

# Lecture 2: Numerical simulation and direct collocation

Moritz Diehl and Armin Nurkanović

Systems Control and Optimization Laboratory (syscop)  
Summer School on Direct Methods for Optimal Control of Nonsmooth Systems  
September 11-15, 2023

**universität freiburg**

# Outline of the lecture



- 1 Basic definitions
- 2 Runge-Kutta methods
- 3 Collocation methods
- 4 Direct collocation for optimal control



Let:

- ▶  $t \in \mathbb{R}$  be the time
- ▶  $x(t) \in \mathbb{R}^{n_x}$  the differential states
- ▶  $u(t) \in \mathbb{R}^{n_u}$  a given control function
- ▶ denote by  $\dot{x}(t) = \frac{dx(t)}{dt}$

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$$F(t, \dot{x}(t), x(t), u(t)) = 0,$$

is called an Ordinary Differential Equation (ODE).



# Ordinary differential equations and controlled dynamical system

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- ▶ Given a function  $f : \mathbb{R} \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \rightarrow \mathbb{R}^{n_x}$  then a system of equations:

$$\dot{x}(t) = f(t, x(t), u(t)) \tag{1}$$

is called an **explicit ODE**.



## Theorem (Picard-Lindelöf / Cauchy–Lipschitz )

*An initial value problem in ODE*

$$\begin{aligned}\dot{x}(t) &= f(t, x(t), u(t)), \quad t \in [0, T], \\ x(0) &= x_0\end{aligned}$$

- ▶ *with given initial state  $x_0$ , and controls  $u(t)$ ,*
- ▶  *$f(t, x(t), u(t)) = \hat{f}(t, x(t))$  is continuous in  $t$  and Lipschitz continuous in  $x$*



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- ▶  $f$  is Lipschitz if  $\|f(x) - f(y)\| \leq L\|x - y\|$
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 $\dot{x}(t) = \sqrt{|x(t)|}$ ,  $x(0) = 0$ , solutions:  $x(t) = 0$  and  $x(t) = \frac{t^2}{4}$



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- ▶ Conditions are only sufficient, ODEs with a non-Lipschitz r.h.s. can have unique solutions

A collection of results in: Agarwal, Ratan Prakash, Ravi P. Agarwal, and V. Lakshmikantham. *Uniqueness and nonuniqueness criteria for ordinary differential equations*.

Vol. 6. World Scientific, 1993.

# ODE Example: harmonic oscillator



Mass  $m$  with spring constant  $k$  and friction coefficient  $c$ :

$$\begin{aligned}\dot{x}_1(t) &= x_2(t) \\ \dot{x}_2(t) &= -\frac{k}{m}(x_2(t) - u(t)) - \frac{\beta}{m}x_1(t)\end{aligned}$$

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- velocity of mass  $x_2(t)$
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Can summarize as  $\dot{x} = f(x, u)$  with

$$f(x, u) = \begin{bmatrix} x_2 \\ -\frac{k}{m}(x_2 - u) - \frac{c}{m}x_1 \end{bmatrix}$$



- ▶ IVPs have only in special cases a closed form solution
- ▶ Instead, compute numerically a **solution approximation**  $\tilde{x}(t)$  that approximately satisfies:

$$\begin{aligned}\dot{\tilde{x}}(t) &\approx f(t, \tilde{x}(t), u(t)), & t \in [0, T] \\ \tilde{x}(0) &= x(0) = x_0\end{aligned}$$



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- ▶ Recursively generate solution approximation  $x_n := \tilde{x}(t_n) \approx x(t_n)$  at  $N$  discrete time points  $0 = t_0 < t_1 < \dots < t_N = T$
- ▶ Integration interval  $[0, T]$  split into subintervals  $[t_n, t_{n+1}]$  where  $h = t_{n+1} - t_n$
- ▶  $h$  - integration step size can be constant, different for every interval, or adaptive



## Single step abstract integration method

$$\begin{aligned}x_{n+1} &= \phi_f(x_n, z_n, u_n), \\ 0 &= \phi_{\text{int}}(x_n, z_n, u_n), \quad n = 0, \dots, N - 1.\end{aligned}$$

- ▶  $\phi_f$  - state transition - compute next integration step
- ▶  $\phi_{\text{int}}$  - internal computations, e.g., stages of a Runge-Kutta method (next section)
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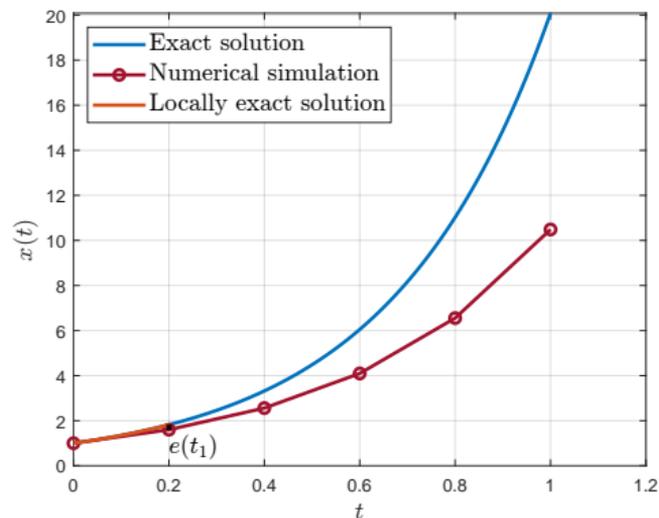
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Is an overkill for simple examples but pays off for complicated methods later.

## Local and global error

- ▶ Local integration error at  $t_{n+1}$ :

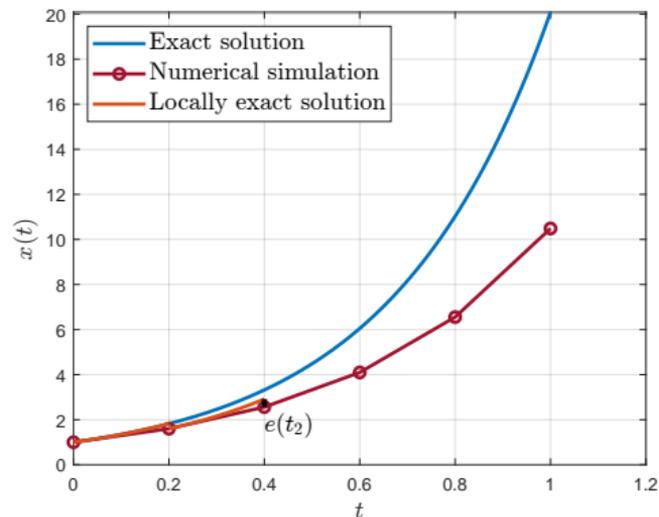
$$e(t_{n+1}) = \|x(t_{n+1}) - \phi_f(x(t_n), z_n, u_0)\|.$$



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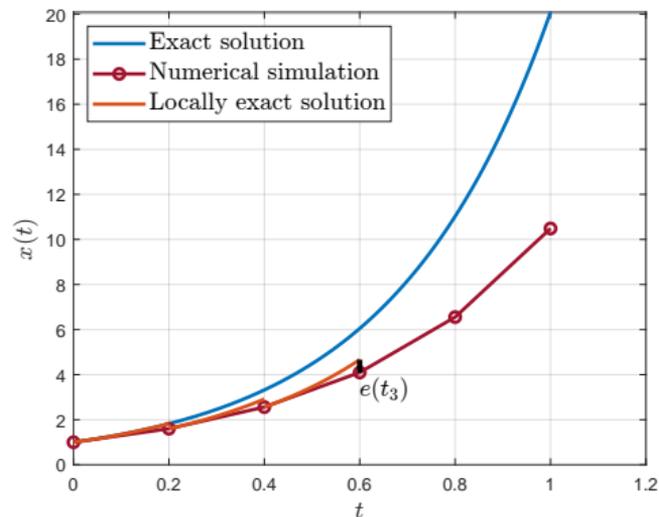
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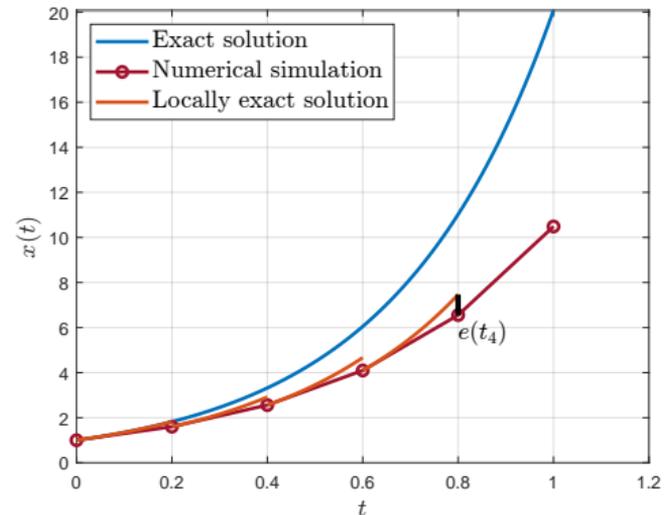
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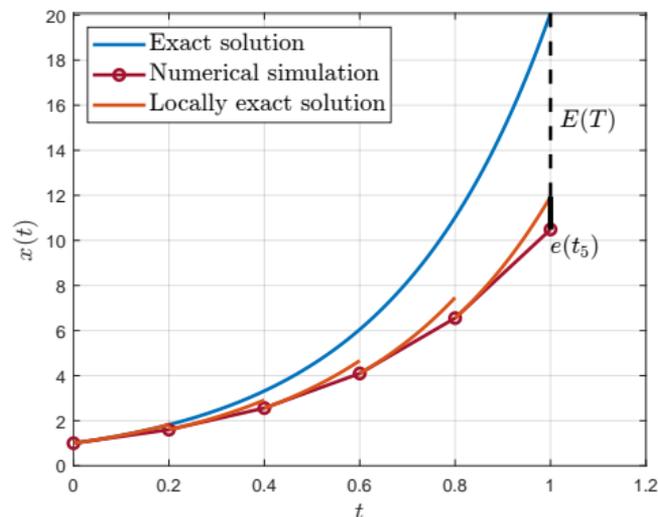
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- ▶ Global integration error at  $t = T$ :

$$E(T) = \|x(T) - x_N\|.$$

- ▶ Global error - accumulation of local errors



## Integrator convergence and accuracy

### ► Convergence

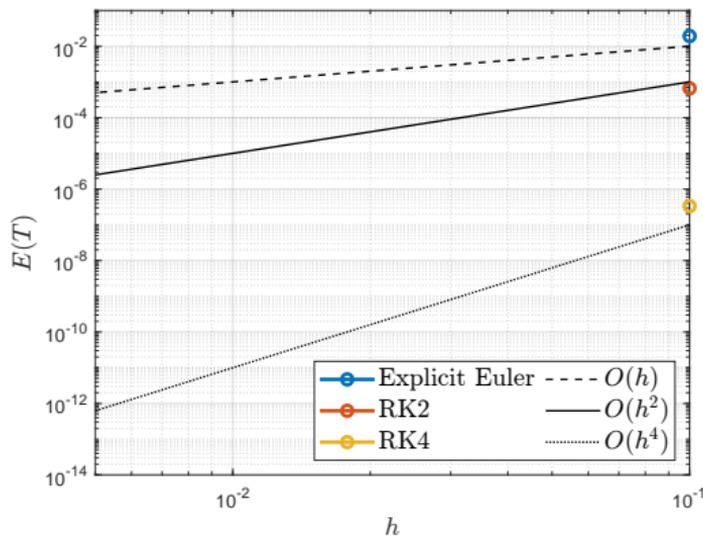
$$\lim_{h \rightarrow 0} E(T) = 0$$

### ► Integrator has order $p$ if

$$\lim_{h \rightarrow 0} e(t_i) \leq Ch^{p+1} = O(h^{p+1}), C > 0$$

### ► Higher order $p$ :

- less, but more expensive steps for same accuracy
- in total fewer r.h.s. evaluations for same accuracy



