

# HPP\_A3

Group20

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[galsim.c](#)

## 1. The Problem

This task require us to implement a program that simulates the gravitational interaction between N particles in a galaxy using Newton's law of gravitation. The simulation involves updating the positions and velocities of the particles over a certain number of timesteps. Based on the given mathematical function and instruction, we wrote the initial version code, and use optimization techniques to do further improvement.

## 2. The Solution

### 2.1 Initial Version Code

The following is the initial version of the code, without any use both compiler optimisation flags and our own code changes.

```
/*Initial Version*/

#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <string.h>

#define EPSILON 0.001

typedef struct {
    double position_x;
    double position_y;
    double mass;
    double velocity_x;
    double velocity_y;
    double brightness;
} Particle;

typedef struct{
    double force_x;
    double force_y;
}Force;

void read_initial_configuration(const char *filename, Particle *particles, int N) {
    // Implement function to read initial configuration from file

    FILE *file = fopen(filename, "rb");
    if (file == NULL) {
        fprintf(stderr, "Error: Could not open file %s\n", filename);
        exit(1);
    }

    // Read the particles from the file
    size_t particles_read = fread(particles, sizeof(Particle), N, file);
```

```

    if (particles_read == 0) {
        fprintf(stderr, "Error: Could not read from file %s\n", filename);
        exit(1);
    }

    fclose(file);
}

void compute_forces(Particle *particles, Force *forces, int N) {
    // Implement function to compute forces between particles
    double G = 100.0/N;
    for (int i = 0; i < N; i++) {
        forces[i].force_x = 0.0;
        forces[i].force_y = 0.0;

        for (int j = 0; j < N; j++) {
            if (j != i) {
                double dx = particles[i].position_x - particles[j].position_x;
                double dy = particles[i].position_y - particles[j].position_y;
                double distance = sqrt(dx * dx + dy * dy);
                double force_magnitude = -G \
* particles[i].mass * particles[j].mass / pow(distance + EPSILON, 3);
                forces[i].force_x += force_magnitude * dx;
                forces[i].force_y += force_magnitude * dy;
            }
        }
    }
}

void update_particle(Particle *particle, Force *force, double delta_t) {
    // Implement function to update position and velocity of a particle
    particle->velocity_x += delta_t * force->force_x / particle->mass;
    particle->velocity_y += delta_t * force->force_y / particle->mass;
    particle->position_x += delta_t * particle->velocity_x;
    particle->position_y += delta_t * particle->velocity_y;
}

void simulate(Particle *particles, Force *forces, int N, int nsteps, double delta_t) {
    for (int step = 0; step < nsteps; step++) {
        compute_forces(particles, forces, N);
        for (int i = 0; i < N; i++) {
            update_particle(&particles[i], &forces[i], delta_t);
        }
    }
}

void write_results(const char *filename, Particle *particles, int N) {
    // Implement function to write results to file
    FILE *file = fopen(filename, "wb");

    size_t particles_written = fwrite(particles, sizeof(Particle), N, file);
    if (particles_written != N) {
        fprintf(stderr, "Error: Could not write to file %s\n", filename);
        exit(1);
    }

    fclose(file);
}

```

```

int main(int argc, char *argv[]) {
    // Parse command line arguments
    if (argc != 6) {
        printf("Usage: %s N filename nsteps delta_t graphics\n", argv[0]);
        return 1;
    }
    int N = atoi(argv[1]);
    char *filename = argv[2];
    int nsteps = atoi(argv[3]);
    double delta_t = atof(argv[4]);
    int graphics = atoi(argv[5]);

    Particle *particles = malloc(N * sizeof(Particle));
    if (particles == NULL) {
        fprintf(stderr, "Memory allocation failed\n");
        return 1;
    }
    Force *forces = malloc(N * sizeof(Force));
    if (forces == NULL) {
        fprintf(stderr, "Memory allocation failed\n");
        return 1;
    }

    read_initial_configuration(filename, particles, N);
    simulate(particles, forces, N, nsteps, delta_t);
    write_results("result.gal", particles, N);

    free(particles);
    free(forces);

    return 0;
}

```

## 2.2 Time Consuming

```

"Initial version time consuming"
time ./galsim 1500 ellipse_N_01500.gal 100 0.00001 1

"PC1"
real    0m9.844s
user    0m9.844s
sys     0m0.000s

"PC2"
real    0m22.830s
user    0m22.818s
sys     0m0.000s

```

## 2.3 Accuracy

```

"Initial version accuracy"

N = 10
fileName1 = '../result.gal'
fileName2 = '../ref_output_data/ellipse_N_00010_after200steps.gal'
pos_maxdiff = 0.000000000000

```

```

N = 3000
fileName1 = '../result.gal'
fileName2 = '../ref_output_data/ellipse_N_03000_after100steps.gal'
pos_maxdiff = 0.000000000000

```

## 3. Performance

### 3.1 Summary

The performance of the code improved significantly after optimizations. By avoiding repeated computations, eliminating the use of `pow()`, loop skipping, merging functions, and using compiler optimizations, we saw a decrease in computation time.

Among the different optimization levels on each PC, the lower real time values indicate better performance.

On PC1, the -O1 and -O4 optimizations have the lowest real time values both at 2.114s. On PC2, the -O3 optimization level has the lowest real time at 10.146s.

### 3.2 CPU Model

```

"PC1 CPU model"
lish6557@LAPTOP-B927FN7A:~/HPP/Assignment3$ lscpu
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Address sizes:          39 bits physical, 48 bits virtual
Byte Order:             Little Endian
CPU(s):                 20
On-line CPU(s) list:   0-19
Vendor ID:              GenuineIntel
Model name:             12th Gen Intel(R) Core(TM) i7-12700H
CPU family:             6
Model:                  154
Thread(s) per core:     2
Core(s) per socket:     10
Socket(s):              1

```

```

"PC1 compiler version"
gcc (Ubuntu 11.4.0-1ubuntu1~22.04) 11.4.0
Copyright (C) 2021 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.

```

```

"PC2 CPU model"
holi6891@arrhenius:~/Assignment3$ lscpu
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Address sizes:          40 bits physical, 48 bits virtual
Byte Order:             Little Endian
CPU(s):                 16
On-line CPU(s) list:   0-15
Vendor ID:              GenuineIntel
Model name:             Intel(R) Xeon(R) CPU                    E5520   @ 2.27GHz
CPU family:             6
Model:                  26
Thread(s) per core:     2
Core(s) per socket:     4
Socket(s):              2

```

```
"PC2 compiler version"
gcc (Ubuntu 11.4.0-1ubuntu1~22.04) 11.4.0
Copyright (C) 2021 Free Software Foundation, Inc.
This is free software; see the source for copying conditions.  There is NO
warranty; not even for MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE.
```

## 3.3 Optimisation

### 3.3.1 Optimisation within Code

When performing in-code optimisations, start with the initial version of the code and don't use any compiler optimisation flags.

```
"makefile used in 3.3.1"

galsim: galsim.c
gcc -o galsim galsim.c -lm
clean:
rm -f galsim
```

#### 1. Avoiding repeat computations

```
/*Avoiding repeat computations*/

//.....

void compute_forces(Particle *particles, Force *forces, int N) {
    // Implement function to compute forces between particles
    double G = 100.0 / N;
    for (int i = 0; i < N; i++) {
        forces[i].force_x = 0.0;
        forces[i].force_y = 0.0;

        double position_x_i = particles[i].position_x;
        double position_y_i = particles[i].position_y;
        double mass_i = particles[i].mass;

        for (int j = 0; j < N; j++) {
            if (j != i) {
                double dx = position_x_i - particles[j].position_x;
                double dy = position_y_i - particles[j].position_y;
                double distance = sqrt(dx * dx + dy * dy);
                double force_magnitude = -G * \
particles[i].mass * particles[j].mass / pow(distance + EPSILON, 3);
                forces[i].force_x += force_magnitude * dx;
                forces[i].force_y += force_magnitude * dy;
            }
        }
    }
}

void update_particle(Particle *particle, Force *force, double delta_t) {
    // Implement function to update position and velocity of a particle
    double delta_t_mass = delta_t / particle->mass;
    particle->velocity_x += delta_t_mass * force->force_x;
    particle->velocity_y += delta_t_mass * force->force_y;
    particle->position_x += delta_t * particle->velocity_x;
    particle->position_y += delta_t * particle->velocity_y;
```

```
}
//.....
```

