Lecture 6: Explicit Runge-Kutta Methods

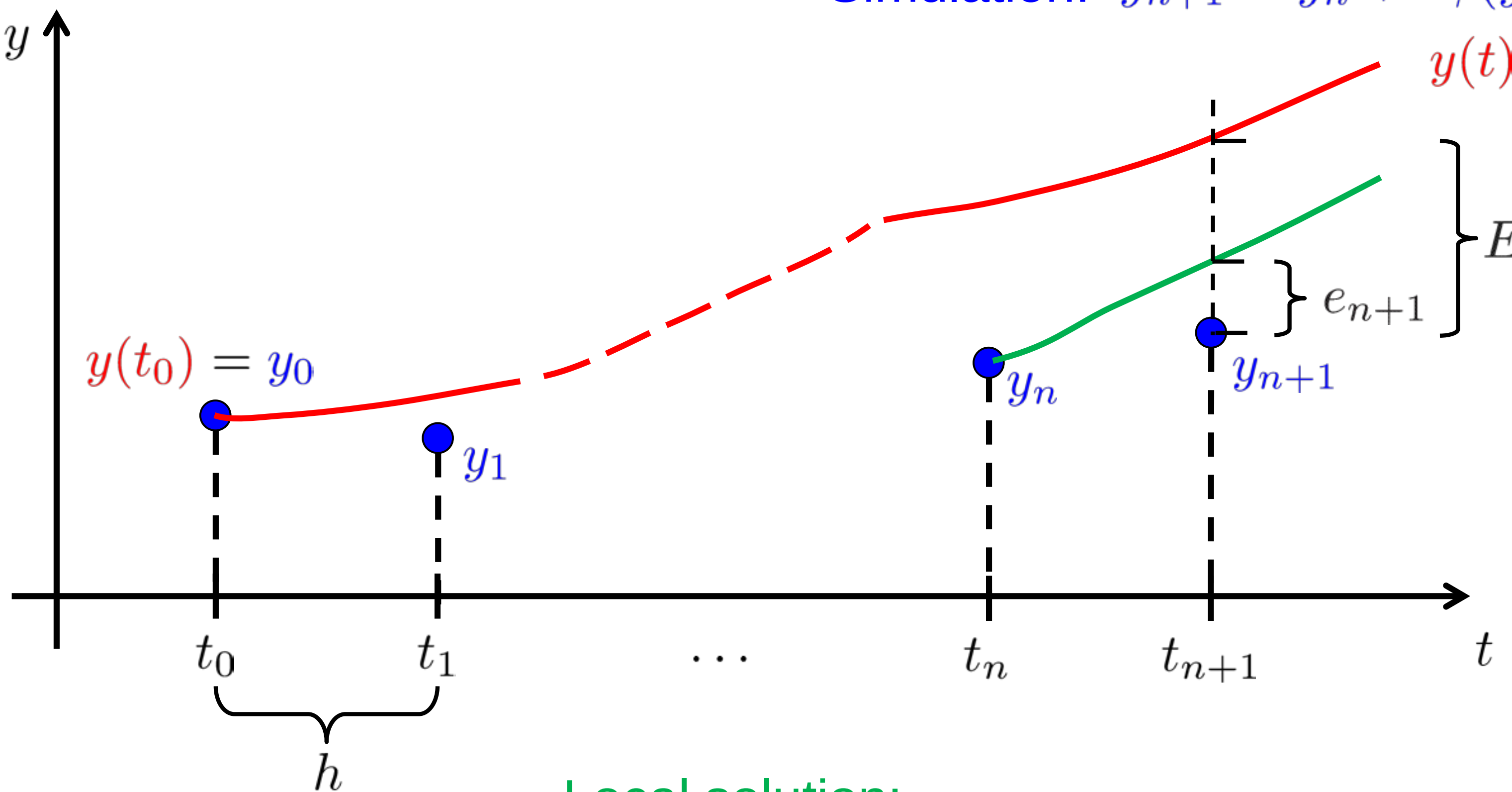
Explicit Runge-Kutta (ERK) methods, and their order and stability

Book: 14.3, 14.4

Recap: Notation

IVP: $\dot{y} = f(y,t), \quad y(t_0) = y_0$

Simulation: $y_{n+1} = y_n + h\phi(y_n, t_n)$



Local solution:

$$\dot{y}_L(t_n;t) = f(y_L(t_n;t),t), \quad y_L(t_n;t_n) = y_n$$

- Local error: $e_{n+1} = y_{n+1} - y_L(t_n;t_{n+1})$
- Global error: $E_{n+1} = y_{n+1} - y(t_{n+1})$
- If local error is $O(h^{p+1})$ then we say method is of order p

Order (accuracy)

- Given IVP:

$$\dot{y} = f(y, t), \quad y(0) = y_0$$

- One-step method:

$$y_{n+1} = y_n + h\phi(y_n, t_n), \quad h = t_{n+1} - t_n$$

- If we can show that

$$y_{n+1} = y_n + hf(y_n, t) + \frac{h^2}{2}\frac{\mathrm{d}f(y_n, t)}{\mathrm{d}t} + \ldots + \frac{h^p}{p!}\frac{\mathrm{d}^{p-1}f(y_n, t)}{\mathrm{d}t^{p-1}} + O(h^{p+1})$$

- Then:
  - Local error is $O(h^{p+1})$
  - Method is order p

Linearization

(14.2.4)

- System $\dot{y} = f(y,t)$, $y = (y_1, \ldots, y_d)^{\mathsf{T}}$
- Linearize around operating point y^*: $\Delta\dot{y} = J\Delta y, \quad J = \left.\frac{\partial f}{\partial y}\right|_{y=y^*}$
- Diagonalize: $Jm_i = \lambda_i m_i, \quad \text{where} \quad \begin{cases} m_i : \text{eigenvectors of } J \\ \lambda_i : \text{eigenvalues of } J \end{cases}$
- Define $q = M^{-1}\Delta y$:

$$\dot{q} = M^{-1}J\Delta y = M^{-1}JMq = \Lambda q, \qquad \Lambda = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_d \end{pmatrix}$$

- That is, $\dot{q}_i = \lambda_i q_i$ from which we can find $\Delta y(t) = Mq = \sum_{i=1}^{d} q_i(t) m_i$

We can study properties of a method used to simulate the system $\Delta\dot{y} = J\Delta y$, by study properties of the method for the systems $\dot{q}_i = \lambda_i q_i, \quad i = 1, \ldots, d$.

