

Computational Physics - Project 5

Johannes Scheller (candidate no. 71), Vincent Noculak (candidate no. 22)
Lukas Powalla (candidate no. 67), Richard Asbah (candidate no. 50)

December 6, 2015

Contents

| | | |
|----------|---|----------|
| 1 | Introduction | 3 |
| 2 | Theory | 3 |
| 2.1 | Newton's law of universal gravitation | 3 |
| 2.2 | Energy | 3 |
| 2.3 | Open Clusters | 4 |
| 2.4 | Verlet algorithm | 4 |
| 2.4.1 | Velocity Verlet algorithm | 4 |
| 2.5 | Runge-Kutta methods | 5 |
| 2.5.1 | Fourth order Runge-Kutta method (RK4) | 5 |
| 2.5.2 | RK4 in this Project | 5 |
| 3 | Execution | 6 |
| 3.1 | General structure and overview | 6 |
| 3.1.1 | constructor | 7 |
| 3.1.2 | constants and objects | 7 |
| 3.1.3 | general functions | 7 |
| 3.2 | Velocity-verlet-algorithm | 9 |
| 3.3 | Runge Kutta-Method | 9 |
| 4 | Discussion | 9 |
| 5 | Source code | 9 |

1 Introduction

In this project we are going to simulate open clusters using Newton's law of universal gravitation. We are going to look at the time an open cluster with a cold collapse would need to collapse into singularity and observe the energy conservation and distribution of potential and kinetic energy. On what properties does it depend how many particles get ejected from the cluster and how do those particles change the energy of the system? The equilibrium state and its radial partial density are going to be observed too.

We are doing these calculation by using the Velocity Verlet algorithm and the fourth order Runge-Kutta method. First we are going to compare both algorithms by simulating a two body system. Then we are going to study, which algorithm is more suitable for doing open cluster simulations and continue to simulate the open cluster with the more fitting algorithm.

2 Theory

2.1 Newton's law of universal gravitation

Newton's law of universal gravitation states that every point mass attracts every single other point mass by a force pointing along the line intersecting both points. The force two points of mass with the masses m_i and m_j and a distance of r_{ij} to each other attract each other is given by

$$\mathbf{F}_G = -G \frac{m_i \cdot m_j}{r_{ij}^3} \cdot \mathbf{r}_{ij} \quad (1)$$

Where G is the gravitational constant. In our project we have a system with n stars which get approximated as points of mass. Hence, to get the gravitational force acting on one star, we just need to sum over all \mathbf{F}_G 's (having the form of equation (1)) that are acting on this star due to the other stars.

$$\mathbf{F}_{Gi} = \sum_{j \neq i}^n -G \frac{m_i \cdot m_j}{r_{ij}^3} \cdot \mathbf{r}_{ij} = -G m_i \sum_{j \neq i}^n m_j \frac{\mathbf{r}_{ij}}{r_{ij}^3} \quad (2)$$

Then the acceleration of star i is given by

$$\mathbf{a} = -G \sum_{j \neq i}^n m_j \frac{\mathbf{r}_{ij}}{r_{ij}^3} \quad (3)$$

2.2 Energy

In the project we are going to observe the kinetic and potential energy of systems of particles, which interact via the gravitational force. The kinetic energy of a mass m with velocity v is given by $E_{Kin} = \frac{1}{2} m v^2$. Because we have n particles we just need to sum over the kinetic energies of all particles to get the kinetic energy of the system.