1. In the `compute_forces` function, the positions and masses of each particle are calculated in advance to avoid repeated retrieval in the inner loop.
2. In the `update_particle` function, the parts of repeated calculations `delta_t_mass` are calculated in advance to avoid repeated calculations.

```
"Time consuming avoiding repeat computation"
time ./galsim 1500 ellipse_N_01500.gal 100 0.00001 1

      before              after
"PC1"
real   0m9.844s          real   0m9.103s
user   0m9.844s          user   0m9.102s
sys    0m0.000s          sys    0m0.000s

"PC2"
real   0m22,830s         real   0m22,113s
user   0m22,818s         user   0m21,969s
sys    0m0,000s          sys    0m0,132s

"Accuracy"
N = 10
fileName1 = '../result.gal'
fileName2 = '../ref_output_data/ellipse_N_00010_after200steps.gal'
pos_maxdiff = 0.000000000000

N = 3000
fileName1 = '../result.gal'
fileName2 = '../ref_output_data/ellipse_N_03000_after100steps.gal'
pos_maxdiff = 0.000000000000
```

## 2.Avoiding use pow()

```
/*Avoiding use pow()*/
//.....

void compute_forces(Particle *particles, Force *forces, int N) {
    // Implement function to compute forces between particles
    double G = 100.0 / N;
    for (int i = 0; i < N; i++) {
        forces[i].force_x = 0.0;
        forces[i].force_y = 0.0;

        double position_x_i = particles[i].position_x;
        double position_y_i = particles[i].position_y;
        double mass_i = particles[i].mass;

        for (int j = 0; j < N; j++) {
            if (j != i) {
                double dx = position_x_i - particles[j].position_x;
                double dy = position_y_i - particles[j].position_y;
                double distance_squared = sqrt(dx * dx + dy * dy) + EPSILON;
            }
        }
    }
}
```

```

        double distance_cubed = distance_squared*
\distance_squared * distance_squared;
        double force_magnitude = -G * mass_i * particles[j].mass / distance_cubed;
        forces[i].force_x += force_magnitude * dx;
        forces[i].force_y += force_magnitude * dy;
    }
}
}
}

//.....

```

1. In the `compute_forces` function, avoid using `pow()`. Arithmetic operations are faster than function calls.

```

"Time consuming avoiding use pow()"
time ./galsim 1500 ellipse_N_01500.gal 100 0.00001 1

          before                after
"PC1"
real      0m9.103s                real      0m2.403s
user      0m9.102s                user      0m2.403s
sys       0m0.000s                sys       0m0.001s

"PC2"
real      0m22,113s                real      0m7,710s
user      0m21,969s                user      0m7,704s
sys       0m0,132s                sys       0m0,000s

"Accuracy"
N = 10
fileName1 = '../result.gal'
fileName2 = '../ref_output_data/ellipse_N_00010_after200steps.gal'
pos_maxdiff = 0.000000000000

N = 3000
fileName1 = '../result.gal'
fileName2 = '../ref_output_data/ellipse_N_03000_after100steps.gal'
pos_maxdiff = 0.000000000000

```

### 3. Loop avoidance

```

/*Loop avoidance*/

//.....

void compute_forces(Particle *particles, Force *forces, int N) {
    double G = 100.0/N;
    for (int i = 0; i < N; i++){
        forces[i].force_x = 0.0;
        forces[i].force_y = 0.0;
    }
    //memset(forces, 0, N * sizeof(Force));
    //memset worse than using loops
    for (int i = 0; i < N; i++) {
        double position_x_i = particles[i].position_x;
        double position_y_i = particles[i].position_y;
        double mass_i = particles[i].mass;

```

```

    for (int j = i + 1; j < N; j++) {
        double dx = position_x_i - particles[j].position_x;
        double dy = position_y_i - particles[j].position_y;
        double distance_squared = sqrt(dx * dx + dy * dy) + EPSILON;
        double distance_cubed = distance_squared * \
                                distance_squared * distance_squared;
        double force_magnitude = -G * mass_i * particles[j].mass / distance_cubed;
        forces[i].force_x += force_magnitude * dx;
        forces[i].force_y += force_magnitude * dy;

        forces[j].force_x -= force_magnitude * dx;
        forces[j].force_y -= force_magnitude * dy;
    }
}

//.....

