h>
#include<sys/time.h>
#include<time.h>

#define CMAX        1496        //+-1 AU * 10e-5
#define CMIN       -1496
#define MMAX        9e2        //approximately mass of Ceres
#define MMIN        14e1        //approximately mass of Bennu
#define AMAX        1000
#define AMIN       -1000
#define VC          299792458    //speed of light

#define EPSILON2    0.5f        //softener used to prevent r^2 -> 0

#define DEF_BODIES 256
#define G           1.0f//6.673e-11f   //gravitational constant
#define DEF_DELTA   0.1f
#define DEF_STEPS   10000

//Lazy programming
int NUM_BODIES, NUM_STEPS;
float DELTA_T;

//tools
int parse_args(int argc, char **argv);
int output = 1;

//parameter functions
float rand_acceleration();
```

```
float rand_coordinate();
float rand_mass();

//timing functions and struct
typedef struct {
        struct timeval start;
        struct timeval end;
} timer;
void start_timer(timer *t);
void stop_timer(timer *t);
float elapsed_time(timer *t);
```

7 Appendix B: Serial version

```
#include "nbody.h"

//CPU-specific structs and functions
typedef struct {
        float x;
        float y;
        float z;
} float3;

typedef struct {
        float x;
        float y;
        float z;
        float w;
} float4;
void interact(float4 *body_i, float4 *body_j, float3 *acc_i, float4 *inter_i);

int main(int argc, char **argv) {
        //Get parameters, if any, from user
        NUM_BODIES = DEF_BODIES;
        NUM_STEPS  = DEF_STEPS;
        DELTA_T    = DEF_DELTA;
        int status = parse_args(argc, argv);
        if(status)
        return status;

        int i, j, t;
        srand(time(NULL));
        timer perf_timer;
        timer total_timer;

        printf("Creating␣bodies...\n");

        float4 *pos_mass;
        float4 *intermediate;
        float3 *acc;

        printf("Allocating␣memory...\n");

        start_timer(&total_timer);
        pos_mass     = (float4 *)malloc(NUM_BODIES * sizeof(float4));
        intermediate = (float4 *)malloc(NUM_BODIES * sizeof(float4));
        acc          = (float3 *)malloc(NUM_BODIES * sizeof(float3));

        printf("Initializing␣bodies...\n");

        for(i = 0; i < NUM_BODIES; i++) {
                pos_mass[i].x = rand_coordinate();
                pos_mass[i].y = rand_coordinate();
                pos_mass[i].z = rand_coordinate();
                pos_mass[i].w = rand_mass();
        }
```

```
	printf("SIMULATION␣SETTINGS:\n");
	printf("␣␣bodies␣␣=␣%d\n", NUM_BODIES);
	printf("␣␣steps␣␣␣=␣%d\n", NUM_STEPS);
	printf("␣␣delta␣t␣=␣%f\n", DELTA_T);

	printf("Running␣simulation...\n");

	start_timer(&perf_timer);
	for(t = 0; t < NUM_STEPS; t++) {
		for(i = 0; i < NUM_BODIES; i++) {
			for(j = 0; j < NUM_BODIES, j != i; j++) {
				interact(&pos_mass[i], &pos_mass[j], &acc[i], &
				    ↪ intermediate[i]);
			}
		}
		//Update positions
		for(i = 0; i < NUM_BODIES; i++) {
			pos_mass[i] = intermediate[i];
		}
	}
	stop_timer(&perf_timer);
	stop_timer(&total_timer);

	printf("Simulation␣runtime:\t%f␣s\n", elapsed_time(&perf_timer));
	printf("Total␣runtime:\t%f␣s\n", elapsed_time(&total_timer));

	if(output) {
		time_t raw_time;
		struct tm *current_time;
		time(&raw_time);
		current_time = localtime(&raw_time);
		char *filename = (char *)malloc(64);
		sprintf(filename, "cpu_%02d%02d%02d_%02d%02d%02d.nbd",
		current_time->tm_year%100, current_time->tm_mon,
		current_time->tm_mday, current_time->tm_hour,
		current_time->tm_min, current_time->tm_sec);

		printf("Saving␣to␣%s...\n", filename);