$$E_{Kin} = \sum_{i=1}^n \frac{1}{2} m_i v_i^2 \quad (4)$$

The potential energy of a system is given by $-\nabla E_{Pot} = \mathbf{F}$. Hence we have $\frac{\partial}{\partial x_i} E_{Pot} = -F_{x_i}$ and can get a potential energy by trough integration:

$$E_{Pot} = - \int dx' F_x(x', y, z) \quad (5)$$

To get the potential energy of our system, we add one particle after an other from an infinite distance to the system. Each time we add a particle i we calculate its potential energy V_i (negative work that is needed to move the particle to an infinite distance to the system) using (5). We do this until we have n particles in the system. Then the potential energy of our system is given by the sum over all V_i . If we add the particle 1 there is no force yet, hence $V_1 = 0$. When adding the second particle there is a force between particle 1 and 2. Adding the particle number i , there are $i - 1$ forces acting on particle i (we write the force between particle i and j , acting on i , as F_{ij}). Hence V_i can simply be calculated by

$$V_i = - \int_{x_i}^{\infty} dx \sum_{j \neq i}^i F_{ijx} \quad (6)$$

And we get

$$V_{System} = \sum_{i=1}^n V_i = - \sum_{i=1}^n \int_{x_i}^{\infty} dx \sum_{j \neq i}^i F_{ijx} = - \frac{1}{2} \sum_{i,j=1; i \neq j}^n \int_{x_i}^{\infty} dx F_{ijx} \quad (7)$$

With (1) we know

$$\int_{x_i}^{\infty} dx F_{ijx} = - \int_{x_i}^{\infty} dx G m_i m_j \frac{(x - x_j)}{((x - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2)^{\frac{3}{2}}} = - \left[G \frac{m_i m_j}{((x - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2)^{\frac{1}{2}}} \right]_{x_i}^{\infty} = G \frac{m_i m_j}{r_{ij}} \quad (8)$$

Setting (8) in (7) we get the potential energy of our system, which is

$$V_{System} = - \frac{1}{2} \sum_{i,j=1; i \neq j}^n G \frac{m_i m_j}{r_{ij}} \quad (9)$$

2.3 Open Clusters

Open clusters are groups of a few thousand stars that were formed from the same giant molecular cloud and have roughly the same age. They have yet only been found in spiral and irregular galaxies, in which active star formation is occurring. Many open clusters are unstable and have a small enough mass that the escape velocity of the system is lower than the average velocity of the constituent stars. These clusters will rapidly disperse within a few million years¹.

The open cluster we simulate in this project will have the starting conditions of a cold collapse. This means, that the particles start with little or no initial velocity. In addition to that, the N particles, we simulate, will be uniformly distributed at the starting time inside a sphere with given radius R_0 . Our particles masses will be distributed by a Gaussian distribution around ten solar masses with a standard deviation of one solar mass.

2.4 Verlet algorithm

The Verlet algorithm is one method that is important for this project to numerically solve the equation of motion having the form of equation (2).

Using a Taylor expansion for a function $x(t)$ around the point $t_0 = t_i$ and then setting $t = t_i + h$ and $t = t_i - h$, we get the equations

$$x(t_i + h) = x_i + h x'(t_i) + \frac{h^2}{2} x''(t_i) + \frac{h^3}{3!} x'''(t_i) + \sigma(h^4) \quad (10)$$

$$x(t_i - h) = x_i - h x'(t_i) + \frac{h^2}{2} x''(t_i) - \frac{h^3}{3!} x'''(t_i) + \sigma(h^4) \quad (11)$$

For an easier overview it is useful to use the notation $x(t_i) = x_i$, $x(t_i \pm h) = x_{i \pm 1}$ and $x'' = a(x, t)$. By adding up equation (10) and (11) we come to the equation

$$x_{i+1} = 2x_i - x_{i-1} + a(x_i, t_i) \cdot h^2 + \sigma(h^4) \quad (12)$$

Which gives us a method to determine all x_i , if the boundary conditions are known. It can be seen that due to the x_{i-1} part, the algorithm is not self-starting. Hence x_1 must be found, using an other method (for example Euler's method).