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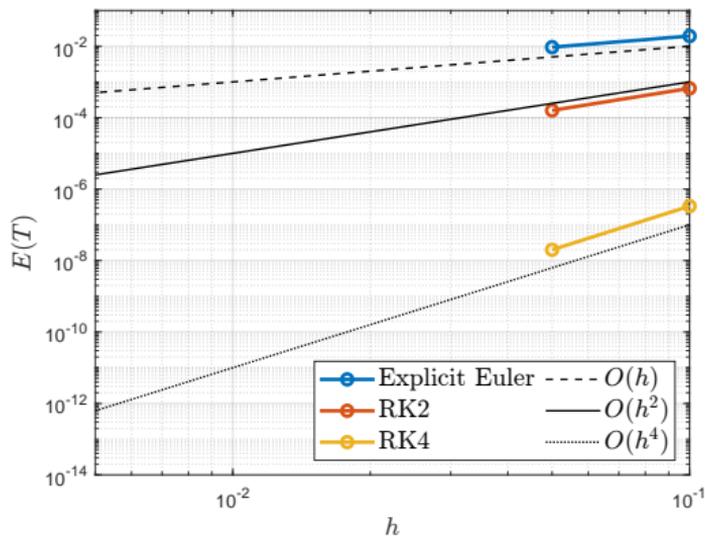
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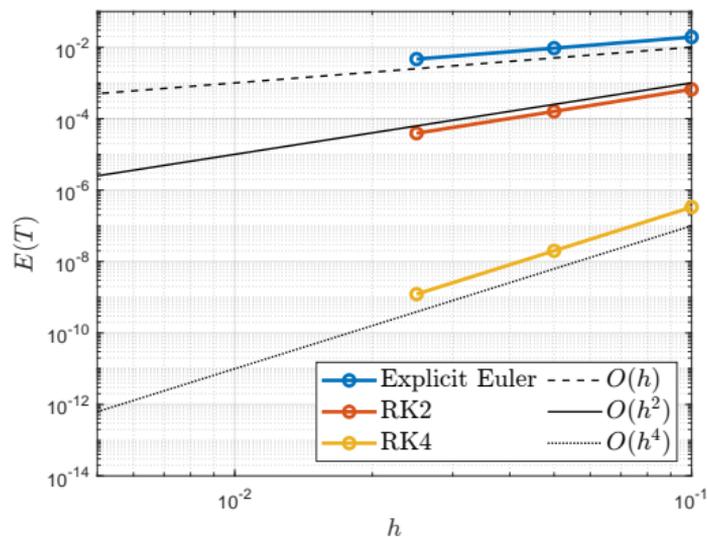
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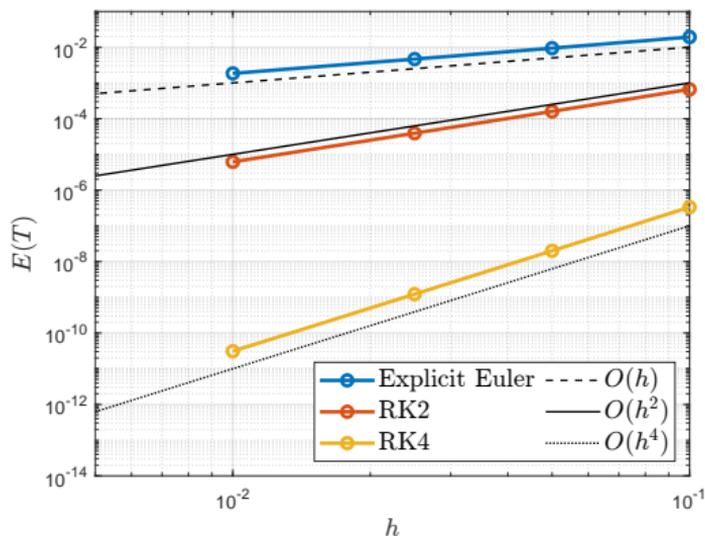
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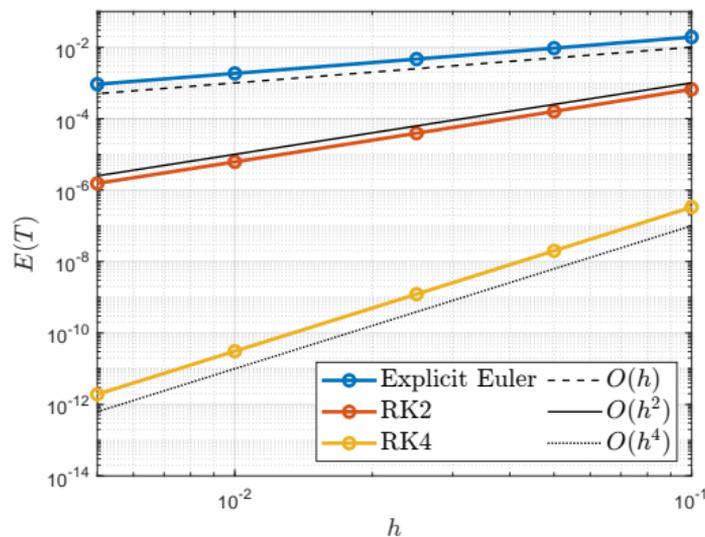
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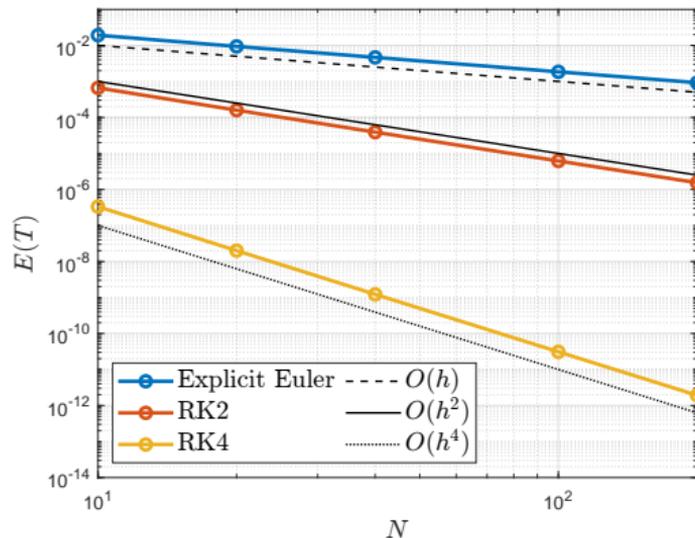
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Alternatively one can plot the error over  $N \propto \frac{1}{h}$  instead of  $h$

# Stability and convergence

## Integrator convergence and accuracy

- ▶ Convergence

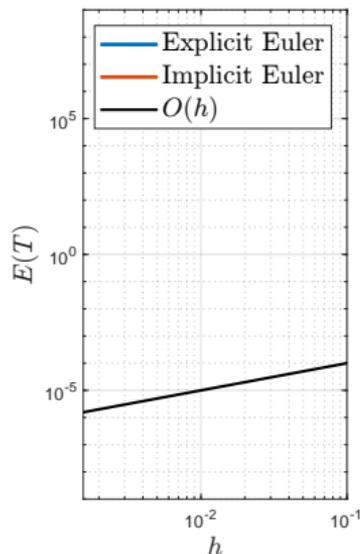
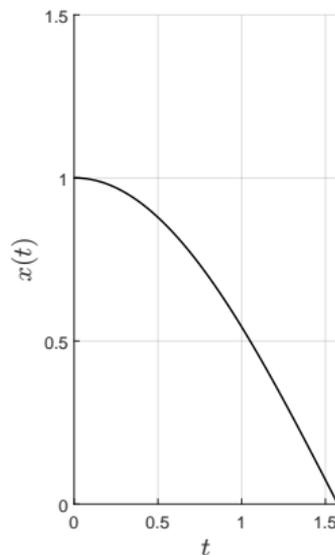
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- ▶ **Stability:** damping of errors, does it work for  $h \gg 0$ ?

- ▶ If integrator is unstable, it does not converge and has  $p = 0$ , unless  $h$  very small



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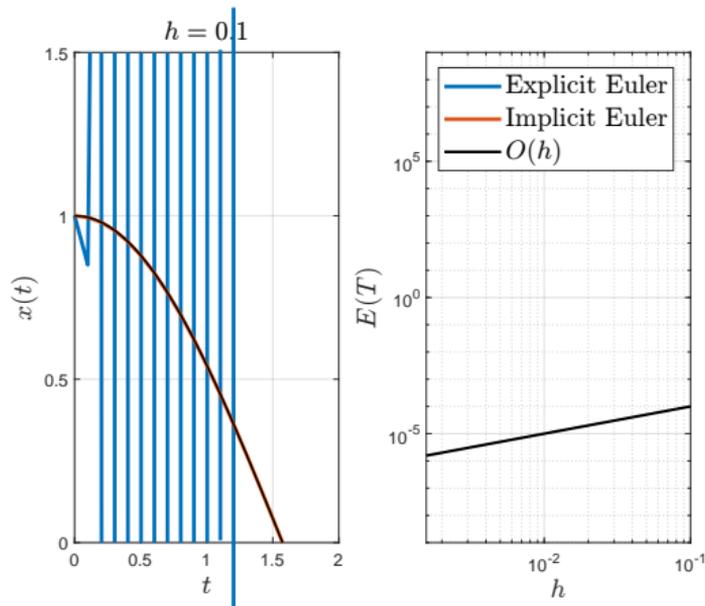
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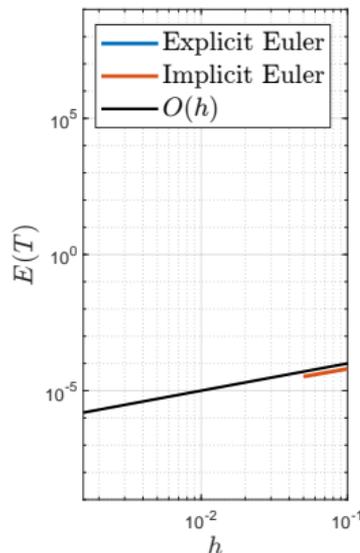
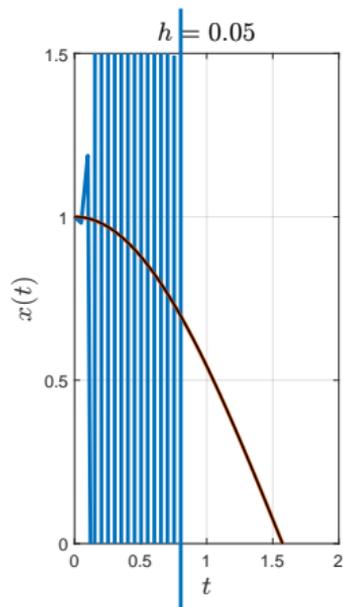
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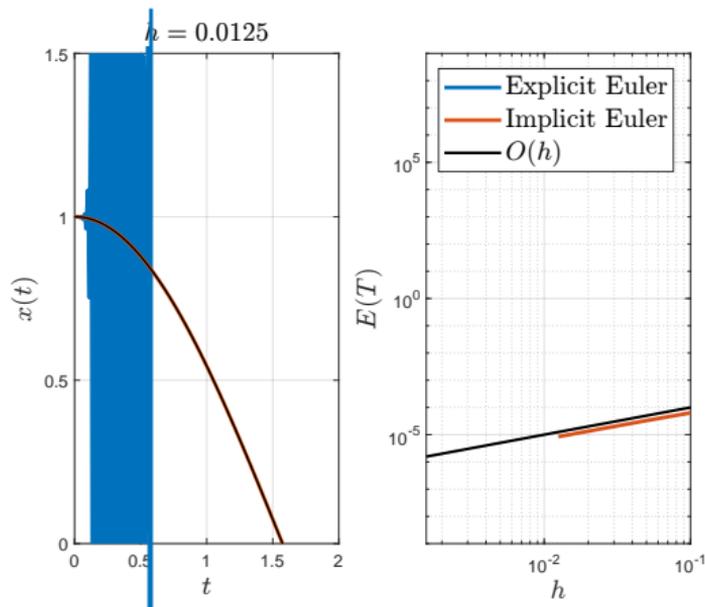
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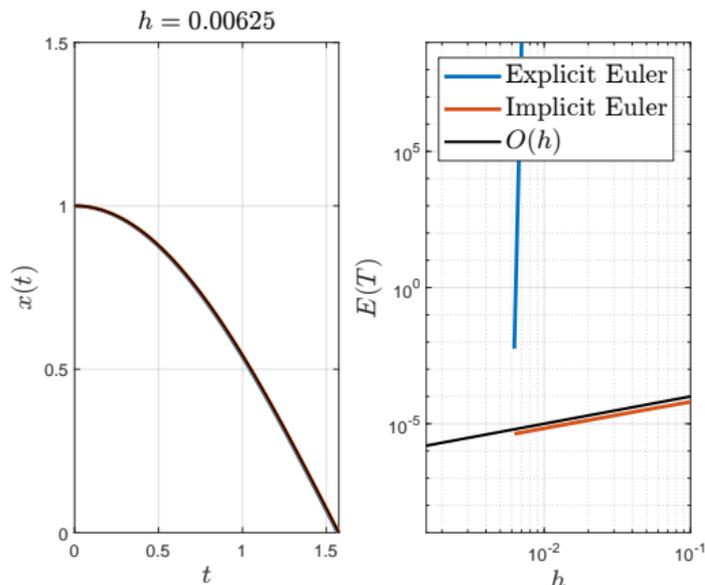
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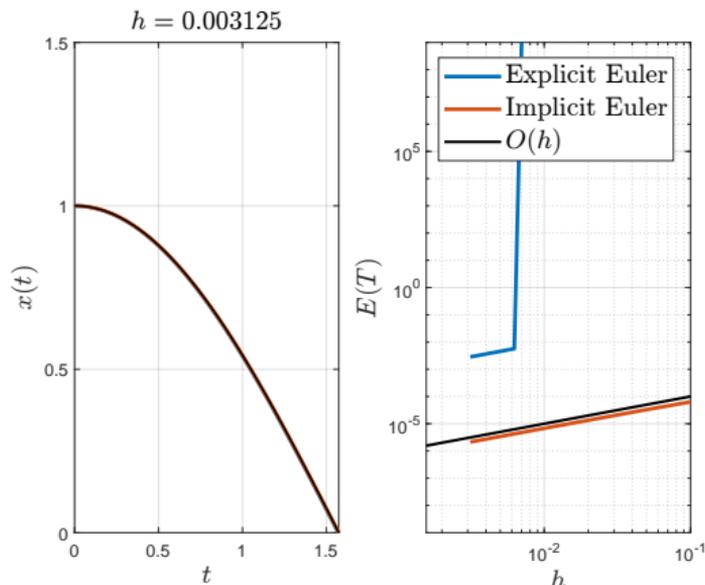
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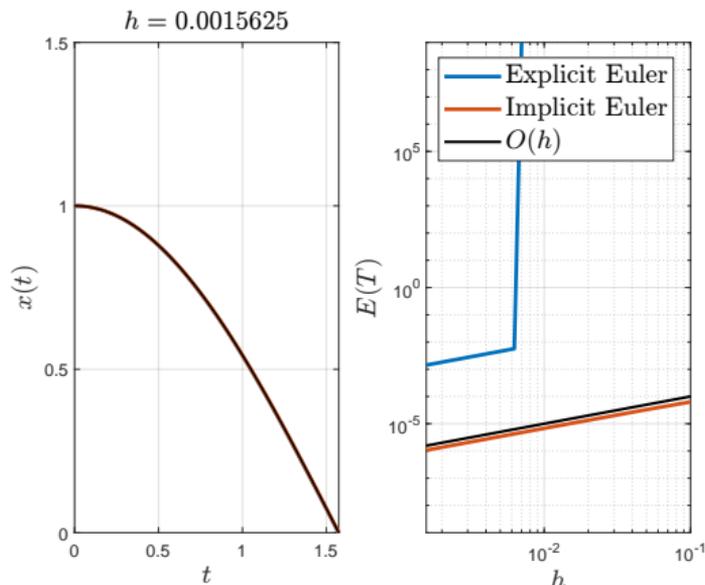
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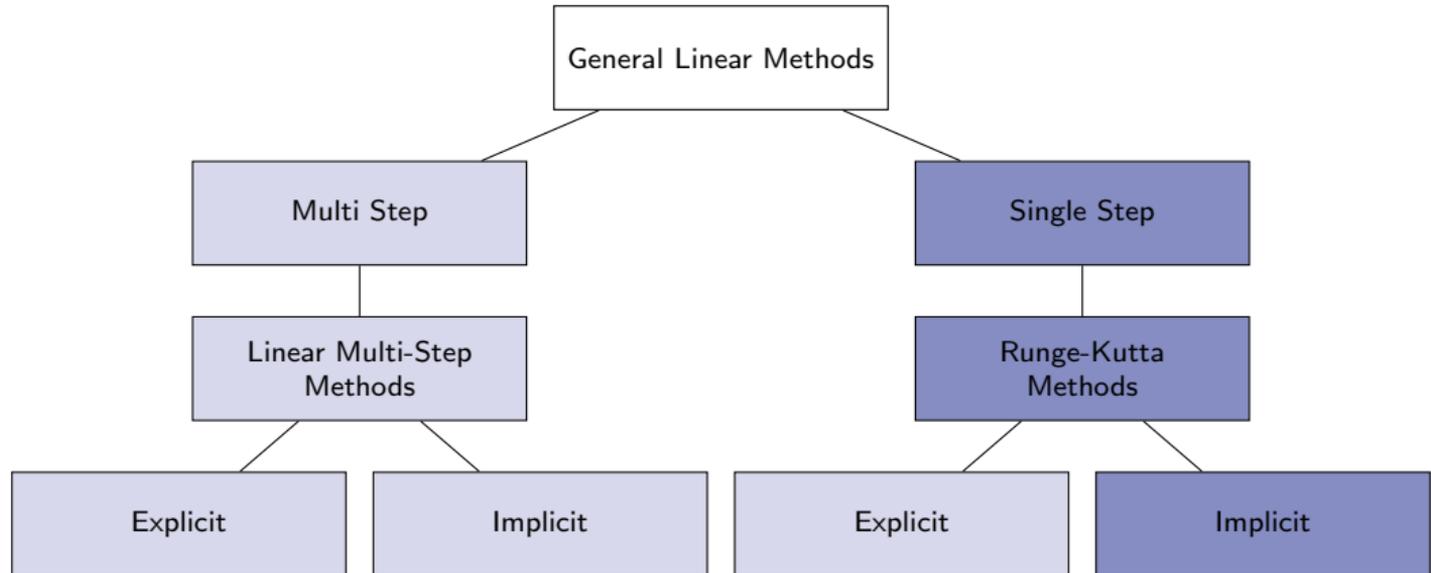