Example linearization

- System:

$$\dot{y}_1 = y_2$$
$$\dot{y}_2 = -y_1^3 - c y_2$$

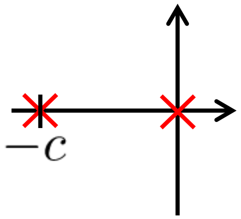
Linearization about $(y_1^*, y_2^*)^\mathsf{T}$:

$$\begin{pmatrix} \Delta\dot{y}_1 \\ \Delta\dot{y}_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -3\left(y_1^*\right)^2 & -c \end{pmatrix} \begin{pmatrix} \Delta y_1 \\ \Delta y_2 \end{pmatrix}$$

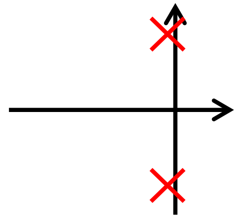
- Eigenvalues:

$$\lambda^2 + c\lambda + 3\left(y_1^*\right) = 0 \qquad \lambda_{1,2} = -\frac{c}{2} \pm \sqrt{\left(\frac{c}{2}\right)^2 - 3\left(y_1^*\right)^2}$$

$$y_1^* = 0: \quad \lambda_1 = 0,\ \lambda_2 = -c$$



$$y_1^* = \text{large}: \quad \lambda_{1,2} \to \pm j\omega_0$$



Test system, stability function

- One step method:

$$y_{n+1} = y_n + h\phi(y_n, t_n)$$

- Apply it to scalar test system:

$$\dot{y} = \lambda y$$

- We get:

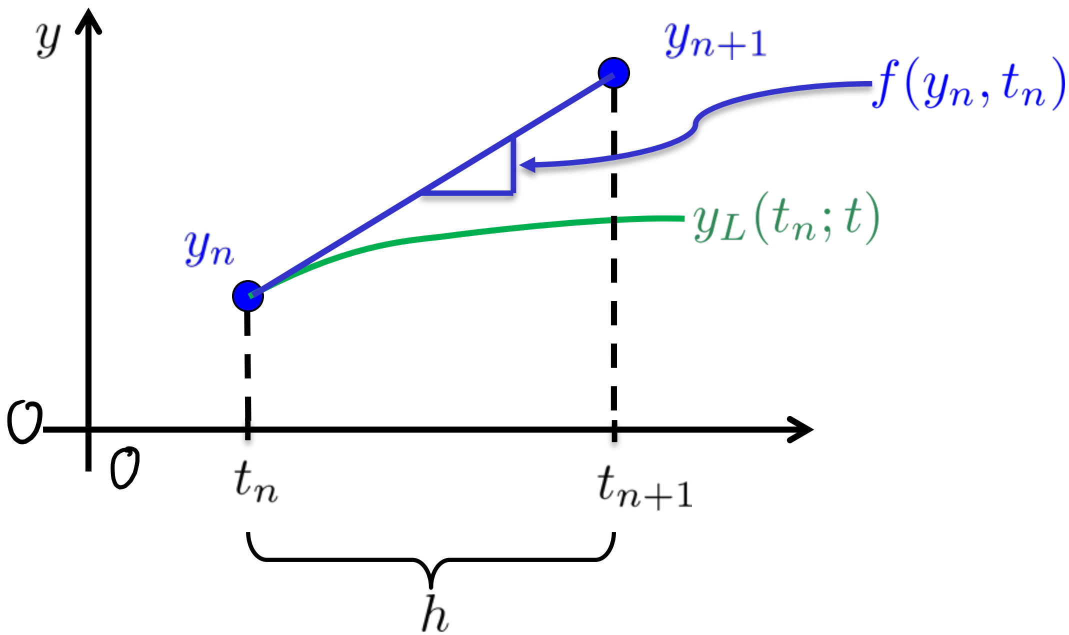
$$y_{n+1} = R(h\lambda)y_n$$

where $R(h\lambda)$ is stability function

- The method is stable (for test system!) if $|y_{n+1}| \leq |y_n|$

$$|R(h\lambda)| \leq 1$$

Simplest method: Euler



- Slope:

$$\frac{y_{n+1} - y_n}{h} = f(y_n, t_n)$$

- Euler's method:

$$y_{n+1} = y_n + hf(y_n, t) + \frac{h^2}{2}\frac{\mathrm{d}f(y_n, t)}{\mathrm{d}t} + \ldots + \frac{h^p}{p!}\frac{\mathrm{d}^{p-1}f(y_n, t)}{\mathrm{d}t^{p-1}} + O(h^{p+1})$$

$e_{n+1} = O(h^2)$

$$y_{n+1} = y_n + hf(y_n, t_n)$$

$\rightarrow$ method $p = 1$

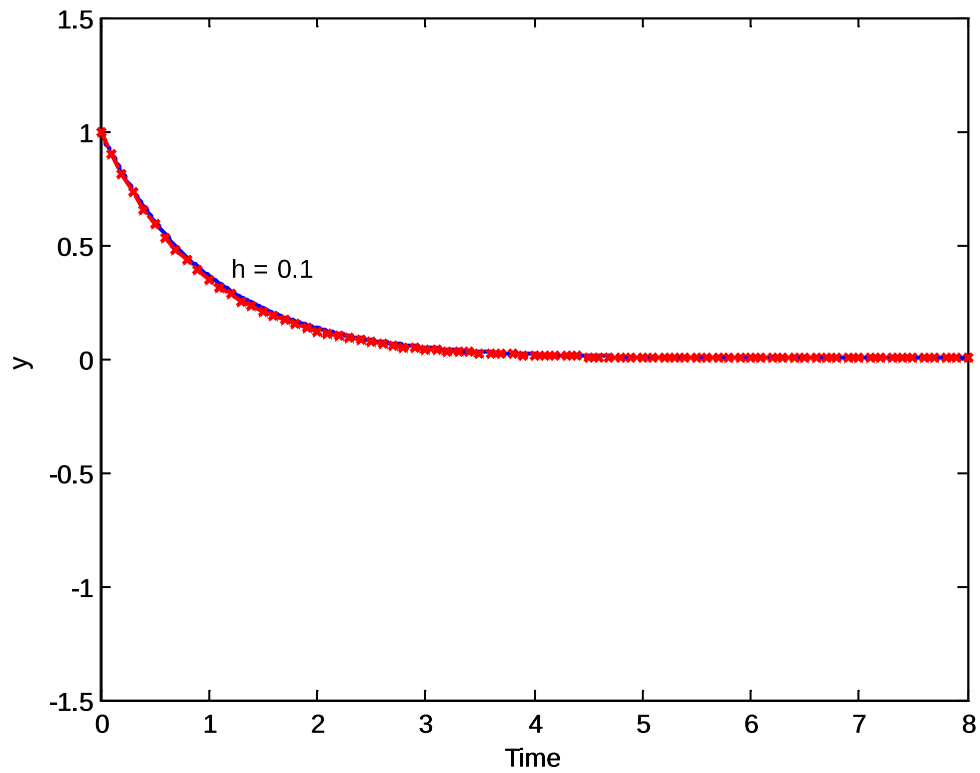
Example Euler's method

ODE: $\dot{y} = -y, \quad y(0) = 1$

Euler simulation: $y_{n+1} = y_n + h\left(-y_n\right), \quad y_0 = 1$

Example, h = 0.1:

n	t_n	y_n
0	0	1
1	0.1	
2	0.2	
3	0.3	
4	0.4	
…	…	…



Example: Euler's method stability

ODE:

$$\dot{y} = -y, \quad y(0) = 1$$

$\lambda = -1$

Euler simulation:

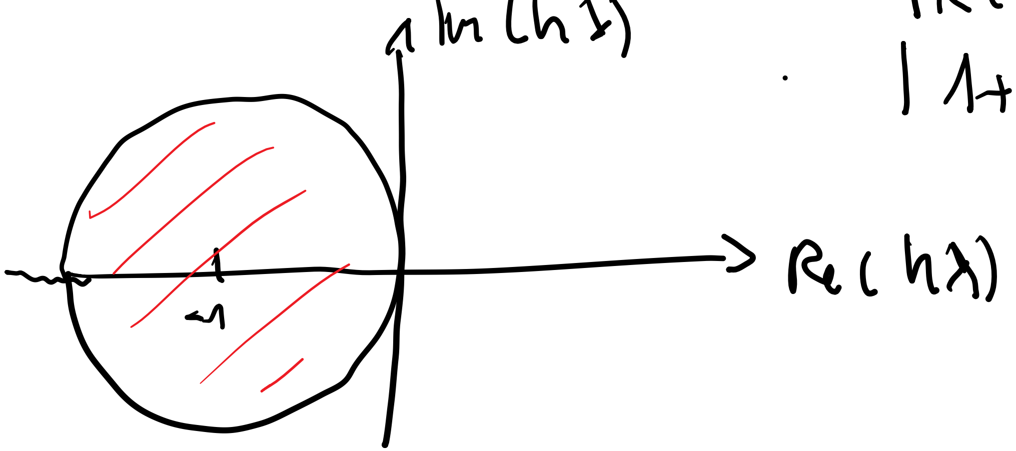
$$y_{n+1} = y_n + h\left(-y_n\right), \quad y_0 = 1$$

Stability of method: $\dot{y} = \lambda y$ (test system)