2.4.1 Velocity Verlet algorithm

The Velocity Verlet is similar to the Verlet algorithm. Here we use the Taylor expansion with $t_0 = t_i$ and $t = t_i + h$ to get the formula:

$$x_{i+1} = x_i + h \cdot v_i + \frac{h^2}{2} a_i(x_i, t_i) + \sigma(h^3) \quad (13)$$

With $v(t) = \frac{dx}{dt}$. And we use the Trapezoidal rule to get the formula:

$$v_{i+1} = v_i + \frac{h}{2} \cdot (a(x_i, t_i) + a(x_{i+1}, t_{i+1})) + \sigma(h^2) \quad (14)$$

The algorithm starts with calculating equation (13) for $i = 0$ to get x_{i+1} . With this value, $a(x_i, t_i)$ and $a(x_{i+1}, t_{i+1})$ can be calculated. Then it is possible to calculate v_{i+1} with equation (14). These steps can now be repeated for $i = i + 1$, allowing to get the values for all x_i and v_i .

¹Source: https://en.wikipedia.org/wiki/Open_cluster

2.5 Runge-Kutta methods

Runge-Kutta methods use the following basic equation of integration to numerically approximate Ordinary differential equations.

$$x_{i+1} = x_i + \int_{t_i}^{t_{i+1}} dt' v(x, t') \quad (15)$$

With $x(t_i) = x_i$, $x(t_i \pm h) = x_{i\pm 1}$ and $\frac{dx}{dt} = v$. The integral can be approximated using numerical integration methods, as for example the trapezoidal rule or Simpson's rule. In Runge-Kutta methods to calculate a step x_{i+1} , an intermediate step between x_i and x_{i+1} gets used.

2.5.1 Fourth order Runge-Kutta method (RK4)

In this project we are going to use the fourth order Runge-Kutta method. This method solves the integral in equation (15) with help of Simpson's method. By applying this method we get

$$\int_{t_i}^{t_{i+1}} dt' v(t', x) = \frac{h}{6} [v(t_i, x_i) + 4v(t_{i+\frac{1}{2}}, x_{i+\frac{1}{2}}) + v(t_{i+1}, x_{i+1})] + \sigma(h^5) \quad (16)$$

By setting (16) in (15):

$$x_{i+1} = x_i + \frac{h}{6} [v(t_i, x_i) + 2v(t_{i+\frac{1}{2}}, x_{i+\frac{1}{2}}) + 2v(t_{i+\frac{1}{2}}, x_{i+\frac{1}{2}}) + v(t_{i+1}, x_{i+1})] + \sigma(h^5) \quad (17)$$

$x_{i+\frac{1}{2}}$ and x_{i+1} are unknown values. Now we define $k_1 = v(t_i, x_i)$, first approximate $x_{i+\frac{1}{2}}$ with Euler's method

$$x_{i+\frac{1}{2}} \approx x_i + \frac{h}{2} v(t_i, x_i) = x_i + \frac{h}{2} k_1 \quad (18)$$

and define

$$k_2 = v(t_{i+\frac{1}{2}}, x_i + \frac{h}{2} k_1) \quad (19)$$

Next we calculate $x_{i+\frac{1}{2}}$ with Euler's method using k_2 instead of k_1 and then define

$$k_3 = v(t_{i+\frac{1}{2}}, x_i + \frac{h}{2} k_2) \quad (20)$$

We predict x_{i+1} with k_3 using Euler's method

$$x_{i+1} = x_i + h k_3 \quad (21)$$

$$k_4 = v(t_{i+1}, x_i + h k_3) \quad (22)$$

Now we can calculate our final x_{i+1} by inserting our k_j 's in equation (17).

$$x_{i+1} = x_i + \frac{h}{6} (k_1 + 2k_2 + 2k_3 + k_4) + \sigma(h^5) \quad (23)$$

2.5.2 RK4 in this Project

In section 2.5.1 it could be seen, that with the fourth order Runge-Kutta method, first-order ODE's (ordinary differential equations) can be solved. In this project however, we need to numerically solve the equation of motion for multiple particles, which is a second-order ODE (see equation (3)). This ODE can be split up into two first-order ODE's by writing

$$\frac{d\mathbf{r}}{dt} = \mathbf{v} \quad (24)$$

$$\frac{d\mathbf{v}}{dt} = G \sum_{j \neq i}^n m_j \frac{\mathbf{r}_{ij}}{r_{ij}^3} \quad (25)$$