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# Runge-Kutta method definition

Unknowns are derivatives at stage points



## Definition (Runge-Kutta method in differential form)

Let  $n_s$  be the number of stages. Given the matrix  $A \in \mathbb{R}^{n_s \times n_s}$  with the entries  $a_{i,j}$  for  $i, j = 1, \dots, n_s$ , and the vectors  $b, c \in \mathbb{R}^{n_s}$ . Let  $t_{n,i} = t_n + c_i h$ . The system of equations:

$$k_{n,i} = f(t_{n,i}, x_n + h \sum_{j=1}^{n_s} a_{i,j} k_{n,j}, u_n), \quad i = 1, \dots, n_s$$

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is called a  $n_s$ -stage Runge-Kutta (RK) method in the *differential form*.

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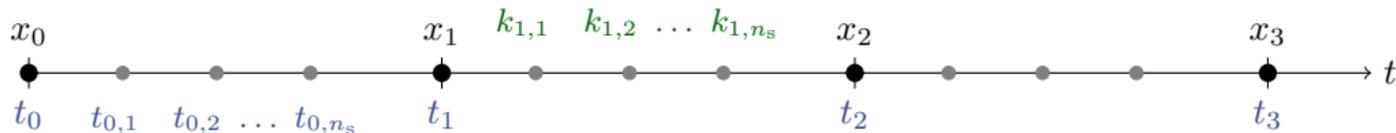
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$$h, t_n, t_{n,i} \\ i = 1, \dots, n_s$$

### Butcher tableau

$$a_{i,j}, b_i, c_i \\ i, j = 1, \dots, n_s$$

### Data

$$x_n, u_n, f(\cdot)$$

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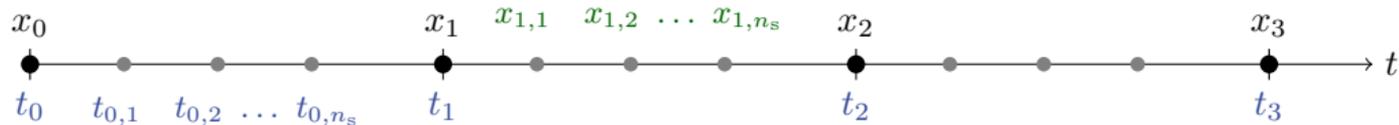
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# Runge-Kutta method examples

## Explicit Runge-Kutta 4

$$k_{n,1} = f(t_n, x_n)$$

$$k_{n,2} = f\left(t_n + \frac{h}{2}, x_n + h \frac{k_{n,1}}{2}\right)$$

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## Implicit Euler Method

$$k_{n,1} = f(t_n, x_n + hk_{n,1})$$

$$x_{n+1} = x_n + hk_{n,1}$$

- ▶ All  $k_{n,1}$  is found implicitly by solving  $k_{n,1} - f(t_n, x_n + hk_{n,1}) = 0$ .

# Explicit vs implicit Runge-Kutta methods

The Butcher tableau



## Explicit Runge-Kutta method

0					
$c_2$	$a_{2,1}$				
$\vdots$	$\vdots$	$\vdots$	$\ddots$		
$c_{n_s}$	$a_{n_s,1}$	$a_{n_s,2}$	$\dots$	$a_{n_s,n_s-1}$	
	$b_1$	$b_2$	$\dots$	$b_{n_s-1}$	$b_{n_s}$

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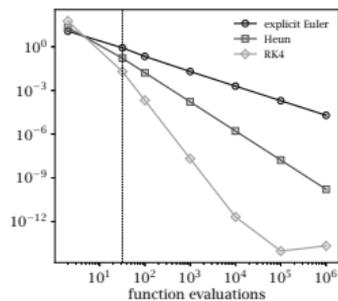
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- ▶ Requires solving nonlinear rootfinding problem with Newton's method
- ▶ Expensive but good for stiff systems
- ▶ Order:  $p = 2n_s, p = 2n_s - 1, \dots$
- ▶ Famous representative: collocation methods - treated next!

# Butcher tableau, six examples



Euler

$$\begin{array}{c|c} 0 & \\ \hline 1 & \end{array}$$

Heun

$$\begin{array}{c|cc} 0 & & \\ \hline 1 & 1 & \\ \hline 1/2 & 1/2 & \end{array}$$

RK4

$$\begin{array}{c|cccc} 0 & & & & \\ 1/2 & 1/2 & & & \\ 1/2 & 0 & 1/2 & & \\ 1 & 0 & 0 & 1 & \\ \hline & 1/6 & 2/6 & 2/6 & 1/6 \end{array}$$

Implicit Euler

$$\begin{array}{c|c} 1 & 1 \\ \hline & 1 \end{array}$$

Midpoint rule (GL2)

$$\begin{array}{c|cc} 1/2 & 1/2 & \\ \hline & & 1 \end{array}$$

Gauss-Legendre of order 4 (GL4)

$$\begin{array}{c|cc} 1/2 - \sqrt{3}/6 & 1/4 & 1/4 - \sqrt{3}/6 \\ 1/2 + \sqrt{3}/6 & 1/4 + \sqrt{3}/6 & 1/4 \\ \hline & 1/2 & 1/2 \end{array}$$

$$\begin{array}{c|cccc} c_1 & a_{11} & \cdots & a_{1s} \\ c_2 & a_{21} & \cdots & a_{2s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \cdots & a_{ss} \\ \hline & b_1 & \cdots & b_s \end{array}$$

# Outline of the lecture



- 1 Basic definitions
- 2 Runge-Kutta methods
- 3 Collocation methods
- 4 Direct collocation for optimal control



## Main ideas:

- ▶ Approximate  $x(t)$  on  $t \in [t_n, t_{n+1}]$  with a **polynomial**  $q_n(t)$  of degree  $n_s$



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- ▶ Polynomial of degree  $n_s$ :  $n_s + 1$  coefficient and  $n_s + 1$  equations
- ▶ Next value - simple evaluation:  $x_{n+1} = q_n(t_{n+1})$

# Collocation - how to implement it?



How to parameterize  $q_n(t)$ ?

Two common (equivalent) choices



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Two common (equivalent) choices

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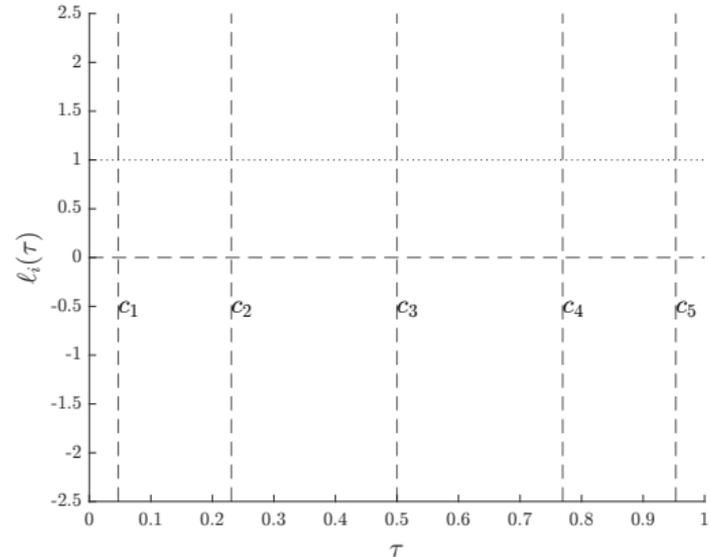
► with:

$$\begin{aligned} \dot{q}_n(t) &= \ell_1 \left( \frac{t - t_n}{h} \right) k_{n,1} + \ell_2 \left( \frac{t - t_n}{h} \right) k_{n,2} + \dots + \ell_{n_s} \left( \frac{t - t_n}{h} \right) k_{n,n_s} \\ &= \sum_{i=1}^{n_s} \ell_i \left( \frac{t - t_n}{h} \right) \underbrace{f(t_n + c_i, q_n(t_n + c_i h), u_0)}_{=k_{n,i}} \end{aligned}$$