$$y_{n+1} = y_n + h\lambda y_n = \underbrace{(1 + h\lambda)}_{R(h\lambda)} y_n$$

Method is stable if $|R(h\lambda)| \le 1$

$$|1 + h\lambda| \le 1$$



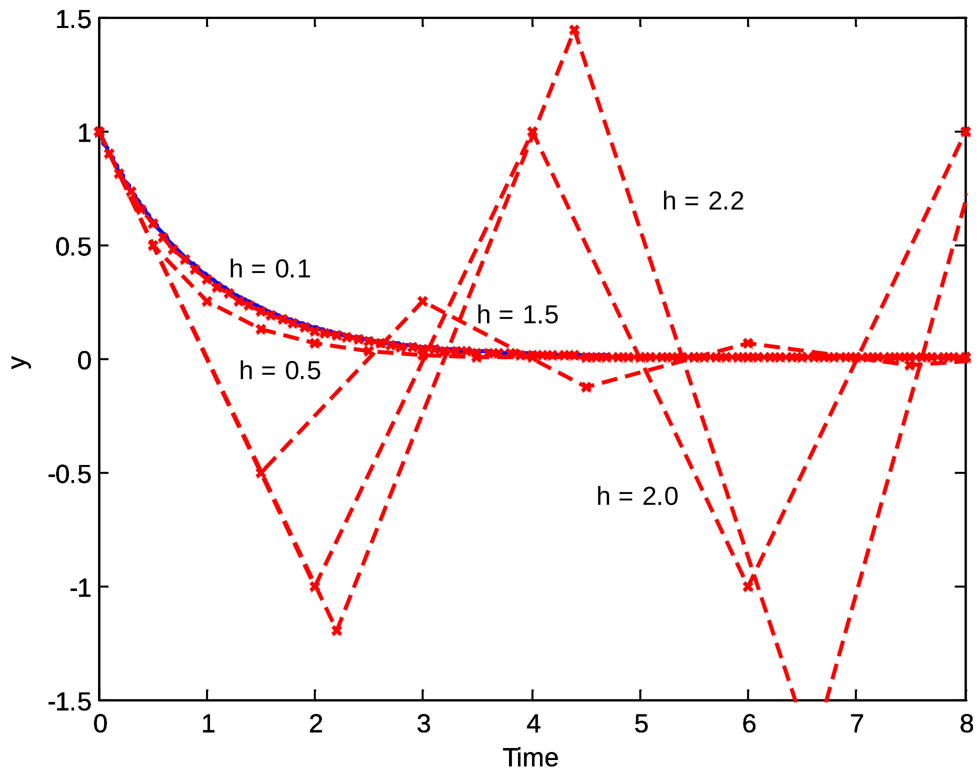
Example Euler's method

$$y_{n+1} = \underbrace{(1 + h\lambda)}_{R(h\lambda)} y_n$$

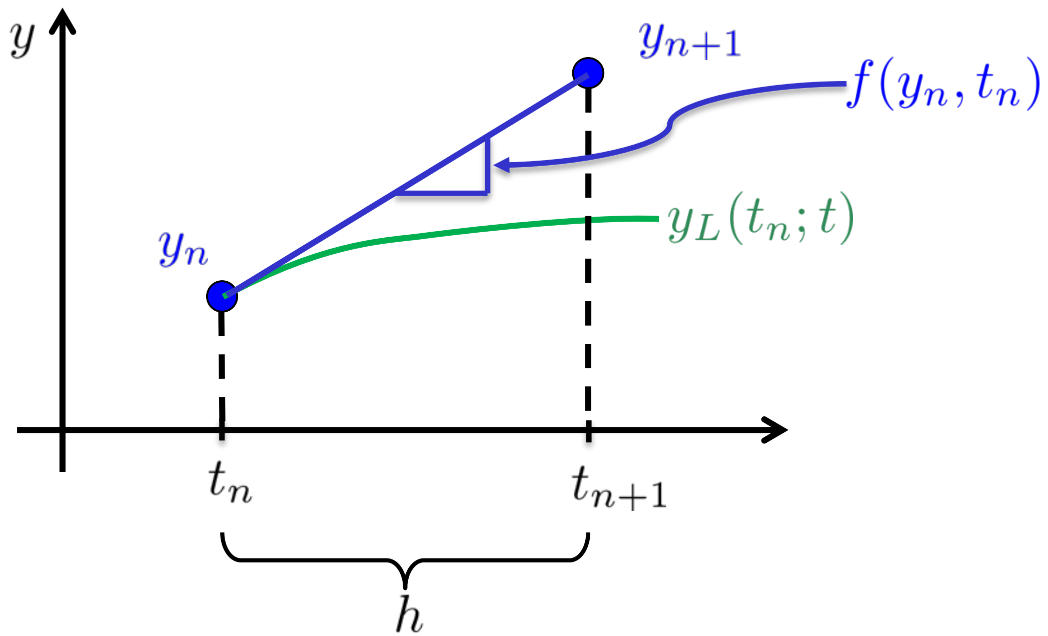
ODE: $\dot{y} = -y, \quad y(0) = 1$

Euler simulation: $y_{n+1} = y_n + h\,(-y_n)\,, \quad y_0 = 1$

Stability: $|R(h\lambda)| = |1 - h| \leq 1 \Rightarrow 0 \leq h \leq 2$



Simplest method: Euler



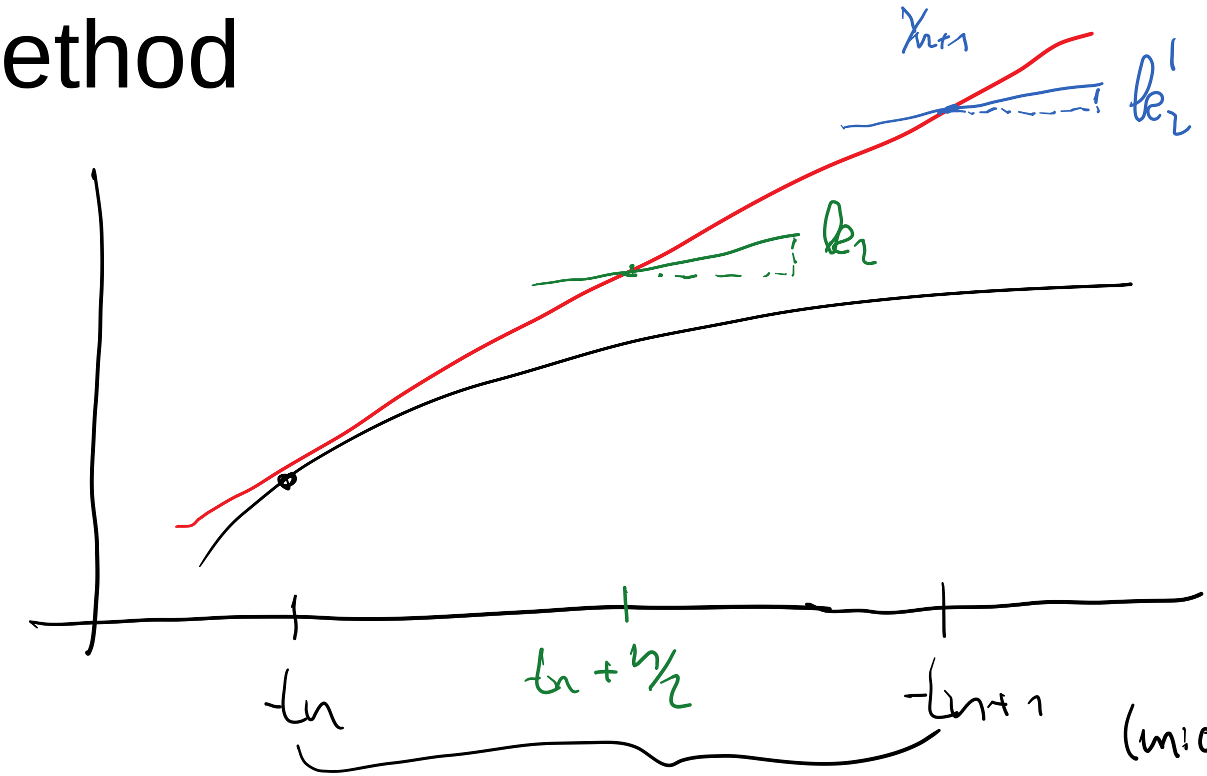
- Slope:

$$\frac{y_{n+1} - y_n}{h} = f(y_n, t_n)$$

- Euler's method:

$$y_{n+1} = y_n + hf(y_n, t_n)$$

Euler method



(midpoint rule)