Now we can use the RK4 method \mathbf{r} and \mathbf{v} simultaneously. Because we use this method in three dimensions and the fact, that we have a second-order ODE, the equations for the RK4 method look different than in section 2.5.1. The following steps give in the right order, how to approach the system, when we do a numerical calculation from the time t_i to t_{i+1} . It has to be noted, that when we do a calculation for one particle, directly after it, the same time the calculation gets performed for the other particles. The index on the upper left side refer to the number of the particle

and the index on the upper right side gives the information, if the value belongs to the RK4 method for the location or the velocity.

$$\mathbf{k}_1^r = \mathbf{v}_i \quad (26)$$

$$\mathbf{k}_1^v = \mathbf{a}({}^1\mathbf{r}_i, {}^2\mathbf{r}_i, \dots, {}^N\mathbf{r}_i) \quad (27)$$

$$\mathbf{k}_2^r = \mathbf{v}_i + \frac{h}{2} \mathbf{k}_1^v \quad (28)$$

$$\mathbf{k}_2^v = \mathbf{a}({}^1\mathbf{r}_i + \frac{h}{2} \cdot {}^1\mathbf{k}_1^r, {}^2\mathbf{r}_i + \frac{h}{2} \cdot {}^2\mathbf{k}_1^r, \dots, {}^N\mathbf{r}_i + \frac{h}{2} \cdot {}^N\mathbf{k}_1^r) \quad (29)$$

$$\mathbf{k}_3^r = \mathbf{v}_i + \frac{h}{2} \mathbf{k}_2^v \quad (30)$$

$$\mathbf{k}_3^v = \mathbf{a}({}^1\mathbf{r}_i + \frac{h}{2} \cdot {}^1\mathbf{k}_2^r, {}^2\mathbf{r}_i + \frac{h}{2} \cdot {}^2\mathbf{k}_2^r, \dots, {}^N\mathbf{r}_i + \frac{h}{2} \cdot {}^N\mathbf{k}_2^r) \quad (31)$$

$$\mathbf{k}_4^r = \mathbf{v}_i + h \cdot \mathbf{k}_3^v \quad (32)$$

$$\mathbf{k}_4^v = \mathbf{a}({}^1\mathbf{r}_i + h \cdot {}^1\mathbf{k}_3^r, {}^2\mathbf{r}_i + h \cdot {}^2\mathbf{k}_3^r, \dots, {}^N\mathbf{r}_i + h \cdot {}^N\mathbf{k}_3^r) \quad (33)$$

The accelerations can always get calculated by using equation (3). After the steps of equations (26) to (33) are executed, the velocity and positions of the particles for the time t_{i+1} can be calculated using formula (23).

3 Execution

In this project we are programming the motion of a n-body system. We are using two different algorithms for calculating the motion of the bodies called the Velocity-Verlet-algorithm and the Runge-Kutta-algorithm. We started to set up an algorithm for a two body system because this is much easier than dealing with n-bodies. However, we think it is sufficient to describe the program for n-bodies because the two body case is there also included. In our case, the bodies are represented by planets.