# The Lagrange polynomials $l_i(\tau)$

## Lagrange polynomial basis

$$l_i(\tau) = \prod_{j=1, j \neq i}^{n_s} \frac{\tau - c_j}{c_i - c_j}.$$



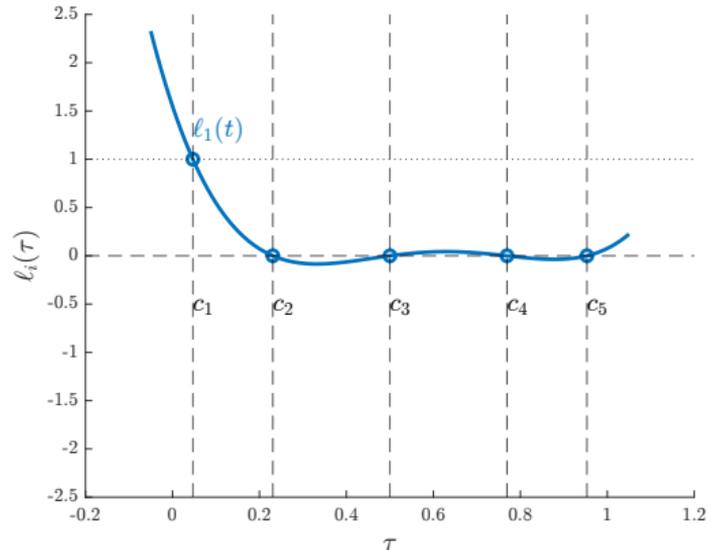
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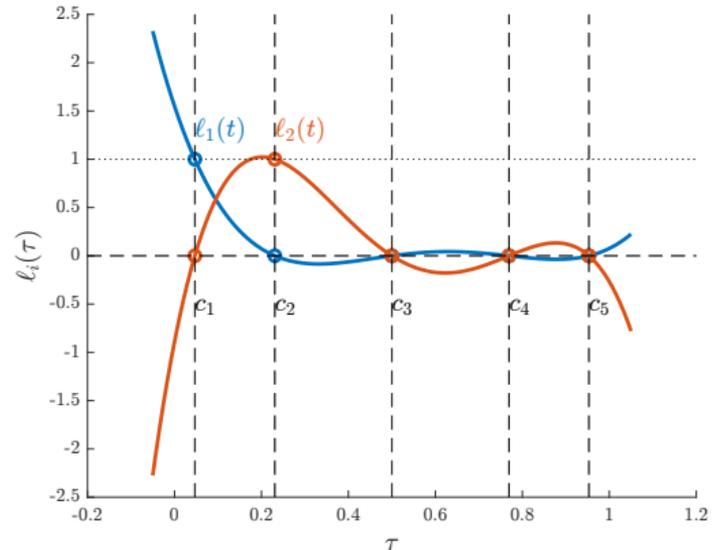
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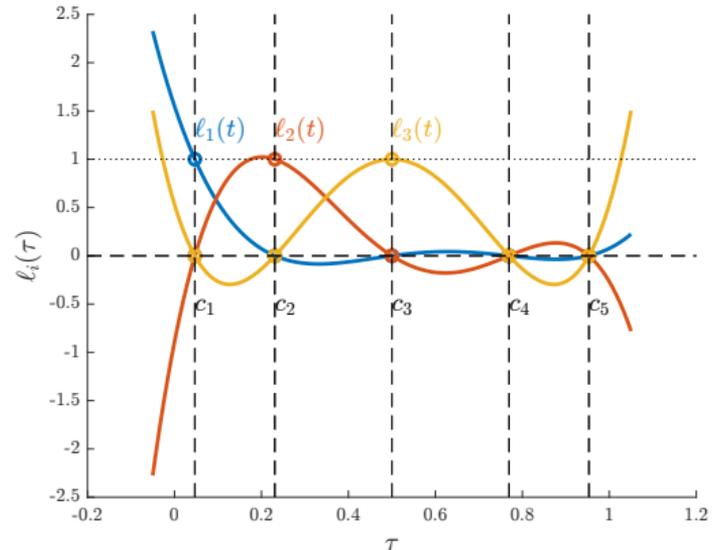
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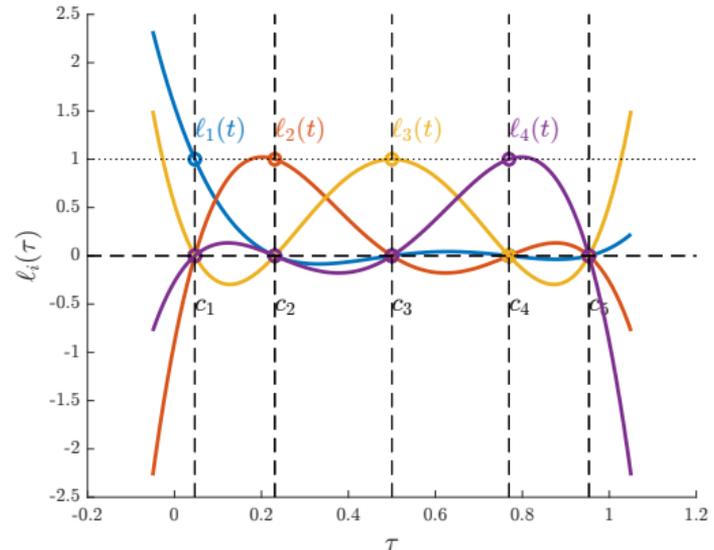
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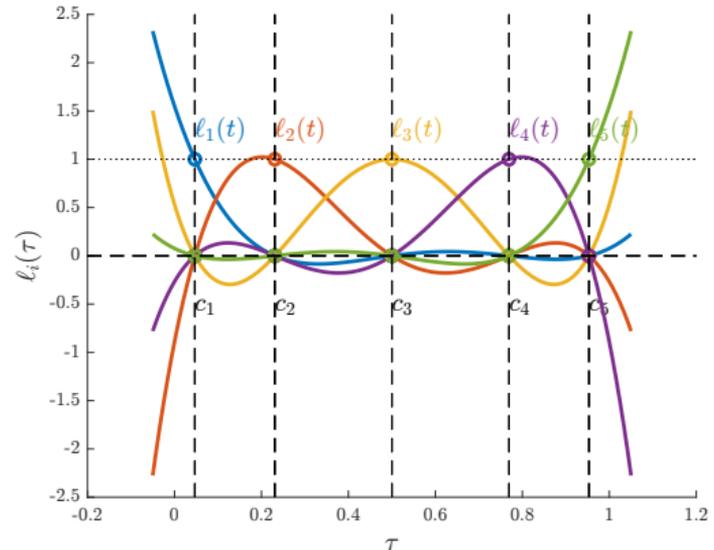
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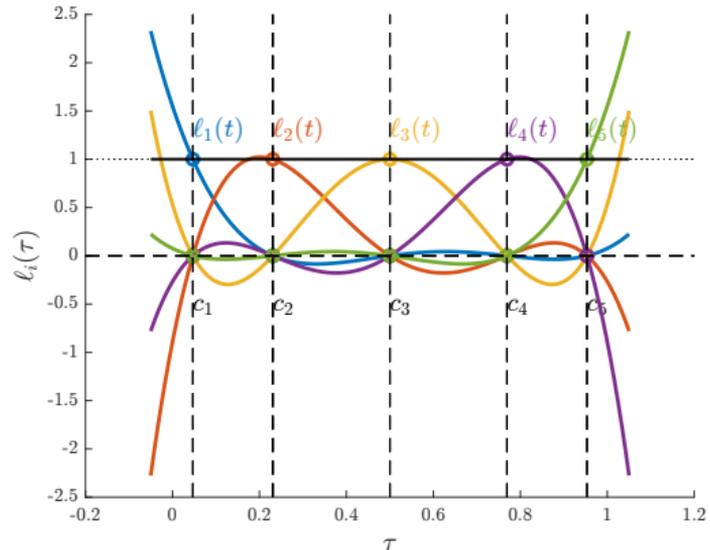
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$$\sum_{i=1}^{n_s} l_i(t) = 1$$





- ▶ Evaluate  $q_n(t)$  at collocation points

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- Evaluate  $q_n(t)$  at collocation points

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Similarly  $q_n(t)$  evaluated at  $t_{n+1} = t_n + h$ :

$$q_n(t_n + h) = x_n + h \sum_{i=1}^{n_s} k_i \underbrace{\int_0^1 \ell_i(\sigma) d\sigma}_{:=b_i} = x_n + h \sum_{i=1}^{n_s} k_i b_i$$

# All collocation methods are implicit Runge-Kuta method



## Collocation equations

$$q_n(t_n) = x_n \quad \text{(initial value)}$$

$$\dot{q}_n(t_n + c_i h) = f(t_n + c_i h, q_n(t_n + c_i h), u_n), \quad i = 1, \dots, n_s \quad \text{(stage eqs.)}$$

$$x_{n+1} = q_n(t_{n+1}) \quad \text{(next value)}$$

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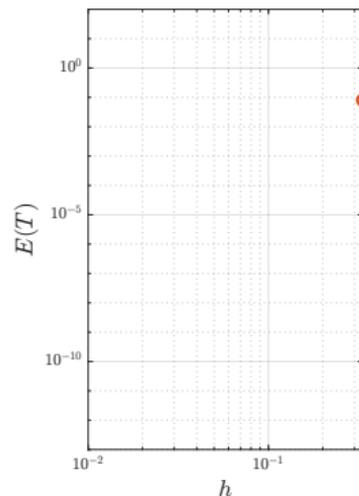
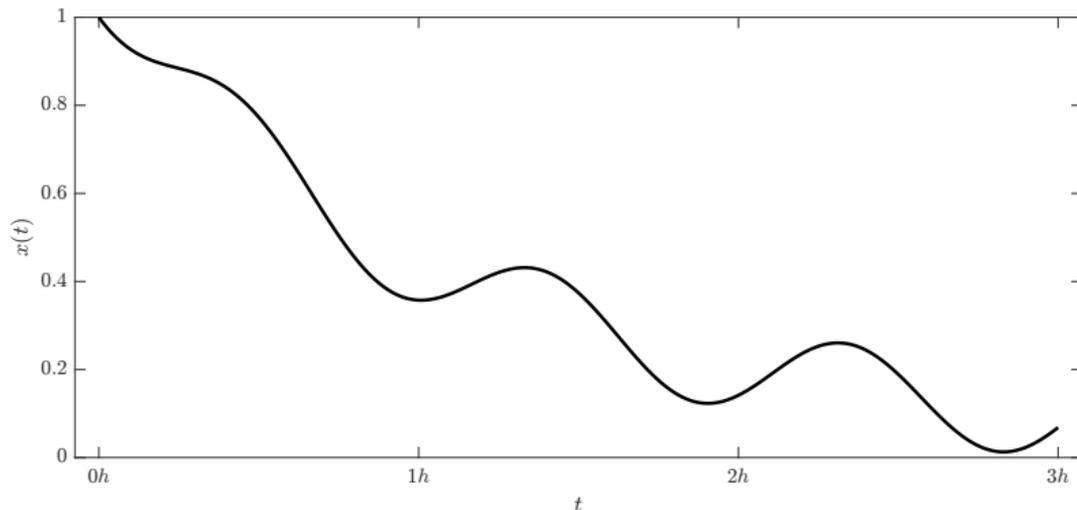
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- ▶ We arrived at the implicit RK equations in differential form
- ▶ Unknowns:  $x_{n+1} \in \mathbb{R}^{n_x}$  and  $z_n = (k_{n,1}, \dots, k_{n,n_s}) \in \mathbb{R}^{n_s n_x}$
- ▶  $(n_s + 1)n_x$  equations and  $(n_s + 1)n_x$  variables - solve via Newton's methods

# Collocation - visualization

- ▶ Choice of points  $c_1, \dots, c_{n_s}$  determines properties of method.
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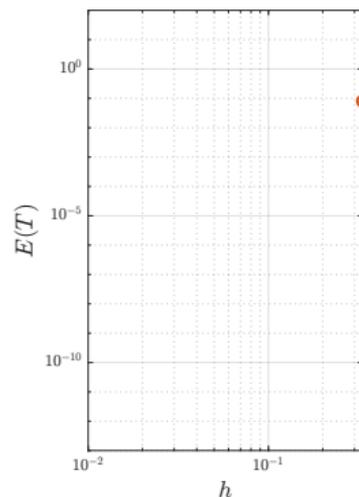
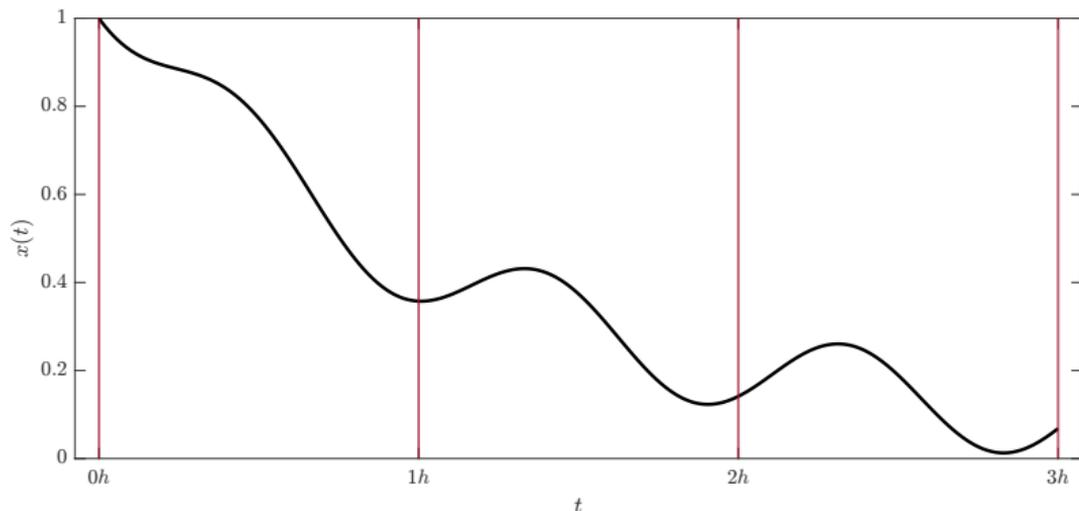


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Visualization inspired by Leo Simpson's talk at the European control conference 2023

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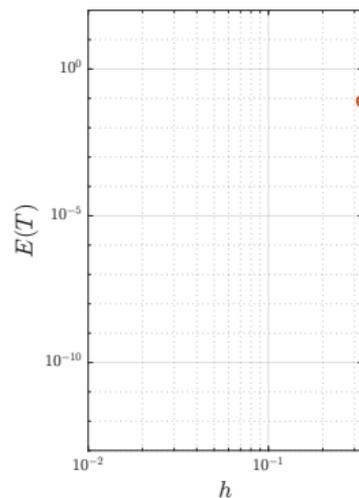
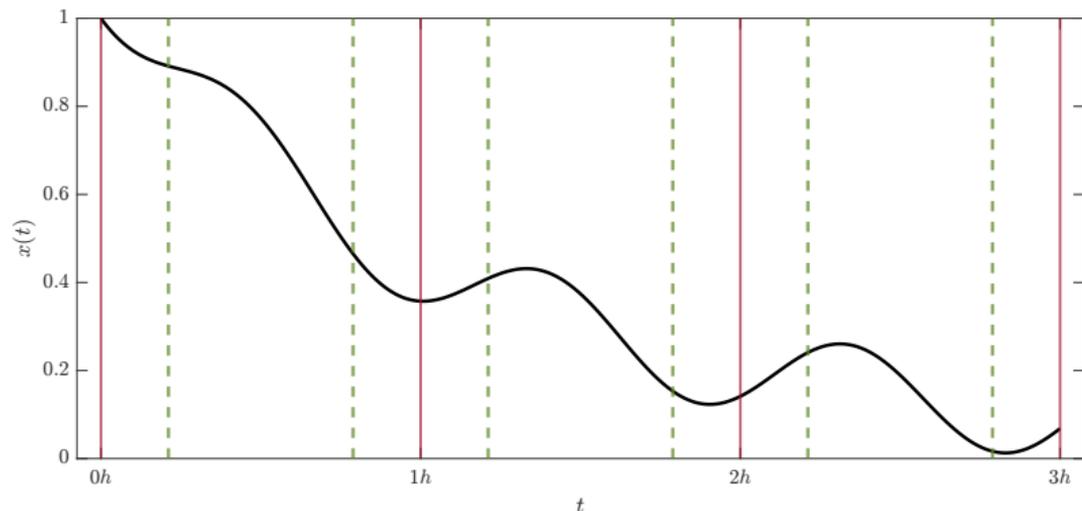


