Summary: Chapter 5

- A one-step numerical scheme $y_{n+1} = \Phi_h(y_n)$ is called *symplectic* if $\Phi_h : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is a symplectic map:
$$\Phi_h'(y)^T J \Phi_h'(y) = J \quad \forall\, y,$$
with $J = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix}$ and where $\Phi_h'(y) := \frac{\partial \Phi_h(y)}{\partial y}$.
Example: Midpoint rule.

- If the coefficients of a Runge-Kutta scheme satisfy
$$b_i a_{ij} + b_j a_{ji} = b_i b_j \qquad \forall\, i, j = 1, \ldots, s,$$
then the numerical scheme is symplectic.
Idea of the proof: We consider a Hamiltonian problem together with its *variational equation*
$$\dot{\Psi} = J^{-1} \nabla^2 H(y) \Psi, \quad \Psi(0) = I.$$
We next observe that $\Psi^T J \Psi$ is a quadratic invariant for the above augmented system and thus every Runge-Kutta schemes with the above condition preserve this invariant.
Example: Gauss collocation methods.

- If the coefficients of a partitioned Runge-Kutta scheme satisfy
$$\begin{aligned} b_i \hat{a}_{ij} + \hat{b}_j a_{ji} &= b_i \hat{b}_j & \forall \quad i, j = 1, \ldots, s \\ b_i &= \hat{b}_i & \forall \quad i = 1, \ldots, s, \end{aligned}$$
then the numerical scheme is symplectic.
Example: Symplectic Euler scheme; Störmer-Verlet method.

- We consider the following problem
$$\begin{aligned} y'(x) &= f(y(x)) \\ y(0) &= y_0. \end{aligned}$$
Hypothesis. The numerical solution reads
$$\Phi_h(y) = y + hf(y) + h^2 d_2(y) + h^3 d_3(y) + \ldots$$
with given $d_j(y)$.
Example: Explicit Euler scheme: $d_j(y) = 0 \quad \forall\, j \geq 2$. B-series methods.

Ansatz. The *modified differential equation* is defined as

$$\begin{aligned} \tilde{y}' &= f_h(\tilde{y}) = f(\tilde{y}) + hf_2(\tilde{y}) + h^2 f_3(\tilde{y}) + \dots \\ \tilde{y}(0) &= y_0. \end{aligned}$$

We ask for the exact solution of the modified differential equation to be equal to the numerical solution:

$$\tilde{y}(nh) = y_n = \Phi_h(y_{n-1}), \quad \forall n \geq 1.$$

A Taylor expansion of the exact solution gives us the coefficients of the modified equation $f_j(y)$ in terms of the coefficients of the numerical scheme $d_j(y)$ and of $f(y)$.

- *Properties of the modified differential equation*:

  If the numerical scheme has order p then one has:

  $$\begin{aligned} \tilde{y}' &= f_h(\tilde{y}) = f(\tilde{y}) + h^p f_{p+1}(\tilde{y}) + h^{p+1} f_{p+2}(\tilde{y}) + \dots \\ \tilde{y}(0) &= y_0, \end{aligned}$$

  where $f_{p+1}(\tilde{y})$ is the main coefficient of the local error.

  The coefficients of the modified differential equation for the adjoint scheme satisfy

  $$f_j^*(y) = (-1)^{j+1} f_j(y).$$

  The coefficients of the modified differential equation for a symmetric scheme satisfy

  $$f_j(y) = 0 \quad \text{for} \quad j \quad \text{even}.$$

  If the problem is Hamiltonian, $y' = J^{-1}\nabla H(y)$, and the numerical scheme is symplectic, then the modified differential equation is also Hamiltonian:

  $$f_j(y) = J^{-1}\nabla H_j(y) \qquad \forall\, j \geq 2.$$

- *Error analysis:*

  Hypothesis. We assume that

  $$\|f^{(k)}(y)\| \;\leq\; k!MR^{-k} \quad \text{for} \quad k = 0, 1, 2, \dots$$

  and $\|y - y_0\| \leq 2R$ in a given norm. Let us consider an s-stage Runge-Kutta scheme with step size h and define the following quantities: $\mu := \sum_{i=1}^{s} |b_i|$, $\kappa := \max_{i=1,\dots,s} \sum_{j=1}^{s} a_{ij}$, $\eta := 2\max(\kappa, \mu/(2\ln(2)-1))$, N an integer such that $Nh \leq \frac{R}{\mathrm{e}\eta M}$, $\gamma := \mathrm{e}(2 + 1.65\eta + \mu)$, $h^* := \frac{R}{4\mathrm{e}\eta M}$.

  Then one has:

  $$\begin{aligned} \|d_j(y)\| &\leq \mu M\left(\frac{2\kappa M}{R}\right)^{j-1} \quad \text{for} \quad j \geq 2 \quad \text{and} \quad \|y - y_0\| \leq R. \\ \|f_j(y)\| &\leq \ln(2)\eta M\left(\frac{\eta M j}{R}\right)^{j-1} \quad \text{for} \quad j \geq 2 \quad \text{and} \quad \|y - y_0\| \leq R/2. \\ \|\Phi_h(y_0) - \varphi_{N,h}(y_0)\| &\leq h\gamma M \mathrm{e}^{-h^*/h}, \end{aligned}$$

where $\varphi_{N,h}(y)$ is the flow of the truncated modified differential equation $\tilde{y}' = F_N(\tilde{y}) := f(\tilde{y}) + hf_2(\tilde{y}) + \ldots + h^{N-1} f_N(\tilde{y}), \tilde{y}(0) = y_0$.

For a Hamiltonian problem $\dot{y} = J^{-1}\nabla H(y)$ and a symplectic numerical integrator of order p, one finally obtains

$$\begin{aligned} \tilde{H}(y_n) &= \tilde{H}(y_0) + \mathcal{O}(\mathrm{e}^{-h^*/(2h)}) \quad \text{for} \quad nh \leq T \\ H(y_n) &= H(y_0) + \mathcal{O}(h^p) \quad \text{for} \quad nh \leq T \end{aligned}$$

for exponential long-time $T = \mathrm{e}^{h^*/(2h)}$.