```

1. In the `compute_forces` function, optimizes this by starting the inner loop (j) from i+1, effectively avoiding redundant force calculations for pairs of particles

```

"Time consuming with loop unrolling"
time ./galsim 1500 ellipse_N_01500.gal 100 0.00001 1

      before              after
"PC1"
real    0m2.403s          real    0m1.511s
user    0m2.403s          user    0m1.510s
sys     0m0.001s          sys     0m0.000s

"PC2"
real    0m7,710s          real    0m5,405s
user    0m7,704s          user    0m5,395s
sys     0m0,000s          sys     0m0,000s

"Accuracy"
N = 10
fileName1 = '../result.gal'
fileName2 = '../ref_output_data/ellipse_N_00010_after200steps.gal'
pos_maxdiff = 0.000000000000

N = 3000
fileName1 = '../result.gal'
fileName2 = '../ref_output_data/ellipse_N_03000_after100steps.gal'
pos_maxdiff = 0.000000000000

```

#### 4. Merge functions

```

/*Merge functions*/

//.....

void simulate(Particle *particles, Force *forces, int N, int nsteps, double delta_t) {
    double G = 100.0/N;
    for (int step = 0; step < nsteps; step++) {
        for (int i = 0; i < N; i++){

```



```

        forces[i].force_x = 0.0;
        forces[i].force_y = 0.0;
    }
    for (int i = 0; i < N; i++) {
        double position_x_i = particles[i].position_x;
        double position_y_i = particles[i].position_y;
        double mass_i = particles[i].mass;

        for (int j = i + 1; j < N; j++) {
            double dx = position_x_i - particles[j].position_x;
            double dy = position_y_i - particles[j].position_y;
            double distance_squared = sqrt(dx * dx + dy * dy) + EPSILON;
            double distance_cubed = distance_squared \
* distance_squared * distance_squared;
            double force_magnitude = -G * mass_i * particles[j].mass / distance_cubed;
            forces[i].force_x += force_magnitude * dx;
            forces[i].force_y += force_magnitude * dy;

            forces[j].force_x -= force_magnitude * dx;
            forces[j].force_y -= force_magnitude * dy;
        }
    }
    for (int i = 0; i < N; i++) {
        update_particle(&particles[i], &forces[i], delta_t);
    }
}

}

//.....

```

1. Merging `compute_forces()` and `simulate()` into one function can improve performance by reducing the overhead of function calls. Every function call involves a certain amount of overhead, including the time it takes to jump to the function's code, push arguments onto the stack, and then pop the results off the stack.

```

"Time consuming after merging functions"
time ./galsim 1500 ellipse_N_01500.gal 100 0.00001 1

      before          after
"PC1"
real    0m1.511s      real    0m1.502s
user    0m1.510s      user    0m1.502s
sys     0m0.000s      sys     0m0.000s

"PC2"
real    0m5,405s      real    0m4,745s
user    0m5,395s      user    0m4,739s
sys     0m0,000s      sys     0m0,001s

"Accuracy"
N = 10
fileName1 = '../result.gal'
fileName2 = '../ref_output_data/ellipse_N_00010_after200steps.gal'
pos_maxdiff = 0.000000000000

N = 3000
fileName1 = '../result.gal'

```

```

fileName2 = '../ref_output_data/ellipse_N_03000_after100steps.gal'
pos_maxdiff = 0.000000000000