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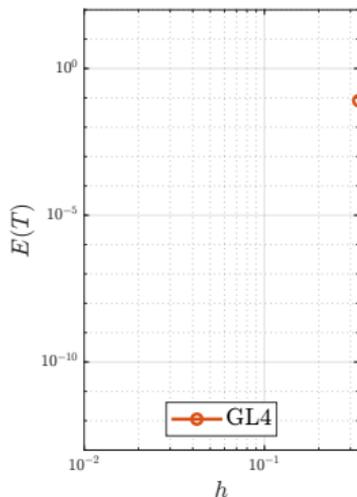
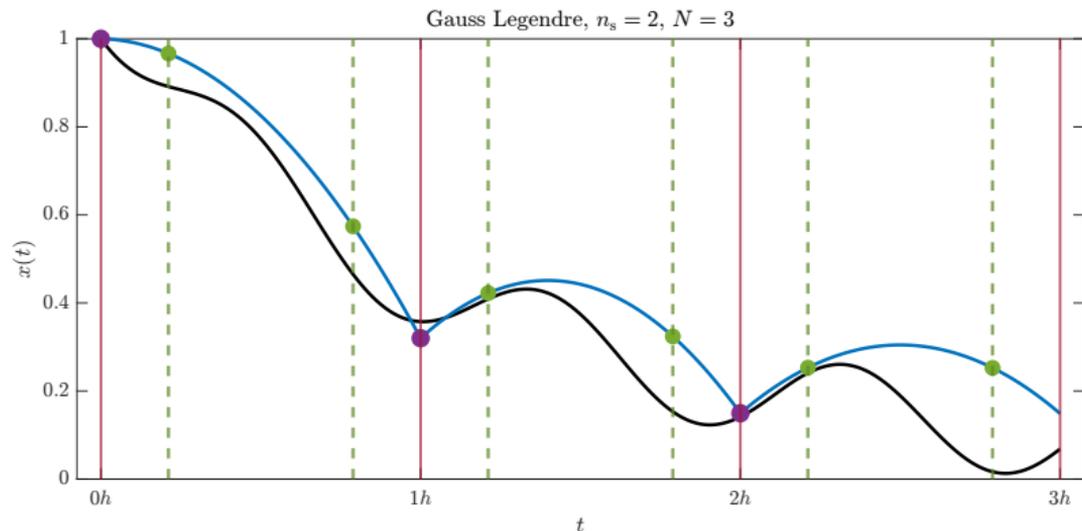


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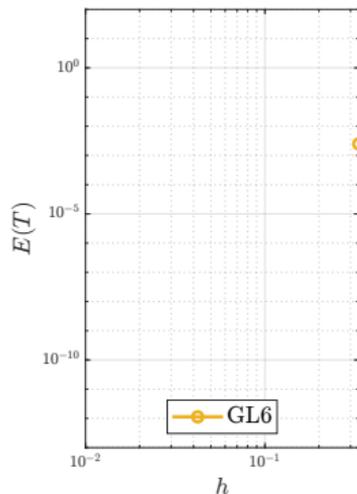
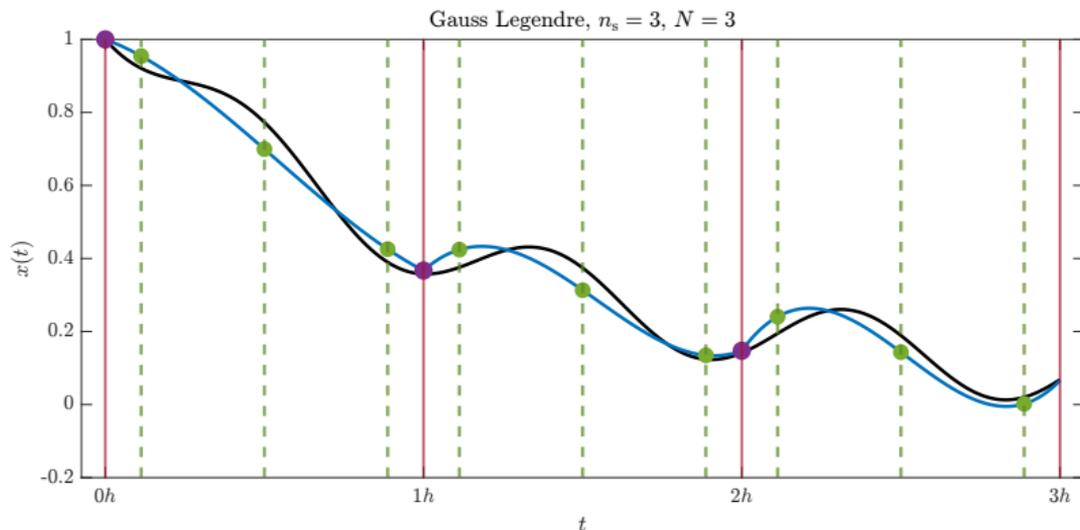


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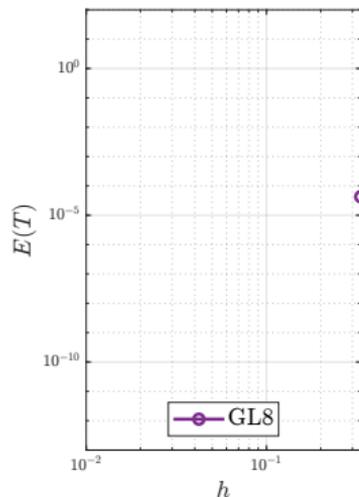
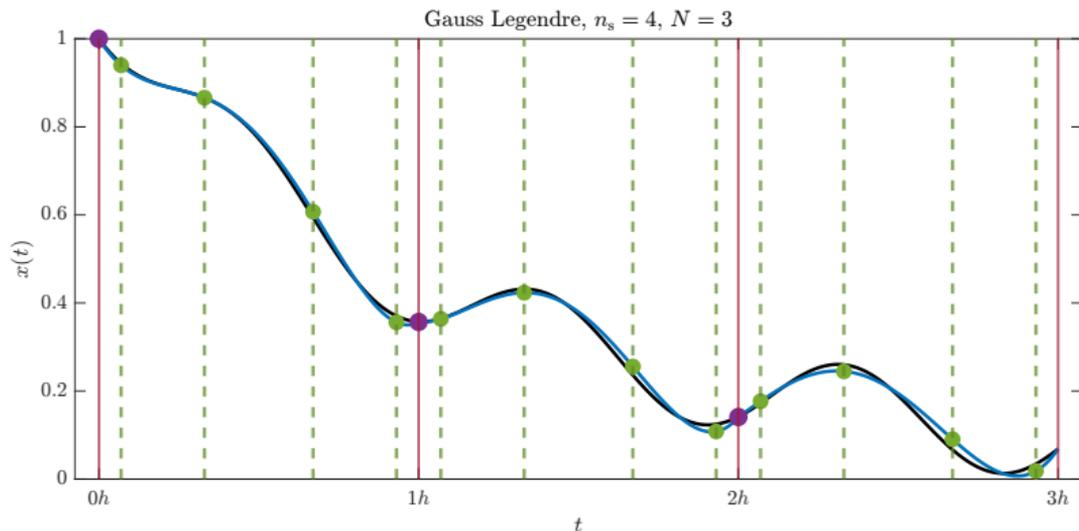


