

Math 4997-3

Lecture 4: N-Body simulations, Structs, Classes, and generic functions

Patrick Diehl 

<https://www.cct.lsu.edu/~pdiehl/teaching/2021/4997/>

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Lecture 3

What you should know from last lecture

- ▶ Iterators
- ▶ Lists
- ▶ Library algorithms
- ▶ Numerical limits
- ▶ Reading and Writing files

Notes

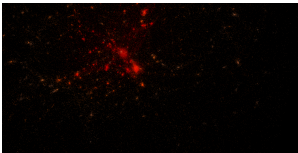
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N -body simulations

N -body simulations¹



The N -body problem is the physically problem of predicting the individual motions of a group of celestial objects interacting with each other gravitationally.

Informal description:

Predict the interactive forces and true orbital motions for all future times of a group of celestial bodies. We assume that we have their quasi-steady orbital properties, e.g. instantaneous position, velocity and time.

¹By Michael L. Umbricht - Own work, CC BY-SA 4.0

Recall: Vectors and basic operations

Vectors

$$\mathbf{u} = (x, y, z) \in \mathbb{R}^3$$

1. Norm: $|\mathbf{u}| = \sqrt{x^2 + y^2 + z^2}$

2. Direction: $\frac{\mathbf{u}}{|\mathbf{u}|}$

Inner product

$$\mathbf{u}_1 \circ \mathbf{u}_2 = x_1 x_2 + y_1 y_2 + z_1 z_2$$

Cross product

$$\mathbf{u}_1 \times \mathbf{u}_2 = |\mathbf{u}_1| |\mathbf{u}_2| \sin(\theta) \mathbf{n}$$

where \mathbf{n} is the normal vector perpendicular to the plane containing \mathbf{u}_1 and \mathbf{u}_2 .

Stepping back: Two-body problem

Let m_i, m_j be the masses of two gravitational bodies at the positions $\mathbf{r}_i, \mathbf{r}_j \in \mathbb{R}^3$

Three definitions:

1. The Law of Gravitation: The force of m_i acting on m_j is

$$\mathbf{F}_{ij} = G m_i m_j \frac{\mathbf{r}_j - \mathbf{r}_i}{|\mathbf{r}_j - \mathbf{r}_i|^3}$$

2. The Calculus:

- 2.1 The velocity of m_i is $\mathbf{v}_i = \frac{d\mathbf{r}_i}{dt}$

- 2.2 The acceleration of m_i is $\mathbf{a}_i = \frac{d\mathbf{v}_i}{dt}$

3. The second Law of Mechanics:

$$\mathbf{F} = m\mathbf{a} \text{ (Force is equal mass times acceleration)}$$

The universal constant of gravitation G was estimated as $6.67408 \cdot 10^{-11} m^3 kg^{-1} s^{-2}$ in 2014 [8].

Put all together: Equation of motion

Derivation for the first body:

$$\mathbf{F}_{ij} = Gm_i m_j \frac{\mathbf{r}_j - \mathbf{r}_i}{|\mathbf{r}_j - \mathbf{r}_i|^3}$$

$$m_i \mathbf{a}_i = Gm_i m_j \frac{\mathbf{r}_j - \mathbf{r}_i}{|\mathbf{r}_j - \mathbf{r}_i|^3}$$

$$\frac{d\mathbf{v}_i}{dt} = Gm_j \frac{\mathbf{r}_j - \mathbf{r}_i}{|\mathbf{r}_j - \mathbf{r}_i|^3}$$

$$\frac{d^2\mathbf{r}_i}{dt^2} = Gm_j \frac{\mathbf{r}_j - \mathbf{r}_i}{|\mathbf{r}_j - \mathbf{r}_i|^3}$$



For the second body follows: $\frac{d^2\mathbf{r}_j}{dt^2} = Gm_i \frac{\mathbf{r}_i - \mathbf{r}_j}{|\mathbf{r}_i - \mathbf{r}_j|^3}$

Note that we used Newton's law of universal gravitation [9].

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The N-body problem

The force for body m_i

$$\mathbf{F}_i = \sum_{j=1, i \neq j}^n \mathbf{F}_{ij} = \sum_{j=1, i \neq j}^n Gm_j \frac{\mathbf{r}_j - \mathbf{r}_i}{|\mathbf{r}_j - \mathbf{r}_i|^3}$$

Law of Conservation:

1. Linear Momentum: $\sum_{i=1}^n m_i \mathbf{v}_i = M_0$

2. Center of Mass: $\sum_{i=1}^n m_i \mathbf{r}_i = M_0 t + M_1$

3. Angular Momentum: $\sum_{i=1}^n m_i (\mathbf{r}_i \times \mathbf{v}_i) = \mathbf{c}$

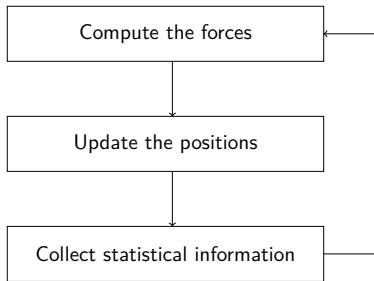
4. Energy: T-U=h with

$$T = \frac{1}{2} \sum_{i=1}^n m_i \mathbf{v}_i \circ \mathbf{v}_i, U = \sum_{i=1}^n \sum_{j=1}^n G \frac{m_i m_j}{|\mathbf{r}_i - \mathbf{r}_j|}$$

More details: Simulations [2] and Astrophysics [1].

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Algorithm



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Complexity of force computation

Force computation: Direct sum

```

for(size_t i = 0; i < bodies.size(); i++)
for(size_t j = 0; j < bodies.size(); j++)
//Compute forces
  
```

Advantage:

Robust, accurate, and completely general

Disadvantage:

1. Computational cost per body $\mathcal{O}(n)$
2. Computational cost for all bodies $\mathcal{O}(n^2)$

Tree-based codes or the Barnes-Hut method [3] reduce the computational costs to $\mathcal{O}(n \log(n))$. More details [6].

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Update of positions

Assume we have computed the forces already, using the direct sum approach and now we want to compute the evolution of the system over the time T :

Discretization in time:

- ▶ Δt the uniform time step size
- ▶ t_0 the beginning of the evolution
- ▶ T the final time of the evolution
- ▶ k the time steps such that $k\Delta t = T$

Question: How can we compute the derivatives dt and dt^2 of the velocity \mathbf{v} and the acceleration \mathbf{a} of a body?

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Finite difference and Euler method

Finite difference

We can use a finite difference method to approximate the derivation by

$$u'(x) \approx \frac{u(x+h)-u(x)}{h}$$

The Euler method

We use the finite difference scheme to approximate the derivations by

$$\mathbf{a}_i(t_k) = \frac{\mathbf{F}_i}{m_i} = \frac{\mathbf{v}_i(t_k) - \mathbf{v}_i(t_k - 1)}{\Delta t} \quad (1)$$

$$\mathbf{v}_i(t_k) = \frac{\mathbf{r}_i(t_{k+1}) - \mathbf{r}_i(t_k)}{\Delta t} \quad (2)$$

More details [10, 7, 5]

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Compute the velocity and updated position

Velocity

$$\mathbf{v}_i(t_k) = \mathbf{v}_i(t_{k-1}) + \Delta t \frac{\mathbf{F}_i}{m_i} \text{ using (1)}$$

Updated position

$$\mathbf{r}_i(t_{k+1}) = \mathbf{r}_{t_k} + \Delta t \mathbf{v}_i(t_k) \text{ using (2)}$$

Note that we used easy methods to update the positions and more sophisticated methods, e.g. Crank-Nicolson method [4], are available

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Structs

Looking at the data structure²

For the N -body simulations, we need three dimensional vectors having

```
▶ x Coordinate      struct vector {
▶ y Coordinate      double x;
▶ z Coordinate      double y;
                   double z;
                   };
```

Initialization

```
struct vector v = {.x=1, .y=1, .z=1};
struct vector v1 = {1,1,1};
```

Reading/Writing elements

```
std::cout << v.x << std::endl;
v.z=42;
```

²<https://en.cppreference.com/w/c/language/struct>

Constructor³

Assign initial values

```
struct A
{
    int x;
    A(int x = 1): x(x) {};
};
```