3.1 General structure and overview

We are using several classes in order to structure our program. The first class is called planet. Objects out of this class represent Planets with properties such as the position, velocity and mass. Originally, we thought that it would be nice to work with the planet objects and its positions and velocities in the algorithms itself. However, the Runge-Kutta method is heavily readable using this representation. Therefore, we used a matrix representation for position and velocity. The important information about position and velocity is kept in the matrix A. The second class is called solarsystem. This class contains all important functions and algorithms used to calculate the motion of the system. The header file for the basic functions looks as follows: (functions to calculate the Energy of the system (kinetic and potential) and to check the Virial theorem will be explained at a later point)

```
class solarsystem
{
public:
    //constructor
    solarsystem();
    //constants and arrays used for Energy-analysis
    double* vecKinpot;
    double* finalEnergy;
    vector<double> average_kin;
    vector<double> average_pot;
    //constants and objects
    double R0=20;
    double averagemass=10;
    int numplanets;
    double G;
    double epsilon=0.002;
    vector<Planet> planets;
    Mat<double> A;
    Mat<double> dA;
    // use of the random class
    std::random_device rd;
```

```

std::mt19937 gen;
std::uniform_real_distribution<> dis;
gaussian_random object;
//general functions
void addplanet(Planet Planet1);
void addrandomplanet(double R0);
void setmatrices();
//functions used only for Velocity-Verlet
void VelocityVerlet(double dt,int n);
void calculateForces();
//Functions used only for Runge-Kutta-method
void RungeKuttamethod(double dt,int n);
mat derivate( Mat<double> B);
// funktions for Energy-analysis
void kinPotEnergy(); //VelocityVerlet
void kinPotEnergy2(); //RK-4
void virial_output();
};

```

We will now briefly explain the use of the constructor, constants and functions of the class solarsystem. The functions, which are specific to Velocity-Verlet or Runge-Kutta method are explained in the section named after the method. The use of the random class itself will not be explained here. We are using a random number generator with a period of 2^{32} . This is sufficient. The random number generator is seeded by default while constructing a object of solarsystem.

3.1.1 constructor

We need a constructor in order to create objects of the class. With constructing the class, we also initialise the random number generator and set the number of planets of the created solarsystem-object to 0.

```

solarsystem::solarsystem() : gen(this->rd()), dis(0,1)
{
    this->numplanets=0;
}

```

3.1.2 constants and objects

We need some constants for the random number generator in order to create random planet-objects with the right properties. R0 is the radius for the sphere in which the planets should be distributed with constant particle density. The average-mass (averagemass) is the averagemass of the random planet-objects. The standard deviation of the planet objects is manually set to a specific value in the function addrandomplanet(double R0). The integer numplanets counts the actual number of planets of a specific planet object. The gravitational constant G is in our case dependent on the number of planets and the average-mass of a planet. Therefore, this constant is recalculated every time you add a planet. (in the function addrandomplanet) The smoothing-factor epsilon is also initialised and defined.

3.1.3 general functions

Our n-body- system can be used in different ways. You can manually add a planet with chosen initial position, initial velocity and mass. This is done by the function addplanet(Planet Planet1). Therefore, this algorithm can also be used to calculate the motion of a given two body system. With small changes, it is also be possible to simulate our solar-system. (G has to be changed)

```

void solarsystem::addplanet(Planet Planet1){
    planets.push_back(Planet1); // adds the planet to the vector of planets
    average_kin.push_back(0);
    average_pot.push_back(0);
    this->numplanets+=1;
    G=4*M_PI*M_PI*R0*R0*R0/(32*this->numplanets*averagemass);
}

```

On the other way, you can choose to add a planet with random position within a sphere and with given Gaussian-distributed mass of the planet. This is done by the function addrandomplanet(double R0). We set the planet-velocities

to 0. With Box–Muller transform, we get a normal-distribution with given mean-value and given standard-deviation. The mass is set to a random Gaussian-distributed value. We want a equal density at $t=0$ within a sphere. Therefore, we have to manipulate a random generated triple (u,v,w between 0 and 1) as follows:

$$\begin{aligned} r &= R0 \cdot \sqrt[3]{u} \\ \theta &= \arccos(1 - 2v) \\ \phi &= 2\pi\omega \end{aligned}$$

