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Highly Oscillatory Problems — Exercise Sheet 02 April 25, 2018

Exercise 4: (Stability Issues of Standard Integration Schemes)

A widely established scheme for the numerical integration of model problems of type

$$y''(t) = -\omega^2 y(t) + \lambda f(y(t)), \quad y(0) = y_0 \in \mathbb{R}, \quad y'(0) = y_0' \in \mathbb{R}, \quad \omega > 0, \quad t \in [0, T], \tag{1}$$

with $\lambda \in \mathbb{R}$ and f being a smooth function, is the classical *Störmer-Verlet* method given through

$$\begin{pmatrix} p^{n+1} \\ q^{n+1} \end{pmatrix} = \Phi_{\mathrm{SV}}^{\tau} \begin{pmatrix} p^n \\ q^n \end{pmatrix}, \quad p^0 = y'(0), \quad q^0 = y(0),$$

with the recursion

$$\begin{cases} p^{n+1/2} = p^n + \frac{\tau}{2}(-\omega^2 q^n + \lambda f(q^n)) & =: \varphi_{\mathrm{p}}^{\tau/2} \begin{pmatrix} p^n \\ q^n \end{pmatrix} \\ q^{n+1} = q^n + \tau p^{n+1/2} & =: \varphi_{\mathrm{q}}^{\tau} \begin{pmatrix} p^{n+1/2} \\ q^n \end{pmatrix} \\ p^{n+1} = p^{n+1/2} + \frac{\tau}{2}(-\omega^2 q^{n+1} + \lambda f(q^{n+1})) & =: \varphi_{\mathrm{p}}^{\tau/2} \begin{pmatrix} p^{n+1/2} \\ q^{n+1} \end{pmatrix}. \end{cases} \tag{2}$$

Note that here q^n and p^n denote numerical approximations to $y(t_n)$ and $y'(t_n)$, respectively, at time $t_n = n\tau$, $n = 0, 1, 2, \ldots, \lfloor T/\tau \rfloor$. Based on [HLW2006] and [Sturm2017], we discuss the following stability issues of the Störmer-Verlet method for large $\omega \gg 1$.

(a) Reformulate (1) as a first order system in time for variables $q(t) = y(t)$ and $p(t) = y'(t) = q'(t)$.

(b) Show that we can interpret the scheme $\Phi_{\mathrm{SV}}^{\tau} \begin{pmatrix} p^n \\ q^n \end{pmatrix}$ from above as a Strang splitting scheme with step size τ applied to the system from part a).

Hint: The mappings $\varphi_{\mathrm{p}}^{\tau}$ and $\varphi_{\mathrm{q}}^{\tau}$ in (2) are the exact flows of subproblems corresponding to the system from part a).

(c) It is well-known that the Strang splitting/ Störmer-Verlet scheme $\Phi_{\mathrm{SV}}^{\tau}$ satisfies second order local error bounds in time. However, it suffers from severe stability issues. In the following, consider the case of vanishing nonlinearity $f \equiv 0$.

α) Derive a compact formulation of the scheme $\Phi_{\mathrm{SV}}^{\tau}$ such that

$$\begin{pmatrix} p^{n+1} \\ q^{n+1} \end{pmatrix} = \Phi_{\mathrm{SV}}^{\tau} \begin{pmatrix} p^n \\ q^n \end{pmatrix} = A \begin{pmatrix} p^n \\ q^n \end{pmatrix} = A^{n+1} \begin{pmatrix} p^0 \\ q^0 \end{pmatrix} \quad \text{for a suitable matrix } A.$$

β) Show that the Störmer-Verlet scheme is stable (i.e. possesses bounded numerical solutions) if and only if the **C**ourant-**F**riedrich-**L**evy (CFL) condition

$$\tau\omega \leq 2 \qquad \text{is satisfied (cf. [HLW2006] and [Sturm2017]).}$$

Hint: Exploit that the scheme $\Phi_{\mathrm{SV}}^{\tau}$ defined via the matrix A is stable if and only if $\|A^n x\| \leq \|x\|$ for all $n \in \mathbb{N}$ and for all $x \in \mathbb{R}^2$ with a constant $\mathcal{M}$ independent of n. What property do the eigenvalues of A have to satisfy?