```

### 3.3.2 Compiler Optimisation

The following is the final version of the code, which has undergone our own code changes.

```

/*Final Version*/

#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <string.h>

#define EPSILON 0.001

typedef struct {
    double position_x;
    double position_y;
    double mass;
    double velocity_x;
    double velocity_y;
    double brightness;
} Particle;

typedef struct{
    double force_x;
    double force_y;
}Force;

void read_initial_configuration(const char *filename, Particle *particles, int N) {
    // Implement function to read initial configuration from file

    char filepath[100];

    strcpy(filepath, "input_data/");
    strcat(filepath, filename);
    FILE *file = fopen(filepath, "rb");
    if (file == NULL) {
        fprintf(stderr, "Error: Could not open file %s\n", filename);
        exit(1);
    }

    // Read the particles from the file
    size_t particles_read = fread(particles, sizeof(Particle), N, file);
    if (particles_read == 0) {
        fprintf(stderr, "Error: Could not read from file %s\n", filename);
        exit(1);
    }

    fclose(file);
}

void update_particle(Particle *particle, Force *force, double delta_t) {
    // Implement function to update position and velocity of a particle
    double delta_t_mass = delta_t / particle->mass;
    particle->velocity_x += delta_t_mass * force->force_x;
    particle->velocity_y += delta_t_mass * force->force_y;
}

```

```

    particle->position_x += delta_t * particle->velocity_x;
    particle->position_y += delta_t * particle->velocity_y;
}

void simulate(Particle *particles, Force *forces, int N, int nsteps, double delta_t) {
    double G = 100.0/N;
    for (int step = 0; step < nsteps; step++) {
        for (int i = 0; i < N; i++){
            forces[i].force_x = 0.0;
            forces[i].force_y = 0.0;
        }
        for (int i = 0; i < N; i++) {
            double position_x_i = particles[i].position_x;
            double position_y_i = particles[i].position_y;
            double mass_i = particles[i].mass;

            for (int j = i + 1; j < N; j++) {
                double dx = position_x_i - particles[j].position_x;
                double dy = position_y_i - particles[j].position_y;
                double distance_squared = sqrt(dx * dx + dy * dy) + EPSILON;
                double distance_cubed = distance_squared * \
distance_squared * distance_squared;
                double force_magnitude = -G * mass_i * particles[j].mass / distance_cubed;
                forces[i].force_x += force_magnitude * dx;
                forces[i].force_y += force_magnitude * dy;

                forces[j].force_x -= force_magnitude * dx;
                forces[j].force_y -= force_magnitude * dy;
            }
        }
        for (int i = 0; i < N; i++) {
            update_particle(&particles[i], &forces[i], delta_t);
        }
    }
}

void write_results(const char *filename, Particle *particles, int N) {
    // Implement function to write results to file
    FILE *file = fopen(filename, "wb");

    size_t particles_written = fwrite(particles, sizeof(Particle), N, file);
    if (particles_written != N) {
        fprintf(stderr, "Error: Could not write to file %s\n", filename);
        exit(1);
    }

    fclose(file);
}

int main(int argc, char *argv[]) {
    // Parse command line arguments
    if (argc != 6) {
        printf("Usage: %s N filename nsteps delta_t graphics\n", argv[0]);
        return 1;
    }
    int N = atoi(argv[1]);
    char *filename = argv[2];

```

```

int nsteps = atoi(argv[3]);
double delta_t = atof(argv[4]);
int graphics = atoi(argv[5]);

Particle *particles = malloc(N * sizeof(Particle));
if (particles == NULL) {
    fprintf(stderr, "Memory allocation failed\n");
    return 1;
}
Force *forces = malloc(N * sizeof(Force));
if (forces == NULL) {
    fprintf(stderr, "Memory allocation failed\n");
    return 1;
}

read_initial_configuration(filename, particles, N);
simulate(particles, forces, N, nsteps, delta_t);
write_results("result.gal", particles, N);

free(particles);
free(forces);

return 0;
}

```

Then trying the ability of different compiler optimisation methods to optimise the final code.

```

"Using final version code"
time ./galsim 3000 ellipse_N_03000.gal 100 0.00001 1

"Without using compiler optimisation"
gcc -o galsim galsim.c -lm

"Using -O1"
gcc -O1 -o galsim galsim.c -lm

"Using -O2"
gcc -O2 -o galsim galsim.c -lm

"Using -O3"
gcc -O3 -o galsim galsim.c -lm

"Using -O4"
gcc -O4 -o galsim galsim.c -lm

"Using -Os"
gcc -Os -o galsim galsim.c -lm

"Using -Ofast"
gcc -Ofast -o galsim galsim.c -lm

```

- **01**: Basic optimization, attempting to reduce code size and execution time, including constant folding and removal of useless code.
- **02**: Further performance improvement, including dead code elimination, function inlining, common subexpression elimination, etc.
- **03**: Higher-level optimizations, including all **02** level optimizations, as well as loop unrolling, vectorization, more function inlining, etc. It may increase code size and compilation time.

