Circuit simulation: transient analysis

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Outline

* Introduction and problem definition
* Taylor series methods
* Runge-Kutta methods
* Specific multi-step methods
* Generalized multi-step methods
* Predictor-corrector methods
* Numerical results
* Stability of numerical methods
* Regions of stability
* Stiff equations
* Adaptive step size
* Miscellaneous topics

Methods for transient analysis

Consider the system of ODE's given by,

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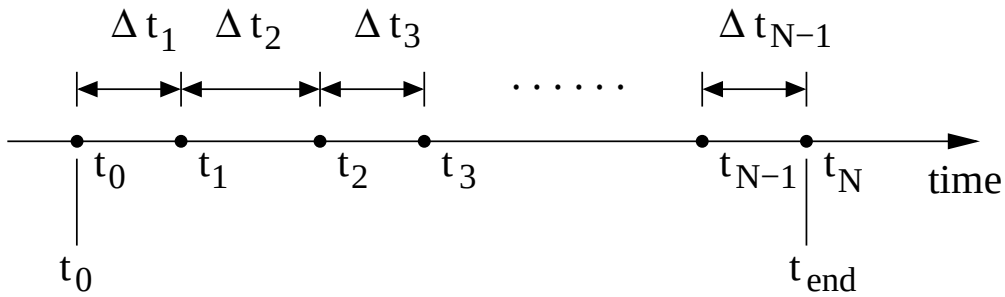
We will consider the special case of a *single* ODE:

$$\frac{dx}{dt} = f(t, x), \quad x(t_0) = x_0 .$$

Discretization of time



* Denote the exact solution of $\dot{x} = f(t, x)$, $x(t_0) = x_0$ on $[t_0, t_{\text{end}}]$, by $x(t)$, and the numerical solution by the sequence $\{x_n\}$, where x_n is the numerical solution computed for $t = t_n$.

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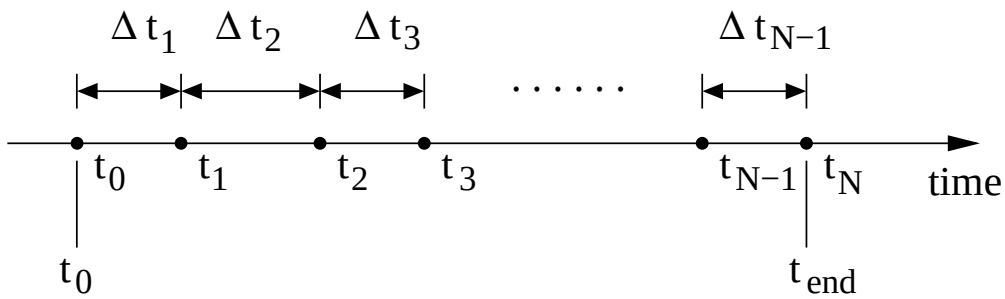

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* The primary objective of a numerical method is to obtain $\{x_n\}$ such that $|x(t_n) - x_n|$ is "small" for all n.

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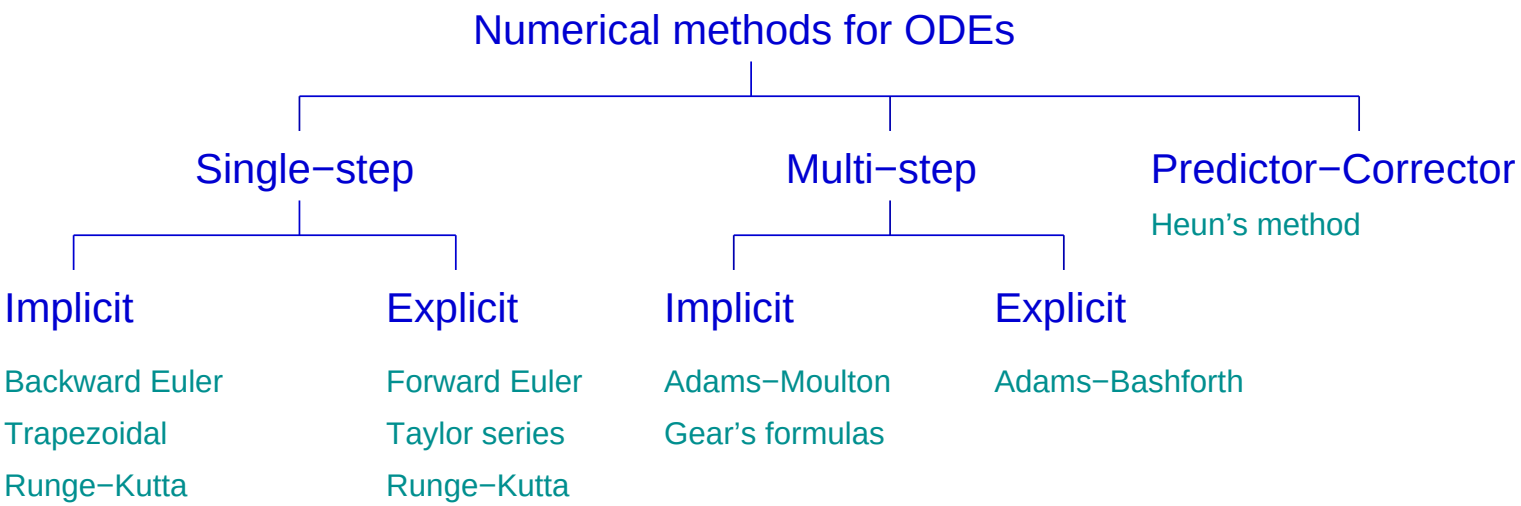
* Numerical methods are expected to work well only for well-posed problems because the problem being solved by these methods is generally a perturbed version of the original problem (due to round-off errors, for example).

Broad classification of methods



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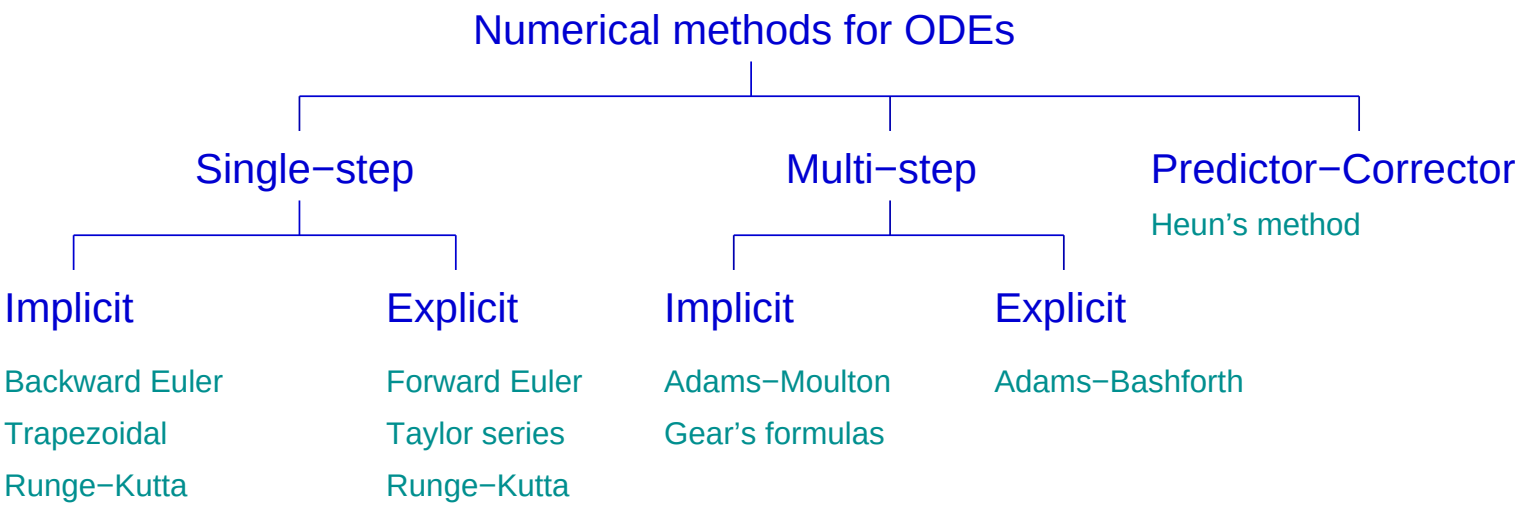

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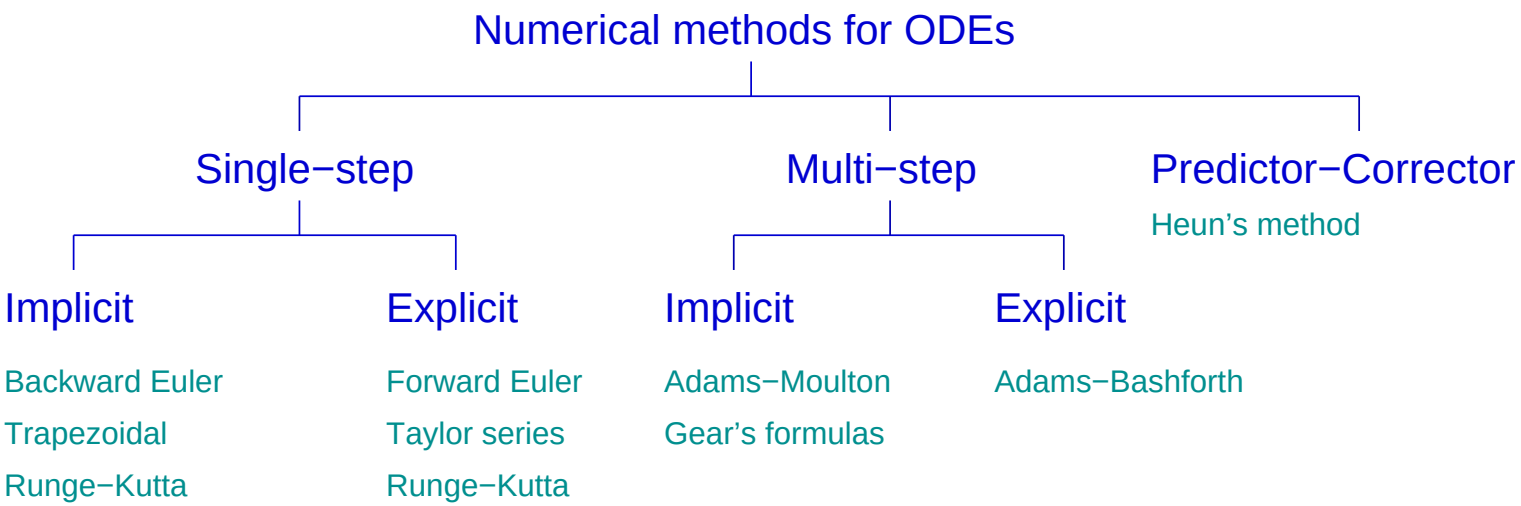

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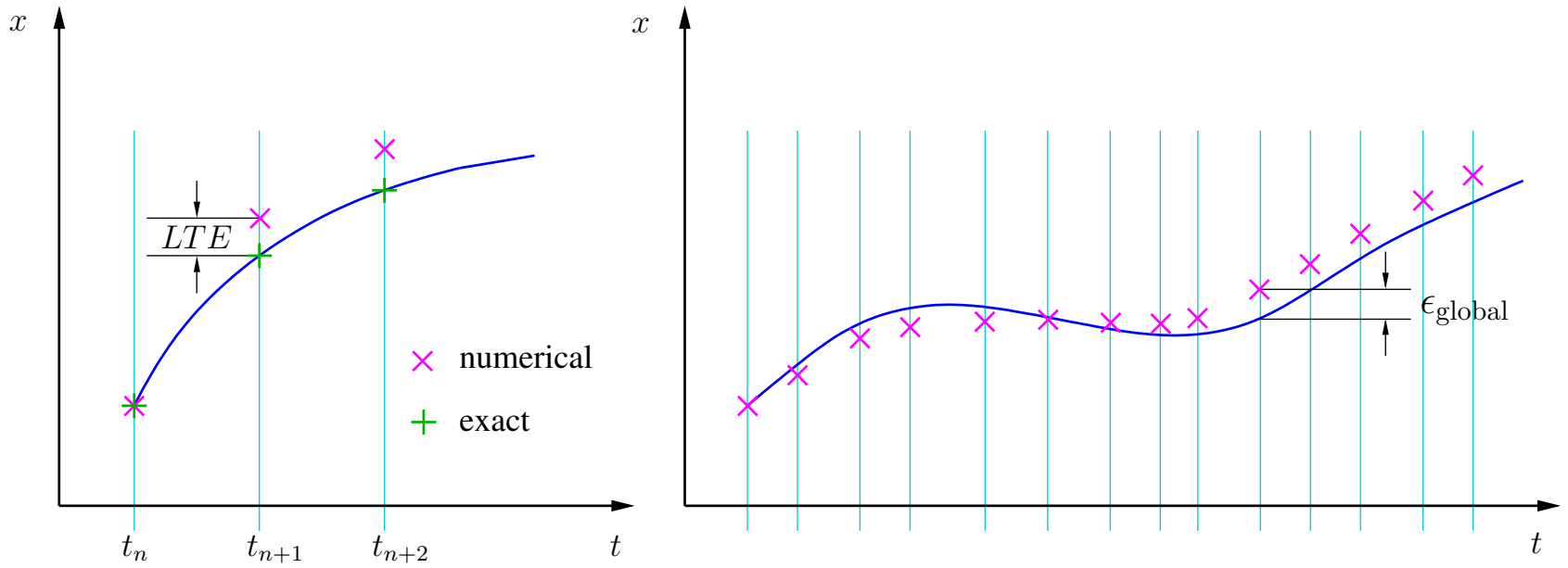
* Other classifications are possible, based on stability and order.

Local Truncation Error (LTE) and Global Error



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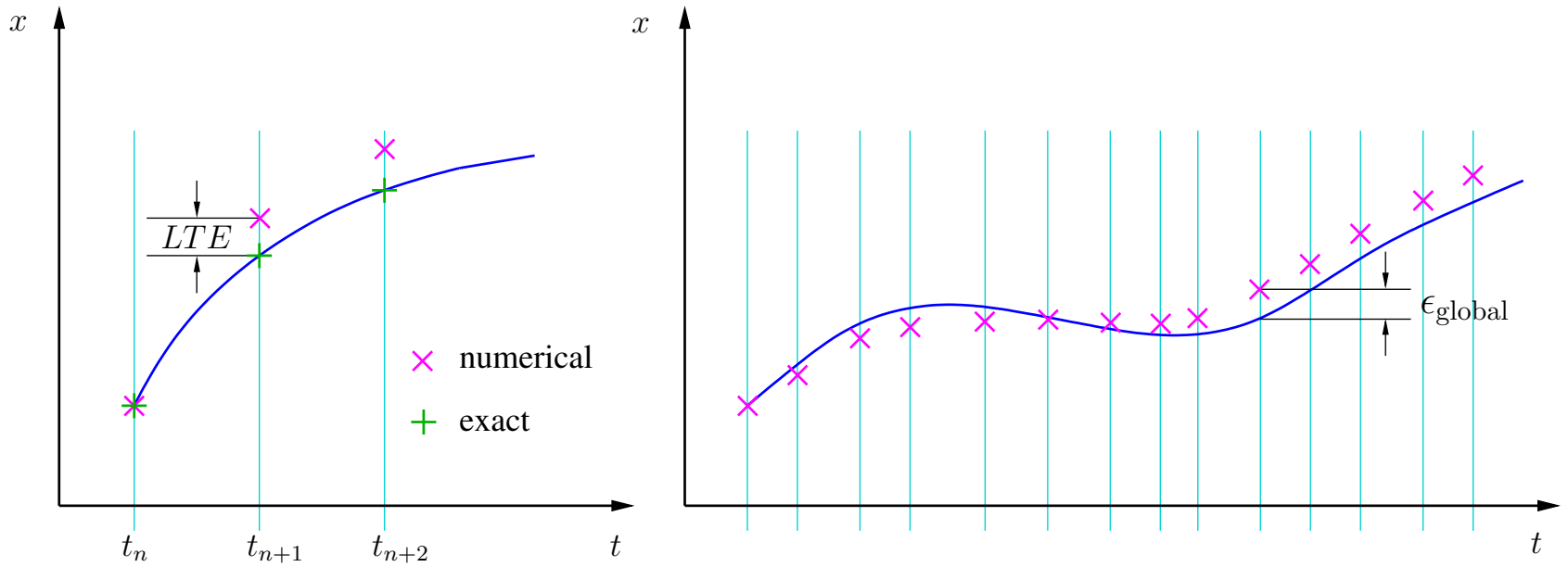

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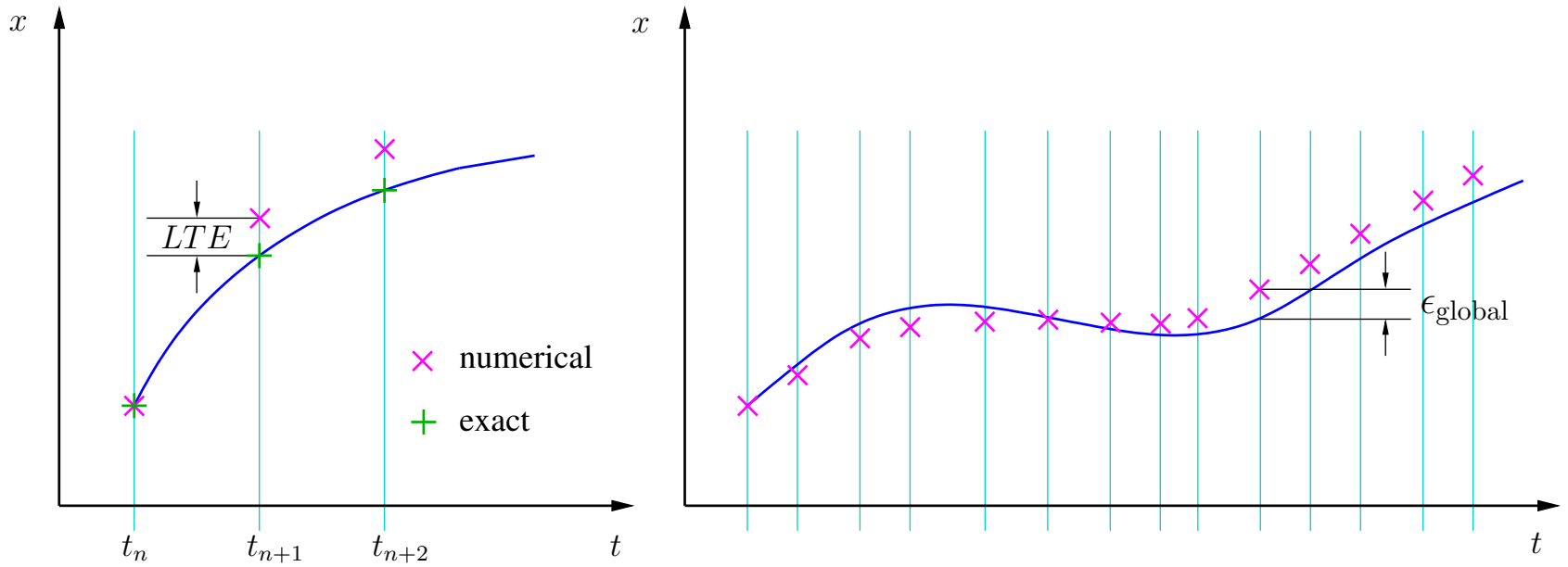

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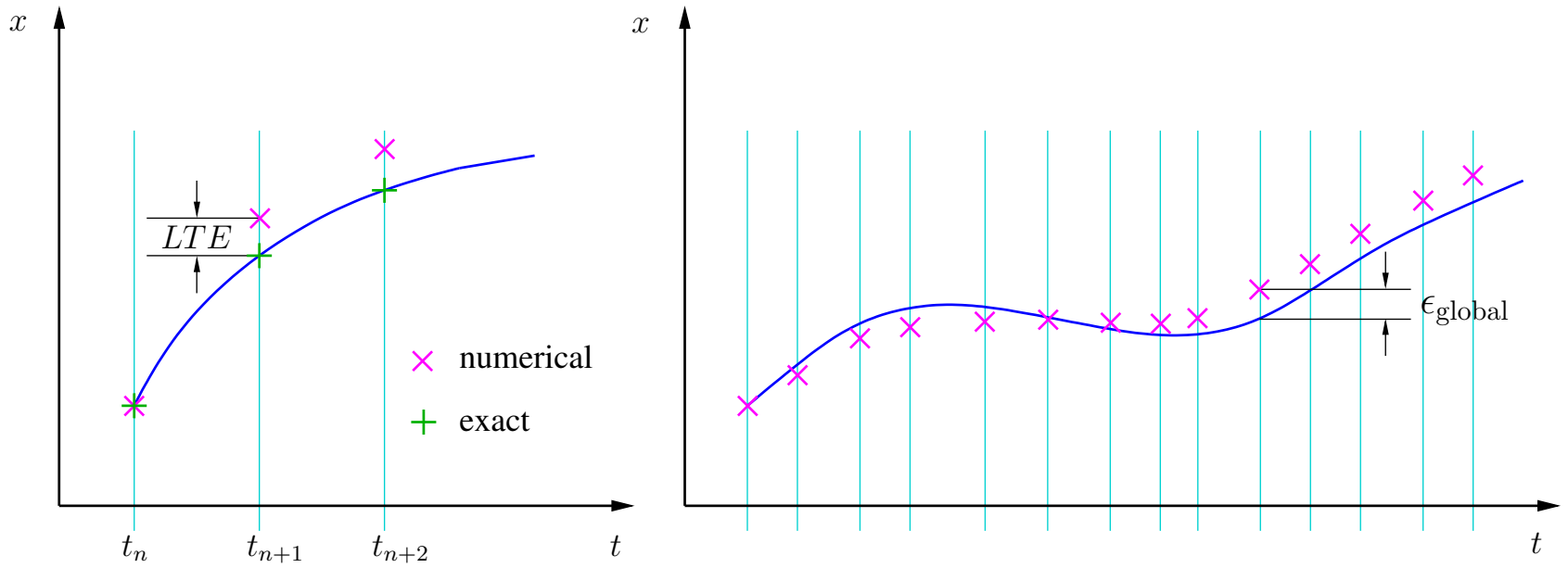

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* Other sources of error: (a) round-off error due to finite precision (b) In case of implicit methods, the equations are not solved exactly but to a certain tolerance.
* If the LTE is $O(h^{k+1})$, the method is said to be of order k.

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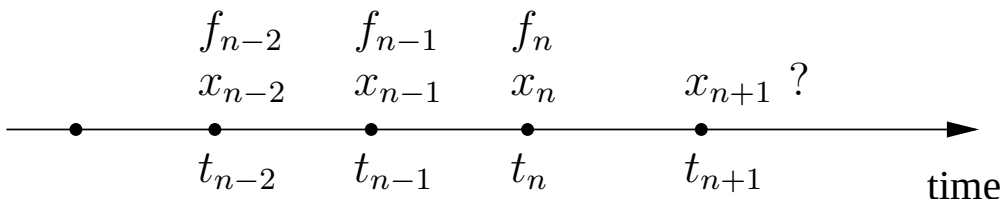

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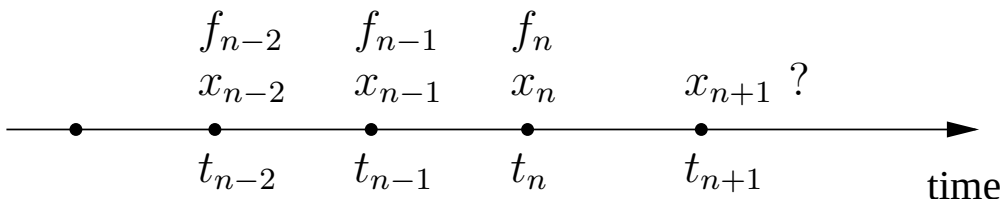

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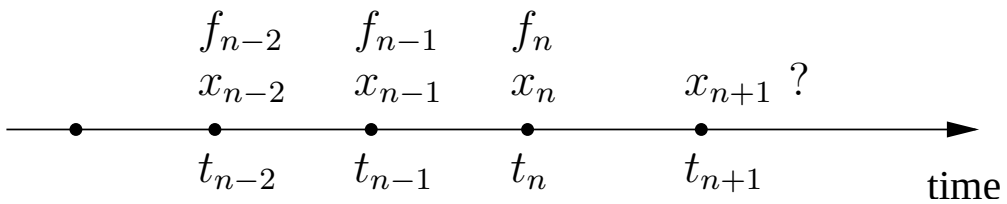

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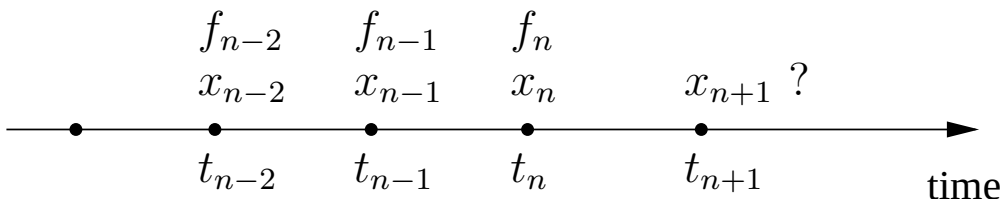

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* Single-step methods: Only the information at t_n is used.
* Multi-step methods: The information at t_n and some others (t_{n-1}, t_{n-2}, ..) is also used.

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* We can rewrite Taylor's theorem as,

$$x(t_{n+1}) = x(t_n) + x'(t_n)\,h + \frac{x''(t_n)}{2\,!}\,h^2 + \cdots + \frac{x^{(k)}(t_n)}{k\,!}\,h^k + O(h^{k+1})\,. \quad (2)$$

Taylor series methods for solving $\dot{x} = f(t, x)$

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$$\begin{aligned} x_{n+1} &= x_n + h f^n\,, \\ x_{n+1} &= x_n + h f^n + \frac{h^2}{2}\left(f_t^n + f^n f_x^n\right)\,, \end{aligned}$$

where $f^n = f(t_n, x_n)$, $f_t^n = \dfrac{\partial f}{\partial t}(t_n, x_n)$, and $f_x^n = \dfrac{\partial f}{\partial x}(t_n, x_n)$.

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x''(t_n) &= \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x} \frac{dx}{dt} = f_t + f\, f_x \,, \\
x^{(3)}(t_n) &= \frac{\partial}{\partial t} \left[f_t + f\, f_x \right] + \frac{\partial}{\partial x} \left[f_t + f\, f_x \right] f \\
&= \left[f_{tt} + f\, f_{xt} + f_t\, f_x \right] + \left[f_{tx} + f_x\, f_x + f\, f_{xx} \right] f \\
&= f_{tt} + 2\, f\, f_{xt} + f_t\, f_x + f\, f_x^2 + f^2\, f_{xx} \,,
\end{aligned}
$$

Taylor series method for solving $\dot{x} = f(t, x)$

The derivatives can be computed as,

$$
\begin{aligned}
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&= f_{tt} + 2\, f\, f_{xt} + f_t\, f_x + f\, f_x^2 + f^2\, f_{xx} \,,
\end{aligned}
$$

Note that computation of the derivatives becomes expensive as the order increases $\rightarrow$ Runge-Kutta methods.

Outline

* Introduction and problem definition
* Taylor series methods
* Runge-Kutta methods
* Specific multi-step methods
* Generalized multi-step methods
* Predictor-corrector methods
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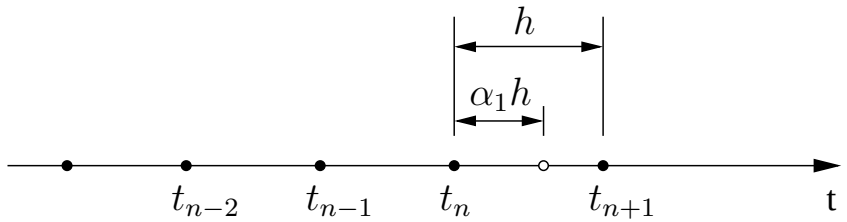
* Miscellaneous topics

Runge-Kutta method for solving $\dot{x} = f(t, x)$



* Basic idea: Instead of evaluating higher-order derivatives (as required in Taylor series method), evaluate the function $f(t, x)$ at some intermediate points such that the resulting formula is equivalent to a Taylor series formula.

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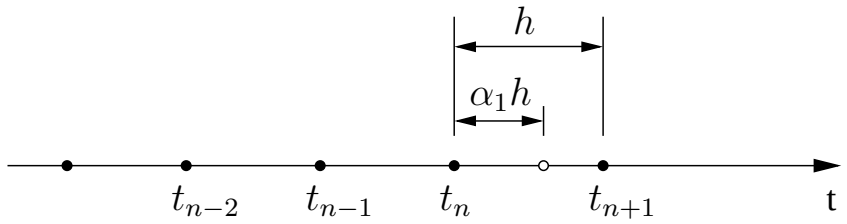
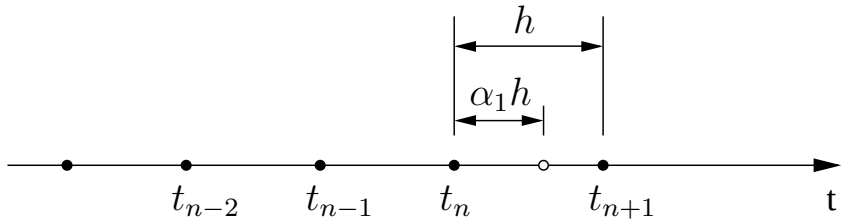


* Basic idea: Instead of evaluating higher-order derivatives (as required in Taylor series method), evaluate the function $f(t, x)$ at some intermediate points such that the resulting formula is equivalent to a Taylor series formula.
* Note that this is still a single-step method since we are using information only at t_n (and not t_{n-1}, t_{n-2}, etc.).

Runge-Kutta method for solving $\dot{x} = f(t, x)$



Consider the algorithm given by,

$$
\begin{aligned}
f_0 &= f(t_n, x_n)\,, \\
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x_{n+1} &= x_n + h[\gamma_0\, f_0 + \gamma_1\, f_1]\,.
\end{aligned}
$$

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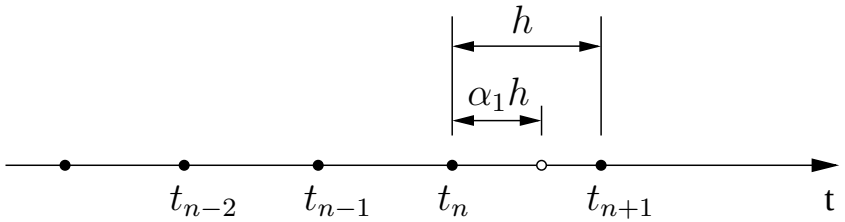

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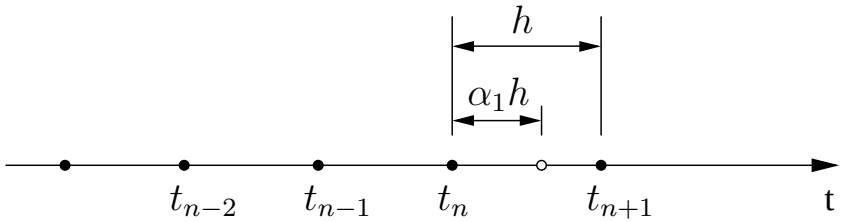

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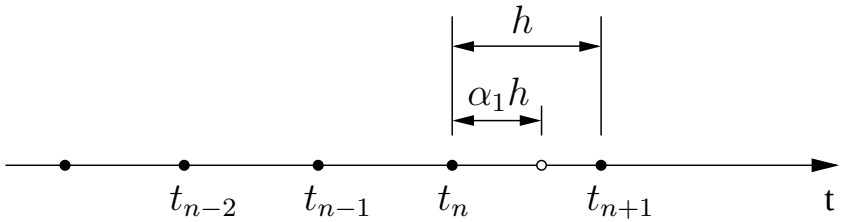

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* The reason for using subscripts for α and β will become clear later.

Runge-Kutta method for solving $\dot{x} = f(t, x)$

* Taylor series for a function of two variables:

$$f(t\,, x) = f(t_n, x_n) + f_t(t_n, x_n)(t - t_n) + f_x(t_n, x_n)(x - x_n)$$
$$+ \frac{1}{2\,!}\left[f_{tt}(t_n, x_n)(t - t_n)^2 + f_{tx}(t_n, x_n)(t - t_n)(x - x_n) + f_{xx}(t_n, x_n)(x - x_n)^2\right]$$
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* Substituting $t = t_n + \alpha_1\, h$ and $x = x_n + h\,\beta_{1,0}\, f_0$, we get

$$\begin{aligned} x_{n+1} &= x_n + h[\gamma_0\, f_0 + \gamma_1\, f(t_n + \alpha_1\, h, x_n + h\,\beta_{1,0}\, f_0)] \\ &= x_n + \gamma_0 hf + \gamma_1 hf + \alpha_1\gamma_1 h^2 f_t + \beta_{1,0}\gamma_1 h^2 f f_x + O(h^3)\,. \end{aligned}$$

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* Compare with the second-order Taylor series method,

$$x_{n+1} = x_n + h\,f + \frac{h^2}{2}\,(f_t + f\,f_x)\,.$$

* With the conditions,

$$\begin{aligned} \gamma_0 + \gamma_1 &= 1\,, \\ \alpha_1\gamma_1 &= 1/2\,, \\ \beta_{1,0}\gamma_1 &= 1/2\,, \end{aligned}$$

the two algorithms are the same to $O(h^2)$.

Runge-Kutta method for solving $\dot{x} = f(t, x)$

* There are four parameters for this method $(\alpha_1, \beta_{1,0}, \gamma_0, \gamma_1)$ and only three constraints:

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* The corresponding algorithm is,

$$\begin{aligned} f_0 &= f(t_n, x_n)\,, \\ f_1 &= f(t_n + \tfrac{2}{3}\,h, x_n + \tfrac{2}{3}\,h f_0)\,, \\ x_{n+1} &= x_n + h\,[\tfrac{1}{4}\,f_0 + \tfrac{3}{4}\,f_1]\,. \end{aligned}$$

Butcher array representation of RK methods [4]

	f_0	f_1	$\cdots$	f_{s-1}	f_s	
α_0	$\beta_{0,0}$	$\beta_{0,1}$		$\beta_{0,s-1}$	$\beta_{0,s}$	X_0
α_1	$\beta_{1,0}$	$\beta_{1,1}$		$\beta_{1,s-1}$	$\beta_{1,s}$	X_1
$\vdots$						$\vdots$
α_s	$\beta_{s,0}$	$\beta_{s,1}$		$\beta_{s,s-1}$	$\beta_{s,s}$	X_s
	γ_0	γ_1	$\cdots$	γ_{s-1}	γ_s	

Interpretation: For $i = 0, 1, \cdots, s$,

$$\begin{aligned} T_i &= t_n + \alpha_i h\,, \\ X_i &= x_n + h \sum_{j=0}^{s} \beta_{i,j} f_j\,, \\ f_i &= f(T_i, X_i)\,. \end{aligned}$$

Finally,

$$x_{n+1} = x_n + h \sum_{i=0}^{s} \gamma_i f_i\,.$$

Explicit RK methods

* When the β matrix in the Butcher array is lower-triangular, the RK method is *explicit*, i.e., the computation of f_i involves only f_1, f_2, $\cdots$, f_{i-1}.

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Examples: second-order formulas [4]

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

$\alpha_1 = \frac{1}{2}$

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

$\alpha_1 = \frac{2}{3}$

(Heun form)

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

$\alpha_1 = 1$

(Improved Euler)

Explicit RK methods

Examples: third-order formulas [4]

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{3}{8} & \frac{2}{3} & \frac{1}{6} \end{array}$$

$\alpha_1 = \frac{1}{2}$, $\alpha_2 = 1$

(Classic form)

$$\begin{array}{c|ccc} 0 & & & \\ \frac{2}{3} & \frac{2}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{1}{4} & \frac{3}{8} & \frac{3}{8} \end{array}$$

$\alpha_1 = \alpha_2 = \frac{2}{3}$

(Nystrom form)

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

$\alpha_1 = \frac{1}{3}$, $\alpha_2 = \frac{2}{3}$

(Heun form)

Explicit RK methods

Examples: fourth-order formulas [4]

0				
$\frac{1}{2}$	$\frac{1}{2}$			
$\frac{1}{2}$	0	$\frac{1}{2}$		
1	0	0	1	
	$\frac{1}{6}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{6}$

$\alpha_1 = \alpha_2 = \frac{1}{2}$ (Classic form)

0				
$\frac{1}{3}$	$\frac{1}{3}$			
$\frac{2}{3}$	$-\frac{1}{3}$	1		
1	1	-1	1	
	$\frac{1}{8}$	$\frac{3}{8}$	$\frac{3}{8}$	$\frac{1}{8}$

$\alpha_1 = \frac{1}{3}$, $\alpha_2 = \frac{2}{3}$ (Kutta form)

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However, implicit methods have some advantages:

* An implicit RK formula may allow a higher order as compared to an explicit RK formula with the same number of stages.
* Implicit formulas generally have better stability properties.

Implicit RK methods [4]

Examples:

$(3-\sqrt{3})/6$	$1/4$	$(3-2\sqrt{3})/12$
$(3+\sqrt{3})/6$	$(3+2\sqrt{3})/12$	$1/4$
	$1/2$	$1/2$

Fourth-order Gauss implicit method

Implicit RK methods [4]

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Fourth-order Gauss implicit method

0	0	0	0	0
$(5-\sqrt{5})/10$	$(5+\sqrt{5})/60$	$1/6$	$(15-7\sqrt{5})/60$	0
$(5+\sqrt{5})/10$	$(5-\sqrt{5})/60$	$(15+7\sqrt{5})/60$	$1/6$	0
1	$1/6$	$(5-\sqrt{5})/12$	$(5+\sqrt{5})/12$	0
	$1/12$	$5/12$	$5/12$	$1/12$

Sixth-order Lobatto implicit method

RK method: system of equations

The RK methods (both explicit and implicit) can be used to solve a system of ODEs,

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(t, \mathbf{x}) , \quad \mathbf{x}(t_0) = \mathbf{x}_0 .$$

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The computation involves the following:

For $i = 0, 1, \cdots, s$,

$$\begin{aligned} T_i &= t_n + \alpha_i h , \\ \mathbf{X_i} &= \mathbf{x_n} + h \sum_{j=0}^{s} \beta_{i,j} \, \mathbf{f_j} , \\ \mathbf{f_j} &= \mathbf{f}\left(T_i, \mathbf{X_i}\right) , \end{aligned}$$

and finally,

$$\mathbf{x_{n+1}} = \mathbf{x_n} + h \sum_{i=0}^{s} \gamma_i \, \mathbf{f_i} .$$

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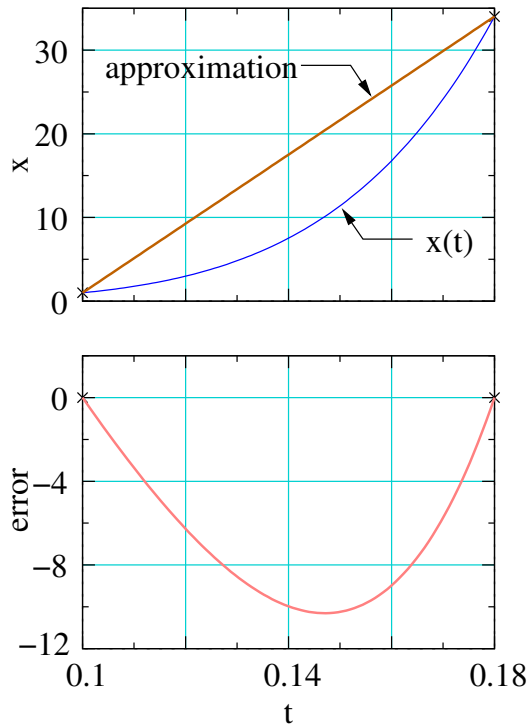
Multi-step methods for solving $\dot{x} = f(t, x)$

Consider fitting the function $x(t)$ with a staight line.



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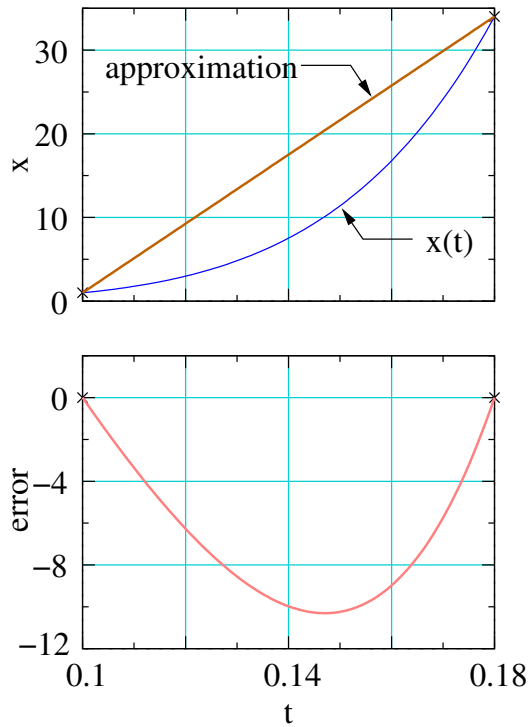

The fit can be improved in two ways:

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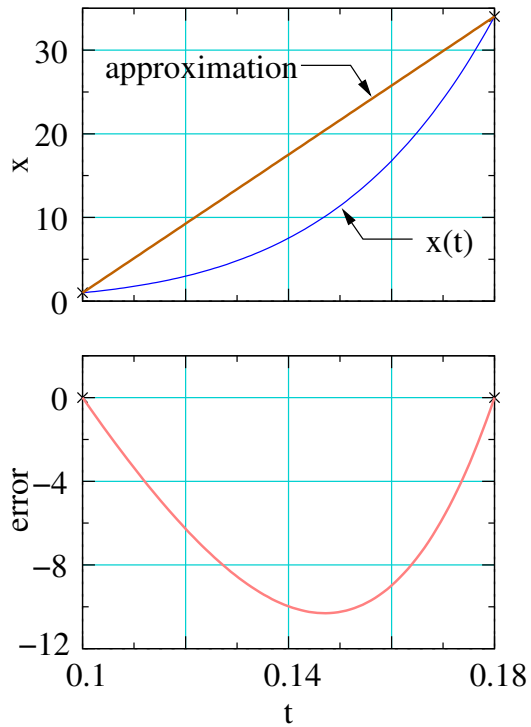

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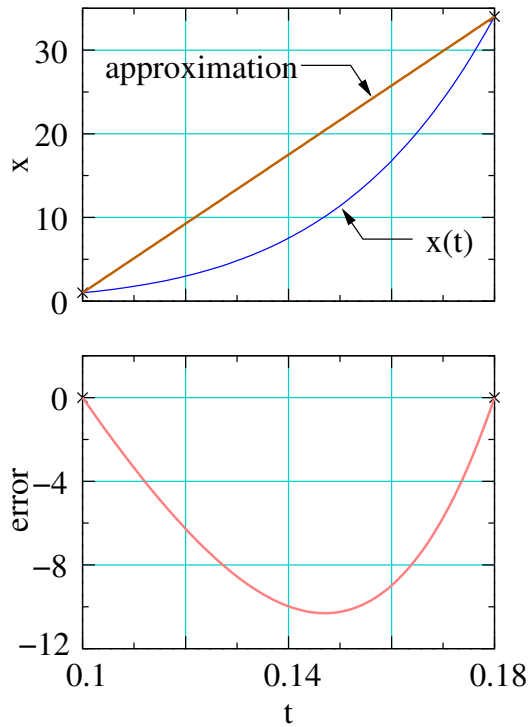
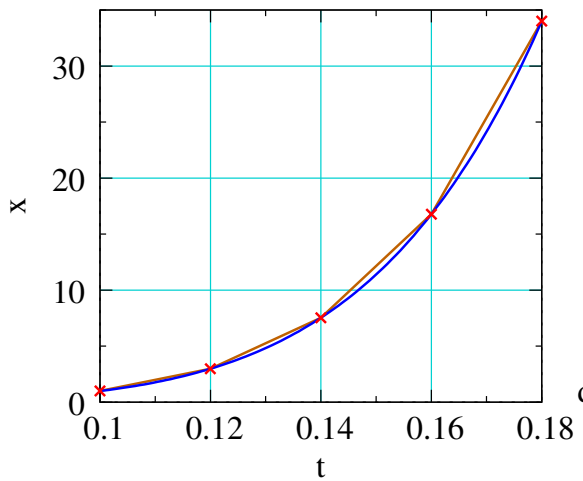


The fit can be improved in two ways:

* Reduce the time step.
* Use a higher-order polynomial.

Multi-step methods for solving $\dot{x} = f(t, x)$

Use of a smaller time step:



solid line: x(t)

dashed line: approximation

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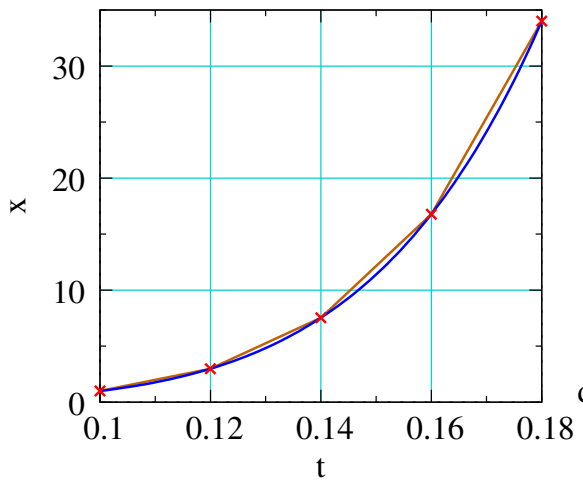

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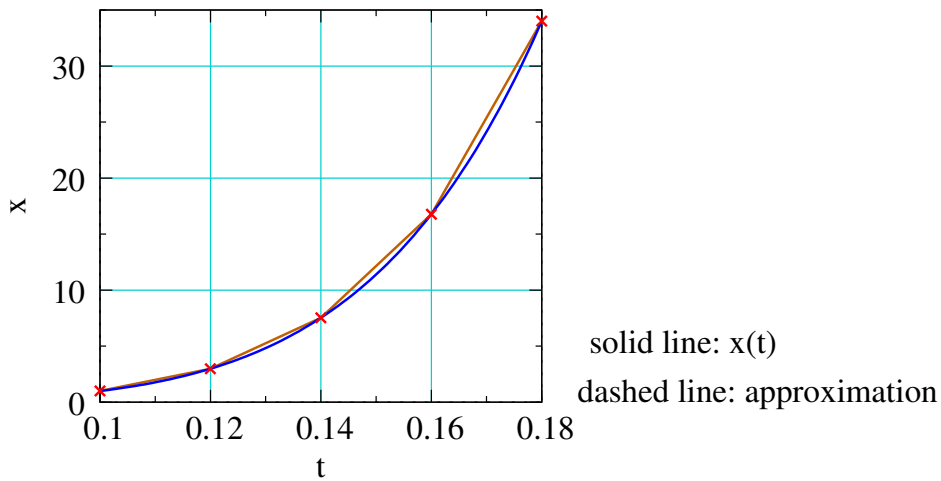
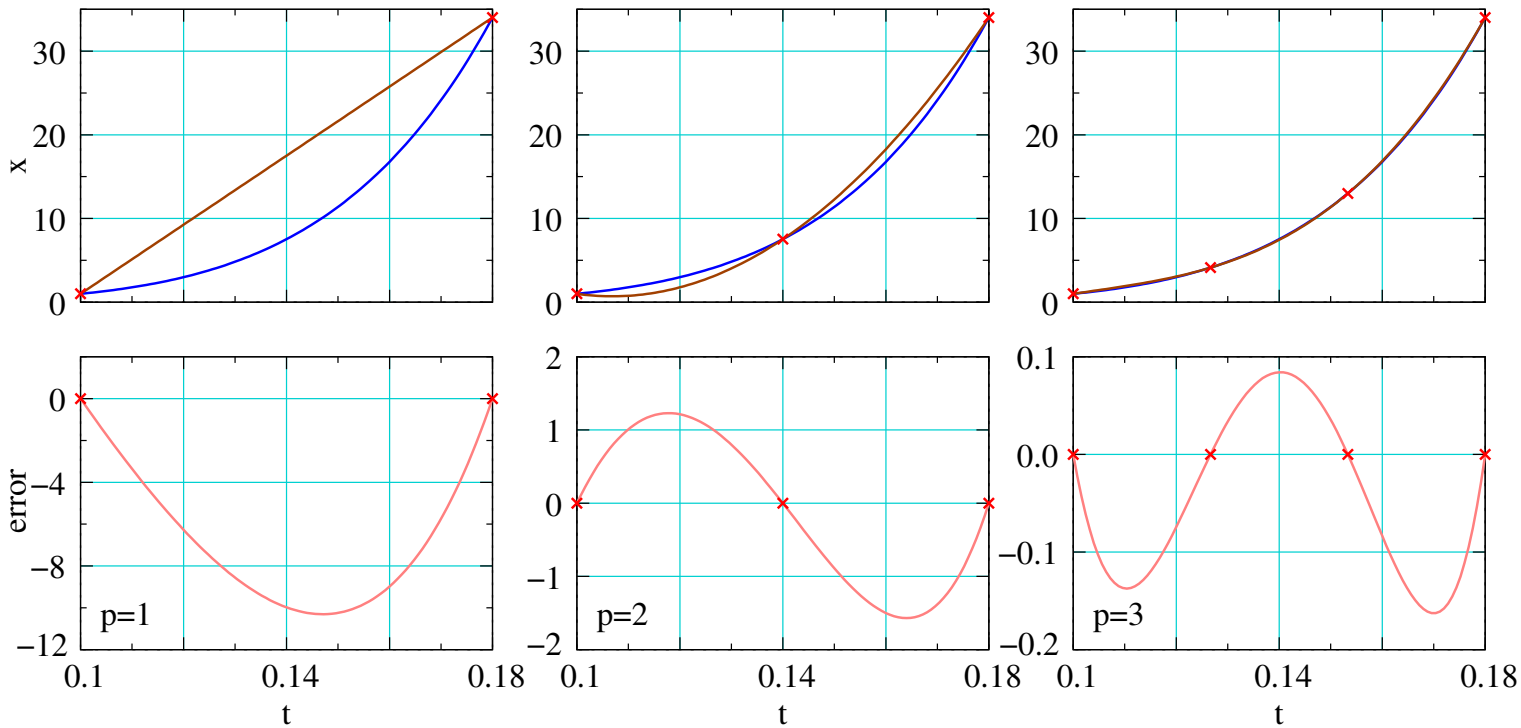


* The approximation is better when the step size is reduced.
* A larger number of time steps $\Rightarrow$ slower simulation

Multi-step methods for solving $\dot{x} = f(t, x)$

Use of a higher-order polynomial:



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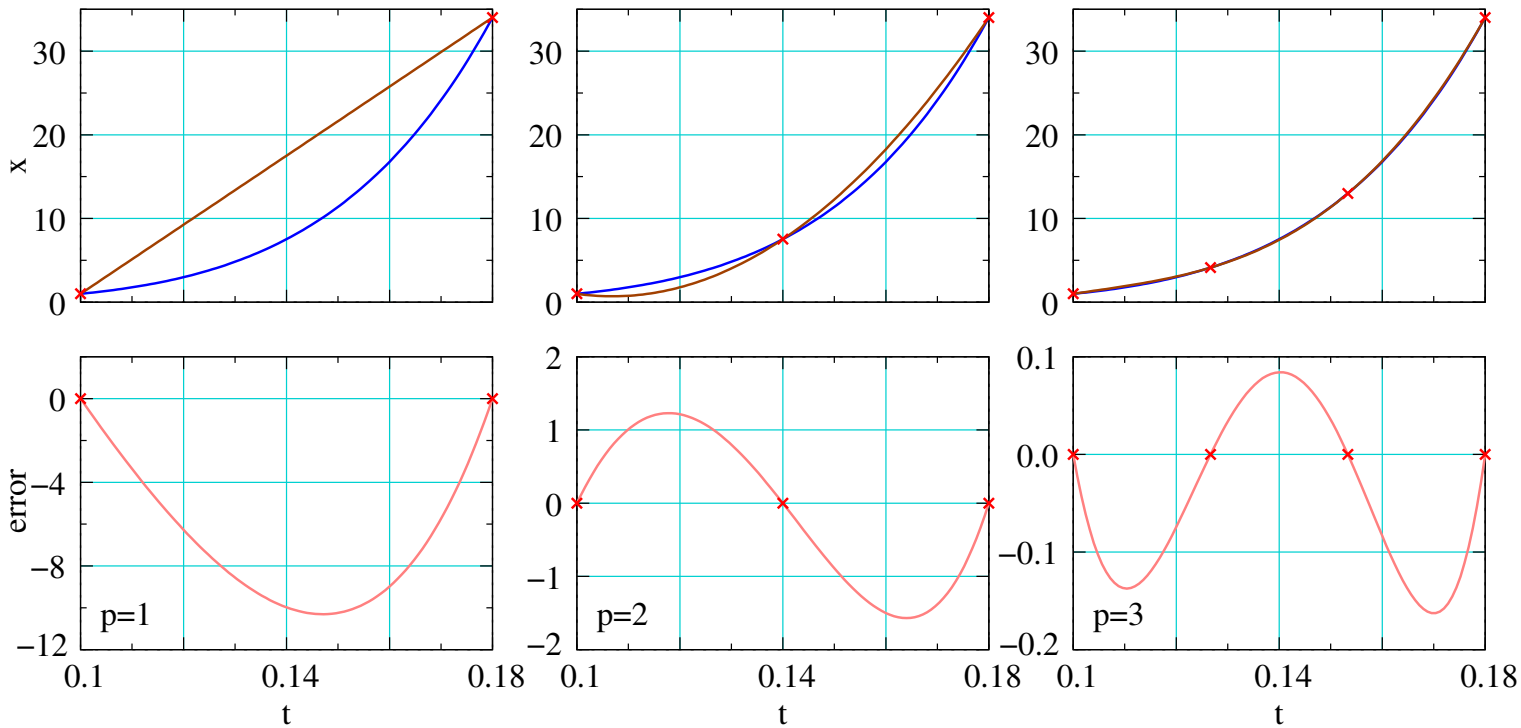

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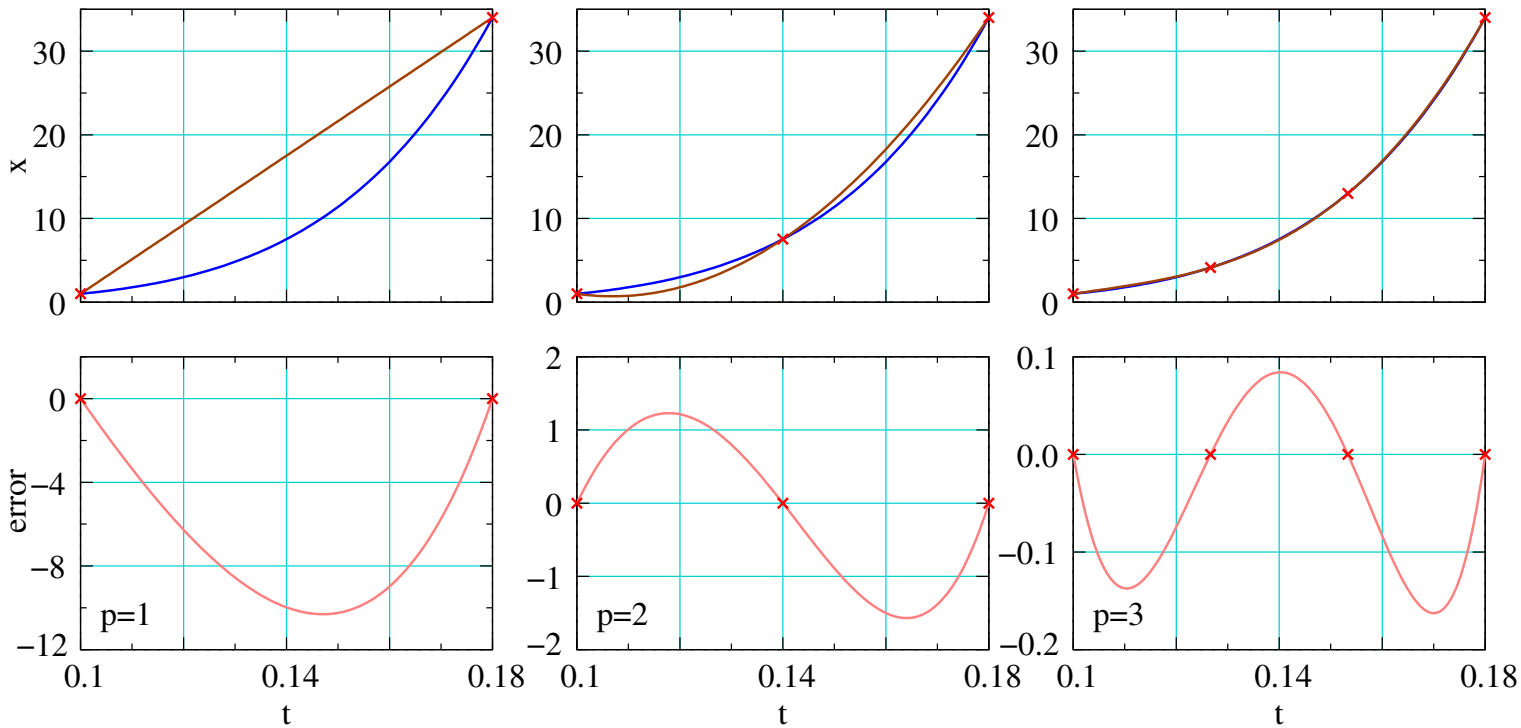

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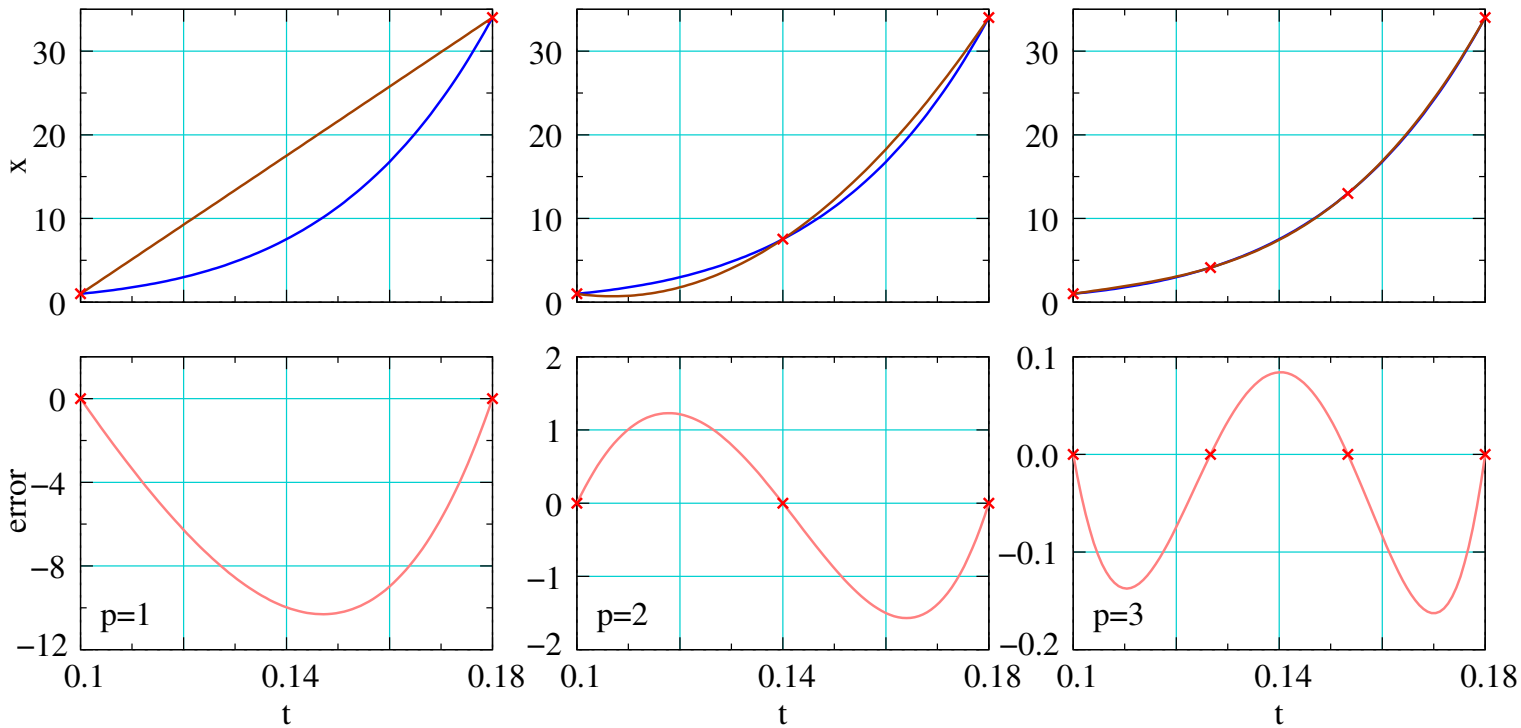
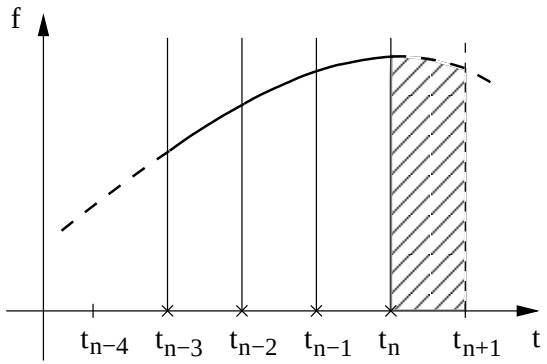
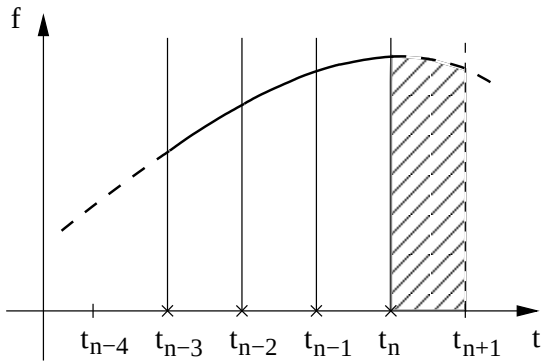


* The approximation is better when the order is increased.
* For fitting with a polynomial of order p, we need $(p + 1)$ points.
* The Adams-Bashforth and Adams-Moulton methods are based on approximating $x(t)$ with a polynomial.

Adams-Bashforth methods for $\dot{x} = f(t, x)$



Adams-Bashforth methods for $\dot{x} = f(t, x)$



* Motivation:

$$\begin{aligned} x(t_{n+1}) &= x(t_n) + \int_{t_n}^{t_{n+1}} x'(t)dt \\ &= x(t_n) + \int_{t_n}^{t_{n+1}} f\, dt\,. \end{aligned} \tag{3}$$

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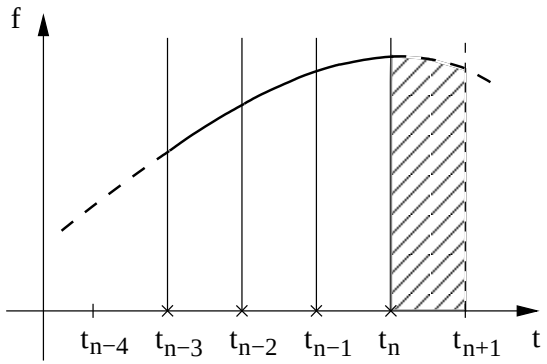

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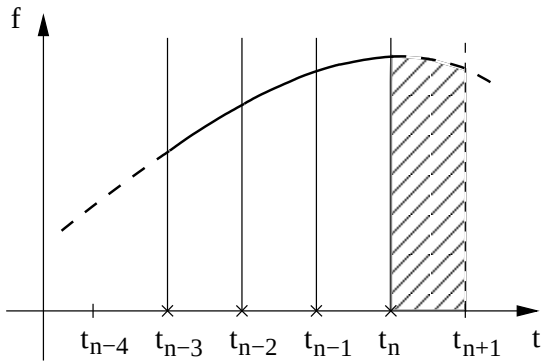

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Adams-Bashforth methods for $\dot{x} = f(t, x)$

The AB formula of order p is given by,

$$x(t_{n+1}) = x(t_n) + h \sum_{i=0}^{p-1} \beta_i \, f_{n-i} \ . \tag{4}$$

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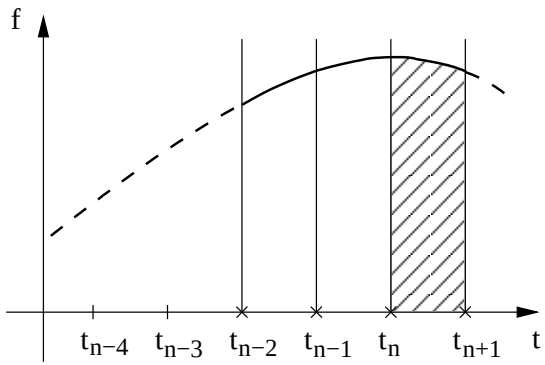
Order	β_0	β_1	β_2	β_3	β_4	β_5	LTE
1	1						$\frac{1}{2} h^2 x''(\xi_0)$
2	$\frac{3}{2}$	$-\frac{1}{2}$					$\frac{5}{12} h^3 x^{(3)}(\xi_0)$
3	$\frac{23}{12}$	$-\frac{16}{12}$	$\frac{5}{12}$				$\frac{9}{24} h^4 x^{(4)}(\xi_0)$
4	$\frac{55}{24}$	$-\frac{59}{24}$	$\frac{37}{24}$	$-\frac{9}{24}$			$\frac{251}{720} h^5 x^{(5)}(\xi_0)$
5	$\frac{1901}{720}$	$-\frac{2774}{720}$	$\frac{2616}{720}$	$-\frac{1274}{720}$	$\frac{251}{720}$		$\frac{475}{1440} h^6 x^{(6)}(\xi_0)$
6	$\frac{4277}{1440}$	$-\frac{7923}{1440}$	$\frac{9982}{1440}$	$-\frac{7298}{1440}$	$\frac{2877}{1440}$	$-\frac{475}{1440}$	$\frac{19,087}{60,480} h^7 x^{(7)}(\xi_0)$

(Note that the AB1 formula is the same as Forward Euler.)

Adams-Moulton methods for $\dot{x} = f(t, x)$



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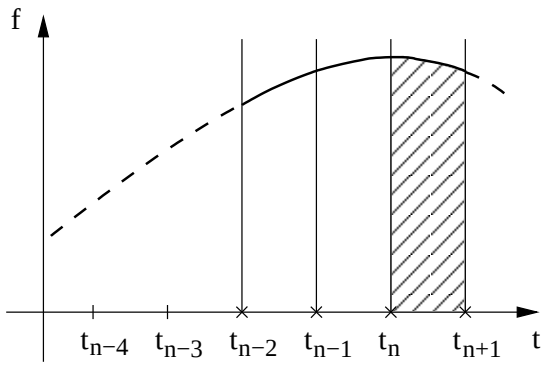

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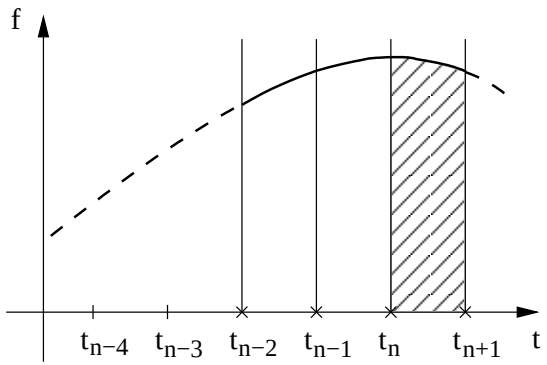

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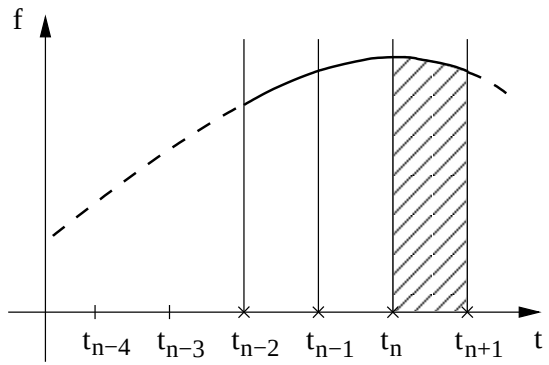

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Adams-Moulton methods for $\dot{x} = f(t, x)$

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* The AM1 and AM2 formulas are the same as the Backward Euler and trapezoidal methods, respectively.
* By comparing the LTE columns in the AB and AM tables, we see that, for the same order, the AM formula is more accurate.

Backward Differentiation Formulas (BDF): Gear's formulas

We are looking for $x(t)$ which will satisfy the ODE at $t = t_{n+1}$, i.e.,

$$\dot{x}(t_{n+1}) = f(t_{n+1}, x_{n+1})\,. \tag{7}$$

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* Replace the LHS of Eq. 7 with $\dot{\tilde{x}}(t)$ at $t = t_{n+1}$. $\Rightarrow$ BDF formula
* BDFs are implicit in nature since $f(t_{n+1}, x_{n+1})$ appears in the formula.

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

The general form of the BDF of order p is,

$$\sum_{i=-1}^{p-1} \alpha_i \, x_{n-i} = h \, f(t_{n+1}, x_{n+1}) \, . \tag{8}$$

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Order	α_{-1}	α_0	α_1	α_2	α_3	α_4	α_5	LTE
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2	$\frac{3}{2}$	-2	$\frac{1}{2}$					$-\frac{2}{9} h^3 x'''(\xi)$
3	$\frac{11}{6}$	-3	$-\frac{3}{2}$	$-\frac{1}{3}$				$-\frac{3}{22} h^4 x^{(4)}(\xi)$
4	$\frac{25}{12}$	-4	3	$-\frac{4}{3}$	$\frac{1}{4}$			$-\frac{12}{125} h^5 x^{(5)}(\xi)$
5	$\frac{137}{60}$	-5	5	$-\frac{10}{3}$	$\frac{5}{4}$	$-\frac{1}{5}$		$-\frac{10}{137} h^6 x^{(6)}(\xi)$
6	$\frac{147}{60}$	-6	$\frac{15}{2}$	$-\frac{20}{3}$	$\frac{15}{4}$	$-\frac{6}{5}$	$\frac{1}{6}$	$-\frac{60}{1029} h^7 x^{(7)}(\xi)$

(Note that the BDF1 formula is the same as the Backward Euler method.)

Outline

* Introduction and problem definition
* Taylor series methods
* Runge-Kutta methods
* Specific multi-step methods
* Generalized multi-step methods
* Predictor-corrector methods
* Numerical results
* Stability of numerical methods
* Regions of stability
* Stiff equations
* Adaptive step size
* Miscellaneous topics

The AB, AM, and BDF methods are special cases of "linear multi-step methods" (LMM) given by,

$$\sum_{i=-1}^{k} \alpha_i \, x_{n-i} = h \sum_{i=-1}^{k} \beta_i \, f(t_{n-i}, x_{n-i}) \, .$$

Method	k	α_i	β_i
AB	$p-1$	$\alpha_i = 0, \quad i = 1$ to k	$\beta_{-1} = 0$
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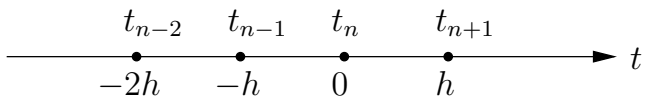
* What is so special about the AM, AB, and BDF methods? (to be discussed)

Exactness constraints for LMMs [6] for solving $\dot{x} = f(t, x)$



As an example, consider the LMM given by,

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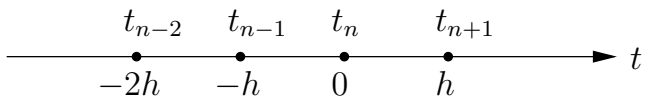

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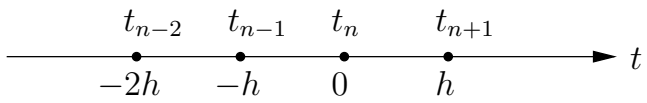

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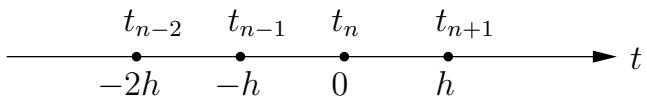

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Similarly, the other two exactness constraints can be derived.

Exactness constraints for LMMs for solving $\dot{x} = f(t, x)$

x	f	x_{n+1}	Constraint
1	0	1	$\alpha_{-1} + \alpha_0 + \alpha_1 = 0$
t	1	h	$\alpha_{-1} - \alpha_1 = \beta_{-1}$
t^2	$2\,t$	h^2	$\alpha_{-1} + \alpha_1 = 2\,\beta_{-1}$

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$$\frac{3}{2}\,x_{n+1} - 2\,x_n + \frac{1}{2}\,x_{n-1} = h\,f_{n+1}\,.$$

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* This is the same as the BDF2 formula.

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& \vdots \qquad\qquad\qquad \vdots \\
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  - Repeat to the desired tolerance.

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* Generally, one or two CE steps give a substantially better accuracy (over the predicted x_{n+1}).

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step size (h)		0.05	0.1	0.2
predicted $x(h)$		1.05	1.1	1.2
corrected $x(h)$	(1)	1.04993750	1.09950000	1.19600000
	(2)	1.04993766	1.09950499	1.19615840
	(3)	1.04993766	1.09950494	1.19615219
	(4)	1.04993766	1.09950494	1.19615243
	(5)	1.04993766	1.09950494	1.19615242
$x(h)$ (TRZ)		1.04993766	1.09950494	1.19615242
$x(h)$ (exact)		1.04995837	1.09966799	1.19737532
LTE		2.0719×10^{-5}	1.6306×10^{-4}	1.2229×10^{-3}

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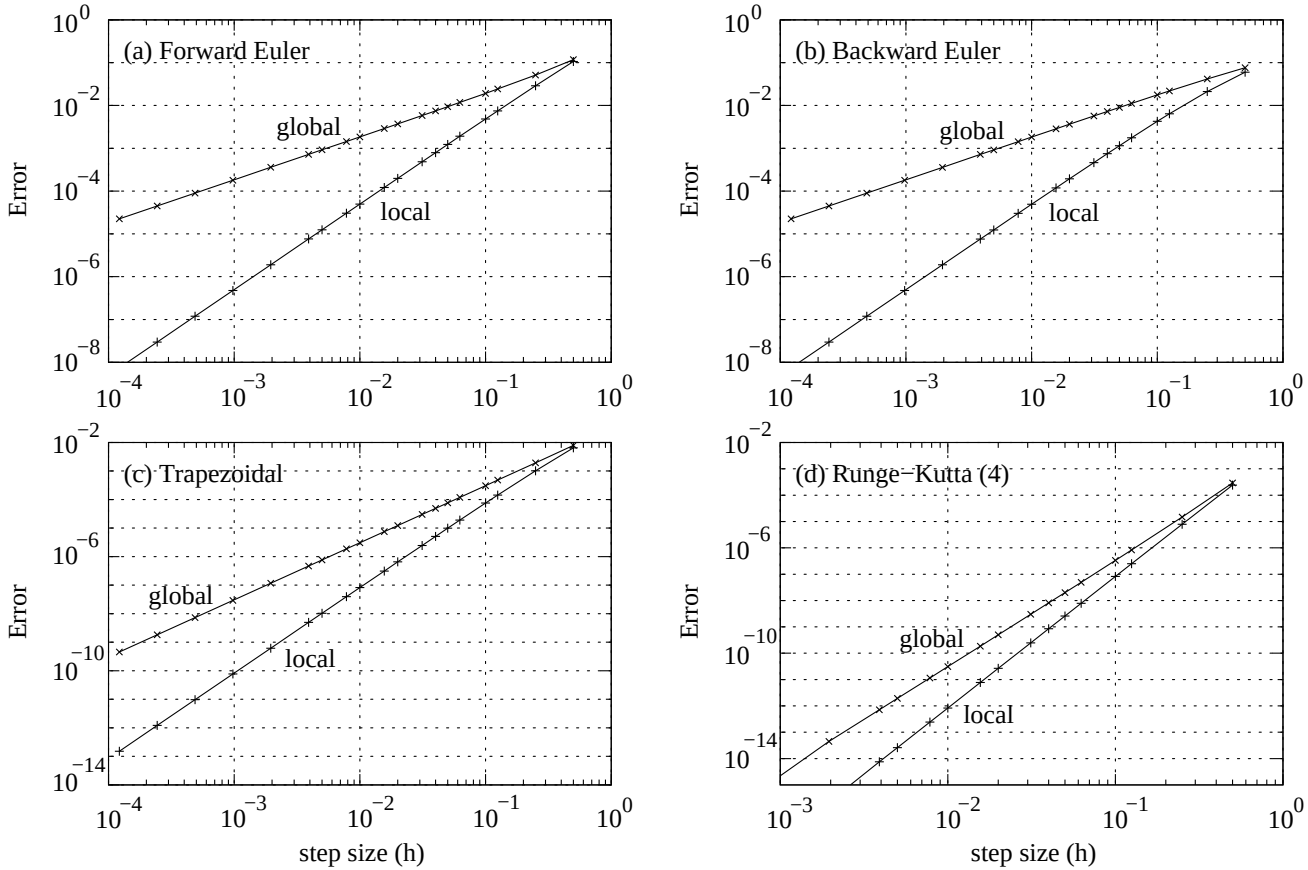
Numerical examples: local/global error versus h



Local and global errors versus step size h for $\dot{x} = -x$, with $x(0) = 1$, for Forward Euler, Backward Euler, Trapezoidal, and Runge-Kutta (4^{th} order) methods. The local error has been computed for the first step, i.e., from $t = 0$ to $t = h$. The global error has been computed at $t = 1$.

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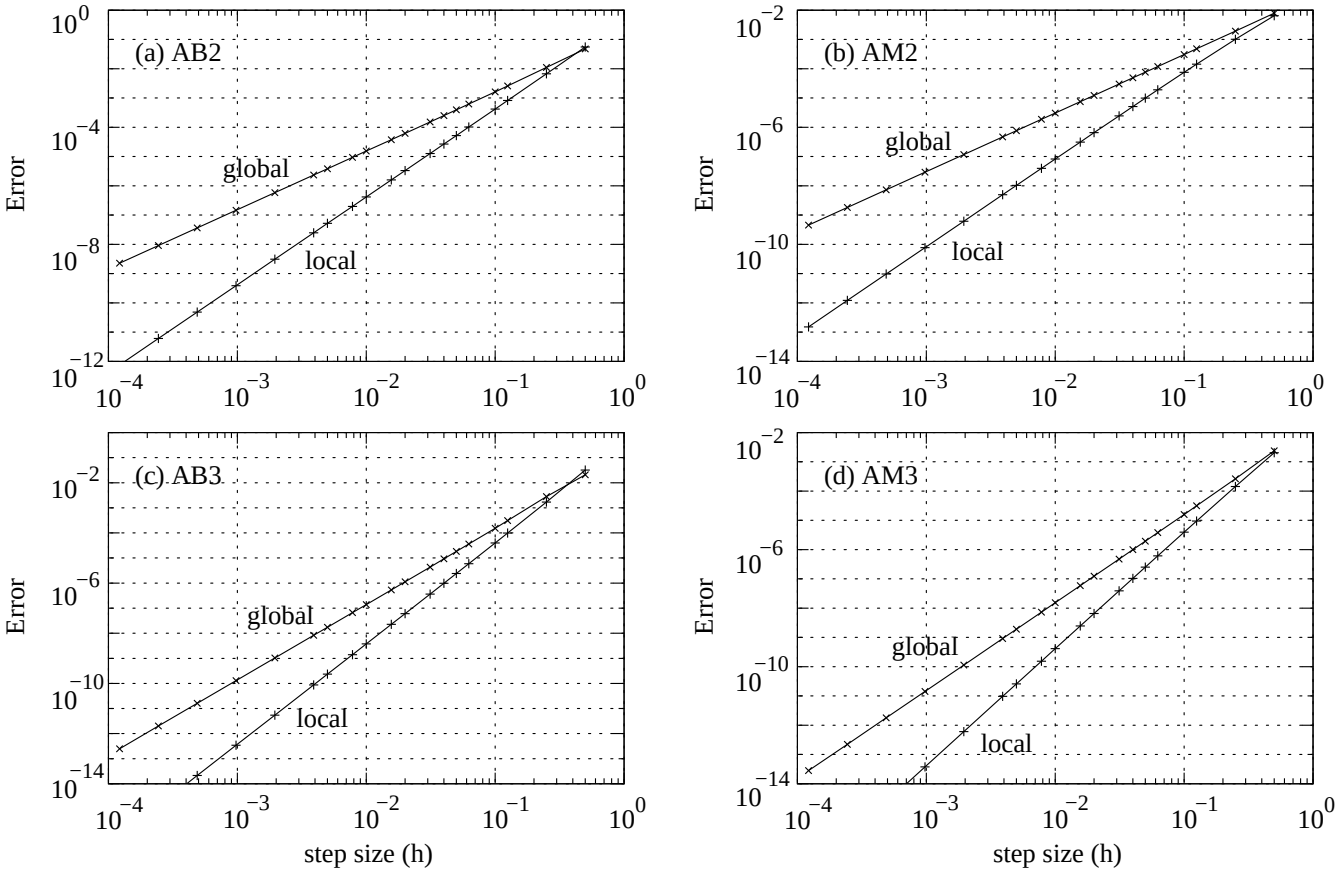

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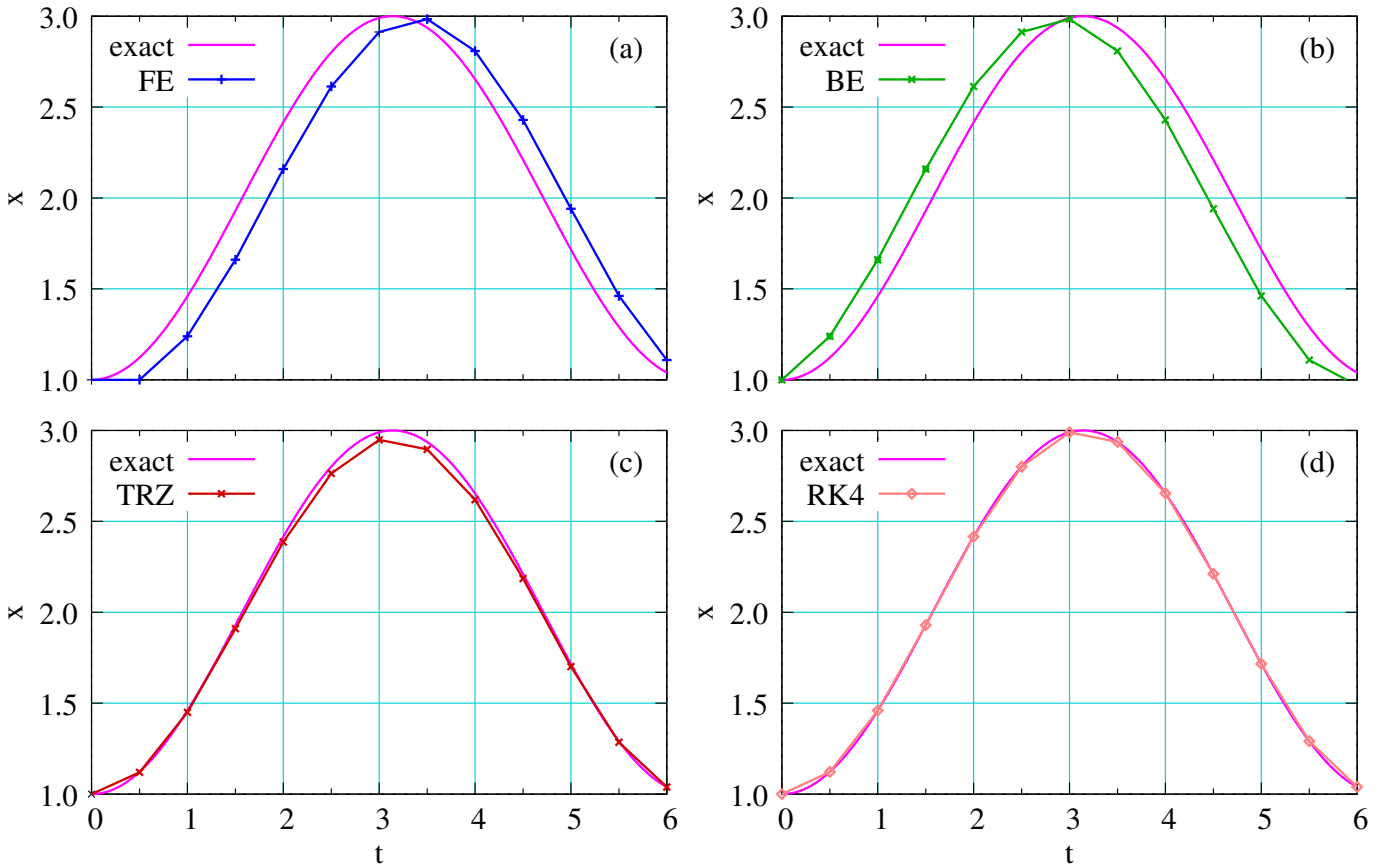
Numerical examples: comparison of methods



Exact and numerical solutions for $\dot{x} = \sin(t)$, with $x(0) = 1$. (a) Forward Euler, (b) Backward Euler, (c) Trapezoidal, and (d) Runge-Kutta (4^{th} order).

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  NO. Need to worry about *stability*.

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Stability of numerical methods for $\dot{x} = f(t, x)$

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* Runge-Kutta methods are stable.
* Linear multi-step methods (LMMs) can be unstable.

Stability for small h: LMMs

Consider a linear multi-step method of order p,

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* If the difference between the original numerical solution (x_n^{orig}) and the numerical solution of the perturbed problem (x_n^{new}) is such that,

$$\max |x_n^{\text{orig}} - x_n^{\text{new}}| \leq S \max(|\Delta|, \max |\delta_n|) \, ,$$

then the method is called *zero-stable* or *D-stable* (after Dahlquist) or simply *stable*.

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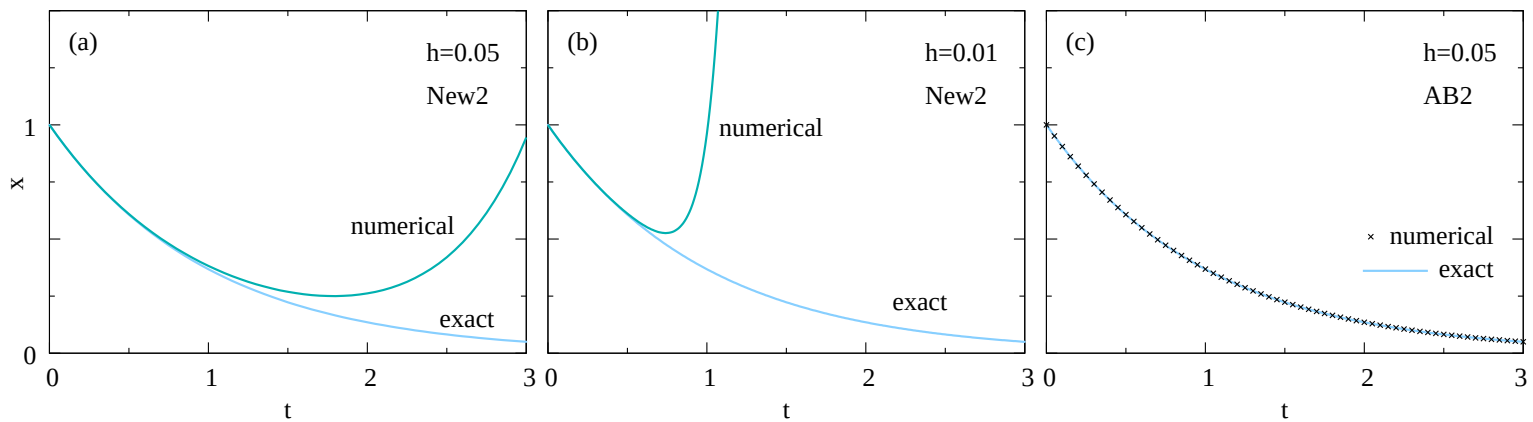

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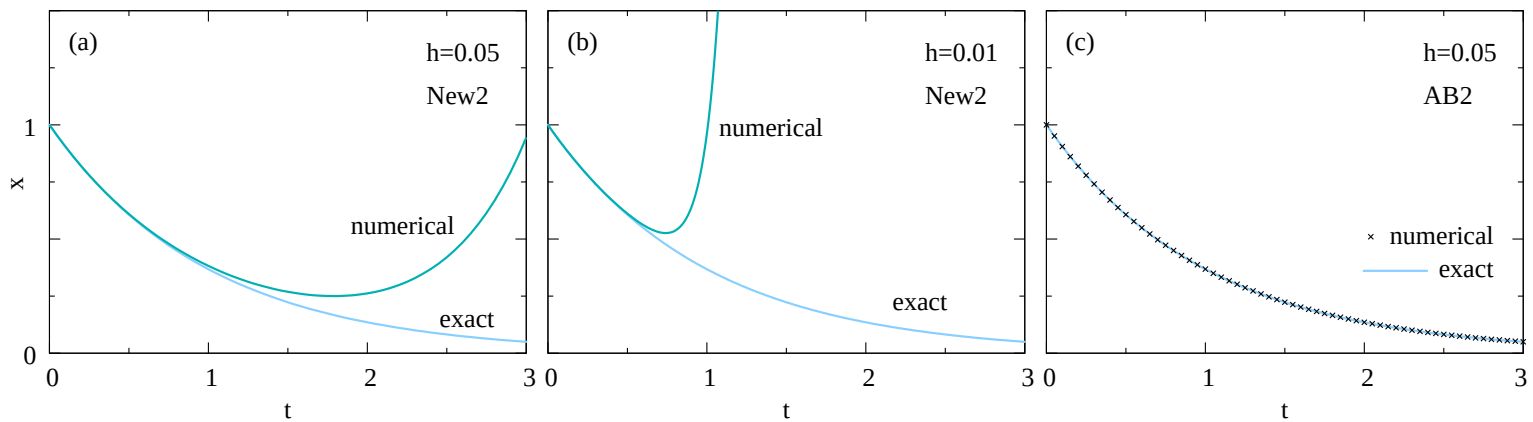

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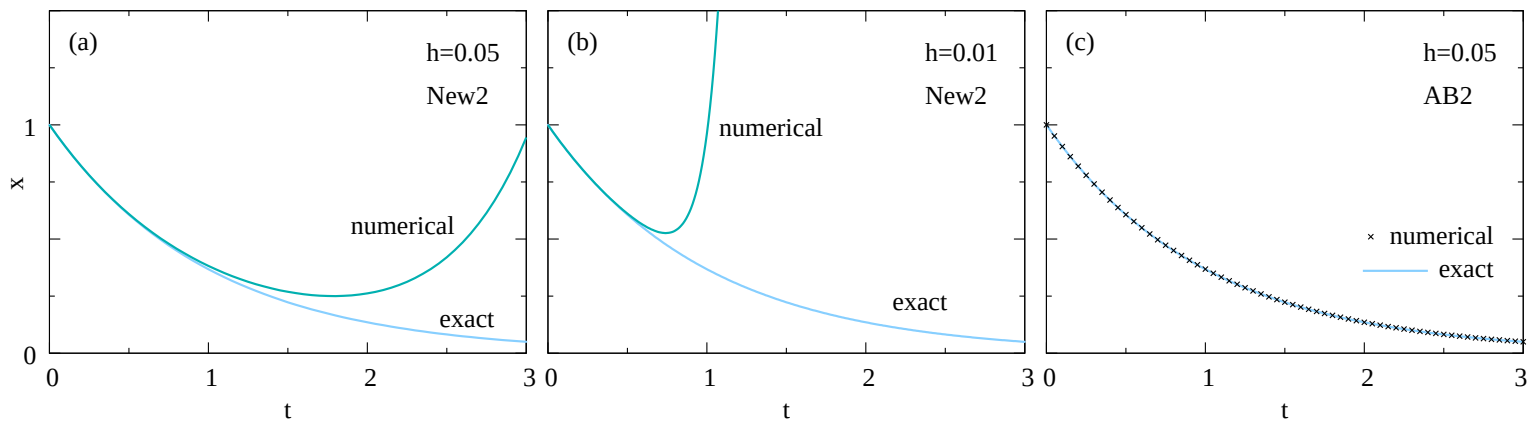

* New2 is unstable while AB2 is stable.
* Why are these two methods so different?

Difference equations: general solution

Consider a linear difference equation with constant (real) coefficients,

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* Eq. 13 is called the *characteristic equation* of the difference equation (Eq. 11).

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* If the roots of the characteristic equation, z_1, $z_2, \cdots$, z_k, are distinct, then the general solution of Eq. 12 is given by

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* The complete solution of Eq. 11 is then given by,

$$x_i = x_i^{(h)} + x_i^{(p)} \,, \tag{16}$$

where $x_i^{(p)}$ is a particular solution. The constants c_1, c_2, etc. can be determined from the initial condition(s), i.e., the starting values in the sequence $\{x_i\}$.

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associated with the LMM,

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Let the roots of Eq. 17 be z_1, $z_2, \cdots$, z_k. If $|z_i| \leq 1$ for all i, and all roots with magnitude 1 are simple, then the LMM is said to satisfy the *root condition*.

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* If an LMM does not satisfy the root condition, it is said to be *unstable*.

Coming back to AB2 and New2,

AB2	$x_{n+1} = x_n + h\,(1.5\,f_n - 0.5\,f_{n-1})$ char. eqn.: $z - 1 = 0$. roots: $z_1 = 1$.
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* Even if c_2 is forced to be zero because of initial conditions, numerical errors can make it non-zero.

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* $h_{\max}$ would depend on the ODE being solved. Generally, it is determined for the *test equation*,

$$\dot{x} = \lambda x, \qquad x(0) = 1\,, \tag{19}$$

where λ is a constant, a complex number in general. Eq. 19 is representative of several problems of practical importance, such as RC circuits.

Stability for large h (for $\dot{x} = \lambda x$, $x(0) = 1$)

Let λ be real and negative. Consider the Forward Euler method,

$$\begin{aligned} x_{n+1} &= x_n + h\, f(t_n, x_n) \\ &= x_n + h\lambda\, x_n \\ &= x_n\,(1 + h\lambda) \end{aligned} \tag{20}$$

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for which the general solution is given by,

$$\begin{aligned} x_i &= c_1\, z_1^i \\ &= (1 + h\lambda)^i\,. \end{aligned} \tag{22}$$

($c_1 = 1$ is required to satisfy the initial condition, $x_0 = 1$.)

Stability for large h (for $\dot{x} = \lambda x$, $x(0) = 1$)

* The exact solution is $x(t) = \exp(\lambda t)$ which, for $t_k = kh$ and $|h\lambda| \ll 1$, is

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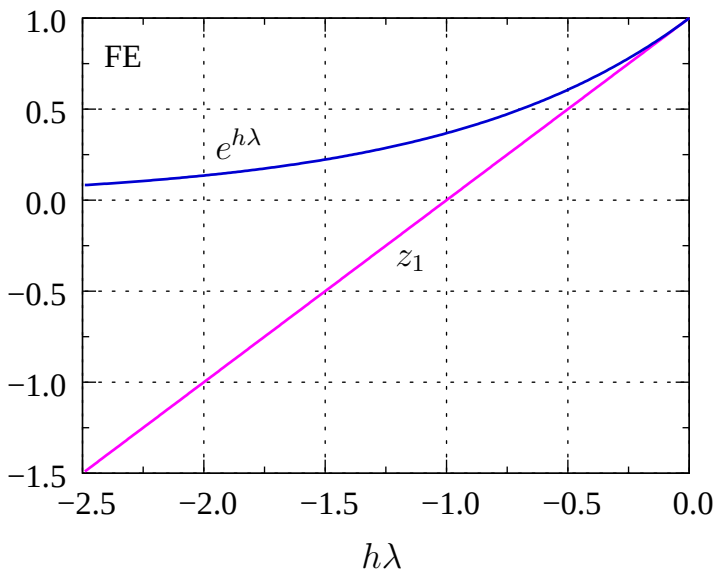
* As h is increased, $z_1 = 1 + h\lambda$ decreases (since $\lambda < 0$), and for $h\lambda = -2$, z_1 becomes equal to -1 (see figure). Beyond this point, $|z_1| > 1$, and the numerical solution ($x_k = c_1 \, z_1^k$) grows indefinitely with $k \Rightarrow$ instability.



Stability for large h (for $\dot{x} = \lambda x$, $x(0) = 1$)

Consider the second-order Adams-Bashforth method. The difference equation is,

$$x_{n+1} = x_n + h\lambda \left[\frac{3}{2} x_n - \frac{1}{2} x_{n-1} \right] .$$

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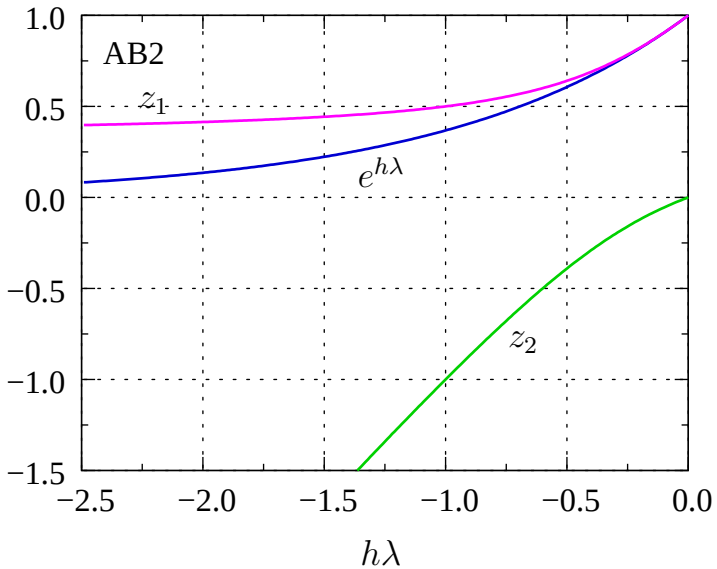
$$z_{1,2} = \frac{1}{2} \left\{ \left(1 + \frac{3h\lambda}{2} \right) \pm \sqrt{\left(1 + \frac{3h\lambda}{2} \right)^2 - 2h\lambda} \right\} ,$$

and the general solution,

$$x_i = c_1 z_1^i + c_2 z_2^i .$$

Stability for large h (AB2 method for $\dot{x} = \lambda x$, $x(0) = 1$)



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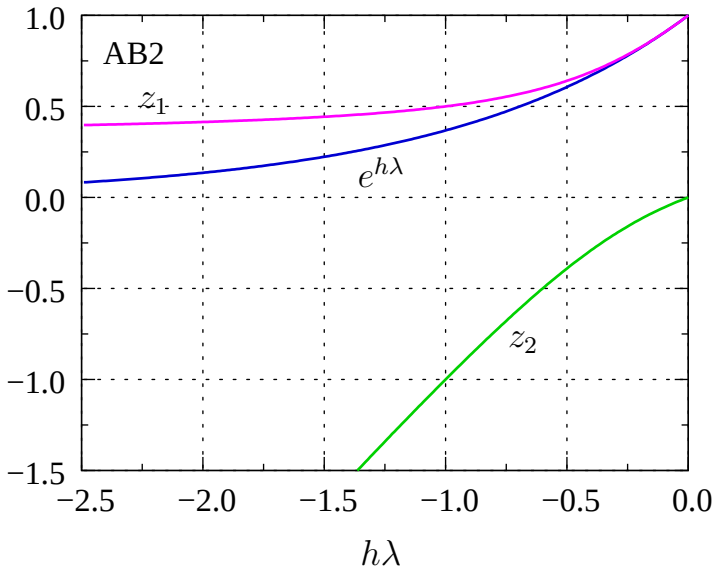

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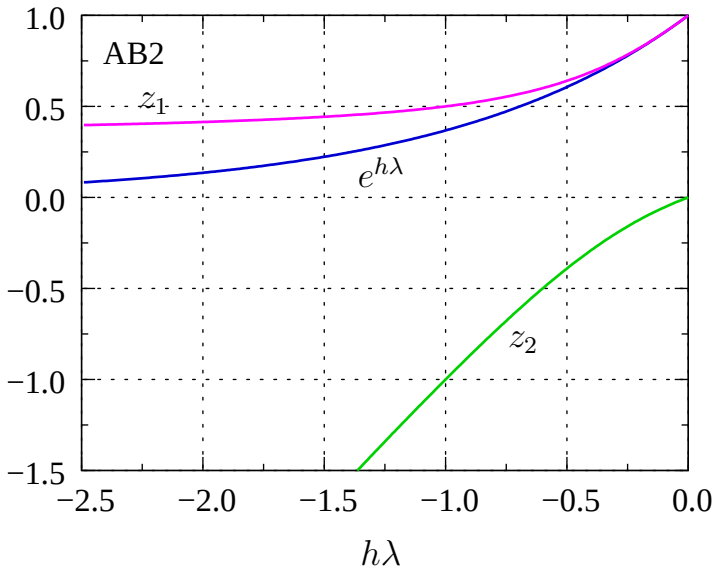

* For small values of $h\lambda$, z_1 represents $e^{h\lambda}$ more closely than in the FE method, as we would expect from a second-order method.
* What is of concern, from the stability angle, is the other root z_2 which starts off at zero, but becomes greater than one in magnitude at $h\lambda = -1$, thus leading to instability.

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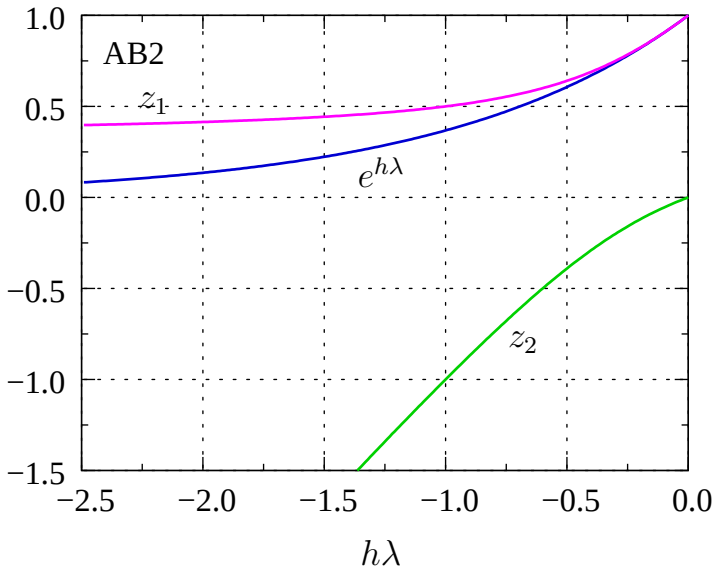

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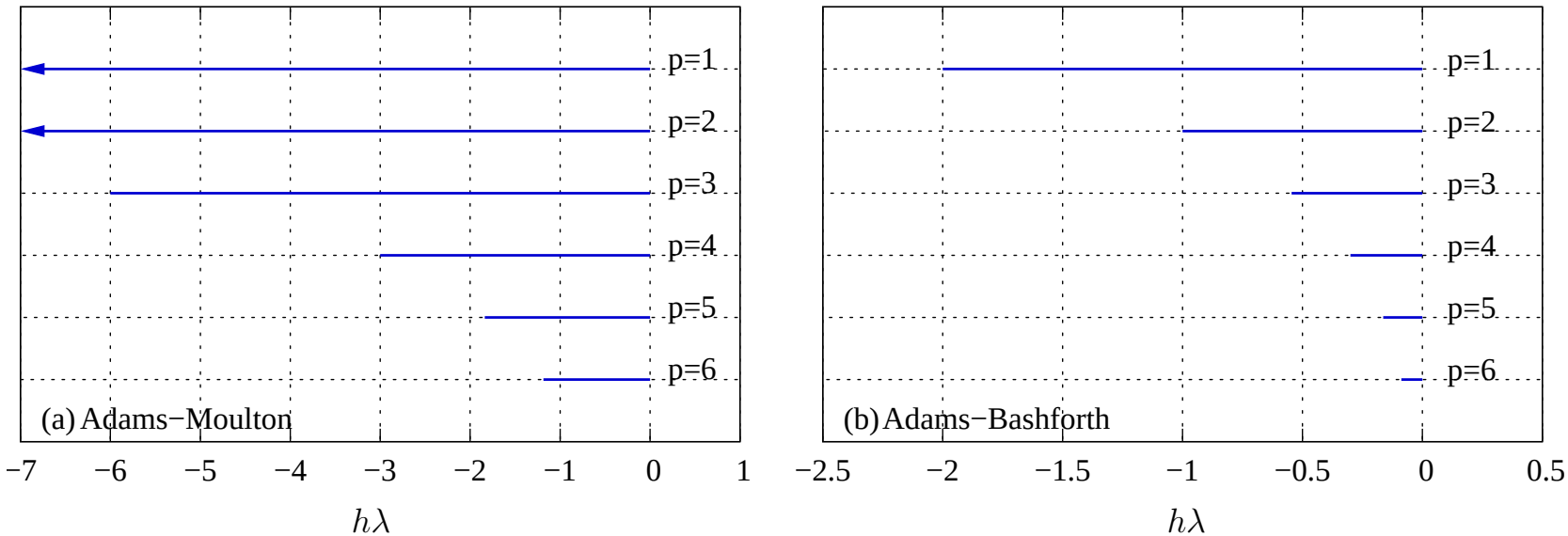
* What is of concern, from the stability angle, is the other root z_2 which starts off at zero, but becomes greater than one in magnitude at $h\lambda = -1$, thus leading to instability.
* This root is not *required* to represent $e^{h\lambda}$, and in that sense, it is a *parasitic* or *spurious* root. In contrast, the root z_1, which approximates $e^{h\lambda}$, is called the *principal* root.

Stability for large h: AB and AM methods for $\dot{x} = \lambda x$, $\lambda < 0$



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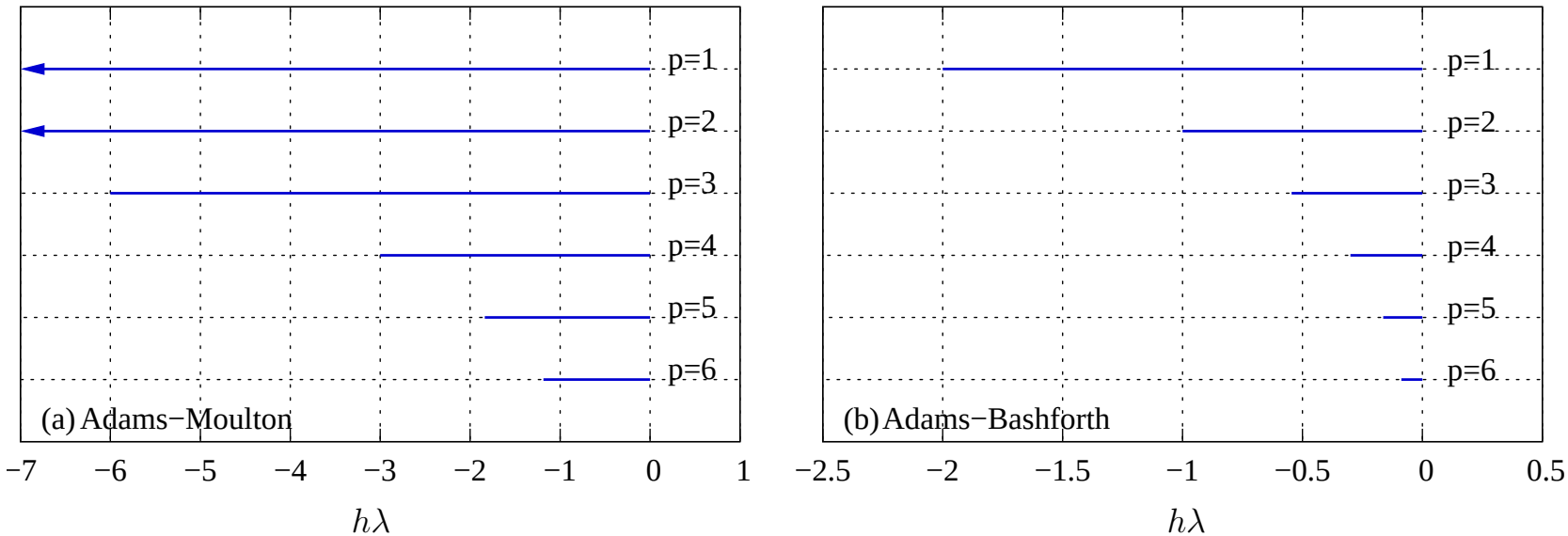

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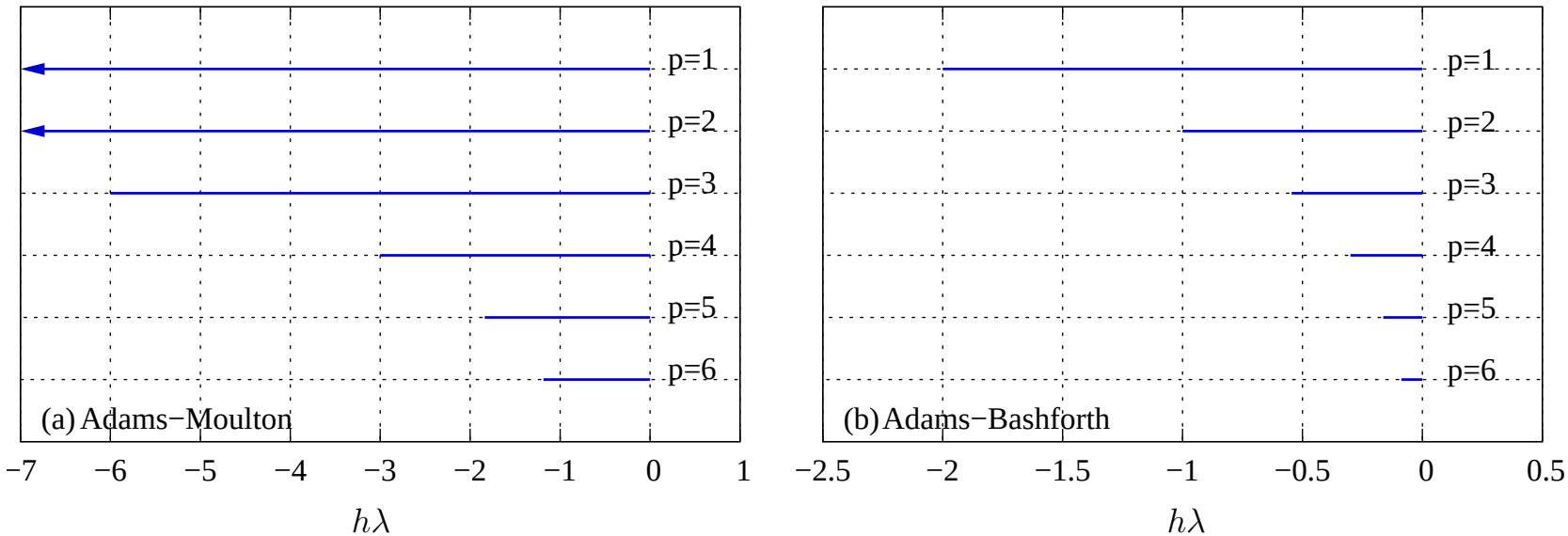

* The AM methods, for the same order, are more stable than the AB methods.
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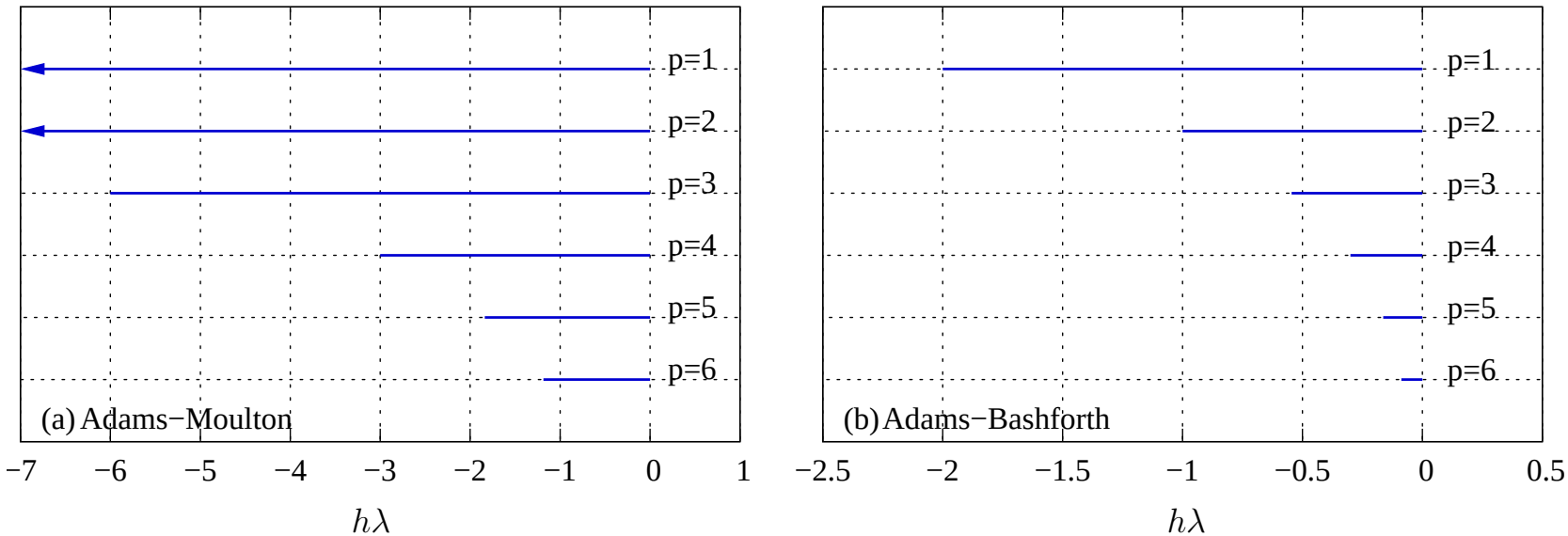
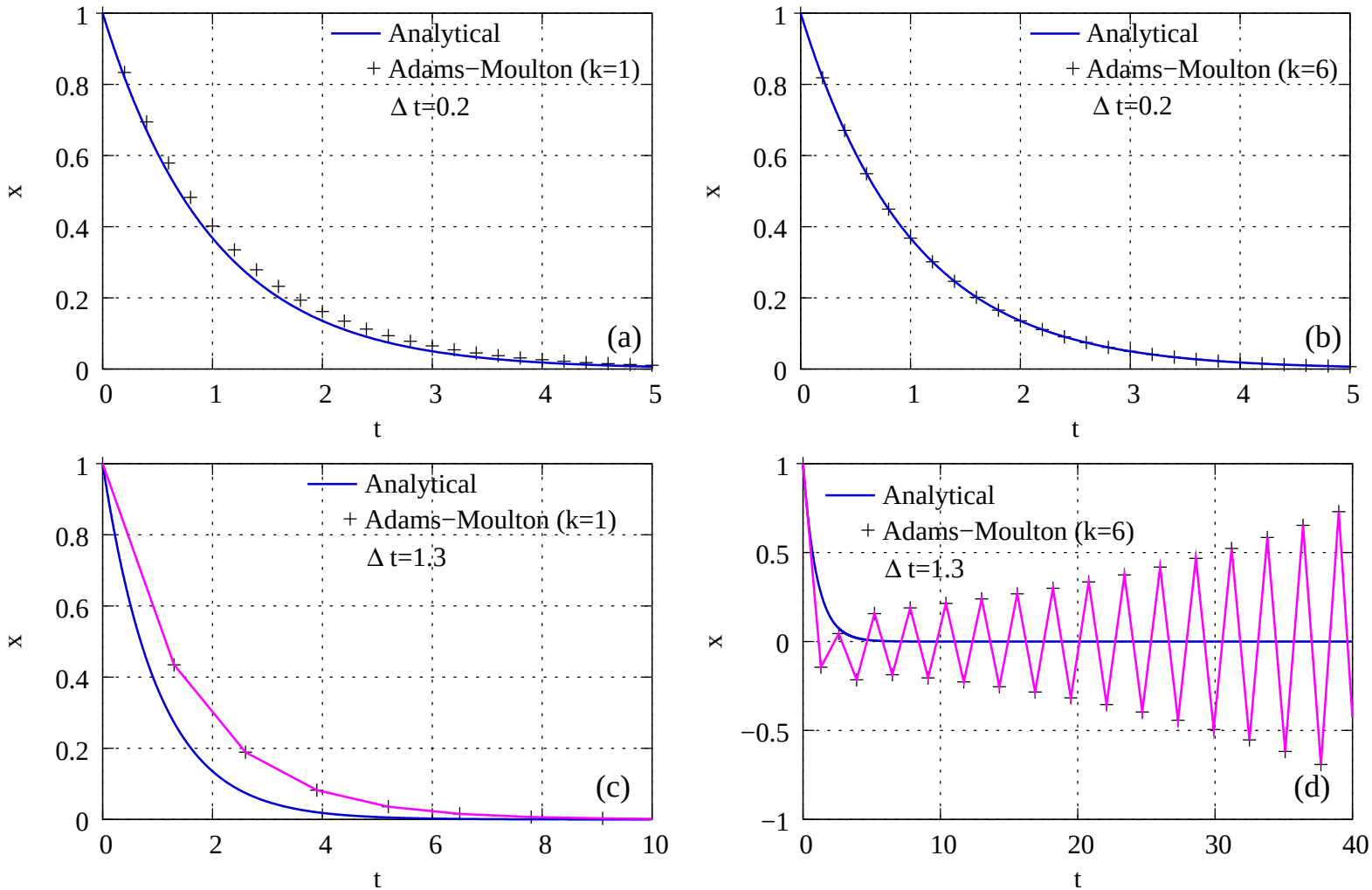


* The AM methods, for the same order, are more stable than the AB methods.
* The AM methods of order 1 and 2 (the BE and TRZ methods) are stable for all values of $h\lambda$.
* As the order increases, the range of stability becomes smaller for both AB and AM methods. This explains why higher-order methods are not used in circuit simulation.

Stability for large h: AM1 and AM6 methods for $\dot{x} = -x$, $x(0) = 1$



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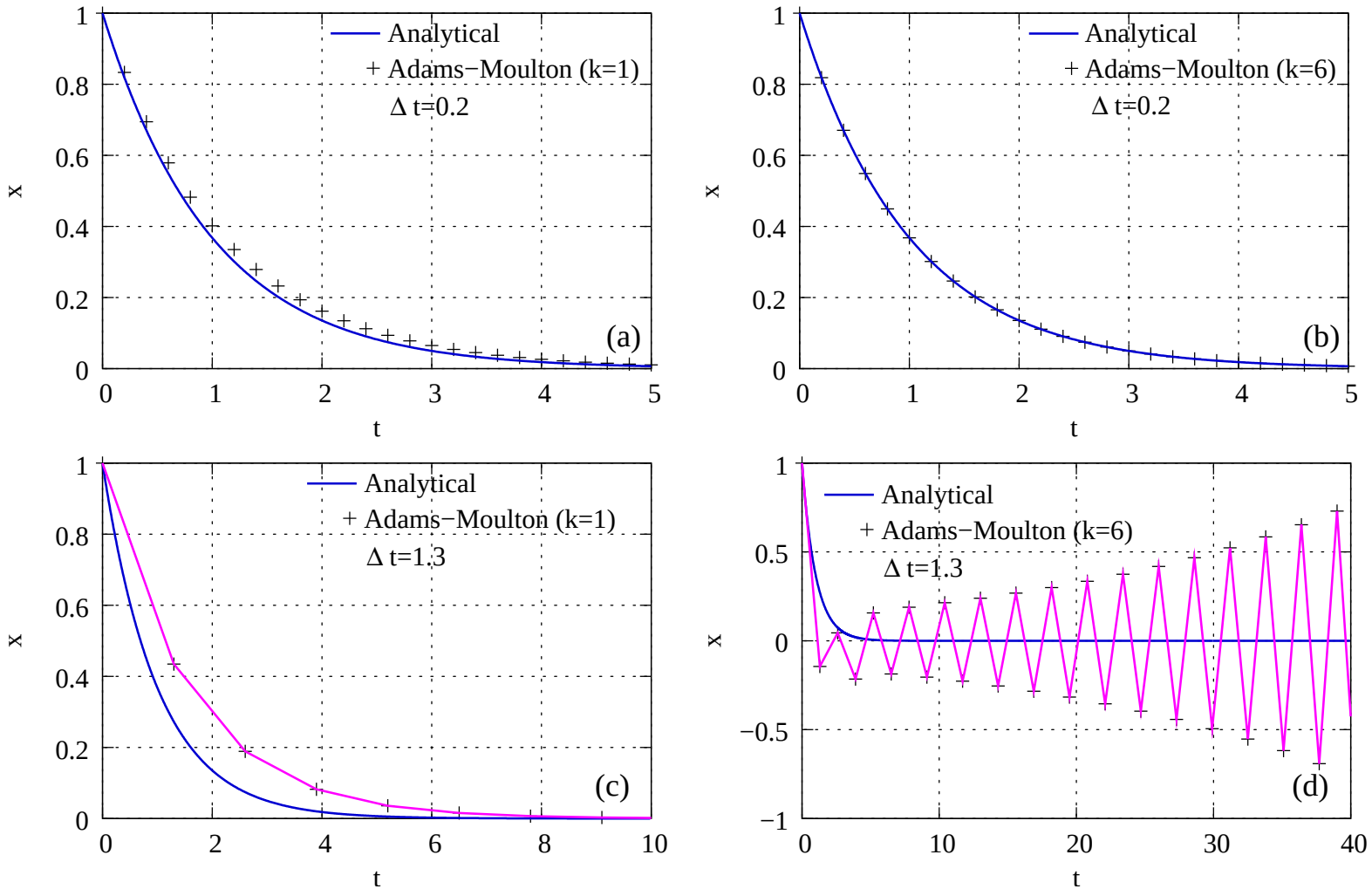

* AM6 is more accurate than AM1 (upper figures).

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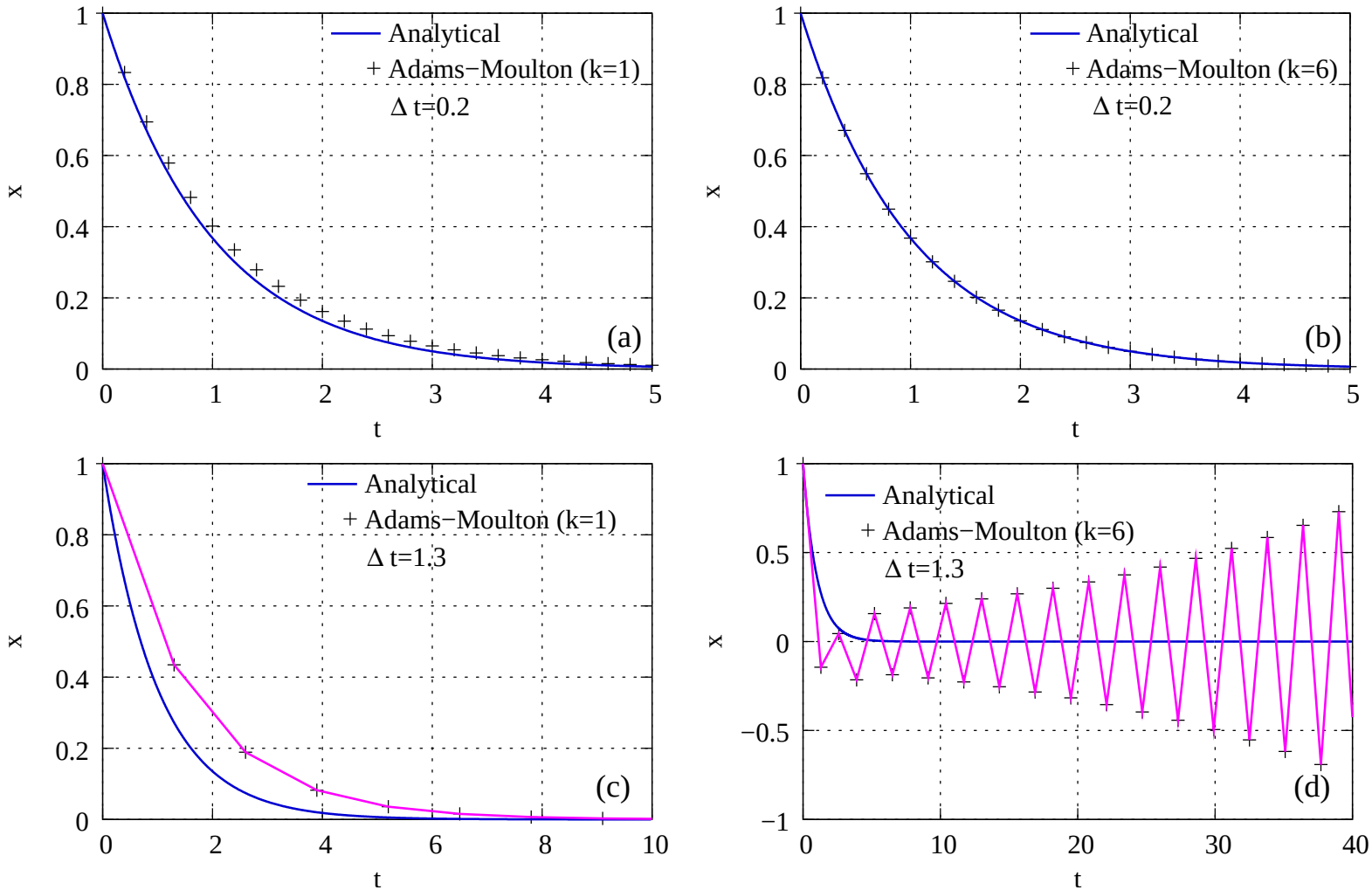

* AM6 is more accurate than AM1 (upper figures).
* For $\Delta t = 1.3$, AM1 is stable, but AM6 is not (lower figures).

Consider the 2×2 system of ODEs, $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$, which may be written in the expanded form,

$$\begin{aligned} \dot{x_1} &= a_{11}x_1 + a_{12}x_2 \,, \\ \dot{x_2} &= a_{21}x_1 + a_{22}x_2 \,, \end{aligned} \tag{23}$$

with $x_1(0) = x_1^0$ and $x_2(0) = x_2^0$.

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Eq. 23 can be re-written in a diagonalized form,

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$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} \mathbf{S_1} & \mathbf{S_2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} . \tag{25}$$

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Solving the system of ODEs, Eq. 23, is thus equivalent to solving two separate ODEs. Since λ_1, λ_2 are generally complex, we are interested in solving $\dot{x} = \lambda x$ when λ is complex.

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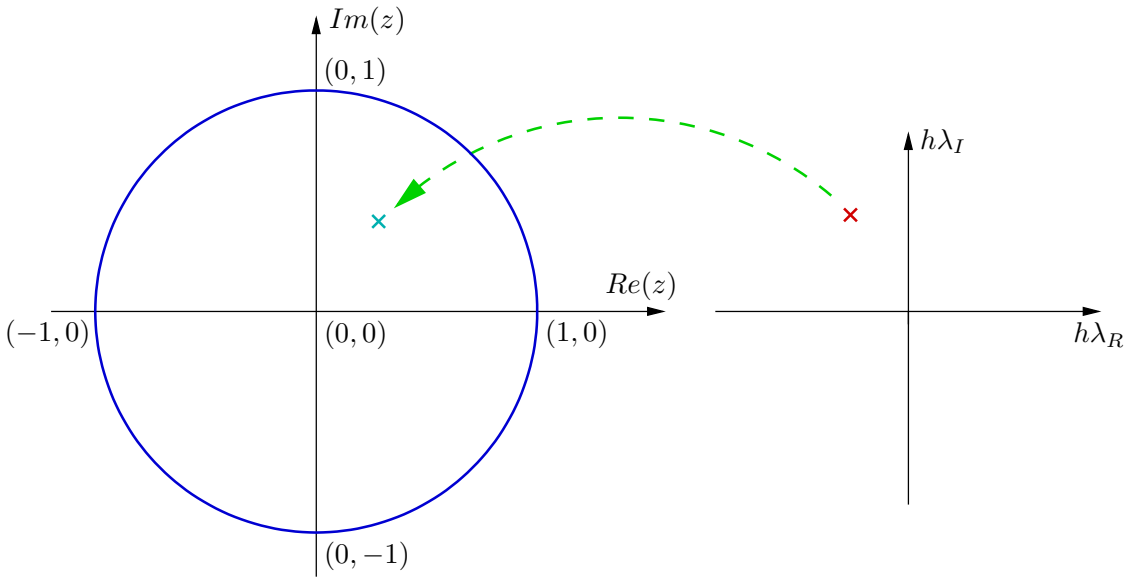
Stability for large h ($\dot{x} = \lambda x$, complex λ)

* A method is said to be *absolutely stable* (with respect to the test equation) for a given $h\lambda$ with $\mathrm{Re}(\lambda) < 0$ if all the roots of the characteristic equation lie inside the unit circle in the $h\lambda$ plane. The set of all such $h\lambda$ is called the *region of absolute stability* of the method [5].