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[HLW2006] - E. Hairer et. al., *Geometric Numerical Integration*, Springer 2006
[Sturm2017] - A. Sturm, *Locally Implicit Time Integration for Linear Maxwell's Equations*, Dissertation 2017

In the following let $c \geq 1$ and let $k \in \mathbb{Z}$. For $T > 0$ and $\lambda \in \mathbb{R}$, we consider the ODE problem

$$y''(t) = -c^2 \langle k \rangle_c^2 y(t) + c^2 \lambda f(y(t)), \quad y(0) = y_0 \in \mathbb{R}, \quad y'(0) = y_0' \in \mathbb{R} \qquad \text{for all} \quad t \in [0, T], \tag{3}$$

where $\langle k \rangle_c := \sqrt{|k|^2 + c^2}$ denotes the *japanese symbol* of k corresponding to the index c and where $f : \mathbb{R} \to \mathbb{R}$ is a smooth function.

Exercise 5: (Exponential Integrator in the Linear 1-dimensional Case)

Consider the linear case with $f(y) = y$ and let $0 \leq \lambda < |k|^2 + c^2$.

(a) Determine the so-called dispersion relation $\omega_k : \mathbb{R} \times (\mathbb{R} \setminus \{0\}) \to \mathbb{R}_{\geq 0}$ of (3), depending on the integer k and on the parameters c and λ. Note that in this notation, the solution of (3) is given by (cf. exercise 1)

$$y(t) = \cos(t\omega_k(c, \lambda)) y_0 + \frac{\sin(t\omega_k(c, \lambda))}{\omega_k(c, \lambda)} y_0', \qquad \text{for all } t \in [0, T].$$

(b) Based on the ansatz (cf. exercise sheet 1)

$$u(t) = y(t) - i \frac{1}{c \langle k \rangle_c} y'(t) \quad \text{and} \quad y(t) = \frac{1}{2}(u(t) + \overline{u(t)})$$

construct a first order exponential time integration scheme for a numerical approximation u^n of $u(t_n)$ at time $t_n = n\tau$, $n = 0, 1, 2, \ldots, \lfloor T/\tau \rfloor =: N_T$, defined via

$$u^{n+1} = \Phi^\tau_{\exp}(u^n), \quad u^0 = u(0).$$

in order to approximate the solution $y(t_n)$ of (3).

Hint: Duhamel's formula for $u(t_n + \tau)$ from exercise 3 and freezing of the nonlinearity at time t_n. Make use of the so-called φ_1 function defined via $\varphi_1(x) = \dfrac{e^x - 1}{x}$.

(c) Prove the following estimates:

$$\alpha) \quad \frac{c}{\langle k \rangle_c} \leq 1 \quad \text{for all } k \in \mathbb{Z} \text{ and for all } c > 0. \qquad \beta) \quad |\varphi_1(ix)| = \frac{|e^{ix} - 1|}{|x|} \leq 1 \quad \text{for all } x \in \mathbb{R}.$$

(d) For the numerical scheme $\Phi^\tau_{\exp}$ from part b) prove the following

α) first order local error bound

$$|u(t_{n+1}) - \Phi^\tau_{\exp}(u(t_n))| \leq \tau^2 c^2 (1 + |k|) \mathcal{M}_u^{\text{loc}},$$

where $\mathcal{M}_u^{\text{loc}}$ depends on $\sup_{t_n \leq t \leq t_n + \tau} |u(t)|$. Note that this error bound heavily depends on c.

β) stability bound

$$|\Phi^\tau_{\exp}(v) - \Phi^\tau_{\exp}(w)| \leq (1 + \tau \mathcal{M}^{\text{stab}})|v - w|,$$

where $\mathcal{M}^{\text{stab}}$ is independent of c and k.

