

Tutorial

1: Equations of motion and integrators

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1 A simple first order integrator: Cannonball

1.1 Introduction

The simplest possible set of equations of motion is one particle with a constant external force. To get some first impressions on C programming, we will solve this one-particle problem by implementing the easiest possible straight forward integrator.

The idea is simply to formulate the Newton equations for finite time steps:

$$v(t + \Delta t) = v(t) + \left(\frac{F(t)}{m} \right) \Delta t \quad (1)$$

$$x(t + \Delta t) = x(t) + v(t) \cdot \Delta t \quad (2)$$

Of course, we still need x_0 and v_0 as initial conditions. As you can easily see, these two equations are nothing but a second order Taylor expansion around the time coordinate:

$$v(t + \Delta t) = v(t) + \frac{\partial v(t)}{\partial t} \Delta t + \mathcal{O}(\Delta t^2) \quad (3)$$

$$x(t + \Delta t) = x(t) + \frac{\partial x(t)}{\partial t} \Delta t + \mathcal{O}(\Delta t^2) \quad (4)$$

Thus the order of numerical steps for our integrator is given: We first have to calculate the force on the particles for their current positions. From this, we can get the new positions and the new velocities. This method will allow us to implement an easy code.

Note: Is this algorithm time-reversible? (...if you do a Taylor expansion to $(t - \Delta t)$...?)

1.2 Task: Implement our simple integrator

In the tutorial's directory, there is the subdirectory "integrator", which contains the prepared code. First, you only need to take a look at the `integrate` function in the `integrate.c` file. It already contains all needed variables to implement your integrator. The function is prepared for gravitational and wind force. Implement the gravitational force first (the particle's mass is 1). Compile the program with

```
./compile_integrator
```

If you have trouble, ask your tutors for help. Run the compiled code for the first time with

```
./integrator
```

You will now see a file called `trajectory.dat` that contains the trajectory of a thrown particle. To view this trajectory, we will need the very useful plotting tool `gnuplot`. In your terminal, start `gnuplot`. Plot the trajectory with the `gnuplot` command

```
plot "trajectory.dat"
```

The result should look like figure 1. If it doesn't, take another look at your integrator. If necessary, get help from your tutors.

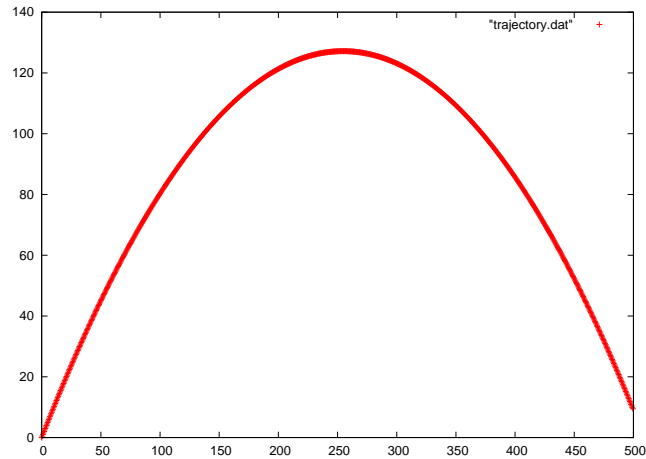


Figure 1: The trajectory as printed with `gnuplot`.

1.3 Homework 1 (2 points): Study the trajectory

Influence of wind

With the program, you have the option to set starting values for your parameters from the console. Take a look at the file `integrator.c`, which contains the information about the possible parameters. Run the program several times with the same starting velocity of $(50, 50)$ and additional wind force.

Does the wind force change the trajectory? Are the changes in a realistic range? If not, take a closer look at your integrator! The implementation for wind force is analogue to the gravitational force, just in another direction.

Note for presenting the homework: Whenever you are asked to produce/compare some results you need to present a plot and a some explanation of it. Send in a file with your solutions or print out the plot.

Influence of starting parameters

You can also change the starting speed of your particle. At an angle of 45 degrees ($v_x = v_y$), try to hit the word “trajectory” in `gnuplot`’s legend. Write down the used starting speed and hand in the plot.

Switch on the graphical user interface

As you can tell from the name of this section, the integrator you have just programmed can be used for a very old computer game called “Cannonball”. After all, the trajectory you just plotted may show the flight of a cannonball! :o) We have prepared a graphical user interface that can be used with your own integrator.