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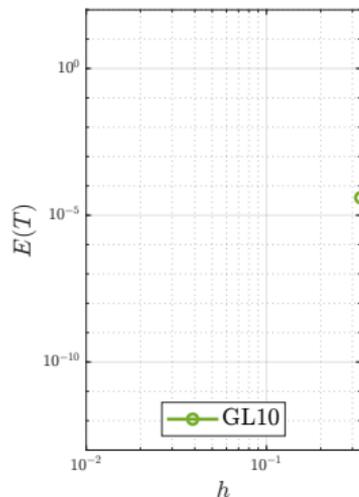
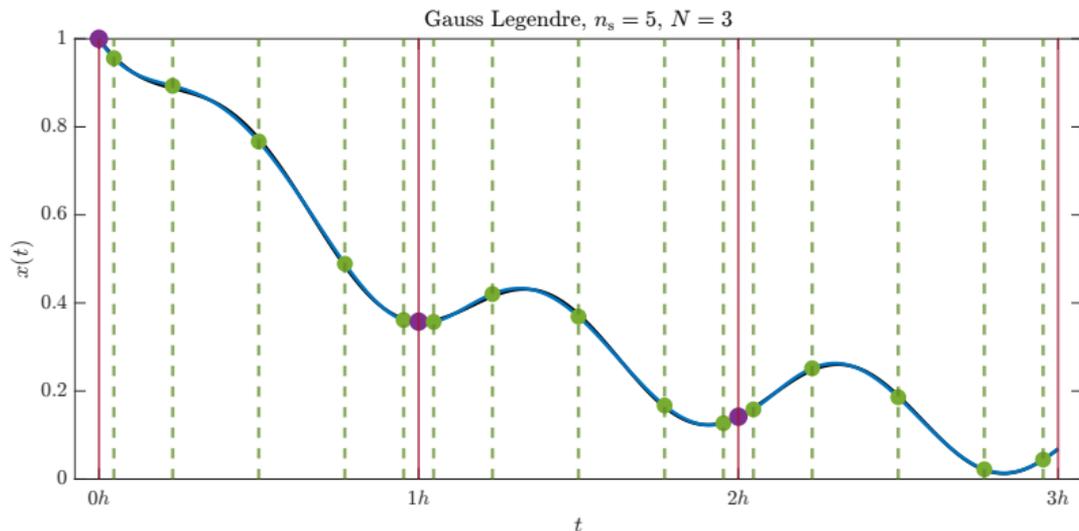
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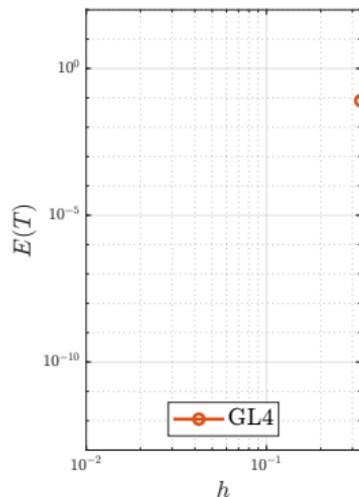
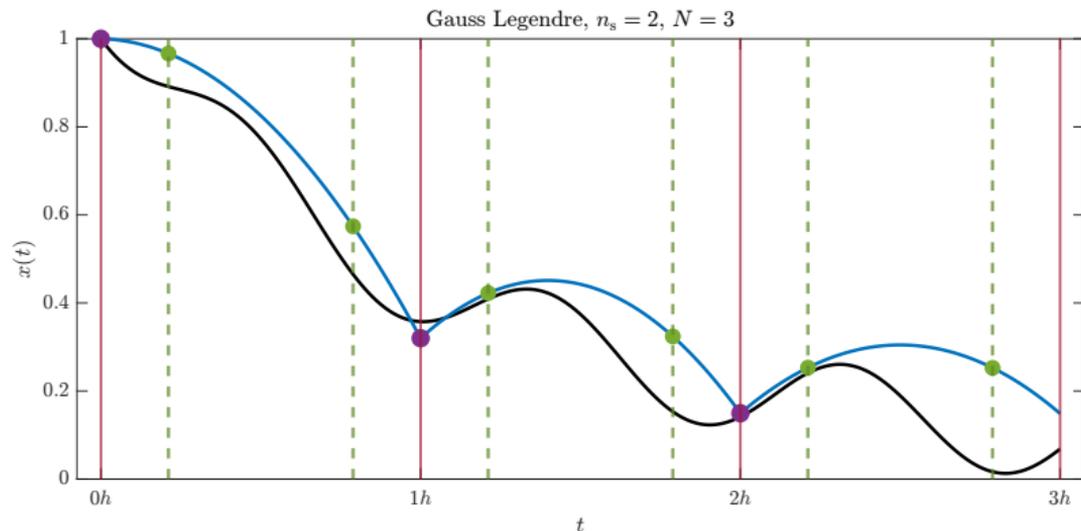
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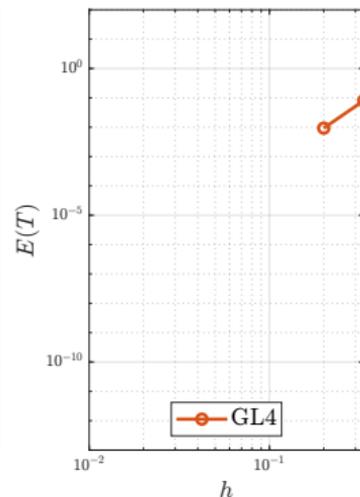
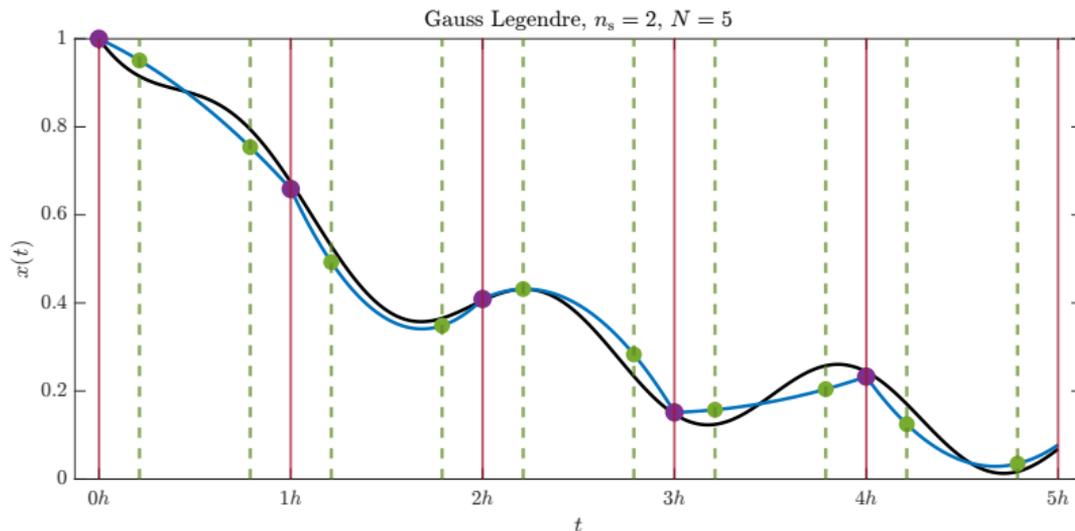
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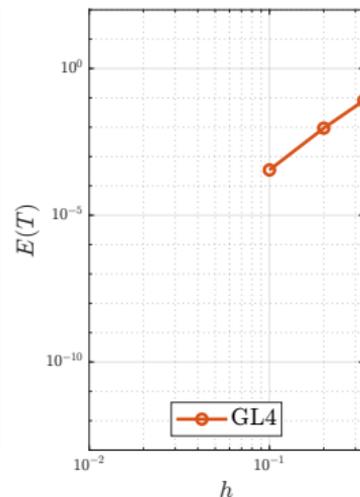
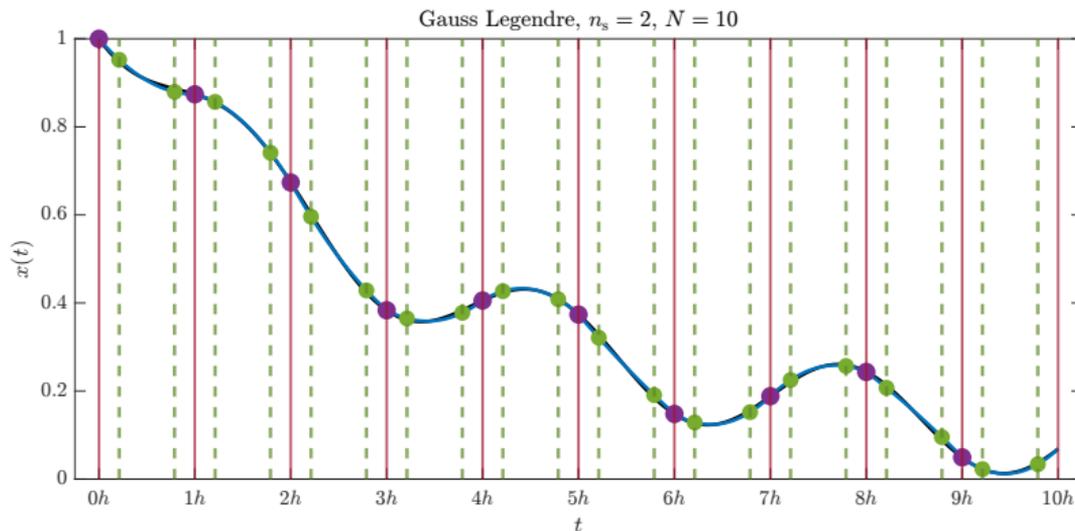
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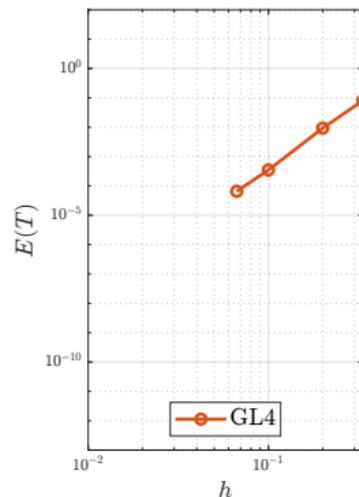
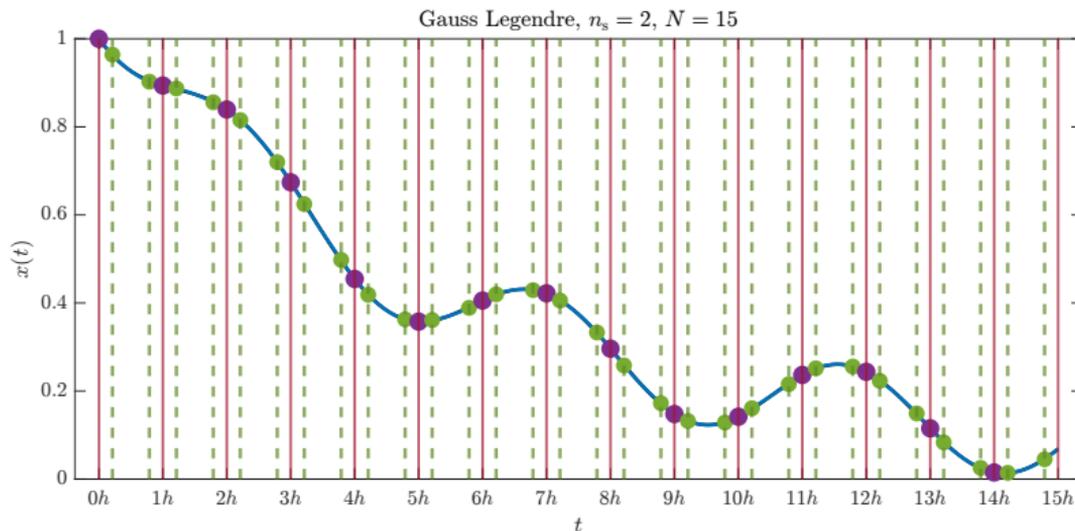
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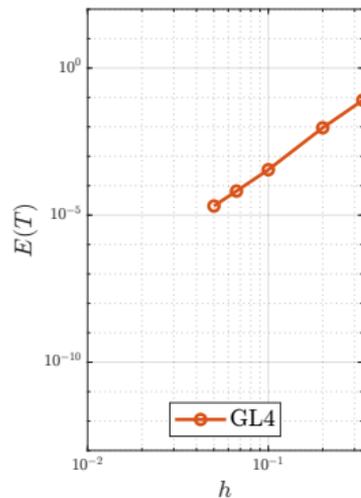
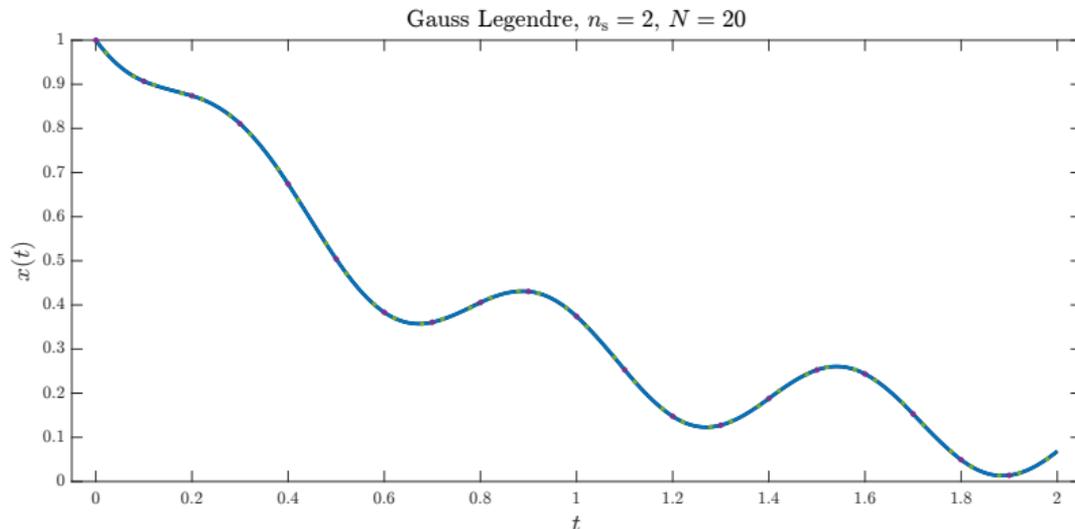
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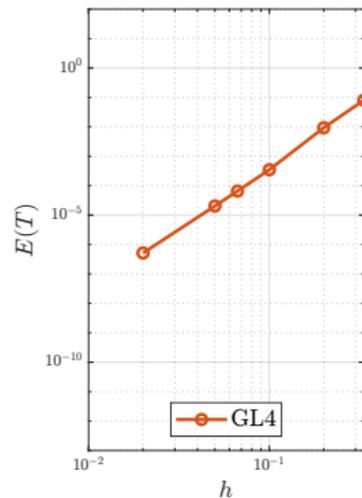
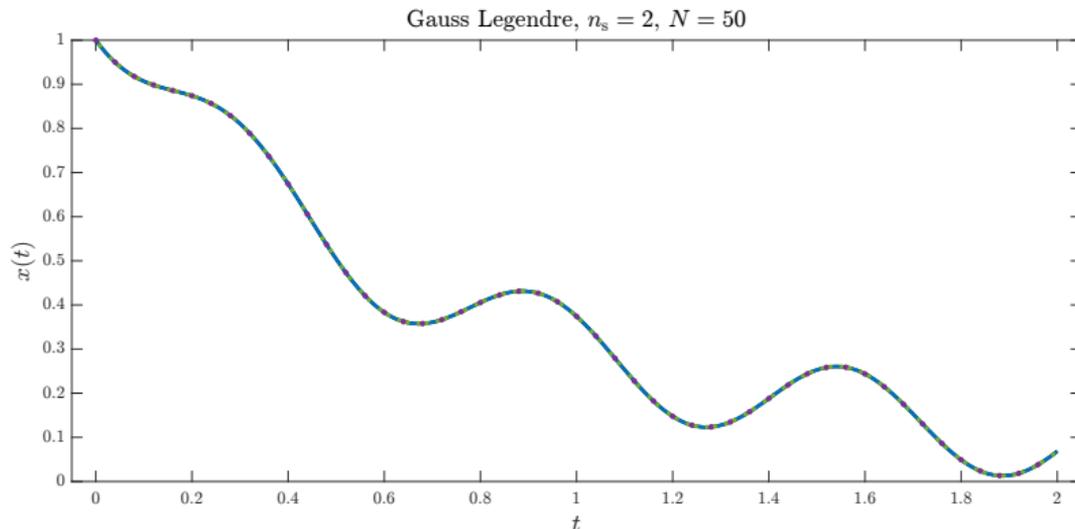
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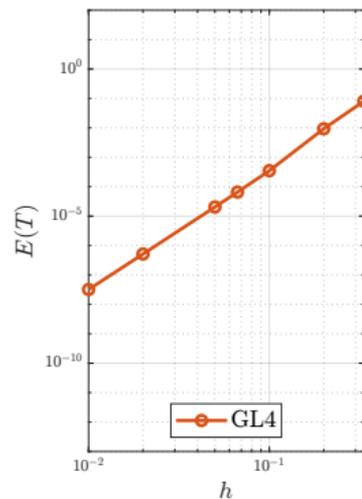
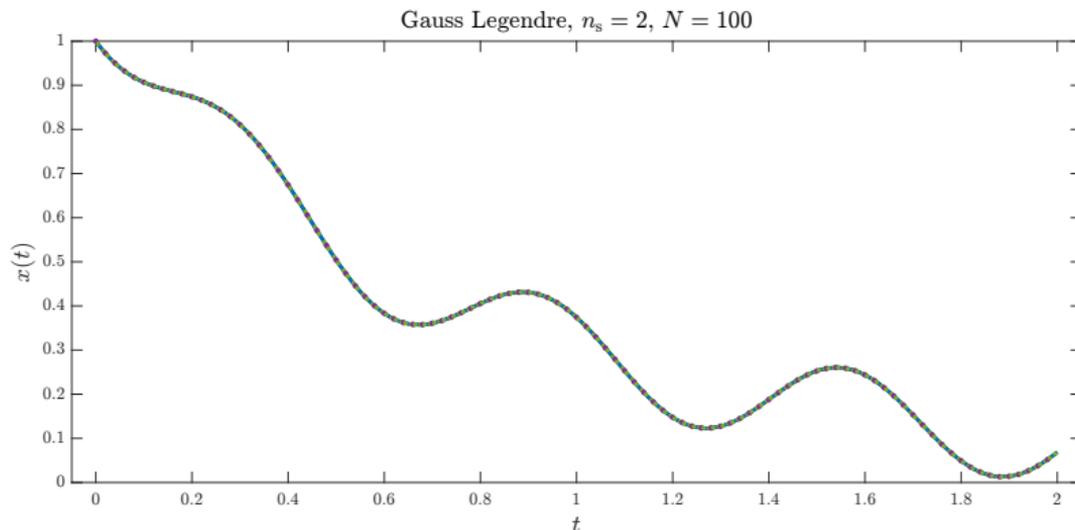
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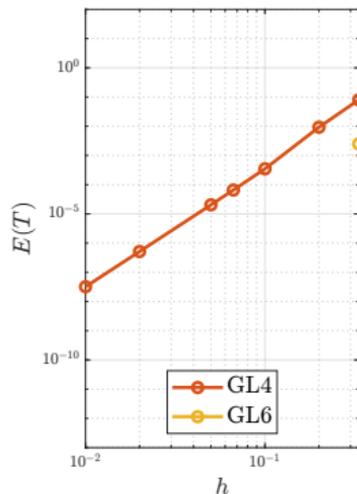