		FILE *outfile = fopen(filename, "w");
		if(outfile == NULL)
		fprintf(stderr, "Error␣opening␣file\n");
		else {
			fprintf(outfile, "Final␣output:\n");

			fprintf(outfile, "i\tx\t\ty\t\tz\n");
			fprintf(outfile, "---\n");
			for(i = 0; i < NUM_BODIES; i++) {
				fprintf(outfile, "%d\t%f\t%f\t%f\n", i, pos_mass[i].
				    ↪ x,
				pos_mass[i].y, pos_mass[i].z);
			}
			fclose(outfile);
		}
	}

	printf("Done.\n");

	return 0;
}

void interact(float4 *body_i, float4 *body_j, float3 *acc_i, float4 *inter_i) {
	//calculate distance components
	float3 d;
	d.x = body_j->x - body_i->x;
	d.y = body_j->y - body_i->y;
	d.z = body_j->z - body_i->z;

	//use episilon softener
	//  r^2 + epsilon^2
```

```
        float denominator = d.x * d.x + d.y * d.y + d.z * d.z + EPSILON2;
        //cube and sqrt to get (r^2 + epsilon^2)^(3/2)
        denominator = sqrt( denominator * denominator * denominator );

        float acc = G * body_j->w / denominator;

        //update acceleration
        acc_i->x += acc * d.x * DELTA_T;
        acc_i->y += acc * d.y * DELTA_T;
        acc_i->z += acc * d.z * DELTA_T;

        //update position of body i
        inter_i->x = body_i->x + acc_i->x;
        inter_i->y = body_i->y + acc_i->y;
        inter_i->z = body_i->z + acc_i->z;
        inter_i->w = body_i->w;
}

int parse_args(int argc, char **argv) {
        int i;
        for(i = 1; i + 1 <= argc; i += 2) {
                if(strcmp(argv[i], "-h") == 0) {
                        printf("Usage:␣%s␣[-b␣num_bodies]␣[-s␣num_steps]␣[-t␣delta_t
                            ↪ ]␣\␣[-o]\n", argv[0]);
                        return 1;
                }
                else if(strcmp(argv[i], "-b") == 0) {
                        NUM_BODIES = atoi(argv[i + 1]);
                }
                else if(strcmp(argv[i], "-s") == 0) {
                        NUM_STEPS  = atoi(argv[i + 1]);
                }
                else if(strcmp(argv[i], "-t") == 0) {
                        DELTA_T    = atof(argv[i + 1]);
                }
                else if(strcmp(argv[i], "-o") == 0) {
                        output     = 0;
                }
                else {
                        fprintf(stderr, "Error:␣unsupported␣flag␣%s\n", argv[i]);
                        return -1;
                }
        }
        return 0;
}

float rand_coordinate() {
        return ((float)rand() / (float)RAND_MAX) * (CMAX - CMIN) + CMIN;
}

float rand_acceleration() {
        return ((float)rand() / (float)RAND_MAX) * (AMAX - AMIN) + AMIN;
}

float rand_mass() {
        return ((float)rand() / (float)RAND_MAX) * (MMAX - MMIN) + MMIN;
}

void start_timer(timer *t) {
        gettimeofday( &(t->start), NULL);
}

void stop_timer(timer *t) {
        gettimeofday( &(t->end), NULL);
}

float elapsed_time(timer *t) {
        return (float) (t->end.tv_sec  - t->start.tv_sec)  +
        (t->end.tv_usec - t->start.tv_usec) /
        1000000.0;
```

```
	}
```

8 Appendix C: Parallel version

```
#include "nbody.h"
#include<cuda.h>

//CUDA-specific vars and functions
__device__ int NBODIES;
__device__ float DT;
__global__ void main_nbody_kernel(float4 *dev_pos_mass, float3 *dev_acc,
float3 *dev_output, int cur_step);
__device__ void tile_nbody_kernel(float4 *my_pos_mass, float3 *my_acc);
__device__ void force_kernel(float4 *body_i, float4 *body_j,
float3 *acc_i);

int main(int argc, char **argv) {
	//Get parameters, if any, from user
	NUM_BODIES = DEF_BODIES;
	NUM_STEPS  = DEF_STEPS;
	DELTA_T    = DEF_DELTA;
	int status = parse_args(argc, argv);
	if(status)
	return status;
	cudaMemcpyToSymbol(NBODIES, &NUM_BODIES, sizeof(int), 0,
	cudaMemcpyHostToDevice);
	cudaMemcpyToSymbol(DT, &DELTA_T, sizeof(int), 0,
	cudaMemcpyHostToDevice);

	int i;
	srand(time(NULL));
	timer perf_timer;
	timer total_timer;

	printf("Creating bodies...\n");

	float4 *host_pos_mass, *dev_pos_mass;
	float3 *host_acc, *dev_acc;
	float3 *host_output, *dev_output;

	printf("Allocating host memory...\n");