- `-O4` : This is not a standard option for the GCC compiler, generally, it is considered equivalent to `-O3`.
- `-Os` : Optimize code size without significantly affecting performance, suitable for embedded systems, etc.
- `-Ofast` : Enable all `-O3` level optimizations and further enable some optimizations that may change program behavior. Allow the compiler to assume no floating-point exceptions, which may enable more optimizations.

"PC1"	Initial	-O1	-O2	-O3	-O4	-Os	-Ofast
real	0m6.299s	0m2.114s	0m2.132s	0m2.136s	0m2.114s	0m2.890s	0m2.115s
user	0m6.299s	0m2.114s	0m2.132s	0m2.135s	0m2.114s	0m2.890s	0m2.115s
sys	0m0.000s	0m0.000s	0m0.001s	0m0.000s	0m0.000s	0m0.000s	0m0.000s

"PC2"	Initial	-O1	-O2	-O3	-O4	-Os	-Ofast
real	0m20,806s	0m10,207s	0m10,538s	0m10,146s	0m10,156s	0m10,541s	0m10,157s
user	0m20,795s	0m10,196s	0m10,528s	0m10,140s	0m10,149s	0m10,530s	0m10,156s
sys	0m0,004s	0m0,004s	0m0,004s	0m0,000s	0m0,001s	0m0,004s	0m0,001s

The difference between the vectorized `-O3` and the non-vectorized `-O1` and `-O2` is not significant, which may be influenced by the following factors:

1. **External functions inside the loop:** In the `simulate` function, the part that updates the particle position and speed includes a call to an external function, namely the `sqrt()` function. Although this is a standard mathematical library function, it will hinder vectorization unless it is inlined.
2. **Conditional statements:** There are conditional statements in the loop `if (j != i)`, which limit the possibility of vectorization, because it is difficult to predict the result of conditional statements during vectorization. In addition, `break` and `continue` statements may also prevent the loop from being vectorized.
3. **Data dependency:** In the inner loop, there are data dependencies in the calculation of forces between particles, i.e., the results of subsequent calculations depend on the results of previous calculations. This dependency may complicate vectorization because vectorization will change the order of operations.
4. **Memory access pattern:** The calculation of forces between particles may lead to non-continuous memory access patterns, which may affect the effect of vectorization.

```
"Final makefile"
"-O3/O4 seems better compared with other optimisation methods"
"All the compiler optimisation methods keep the code accuracy 0.0000"

galsim: galsim.c
gcc -O4 -o galsim galsim.c -lm
clean:
rm -f galsim
```