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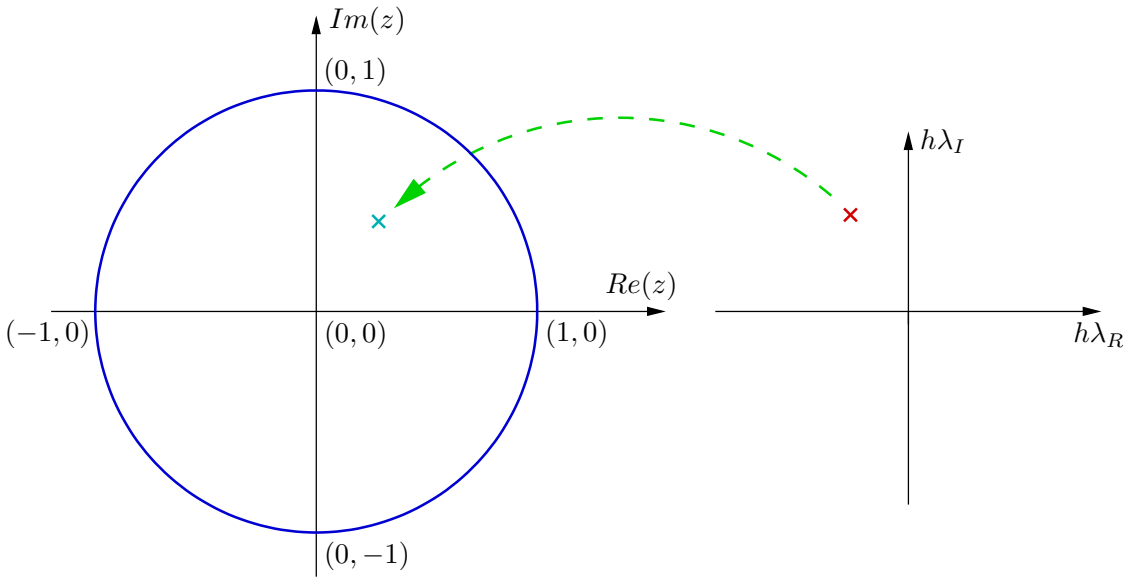
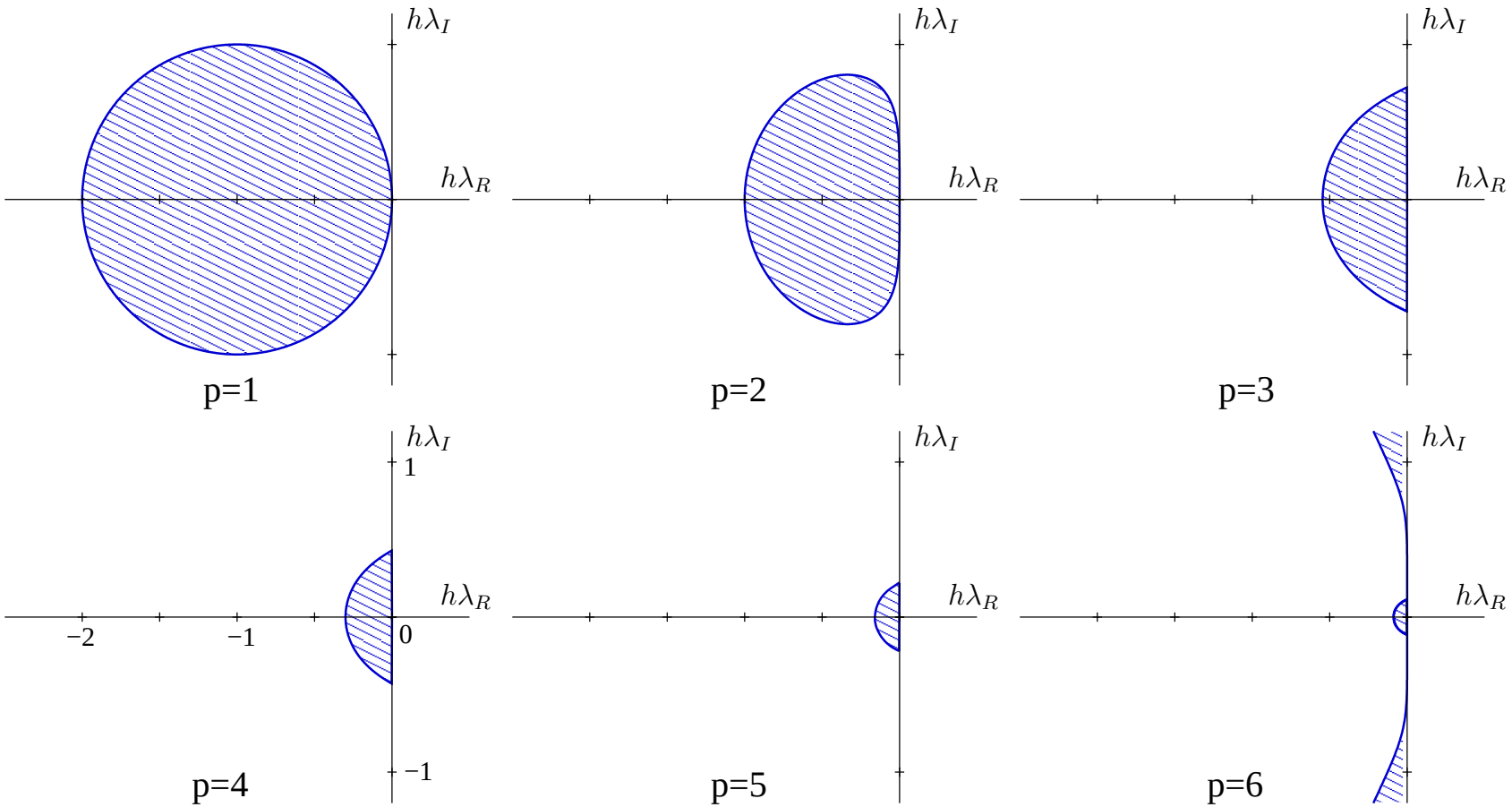
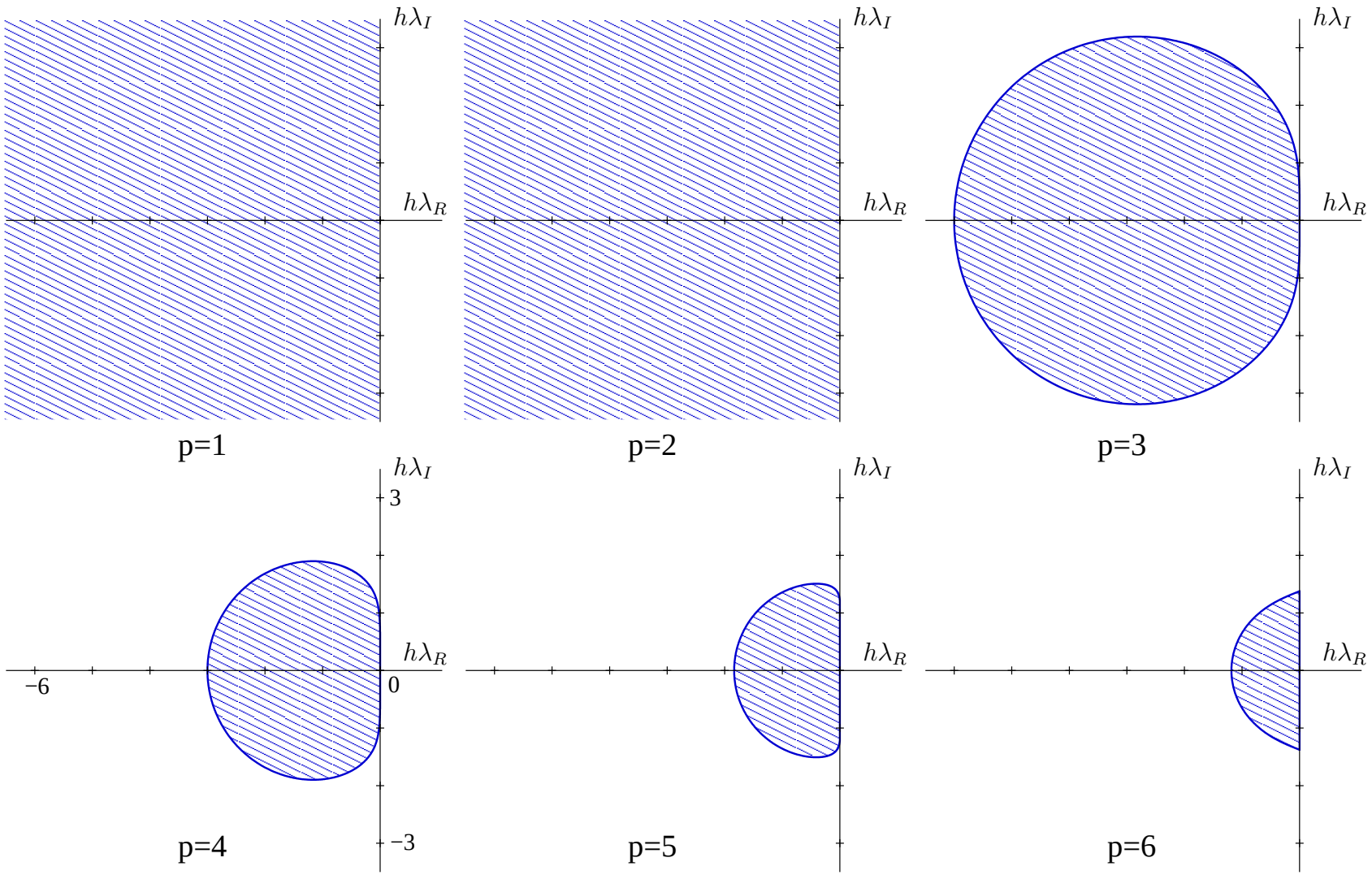


* Methods that are stable for all λ with $\mathrm{Re}(\lambda) < 0$ are called *A-stable*.

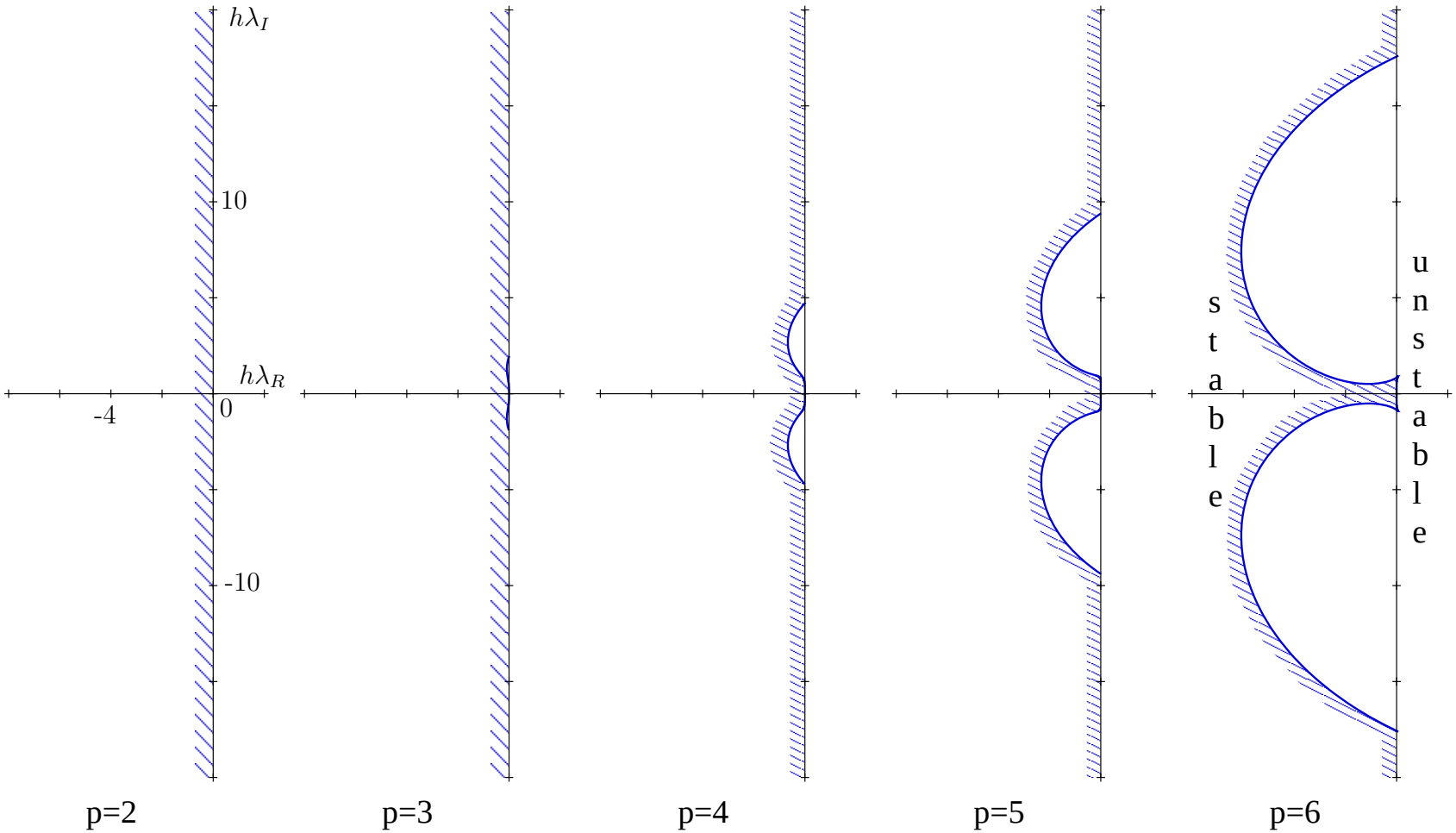
Region of stability for AB methods



Region of stability for AM methods



Region of stability for BDF methods



Stability for large h ($\dot{x} = \lambda x$, complex λ)

* The AM1 (Backward Euler), AM2 (Trapezoidal), and second-order BDF methods are A-stable; other methods are *conditionally* stable.

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* For purely real values of λ, the BDF methods (up to order six) are unconditionally stable, while the AB and AM (except AM1 and AM2) methods are conditionally stable.

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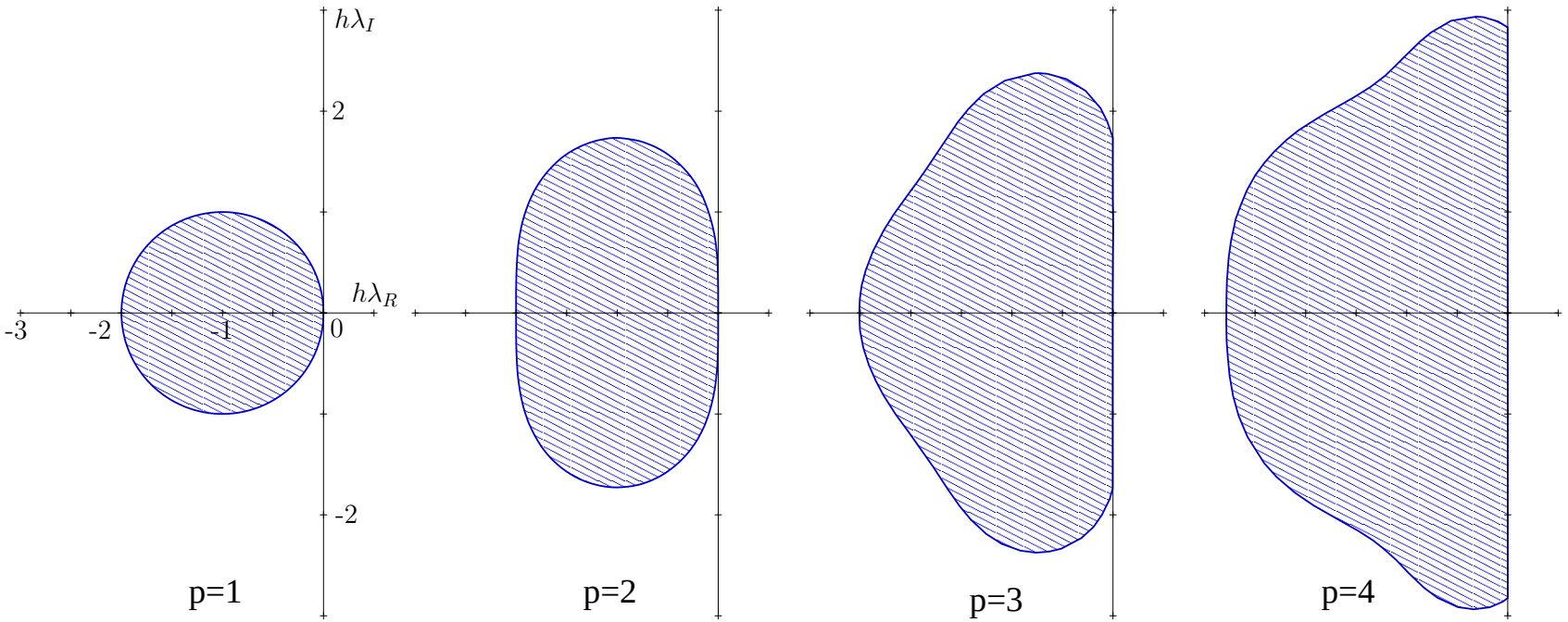
* Stability conditions impose restrictions on the choice of methods for circuit simulation.

Region of stability for explicit Runge-Kutta methods



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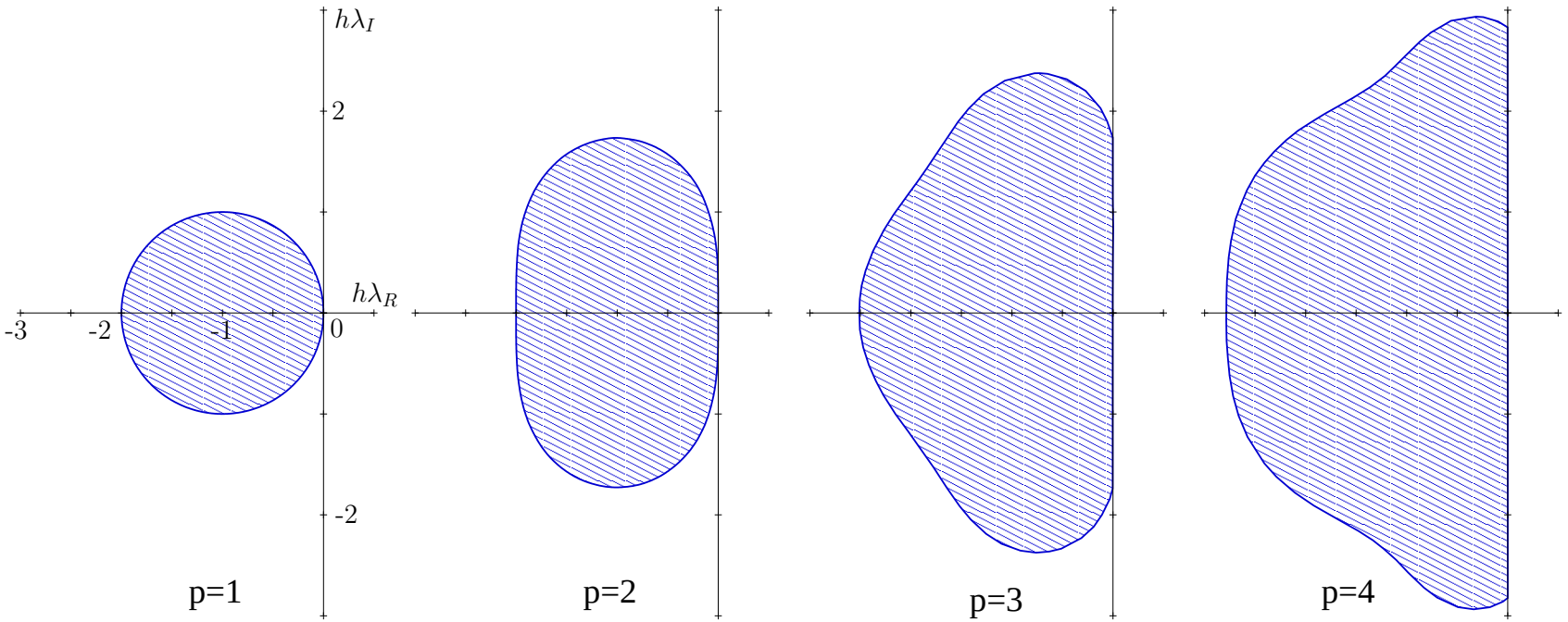

* Explicit Runge-Kutta methods are conditionally stable.

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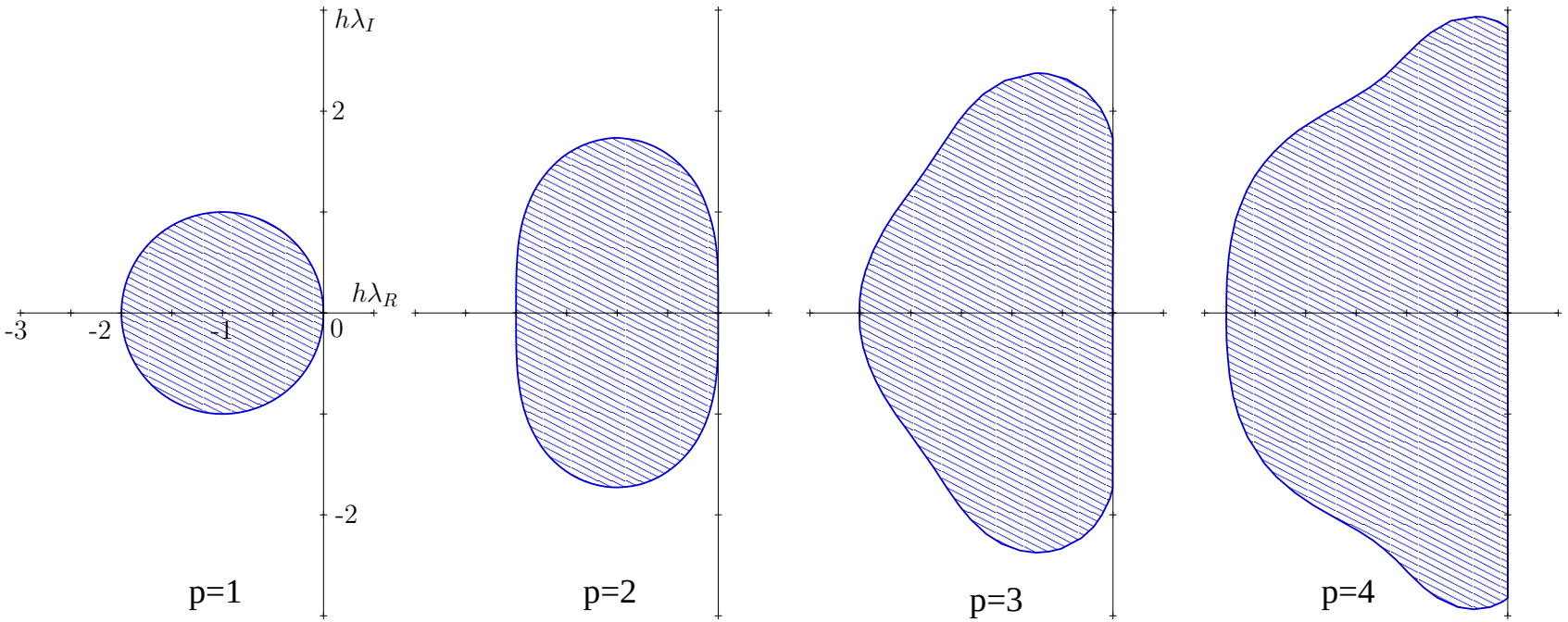

* Explicit Runge-Kutta methods are conditionally stable.
* On the other hand, implicit Runge-Kutta methods are A-stable [4].

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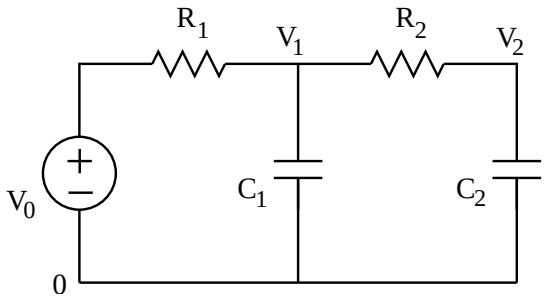
* There are several physical examples of stiff systems, such as motion of masses connected by springs, chemical reactions involving several reactants, and electrical circuits.
* Stiff equations present a challenge because they involve vastly different time constants. In some cases, it is important for the numerical method to be able to resolve transients on a time scale corresponding to the smallest time constant.

Stiff equations: *RC* circuit example



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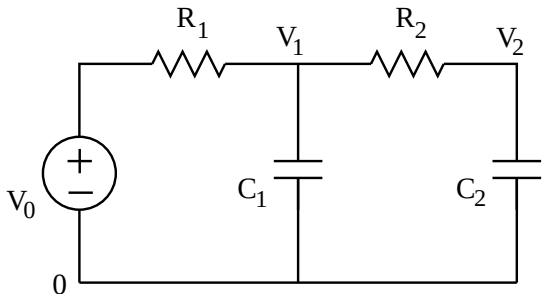
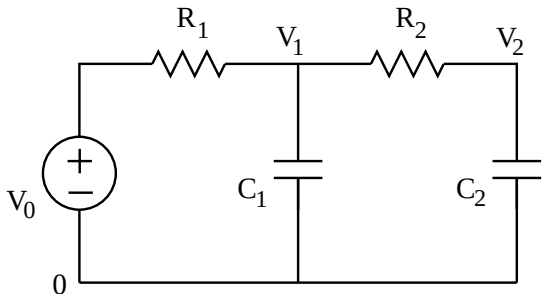


$$\begin{aligned} \frac{dV_1}{dt} &= \left(\frac{-1}{C_1}\right)\left(\frac{1}{R_1}+\frac{1}{R_2}\right)V_1 + \left(\frac{1}{C_1R_2}\right)V_2 + \left(\frac{V_0}{C_1R_1}\right), \\ \frac{dV_2}{dt} &= \left(\frac{1}{C_2R_2}\right)V_1 - \left(\frac{1}{C_2R_2}\right)V_2 . \end{aligned} \tag{27}$$

Stiff equations: *RC* circuit example



$$\begin{aligned} \frac{dV_1}{dt} &= \left(\frac{-1}{C_1}\right)\left(\frac{1}{R_1}+\frac{1}{R_2}\right)V_1 + \left(\frac{1}{C_1R_2}\right)V_2 + \left(\frac{V_0}{C_1R_1}\right), \\ \frac{dV_2}{dt} &= \left(\frac{1}{C_2R_2}\right)V_1 - \left(\frac{1}{C_2R_2}\right)V_2 . \end{aligned} \tag{27}$$

* This is a coupled system of ODEs (see Eq. 26).

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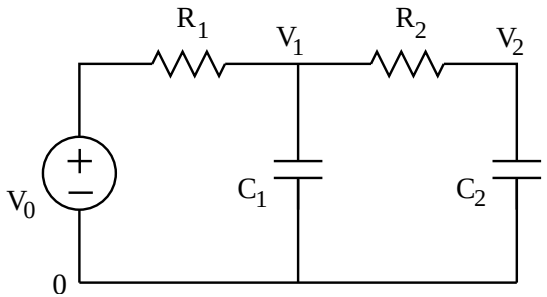

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* This is a coupled system of ODEs (see Eq. 26).
* For $R_1 = 0.5\,\Omega$, $R_2 = 5\,\Omega$, $C_1 = 0.01\,F$, $C_2 = 1\,F$, the eigenvalues are, $\lambda_1 = -0.182\,s^{-1}$, $\lambda_2 = -220\,s^{-1}$, and the time constants are $\tau_1 = 5.5\,s$, $\tau_2 = 0.0045\,s$.