	start_timer(&total_timer);
	host_pos_mass = (float4 *)malloc(NUM_BODIES * sizeof(float4));
	host_acc      = (float3 *)malloc(NUM_BODIES * sizeof(float3));
	host_output   = (float3 *)malloc(NUM_BODIES * NUM_STEPS * sizeof(float3));

	printf("Allocating device memory...\n");

	cudaMalloc((void **)&dev_pos_mass, NUM_BODIES * sizeof(float4));
	cudaMalloc((void **)&dev_acc, NUM_BODIES * sizeof(float3));
	cudaMalloc((void **)&dev_output, NUM_BODIES * NUM_STEPS * sizeof(float3));

	printf("Initializing bodies...\n");

	for(i = 0; i < NUM_BODIES; i++) {
		host_pos_mass[i].x = rand_coordinate();
		host_pos_mass[i].y = rand_coordinate();
		host_pos_mass[i].z = rand_coordinate();
		host_pos_mass[i].w = rand_mass();
	}

	printf("SIMULATION SETTINGS:\n");
	printf("  bodies  = %d\n", NUM_BODIES);
	printf("  steps   = %d\n", NUM_STEPS);
	printf("  delta t = %f\n", DELTA_T);
```

```
/*
printf("Initial positions and masses:\n");
for(i = 0; i < NUM_BODIES; i++) {
        printf("%d:\t%f\t%f\t%f\n", i, host_pos_mass[i].x, host_pos_mass[i].y,
        host_pos_mass[i].z, host_pos_mass[i].w);
}
*/

printf("Copying␣to␣device...\n");

cudaMemcpy(dev_pos_mass, host_pos_mass, NUM_BODIES * sizeof(float3),
cudaMemcpyHostToDevice);
cudaMemcpy(dev_acc, host_acc, NUM_BODIES * sizeof(float3),
cudaMemcpyHostToDevice);
cudaMemcpy(dev_output, host_output, NUM_BODIES * NUM_STEPS * sizeof(float3),
cudaMemcpyHostToDevice);

printf("Running␣kernel...\n");

start_timer(&perf_timer);
int block_size = (NUM_BODIES < 16) ? 4 : (NUM_BODIES < 256) ? 16 : 32;
int grid_size  = NUM_BODIES / block_size;
int mem_size = (block_size+1) * sizeof(float4);
printf("KERNEL␣SETTINGS:\n");
printf("␣␣bodies␣␣␣␣␣=␣%d\n", NUM_BODIES);
printf("␣␣tile␣size␣=␣%d\n", block_size);
printf("␣␣grid␣size␣=␣%d\n", grid_size);
for(i = 0; i < NUM_STEPS; i++) {
        main_nbody_kernel<<<grid_size, block_size, mem_size>>>(dev_pos_mass,
        dev_acc, dev_output, i);
}
stop_timer(&perf_timer);

printf("Simulation␣runtime:\t%f␣s\n", elapsed_time(&perf_timer));

printf("Copying␣to␣host...\n");

cudaMemcpy(host_output, dev_output, NUM_BODIES * NUM_STEPS * sizeof(float3),
cudaMemcpyDeviceToHost);
cudaFree(dev_pos_mass);
cudaFree(dev_acc);
cudaFree(dev_output);
stop_timer(&total_timer);

printf("Total␣runtime:\t%f␣s\n", elapsed_time(&total_timer));

if(output) {
        time_t raw_time;
        struct tm *current_time;
        time(&raw_time);
        current_time = localtime(&raw_time);
        char *filename = (char *)malloc(64);
        sprintf(filename, "cuda_%02d%02d%02d_%02d%02d%02d.nbd",
        current_time->tm_year%100, current_time->tm_mon,
        current_time->tm_mday, current_time->tm_hour,
        current_time->tm_min, current_time->tm_sec);

        printf("Saving␣to␣%s...\n", filename);

        FILE *outfile = fopen(filename, "w");
        if(outfile == NULL)
        fprintf(stderr, "Error␣opening␣file\n");
        else {
                //printf("%f\n", host_output[0].x);
                fprintf(outfile, "%d,%d\n", NUM_BODIES, NUM_STEPS);
                for(i = 0; i < NUM_BODIES * NUM_STEPS; i++) {
                        fprintf(outfile, "%f,%f,%f\n", host_output[i].x,
                        host_output[i].y, host_output[i].z);
                }
```

```
                        fclose(outfile);
                }
        }

        printf("Done.\n");
        return 0;
}

__global__ void main_nbody_kernel(float4 *dev_pos_mass, float3 *dev_acc,
float3 *dev_output, int cur_step) {
        //index into global arrays for this thread's body
        int global_id = blockIdx.x * blockDim.x + threadIdx.x;

