

# Lecture 7: Implicit Runge-Kutta Methods

- Recap Explicit Runge-Kutta (ERK) methods
- Stiff systems
- Implicit Runge-Kutta (IRK) ODE solvers

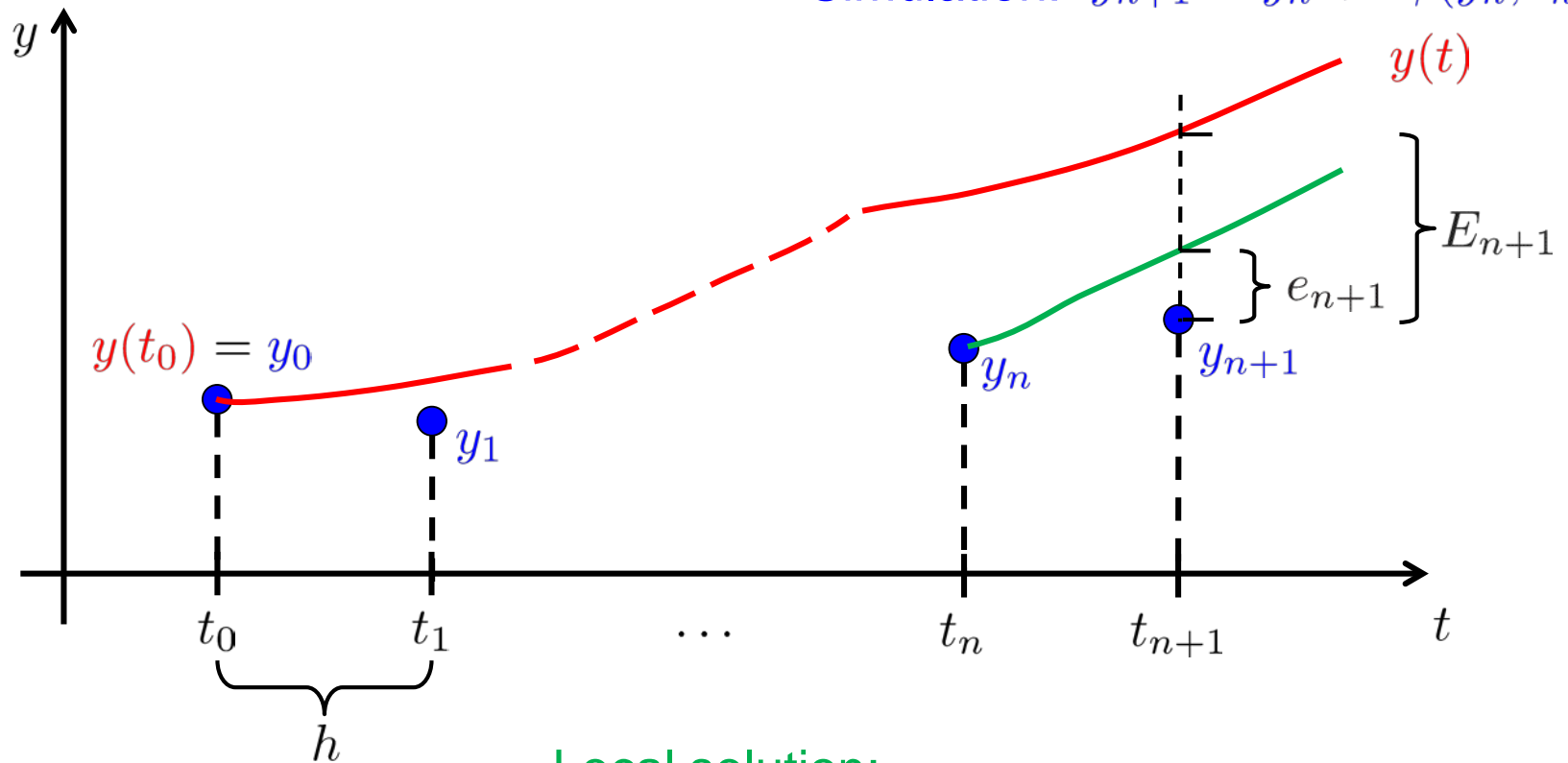
Book: 14.5 (+ 14.8.1)

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# 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  $p$

# Recap: Explicit Runge-Kutta (ERK) methods

- IVP:  $\dot{y} = f(y, t), \quad y(0) = y_0$
- One-step methods:  $y_{n+1} = y_n + h\phi(y_n, t_n), \quad h = t_{n+1} - t_n$
- ERK:
 
$$\begin{aligned}
 k_1 &= f(y_n, t_n) \\
 k_2 &= f(y_n + ha_{21}k_1, t_n + c_2h) \\
 k_3 &= f(y_n + h(a_{31}k_1 + a_{32}k_2), t_n + c_3h) \\
 &\vdots \\
 k_\sigma &= f(y_n + h(a_{\sigma,1}k_1 + a_{\sigma,2}k_2 + \dots + a_{\sigma,\sigma-1}k_{\sigma-1}), t_n + c_\sigma h) \\
 y_{n+1} &= y_n + h(b_1k_1 + b_2k_2 + \dots + b_\sigma k_\sigma)
 \end{aligned}$$

- Butcher array:

<b>c</b>	<b>A</b>				
	<b>b<sup>T</sup></b>				
0					
c <sub>2</sub>	a <sub>21</sub>				
c <sub>3</sub>	a <sub>31</sub>	a <sub>32</sub>			
⋮	⋮	⋮	⋱		
c <sub>σ</sub>	a <sub>σ,1</sub>	a <sub>σ,2</sub>	⋯	a <sub>σ,σ-1</sub>	
	b <sub>1</sub>	b <sub>2</sub>	⋯	b <sub>σ-1</sub>	b <sub>σ</sub>

# Recap: 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

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

# Stability function for RK-methods

- Two alternative, equivalent expressions can be derived:

- Either

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

- or

$$R(h\lambda) = \frac{\det [\mathbf{I} - h\lambda (\mathbf{A} - \mathbf{1b}^T)]}{\det [\mathbf{I} - h\lambda \mathbf{A}]}$$

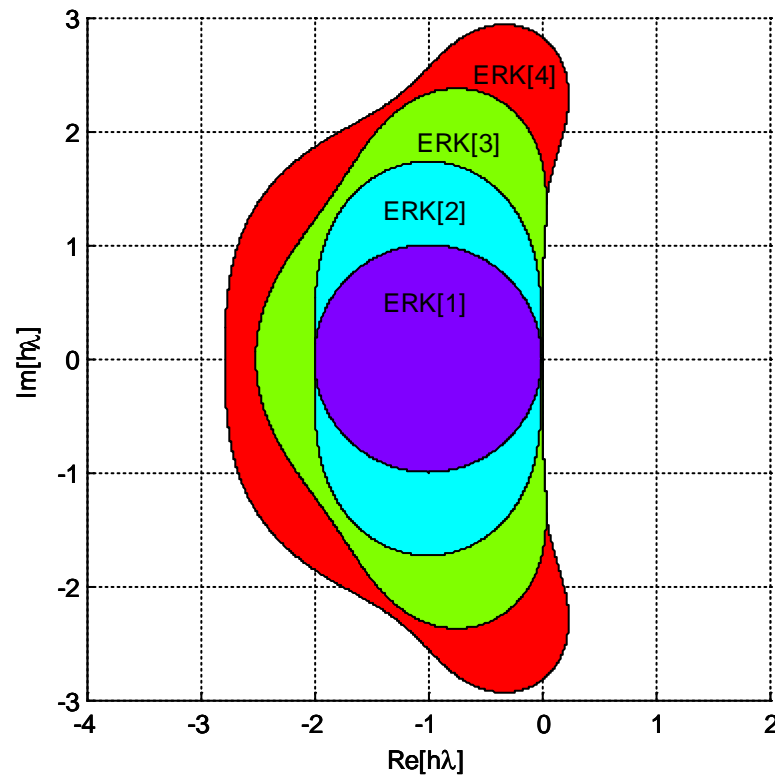
- The latter can be simplified for ERK (since A is lower triangular):

$$R_E(h\lambda) = \det [\mathbf{I} - h\lambda (\mathbf{A} - \mathbf{1b}^T)]$$

- Two observations can be made

1.  $|R_E(h\lambda)|$  will tend to infinity when  $h\lambda$  goes to infinity.
2.  $R_E(h\lambda)$  is a polynomial in  $h\lambda$  of order less than or equal to  $\sigma$ .