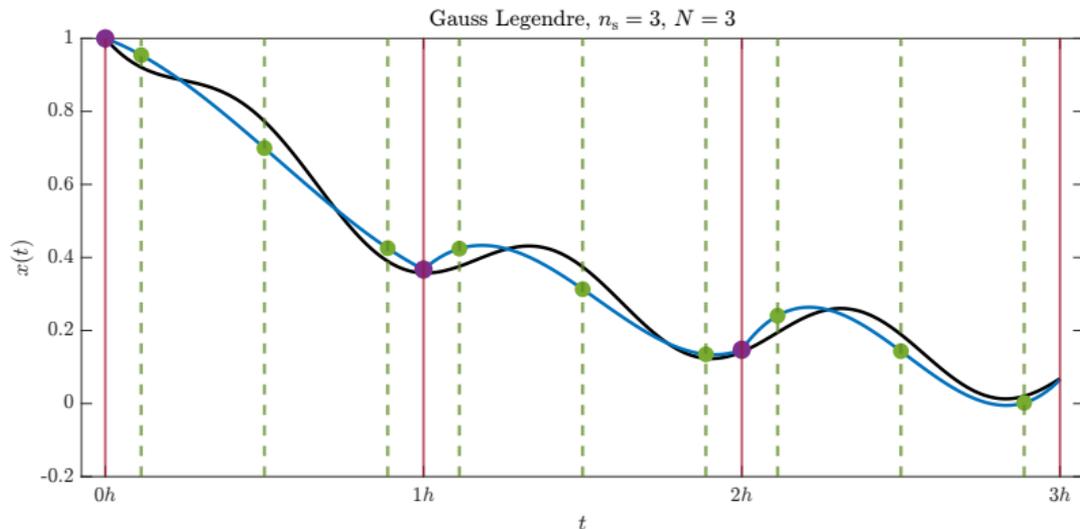
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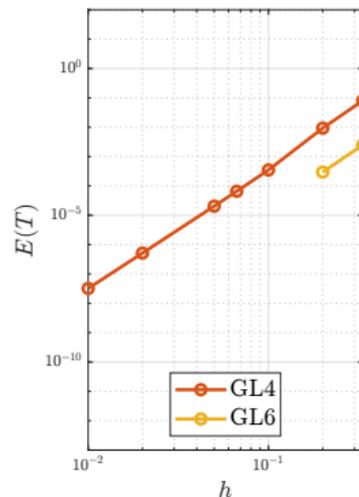
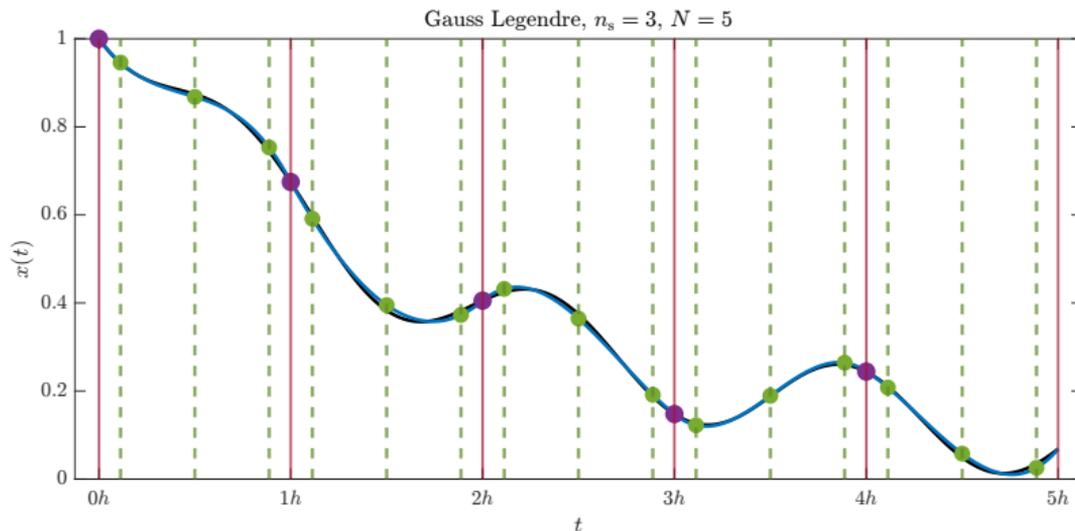
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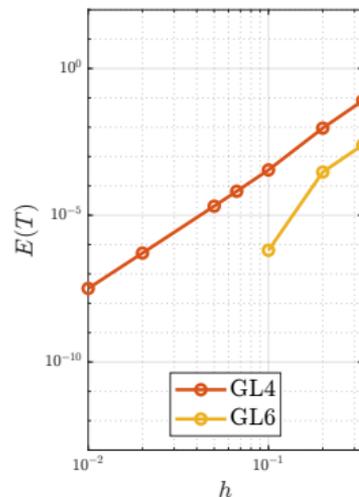
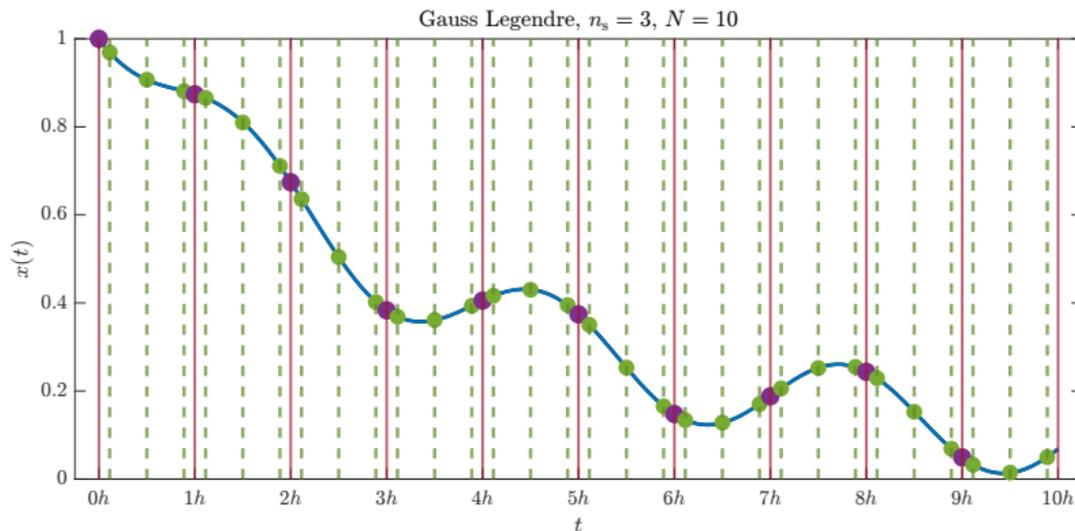
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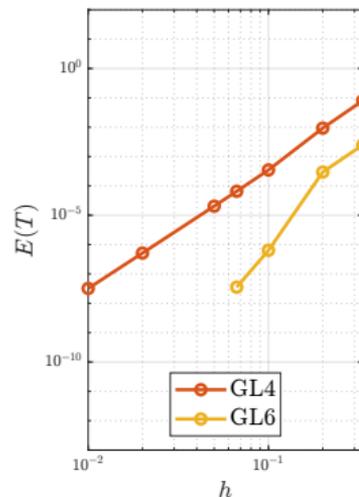
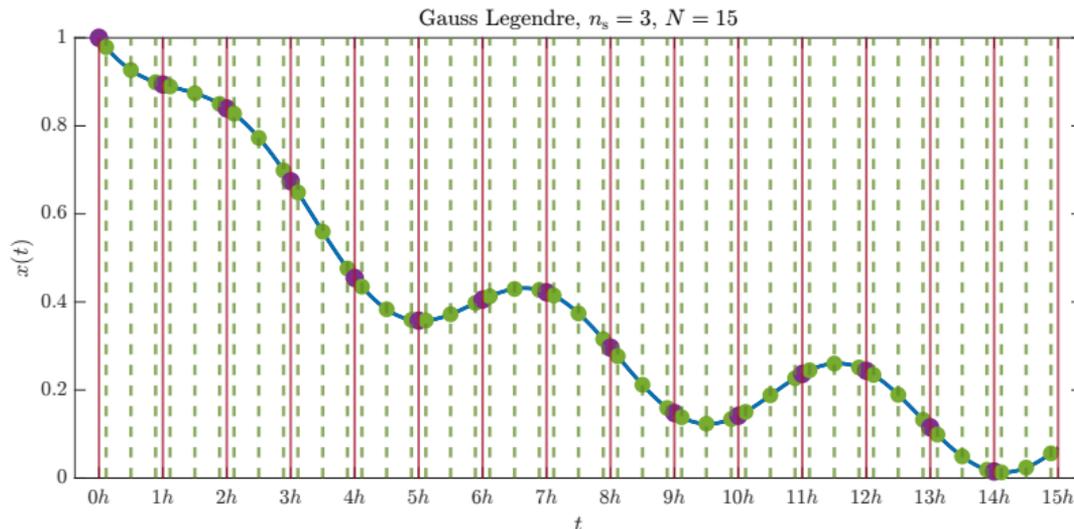
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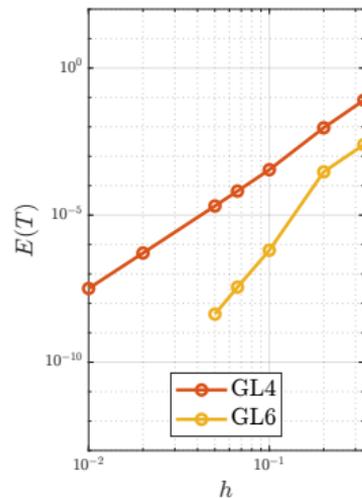
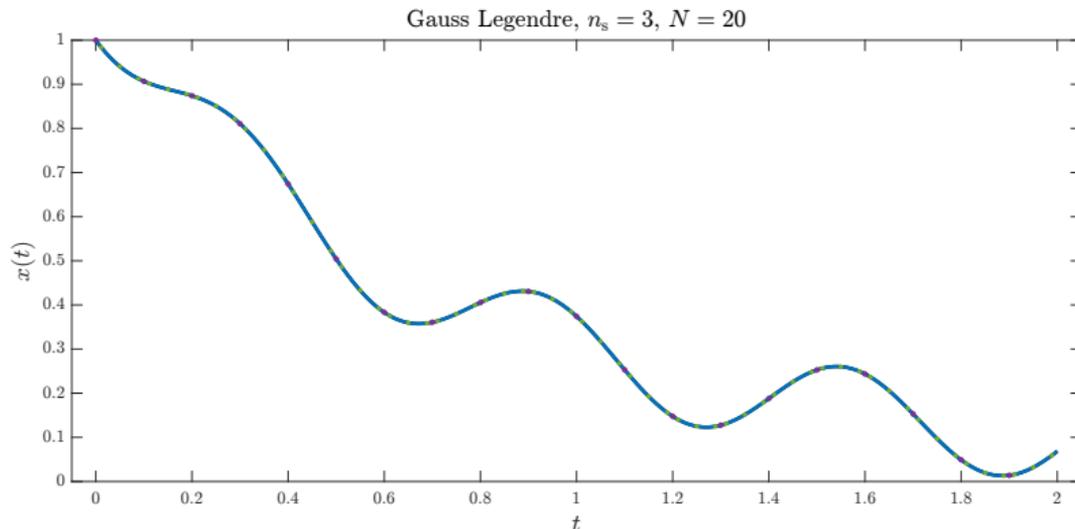
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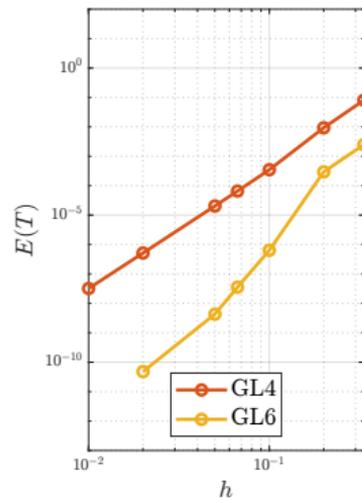
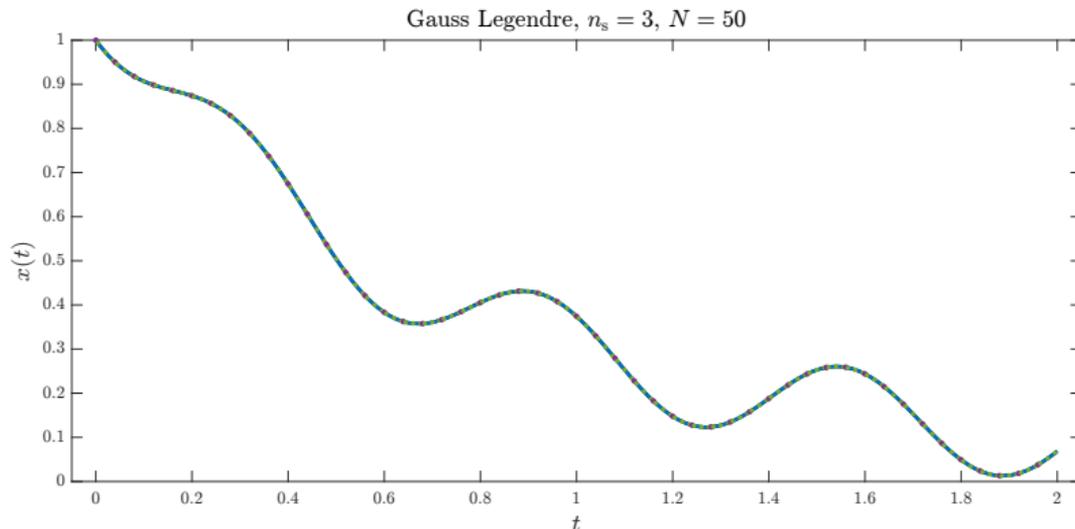
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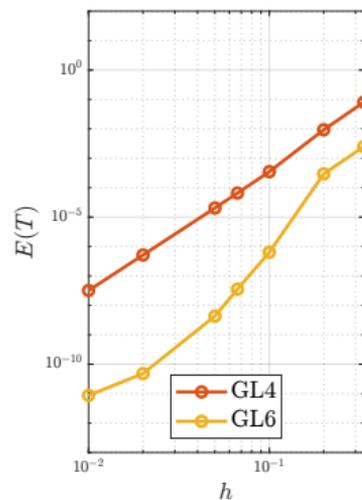
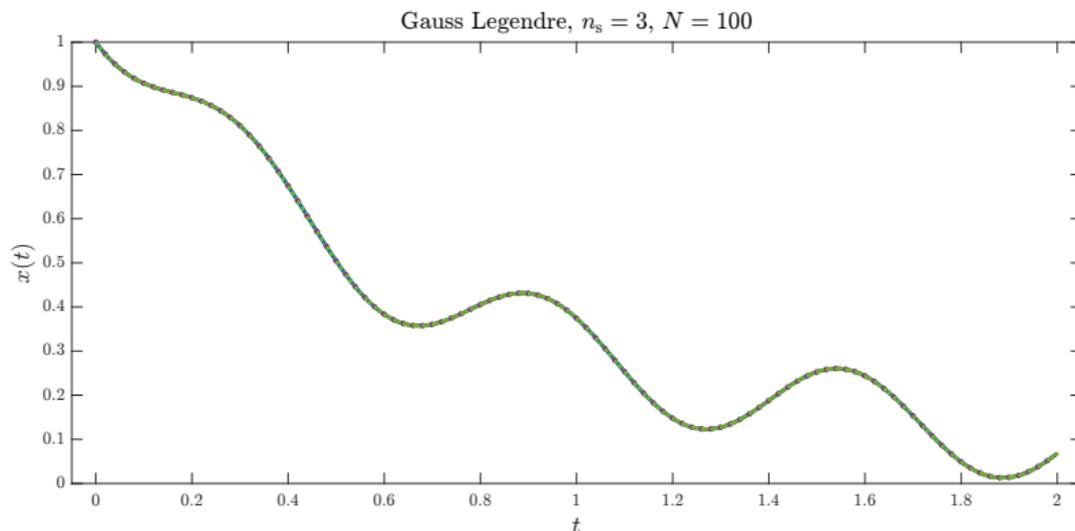
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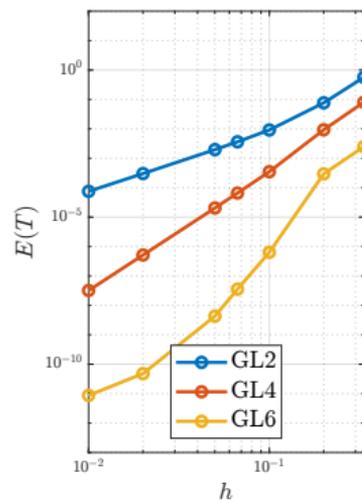
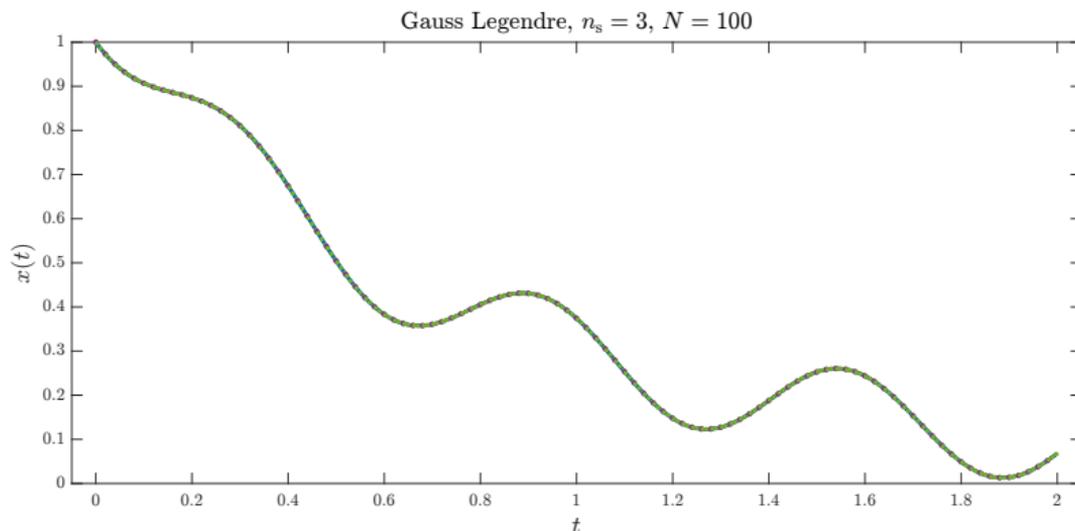
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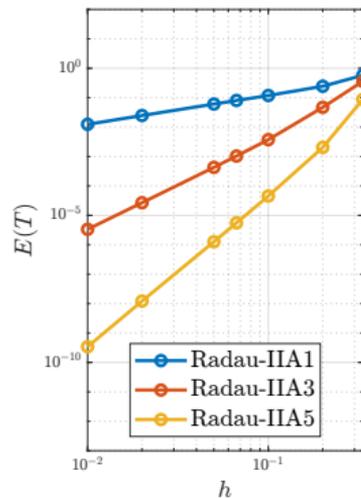
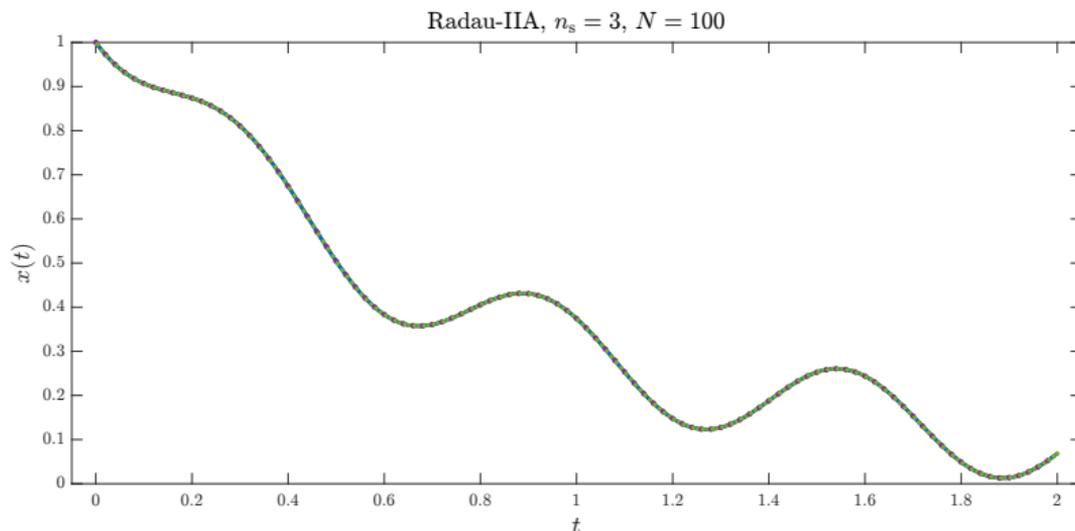
$$\dot{x}(t) = -0.5x(t)^2 - x(t) + \sin(10t), x(0) = 1$$