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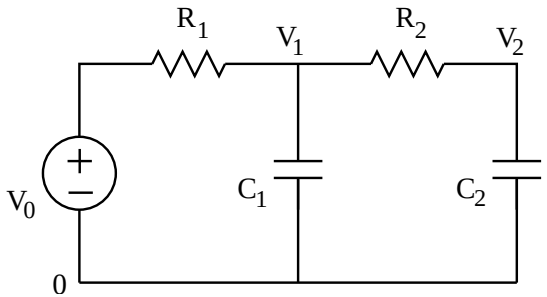

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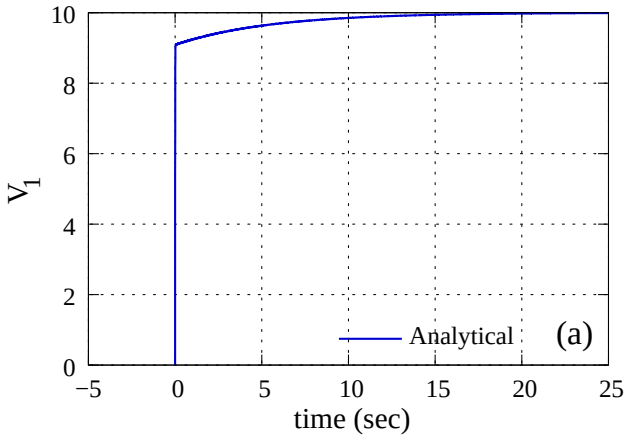

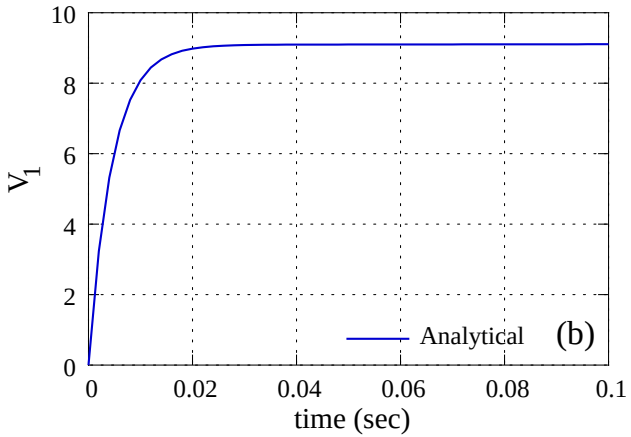

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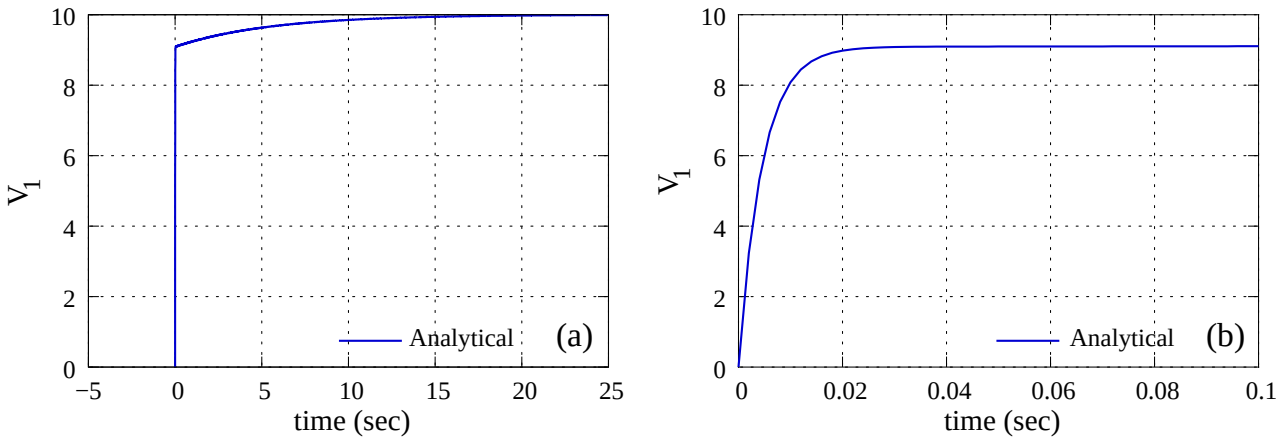

* The currents and voltages in the circuit are given by the general form,

$$x(t) = Ae^{-t/\tau_1} + Be^{-t/\tau_2} + C\,. \tag{28}$$

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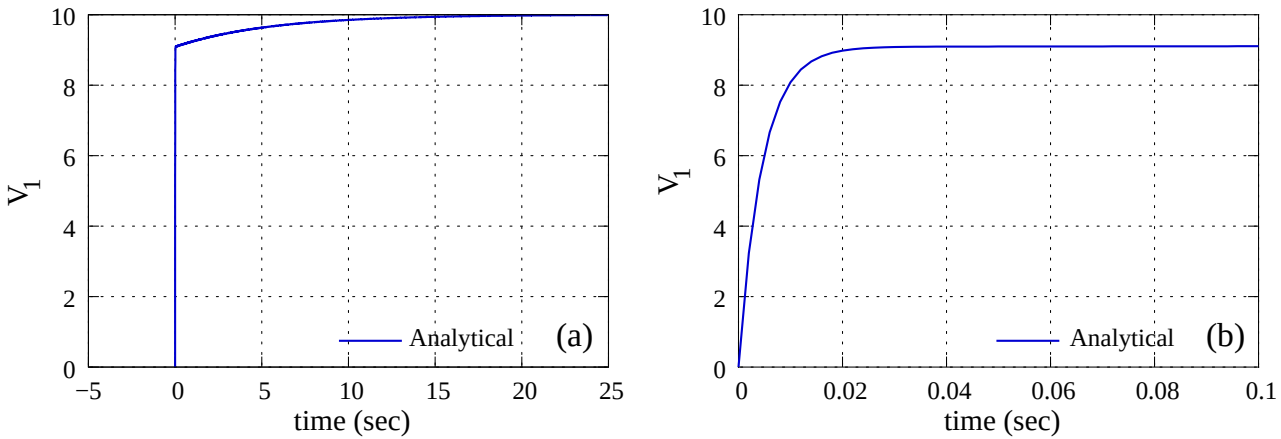

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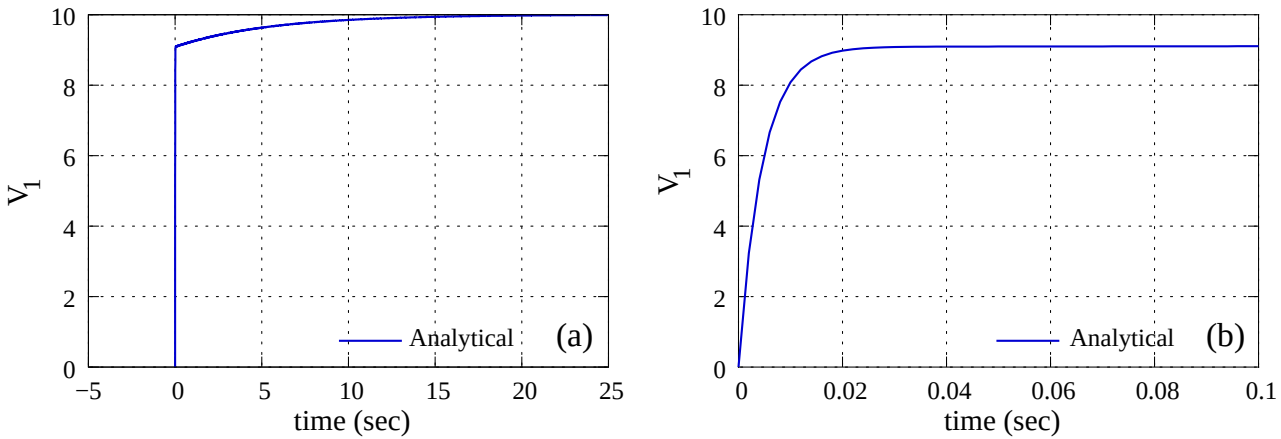

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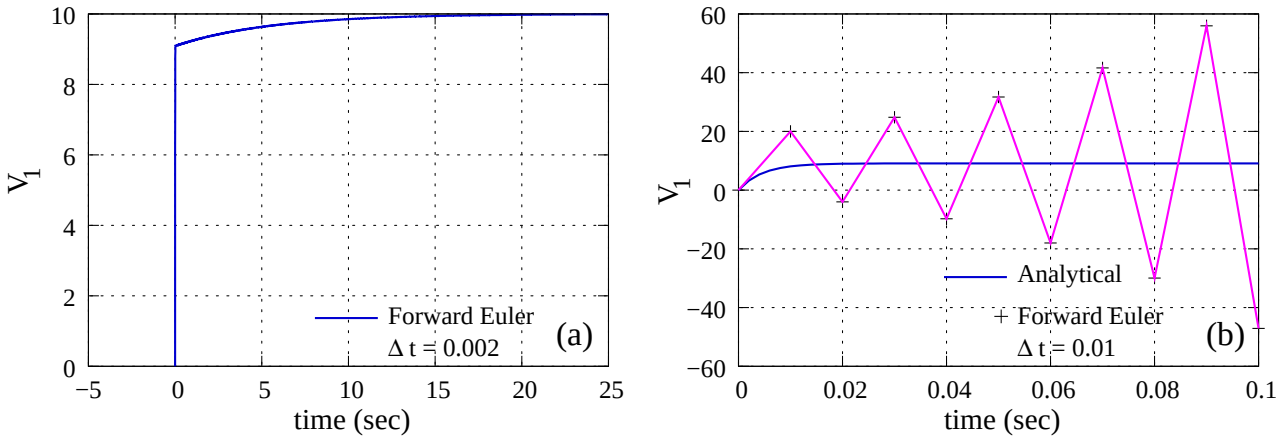
* An expanded view of the fast transient is shown in (b).

Stiff equations: *RC* circuit example (FE results)



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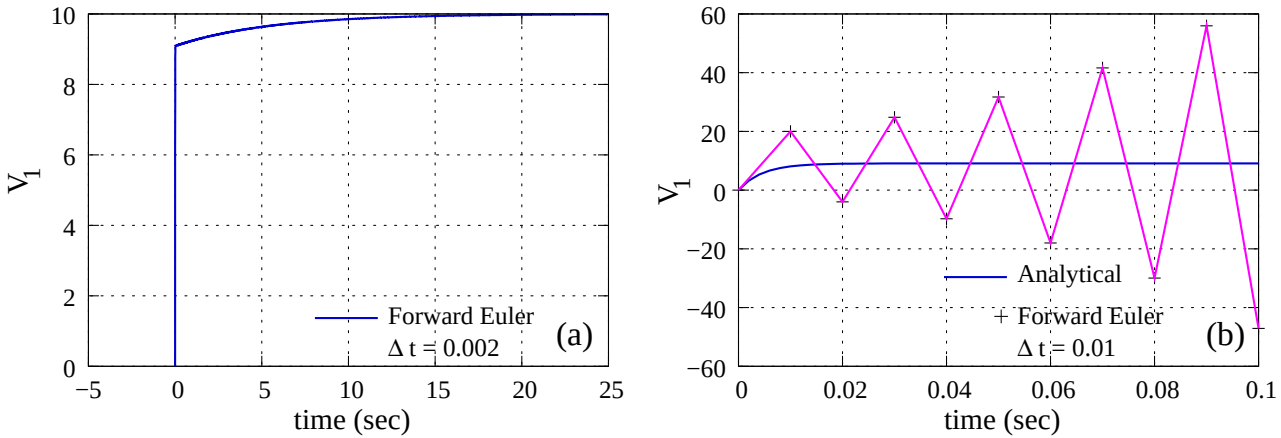

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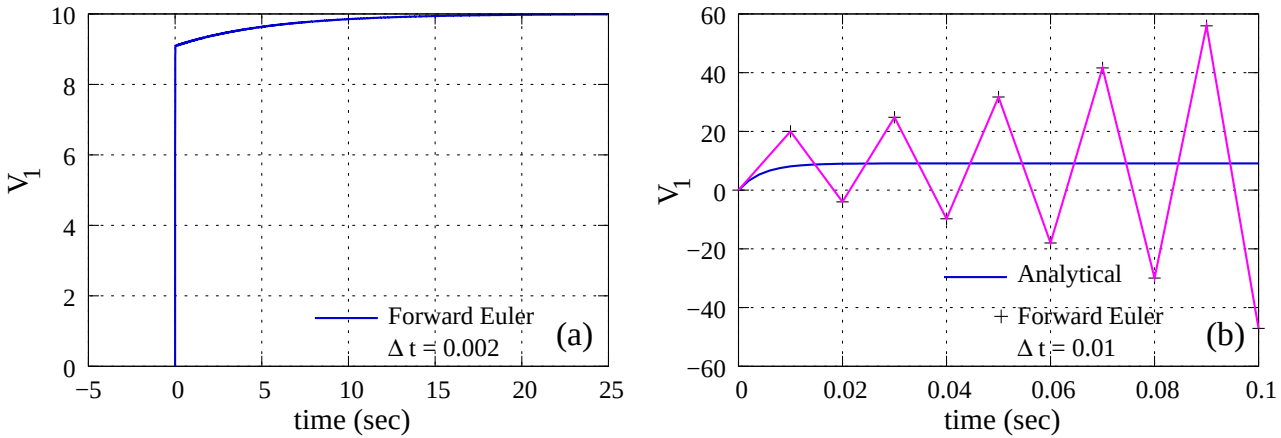

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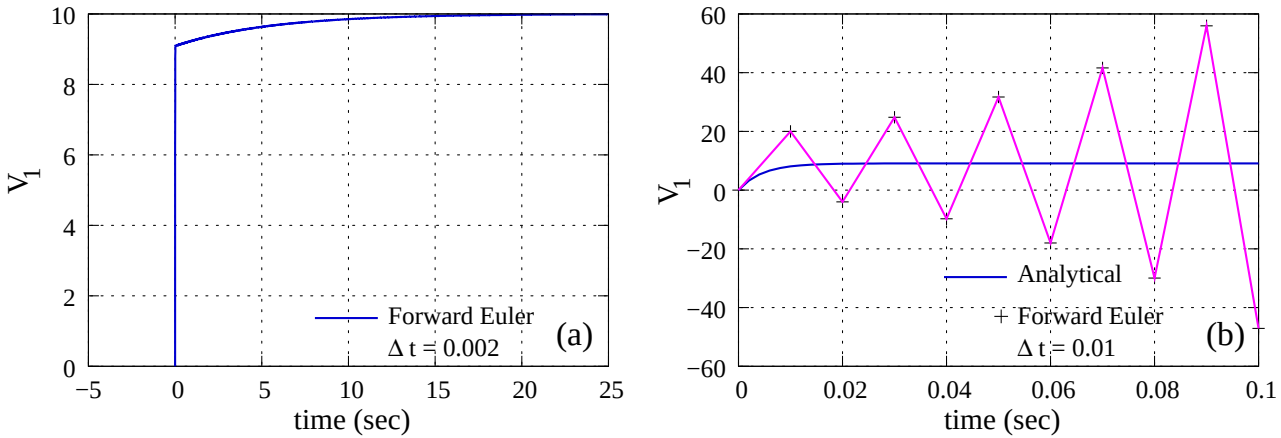
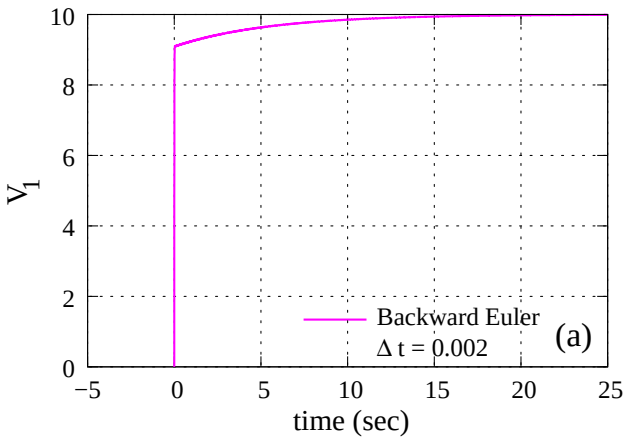
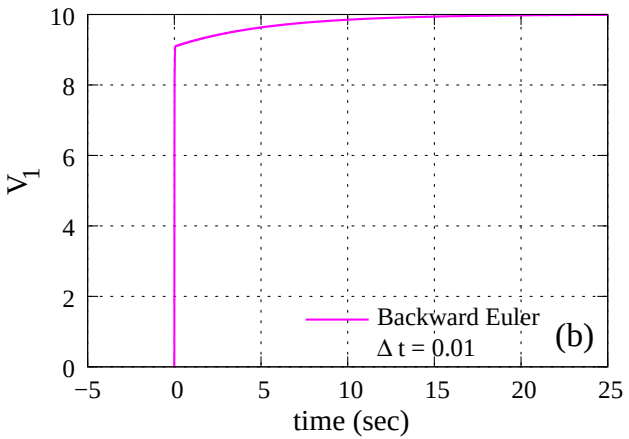


* For $\Delta t = 0.002$ s, Forward Euler results are acceptable.
* For $\Delta t = 0.01$ s, which is large than $2\,\tau_2$ but much smaller than τ_1, the Forward Euler method is unstable.
* To prevent the unstable behaviour, a small time step is required *throughout*, i.e., even *after* the fast transient has vanished $\Rightarrow$ extremely inefficient simulation.

Stiff equations: *RC* circuit example (BE results)





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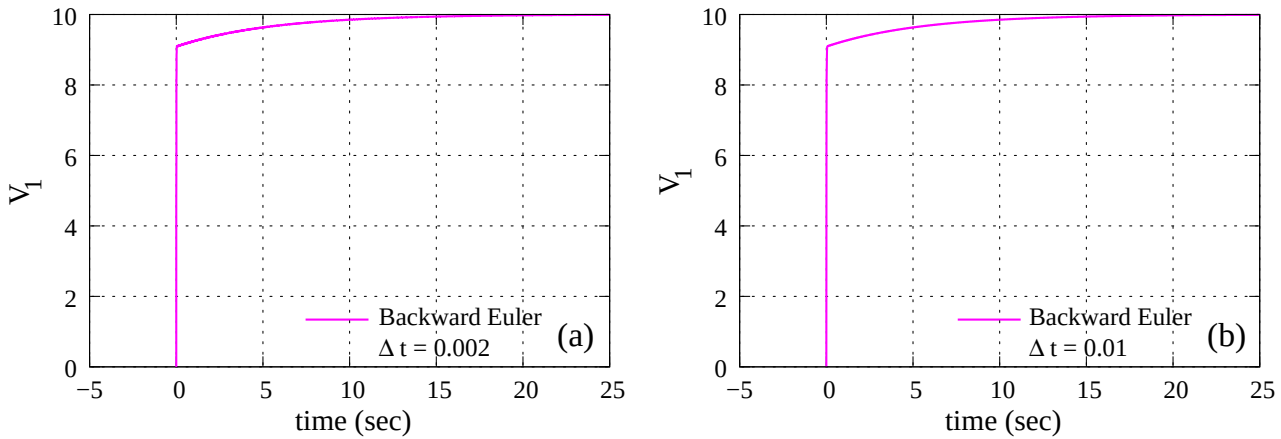

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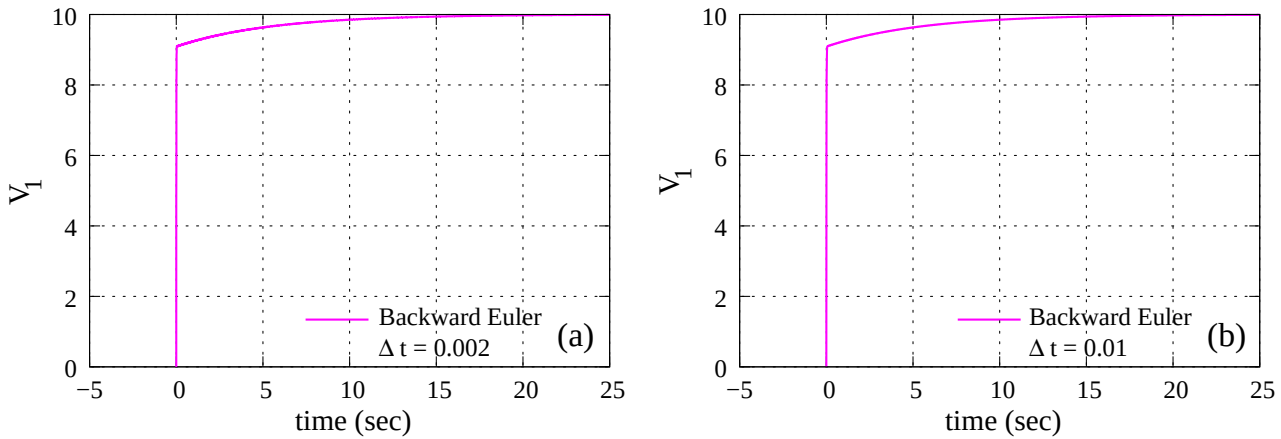

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* The BE method allows much larger time steps than the FE method.

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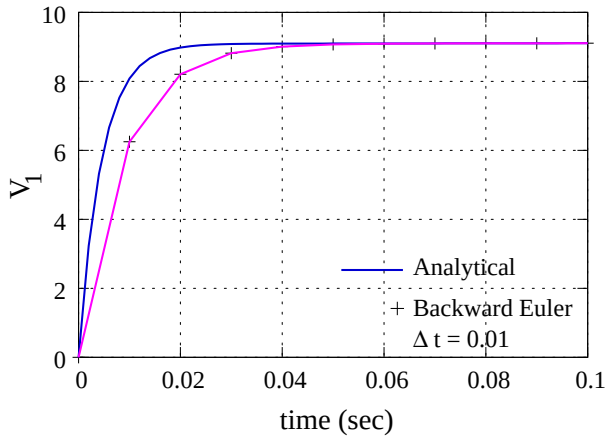

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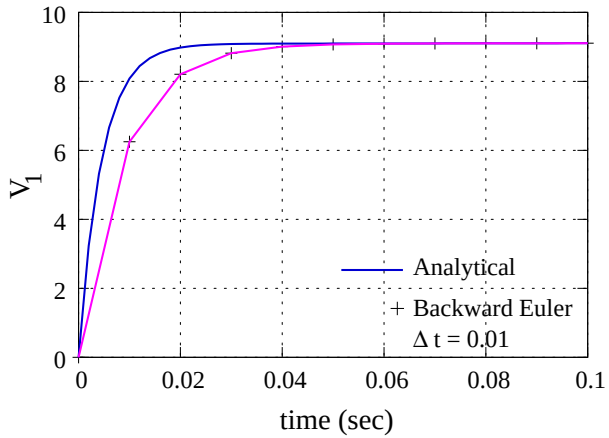

* Although the BE method with $\Delta t = 0.01$ s works well for the slow transient, it does not capture the fast transient accurately, as shown in this expanded view.

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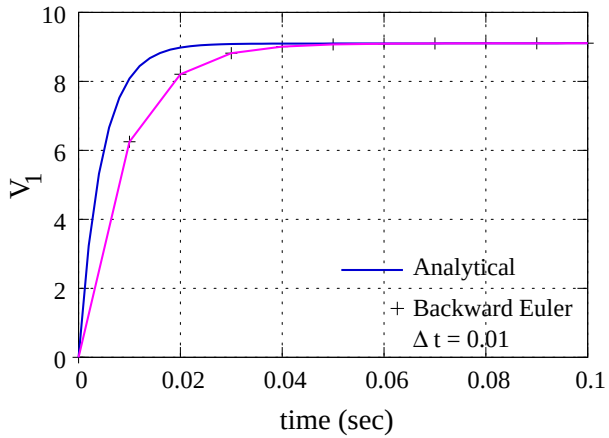
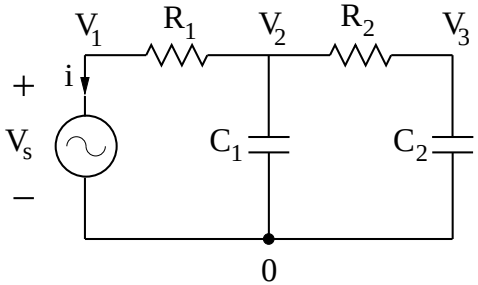
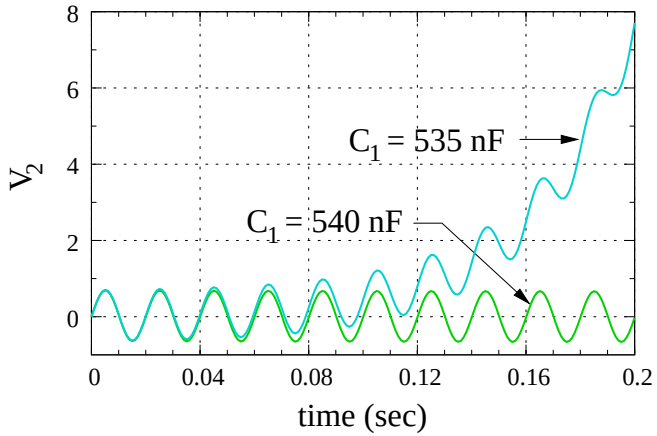


* Although the BE method with $\Delta t = 0.01$ s works well for the slow transient, it does not capture the fast transient accurately, as shown in this expanded view.
* In practice, the time step is made small when things are changing rapidly, and large otherwise. This strategy makes the simulation faster without compromising on accuracy.

