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**Exercise 18:** Complete the proof of the following Theorem from the lecture.

Let $f(y)$ be analytic in $B_{2R}(y_0)$, let the coefficients $d_j(y)$ of the numerical scheme be analytic in $B_R(y_0)$ and assume that

$$\|f(y)\| \leq M \quad \text{for} \quad \|y - y_0\| \leq 2R$$

and

$$\|d_j(y)\| \leq \mu M \Big(\frac{2\kappa M}{R}\Big)^{j-1} \quad \text{for} \quad \|y - y_0\| \leq R$$

hold. If $h \leq h_0/4$ with $h_0 = R/(\mathrm{e}\eta M)$, then there exists $N = N(h)$ (namely $N$ equals the largest integer satisfying $hN \leq h_0 < h(N+1)$) such that the difference between the numerical solution $y_1 = \Phi_h(y_0)$ and the exact solution $\varphi_{N,t}(y_0)$ of the truncated modified equation satisfies

$$\|\Phi_h(y_0) - \varphi_{N,h}(y_0)\| \leq h\gamma M \mathrm{e}^{-h_0/h}$$

where $\gamma = \mathrm{e}(2 + 1.65\eta + \mu)$ depends only on the method.

The proof proceeded in the following steps, where all parts except for part (d) were done in the lecture.

(a) Show that for $g(h) := \Phi_h(y_0) - \varphi_{N,h}(y_0)$ the bound

$$\|g(h)\| \leq \Big(\frac{h}{\varepsilon}\Big)^{N+1} \max_{|z|\leq\varepsilon} \|g(z)\|$$

holds for $0 \leq h \leq \varepsilon := \mathrm{e}h_0/N$.

(b) Split the error in two parts,

$$\|g(z)\| \leq \|\Phi_z(y_0) - y_0\| + \|\varphi_{N,z}(y_0) - y_0\| ,$$

which are estimated separately in the following two steps of the proof.

(c) Show that

$$\|\Phi_z(y_0) - y_0\| \leq \varepsilon M(1 + \mu)$$

holds.

(d) Show that

$$\|\varphi_{N,z}(y_0) - y_0\| \leq \varepsilon M(1 + 1.65\eta)$$

for $\varphi_{N,z}(y_0) \in B_{R/2}(y_0)$.

(e) Finally combine both bounds to obtain the desired result.

**Exercise 19:**

Consider a differential equation

$$y'(t) = f(y(t)) , \quad y(0) = y_0 ,$$

which possesses the invariant $I(y)$. We solve this equation numerically with a scheme $\Phi_h(y)$, that also conserves the invariant. Show that the modified equation conserves $I(y)$ as well.

Hint: Show via induction that $\nabla I(y) f_j(y) = 0$, $j = 1, \ldots, r$ holds. For this purpose let $\varphi_{r,t}^{(h)}$ be the flow of the truncated modified equation $\tilde{y}' = f(\tilde{y}) + hf_2(\tilde{y}) + \ldots + h^{r-1} f_r(\tilde{y})$, $\tilde{y}(0) = y_0$.

**Programming Exercise 7:**

(a) Show that for a nonsymplectic method of order $r$ applied to a Hamilton system the error in the energy grows linearly with the time, namely

$$H(y_n) - H(y_0) = \mathcal{O}(th^r)\,,$$

where $t = nh$.

Hint: Use that the local error of the method is of the order $h^{r+1}$.

(b) Consider the pendulum equation given by the Hamiltonian

$$H(p,q) = \frac{p^2}{2} - \cos(q)$$

with initial condition $(p_0, q_0) = (2.5, 0)$. Solve this equation with the explicit and the symplectic Euler method on the time interval $[0, T] = [0, 50]$ using the time step size $h = 0.005$. Plot the error in the energy $H$ of both methods over time.

**Programming Exercise 8:**

Consider the pendulum equation given by the Hamilton function

$$H(p,q) = \frac{p^2}{2} - \cos(q)\,.$$

(a) Let $K$ be a compact subset of $\{(x,y) \in \mathbb{R}^2; |x| \leq c\}$. Show that

$$\|f(p,q)\| \leq \sqrt{(c+2R)^2 + e^{4R}} = M$$

for $f(p,q) = -J\nabla H(p,q)$ and $||(p,q) - (p_0,q_0)|| \leq 2R$ with $(p_0,q_0) \in K$.

