L9 Structural Bioinformatics

In this exercise we will try to solve some simple differential equations, the keyword here is „try“ as you will find out on your journey. Don't be intimidated by the word „differential equation“, this is nothing new to you. You have done this in Physik A already. We consider a 2-dimensional space with the potential:

$$V = x_1^2 + x_2^2 \tag{1}$$

We neglect units as they are tedious and in the world of simulations physicists have found systems which allow things like this.

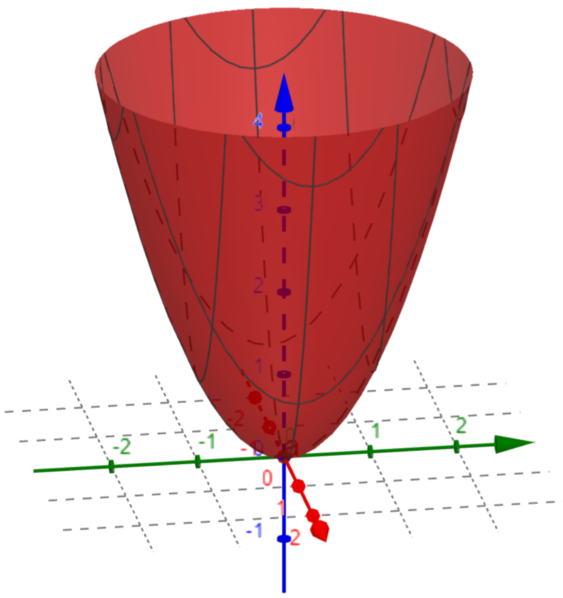

Abbildung 1: The potential given by equation 1

a) For now consider any particle with mass $m = 1$ moving without friction in this 2-dimensional space. At time $t = 0$ the particle is at the position $\vec{x}_0$ with the speed $\vec{v}_0$.

$$\vec{x}_0 = \begin{pmatrix} -1 \\ 1 \end{pmatrix}; \quad \vec{v}_0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{2}$$

The differential equation you have to solve now is Newtons equation of motion.

$$\ddot{\vec{x}} = \frac{\vec{F}}{m} = -\frac{\nabla V}{m} \tag{3}$$

In vector notation this comes down to

$$\begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{pmatrix} = -\frac{2}{m} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}. \tag{4}$$

Which shows us that the equations are decoupled. Can you guess the solution? Remember for solving differential equations, you first find a general solution which is a function with parameters. The parameters then become specified by initial conditions.

b) Now we consider a more complicated case. Imagine now two singly charged particles with the same charge in the given 2-dimensional space, they interact by Coulombs law:

$$\vec{F}_C = k_C \frac{\vec{d}}{\left|\vec{d}\right|^3} \tag{5}$$

Where d is the distance vector between the particles. We now call the particles A and B and place them at the positions

$$\vec{x}_{A,0} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}; \quad \vec{v}_{A,0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{6}$$

$$\vec{x}_{B,0} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}; \quad \vec{v}_{B,0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{7}$$

Before you continue, hold a moment and think about how you would solve Newtons equation of motion now?

We now explore something what physicists call phase space, the phase space of this system is 8-dimensional. What are these 8 dimensions? Well, every particle has a position and a velocity, each defined by 2 numbers. As we have two particles, we have 8 numbers defining the system. We now assign the indices 1 and 2 to the coordinates of the first particle and the indices 3 and 4 to the respective coordinates of the second particle.

$$\vec{x}_A = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}; \quad \vec{v}_A = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \tag{8}$$

$$\vec{x}_B = \begin{pmatrix} x_3 \\ x_4 \end{pmatrix}; \quad \vec{v}_B = \begin{pmatrix} v_3 \\ v_4 \end{pmatrix} \tag{9}$$

Given these definitions, we can find an expression for d:

$$\left|\vec{d}\right| = \sqrt{(x_1 - x_3)^2 + (x_2 - x_4)^2} \tag{10}$$

Make a sketch if you can't follow the formula. Furthermore, we can rewrite our initial conditions as

$$\vec{x}_0 = \begin{pmatrix} -1 \\ 1 \\ 1 \\ 1 \end{pmatrix}; \quad \vec{v}_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{11}$$

Now we reconsider equation 3. Without the interaction, the particles would move separate of each other we would be able to solve the equations just like we did in task a). But this is not the case, our governing equations of motion are now

$$\ddot{\vec{x}} = \frac{\vec{F}}{m} = \frac{k_C}{m} \frac{\vec{d}}{\left|\vec{d}\right|^3} - \frac{\nabla V}{m} \tag{12}$$

or in vector notation:

$$\begin{pmatrix} \ddot{x}_1 \\ \ddot{x}_2 \\ \ddot{x}_3 \\ \ddot{x}_4 \end{pmatrix} = \frac{1}{m} \begin{pmatrix} k_C \frac{x_1 - x_3}{((x_1-x_3)^2+(x_2-x_4)^2)^{1.5}} - 2x_1 \\ k_C \frac{x_2 - x_4}{((x_1-x_3)^2+(x_2-x_4)^2)^{1.5}} - 2x_2 \\ k_C \frac{x_3 - x_1}{((x_1-x_3)^2+(x_2-x_4)^2)^{1.5}} - 2x_3 \\ k_C \frac{x_4 - x_2}{((x_1-x_3)^2+(x_2-x_4)^2)^{1.5}} - 2x_4 \end{pmatrix}. \tag{13}$$

These differential equations are highly coupled. Try to find a solution!