Improved Euler

$k_1 = f(y_n, t_n)$

$k_2' = f(y_n + h k_1, t_n + h)$

$y_{n+1} = y_n + \frac{h}{2}(k_1 + k_2')$

Modified Euler

$k_1 = f(y_n, t_n)$

$k_2 = f(y_n + \frac{h}{2} k_1, t_n + \frac{h}{2})$

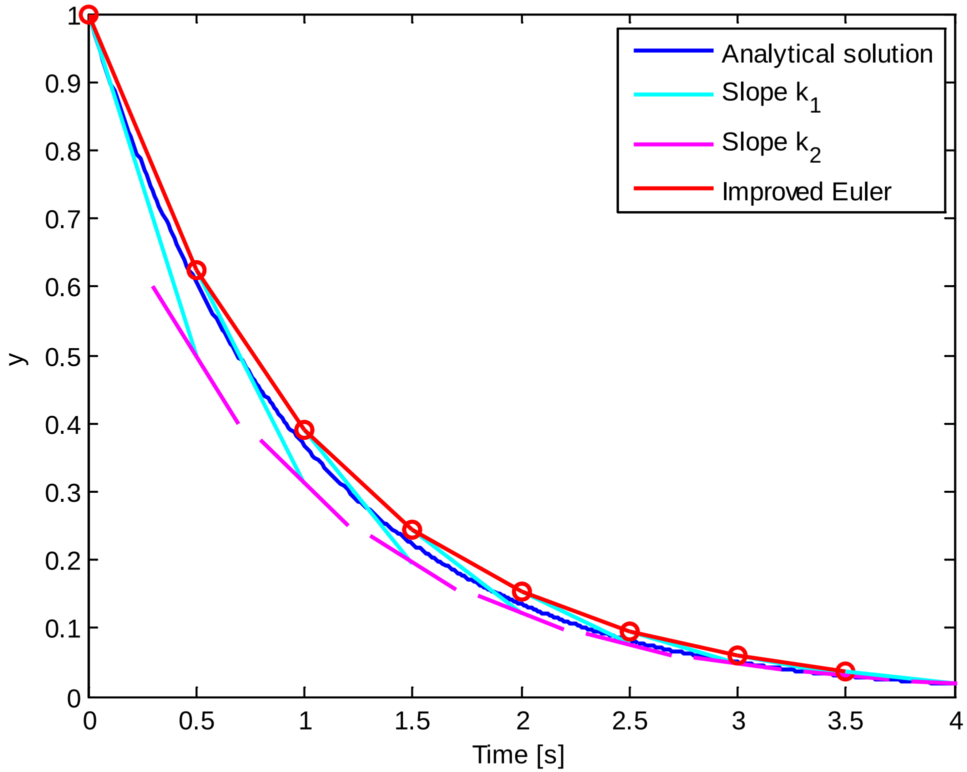
$y_{n+1} = y_n + h k_2$

Improved Euler illustration

$$\dot{y} = -y, \quad y(0) = 1$$

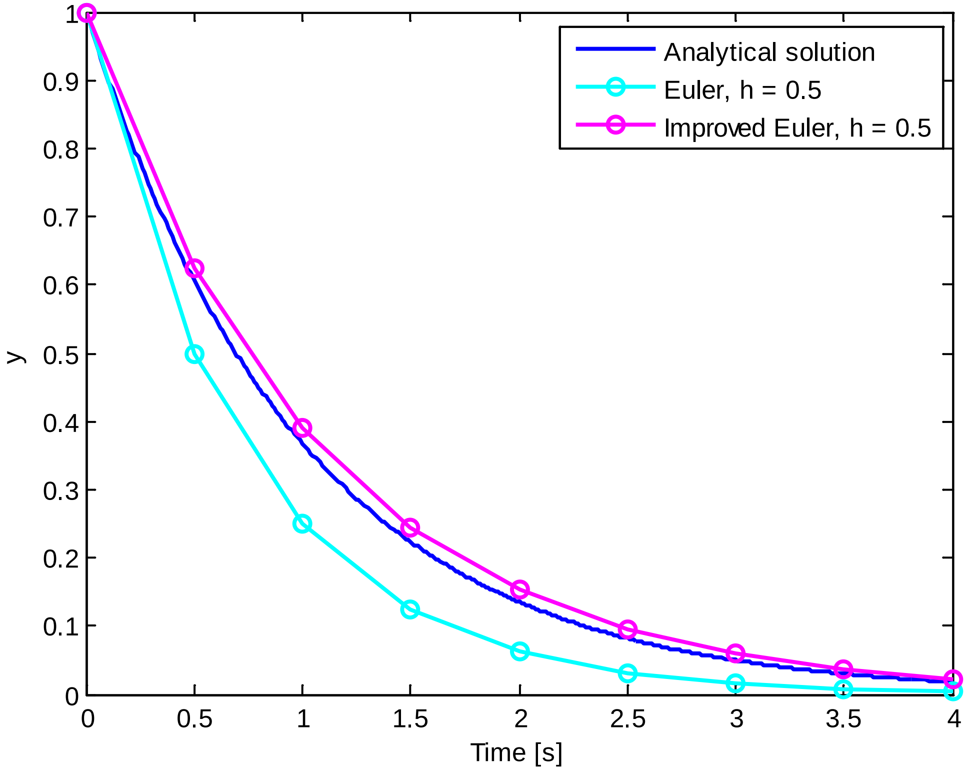
Improved Euler: $k_1 = f(y_n), \quad k_2 = f(y_n + hk_1)$

$$y_{n+1} = y_n + \frac{h}{2}(k_1 + k_2)$$



Improved Euler vs Euler

$$\dot{y} = -y, \quad y(0) = 1$$



Order of improved Euler method

$$k_1 = f(y_n), \quad k_2 = f(y_n + hk_1)$$

$$y_{n+1} = y_n + \frac{h}{2}(k_1 + k_2)$$

- Taylor series expansion of k_2:

$$k_2 = f(y_n, t_n) + h\frac{df(y_n, t_n)}{dt} + \frac{h^2}{2}\frac{d^2 f(y_n, t_n)}{dt^2} + O(h^3)$$

$$y_{n+1} = y_n + hf(y_n, t) + \frac{h^2}{2}\frac{\mathrm{d}f(y_n, t)}{\mathrm{d}t} + \ldots + \frac{h^p}{p!}\frac{\mathrm{d}^{p-1}f(y_n, t)}{\mathrm{d}t^{p-1}} + O(h^{p+1})$$