(b) Now choose $c = 2$ and $R = 1/2$ and compute the corresponding time step size $h_0$ for the midpoint rule to obtain good energy conservation.

(c) Numerically compute the solution of the pendulum equations with the different initial conditions

$$(p_0,q_0) = (0,-1.5)\,,\quad (0,-2.5)\,,\quad (1.5,-\pi)\,,\quad (2.5,-\pi)\,.$$

Therefore use the midpoint rule with the time step size $h_0$ computed in the previous part on the time interval $[0, 200.000h_0]$ and plot the components $p$ and $q$ against each other. What happens to the results, if the time step size is increased?

**Programming Exercise 9:** *Oscillatory example – Fermi-Pasta-Ulam problem*

Consider the equation

$$x''(t) = -\omega^2 x(t)\,,\quad \omega \gg 1$$

with initial conditions $x(0) = x_0$ and $x'(0) = x'_0$.

(a) Show, that the exact solution of the system is given by

$$\begin{pmatrix} \omega x(t) \\ x'(t) \end{pmatrix} = \begin{pmatrix} \cos\omega t & \sin\omega t \\ -\sin\omega t & \cos\omega t \end{pmatrix} \begin{pmatrix} \omega x_0 \\ x'_0 \end{pmatrix}\,.$$

(b) We consider the midpoint rule

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

for $y' = f(y)$ as well as the Störmer-Verlet method

$$\begin{aligned} x'_{n+1/2} &= x'_n + \frac{h}{2}g(x_n) \\ x_{n+1} &= x_n + hx'_{n+1/2} \\ x'_{n+1} &= x'_{n+1/2} + \frac{h}{2}g(x_{n+1}) \end{aligned}$$

for $x'' = g(x)$. Compute one step of each method applied to the above problem. Note that for the midpoint rule, the problem needs to be rewritten as a first order system. Analyze the stability of the methods with respect to the time step size $h$.

Hint: Write the numerical solution as

$$\begin{pmatrix} \omega x_{n+1} \\ x'_{n+1} \end{pmatrix} = M(h\omega) \begin{pmatrix} \omega x_n \\ x'_n \end{pmatrix}$$

and consider the eigenvalues of $M(h\omega)$.

(c) The Hamiltonian of the Fermi-Pasta-Ulam problem in the scaled expansions of the springs is given by

$$\begin{aligned} H(y,x) = {} & \frac{1}{2}\sum_{i=1}^{m}(y_{0i}^2 + y_{1i}^2) + \frac{\omega^2}{2}\sum_{i=1}^{m} x_{1i}^2 \\ & + \frac{1}{4}(x_{01} - x_{11})^4 + \frac{1}{4}\sum_{i=1}^{m-1}(x_{0i+1} - x_{1i+1} - x_{0i} - x_{1i})^4 + \frac{1}{4}(x_{0m} + x_{1m})^4 , \end{aligned}$$

the oscillatory energy of the stiff springs is given by

$$I_j(x_{1j}, y_{1j}) = \frac{1}{2}(y_{1j}^2 + \omega^2 x_{1j}^2)$$

and the total oscillatory energy is $I = I_1 + \ldots + I_m$. Consider for $m = 3$ and $\omega = 50$ the initial values

$$\begin{aligned} & x_{01}(0) = 1 , \quad y_{01}(0) = 1 , \quad x_{11}(0) = \omega^{-1} , \quad y_{11}(0) = 1 \\ & x_{0i}(0) = y_{0i}(0) = x_{1i}(0) = y_{1i}(0) = 0 , \quad i = 2, 3 . \end{aligned}$$

Solve this problem numerically on the time interval $[0, 225]$ with

(i) the implicit midpoint rule,

(ii) the symplectic Euler method and

(iii) the Störmer-Verlet method.

Employ the time step sizes $h = 0.001$ and $h = 0.03$ and plot the shifted Hamiltonian $H(y, x) - 0.8$ as well as the total oscillatory energy $I$ and the energies of the three stiff springs $I_j$, $j = 1, 2, 3$.

**Discussion in the exercise class on 12.7.2012.**