        //local copies of this body's position, mass, and acceleration
        float4 my_pos_mass = dev_pos_mass[global_id];
        float3 my_acc = dev_acc[global_id];

        //copy of position and mass for bodies in the current tile
        extern __shared__ float4 tile_pos_mass[];

        //iterate over all tiles and update position and acceleration
        //each iteration loads one tile's worth of data from global memory
        //these reads should be coalesced
        int i, tile;
        for(i = 0, tile = 0; i < NBODIES; i += blockDim.x, tile++) {
                //index into global for this thread's body *for this tile*
                int tile_id = tile * blockDim.x + threadIdx.x;

                //threads collaborate to load from global for this tile
                tile_pos_mass[threadIdx.x] = dev_pos_mass[tile_id];
                __syncthreads();

                //update acceleration for this thread's body for this tile
                tile_nbody_kernel(&my_pos_mass, &my_acc);
                __syncthreads();
        }

        //update position for this body
        my_pos_mass.x += my_acc.x;
        my_pos_mass.y += my_acc.y;
        my_pos_mass.z += my_acc.z;

        //update global position array
        dev_pos_mass[global_id] = my_pos_mass;
        dev_acc[global_id] = my_acc;

        //update global output
        dev_output[cur_step * NBODIES + global_id].x = my_pos_mass.x;
        dev_output[cur_step * NBODIES + global_id].y = my_pos_mass.y;
        dev_output[cur_step * NBODIES + global_id].z = my_pos_mass.z;
}

__device__ void tile_nbody_kernel(float4 *my_pos_mass, float3 *my_acc) {
        //tile position array from the outer kernel
        //pre-loaded with this tile's positions and masses
        extern __shared__ float4 tile_pos_mass[];

        //iterate over each body in the tile and calculate its effect on
        //this thread's body
        int i;
        for(i = 0; i < blockDim.x; i++) {
                force_kernel(my_pos_mass, &tile_pos_mass[i], my_acc);
        }
}

__device__ void force_kernel(float4 *body_i, float4 *body_j, float3 *acc_i) {
        //calculate distance components
        float3 d;
        d.x = body_j->x - body_i->x;
        d.y = body_j->y - body_i->y;
```

```
            d.z = body_j->z - body_i->z;

            //use epsilon softener
            //  r^2 + epsilon^2
            float denominator = d.x * d.x + d.y * d.y + d.z * d.z + EPSILON2;
            //cube and sqrt to get (r^2 + epsilon^2)^(3/2)
            denominator = sqrt( denominator * denominator * denominator );

            float acc = G * body_j->w / denominator;

            //update acceleration
            acc_i->x += acc * d.x * DT;
            acc_i->y += acc * d.y * DT;
            acc_i->z += acc * d.z * DT;
    }

    int parse_args(int argc, char **argv) {
            int i;
            for(i = 1; i + 1 <= argc; i += 2) {
                    if(strcmp(argv[i], "-h") == 0) {
                            printf("Usage: %s [-b num_bodies] [-s num_steps] [-t delta_t ] \
                                    [-o]\n", argv[0]);
                            return 1;
                    }
                    else if(strcmp(argv[i], "-b") == 0) {
                            NUM_BODIES = atoi(argv[i + 1]);
                    }
                    else if(strcmp(argv[i], "-s") == 0) {
                            NUM_STEPS  = atoi(argv[i + 1]);
                    }
                    else if(strcmp(argv[i], "-t") == 0) {
                            DELTA_T    = atof(argv[i + 1]);
                    }
                    else if(strcmp(argv[i], "-o") == 0) {
                            output     = 0;
                    }
                    else {
                            fprintf(stderr, "Error: unsupported flag %s\n", argv[i]);
                            return -1;
                    }
            }
            return 0;
    }

    float rand_coordinate() {
            return ((float)rand() / (float)RAND_MAX) * (CMAX - CMIN) + CMIN;
    }

    float rand_acceleration() {
            return ((float)rand() / (float)RAND_MAX) * (AMAX - AMIN) + AMIN;
    }

    float rand_mass() {
            return ((float)rand() / (float)RAND_MAX) * (MMAX - MMIN) + MMIN;
    }

    void start_timer(timer *t) {
            gettimeofday( &(t->start), NULL);
    }

    void stop_timer(timer *t) {
            gettimeofday( &(t->end), NULL);
    }

    float elapsed_time(timer *t) {
            return (float) (t->end.tv_sec  - t->start.tv_sec)  +
            (t->end.tv_usec - t->start.tv_usec) /
            1000000.0;
    }
```