# Stability regions for ERK methods



# Order and stages

- For number of stages less than or equal to 4 it is possible to develop ERK methods (**find combinations of  $a_{ij}$ ,  $c_i$ ,  $b_i$** ) with order equal to number of stages. **These are the ones that are used.**

- These methods have stability function of the type

$$R_E(h\lambda) = 1 + h\lambda + \frac{(h\lambda)^2}{2} + \dots + \frac{(h\lambda)^p}{p!}$$

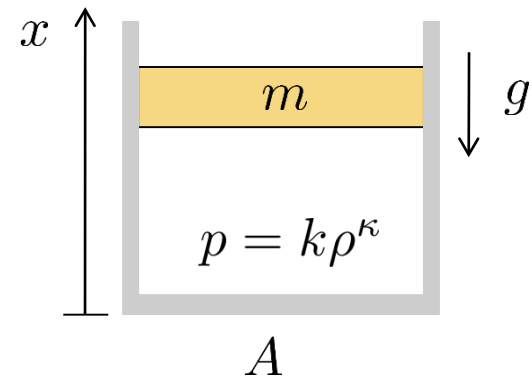
- To obtain higher order, requires more stages:
  - Order 5 requires 6 stages
  - Order 6 requires 7 stages
  - Order 7 requires 9 stages
  - Order 8 requires 11 stages
  - ...

# ERK example: Pneumatic spring

- Model from Newton's 2nd law:

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

"mass-spring-damper with nonlinear spring"



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

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

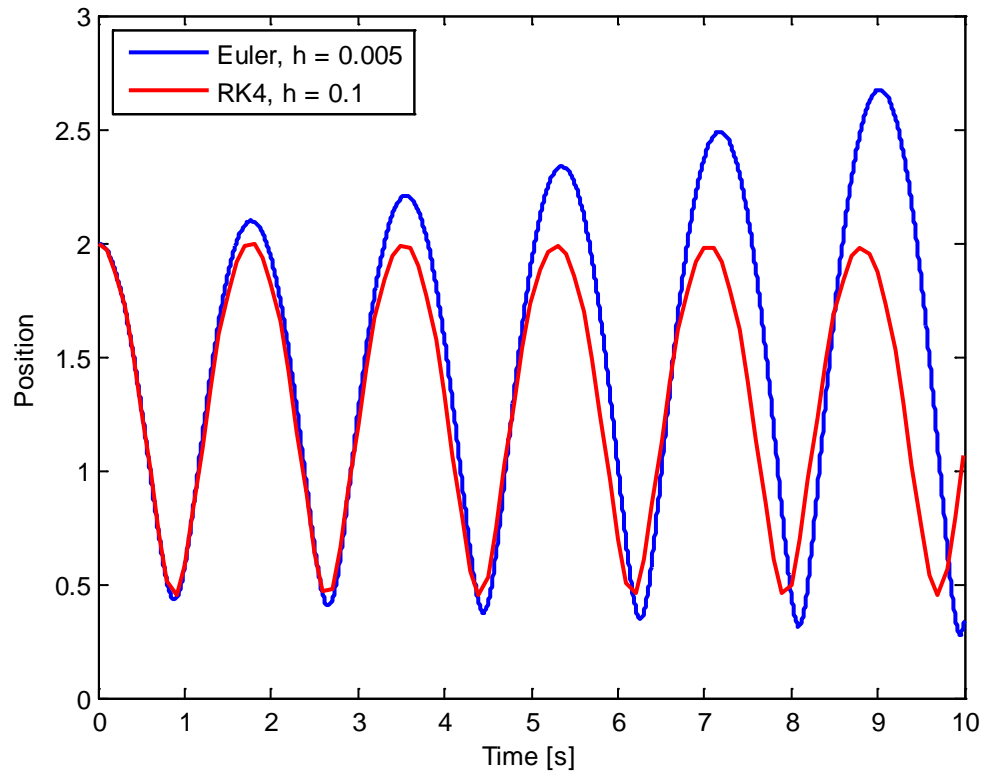
- Linearization about equilibrium ( $y_1 = 1$ ):

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



# Simulation

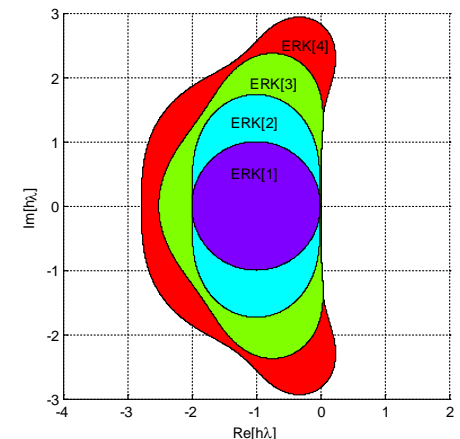
Euler: 2000 function evaluations  
RK4: 400 function evaluations



- Stability, RK4

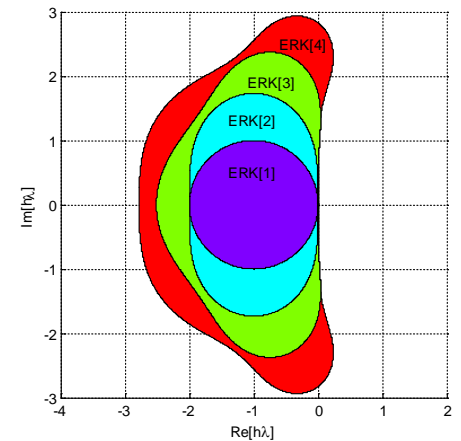
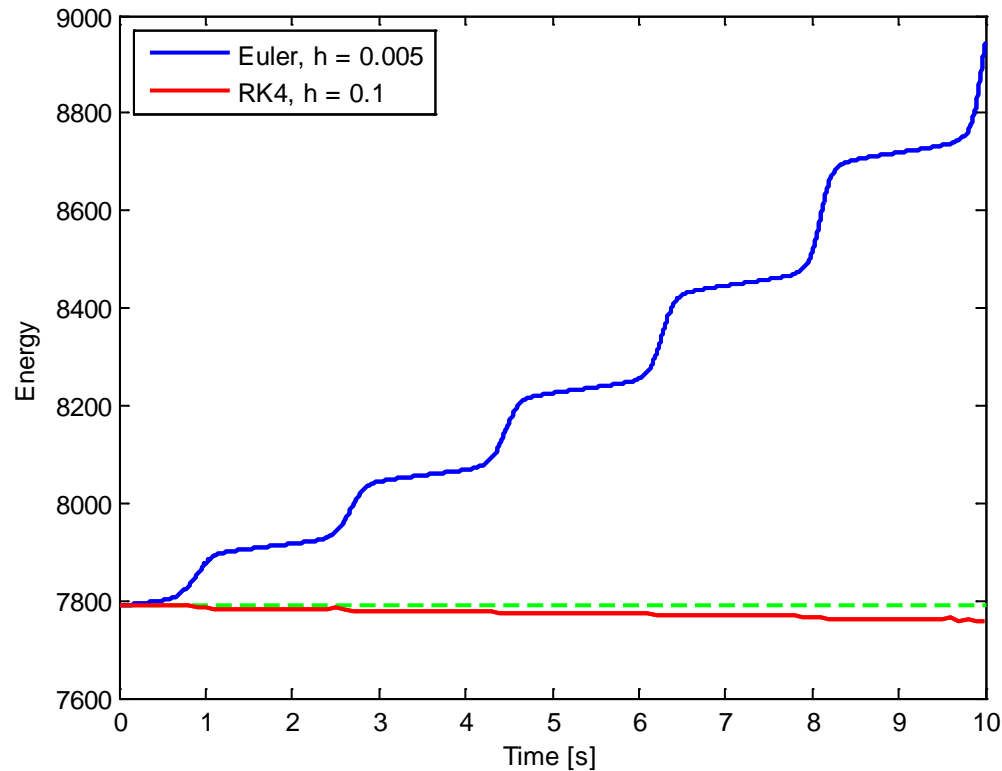
- Theoretical:  $\omega_0 h \approx 2.83 \Rightarrow h \approx 0.76$