We want to use spherical coordinate. Therefore, we transform back to spherical coordinates, simplify and get:

$$\begin{aligned} x &= R0 \cdot \sqrt[3]{u} \cdot \sqrt{1 - (1 - 2v)^2} \cdot \cos(2\pi \cdot \omega) \\ y &= R0 \cdot \sqrt[3]{u} \cdot \sqrt{1 - (1 - 2v)^2} \cdot \sin(2\pi \cdot \omega) \\ z &= R0 \cdot \sqrt[3]{u} \cdot (1 - 2v) \end{aligned}$$

In the end, we add the new planet with the function `addplanet` to the `solarsystem`.

```
void solarsystem::addrandomplanet() {
    Planet randomplanet;
    // set andom mass with Gaussian-distribution
    randomplanet.m=object.generateGaussianNoise(10,1);
    // set velocities to 0
    randomplanet.velocity[0]=0;
    randomplanet.velocity[1]=0;
    randomplanet.velocity[2]=0;
    //generate random position
    double r=dis(gen);
    double theta=dis(gen);
    double phi=dis(gen);
    //transform random position in order to get
    //Cartesian coordinates with constant density
    randomplanet.position[0]=R0*pow(r,(1.0/3.0))*sqrt((1-(pow(1-2*theta,2))))*cos(2*M_PI*phi);
    randomplanet.position[1]=R0*pow(r,(1.0/3.0))*sqrt((1-(pow(1-2*theta,2))))*sin(2*M_PI*phi);
    randomplanet.position[2]=R0*pow(r,(1.0/3.0))*(1-(2*theta));
    addplanet(randomplanet);
}
```

To use the matrix-representation of position and velocity, we wrote the function `setmatrices()`, which constructs a matrix A , which contains all positions and velocities of the planets, which has been added to the system so far. The position of the planets can be found in the first column and the velocity in the second column. Every planet has 3 Coordinates. In addition to that, we construct the matrix dA , which is the derivative of the matrix A . This means that in the first column are velocities and in the second column are accelerations. For RK4, this is really useful because we can perform very understandable operations like $A = A + dA \cdot dt$.

$$A = \begin{bmatrix} r_{x_1} & v_{x_1} \\ r_{y_1} & v_{y_1} \\ r_{z_1} & v_{z_1} \\ r_{x_2} & v_{x_2} \\ \dots & \dots \\ r_{x_n} & v_{x_n} \\ r_{y_n} & v_{y_n} \\ r_{z_n} & v_{z_n} \end{bmatrix} \quad dA = \begin{bmatrix} v_{x_1} & a_{x_1} \\ v_{y_1} & a_{y_1} \\ v_{z_1} & a_{z_1} \\ v_{x_2} & a_{x_2} \\ \dots & \dots \\ v_{x_n} & a_{x_n} \\ v_{y_n} & a_{y_n} \\ v_{z_n} & a_{z_n} \end{bmatrix} \quad (34)$$

```
void solarsystem::setmatrices() {
    A=Mat<double>(this->numplanets*3,2);
    dA=Mat<double>(this->numplanets*3,2);

    for (int i=0; i<this->numplanets; i+=1) {
        for (int j=0; j<3; j++) {
            A(3*i+j,0)=planets[i].position[j];
            A(3*i+j,1)=planets[i].velocity[j];
        }
    }
```



```

    }

    for(int i=0;i<this->numplanets;i+=1){
        for(int j=0;j<3;j++){
            dA(3*i+j,0)=planets[i].velocity[j];
            dA(3*i+j,1)=planets[i].force[j]/planets[i].m;
        }
    }
}

```

3.2 Velocity-verlet-algorithm

```

...
setmatrices();
calculateForces();
A.col(1)=A.col(1)+0.5*dt*dA.col(1); // v(t)->v(t+0.5dt)
for(int k=0;k<n;k++){
    A.col(0)=A.col(0)+A.col(1)*dt; // r(t+dt)
    calculateForces(); // a(t+dt)
    A.col(1)=A.col(1)+dt*dA.col(1); // v(t+0.5dt) -> v(t+3/2dt)
}
...

```

3.3 Runge Kutta-Method

4 Discussion

5 Source code