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$$\dot{x}(t) = -0.5x(t)^2 - x(t) + \sin(10t), x(0) = 1$$

# Outline of the lecture



- 1 Basic definitions
- 2 Runge-Kutta methods
- 3 Collocation methods
- 4 Direct collocation for optimal control

Variables  $x_{n+1} \in \mathbb{R}^{n_x}$  and  $z_n = (k_{n,1}, \dots, k_{n,n_s}) \in \mathbb{R}^{n_s n_x}$

## Collocation equations

$$x_{n+1} = x_n + h \sum_{i=1}^{n_s} k_i b_i \quad (\text{next value})$$

$$k_{n,1} = f(t_n + c_1 h, x_n + h \sum_{j=1}^{n_s} k_{n,j} a_{1,j}, u_n) \quad (\text{stage Eq. 1})$$

$\vdots$

$$k_{n,n_s} = f(t_n + c_{n_s} h, x_n + h \sum_{j=1}^{n_s} k_{n,j} a_{n_s,j}, u_n), \quad (\text{stage Eq. } n_s)$$

# Direct collocation in optimal control

Variables  $x_{n+1} \in \mathbb{R}^{n_x}$  and  $z_n = (k_{n,1}, \dots, k_{n,n_s}) \in \mathbb{R}^{n_s n_x}$

## Collocation equations

$$x_{n+1} = x_n + h \sum_{i=1}^{n_s} k_i b_i \quad (\text{next value})$$

$$0 = k_{n,1} - f(t_n + c_1 h, x_n + h \sum_{j=1}^{n_s} k_{n,j} a_{1,j}, u_n) \quad (\text{stage Eq. 1})$$

$\vdots$

$$0 = k_{n,n_s} - f(t_n + c_{n_s} h, x_n + h \sum_{j=1}^{n_s} k_{n,j} a_{n_s,j}, u_n), \quad (\text{stage Eq. } n_s)$$



Variables  $x_{n+1} \in \mathbb{R}^{n_x}$  and  $z_n = (k_{n,1}, \dots, k_{n,n_s}) \in \mathbb{R}^{n_s n_x}$

## Collocation equations

$$x_{n+1} = x_n + h \sum_{i=1}^{n_s} k_i b_i =: \phi_f(x_n, z_n, u_n) \quad (\text{next value})$$

$$0 = \begin{bmatrix} k_{n,1} - f(t_n + c_1 h, x_n + h \sum_{j=1}^{n_s} k_{n,j} a_{1,j}, u_n) \\ \vdots \\ k_{n,n_s} - f(t_n + c_{n_s} h, x_n + h \sum_{j=1}^{n_s} k_{n,j} a_{n_s,j}, u_n) \end{bmatrix} =: \phi_{\text{int}}(x_n, z_n, u_n) \quad (\text{stage Eqs.})$$

# Direct collocation in optimal control

Variables  $x_{n+1} \in \mathbb{R}^{n_x}$  and  $z_n = (k_{n,1}, \dots, k_{n,n_s}) \in \mathbb{R}^{n_s n_x}$

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$$x_{n+1} = \phi_f(x_n, z_n, u_n) \quad (\text{next value})$$

$$0 = \phi_{\text{int}}(x_n, z_n, u_n) \quad (\text{stage Eqs.})$$

- Use to discretize optimal control problem



## Continuous time OCP

$$\min_{x(\cdot), u(\cdot)} \int_0^T L_c(x(t), u(t)) dt + E(x(T))$$

$$\text{s.t. } x(0) = \bar{x}_0$$

$$\dot{x}(t) = f(x(t), u(t))$$

$$0 \geq h(x(t), u(t)), t \in [0, T]$$

$$0 \geq r(x(T))$$

- ▶ Direct methods: first discretize, then optimize



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- ▶ Direct methods: first discretize, then optimize

1. Parametrize controls, e.g.  
 $u(t) = u_n, t \in [t_n, t_{n+1}]$ .

# Continuous time OCP into Nonlinear Programs (NLP)

## Continuous time OCP

$$\min_{x(\cdot), u(\cdot)} \int_0^T L_c(x(t), u(t)) dt + E(x(T))$$

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- Direct methods: first discretize, then optimize

1. Parametrize controls, e.g.  
 $u(t) = u_n, t \in [t_n, t_{n+1}]$ .
2. Discretize cost and dynamics via collocation

$$L_d(x_n, u_n) = \int_{t_n}^{t_{n+1}} L_c(x(t), u(t)) dt.$$

Replace  $\dot{x} = f(x, u)$  by

$$x_{n+1} = \phi_f(x_n, z_n, u_n),$$

$$0 = \phi_{\text{int}}(x_n, z_n, u_n).$$



## Continuous time OCP

$$\min_{x(\cdot), u(\cdot)} \int_0^T L_c(x(t), u(t)) dt + E(x(T))$$

$$\text{s.t. } x(0) = \bar{x}_0$$

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3. Relax path constraints, e.g., evaluate only at  $t = t_n$

$$0 \geq h(x_n, u_n), n = 0, \dots, N - 1.$$



## Continuous time OCP

$$\begin{aligned} \min_{x(\cdot), u(\cdot)} \quad & \int_0^T L_c(x(t), u(t)) dt + E(x(T)) \\ \text{s.t.} \quad & x(0) = \bar{x}_0 \\ & \dot{x}(t) = f(x(t), u(t)) \\ & 0 \geq h(x(t), u(t)), t \in [0, T] \\ & 0 \geq r(x(T)) \end{aligned}$$

- Direct methods: first discretize, then optimize

## Discrete time OCP (an NLP)

$$\begin{aligned} \min_{\mathbf{x}, \mathbf{z}, \mathbf{u}} \quad & \sum_{k=0}^{N-1} L_d(x_k, u_k) + E(x_N) \\ \text{s.t.} \quad & x_0 = \bar{x}_0 \\ & x_{n+1} = \phi_f(x_n, z_n, u_n) \\ & 0 = \phi_{\text{int}}(x_n, z_n, u_n) \\ & 0 \geq h(x_n, u_n), n = 0, \dots, N-1 \\ & 0 \geq r(x_N) \end{aligned}$$

Variables  $\mathbf{x} = (x_0, \dots, x_N)$ ,  $\mathbf{z} = (z_0, \dots, z_N)$   
and  $\mathbf{u} = (u_0, \dots, u_{N-1})$ .



## Discrete time OCP (an NLP)

$$\min_{\mathbf{x}, \mathbf{z}, \mathbf{u}} \sum_{k=0}^{N-1} L_d(x_k, u_k) + E(x_N)$$

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$$x_{n+1} = \phi_f(x_n, z_n, u_n)$$

$$0 = \phi_{\text{int}}(x_n, z_n, u_n)$$

$$0 \geq h(x_n, u_n), \quad n = 0, \dots, N-1$$

$$0 \geq r(x_N)$$

Variables  $w = (\mathbf{x}, \mathbf{z}, \mathbf{u})$



## Discrete time OCP (an NLP)

$$\begin{aligned} \min_{\mathbf{x}, \mathbf{z}, \mathbf{u}} \quad & \sum_{k=0}^{N-1} L_d(x_k, u_k) + E(x_N) \\ \text{s.t.} \quad & x_0 = \bar{x}_0 \\ & x_{n+1} = \phi_f(x_n, z_n, u_n) \\ & 0 = \phi_{\text{int}}(x_n, z_n, u_n) \\ & 0 \geq h(x_n, u_n), \quad n = 0, \dots, N-1 \\ & 0 \geq r(x_N) \end{aligned}$$

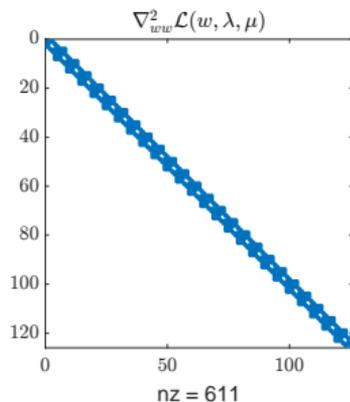
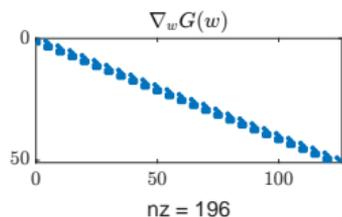
Variables  $w = (\mathbf{x}, \mathbf{z}, \mathbf{u})$

## Nonlinear Program (NLP)

$$\begin{aligned} \min_{w \in \mathbb{R}^{n_x}} \quad & F(w) \\ \text{s.t.} \quad & G(w) = 0 \\ & H(w) \geq 0 \end{aligned}$$

Obtain large and sparse  
NLP

# Direct optimal control methods solve Nonlinear Programs (NLP)



Variables  $w = (\mathbf{x}, \mathbf{z}, \mathbf{u})$

## Nonlinear Program (NLP)

$$\begin{aligned} \min_{w \in \mathbb{R}^{n_x}} \quad & F(w) \\ \text{s.t.} \quad & G(w) = 0 \\ & H(w) \geq 0 \end{aligned}$$

Obtain large and sparse NLP



- ▶ Numerical simulation methods used to solve ODEs approximately.
- ▶ Integration accuracy order and stability play key roles.
- ▶ Collocation methods are implicit Runge-Kutta methods with favorable properties.
- ▶ All collocation methods are IRK methods, the converse is not true.
- ▶ Collocation methods can be used to discretize an OCP into an NLP.
- ▶ Choice of discretization method has huge influence on efficacy and reliability of NLP solution.
- ▶ Best choice is problem dependent and often requires lot of care.
- ▶ Used for practical problems and straightforward to apply.
- ▶ Many good software packages exist.



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