Order of improved Euler method

$$y_{n+1} = y_n + hf(y_n,t) + \frac{h^2}{2}\frac{\mathrm{d}f(y_n,t)}{\mathrm{d}t} + \ldots + \frac{h^p}{p!}\frac{\mathrm{d}^{p-1}f(y_n,t)}{\mathrm{d}t^{p-1}} + O(h^{p+1})$$

$$y_{n+1} = y_n + \frac{h}{2}\left(k_1 + k_2\right)$$

$$= y_n + \frac{h}{2}\left[f(y_n,t_n) + f(y_n,t_n) + h\frac{df}{dt}(y_n,t_n) + \frac{h^2}{2}\frac{d^2f}{dt^2}(y_n,t_n) + O(h^3)\right]$$

$$= \underbrace{y_n + h f(y_n,t_n)}_{\checkmark} + \underbrace{\frac{h^2}{2}\frac{df}{dt}(y_n,t_n)}_{\checkmark} + \underbrace{\frac{h^3}{4}\frac{d^2f}{dt^2}(y_n,t_n)}_{} + O(h^4)$$

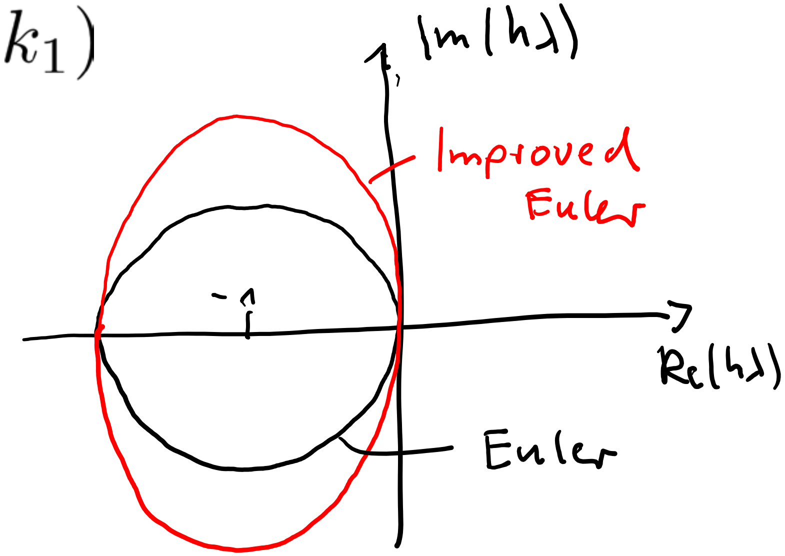
$$\rightarrow e_{n+1} = O(h^3)$$

$\rightarrow$ method is of order 2

Stability of improved Euler method

$$k_1 = f(y_n), \quad k_2 = f(y_n + hk_1)$$

$$y_{n+1} = y_n + \frac{h}{2}(k_1 + k_2)$$



- Test system: $\dot{y} = \lambda y$

$$k_1 = \lambda y_n$$

$$k_2 = \lambda (y_n + h\lambda y_n)$$

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

$$= \underbrace{\left(1 + h\lambda + \frac{(h\lambda)^2}{2}\right)}_{R(h\lambda)} y_n$$

Stable : $\left|1 + h\lambda + \frac{(h\lambda)^2}{2}\right| \leq 1$

Accuracy and stability

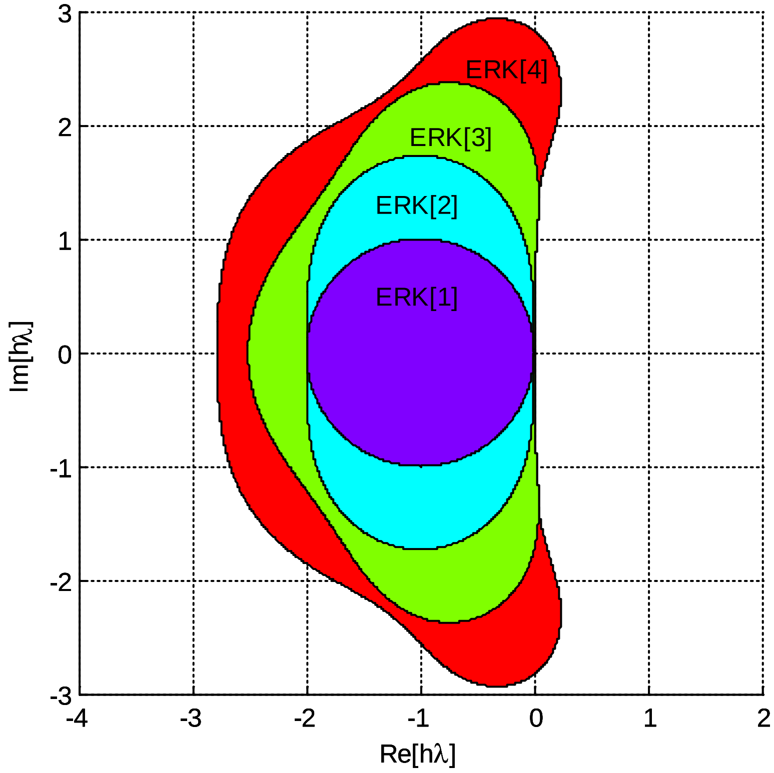
- Lots of different methods, with different complexity. How to quantify their behaviour?

- Two aspects are important: accuracy and numerical stability.
  - Accuracy: How does the local error vary with step-size?
  - Numerical stability: How to avoid that the simulation diverges?

- What decides accuracy and numerical stability?
  - Accuracy: Method and choice of step-size
  - Stability: Method, system eigenvalues, and choice of step-size

- Why are we interested in both accuracy and numerical stability?
  - We always need stability, but stability not enough: Many stable methods are not very accurate!

Stability regions for ERK methods



Explicit Runge-Kutta method I

$$\dot{y} = f(y,t) \qquad y(t_0) = y_0$$

ERK method with σ-steps

$$k_1 = f(y_n, t_n)$$

$$k_2 = f(y_n + h a_{21} k_1 , t_n + c_2 h)$$

$$k_3 = f(y_n + h a_{31} k_1 + h a_{32} k_2 , t_n + c_3 h)$$

$$\vdots$$

$$k_\sigma = f(y_n + h a_{\sigma 1} k_1 + \dots + a_{\sigma \sigma-1} k_{\sigma-1} , t_n + c_\sigma h)$$

$$y_{n+1} = y_n + h (b_1 k_1 + \dots + b_\sigma k_\sigma)$$

c_i $\quad 0 \leq c_i \leq 1$, $\quad c_1 \leq c_2 \leq \dots \leq c_\sigma$ } interpolation parameter

a_{ij} , $\quad \sum_{j=1}^{i-1} a_{ij} = c_i \leq 1$ $\quad$ weighting parameters of stage i

b_i , $\quad \sum_{i=1}^{\sigma} b_i = 1$ $\quad$ weighting parameters of solution

