

Summary: Chapter 3

- We consider problems of the form

$$\begin{aligned}\dot{y} &= f(y), \\ y(t_0) &= y_0.\end{aligned}$$

A non-constant function $I(y)$ is called an *invariant* or *first integral* if

$$I'(y)f(y) = 0 \quad \forall y.$$

From this definition, it follows $I(y(t)) = I(y(t_0)) = \text{Const.}$ along solutions of our problem.

Examples: The total energy $H(p, q)$ of a Hamiltonian system, the total mass in a chemical reaction, etc.

- All Runge-Kutta methods preserve linear invariants $I(y) = d^T y$, where d is a constant vector: $I(y_n) = I(y_0)$ for all $n \geq 1$.

A partitioned Runge-Kutta method for

$$\begin{aligned}\dot{p} &= f(p, q) \\ \dot{q} &= g(p, q)\end{aligned}$$

preserves linear invariants $I(p, q)$, if $b_i = \hat{b}_i$ or, if $I(p, q)$ only depends on p or only depends on q .

- For matrix equations

$$\begin{aligned}\dot{Y} &= B(Y)Y \\ Y(0) &= Y_0\end{aligned}$$

with $B(Y)$ skew-symmetric, we have that the function $g(Y) := Y^T Y$ is an invariant.

Example: Rigid body.

- Gauß (collocation) methods preserve *quadratic invariants*, i.e.

$$y_n^T C y_n = y_0^T C y_0 \quad \forall n,$$

where C is a symmetric matrix.

Runge-Kutta methods with coefficients satisfying

$$b_i a_{ij} + b_j a_{ji} = b_i b_j \quad \forall i, j = 1, \dots, s$$

preserve quadratic invariants $I(y) = y^T C y$, where C is a symmetric matrix.

We have seen similar results for partitioned Runge-Kutta methods.

- Polynomial invariants: For $n \geq 3$, no Runge-Kutta method can preserve all polynomial invariants of degree n .
- We consider *differential equations on manifolds*: Let

$$\mathcal{M} := \{y \in \mathbb{R}^n : g(y) = 0\}$$

a $(n - m)$ -manifold of \mathbb{R}^n with $g : \mathbb{R}^n \rightarrow \mathbb{R}^m$, $g'(y)$ has full rank, and a differential equation $\dot{y} = f(y)$ such that

$$y_0 \in \mathcal{M} \implies y(t) \in \mathcal{M}.$$

We define a *projection method* as follows:

1. Let $y_n \in \mathcal{M}$.
2. We define $\tilde{y}_{n+1} := \tilde{\Phi}_h(y_n)$, where $\tilde{\Phi}_h$ is an arbitrary one-step numerical scheme.
3. To find y_{n+1} , we just project \tilde{y}_{n+1} onto the manifold \mathcal{M} . At this step, one has to solve a nonlinear system (with simplified Newton for example).

The projection method has the same order of convergence as the scheme $\tilde{\Phi}_h$.

Warning: It is important to project onto the correct manifold. If one is not aware of all invariants of the system and only projects onto certain invariants, the method could produce bad results.

Example: Numerical solutions given by the explicit Euler and symplectic Euler methods for the perturbed Kepler problem with invariants $H(p, q) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}$ and $L(p, q) = q_1 p_2 - q_2 p_1$.

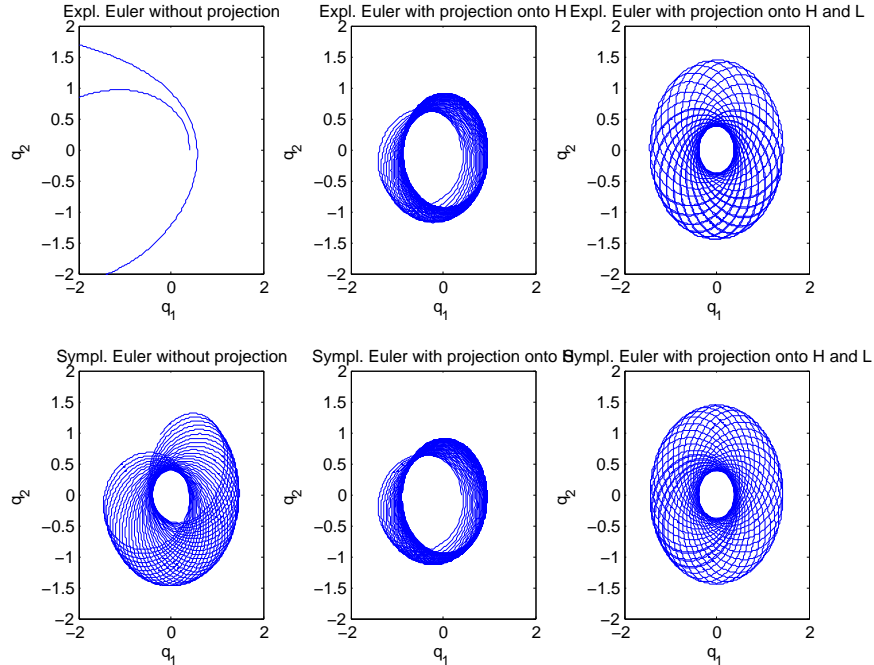


Figure 1: Projection methods for the perturbed Kepler problem.

We have also seen a symmetric version of this projection scheme (with better longtime properties).