A constructor has a

- ▶ Name A
- ▶ Arguments `int x = 1`
- ▶ Assignment : `x(x)`

Now `struct A a;` is equivalent to `struct A a = {1};`

³https://en.cppreference.com/w/cpp/language/default_constructor

Access specifiers⁴

```
struct A
{
    public:
    A(int x = 1): x(x) {};

    private:
    int x;
};
```

- ▶ `public` - The function and members have public access
- ▶ `private` - The function and members are only accessible within the struct

⁴https://en.cppreference.com/w/cpp/language/operator_member_access

Access specifiers⁵: Example

```
struct A
{
    public:
    A(int x = 1): x(x) {};

    private:
    int x;
};
```

```
A a = A(10);
// Will not work since x is declared private
A.x = 1;
```

Solution: Providing `public` method to read and write the variable `a`.

⁵https://en.cppreference.com/w/cpp/language/operator_member_access

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Access specifiers⁶: Access methods

```
struct A
{
    public:
        A(int x = 1): x(x) {};

        // So-called get method
        int getX(){ return x;}

        // So-called set method
        void setX(int value){ x = vlaue;}

    private:
        int x;
};
```

⁶https://en.cppreference.com/w/cpp/language/operator_member_access

Functions⁸

Compute the norm of the vector

```
#include <cmath>
struct vector2 {
    double x , y , z;
    vector2(double x = 0, double y=0, double z=0)
        : x(x) , y(y) ,z(z) {}
    double norm(){ return std::sqrt(x*x+y*y+z*z);}
};
```

Usage

```
struct vector2 v;
std::cout << v.norm() << std::endl;
```

`#include <cmath>`⁷ provides mathematical expressions

⁷<https://en.cppreference.com/w/cpp/header/cmath>

⁸<https://en.cppreference.com/w/cpp/language/functions>

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Generic programming

Why we need generic functions?

Example

```
//Compute the sum of two double values
double add(double a, double b) {
    return a + b;
}
//Compute the sum of two float values
float add(float a, float b) {
    return a + b;
}
```

Reasons:

- ▶ We have less redundant code
- ▶ The C++ standard library makes large usage of generic programming, e.g. `std::vector<double>`, `std::vector<float>`

Notes

Function template⁹

Writing a generic function:

```
template<typename T>
T add(T a, T b)
{
    return a + b;
}
```

Using the generic function:

```
std::cout << add<double>(2.0,1.0) << std::endl;
std::cout << add<int>(2,1) << std::endl;
std::cout << add<float>(2.0,1.0) << std::endl;
```

Additional way to use the generic function:

```
std::cout << add(2,1) << std::endl;
```

⁹https://en.cppreference.com/w/cpp/language/function_template

Generic structs¹⁰

Writing a generic vector type

```
template<typename T>
struct vector {
    T x;
    T y;
    T z;
};
```

Using a generic vector type

```
struct vector<double> vd = {1.5,2.0,3.25};
struct vector<float> vf = {1.25,2.0,3.5};
struct vector<int> vi = {1,2,3};
```

¹⁰<https://en.cppreference.com/w/cpp/language/templates>

Example

Generic struct having functions

```
#include <cmath>

template<typename T>
struct vector {
    T x, y, z;
    vector( T x = 0, T y=0, T z=0)
        : x(x), y(y), z(z) {};
    T norm() { return std::sqrt(x*x+y*y+z*z);}
    T cross(struct vector<T> b)
    {return x*b.y-y*b.x+z*b.z;}
};
```

What we need to define the vector data structure:

- ▶ Structs
- ▶ Generic functions

Summary

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Summary

After this lecture, you should know

- ▶ *N*-Body simulations
- ▶ Structs
- ▶ Generic programming (Templates)

Further reading:

- ▶ C++ Lecture 2 - Template Programming¹¹
- ▶ C++ Lecture 4 - Template Meta Programming¹²

¹¹<https://www.youtube.com/watch?v=iU3vsiJ5mts>

¹²<https://www.youtube.com/watch?v=6PWUByLZ00g>

References

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