- Practically:  $h \approx 0.52$



# Pneumatic spring: Accuracy

- Energy should be constant



# Kahoot

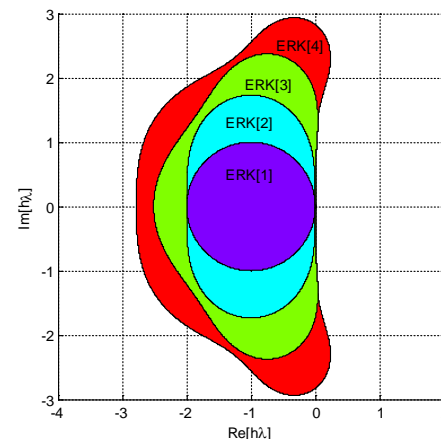
- <https://play.kahoot.it/#/k/5919b1ba-e564-400e-b63e-d9b2d3fa75cc>

# Motivation: Implicit RK

Example :

$$\dot{y}_1 = -y_1$$

$$\dot{y}_2 = -10^6 y_2$$



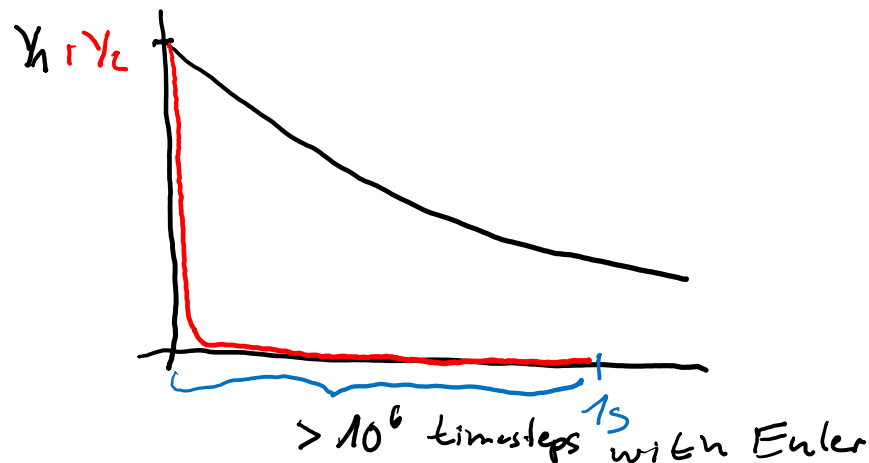
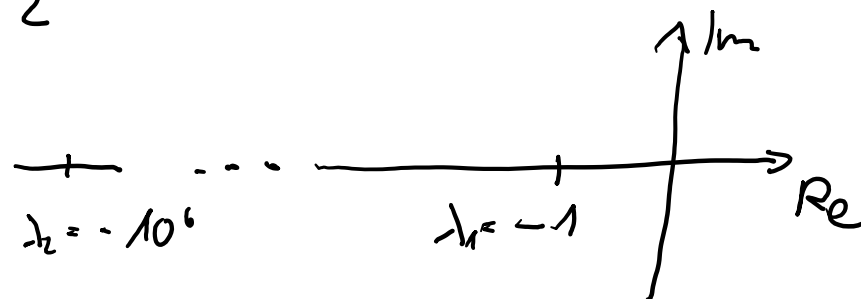
stability condition Euler :  $h|\lambda| \leq 2$

$$\lambda_1 \rightarrow h \leq 2$$

$$\lambda_2 \rightarrow h \leq 2 \cdot 10^{-6}$$

We have to choose

$$h < 2 \cdot 10^{-6}$$



# Motivation IRK: Stiff systems

## **Stiff system:**

*System that cannot be simulated effectively with explicit methods (system with large spread of eigenvalues of Jacobian)*

# Example: Curtiss-Hirschfelder

- IVP:

$$\dot{y} = -50(y - \cos(t)) \quad y(t_0) = 0$$

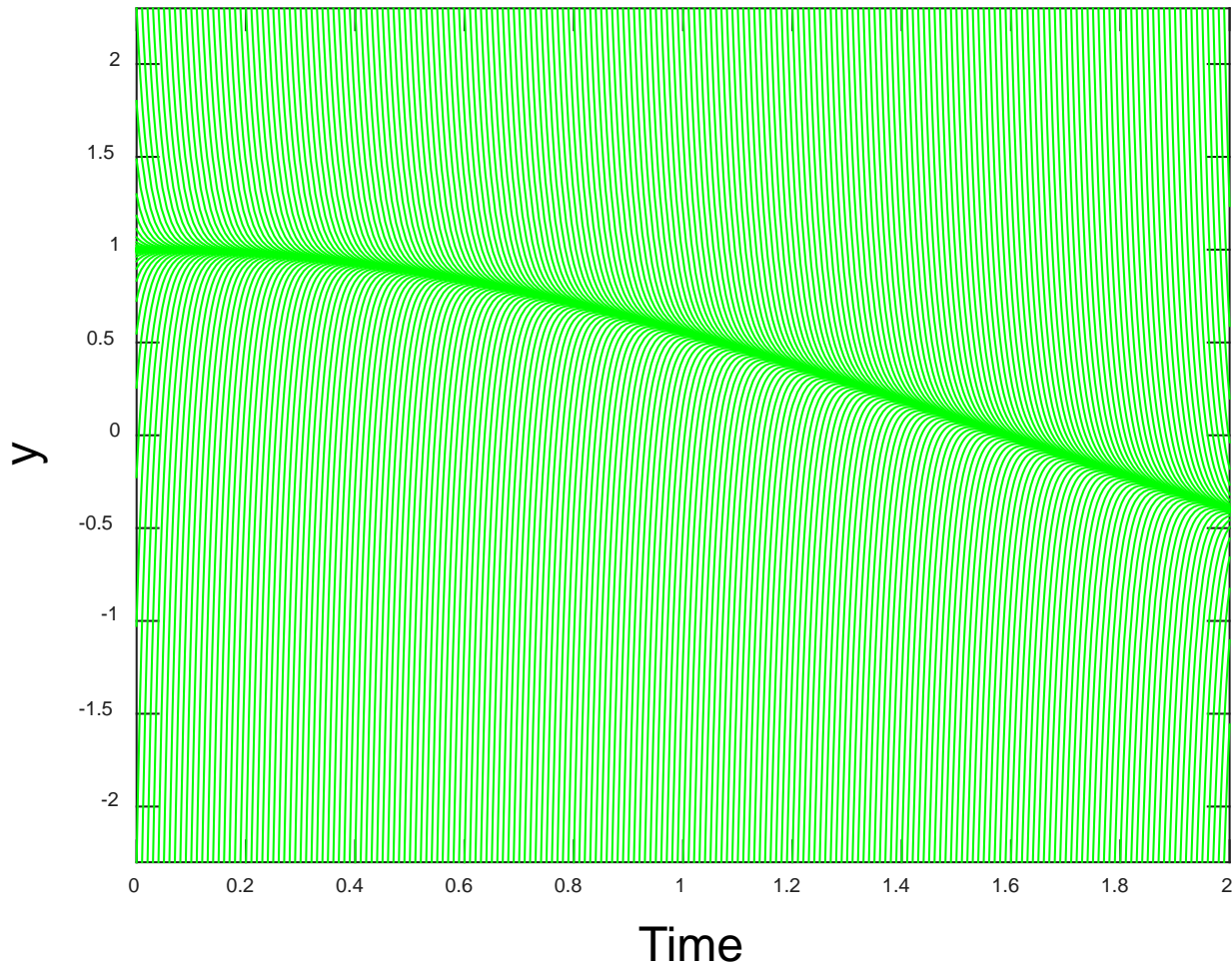
- Task Simulate from  $t = 0$  s to  $t = 2$  s
- Two widely different time scales:
  - Slow manifold

