

Problem set4 ODE, methods

1. Show that the implicit midpoint method is indeed symplectic.
2. Solve the Hamiltonian system for the Hamiltonian $H(p, q) = \frac{|p|^2}{2} - \frac{1}{|q|}$, where p and q are vectors of two components each. The components of p and q can be interpreted components of momentum and position, respectively. Use initial data $q(0) = (0.4, 0)^T, p(0) = (0, 2)^T$
Simulate the solutions using the Störmer-Verlet method, the standard 4th order RK and a symplectic 4th order RK method (for example use the PRK Lobatto III A-B pair, see page 40 in [HLW]), and the modified midpoint method. The latter should conserve both L and H. Plot the solutions in the q -plane, and the value of the Hamiltonian as a function of time. Run for long time and comment on the behavior of the methods. Is there anything wrong with the modified midpoint method?
3. Consider the corresponding constrained problem in 3D, where $0=g(q):=|q|-1$ is the constraint, see p 239 of [HLW], eq (1.9). Use initial data $q(0)=(1,0,0)^T, p(0)=(0,0.1,0.2)^T$, and simulate solutions using the SHAKE algorithm and the symplectic Euler with projection. Plot the solutions in q -space, as well as the Hamiltonian as a function of t . The Shake algorithm is supposed to suffer from long time accumulation of error. Do you observe this?
4. Consider again the same problem as in 3. It is possible to eliminate the lagrange variable λ by deriving an expression $\lambda(p,q)$. This is done by differentiate the constraint $g(q)=0$ twice with respect to time. (See p 239-240 in[HLW]). What happens with the Hamiltonian structure? Simulate using the symplectic Euler method, and the standard 4th order RK. Plot the Hamiltonian and the constraint as functions of t .

[HLW]:

