8 Integration of Ordinary Differential Equations (ODEs)

8.1 ODEs and initial value problems (IVPs) for ODEs

Definition 8.1.1 (ODEs and IVPs for ODEs)**.** *Let* $d \in \mathbb{N}$, $D \subset \mathbb{R}^d$, $y_0 \in D$, $I \in \{[0,\infty)\} \cup \{[0,T] : T \in (0,\infty)\}$ *and let* $f : D \to \mathbb{R}^d$ *be a continuous function. Then a function* $y : I \to D$ *is called solution of the ODE*

$$\dot{y}(t) = f(y(t)), \qquad t \in I \tag{8.1.1}$$

if y *is continuously differentiable and if it holds that* $\forall\, t \in I : \dot{y}(t) := y'(t) = f(y(t))$*. Equation* (8.1.2a) *is called ODE, the function* f *is called right hand side (or vector field) of (the ODE)* (8.1.2a) *and the set* D *is called state space of (the ODE)* (8.1.2a)*. Moreover, a function* $y : I \to D$ *is called solution of the IVP (ger.: Anfangswertproblem (AWP))*

$$\dot{y}(t) = f(y(t)), \qquad t \in I, \tag{8.1.2a}$$

$$y(0) = y_0 \tag{8.1.2b}$$

if y *is continuously differentiable and if it holds that* $y(0) = y_0$ *and* $\forall\, t \in [0,T] : y'(t) = f(y(t))$*.* (8.1.2) *is called IVP,* (8.1.2b) *is called initial condition of (the IVP)* (8.1.2) *and* y_0 *is called initial value of (the IVP)* (8.1.2)*.*

Example 8.1.1 (Scalar linear ODEs). Let $\alpha, y_0 \in \mathbb{R}$. Then the function $y\colon [0,\infty) \to \mathbb{R}$ given by $y(t) = e^{\alpha t} y_0$ for all $t \in [0,\infty)$ is a solution of the IVP

$$\begin{aligned} \dot{y}(t) &= \alpha \cdot y(t), \qquad t \in [0,\infty), \\ y(0) &= y_0 \ . \end{aligned} \tag{8.1.3}$$

<u>Notation:</u> Instead of

$$\dot{y}(t) = f(y(t)), \qquad t \in I \tag{8.1.4}$$

in Definition 8.1.1 one sometimes also writes

$$\dot{y} = f(y), \qquad t \in I \tag{8.1.5}$$

for short. Moreover, note in the setting of Definition 8.1.1 that a continuous function $y\colon I \to \mathbb{R}$ is a solution of the IVP (8.1.2) if and only if it satisfies

$$\forall\, t \in I\colon \qquad y(t) = y_0 + \int_0^t f(y(s))\, ds \ . \tag{8.1.6}$$

Equation (8.1.6) is called integral representation of the IVP (8.1.2).

Theorem 8.1.2 (Existence and uniqueness of solutions of IVPs)**.** *Let $d \in \mathbb{N}$, let $D \subset \mathbb{R}^d$ be an open set, let $y_0 \in D$, let $I \in \{[0,\infty)\} \cup \{[0,T] : T \in (0,\infty)\}$ and let $f : D \to \mathbb{R}^d$ be a locally Lipschitz continuous function. Then there exit at most one solution of the IVP*

$$\begin{aligned} \dot{y}(t) &= f(y(t)), \qquad t \in I, \\ y(0) &= y_0 \end{aligned} \tag{8.1.7}$$

and there exists a real number $T \in (0,\infty)$ such that the IVP

$$\begin{aligned} \dot{y}(t) &= f(y(t)), \qquad t \in [0,T], \\ y(0) &= y_0 \end{aligned} \tag{8.1.8}$$

has a unique solution.

Remark 8.1.2 (Conversion of non-autonomous ODEs into autonomous ODEs). Let $d \in \mathbb{N}$, $T \in (0,\infty)$, $O \subset \mathbb{R}^d$, $D := [0,T] \times O$, let $g\colon [0,T] \times O \to \mathbb{R}^d$ be a continuous function, let $x\colon [0,T] \to O$, $f\colon D \to \mathbb{R}^{d+1}$ and $y\colon [0,T] \to D$ be functions satisfying

$$f(t,v) = (1, g(t,v)) \qquad \text{and} \qquad y(t) = (t, x(t)) \tag{8.1.9}$$

for all $(t,v) \in D$. Then x is continuously differentiable and satisfies

$$\forall\, t \in [0,T]\colon \qquad \dot{x}(t) = g(t, x(t)) \tag{8.1.10}$$

if and only if the function y is a solution of the ODE

$$\dot{y}(t) = f(y(t)), \qquad t \in [0,T]\,. \tag{8.1.11}$$

Clearly, this conversion can also be used to convert a "non-autonomous IVP" to an autonomous IVP in the sense of Definition 8.1.1.

△

Remark 8.1.3 (From higher order ODEs to first order systems). Let $n, d \in \mathbb{N}$, $T \in (0, \infty)$, let $x\colon [0,T] \to \mathbb{R}^d$ be an n-times continuously differentiable function and let $g\colon \mathbb{R}^{nd} \to \mathbb{R}^d$, $f\colon \mathbb{R}^{nd} \to \mathbb{R}^{nd}$ and $y\colon [0,T] \to \mathbb{R}^{nd}$ be continuous functions satisfying

$$f\begin{pmatrix} v_0 \\ v_1 \\ \vdots \\ v_{n-2} \\ v_{n-1} \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_{n-1} \\ g(v_1, \dots, v_{n-1}) \end{pmatrix} \quad \text{and} \quad y(t) = \begin{pmatrix} x(t) \\ x'(t) \\ \vdots \\ x^{(n-2)}(t) \\ x^{(n-1)}(t) \end{pmatrix} \tag{8.1.12}$$

for all $v = (v_0, v_1, \dots, v_{n-1}) \in \mathbb{R}^{nd}$ and all $t \in [0,T]$. Then

$$\forall\, t \in [0,T]\colon \qquad \boxed{x^{(n)}(t) = g\Big(x(t), x'(t), x''(t), \dots, x^{(n-1)}(t)\Big)} \tag{8.1.13}$$

if and only if y is a solution of the ODE

$$\dot{y}(t) = f(y(t)), \qquad t \in [0,T]\,. \tag{8.1.14}$$

Clearly, this conversion can also be used to convert a “higher order IVP” to an IVP in the sense of Definition 8.1.1.

△

Example 8.1.4 (Predator-prey model). [**?**, Sect. 1.1] & [7, Sect. 1.1.1] initially proposed by Alfred J. Lotka in "The theory of autocatalytic chemical reactions" in 1910. Let $\alpha, \beta, \gamma, \delta \in (0, \infty)$. Then the Lotka-Volterra ODE reads as

$$\begin{pmatrix} \dot{y}_1(t) &= (\alpha - \beta y_2(t))\, y_1(t) \\ \dot{y}_2(t) &= (\delta y_1(t) - \gamma)\, y_2(t) \end{pmatrix}, \qquad t \in [0, \infty)\,. \tag{8.1.15}$$

The vector field $f\colon (0,\infty)^2 \to \mathbb{R}^2$ satisfies $f(x) = \big(\alpha x_1 - \beta x_1 x_2, \delta x_1 x_2 - \gamma x_2\big)$ for all $x = (x_1, x_2) \in (0,\infty)^2$ here.

A solution $y = (y_1, y_2)\colon [0,\infty) \to (0,\infty)^2$ of (8.1.15) describes population sizes:

$u(t) := y_1(t) \to$ no. of prey at time $t \in [0,\infty)$,
$v(t) := y_2(t) \to$ no. of predators at time $t \in [0,\infty)$

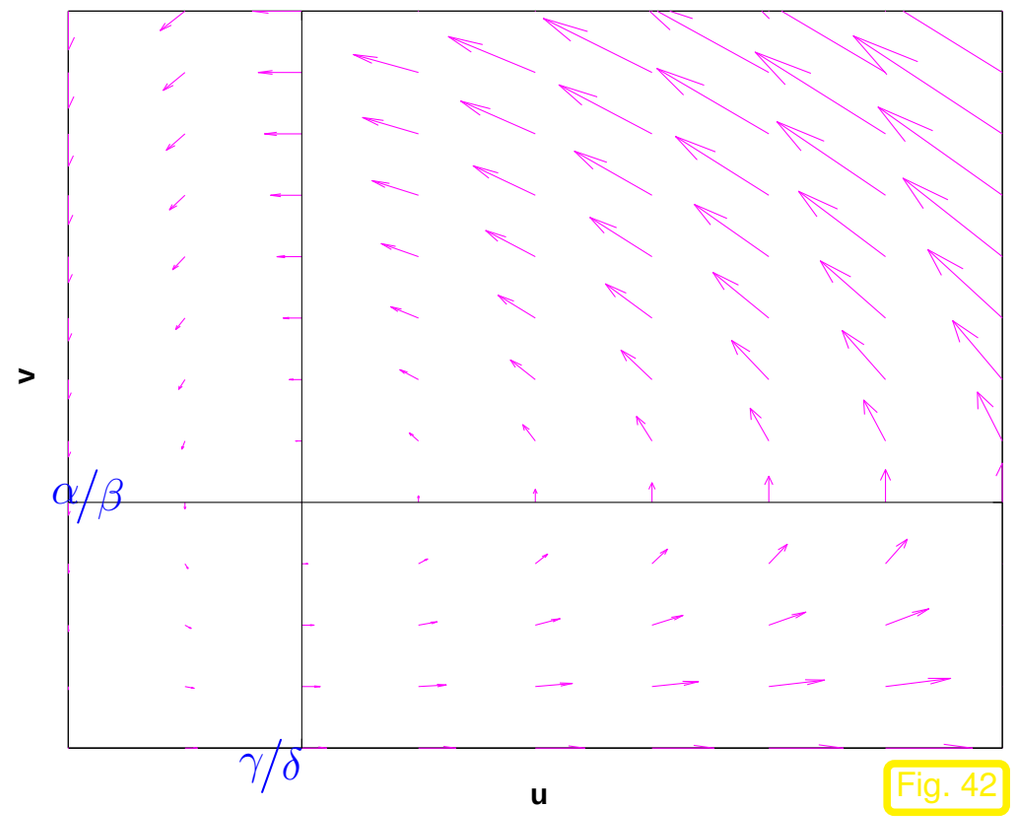
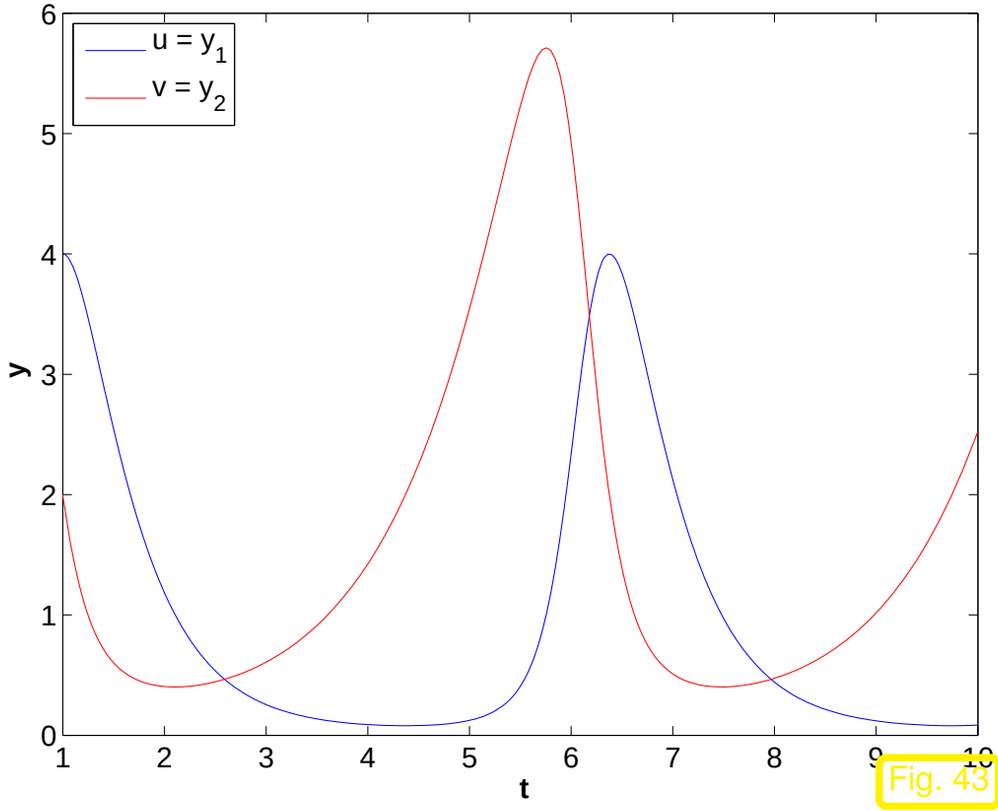


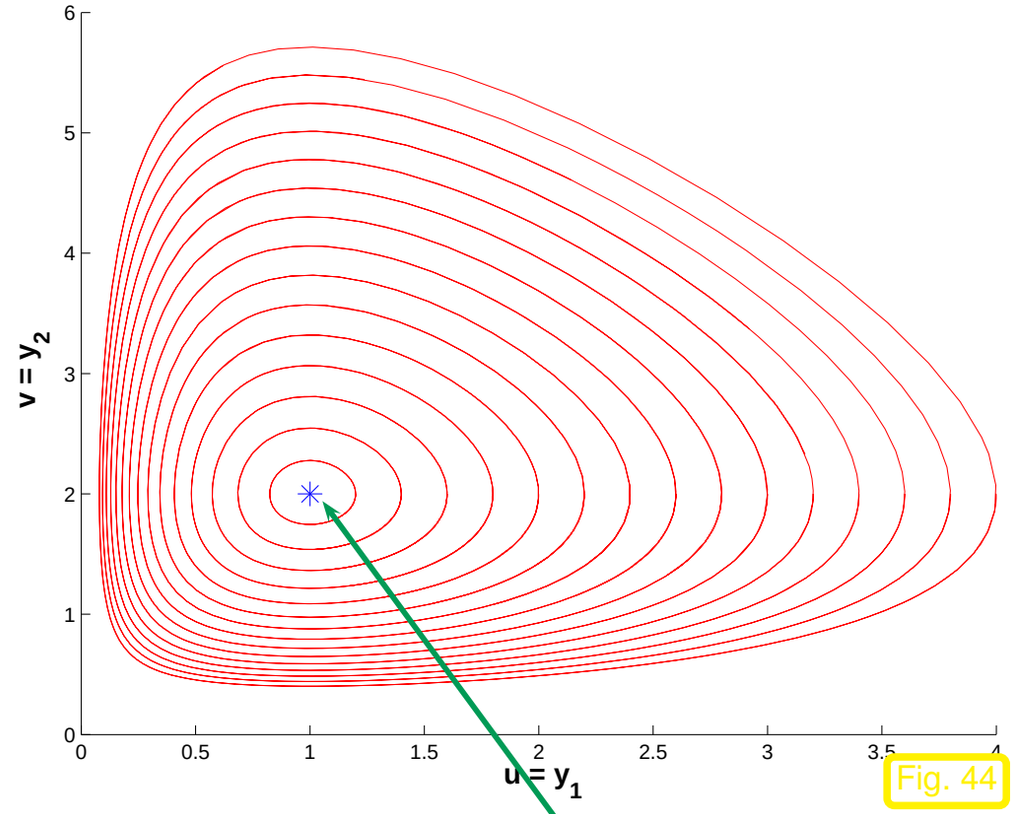
Fig. 42

vector field f for Lotka-Volterra ODE $\triangleright$

Parameter values for Fig. 42: $\alpha = 2, \beta = 1, \delta = 1, \gamma = 1$



Solution $y(t) = (y_1(t), y_2(t))$, $t \in [0, 10]$, with initial condition $y(0) = (4, 2)$



Solution curves for (8.1.15)

stationary point

Parameter values for Figs. 44, 43: $\alpha = 1, \beta = 1, \delta = 1, \gamma = 2$

◇

8.2 Euler methods

In this section assume that $T \in (0,\infty)$, $d \in \mathbb{N}$, $y_0 \in \mathbb{R}^d$, $f \in C(\mathbb{R}^d, \mathbb{R}^d)$ and consider the IVP

$$\begin{aligned} \dot{y}(t) &= f(y(t)), \qquad t \in [0,T] \\ y(0) &= y_0 \ . \end{aligned} \tag{8.2.1}$$

Note that if $0 \le t_0 < t_1 \le T$ and if $y\colon I \to \mathbb{R}^d$ is a solution of the IVP (8.2.1), then the left rectangle quadrature formula gives the approximation

$$\begin{aligned} y(t_1) = y(t_0) + \int_{t_0}^{t_1} f(y(s))\,ds &\approx y(t_0) + \int_{t_0}^{t_1} f(y(t_0))\,ds \\ &= y(t_0) + (t_1 - t_0)\cdot f\big(y(t_0)\big) \ . \end{aligned} \tag{8.2.2}$$

This approximation motivates the next definition.

Definition 8.2.1 ((Explicit) Euler method (Euler 1768)). *Let* $T \in (0,\infty)$, $d, n \in \mathbb{N}$, $0 = t_0 < t_1 < \ldots < t_{n-1} < t_n = T$, $y_0 \in \mathbb{R}^d$ *and let* $f\colon \mathbb{R}^d \to \mathbb{R}^d$ *be a continuous function. Then a sequence* $Y_k \in \mathbb{R}^d$, $k \in \{0,1,\ldots,n\}$, *satisfying*

$$Y_0 = y_0 \qquad \text{and} \qquad \forall\, k \in \{0,1,\ldots,n-1\}\colon \quad Y_{k+1} = Y_k + (t_{k+1} - t_k)\cdot f(Y_k) \tag{8.2.3}$$

is called the explicit Euler approximation for the IVP (8.2.1) *on (the grid)* $\{t_0, t_1, \ldots, t_n\}$. *Moreover, if* $h = t_{k+1} - t_k$ *for all* $k \in \{0,1,\ldots,n-1\}$, *then a sequence* $Y_k \in \mathbb{R}^d$, $k \in \{0,1,\ldots,n\}$, *satisfying* (8.2.3) *is also called the explicit Euler approximation for the IVP* (8.2.1) *with step size* h.

Next note that if $0 \le t_0 < t_1 \le T$ and if $y\colon I \to \mathbb{R}^d$ is a solution of the IVP (8.2.1), then a forward difference approximation of $y'(t_0)$ gives that

$$\frac{y(t_1) - y(t_0)}{(t_1 - t_0)} \approx y'(t_0) = f\big(y(t_0)\big) \tag{8.2.4}$$

and this demonstrates that

$$y(t_1) \approx y(t_0) + (t_1 - t_0)\cdot f\big(y(t_0)\big) \tag{8.2.5}$$

This illustrates why the explicit Euler method is also called forward Euler method.

Moreover, if $0 \le t_0 < t_1 \le T$ and if $y\colon I \to \mathbb{R}^d$ is a solution of the IVP (8.2.1),

then the right rectangle quadrature formula gives the approximation

$$y(t_1) = y(t_0) + \int_{t_0}^{t_1} f(y(s))\,ds \approx y(t_0) + \int_{t_0}^{t_1} f(y(t_1))\,ds \tag{8.2.6}$$
$$= y(t_0) + (t_1 - t_0)\cdot f\big(y(t_1)\big)\ .$$

This approximation motivates the next definition.

Definition 8.2.2 (Implicit Euler method). *Let $T \in (0,\infty)$, $d, n \in \mathbb{N}$, $0 = t_0 < t_1 < \ldots < t_{n-1} < t_n = T$, $y_0 \in \mathbb{R}^d$ and let $f\colon \mathbb{R}^d \to \mathbb{R}^d$ be a continuous function. Then a sequence $Y_k \in \mathbb{R}^d$, $k \in \{0,1,\ldots,n\}$, satisfying*

$$Y_0 = y_0 \qquad \text{and} \qquad \forall\, k \in \{0,1,\ldots,n-1\}\colon \quad Y_{k+1} = Y_k + (t_{k+1} - t_k)\cdot f(Y_{k+1}) \tag{8.2.7}$$

is called an implicit Euler approximation for the IVP (8.2.1) *on (the grid) $\{t_0, t_1, \ldots, t_n\}$. Moreover, if $h = t_{k+1} - t_k$ for all $k \in \{0,1,\ldots,n-1\}$, then a sequence $Y_k \in \mathbb{R}^d$, $k \in \{0,1,\ldots,n\}$, satisfying* (8.2.7) *is also called an implicit Euler approximation for the IVP* (8.2.1) *with step size h.*

If $0 \le t_0 < t_1 \le T$ and if $y\colon I \to \mathbb{R}^d$ is a solution of the IVP (8.2.1),

then a backward difference approximation of $y'(t_1)$ gives that

$$\frac{y(t_1) - y(t_0)}{(t_1 - t_0)} \approx y'(t_1) = f\big(y(t_1)\big) \tag{8.2.8}$$

and this demonstrates that

$$y(t_1) \approx y(t_0) + (t_1 - t_0) \cdot f\big(y(t_1)\big) \tag{8.2.9}$$

This illustrates why the implicit Euler method is also called backward Euler method.

The explicit and the implicit Euler method are under suitable assumptions special cases of so-called numerical one-step schemes for IVPs. More formally, for a function $\Psi\colon [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ and $n \in \mathbb{N}$, $0 = t_0 < t_1 < \cdots < t_n = T$, $y_0 \in \mathbb{R}^d$ consider $Y_k \in \mathbb{R}^d$, $k \in \{0, 1, \ldots, n\}$, given by

$$Y_0 = y_0 \qquad \text{and} \qquad \forall\, k \in \{0, 1, \ldots, n-1\}\colon \quad Y_{k+1} = \Psi(t_{k+1} - t_k, Y_k)\ . \tag{8.2.10}$$

The function Ψ is called one-step function and defines a numerical one-step scheme for the IVP (8.2.1). For instance, if

$$\forall\, (t, y) \in [0,T] \times \mathbb{R}^d\colon \qquad \Psi(t, y) = y + t \cdot f(y)\ , \tag{8.2.11}$$

then $(Y_k)_{k \in \{0,1,\ldots,n\}}$ is the explicit Euler approximation for the IVP (8.2.1) on $\{t_0, t_1, \ldots, t_n\}$.

8.3 Convergence of numerical one-step step methods

In this section assume that $T \in (0,\infty)$, $d \in \mathbb{N}$, $f \in C(\mathbb{R}^d, \mathbb{R}^d)$, $y_0 \in \mathbb{R}^d$ and consider the IVP

$$\begin{aligned} \dot{y}(t) &= f(y(t)), \qquad t \in [0,T] \\ y(0) &= y_0 \,. \end{aligned} \tag{8.3.1}$$

Definition 8.3.1 (Algebraic convergence order of a numerical one-step scheme for IVPs)**.** *Let $T, p \in (0,\infty)$, $d \in \mathbb{N}$, $f \in C(\mathbb{R}^d, \mathbb{R}^d)$, $y_0 \in \mathbb{R}^d$, let $y\colon [0,T] \to \mathbb{R}^d$ be a solution of the IVP* (8.3.1) *and let $\Psi\colon [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ be a function. Then we say that the numerical one-step scheme described by Ψ converges with algebraic order p to y if there exist $c, C \in (0,\infty)$ such that for all $n \in \mathbb{N}$, for all $0 = t_0 < t_1 < \cdots < t_n = T$ fulfilling $\max_{k\in\{0,1,\dots,n-1\}} |t_{k+1} - t_k| \leq c$ and for all $Y_k \in \mathbb{R}^d$, $k \in \{0,1,\dots,n\}$, fulfilling* (8.2.10) *it holds that*

$$\max_{k\in\{0,1,\dots,n\}} \|y(t_k) - Y_k\| \leq C \left[\max_{k\in\{0,1,\dots,n-1\}} |t_{k+1} - t_k|\right]^p \,. \tag{8.3.2}$$

Be aware of the differences between the notion "convergence with order p" (Chapter 1) and "convergence with algebraic order p" (Chaper 8) in the sense of Definition 8.3.1!

Theorem 8.3.2 (Determination of the convergence speed of a numerical one-step method for IVPs)**.** *Let* $T \in (0,\infty)$, $d, p \in \mathbb{N}$, $y_0 \in \mathbb{R}^d$, *let* $f\colon \mathbb{R}^d \to \mathbb{R}^d$ *and* $\Psi\colon [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ *be smooth functions satisfying*

$$\forall\, k \in \{0,1,\dots,p\}\colon \quad \left(\frac{\partial^k}{\partial t^k}\Psi\right)(0,x) = \begin{cases} x & : k = 0 \\ f(x) & : k = 1 \\ f'(x)\,f(x) & : k = 2 \\ f''(x)\big(f(x), f(x)\big) + f'(x)\,f'(x)\,f(x) & : k = 3 \\ \vdots & \vdots \end{cases}$$

and let $y\colon [0,T] \to \mathbb{R}^d$ *be a solution of the IVP* (8.3.1)*. Then the numerical one-step scheme described by* Ψ *converges with algebraic order* p *to* y*.*

An idea in the proof of Theorem 8.3.2: Note in the setting of Theorem 8.3.2 that a Taylor expansion of $y(t)$, $t \in [0,T]$, in $t_0 \in [0,T]$ gives

$$
\begin{aligned}
&y(t_0+h)\\
&= y(t_0) + h\,y'(t_0) + \frac{h^2}{2!}y''(t_0) + \frac{h^3}{3!}\,y^{(3)}(t_0) + \ldots + \frac{h^n}{n!}\,y^{(n)}(t_0) + O(h^{(n+1)})\\
&= y(t_0) + f(y(t_0))h + \frac{h^2}{2!}\,f'(y(t_0))\,f(y(t_0))\\
&\quad + \frac{h^3}{3!}\Big[f''(y(t_0))\big(f(y(t_0)), f(y(t_0))\big) + f'(y(t_0))\,f'(y(t_0))\,f(y(t_0))\Big] + \ldots + \frac{h^n}{n!}\,y^{(n)}(t_0)\\
&\quad + O(h^{(n+1)})
\end{aligned}
\tag{8.3.3}
$$

and that a Taylor expansion of $\Psi(t, y(t_0))$, $t \in [0,T]$, in 0 gives

$$
\begin{aligned}
&\Psi(h, y(t_0))\\
&= \Psi(0, y(t_0)) + h\,\big(\tfrac{\partial}{\partial t}\Psi\big)(0, y(t_0)) + \frac{h^2}{2!}\,\big(\tfrac{\partial^2}{\partial t^2}\Psi\big)(0, y(t_0)) + \ldots + \frac{h^n}{n!}\,\big(\tfrac{\partial^n}{\partial t^n}\Psi\big)(0, y(t_0)) + O(h^{(n+1)})
\end{aligned}
\tag{8.3.4}
$$

Comparing (8.3.3) and (8.3.4) sketches the proof and illustrates the assumptions of Theorem 8.3.2.

Example 8.3.1 (Speed of convergence of the explicit Euler method). Let $T \in (0,\infty)$, $d \in \mathbb{N}$, $y_0 \in \mathbb{R}^d$, let $f\colon \mathbb{R}^d \to \mathbb{R}^d$ be a smooth function and let $y\colon [0,T] \to \mathbb{R}^d$ be a solution of the IVP (8.3.1). Then the explicit Euler method for the IVP (8.3.1) converges with algebraic order 1 to y. Indeed, note that $\Psi\colon [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ given by

$$\forall\,(t,x) \in [0,T] \times \mathbb{R}^d\colon \qquad \Psi(t,x) = x + t \cdot f(x) \qquad \text{(Explicit Euler method)} \tag{8.3.5}$$

satisfies

$$\forall\, x \in \mathbb{R}^d\colon \qquad \Psi(0,x) = x, \qquad \left(\frac{\partial}{\partial t}\Psi\right)(0,x) = f(x), \qquad \left(\frac{\partial^2}{\partial t^2}\Psi\right)(0,x) = 0 \tag{8.3.6}$$

and Theorem 8.3.2 hence shows that the numerical one-step scheme described by Ψ, i.e., the explicit Euler method, converges with algebraic order 1 to y.

8.4 Runge-Kutta methods

In this section assume that $T \in (0,\infty)$, $d \in \mathbb{N}$, $y_0 \in \mathbb{R}^d$, $f \in C(\mathbb{R}^d, \mathbb{R}^d)$ and consider the IVP

$$\begin{aligned} \dot{y}(t) &= f(y(t)), \qquad t \in [0,T] \\ y(0) &= y_0\,. \end{aligned} \tag{8.4.1}$$

Let $0 \leq t_0 < t_0 + h \leq T$ and let $y\colon I \to \mathbb{R}^d$ be a solution of the IVP (8.4.1). Then

$$y(t_0+h) = y(t_0) + \int_{t_0}^{t_0+h} f\big(y(s)\big)\,ds = y(t_0) + h\int_0^1 f\big(y(t_0+sh)\big)\,ds\,. \tag{8.4.2}$$

Idea of Runge-Kutta methods: approximate integral in (8.4.2) by means of m-point quadrature formula ($\to$ Sect. 7.1, defined on reference interval $[0,1]$) with quadrature nodes $c_1,\dots,c_m \in [0,1]$ and quadrature weights $b_1,\dots,b_m \in \mathbb{R}$ to obtain

$$y(t_0+h) = y(t_0) + h\int_0^1 f\big(y(t_0+sh)\big)\,ds \approx y(t_0) + h\left[\sum_{i=1}^m b_i\, f\big(\underbrace{y(t_0+c_ih)}_{\substack{\text{approximate}\\ \text{these vectors via}\\ \text{bootstrapping or}\\ \text{implicitness}}}\big)\right]. \tag{8.4.3}$$

Example 8.4.1 (Explicit Euler method). If $m=1$, $c_1=0$, $b_1=1$ in (8.4.3) (Left rectangle rule), then (8.4.3) reduces to

$$y(t_0+h) \approx y(t_0) + h\cdot f\big(y(t_0)\big) \tag{8.4.4}$$

and this approximation defines the explicit Euler scheme.

Example 8.4.2 (Heun method). If $m = 2$, $c_1 = 0$, $c_2 = 1$, $b_1 = b_2 = \frac{1}{2}$ in (8.4.3) (Trapezoidal rule), then (8.4.3) reduces to

$$y(t_0 + h) \approx y(t_0) + \frac{h}{2}\Big[f\big(y(t_0)\big) + f\big(y(t_0 + h)\big)\Big] \tag{8.4.5}$$

and using Example 8.4.1 results in

$$y(t_0 + h) \approx y(t_0) + \frac{h}{2}\Big[f\big(y(t_0)\big) + f\big(y(t_0) + h \cdot f\big(y(t_0)\big)\big)\Big] \ . \tag{8.4.6}$$

This approximation defines the Heun scheme (a Runge-Kutta method). If $f\colon \mathbb{R}^d \to \mathbb{R}^d$ in (8.4.1) is smooth, then the Heun scheme for the IVP (8.4.1) converges with algebraic order 2 to the solution y of (8.4.1). Indeed, $\Psi\colon [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ given by

$$\forall\,(t,x) \in [0,T] \times \mathbb{R}^d\colon \qquad \Psi(t,x) = x + \frac{t}{2}\Big[f\big(x\big) + f\big(x + t\,f(x)\big)\Big] \tag{8.4.7}$$

satisfies

$$\forall\, x \in \mathbb{R}^d\colon \quad \begin{aligned} \Psi(0,x) &= x, & \big(\tfrac{\partial}{\partial t}\Psi\big)(0,x) &= f(x), \\ \big(\tfrac{\partial^2}{\partial t^2}\Psi\big)(0,x) &= f'(x)\,f(x), & \big(\tfrac{\partial^3}{\partial t^3}\Psi\big)(0,x) &= \tfrac{3}{2}f''(x)\big(f(x), f(x)\big) \end{aligned} \tag{8.4.8}$$

and Theorem 8.3.2 hence shows that the numerical one-step scheme described by Ψ, i.e., the Heun method, converges with algebraic order 2 to y.

Definition 8.4.1 (Heun method)**.** *Let* $T \in (0,\infty)$, $d,n \in \mathbb{N}$, $0 = t_0 < t_1 < \ldots < t_{n-1} < t_n = T$, $y_0 \in \mathbb{R}^d$, $f \in C(\mathbb{R}^d,\mathbb{R}^d)$ *and let* $Y_l \in \mathbb{R}^d$, $l \in \{0,1,\ldots,n\}$, *satisfy*

$$Y_0 = y_0,\ \forall\, l \in \{0,1,\ldots,n-1\}\colon\ Y_{l+1} = Y_l + \frac{(t_{l+1}-t_l)}{2}\left[f(Y_l) + f\Big(Y_l + (t_{l+1}-t_l)\,f(Y_l)\Big)\right]. \tag{8.4.9}$$

Then $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *is called the Heun approximation for the IVP* (8.4.1) *on (the grid)* $\{t_0,t_1,\ldots,t_n\}$. *Moreover, if* $h = t_{l+1} - t_l$ *for all* $l \in \{0,1,\ldots,n-1\}$, *then* $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *is called the Heun approximation for the IVP* (8.4.1) *with step size* h.

Definition 8.4.2 (Runge-Kutta scheme (RK scheme)). *Let* $T \in (0,\infty)$, $d,n,m \in \mathbb{N}$, $0 = t_0 < t_1 < \ldots < t_{n-1} < t_n = T$, $y_0 \in \mathbb{R}^d$, $f \in C(\mathbb{R}^d,\mathbb{R}^d)$, $b = (b_1,\ldots,b_m) \in \mathbb{R}^m$, $A = (a_{i,j})_{i,j\in\{1,\ldots,m\}} \in \mathbb{R}^{m,m}$ *and let* $Y_l \in \mathbb{R}^d$, $l \in \{0,1,\ldots,n\}$, *and* $\mathbf{K}_{l,1},\ldots,\mathbf{K}_{l,m} \in \mathbb{R}^d$, $l \in \{0,1,\ldots,n\}$, *satisfy*

$$Y_0 = y_0 \quad \text{and} \quad \forall\, l \in \{0,1,\ldots,n-1\}: \quad Y_{l+1} = Y_l + \sum_{i=1}^{m} b_i\,\mathbf{K}_{l,i} \quad \text{and}$$

$$\forall\, l \in \{0,1,\ldots,n-1\}, i \in \{1,2,\ldots,m\}: \quad \mathbf{K}_{l,i} = (t_{l+1}-t_l)\cdot f\left(Y_l + \sum_{j=1}^{m} a_{i,j}\,\mathbf{K}_{l,j}\right). \tag{8.4.10}$$

Then $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *is called an* (A,b)*-Runge-Kutta approximation for the IVP* (8.4.1) *on (the grid)* $\{t_0,t_1,\ldots,t_n\}$. *Moreover, if* $h = t_{l+1}-t_l$ *for all* $l \in \{0,1,\ldots,n-1\}$, *then* $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *is called an* (A,b)*-Runge-Kutta approximation for the IVP* (8.4.1) *with step size* h.

If $a_{i,j} = 0$ for all $1 \le i \le j \le m$ in Definition 8.4.2 (A is a lower triangle matrix with zeros on the diagonal), then the RK scheme is explicit (otherwise implicit) and it holds for every

$l \in \{0, 1, \ldots, n-1\}$ that

$$
\begin{aligned}
\mathbf{K}_{l,1} &= (t_{l+1} - t_l) \cdot f(Y_l) \\
\mathbf{K}_{l,2} &= (t_{l+1} - t_l) \cdot f\Big(Y_l + a_{2,1}\,\mathbf{K}_{l,1}\Big) \\
\mathbf{K}_{l,3} &= (t_{l+1} - t_l) \cdot f\Big(Y_l + a_{3,1}\,\mathbf{K}_{l,1} + a_{3,2}\,\mathbf{K}_{l,2}\Big) \\
\vdots \quad & \quad \vdots \\
\mathbf{K}_{l,m} &= (t_{l+1} - t_l) \cdot f\Big(Y_l + a_{m,1}\,\mathbf{K}_{l,1} + \ldots + a_{m,m-1}\,\mathbf{K}_{l,m-1}\Big) \\
Y_{l+1} &= Y_l + b_1\,\mathbf{K}_{l,1} + \ldots + b_m\,\mathbf{K}_{l,m}\,.
\end{aligned}
\tag{8.4.11}
$$

The table

$$
\begin{array}{c|ccc}
a_{1,1} & & \cdots & a_{1,m} \\
a_{2,1} & \ddots & & \vdots \\
\vdots & & \ddots & \vdots \\
a_{m,1} & \cdots & a_{m,m-1} & a_{m,m} \\
\hline
b_1 & & \cdots & b_m
\end{array}
\tag{8.4.12}
$$

describing the RK scheme is called Butcher tableau (RK tableau) and m is called the number of stages of the RK scheme. For instance,

the RK scheme with 2 stages described through $\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}$ is the Heun method, (8.4.13)

the Runge-Kutta scheme with 1 stage described through $\begin{array}{c|c} 0 \\ \hline 1 \end{array}$ is the explicit Euler method,

(8.4.14)

the Runge-Kutta scheme with 1 stage described through $\begin{array}{c|c} 1 \\ \hline 1 \end{array}$ is the implicit Euler method.

(8.4.15)

Definition 8.4.3 ((Explicit) Midpoint method). *Let* $T \in (0,\infty)$, $d, n \in \mathbb{N}$, $0 = t_0 < t_1 < \ldots < t_{n-1} < t_n = T$, $y_0 \in \mathbb{R}^d$, $f \in C(\mathbb{R}^d, \mathbb{R}^d)$ *and let* $Y_l \in \mathbb{R}^d$, $l \in \{0,1,\ldots,n\}$, *satisfy*

$$Y_0 = y_0 \quad \text{and} \quad \forall\, l \in \{0,1,\ldots,n-1\}: \quad Y_{l+1} = Y_l + (t_{l+1} - t_l)\, f\Big(Y_l + \tfrac{(t_{l+1}-t_l)}{2}\, f(Y_l)\Big). \tag{8.4.16}$$

Then $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *is called the (explicit) midpoint approximation for the IVP* (8.4.1) *on (the grid)* $\{t_0, t_1, \ldots, t_n\}$. *Moreover, if* $h = t_{l+1} - t_l$ *for all* $l \in \{0,1,\ldots,n-1\}$, *then* $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *is called the (explicit) midpoint approximation for the IVP* (8.4.1) *with step size* h.

Definition 8.4.4 (Implicit midpoint method). *Let* $T \in (0,\infty)$, $d,n \in \mathbb{N}$, $0 = t_0 < t_1 < \ldots < t_{n-1} < t_n = T$, $y_0 \in \mathbb{R}^d$, $f \in C(\mathbb{R}^d,\mathbb{R}^d)$ *and let* $Y_l \in \mathbb{R}^d$, $l \in \{0,1,\ldots,n\}$, *satisfy*

$$Y_0 = y_0 \quad \text{and} \quad \forall\, l \in \{0,1,\ldots,n-1\}: \quad Y_{l+1} = Y_l + (t_{l+1} - t_l)\, f\left(\frac{Y_l + Y_{l+1}}{2}\right). \tag{8.4.17}$$

Then $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *is called an implicit midpoint approximation for the IVP* (8.4.1) *on (the grid)* $\{t_0,t_1,\ldots,t_n\}$. *Moreover, if* $h = t_{l+1} - t_l$ *for all* $l \in \{0,1,\ldots,n-1\}$, *then* $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *is called an implicit midpoint approximation for the IVP* (8.4.1) *with step size* h.

Definition 8.4.5 (Implicit trapezoidal method). *Let* $T \in (0,\infty)$, $d,n \in \mathbb{N}$, $0 = t_0 < t_1 < \ldots < t_{n-1} < t_n = T$, $y_0 \in \mathbb{R}^d$, $f \in C(\mathbb{R}^d,\mathbb{R}^d)$ *and let* $Y_l \in \mathbb{R}^d$, $l \in \{0,1,\ldots,n\}$, *satisfy*

$$Y_0 = y_0 \quad \text{and} \quad \forall\, l \in \{0,1,\ldots,n-1\}: \quad Y_{l+1} = Y_l + \frac{(t_{l+1}-t_l)}{2}\Big[f(Y_l) + f(Y_{l+1})\Big]. \tag{8.4.18}$$

Then $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *is called an implicit trapezoidal approximation for the IVP* (8.4.1) *on (the grid)* $\{t_0,t_1,\ldots,t_n\}$. *Moreover, if* $h = t_{l+1} - t_l$ *for all* $l \in \{0,1,\ldots,n-1\}$, *then* $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *is called an implicit trapezoidal approximation for the IVP* (8.4.1) *with step size* h.

Remark 8.4.3 (Explicit ODE integrator in MATLAB).

Syntax:

```
[t,Y] = ode45(odefun,tspan,y0);
```

`odefun`	:	Handle to a function of type `@(t,y)` $\leftrightarrow$ r.h.s. $f(t,\mathbf{y})$, $(t,y) \in [t_0,T] \times \mathbb{R}^d$,
`tspan`	:	vector (t_0,T) specifyings initial t_0 and final time $T > t_0$ for numerical integration
`y0`	:	(vector) passing initial value $\mathbf{y}_0$

Return values:

`t`	:	vector $(t_0,t_1,\dots,t_n)$ temporal grid with $t_0 < t_1 < t_2 < \cdots < t_{n-1} = t_n = T$
`Y`	:	vector $(Y_0,Y_1,\dots,Y_n)$ with $Y_0,Y_1,\dots,Y_n \in \mathbb{R}^d$ approximating under suitable assumptions the solution $y\colon [t_0,T] \to \mathbb{R}^d$ of corresponding IVP in the sense that $Y_0 \approx y(t_0)$, $Y_1 \approx y(t_1)$, ..., $Y_n \approx y(t_n) = y(T)$

See help ode45 and `http://www.mathworks.ch/ch/help/matlab/ref/ode45.html` for further details.

$\triangle$

8.5 Stiff problems

8.5.1 Scalar linear model problem

Let $T, \alpha, y_0 \in (0, \infty)$ and let $y\colon [0,T] \to \mathbb{R}$ be the solution of the IVP

$$\begin{aligned} \dot{y}(t) &= -\alpha \cdot y(t), \qquad t \in [0,T], \\ y(0) &= y_0 \,. \end{aligned} \tag{8.5.1}$$

It holds that $y(t) = e^{-\alpha t}$ for all $t \in [0,T]$ (cf. Example 8.1.1).
Thus $y(t) \geq 0$ decreases as t becomes larger.

Next for every $n \in \mathbb{N}$ let $(Y_l^n)_{l \in \{0,1,\dots,n\}}$ be the explicit Euler approximation for the IVP (8.5.1) with step size $\frac{T}{n}$. Let $n \in \mathbb{N}$ and note that

$$\begin{aligned} Y_{l+1}^n &= Y_l^n - \tfrac{T}{n} \cdot \alpha \cdot Y_l^n = \left[1 - \tfrac{T\alpha}{n}\right] Y_l^n = \left[1 - \tfrac{T\alpha}{n}\right]^2 Y_{l-1}^n \\ &= \ldots = \left[1 - \tfrac{T\alpha}{n}\right]^{(l+1)} Y_0^n = \left[1 - \tfrac{T\alpha}{n}\right]^{(l+1)} y_0 \end{aligned} \tag{8.5.2}$$

for all $l \in \{0, 1, \ldots, n-1\}$. If $\alpha \in (0, \infty)$ is large so that $\frac{T\alpha}{n} > 2$, then $|Y_l^n| \geq 0$ increases as l becomes larger. Thus, if $\alpha \in (0, \infty)$ is large, then the explicit Euler method applied to (8.5.1) does

not produces good approximation results unless the step size $\frac{T}{n}$ is extremly small (see `http://en.wikipedia.org/wiki/Stiff_equation`).

One way to overcome this lack of approximation is appropriate implicitness in the numerical scheme. For instance, for every $n \in \mathbb{N}$ let $(Z_l^n)_{l \in \{0,1,\dots,n\}}$ be an (the!) implicit Euler approximation for the IVP (8.5.1) with step size $\frac{T}{n}$. Then note that

$$\forall\, n \in \mathbb{N}: \quad \forall\, l \in \{0,1,\dots,n-1\}: \qquad Z_{l+1}^n = Z_l^n - \frac{T}{n} \cdot \alpha \cdot Z_{l+1}^n \qquad \text{implies that}$$

$$\forall\, n \in \mathbb{N}: \quad \forall\, l \in \{0,1,\dots,n-1\}: \qquad Z_{l+1}^n = \frac{Z_l^n}{[1 + \frac{T\alpha}{n}]} \qquad \text{and this shows that}$$

$$\forall\, n \in \mathbb{N}: \quad \forall\, l \in \{0,1,\dots,n\}: \qquad Z_l^n = \frac{y_0}{\left[1 + \frac{T\alpha}{n}\right]^l}$$

Thus, for every $\alpha \in (0,\infty)$ and every $n \in \mathbb{N}$ it holds that $Z_l^n \geq 0$ decreases as l becomes larger. The implicit Euler method thus preserves this behavior of the exact solution of the IVP (8.5.1).

8.5.2 Semi-implicit Runge-Kutta methods

Let $T \in (0,\infty)$, $d, n \in \mathbb{N}$, $y_0 \in \mathbb{R}^d$, $A \in \mathbb{R}^{d,d}$, $g \in C(\mathbb{R}^d, \mathbb{R}^d)$,

let $f \in C(\mathbb{R}^d, \mathbb{R}^d)$ satisfy $f(x) = Ax + g(x)$ for all $x \in \mathbb{R}^d$ and consider the IVP

$$\begin{aligned} \dot{y}(t) &= f(y(t)), \qquad t \in [0,T], \\ y(0) &= y_0 \end{aligned} \tag{8.5.3}$$

which can also be written as

$$\begin{aligned} \dot{y}(t) &= A\,y(t) + g(y(t)), \qquad t \in [0,T], \\ y(0) &= y_0\,. \end{aligned} \tag{8.5.4}$$

Definition 8.5.1 (Linear implicit Euler method)**.** *Let* $T \in (0,\infty)$, $d, n \in \mathbb{N}$, $0 = t_0 < t_1 < \ldots < t_{n-1} < t_n = T$, $y_0 \in \mathbb{R}^d$, $g \in C(\mathbb{R}^d, \mathbb{R}^d)$, $A \in \mathbb{R}^{d,d}$ *and let* $Y_l \in \mathbb{R}^d$, $l \in \{0,1,\ldots,n\}$, *satisfy*

$$Y_0 = y_0 \quad \text{and} \quad \forall\, l \in \{0,1,\ldots,n-1\}\colon\; Y_{l+1} = Y_l + (t_{l+1} - t_l)\,A\,Y_{l+1} + (t_{l+1} - t_l)\,g(Y_l). \tag{8.5.5}$$

Then $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *is called an linear implicit Euler method for the IVP* (8.4.1) *on (the grid)* $\{t_0, t_1, \ldots, t_n\}$. *Moreover, if* $h = t_{l+1} - t_l$ *for all* $l \in \{0,1,\ldots,n-1\}$, *then* $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *is called an linear implicit Euler method for the IVP* (8.4.1) *with step size* h.

Definition 8.5.2 (Linear implicit trapezoidal (linear implicit Crank-Nicolson) combined with Heun method)**.** *Let* $T \in (0,\infty)$, $d,n \in \mathbb{N}$, $0 = t_0 < t_1 < \ldots < t_{n-1} < t_n = T$, $y_0 \in \mathbb{R}^d$, $g \in C(\mathbb{R}^d,\mathbb{R}^d)$, $A \in \mathbb{R}^{d,d}$ *and let* $Y_l \in \mathbb{R}^d$, $l \in \{0,1,\ldots,n\}$, *satisfy*

$$Y_0 = y_0 \quad \text{and} \quad \forall\, l \in \{0,1,\ldots,n-1\}:$$
$$Y_{l+1} = Y_l + \frac{(t_{l+1}-t_l)}{2}\Big[A\,[Y_l + Y_{l+1}] + g(Y_l) + g\Big(Y_l + (t_{l+1}-t_l)\,g(Y_l)\Big)\Big]. \tag{8.5.6}$$

Then we call $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *an linear implicit trapezoidal-Heun approximation for the IVP* (8.4.1) *on (the grid)* $\{t_0,t_1,\ldots,t_n\}$. *Moreover, if* $h = t_{l+1} - t_l$ *for all* $l \in \{0,1,\ldots,n-1\}$, *then we call* $(Y_l)_{l\in\{0,1,\ldots,n\}}$ *an linear implicit trapezoidal-Heun approximation for the IVP* (8.4.1) *with step size* h.

A standard monograph for the numerical integration of stiff ODEs is [E. Hairer and G. Wanner, *Solving ordinary differential equations. II. Stiff and differential-algebraic problems.* Springer Series in Computational Mathematics, 14. Springer-Verlag, Berlin, 1991 [9]].

8.6 Structure preserving numerical integration

Example 8.6.1 (Explicit and implicit Euler method for long-time evolution for a specific idealized frictionless spring pendulum without mass). Let $T \in (0,\infty)$, $y_0 \in \mathbb{R}^2$, let $f\colon \mathbb{R}^2 \to \mathbb{R}^2$ be given by $f(x_1,x_2) = (x_2,-x_1)$ for all $x = (x_1,x_2) \in \mathbb{R}^2$ and let $y = (y_1,y_2)\colon [0,T] \to \mathbb{R}^2$ be the solution of the IVP

$$\begin{aligned} \dot{y}(t) &= f(y(t)), \qquad t \in [0,T], \\ y(0) &= y_0 \,. \end{aligned} \tag{8.6.1}$$

Then note that the identity

$$\forall\, x \in \mathbb{R}^2\colon \quad \langle x, f(x)\rangle = 0 \tag{8.6.2}$$

implies that $\forall\, t \in [0,T]\colon \|y(t)\|_2^2 = \|y(0)\|_2^2$ (Enegery $\frac{1}{2}\|\cdot\|_2^2$ remains constant).

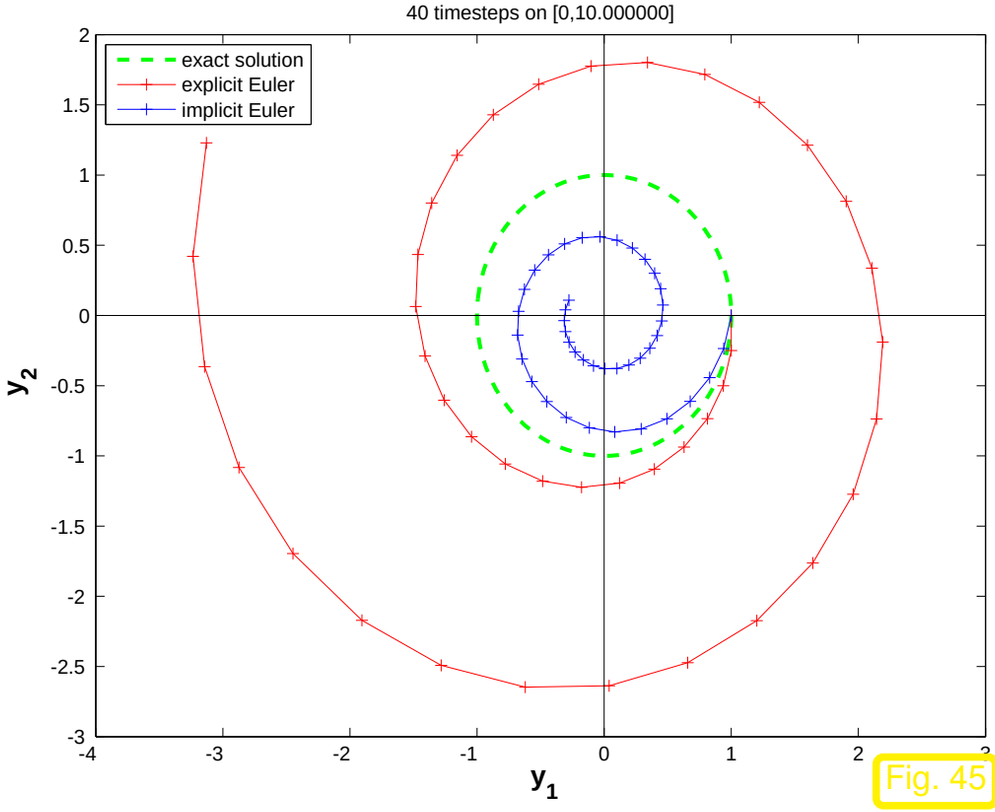


Fig. 45

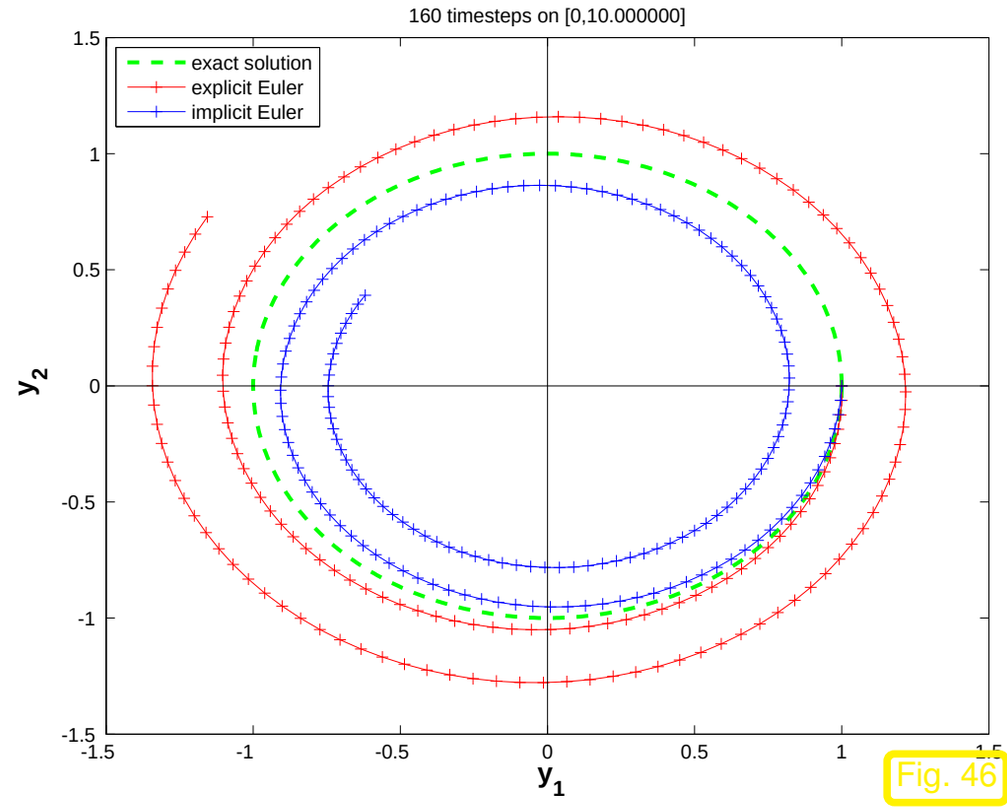


Fig. 46

☞ explicit Euler: numerical solution flyes away

☞ implicit Euler: numerical solution falls off into the center

◇

Can we avoid the energy drift ?

Yes: by using other suitable numerical methods instead of the explicit/implicit Euler method.

8.6.1 Implicit midpoint method

Consider the setting of Example 8.6.1, let $n \in \mathbb{N}$, $0 = t_0 < t_1 < \cdots < t_n = T$ and let $Y_l \in \mathbb{R}^2$, $l \in \{0, 1, \ldots, n\}$, be an implicit midpoint approximation for the IVP (8.6.1) on the grid $\{t_0, t_1, \ldots, t_n\}$. Then note that the identity (8.6.2) implies that for every $l \in \{0, 1, \ldots, n\}$ it holds that

$$\begin{aligned}
\|Y_{l+1}\|_2^2 &= \langle Y_{l+1}, Y_{l+1}\rangle = \langle Y_l + Y_{l+1}, Y_{l+1}\rangle - \langle Y_l, Y_{l+1}\rangle = 2\left\langle \tfrac{Y_l+Y_{l+1}}{2}, Y_{l+1}\right\rangle - \langle Y_l, Y_{l+1}\rangle \\
&= 2\left\langle \tfrac{Y_l+Y_{l+1}}{2}, Y_l + (t_{l+1} - t_l)\, f\left(\tfrac{Y_l+Y_{l+1}}{2}\right)\right\rangle - \langle Y_l, Y_{l+1}\rangle \\
&= 2\left\langle \tfrac{Y_l+Y_{l+1}}{2}, Y_l\right\rangle + 2\,(t_{l+1} - t_l)\left\langle \tfrac{Y_l+Y_{l+1}}{2}, f\left(\tfrac{Y_l+Y_{l+1}}{2}\right)\right\rangle - \langle Y_l, Y_{l+1}\rangle \\
&= 2\left\langle \tfrac{Y_l+Y_{l+1}}{2}, Y_l\right\rangle - \langle Y_l, Y_{l+1}\rangle = \langle Y_l + Y_{l+1}, Y_l\rangle - \langle Y_l, Y_{l+1}\rangle \\
&= \|Y_l\|_2^2 \;. \qquad \text{(Energy remains constant!)}
\end{aligned} \tag{8.6.3}$$

Example 8.6.2 (Implicit midpoint method for long-time evolution for a specific idealized frictionless spring pendulum without mass).

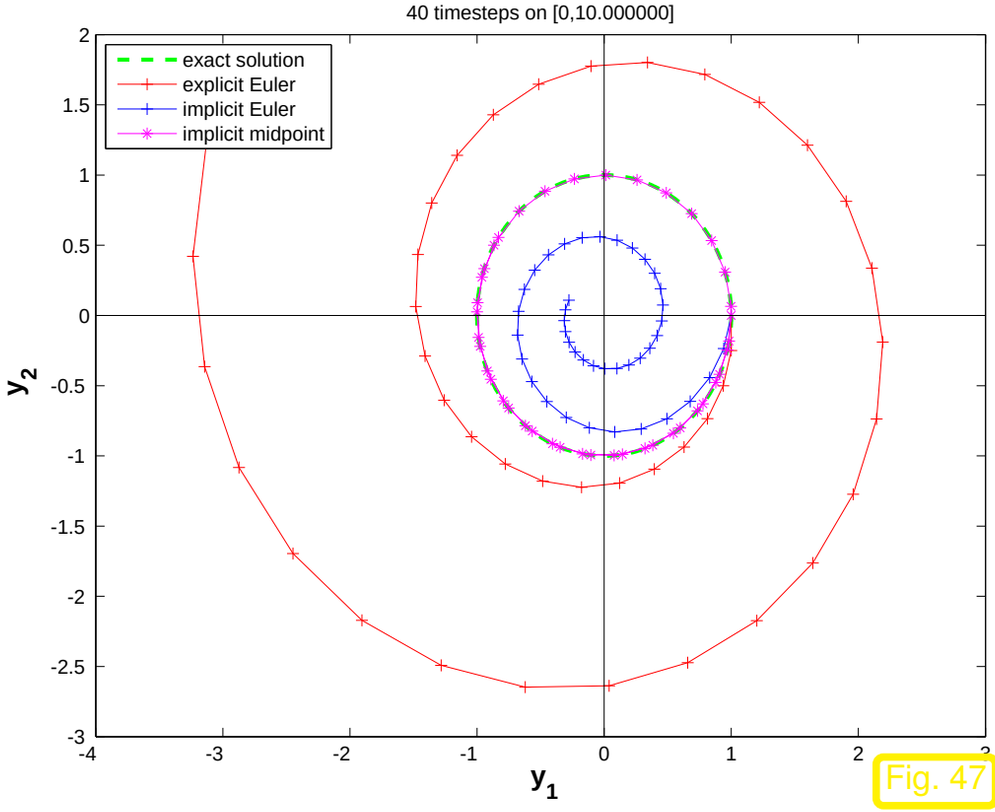


Fig. 47

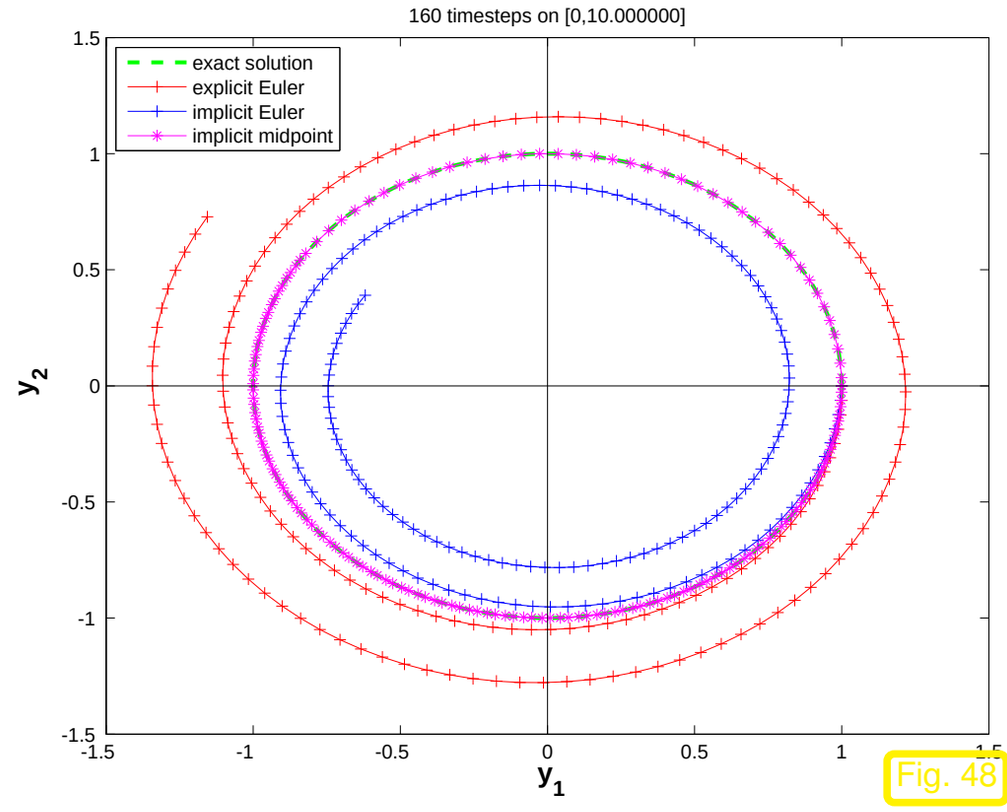


Fig. 48

☞ Implicit midpoint rule: perfect conservation of energy **!**

◇

8.6.2 Störmer-Verlet method [8]

E. Hairer, C. Lubich and G. Wanner, *Geometric numerical integration illustrated by the Störmer-Verlet method.* Acta Numer. 12 (2003), 399–450 [8].

Let $T \in (0,\infty)$, $d \in \mathbb{N}$, $q_0, p_0 \in \mathbb{R}^d$, $g \in C(\mathbb{R}^d, \mathbb{R}^d)$, let $f \in C(\mathbb{R}^{2d}, \mathbb{R}^{2d})$ satisfy $f(q,p) = (p, g(q))$ for all $q, p \in \mathbb{R}^d$ and consider the IVP

$$\begin{aligned} \dot{y}(t) &= f\big(y(t)\big), \qquad t \in [0,T], \\ y(0) &= (q_0, p_0)\ . \end{aligned} \tag{8.6.4}$$

According to Remark 8.1.3, the IVP (8.6.4) can be reformulated as the second-order IVP

$$\begin{aligned} \ddot{q}(t) &= g\big(q(t)\big), \qquad t \in [0,T], \\ q(0) &= q_0 \\ \dot{q}(0) &= p_0\ . \end{aligned} \tag{8.6.5}$$

If $t \in (0,T)$ and if $h \in (0,\infty)$ is sufficiently small, then

$$g\big(q(t)\big) = \ddot{q}(t) \approx \frac{\dot{q}(t+h) - \dot{q}(t)}{h} \approx \frac{\left[\frac{q(t+h)-q(t)}{h}\right] - \left[\frac{q(t)-q(t-h)}{h}\right]}{h} = \frac{q(t+h) - 2q(t) + q(t-h)}{h^2}$$

(Second order central difference approximation). This motivates the next definition.

Definition 8.6.1 (Störmer-Verlet method for second-order IVPs). *Let* $T \in (0,\infty)$, $d,n \in \mathbb{N}$, $h = \frac{T}{n}$, $q_0, p_0 \in \mathbb{R}^d$, $g \in C(\mathbb{R}^d,\mathbb{R}^d)$ *and let* $Q_l \in \mathbb{R}^d$, $l \in \{0,1,\dots,n\}$, *satisfy*

$$\begin{aligned} Q_0 = q_0 \quad , \qquad Q_1 &= q_0 + h\,p_0 + h^2\,g(q_0) \qquad \text{and} \\ \forall\, l \in \{1,\dots,n-1\}: \qquad Q_{l+1} &= -Q_{l-1} + 2\,Q_l + h^2\,g(Q_l)\ . \end{aligned} \tag{8.6.6}$$

Then $(Q_l)_{l\in\{0,1,\dots,n\}}$ *is called the Störmer-Verlet approximation for the IVP* (8.6.5) *with step size* h.

8.7 Splitting methods

See, e.g., [P. Imkeller and C. Lederer, *On the cohomology of flows of stochastic and random differential equations.* Probab. Theory Related Fields 120 (2001), no. 2, 209–235 [11]] for the notion of completeness for vector fields.

Definition 8.7.1 (Forward completeness). *Let $d \in \mathbb{N}$. A function $f \in C(\mathbb{R}^d, \mathbb{R}^d)$ is called forward complete if it holds for every $y_0 \in \mathbb{R}^d$ that the IVP*

$$\begin{aligned} \dot{y}(t) &= f(y(t)), \qquad t \in [0, \infty), \\ y(0) &= y_0 \end{aligned} \tag{8.7.1}$$

has a unique solution $y \colon [0, \infty) \to \mathbb{R}^d$.

Definition 8.7.2 (Solution flows of forward complete vector fields). *Let $d \in \mathbb{N}$ and let $f \in C(\mathbb{R}^d, \mathbb{R}^d)$ be forward complete. Then we denote by $\Phi^f : [0, \infty) \times \mathbb{R}^d \to \mathbb{R}^d$ the unique function with the property that for every $y_0 \in \mathbb{R}^d$ it holds that the function $[0, \infty) \ni t \mapsto \Psi_t^f(y_0) \in \mathbb{R}^d$ is the solution of the IVP*

$$\begin{aligned} \dot{y}(t) &= f(y(t)), \qquad t \in [0, \infty), \\ y(0) &= y_0 \,. \end{aligned} \tag{8.7.2}$$

The function Ψ^f is called forward solution flow associated to (the vector field) f.

Idea of splitting methods: Let $d \in \mathbb{N}$, $T \in (0, \infty)$, $y_0 \in \mathbb{R}^d$ let $f \in C(\mathbb{R}^d, \mathbb{R}^d)$ be *forward complete* and suppose we want to derive a one-step numerical scheme to approximate

the solution $y\colon [0,T] \to \mathbb{R}^d$ of the IVP

$$\begin{aligned} \dot{y}(t) &= f(y(t)), \qquad t \in [0,T], \\ y(0) &= y_0 \ . \end{aligned} \tag{8.7.3}$$

We are thus interested in an approximation of Φ_h^f for small $h \in (0,T]$. For instance, the explicit Euler method uses the approximation

$$\Phi_h^f(x) \approx x + h \cdot f(x) \tag{8.7.4}$$

for small $h \in (0,T]$. Splitting-approach: Assume that there are $a, b \in C(\mathbb{R}^d, \mathbb{R}^d)$ such that

$$f = a + b \ . \tag{8.7.5}$$

Then the so-called Lie-Trotter splitting suggests the approximation

$$\Phi_h^f(x) \approx \Phi_h^a\Big(\Phi_h^b(x)\Big) \qquad \text{(i.e., } \Phi_h^f \approx \Phi_h^a \circ \Phi_h^b \text{ Lie-Trotter splitting; H. F. Trotter 1959)} \tag{8.7.6}$$

for $x \in \mathbb{R}^d$ and small $h \in (0,T]$ and the so-called Strang splitting suggests the approximation

$$\Phi_h^f(x) \approx \Phi_{h/2}^a\Big(\Phi_h^b\Big(\Phi_{h/2}^a(x)\Big)\Big) \qquad \text{(i.e., } \Phi_h^f \approx \Phi_{h/2}^a \circ \Phi_h^b \circ \Phi_{h/2}^a \text{ Strang splitting; G. Strang 1968)} \tag{8.7.7}$$

for $x \in \mathbb{R}^d$ and small $h \in (0,T]$. For example, let $A \in \mathbb{R}^{d\times d}$ and suppose that $a(x) = Ax$ for all $x \in \mathbb{R}^d$. Combining the approximation (8.7.6) with the explicit Euler method then results in the numerical one-step scheme

$$\Phi_h^f(x) \approx e^{Ah}\,(x + h \cdot b(x)) \tag{8.7.8}$$

for $x \in \mathbb{R}^d$ and $h \in (0,T]$. Moreover, combining the approximation (8.7.7) with the explicit midpoint method results in the numerical one-step scheme

$$\Phi^f(x) \approx e^{A\frac{h}{2}}\left(e^{A\frac{h}{2}}x + h \cdot b\left(e^{A\frac{h}{2}}x + \frac{h}{2} \cdot b\left(e^{A\frac{h}{2}}x\right)\right)\right) \qquad \text{for } x \in \mathbb{R}^d \text{ and } h \in (0,T]. \tag{8.7.9}$$

See, e.g., Section II.5 in [E. Hairer, C. Lubich and G. Wanner, *Geometric numerical integration. Structure-preserving algorithms for ordinary differential equations.* Springer Series in Computational Mathematics, 31. Springer-Verlag, Berlin, 2002. [7]] for a more elaborate and appropriate treatment of splitting methods.