FINAL EXAM FOR THE AARMS/PIMS SUMMER SCHOOL
Structure-preserving discretization of differential equations
Halifax, Nova Scotia, July 30, 2015

Instructions and guidelines

- This is a take-home exam, it is expected that you do the problems without help of any other person
- You can use any written material to aid you in solving the problems, including the course material
- The exam consists of two parts. The first part is a google form that you reach via a link on the course home page. The second part consists of Problem 1-3 below
- You can start doing the exam immediately after it is available on the course web page
- The deadline for submission of the two parts of the exam is Monday, August 3, 10pm (Halifax time). The answers to part 2 should be sent by email to Elena Celledoni (`elenac@math.ntnu.no`), with your name clearly indicated on the document. pdf-format is preferred.

Problem 1

a) Find the adjoint of the Runge-Kutta method

$$y_{n+1} = y_n + h\left[-\frac{1}{2}f(y_n) + 2f\big(\frac{y_n + y_{n+1}}{2}\big) - \frac{1}{2}f(y_{n+1})\right]. \qquad (1)$$

Answer: By interchanging index n and $n+1$, replacing h by $-h$ and solving for y_{n+1}, we get the same method back, so the method is symmetric, the adjoint is the method itself. This is the Kahan method.

b) Explain why the midpoint method applied to linear Hamiltonian vector fields is both energy preserving and symplectic.

Answer: For linear Hamiltonian systems of the form $\dot{y} = J\nabla H(y)$ the gradient ∇H must be a linear function of y, and therefore the function $H(y)$ itself is quadratic. The midpoint rule is known to preserve all quadratic invariants, so it must in particular preserve $H(y)$. It is also symplectic for all Hamiltonian systems.

c) Show that the method (1) is symplectic and energy-preserving when applied to linear Hamiltonian vector fields. Does any of these two properties hold true when the Hamiltonian vector field is quadratic?

Answer: The first question is best answered by recognizing that if the problem is linear, i.e. $\dot{y} = Ay$, then the method (1) reduces to

$$y_{n+1} = y_n + hA\left(\frac{y_n + y_{n+1}}{2}\right)$$

which is nothing else than the midpoint rule for the linear problem, thus it is both symplectic and energy preserving as previously found.

For the second question, we obviously ask whether any of the two properties hold for *all* quadratic Hamiltonian problems. The answer is that none of the properties hold since Kahans method is known to be non-symplectic even for quadratic problems, and because it preserves only a perturbed version of the Hamiltonian function in the quadratic case. But to answer the question rigorously, one could use an example, say in $2d$ such as

$$H(y) = H(q,p) = \frac{1}{3}(q^3 + p^3),$$

proceed to compute the method map $\Phi_h(q,p)$ and its Jacobian and thereafter check the symplecticity condition. Similarly, with the energy, just compute $H(\Phi_h(q,p)) - H(q,p)$ and show that it is nonzero.

We end this discussion by noting that there exist quadratic Hamiltonian vector fields for which Kahan's method preserve both symplecticity and energy, one such example is obtained from the Hamiltonian

$$H(q,p) = \frac{1}{3}q^3$$

Problem 2 We are given a system of ordinary differential equations

$$\begin{aligned} \dot{x} &= 2xy - x^2 \\ \dot{y} &= 2yz - y^2 \\ \dot{z} &= 2xz - z^2 \end{aligned} \tag{2}$$

a) Show that the system is divergence free and use the method of Feng and Shang to write down the corresponding two Hamiltonian vector fields $f_{1,2}$ and $f_{2,3}$ as well as the matching Hamiltonians $H_{1,2}$ and $H_{2,3}$.

Answer: It is easily checked that the problem is divergence free, such that its flow is volume preserving. Following the procedure of Feng and Shang, we look for vector fields $f_{1,2}, f_{2,3}$ such that $f = f_{1,2} + f_{2,3}$ and which are of the form

$$f_{1,2} = (-\frac{\partial H_{1,2}}{\partial y}, \frac{\partial H_{1,2}}{\partial x}, 0)^T, \quad f_{2,3} = (0, -\frac{\partial H_{2,3}}{\partial z}, \frac{\partial H_{2,3}}{\partial y})^T,$$

For some functions $H_{1,2}$ and $H_{2,3}$ Then compute by integration $H_{1,2} = x^2y - xy^2$ and $H_{2,3} == 2xyz - z^2y$. The split vector fields are then

$$f_{1,2} = (2xy - x^2, -y^2 + 2xy, 0)^T, \quad f_{2,3} = (0, 2yz - 2xy, 2xz - z^2)^T.$$

A volume preserving method is now obtained by applying a symplectic integrator to each of the two vector fields $f_{1,2}$ and $f_{2,3}$ and to compose these method maps. Suppose Φ_h and Ψ_h are consistent symplectic integrators for the hamiltonian vector fields $f_{1,2}$ and $f_{2,3}$ respectively. Then the maps

$$\Psi_h \circ \Phi_h,\ \Phi_h \circ \Psi_h,\ \Psi_{h/2} \circ \Phi_h \circ \Psi_{h/2}$$

will all be volume preserving, the last one is Strang splitting and has order two.

b) Write down a a consistent volume preserving integrator for this problem.

Problem 3 If we apply the method of Kahan (1) to the problem

$$\begin{aligned}\dot{x} &= y \\ \dot{y} &= -x^2\end{aligned}$$

it results in the method map

$$\Phi_h \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \frac{x+hy}{1+\frac{1}{2}h^2x} \\ \frac{y-(hx^2+\frac{1}{2}h^2xy)}{1+\frac{1}{2}h^2x} \end{pmatrix}$$

which has the following expansion in terms of the stepsize h

$$\Phi_h \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} x \\ y \end{pmatrix} + h \begin{pmatrix} y \\ -x^2 \end{pmatrix} + h^2 \begin{pmatrix} -\frac{1}{2}x^2 \\ -xy \end{pmatrix} + h^3 \begin{pmatrix} -\frac{1}{2}xy \\ \frac{1}{2}x^3 \end{pmatrix} + \cdots$$

Find the coefficient functions f_2 and f_3 in the expansion for the modified vector field.

Answer: The given expansion of Φ_h gives us directly the d_k-coefficients. We compute the elementary differentials

$$f'f = -\begin{pmatrix} x^2 \\ 2xy \end{pmatrix}, \quad f''(f,f) = \begin{pmatrix} 0 \\ -2y^2 \end{pmatrix}, \quad f'f'f = \begin{pmatrix} -2xy \\ 2x^3 \end{pmatrix}$$

We then find that

$$f_2 = d_2 - \frac{1}{2}f'f = 0$$

So the terms in f_3 involving f_2 can be discarded and we get

$$f_3 = d_3 - \frac{1}{6}(f''(f,f) + f'f'f) = \frac{1}{6}(-xy, x^3 + 2y^2)^T$$