$$y^S(t) = \cos(t)$$

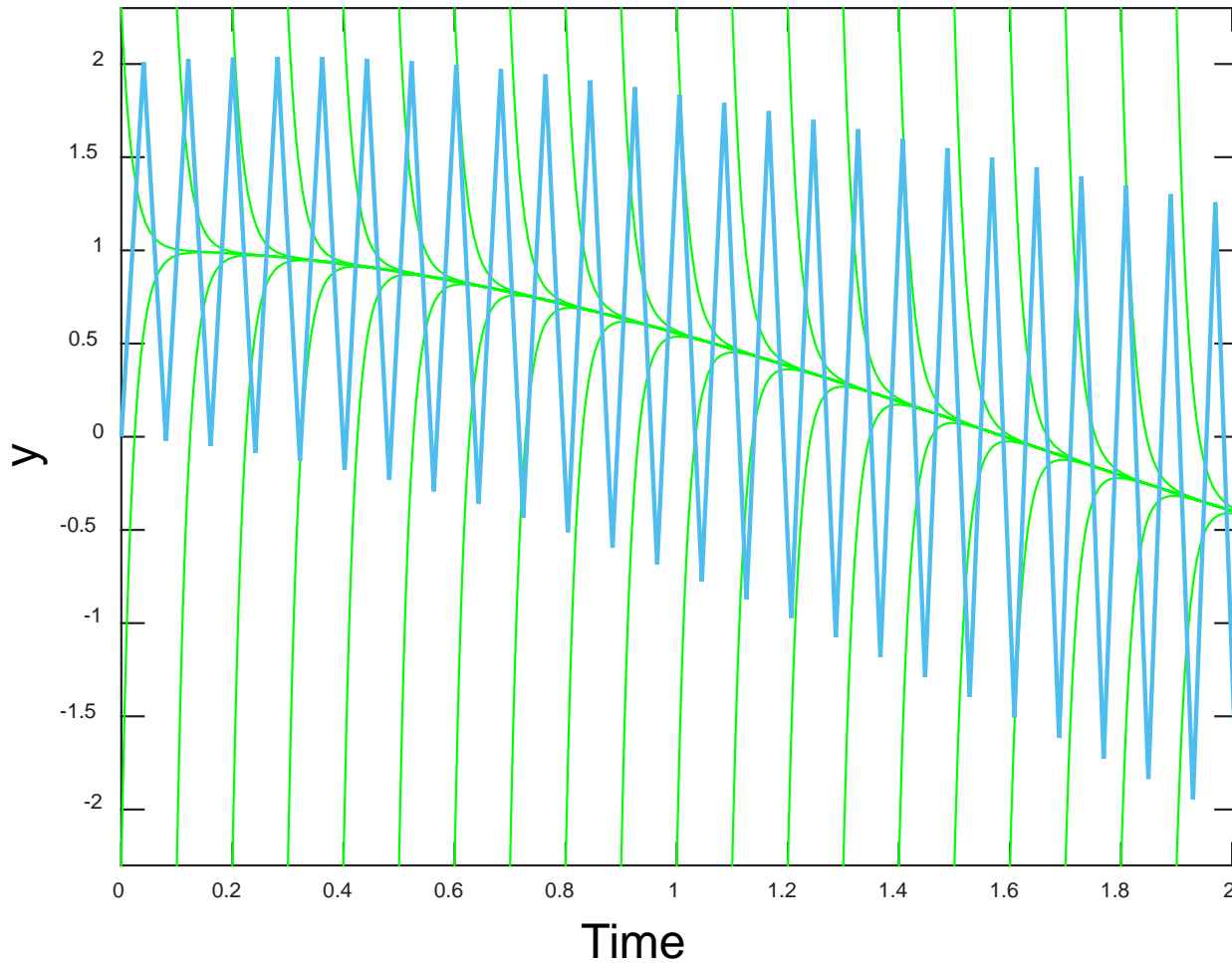
- Strongly damped mode

$$\exp(-50t)$$

# Solution manifold

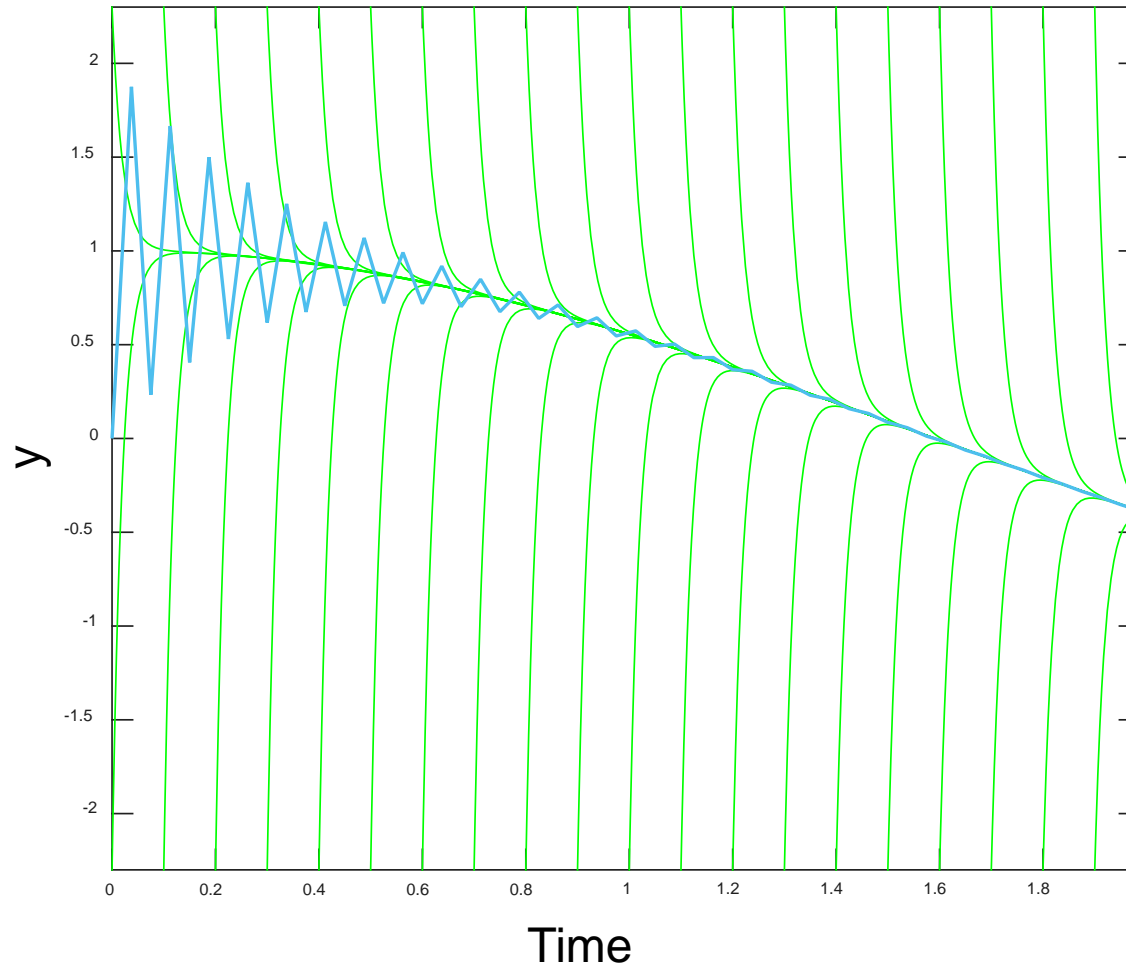