Go to the directory “`canonball`” and copy the integration algorithm you just programmed:

```
cp ../integrate.* .
```

Now you can compile the code with

```
./compile-it.sh
```

Start the game with `. canonball`, make a screenshot and hand it in with your homework.

1.4 Homework 2: Play the game!

If you now start the executable, you can really play the game with random wind and adjustable angle and initial velocity. And all with your integrator.

2 Advanced integrators: Solar system

2.1 Introduction

One of the basic concepts of MD simulations is the integration of classical equations of motion. Therefore a suitable algorithm is required. Since the equations of motion are **time-reversible**, we have to use an appropriate integration scheme. A simple approach to do this is the so called Verlet algorithm:

$$x(t + \Delta t) = 2x(t) - x(t - \Delta t) + a(t) \cdot \Delta t^2 + \mathcal{O}(\Delta t^4) \quad (5)$$

Positions, velocities and the acceleration at time t are denoted by $x(t)$, $v(t)$, and $a(t)$, respectively.

However this algorithm comes with a difficulty during the first time step (think about it!). To overcome this problem, a wide range of methods exists. A widely used approach is named Velocity-Verlet algorithm, that includes the contributions of the velocities directly in every integration step:

$$x(t + \Delta t) = x(t) + v(t) \cdot \Delta t + \frac{a(t)}{2} \Delta t^2 + \mathcal{O}(\Delta t^4) \quad (6)$$

$$v(t + \Delta t) = v(t) + \frac{a(t + \Delta t) + a(t)}{2} \Delta t + \mathcal{O}(\Delta t^3). \quad (7)$$

Of course, to implement the algorithm like this, we would have to access the old and new forces in one timestep. To make the code less complicated, the following scheme is mostly used:

1. Update positions by simple Taylor expansion:

$$x(t + \Delta t) = x(t) + v(t) \cdot \Delta t + \frac{a(t)}{2} \Delta t^2$$

2. Save half time step in temporary velocity variable:

$$v\left(t + \frac{\Delta t}{2}\right) = v(t) + a(t) \frac{\Delta t}{2}$$

3. Derive $a(t + \Delta t)$ (call forces routine)

4. Update velocities:

$$v(t + \Delta t) = v\left(t + \frac{\Delta t}{2}\right) + a(t + \Delta t) \frac{\Delta t}{2}$$

This simply means shifting the algorithm's order in a way that we don't need two values for the force but a temporary velocity instead. As we have seen, the error for our Verlet update is $\mathcal{O}(\Delta t^4)$. What is the error order of our first calculation step here?

Another way to deal with this problem is the Leapfrog Verlet algorithm, whose name comes from the leapfrog-looking integration scheme as seen in figure 2.

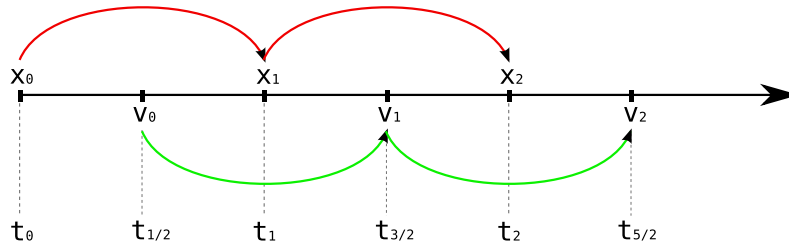


Figure 2: Illustration of the Leapfrog integration method

The basic idea is to give up the synchronous modification of position and velocity data. Instead we introduce velocity update points at half timesteps:

$$v\left(t + \frac{1}{2}\Delta t\right) = v(t) + \left(\frac{F(t)}{2m}\right) \Delta t + \mathcal{O}(\Delta t^2) \quad (8)$$

$$x(t + \Delta t) = x(t) + v\left(t + \frac{1}{2}\Delta t\right) \Delta t + \mathcal{O}(\Delta t^2) \quad (9)$$

$$v\left(t + \frac{3}{2}\Delta t\right) = v\left(t + \frac{1}{2}\Delta t\right) + \left(\frac{F(t + \Delta t)}{2m}\right) \Delta t + \mathcal{O}(\Delta t^2) \quad (10)$$

It has the advantage of being totally symmetric (time-reversibility!) and also avoids the initialization problem.

As you can see, we now have first, third and second order integration algorithms. Each has its advantages when it comes to speed, numerical precision and error calculation. We will examine this later.

2.2 Compilation and tools

The prepared code you need for this exercise is placed in the directory `simple_md`. The file you want to edit is `smd.c`. The `Makefile` in the directory lets you compile the code by simply typing `make`. When you compile and run the code (`./smd`), it produces two files `traj.pdb` and `energy.dat`. The second one contains the total energy of your system and can be plotted with `gnuplot`. The first one is a PDB-file (particle database) and can be viewed with the tool

VMD (Visual Molecular Dynamics). An interesting feature will certainly be the possibility to change the appearance of your particles via menu “Graphics” → “Representations”. Try e.g. a Van-Der-Waals Drawing method (VDW) with a smaller sphere scale, and set the coloring method to “SegName”, which has proven to look nicely. :o) Attention: If your particles spread too far because you are using a less accurate integrator over a very long simulation time, you won’t see your very small particles anymore because VMD zooms out automatically!

You need to take a look at the loop within the `main` function, where you can decide which function to call for your integration. When compiling and running the code for several different integrators, be sure to move the resulting files to suitable names in between the runs, before you overwrite them! In this function, you can also choose values for the main variables to influence the simulation later.

2.3 Task: Implementation

- Implement the Velocity Verlet algorithm in the function `integrate_verlet` in the code file `smd.c`. All required variables are already declared, just fill in the correct lines. If unsure how to use the variables, you can take a quick look at the function `integrate`, which is nothing but the first simple integrator you just implemented.

2.4 Homework (2 points)

- Derive the Verlet algorithm.
Hint: equation 5 consists of two Taylor expansions to include time reversibility.
- Which differences will you expect using our non time-reversible simple integrator and a time reversible integration scheme like the Verlet algorithm?
Think about the influence on energy and momentum of the system!

2.5 Homework 2 (2 points): Implement the Leapfrog Integrator

- Implement the Leapfrog algorithm in the function `integrate_leapfrog` in the code file `smd.c`. All required variables are already declared, just fill in the correct lines.

2.6 Optional Homework: Implement an advanced integrator

- If you are already an advanced programmer, you can implement an integration algorithm of even higher order (≥ 4) and later compare it with the other integration schemes.

2.7 Homework 3 (4 points): Quality of the integrators

You now have a simple code with which you can apply integrators to your problem, each having its advantages and disadvantages! Your homework is to find out the advantages in speed, reliability and long-term stability of each integrator. You will want to adapt the values for the variables `timestep`, `duration` and `update_interval` in your function `main` later.

Long-term stability (1 point)

You can choose which integrator to use by, in the main routine, calling one of the functions `integrate`, `integrate_leapfrog` or `integrate_verlet`. Open the written pdb-files with VMD. You can see some parts of our solar system: The sun, Venus, Earth, Mars and Jupiter. We also implemented the earth's moon as the first thing to fall apart with a less exact integrator.

- For our initial value of 0.012 for the timestep, after how many earth years does the moon leave the earth's orbit for the three different integrators?
- What happens when you decrease or increase the timestep of your integration?

Energy conservation (3 points)

To find out more about your system and the time evolution, it is usually helpful to take a look at some other observables, not just the particle trajectories. As you know, our program already calculates the system's total energy (potential and kinetic) and prints it into a file.

When you have produced energy files for all three integrators, take a look at them with `gnuplot`. You can squeeze several data files into one plot by separating them with commas:

```
plot "data1", "data2", "data3"
```

Take a look at the energy files of the simple and the leapfrog integrator and compare each in one plot together with the Velocity Verlet integrator.

- Why do the graphs look like this? Explain! Think about conservation laws and check what you can see with VMD at the interesting points in the graph. Hand in your explanation and the graphs.
- How does each integrator perform when it comes to speed? You can measure the runtime on your computer by using the tool `time ./smd`.
Hint: Writing to the hard drive takes a lot of time. So be sure to make the "update interval" as long as your whole simulation time. If your simulation runs too fast and there is hardly any difference between the integrators, what are the two main things you can do to increase the runtime?
- How much smaller do you have to make your timestep to reach the stability of the Velocity Verlet algorithm with the Leap Frog integrator?
- Which integrator would you use for this particular system when you want to simulate the solar system for a million years? For ten years without the moon on a really slow computer? Include the reasons for your decision.