Explicit Runge-Kutta method II

Butcher array

$$
\begin{array}{c|cccccc}
0 & 0 & 0 & \cdots & & 0 & 0 \\
c_2 & a_{21} & 0 & & & & \\
\vdots & \vdots & & \ddots & & & \\
c_\sigma & a_{\sigma 1} & a_{\sigma 2} & \cdots & & a_{\sigma \sigma-1} & 0 \\
\hline
 & b_1 & b_2 & \cdots & & b_{\sigma-1} & b_\sigma
\end{array}
\quad = \quad
\begin{array}{c|c}
c & A \\
\hline
 & b^T
\end{array}
$$

$A \to$ singular for ERK

Butcher array: Examples

1. Explicit Euler:

$$k_1 = f(y_n, t_n)$$
$$y_{n+1} = y_n + hk_1$$

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

2. Improved Euler:

$$k_1 = f(y_n, t_n)$$
$$k_2 = f(y_n + hk_1, t_n + h)$$
$$y_{n+1} = y_n + {}^{h}\!/_{2}(k_1 + k_2)$$

3. Heun's method:

$$k_1 = f(y_n, t_n)$$
$$k_2 = f(y_n + {}^{1}\!/_{3}hk_1, t_n + {}^{1}\!/_{3}h)$$
$$k_3 = f(y_n + {}^{2}\!/_{3}hk_2, t_n + {}^{2}\!/_{3}h)$$
$$y_{n+1} = y_n + {}^{1}\!/_{4}hk_1 + {}^{3}\!/_{4}hk_3$$

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 1/3 & 1/3 & 0 & 0 \\ 2/3 & 0 & 2/3 & 0 \\ \hline & 1/4 & 0 & 3/4 \end{array}$$

Butch array: Try yourself

- Write down the equations of the method!

- ERK 4:

0	0	0	0	0
$1/2$	$1/2$	0	0	0
$1/2$	0	$1/2$	0	0
1	0	0	1	0
0	$1/6$	$1/3$	$1/3$	$1/6$

$k_1 \stackrel{?}{=}$

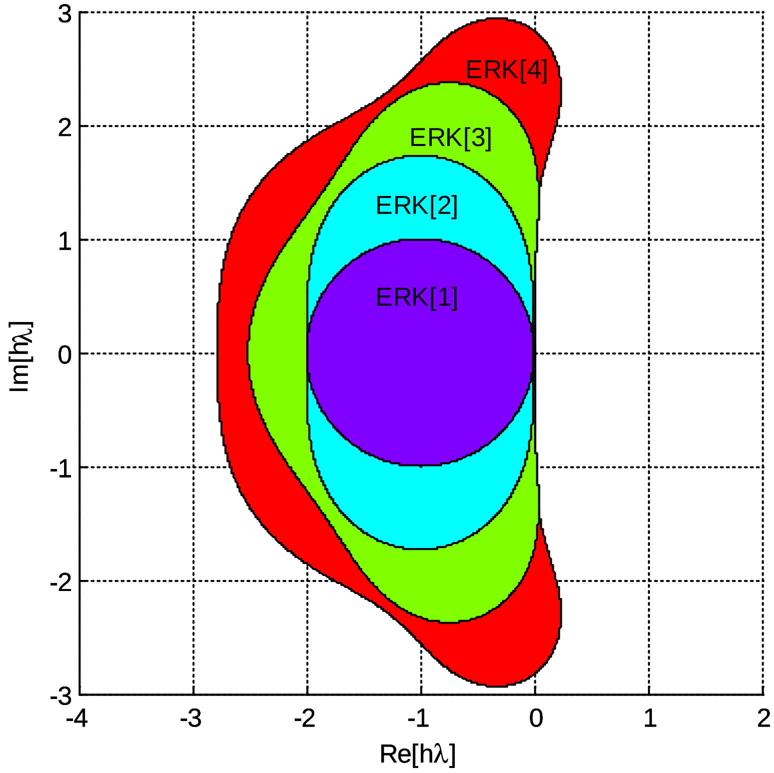
$k_2 \stackrel{?}{=}$

$k_3 \stackrel{?}{=}$

$k_4 \stackrel{?}{=}$

$y_{n+1} \stackrel{?}{=}$

Stability regions for ERK methods



Stability of ERK I

Test function $\dot{y} = \lambda y$

$$k_1 = \lambda y_n$$

$$k_2 = \lambda \left(y_n + h a_{21} k_1 \right)$$

$$\vdots$$

$$k_\sigma = \lambda \left(y_n + h \left(a_{\sigma 1} k_1 + \dots + a_{\sigma \sigma-1} k_{\sigma-1} \right) \right)$$

$$K = \begin{pmatrix} k_1 \\ \vdots \\ k_\sigma \end{pmatrix} \qquad \mathbb{I} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

Then :

$$K = \lambda \left(\mathbb{I} y_n + h A K \right)$$

$$y_{n+1} = y_n + h b^T K$$

Stability of ERK II

solve for k

$$(I - h\lambda A)\, k = \lambda \mathbb{1}\, y_n$$

$$k = (I - h\lambda A)^{-1} \lambda \mathbb{1}\, y_n$$

$$y_{n+1} = y_n + h b^T (I - h\lambda A)^{-1} \lambda \mathbb{1}\, y_n$$

$$R(h\lambda) = 1 + \lambda h b^T (I - h\lambda A)^{-1} \mathbb{1}$$

Stability of ERK III

$$(I - h\lambda A)\kappa = \lambda \mathbf{1} y_n$$
$$y_{n+1} = y_n + h b^T \kappa$$

$$\begin{pmatrix} I - h\lambda A & 0 \\ -hb^T & 1 \end{pmatrix} \begin{pmatrix} \kappa \\ y_{n+1} \end{pmatrix} = \begin{pmatrix} \lambda \mathbb{1} y_n \\ y_n \end{pmatrix}$$