# Attempt 1: Euler (explicit), $h = 0.0402$

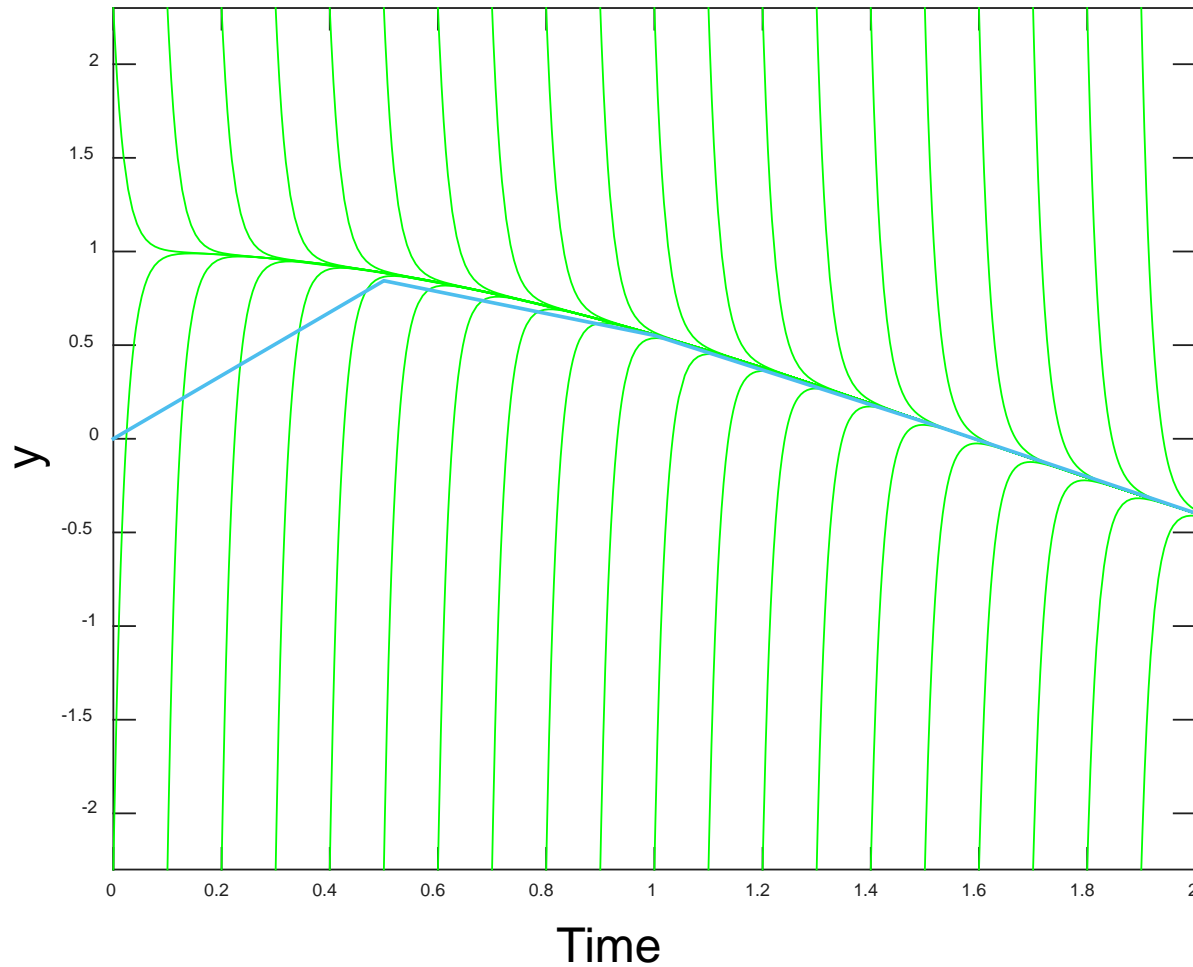




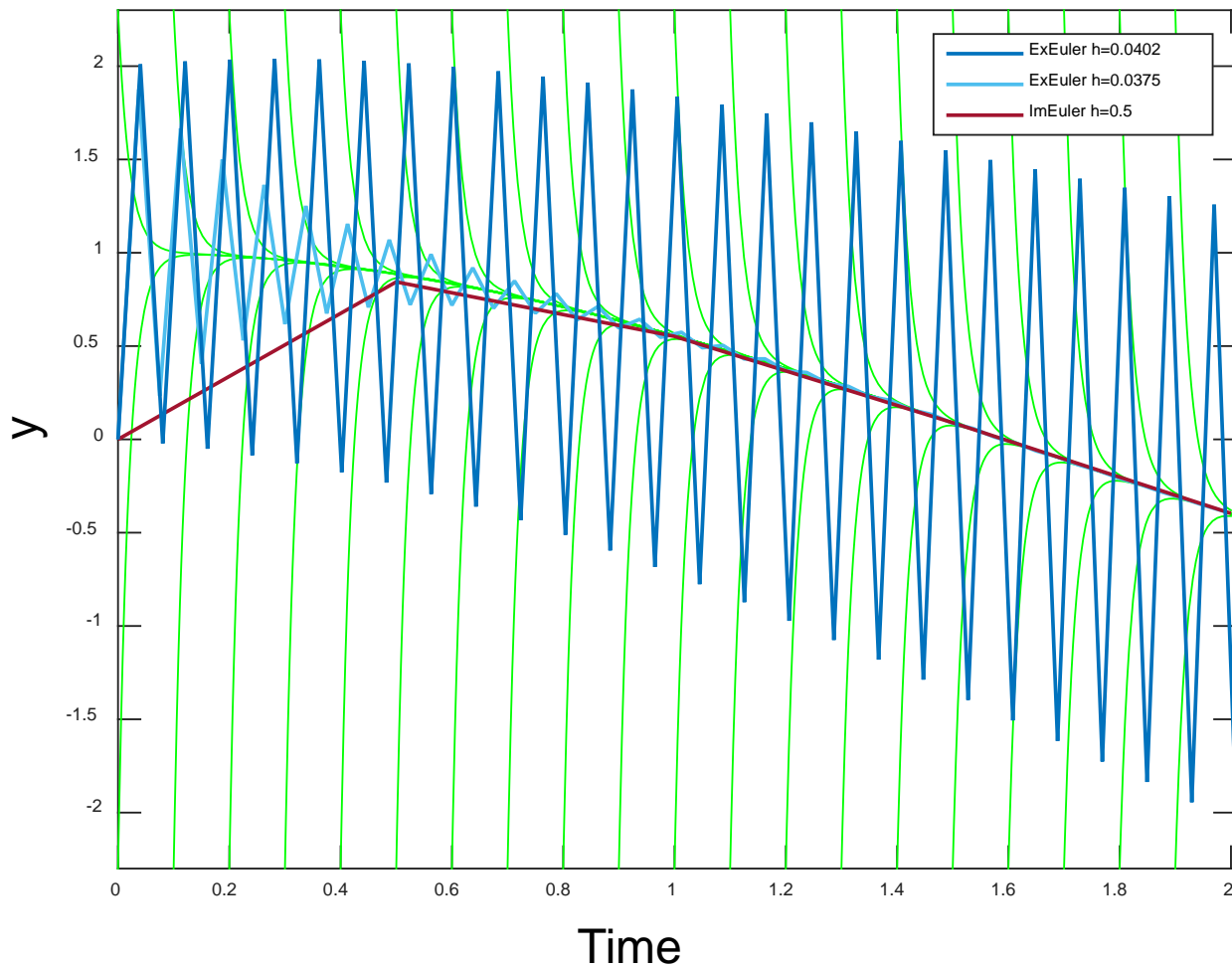
# Attempt 2: Euler (explicit), $h = 0.0375$