γ) global first order error bound

$$|u(t_{n+1}) - u^{n+1}| \leq \tau c^2 \mathcal{M}_u^{\text{glob}}(T, k),$$

where $\mathcal{M}_u^{\text{glob}}(T, k)$ depends on $\sup_{0 \leq t \leq T} |u(t)|$, the time T and on the integer k but is **independent** of c and n.

Hint: Exploit the results from part c). For γ) combine the results from α) and β) and use a Lady Windermere's fan argument.

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Programming Exercise 2: (Störmer-Verlet vs. Exponential Integrator)

Consider the setting from exercise 5, i.e.

$$y''(t) = -c^2 \langle k \rangle_c^2 y(t) + c^2 \lambda y(t), \quad y(0) = y_0 \in \mathbb{R}, \quad y'(0) = y_0' \in \mathbb{R} \qquad \text{for all} \quad t \in [0, T], \tag{4}$$

with $0 \leq \lambda < |k|^2 + c^2$. The aim is now to implement and test the schemes from the previous exercises.

(a) Fix the values $T = 1$, $c = 6$ and $k = 3$, $\lambda = 0.5$ and for these values fix the initial data

$$y_0 = 0.5, \qquad y_0' = 0.5c \langle k \rangle_c .$$

Consider the discretization $t_n = n\tau$, $n = 0, 1, 2, \dots \lfloor T/\tau \rfloor =: N_T$ for step sizes

$$\tau_m = \frac{0.1 \cdot m}{c \langle k \rangle_c}, \qquad m = 1, 2, \dots, 21, \qquad \langle k \rangle_c = \sqrt{|k|^2 + c^2}.$$

α) In view of the construction of our exponential integrator, write a function file `phi1(z)` which takes an array `z` and which returns an array with the **elementwise** evaluations $\phi_1(z_j)$. Take care of the values in the array `z` which take the value 0.

β) Implement the Störmer-Verlet and exponential time integration schemes Φ_{SV}^τ and $\Phi_{\exp}^\tau$ from the previous exercises for this problem in MATLAB or Python.

γ) Plot the exact solution $y(t_n)$ (cf. Ex.5a)) for all times t_n together with the numerical approximations obtained with the schemes Φ_{SV}^τ and $\Phi_{\exp}^\tau$ in one figure.

δ) Discuss the behaviour of the Störmer-Verlet solution for τ_{19}, τ_{20} and for τ_{21}, i.e. for the cases, when the time step size satisfies the CFL condition $\tau \cdot (c \langle k \rangle_c) \leq 2$ from Ex.4c)β) and for the case when this condition is violated. Note, that corresponding to the notation from exercise 4, in the problem (4) we identify ω and f as $c \langle k \rangle_c = \omega$ and $f(y(t)) = c^2 y(t)$.

(b) Create double-logarithmic order plots for the schemes Φ_{SV}^τ and $\Phi_{\exp}^\tau$:

α) Create an array `tau_array` containing all time step sizes τ_m, $m = 1, 2, \dots, 21$ and in additional arrays `errSV_array` and `errEX_array` for the Störmer-Verlet and Exponential time integration scheme, respectively, save for each τ_m the maximum error over all times t

$$\text{err}_{\max} = \max_{t_n \in [0,T]} |y(t_n) - y^n|,$$

where y^n denotes the numerical approximation to the exact solution $y(t_n)$ at time t_n. Plot the errors `err{X}_array` versus the time steps `tau_array` in a `loglog` plot and add lines of slope 1 and 2 corresponding to order 1 and order 2 convergence, respectively. Why may it not be enough for highly-oscillatory to only consider the error at the end time $t_{N_T} \approx T$?

β) Modify your code such that in the previous order plots the error data corresponding to additional values of $c = 1, 6, 11, 16, 21$ are plotted.

Discussion in the problem class friday 11:30 am, in room 2.058 in the Kollegiengebäude Mathematik 20.30.