Norwegian University of Science and Technology
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MA8404 Numerical solution of time dependent differential equations
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Exercise set 4

1 For a given Hamiltonian

$$H(p,q) = \frac{1}{2}p^2 + V(q)$$

the Hamiltons equations becomes

$$q' = p, \qquad p' = -V'(q)$$

Use the Morse potential $V(q) = (1-e^{-q})^2$. Solve this problem by the explicit Euler method, RK4 (the classical 4th order method) and Störmer-Verlet's method. Plot the solution in the $p-q$ plane. Examine the energy conservation H for the different methods. Experiment with different stepsizes. As initial values, choose e.g. $q_0 = 1$, $p_0 = 1$ and integrate from 0 to 20 (for example). You may very well also experiment with different initial values.

2 In GNI IV, Example 1.3, conservation of total linear and angular momentum is discussed. Prove that in the case of a Kepler problem, with the Hamiltonian

$$H(p,q) = \frac{1}{2}p^T M^{-1} p - \frac{1}{\|q\|_2}$$

also the vector

$$A = p \times L - M\frac{q}{\|q\|_2}$$

is conserved. Here, $L = q \times p$ is the angular momentum, red $q, p \in \mathbb{R}^3$ and $M \in \mathbb{R}^+$ is the mass of the body.

Hint: Use the identity $x \times (y \times z) = (x^T z)y - (x^T y)z$.

If you want, solve the problem with some appropriate methods, and see how well the constraints are preserved.

3 Prove that the flow of the problem

$$y' = \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} y$$

is volume preserving, but not symplectic for any possible pairs of variables.

4 **a)** Given 3 matrices $A, B, C \in \mathbb{R}^{m\times m}$. Prove the Jacobi identity

$$[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0.$$

b) Prove that the same hold for the Lie derivatives, that is

$$[D_A,[D_B,D_C]] + [D_B,[D_C,D_A]] + [D_C,[D_A,D_B]] = 0,$$

where the Lie derivate D_A is defined as

$$D_A = \sum_{i=1}^{m} f_i^A(y)\frac{\partial}{\partial y_i}$$

and similar for D_B and D_C.

5 *Time-dependent Hamiltonian systems:*

This exercise is a slightly modified version of an exercise taken from Leimkuhler and Reich, *Simulating Hamiltonian dynamics.*

Given a time-dependent Hamiltonian

$$H = H(p, q, t)$$

with the corresponding differential equations

$$q' = H_p(p, q, t), \qquad p' = -H_q(p, q, t) \tag{1}$$

We can write this differential equation in the autonomous form by as usual adding one extra equation, e.g. $Q' = 1$ or $Q = t$ to the system. To make it Hamiltonian, we can add an additional corresponding momentum P, so that the extended Hamiltonian is given by

$$\tilde{H} = H(q, p, Q) + P. \tag{2}$$

a) Write out the differential equations corresponding to the the extended Hamiltonian $\tilde{H}$, and show that if the extended system is solved with initial conditions $q(t_0) = q_0$, $p(t_0) = p_0$, $Q(t_0) = t_0$ and $P(t_0) = 0$, the solution is the same as that of (1) for the original Hamiltonian.

b) Prove that applying symplectic Euler to the extended system is equivalent to the following method for the original problem:

$$q_{n+1} = q_n + hH_p(p_{n+1}, q_n, t_n), \qquad p_{n+1} = p_n - hH_q(p_{n+1}, q_n, t_n)$$

NB! There are two versions of the symplectic Euler method. Pick the right one.

c) Find the appropriate generalization of the Störmer-Verlet method to Hamiltonian systems of the form

$$H(p, q, t) = \frac{1}{2}p^T M^{-1} p + V(q, t).$$

d) Test the two methods on the problem with Hamiltonian

$$H(p, q, t) = \frac{1}{2}p^T p + \frac{1}{2}(1 + \varepsilon \sin(\alpha t))q^T q$$

using e.g. $q_0 = (1, 2, 3, 4)$, $p_0 = (4, 1, 2, 3)$, $t_0 = 0$, $\alpha = 0.1$ and $\varepsilon = 0.25$. Use stepsize $h = 0.25$ and integrate from 0 to 1000. Plot the Hamiltonian. Experiment a bit with the parameters, and the stepsize.