# Attempt 3: Euler (implicit), $h = 0.5$



# Comparison



# Recap: Explicit Runge-Kutta (ERK) methods

- IVP:  $\dot{y} = f(y, t), \quad y(0) = y_0$
- One-step methods:  $y_{n+1} = y_n + h\phi(y_n, t_n), \quad h = t_{n+1} - t_n$
- ERK:
 
$$\begin{aligned}
 k_1 &= f(y_n, t_n) \\
 k_2 &= f(y_n + ha_{21}k_1, t_n + c_2h) \\
 k_3 &= f(y_n + h(a_{31}k_1 + a_{32}k_2), t_n + c_3h) \\
 &\vdots \\
 k_\sigma &= f(y_n + h(a_{\sigma,1}k_1 + a_{\sigma,2}k_2 + \dots + a_{\sigma,\sigma-1}k_{\sigma-1}), t_n + c_\sigma h) \\
 y_{n+1} &= y_n + h(b_1k_1 + b_2k_2 + \dots + b_\sigma k_\sigma)
 \end{aligned}$$

- Butcher array:

<b>c</b>	<b>A</b>				
	<b>b<sup>T</sup></b>				
0					
c <sub>2</sub>	a <sub>21</sub>				
c <sub>3</sub>	a <sub>31</sub>	a <sub>32</sub>			
⋮	⋮	⋮	⋱		
c <sub>σ</sub>	a <sub>σ,1</sub>	a <sub>σ,2</sub>	⋯	a <sub>σ,σ-1</sub>	
	b <sub>1</sub>	b <sub>2</sub>	⋯	b <sub>σ-1</sub>	b <sub>σ</sub>

# Implicit Runge-Kutta (IRK) methods

- IVP:  $\dot{y} = f(y, t), \quad y(0) = y_0$
- IRK:
 
$$\begin{aligned}
 k_1 &= f(y_n + h(a_{1,1}k_1 + a_{1,2}k_2 + \dots + a_{1,\sigma}k_\sigma), t_n + c_1h) \\
 k_2 &= f(y_n + h(a_{2,1}k_1 + a_{2,2}k_2 + \dots + a_{2,\sigma}k_\sigma), t_n + c_2h) \\
 k_3 &= f(y_n + h(a_{3,1}k_1 + a_{3,2}k_2 + \dots + a_{3,\sigma}k_\sigma), t_n + c_3h) \\
 &\vdots \\
 k_\sigma &= f(y_n + h(a_{\sigma,1}k_1 + a_{\sigma,2}k_2 + \dots + a_{\sigma,\sigma}k_\sigma), t_n + c_\sigma h) \\
 y_{n+1} &= y_n + h(b_1k_1 + b_2k_2 + \dots + b_\sigma k_\sigma)
 \end{aligned}$$

$$0 \leq c_i \leq 1$$

$$\sum_{i=1}^{\sigma} b_i = 1$$

$$\sum_{j=1}^{\sigma} a_{ij} = c_i$$

(usually)

- Butcher array:

c	A				
	b <sup>T</sup>				
c <sub>1</sub>	a <sub>11</sub>	a <sub>12</sub>	⋯	a <sub>1,σ-1</sub>	a <sub>1,σ</sub>
c <sub>2</sub>	a <sub>21</sub>	a <sub>22</sub>	⋯	a <sub>2,σ-1</sub>	a <sub>2,σ</sub>
⋮	⋮	⋮	⋱	⋮	⋮
c <sub>σ</sub>	a <sub>σ,1</sub>	a <sub>σ,2</sub>	⋯	a <sub>σ,σ-1</sub>	a <sub>σ,σ</sub>
	b <sub>1</sub>	b <sub>2</sub>	⋯	b <sub>σ-1</sub>	b <sub>σ</sub>

# Recap: 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 you can show that

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

- Then:

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

# Implicit Euler method: Order

$$k_1 = f(y_n + hk_1, t_n + h)$$

$$y_{n+1} = y_n + hk_1$$

- Taylor series expansion of  $k_1$ :

$$k_1 = f(y_n, t_n) + h \frac{df(y_n, t_n)}{dt} + O(h^2)$$

- Solution:

$$y_{n+1} = y_n + hf(y_n, t_n) + h^2 \frac{f(y_n, t_n)}{dt} + O(h^3)$$

- Error:  $O(h^2)$   
→ method of order 1

# Recap: 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

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



# Implicit Euler method: Stability

$$k_1 = f(y_n + hk_1, t_n + h)$$

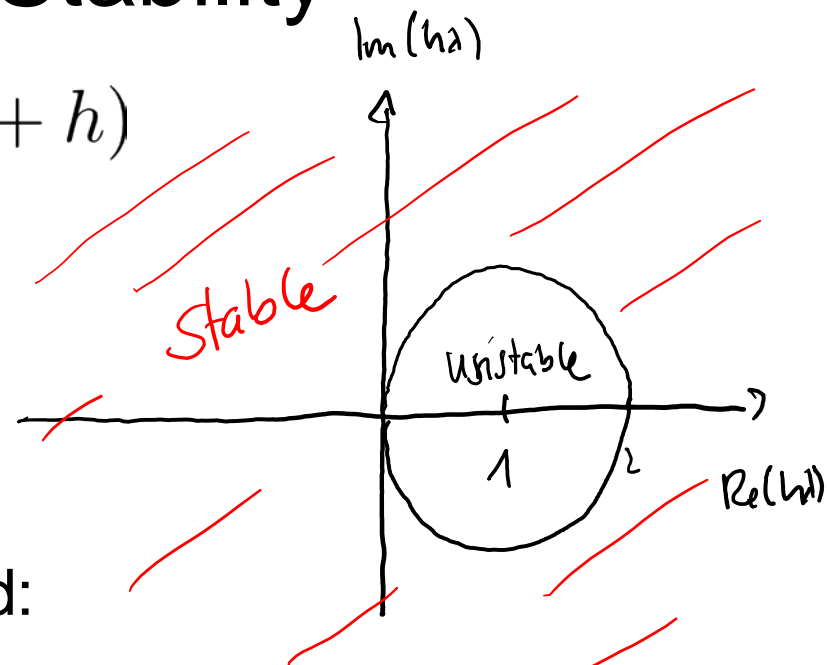
$$y_{n+1} = y_n + hk_1$$

- Test function:  $\dot{y} = \lambda y$
- Applied to Implicit Euler method:

$$k_1 = \lambda(y_n + hk_1) = \lambda y_{n+1}$$

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

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



$$|R(h\lambda)| \leq 1 \rightarrow |1 - h\lambda| \geq 1$$

# IRK: Trapezoidal rule

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

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

$$\begin{aligned} y_{n+1} &= y_n + \frac{h}{2}(k_1 + k_2) \\ &= y_n + \frac{h}{2}[f(y_n, t_n) + f(y_{n+1}, t_{n+1})] \end{aligned}$$