Cramers rule : $Ax = b \Rightarrow x_i = \dfrac{\det(A_i)}{\det(A)}$

A_i : A with column i replaced by b

$$A_i = \begin{pmatrix} I - h\lambda A & \lambda \mathbb{1} y_n \\ -hb^T & y_n \end{pmatrix} \qquad A = \begin{pmatrix} I - h\lambda A & 0 \\ -hb^T & 1 \end{pmatrix}$$

$$\Rightarrow y_{n+1} = \underbrace{\frac{\det(I - h\lambda(A - \mathbb{1} b^T))}{\det(I - h\lambda A)}}_{R(h\lambda)} \cdot y_n$$

Stability of ERK IV

$$\text{ERK}: \quad \det(I - h\lambda A) = \det\begin{pmatrix} 1 & & & 0 \\ \times & 1 & & \\ \times & \times & \ddots & \\ \times & \times & & 1 \end{pmatrix}$$

$$\underline{= 1}$$

$$\rightarrow R_E(h\lambda) = \det\left(I - h\lambda\left(A - \mathbb{1} b^T\right)\right)$$

Observe:

1) $|R_E(h\lambda)| \to \infty$ if $|\lambda h| \to \infty$

2) $R_E(h\lambda)$ polynominal λh of order less or equal to σ

Homework

- Write the Butcher array for the improved Euler method (Slide 24)
- Write down the equations of the ERK4 method on slide 25.

- For Monday: Read 14.12 (only until 14.12.1)

- For Thursday: Read 14.5

Next lecture …

Fact: For $1 \leq \sigma \leq 4$, one can devise ERK methods with order $p = \sigma$

- For these methods, per definition

$$y_{n+1} = y_n + hf(y_n, t_n) + \ldots + \frac{h^p}{p!}\frac{\mathrm{d}^{p-1}}{\mathrm{d}t^{p-1}} f(y_n, t_n) + O(h^{p+1})$$

- For test system $\dot{y} = \lambda y$,

$$\begin{aligned} y_{n+1} &= y_n + h\lambda y_n + \ldots + \frac{h^p \lambda^p}{p!} y_n + O(h^{p+1}) \\ &= \left(1 + h\lambda + \ldots + \frac{h^p \lambda^p}{p!}\right) y_n + O(h^{p+1}) \end{aligned}$$

- From before, we know that $y_{n+1} = R_E(h\lambda) y_n$, where $R_E(h\lambda)$ is polynomial of degree less than or equal to $\sigma = p$

That is: For ERK methods with order $p = \sigma$, for $\sigma \leq 4$:

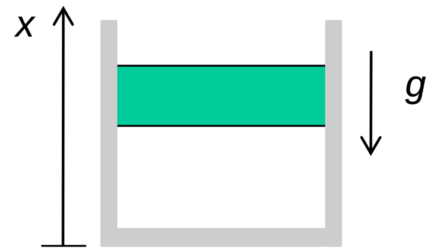
$$R_E(h\lambda) = 1 + h\lambda + \ldots + \frac{h^p \lambda^p}{p!}$$

Case: Pneumatic spring

- Model from Newton's 2nd law:

$$\ddot{x} + g(1 - x^{-\kappa}) = 0$$

  "mass-spring-damper with nonlinear spring and no damping"



- On states-space form $\dot{y} = f(y, t)$

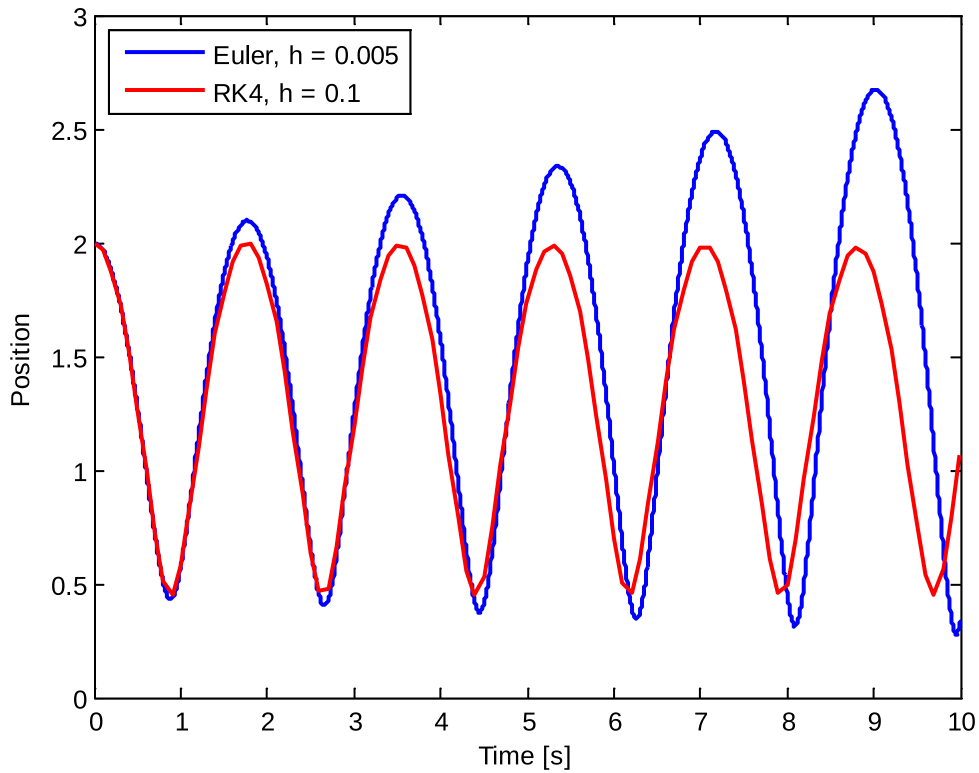
$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \end{pmatrix} = \begin{pmatrix} y_2 \\ -g(1 - y_1^{-\kappa}) \end{pmatrix}$$

- Linearization about equilibrium ($y_1 = 1$) :

$$\frac{\partial f}{\partial y} = \begin{pmatrix} 0 & 1 \\ -g\kappa & 0 \end{pmatrix}, \qquad \lambda_{1,2} = \pm j\omega_0, \quad \omega_0 = \sqrt{g\kappa} \approx 3.7$$

Simulation

Euler: 2000 function evaluations
RK4: 400 function evaluations



- Stability, RK4
  - Theoretical: $\omega_0 h \approx 2.83 \quad \Rightarrow \quad h \approx 0.76$
  - Practically: $h \approx 0.52$

Accuracy: Energy should be constant