## 4. Discussion

### 4.1. Time complexity

How the computational time depends on N?

```
"Final version code with -O4 compiler optimisation"

"PC1"
time ./galsim 3000 ellipse_N_03000.gal 100 0.00001 1
real    0m2.158s
user    0m2.158s
sys     0m0.000s

time ./galsim 1500 ellipse_N_01500.gal 100 0.00001 1
real    0m0.539s
user    0m0.539s
```

```

sys      0m0.000s

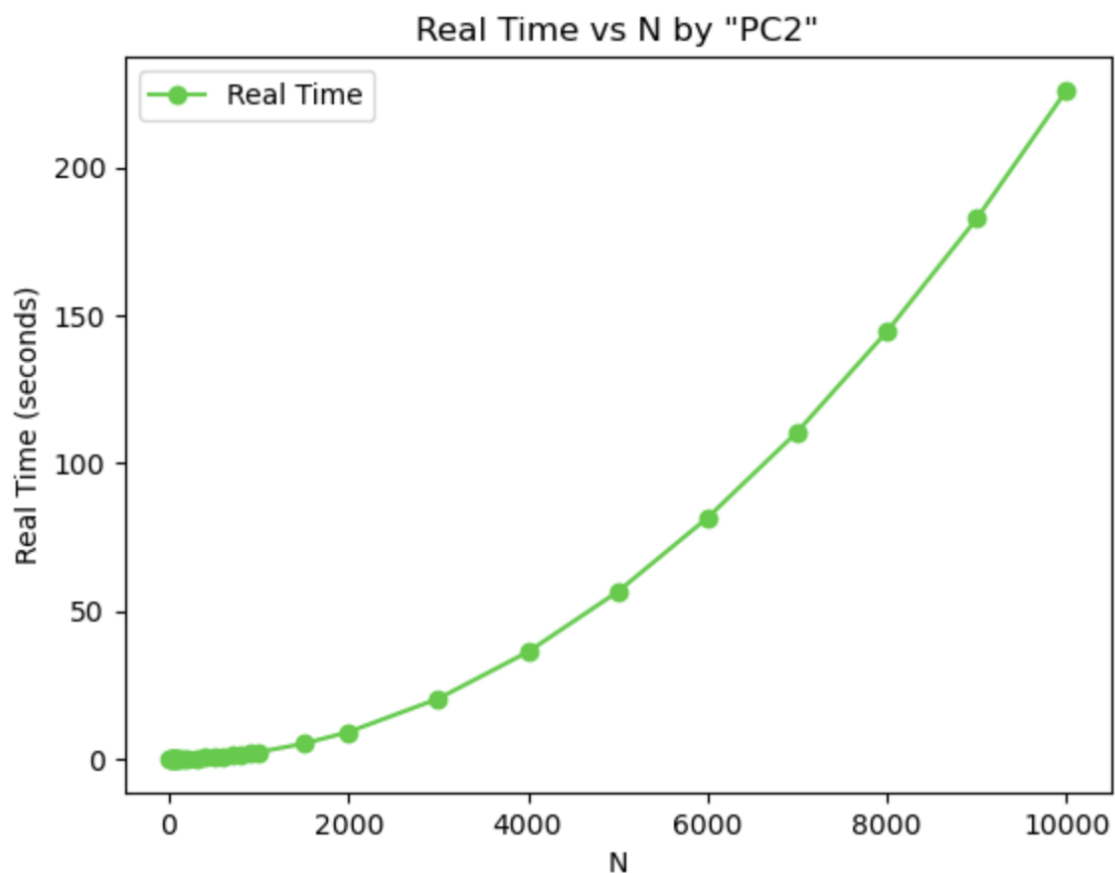
"PC2"
time ./galsim 3000 ellipse_N_03000.gal 200 0.00001 1
real      0m20,299s
user      0m20,291s
sys      0m0,001s

time ./galsim 1500 ellipse_N_03000.gal 200 0.00001 1

real      0m5,089s
user      0m5,081s
sys      0m0,005s

```

The real time to run 3000 particles is always around 4 times that of running 1500 particles, which proves that the time complexity of the code is  $O(N^2)$ .



## 4.2 Accuracy

```

"Final version accuracy"

N = 10
fileName1 = '../input_data/ellipse_N_00010.gal'
fileName2 = '../ref_output_data/ellipse_N_00010_after200steps.gal'
pos_maxdiff = 0.000000000000

N = 3000
fileName1 = '../input_data/ellipse_N_03000.gal'

```

```
fileName2 = '../ref_output_data/ellipse_N_03000_after100steps.gal'  
pos_maxdiff = 0.000000000000
```

We notice that the maximum difference in position ( `pos_maxdiff` ) is equal to 0 for both simulations with 10 and 3000 particles, indicating that the simulation is quite accurate.

### 4.3 Limitations and Further Improvements

Despite the significant performance improvements, there are still some limitations and potential areas for further optimization. For example, the current code does not take advantage of parallel computing, which could further speed up the calculations. Also, more sophisticated algorithms for handling particle interactions, such as the Barnes-Hut algorithm, could be used to improve performance for large particle numbers.