# IRK: Trapezoidal rule: Order: 2

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

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

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

$$= y_n + \frac{h}{2}[f(y_n, t_n) + f(y_{n+1}, t_{n+1})]$$

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

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

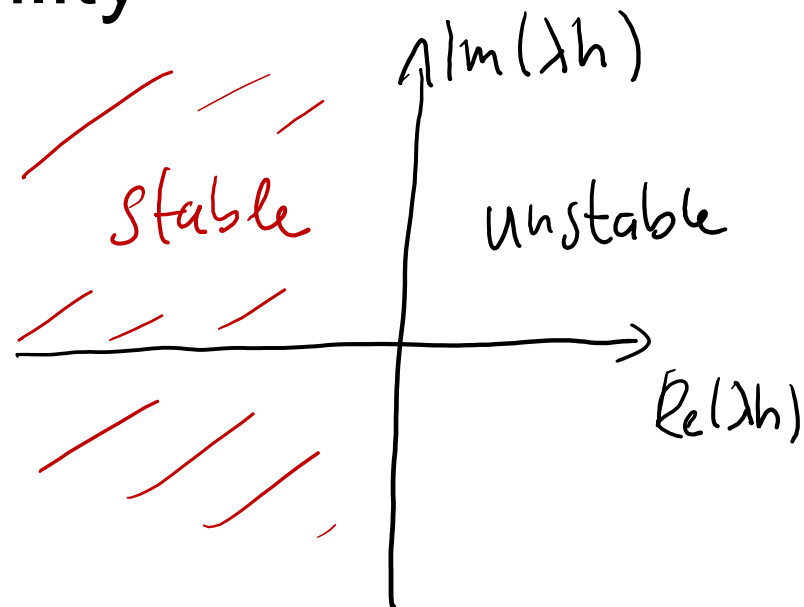
# Trapezoidal rule – stability

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

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

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

$$= y_n + \frac{h}{2}[f(y_n, t_n) + f(y_{n+1}, t_{n+1})]$$



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

$$y_{n+1} \approx y_n + \frac{h\lambda}{2} (y_n + y_{n+1})$$

$$y_{n+1} \approx \underbrace{\frac{1 + \frac{h\lambda}{2}}{1 - \frac{h\lambda}{2}}}_{R(h\lambda)} y_n$$

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

# IRK: Implicit midpoint rule

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

$$y_{n+1} = y_n + hk_1$$

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

- Order ?
- Order: 2

# Stability of Implicit midpoint rule

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

$$y_{n+1} = y_n + hk_1$$

trick:

$$\begin{aligned}
 y_n + \frac{h}{2}k_1 &= \frac{y_n}{2} + \frac{y_n}{2} + \frac{h}{2}k_1 \\
 &= \frac{1}{2}(y_n + y_{n+1}) \\
 \Rightarrow k_1 &= f\left(\frac{y_n + y_{n+1}}{2}, t_n + \frac{h}{2}\right)
 \end{aligned}$$

# Stability function of IRK

- As for ERK:

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

- Or:

$$R(h\lambda) = \frac{\det [\mathbf{I} - h\lambda (\mathbf{A} - \mathbf{1}\mathbf{b}^T)]}{\det [\mathbf{I} - h\lambda \mathbf{A}]}$$

- $\rightarrow R(h\lambda) = \frac{\text{polynomial of } h\lambda \text{ of order } \leq \sigma}{\text{polynomial of } h\lambda \text{ of order } \leq \sigma}$

# Some implicit Runge-Kutta methods

- Implicit Euler:

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

Implicit midpoint rule

- Gauss (or Gauss-Legendre) methods:

Trapezoidal rule

Order 2	Order 4	Order 6
$\begin{array}{c c} 1/2 & 1/2 \\ \hline & 1 \end{array}$	$\begin{array}{c c} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} \\ \hline & \frac{1}{2} \end{array}$	$\begin{array}{c c} \frac{1}{2} - \frac{\sqrt{15}}{10} & \frac{5}{36} \\ \hline \frac{1}{2} + \frac{\sqrt{15}}{10} & \frac{5}{36} + \frac{\sqrt{15}}{24} \\ \hline & \frac{5}{18} \end{array}$

- Lobatto methods:

	Order 2	Order 4
Lobatto IIIA	$\begin{array}{c c} 0 & 0 \\ \hline 1 & 1/2 \\ \hline & 1/2 \end{array}$	$\begin{array}{c c} 0 & 0 \\ \hline 1/2 & 5/24 \\ \hline & 1/6 \end{array}$
Lobatto IIIB	$\begin{array}{c c} 0 & 1/2 \\ \hline 1 & 1/2 \\ \hline & 1/2 \end{array}$	$\begin{array}{c c} 0 & 1/6 \\ \hline 1/2 & 1/6 \\ \hline & 1/6 \end{array}$
Lobatto IIIC	$\begin{array}{c c} 0 & 1/2 \\ \hline 1 & 1/2 \\ \hline & 1/2 \end{array}$	$\begin{array}{c c} 0 & 1/6 \\ \hline 1/2 & 1/6 \\ \hline & 1/6 \end{array}$

- Radau methods:

	Order 3	Order 5
Radau IA	$\begin{array}{c c} 0 & 1/4 \\ \hline 2/3 & 1/4 \end{array}$	$\begin{array}{c c} 0 & 1/9 \\ \hline 2/3 & 1/9 \end{array}$
Radau IIA	$\begin{array}{c c} 1/3 & 5/12 \\ \hline 1 & 3/4 \end{array}$	$\begin{array}{c c} 2/5 & 11/45 \\ \hline 1 & 3/5 \end{array}$

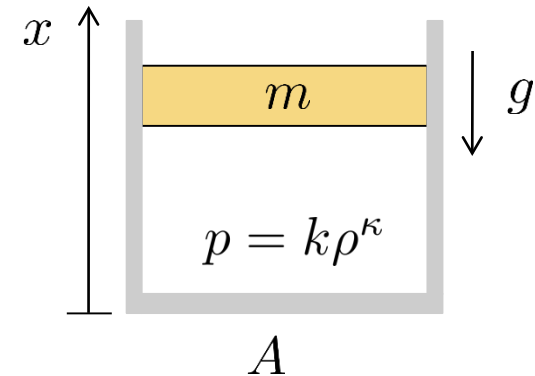


# Pneumatic spring example, again (preview)

- Model from Newton's 2nd law:

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

"mass-spring-damper with nonlinear spring"



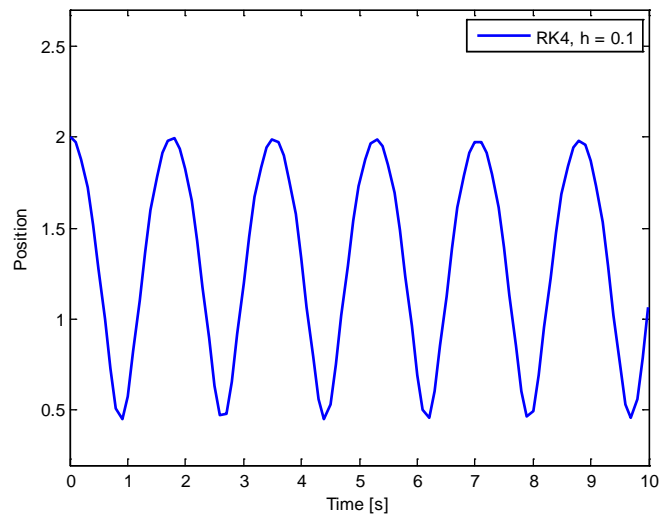
- On state-space form  $\dot{y} = f(y, t)$

