FB 08 Informatik
Lehrstuhl f. Software-Technik und Bioinformatik

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BIOINFORMATICS II - SS 16

4. EXERCISE SHEET

TO BE DELIVERED NOT LATER THAN 22-05-2016

	Exercise	Points
Theoretical	1	10
Theoretical	2	10
Practical	3	20

Exercise 1: Solving a simple model – System differential equations (10 Points)
Consider the system composed by a water molecule; assume for simplicity that the position of the oxygen atoms is fixed (without loss of generalization, as this corresponds to the the choice of the system of reference). Assuming that the angle between the hydrogen atoms is fixed (i.e., only the distance between atoms can change, but not the angle), solve the equation of motion for the hydrogen atoms. Name the distances between oxygen and hydrogen atoms ρ_1 and ρ_2, and use as initial conditions:

$$\rho_1(0) = \tilde{\rho}_1$$

$$\dot{\rho}_1(0) = v_1$$

$$\rho_2(0) = \tilde{\rho}_2$$

$$\dot{\rho}_2(0) = v_2$$

Exercise 2: Lennard-Jones (10 Points)
Let's consider two particles whose positions are given by vectors $\mathbf{r_1}$ and $\mathbf{r_2}$ and the vector

$$\mathbf{r} = \mathbf{r_1} - \mathbf{r_2},$$

with the modulus denoted by:

$$r = \|\mathbf{r_1} - \mathbf{r_2}\|.$$

The Lennard-Jones potential energy can be written as:

$$V(\mathbf{r_1}, \mathbf{r_2}) = V(r) = \varepsilon \left[\left(\frac{r_0}{r} \right)^{12} - 2 \left(\frac{r_0}{r} \right)^{6} \right], \tag{1}$$

and the corresponding force (directed along the direction of $\mathbf{r}$) turns to be

$$\mathbf{F}(\mathbf{r_1}, \mathbf{r_2}) = -\nabla V = \frac{12\varepsilon}{r}\left[\left(\frac{r_0}{r}\right)^{12} - \left(\frac{r_0}{r}\right)^{6}\right]\frac{\mathbf{r}}{r}.$$

A Taylor expansion of the potential energy close to a fixed point $\tilde{r}$ can be written as:

$$V(r) = V(\tilde{r}) + \frac{\mathrm{d}V(\tilde{r})}{\mathrm{d}r}(r-\tilde{r}) + \frac{1}{2}\frac{\mathrm{d}^2V(\tilde{r})}{\mathrm{d}r^2}(r-\tilde{r})^2 + o((r-\tilde{r})^2);$$

if we are looking for a minimum of the potential (i.e. an equilibrium point) we have to solve the equation:

$$\frac{\mathrm{d}V}{\mathrm{d}r} = 0 = -\frac{12\varepsilon}{r}\left[\left(\frac{r_0}{r}\right)^{12} - \left(\frac{r_0}{r}\right)^{6}\right] \quad \Leftrightarrow \quad \tilde{r} = r_0;$$

the second derivative, evaluated in the equilibrium point, is equal to:

$$\left.\frac{\mathrm{d}^2V}{\mathrm{d}r^2}\right|_{r=r_0} = \left.\frac{12\varepsilon}{r^2}\left[13\left(\frac{r_0}{r}\right)^{12} - 7\left(\frac{r_0}{r}\right)^{6}\right]\right|_{r=r_0},$$

which is positive (thus the equilibrium is stable). Hence, if we stay close enough to r_0,

$$V(r) = V(r_0) + \cancel{\frac{\mathrm{d}V(r_0)}{\mathrm{d}r}(r-r_0)} + \frac{1}{2}\frac{\mathrm{d}^2V(r_0)}{\mathrm{d}r^2}(r-r_0)^2 + o((r-r_0)^2)$$

$$V(r) \simeq -\varepsilon + \frac{6\varepsilon}{r_0^2}(13-7)(r-r_0)^2$$

$$\mathbf{F} = -\nabla V \simeq -\underbrace{\frac{72\varepsilon}{r_0^2}}_{k_{LJ}}(r-r_0)\frac{\mathbf{r}}{r}$$

So we can approximate the force with a kind of Hooke force (linear force) as long as we consider positions close to the equilibrium.
Take a system of two particles, one of which fixed at the origin of the coordinate system; assume that the interaction is described by a Lennard-Jones potential energy with parameters $r_0 = 12$, $\varepsilon = 2$. Make a plot of both potential energy and force close to equilibrium point (comparing them with approximated functions) via `gnuplot`. Given a Morse potential:

$$V(r) = \varepsilon\left(1 - \mathrm{e}^{-\sigma(r-r_0)}\right)^2,$$

determine a linear approximation of the force (i.e., determine for the Morse potential a constant k_M as it was done for Lennard-Jones).

Exercise 3: Euler method – `C++` (20 Points)
Given a starting location $\mathbf{x}(0)$ and an initial velocity $\mathbf{v}(0)$, the Newton's second law of motion takes the following form:

$$\begin{cases} m\frac{\mathrm{d}^2\mathbf{x}(t)}{\mathrm{d}t^2} = \mathbf{F}(\mathbf{x}(t)) \\ \mathbf{x}(0) = \mathbf{x}_0 \\ \mathbf{v}(0) = \mathbf{v}_0 \end{cases} \tag{2}$$

This formulation, by means of ordinary differential equations, is generally refered to as the *initial value problem*, a special case of the *Cauchy problem*. The first equation can also be represented as:

$$m\frac{\mathrm{d}^2\mathbf{x}(t)}{\mathrm{d}t^2} = \mathbf{F}(\mathbf{x}(t)) \quad \Leftrightarrow \quad m\frac{\mathrm{d}}{\mathrm{d}t}\frac{\mathrm{d}\mathbf{x}(t)}{\mathrm{d}t} = \mathbf{F}(\mathbf{x}(t))$$

The definition of acceleration:

$$\frac{\mathrm{d}\mathbf{v}(t)}{\mathrm{d}t} = \lim_{\Delta t \to 0} \frac{\mathbf{v}(t+\Delta t) - \mathbf{v}(t)}{\Delta t}.$$

If we approximate the derivative (slope of tangent) by a difference quotient (Δt), we get the formula:

$$\frac{\mathrm{d}\mathbf{v}(t)}{\mathrm{d}t} \approx \frac{\mathbf{v}(t+\Delta t) - \mathbf{v}(t)}{\Delta t}$$

This leads to:

$$m\frac{\mathbf{v}(t+\Delta t) - \mathbf{v}(t)}{\Delta t} \approx \mathbf{F}(\mathbf{x}(t))$$

Solving for $\mathbf{v}(t+\Delta t)$ gives:

$$\mathbf{v}(t+\Delta t) \approx \mathbf{v}(t) + \frac{\Delta t}{m}\mathbf{F}(\mathbf{x}(t)).$$

Similarly, we can proceed with the definition of velocity and obtain:

$$\mathbf{v}(t) = \frac{\mathrm{d}\mathbf{x}(t)}{\mathrm{d}t} = \lim_{\Delta t \to 0} \frac{\mathbf{x}(t+\Delta t) - \mathbf{x}(t)}{\Delta t},$$

$$\mathbf{v}(t) \approx \frac{\mathbf{x}(t+\Delta t) - \mathbf{x}(t)}{\Delta t},$$

$$\mathbf{x}(t+\Delta t) \approx \mathbf{x}(t) + \Delta t\mathbf{v}(t).$$

In order to solve these equations, we divide the interval $[0, T]$ into N subintervals of the same length Δt. Then we can evaluate the solution for the (current) n^{th} time interval based on the (previous) $n-1^{th}$ time interval. Using the standard notation:

$$\mathbf{x}(t+n\Delta t) := \mathbf{x}_n,$$

$$\mathbf{v}(t+n\Delta t) := \mathbf{v}_n,$$

$$\Delta t := h,$$

the force, velocity and position at n^{th} time inteval can be formulated as follows:

(a) Force: $\mathbf{F}_n = \mathbf{F}(\mathbf{x}_{n-1})$,

(b) Velocity: $\mathbf{v}_n = \mathbf{v}_{n-1} + \frac{h}{m}\mathbf{F}_n$,

(c) Position: $\mathbf{x}_n = \mathbf{x}_{n-1} + h\mathbf{v}_{n-1}$.

In order to evaluate these equations, we require starting values for $\mathbf{x}$ and $\mathbf{v}$, as $\mathbf{x}_0$ and $\mathbf{v}_0$ respectively. We get them from the initial conditions:

$$\mathbf{x}_{n=0} = \mathbf{x}(0) = \mathbf{x}_0,$$

$$\mathbf{v}_{n=0} = \mathbf{v}(0) = \mathbf{v}_0.$$

Implement this procedure for numerical integration, so called *Euler method*, in `C++`. Assume for the force a formula:

$$\mathbf{F} = -k\mathbf{x}$$

Choose $k = 1, m = 1, h = 0.01$ and give the time, force, velocity and position of each step in a file. Run your program for 1000 steps and plot the three variables in a graph (with `gnuplot`).