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

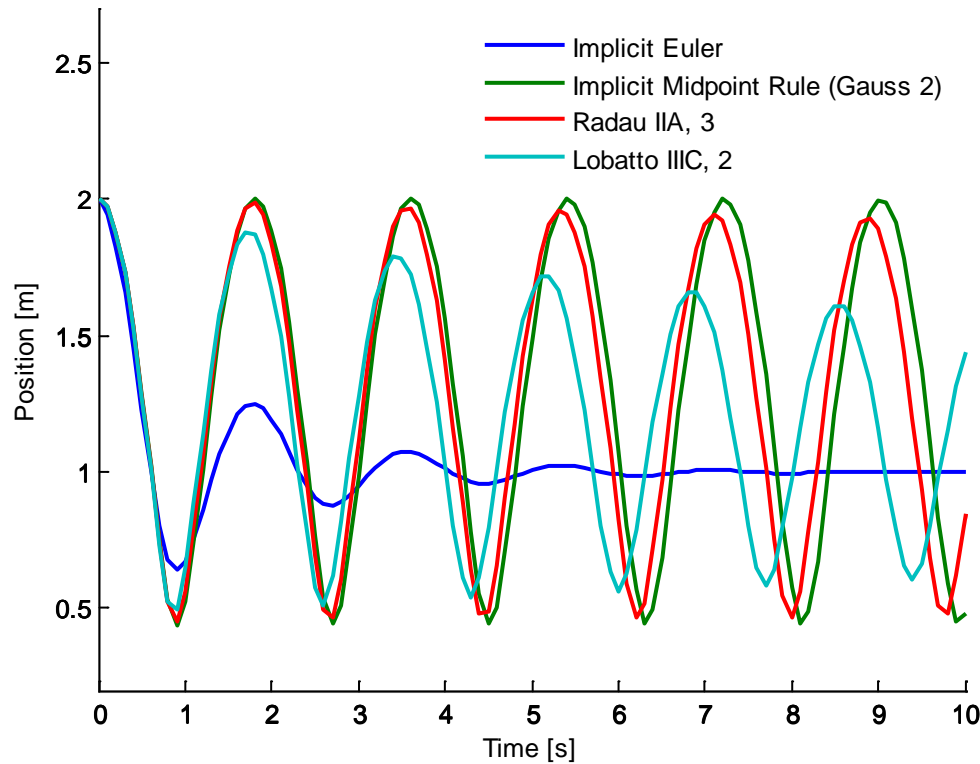
- Linearization about equilibrium:

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

# Simulation

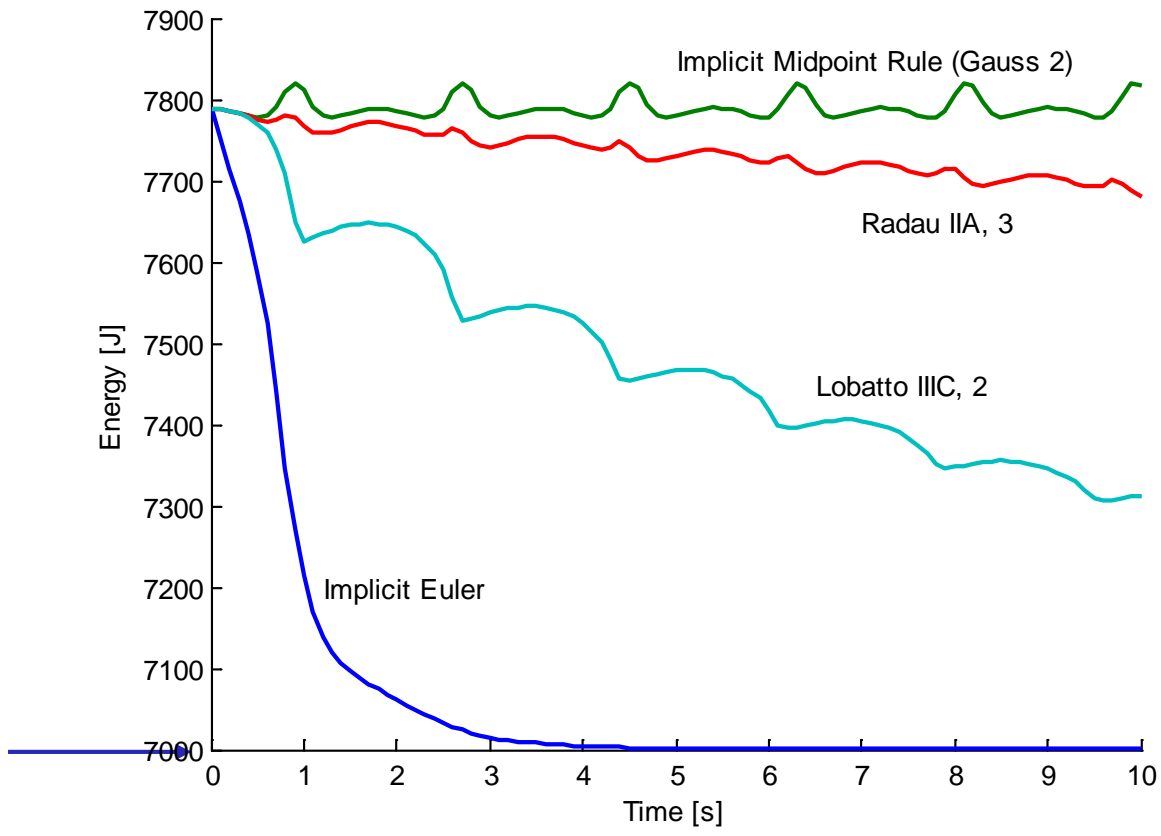


$h = 0.5$  (stability limit for RK4)



# Energy

Equilibrium energy



# How to solve implicit equations? I

- Define  $z_i$  with:

$$k_i = f(y_n + h(a_{i1}k_1 + \dots + a_{i\sigma}k_\sigma)) = f(y_n + z_i)$$

$$z_i = ha_{i1}f(y_n + z_1) + \dots + ha_{i\sigma}f(y_n + z_\sigma)$$

$$\begin{pmatrix} z_1 \\ \vdots \\ z_\sigma \end{pmatrix} = h \begin{pmatrix} a_{11}I_\sigma & \dots & a_{1\sigma}I_\sigma \\ \vdots & \ddots & \vdots \\ a_{\sigma 1}I_\sigma & \dots & a_{\sigma\sigma}I_\sigma \end{pmatrix} \begin{pmatrix} f(y_n + z_1) \\ \vdots \\ f(y_n + z_\sigma) \end{pmatrix}$$

$$z = h(A \otimes I_\sigma)F(z)$$

- Use methods from optimal control to solve:

$$r(z) = z - h(A \otimes I_\sigma)F(z) = 0$$

# How to solve implicit equations? II

$$r(z) = z - h(A \otimes I_\sigma)F(z) = 0$$

$$\frac{\partial r}{\partial z} = I - h(A \otimes I_\sigma) \begin{bmatrix} \frac{\partial f(y_n + z_n)}{\partial z_n} & 0 \\ 0 & \frac{\partial f(y_n, z_n)}{\partial z_\sigma} \end{bmatrix}$$

$$\approx I - h(A \otimes J)$$

$$\frac{\partial f(y_n)}{\partial y} = J$$

# How to solve implicit equations? III

- If  $z$  is found:

$$y_{n+1} = y_n h b_1 f(y_n, z_1) + \dots + h b_\sigma f(y_n + z_\sigma)$$

$$= y_n + h b^T F(z)$$

$$= y_n + \underbrace{h b^T \frac{1}{h} (A \otimes I_\sigma)^{-1}}_{\text{evaluate a priori}} z$$

- Special case: (S)DIRK: (single) diagonal IRK

$$A = \begin{pmatrix} \gamma & 0 & 0 \\ x & \ddots & 0 \\ x & x & \gamma \end{pmatrix}$$

$$z_1 = h f(y_n + z_1) \rightarrow \text{solve } z_1$$

$$z_2 = \dots \rightarrow \text{solve } z_2$$

$\sigma$  equation system : dimension  $d \times d$

$\rightarrow$  Much faster than solving  $(\sigma d \times \sigma d)$  equation system

# Homework

- Implement in matlab the Euler method for the Curtiss-Hirschfelder example (slide 14)
- Write down the Butcher array of the trapezoidal rule (slide 31) and midpoint rule (slide 34)
  - Check on slide 37
- Find the stability function of the implicit midpoint rule (use hint on slide 35)
- Read 14.6.1 – 14.6.5

# Kahoot

- <https://play.kahoot.it/#/k/87256f68-7b17-4aa0-9c9c-c30869da5639>