Stiff equations: *RC* circuit example (RK4 results)





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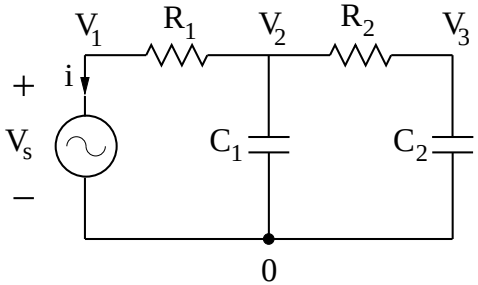

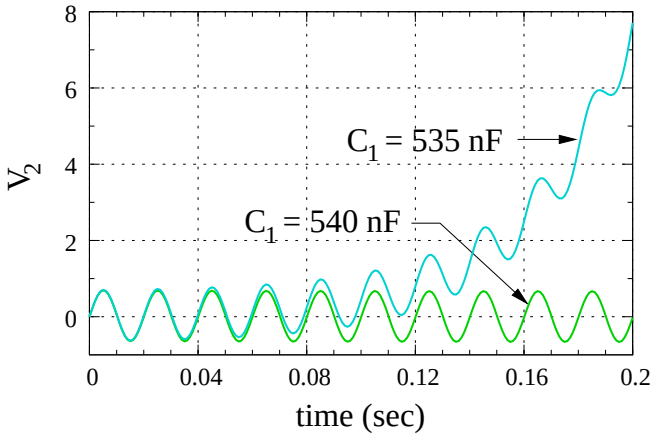

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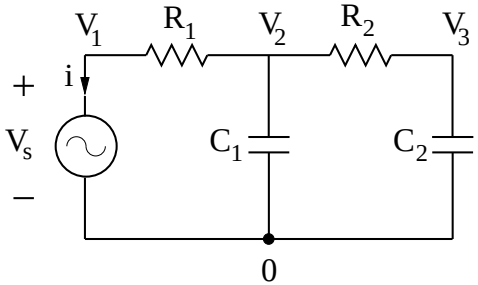

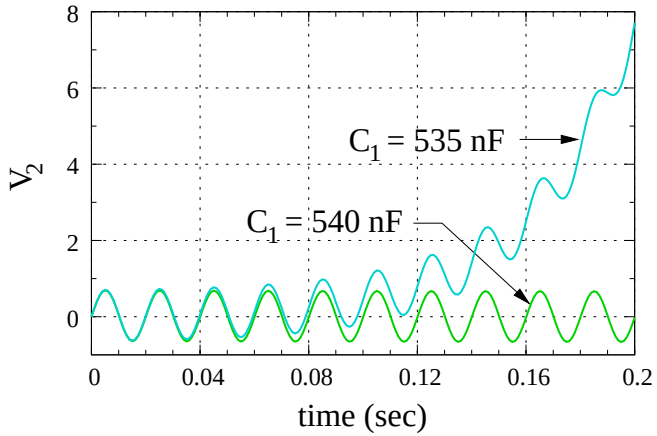

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* For $f = 50$ Hz, $X_{C1} = 295$ kΩ, and $X_{C2} = 160$ Ω. $\Rightarrow$ C_1 is effectively an open circuit, and its exact value should have no effect on the results.

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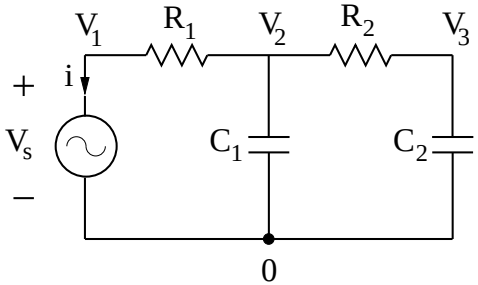

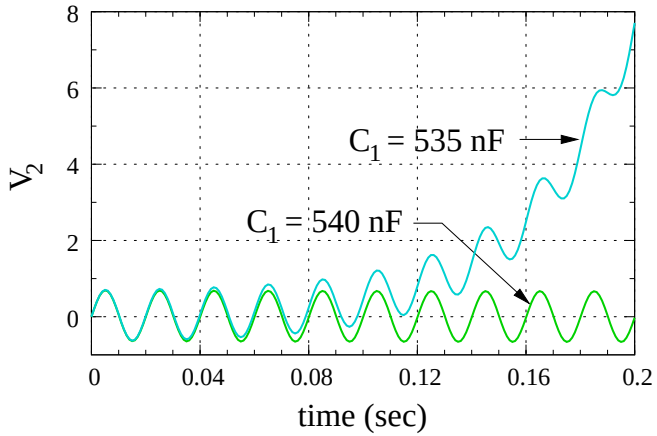

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* However, for $C_1 = 540$ nF and $C_1 = 535$ nF, the RK4 results are dramatically different. Why?

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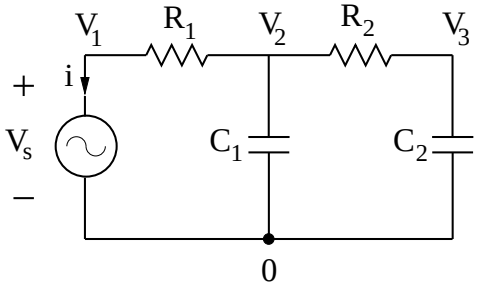

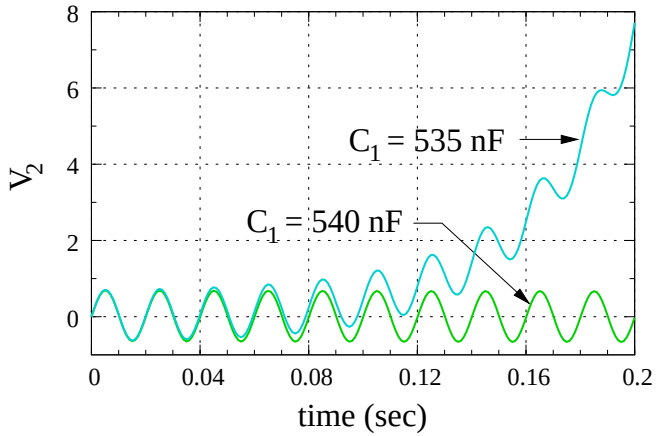

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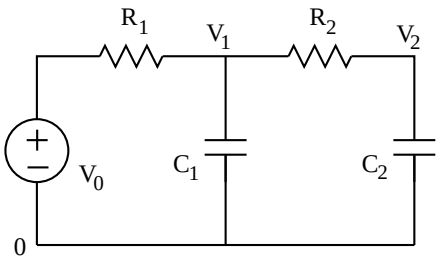
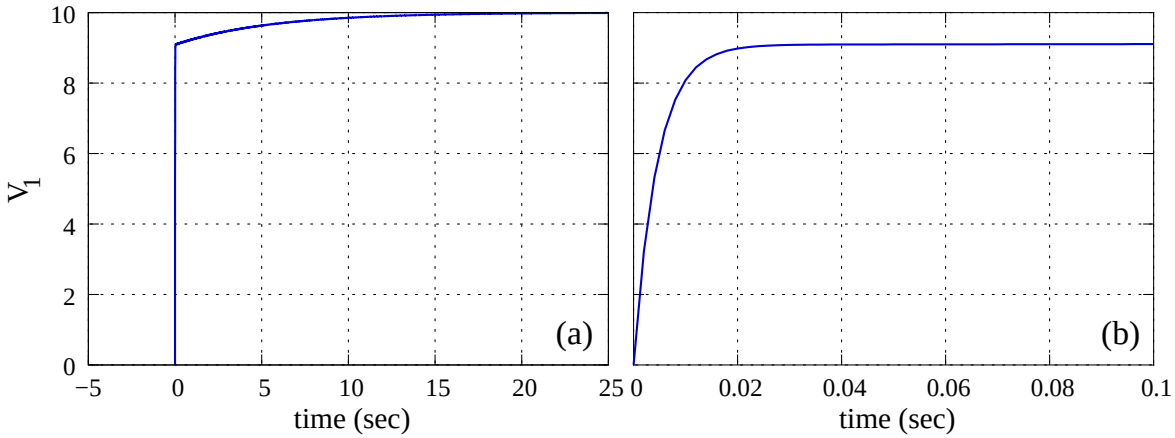
* $C_1 = 535$ nF makes one of the time constants in the circuit small enough (with respect to $h = 1$ ms) to make the RK4 method unstable.

Outline

* Introduction and problem definition
* Taylor series methods
* Runge-Kutta methods
* Specific multi-step methods
* Generalized multi-step methods
* Predictor-corrector methods
* Numerical results
* Stability of numerical methods
* Regions of stability
* Stiff equations
* Adaptive step size
* Miscellaneous topics

Adaptive step size





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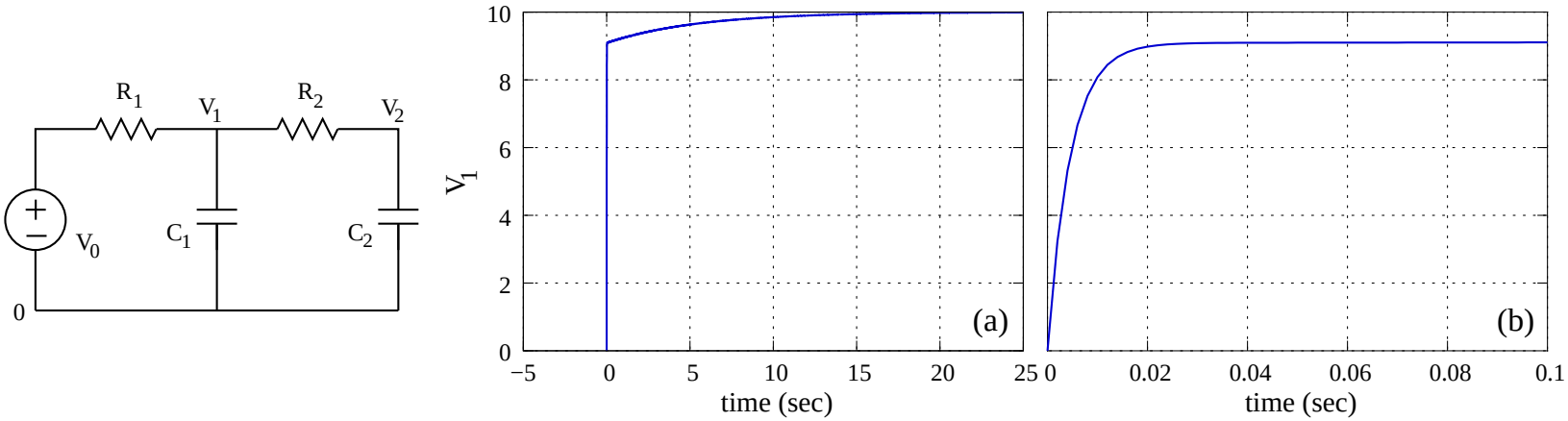

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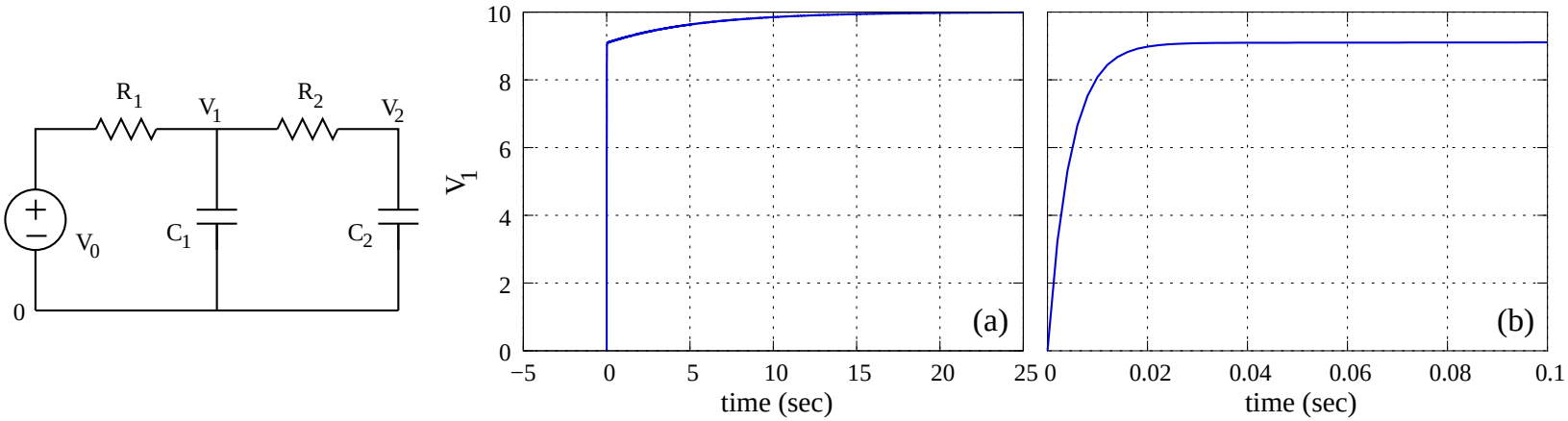

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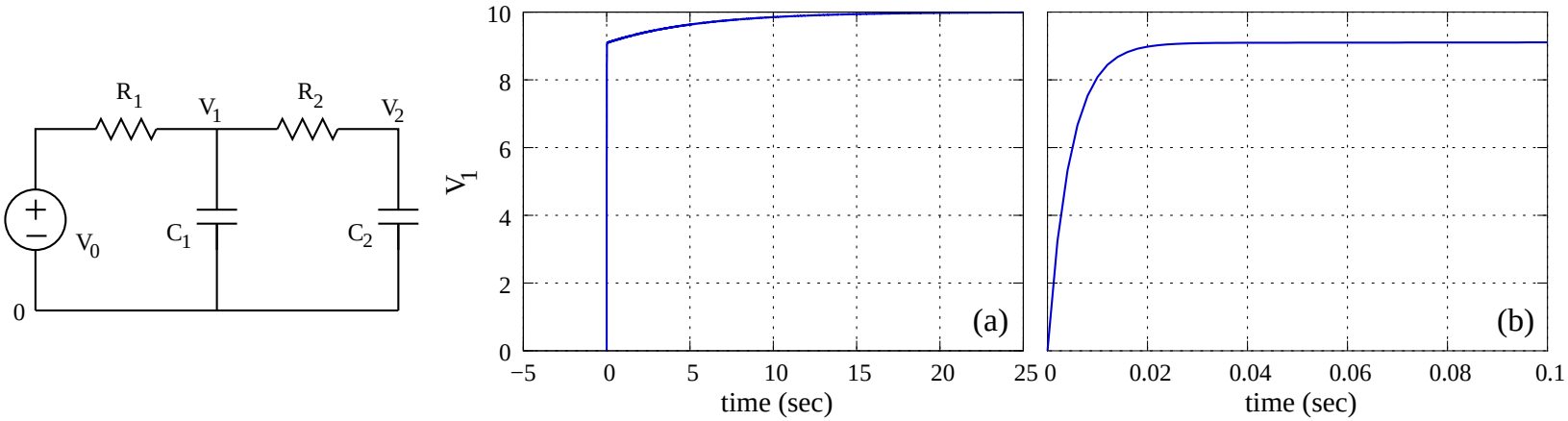

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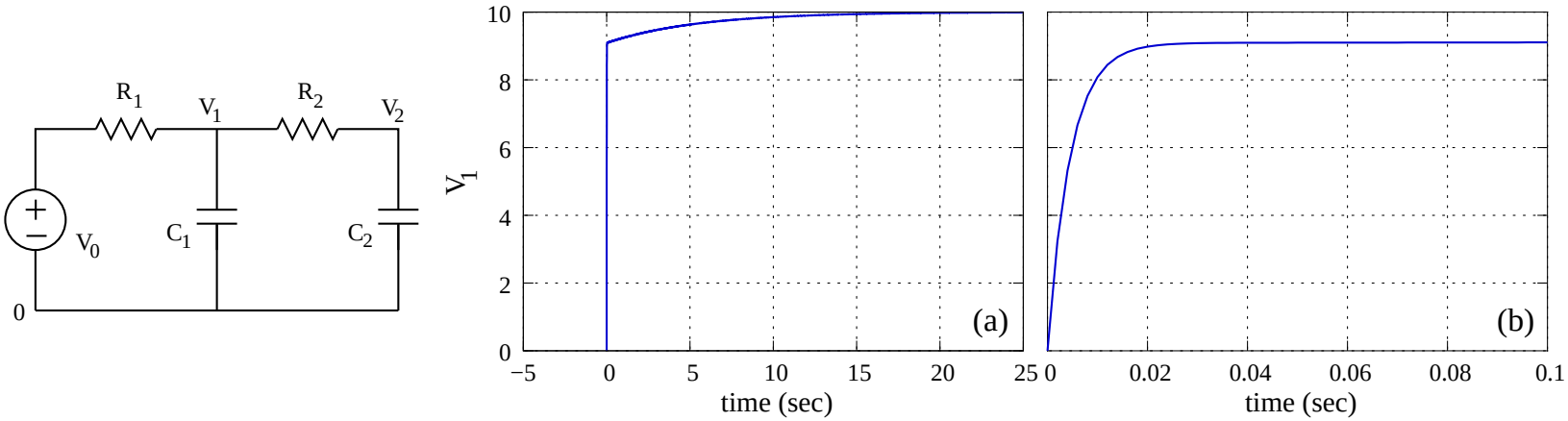

* It is desirable to use small time steps when the solution is changing rapidly, and large time steps otherwise.
* For automatic time step computation, the next time step can be computed on the basis of
  - an estimate of the local truncation error (LTE)
  - convergence behaviour of Newton-Raphson algorithm (for nonlinear problems)

LTE estimation: use of two time steps

* The local error of a numerical method of order p is given by,

$$x(t_n + h) - x_{n+1} = h^{p+1}\psi(t_n, x_n) + O(h^{p+2}), \tag{29}$$

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* By subtracting Eq. 29 from Eq. 30, we get an estimate for the LTE,

$$\text{LTE}^{\text{est}} = \left(\frac{2^p}{2^p - 1}\right)|\tilde{x}_{n+1} - x_{n+1}|. \tag{31}$$

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* LTE^{est} may also be used to improve the accuracy of the solution.

LTE estimation: use of methods of different orders

Consider two methods of orders p and $(p+1)$. If $x_n = x(t_n)$ is assumed, we get

$$\text{LTE}^{(p)} = x(t_{n+1}) - x_{n+1}\,, \tag{33}$$

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Subtracting Eq. 34 from Eq. 33 yields,

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Note that an additional cost of computing $\tilde{x}_{n+1}$ with a higher-order method is involved here. In practice, the low- and high-order methods are chosen so that some of the computation of the low-order method can be used for the high-order method.

Runge-Kutta-Fehlberg 4/5 method

0					0					
$\frac{1}{4}$	$\frac{1}{4}$				$\frac{1}{4}$	$\frac{1}{4}$				
$\frac{3}{8}$	$\frac{3}{32}$	$\frac{9}{32}$			$\frac{3}{8}$	$\frac{3}{32}$	$\frac{9}{32}$			
$\frac{12}{13}$	$\frac{1932}{2197}$	$-\frac{7200}{2197}$	$\frac{7296}{2197}$		$\frac{12}{13}$	$\frac{1932}{2197}$	$-\frac{7200}{2197}$	$\frac{7296}{2197}$		
1	$\frac{439}{216}$	-8	$\frac{3680}{513}$	$-\frac{845}{4104}$	1	$\frac{439}{216}$	-8	$\frac{3680}{513}$	$-\frac{845}{4104}$	
					$\frac{1}{2}$	$-\frac{8}{27}$	2	$-\frac{3544}{2565}$	$\frac{1859}{4104}$	$-\frac{11}{40}$
	$\frac{25}{216}$	0	$\frac{1408}{2565}$	$\frac{2197}{4104}$	$-\frac{1}{5}$	$\frac{16}{135}$	0	$\frac{6656}{12825}$	$\frac{28561}{56430}$	$-\frac{9}{50}$	$\frac{2}{55}$

4^{th}-order array

5^{th}-order array

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4^{th}-order array 5^{th}-order array

* Since the function values, $f_0, f_1, \cdots, f_4$ are the same in the two methods, only six function evaluations are required in each time step.

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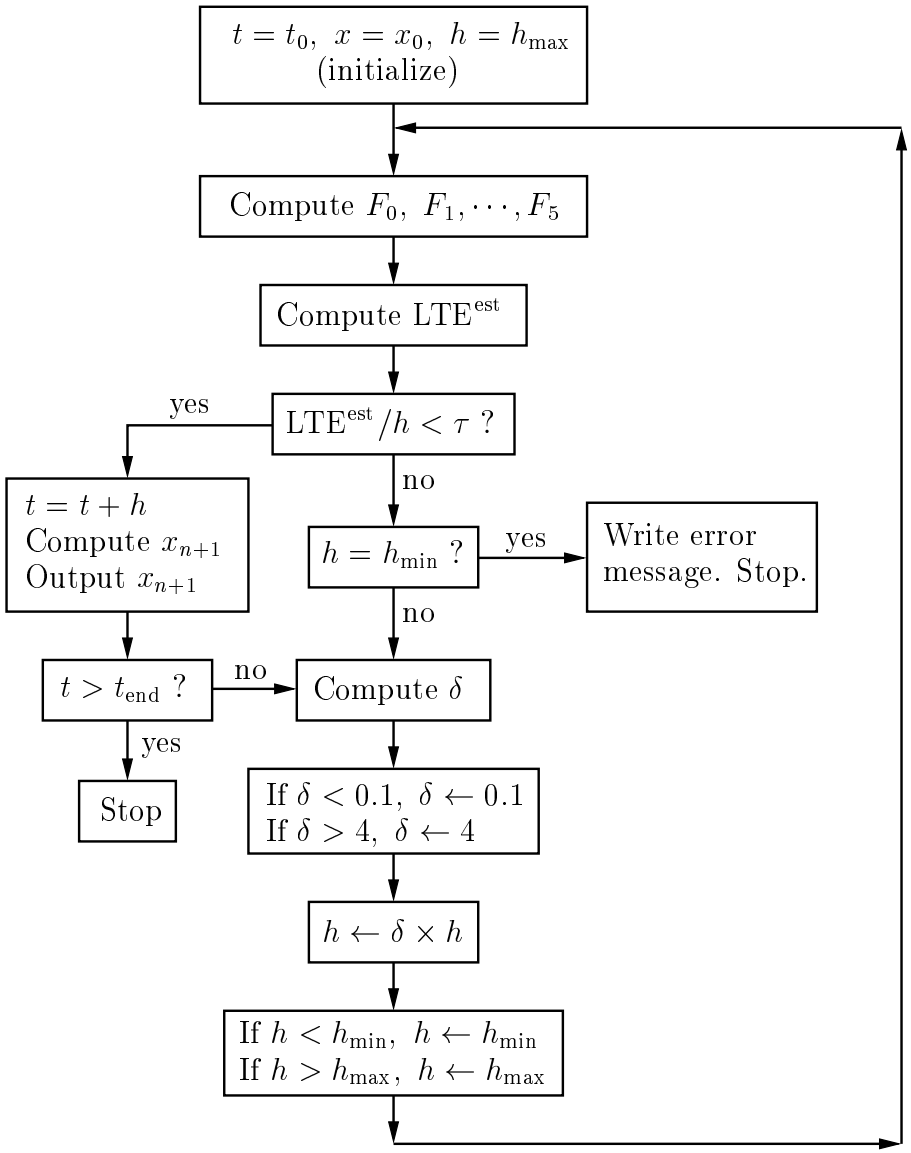
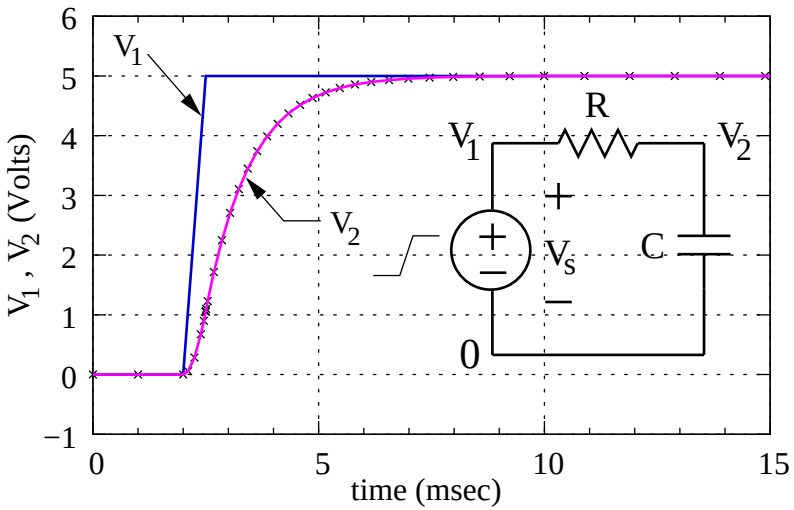
* Since the function values, $f_0, f_1, \cdots, f_4$ are the same in the two methods, only six function evaluations are required in each time step.
* The estimated LTE of the fourth-order formula is given by,

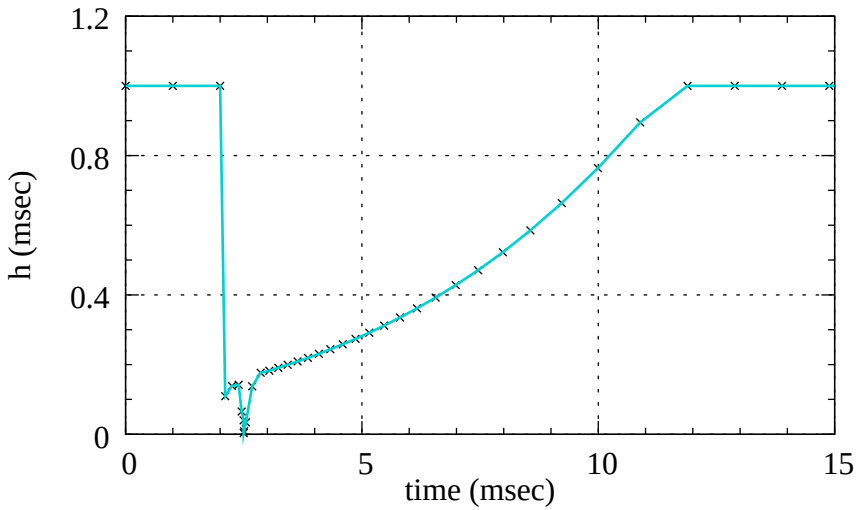
$$\text{LTE}^{\text{est}} = h\left[\frac{1}{360}f_0 - \frac{128}{4275}f_2 - \frac{2197}{25740}f_3 + \frac{1}{50}f_4 + \frac{2}{55}f_5\right]. \qquad (36)$$

Runge-Kutta-Fehlberg 4/5 method: flow chart [1]



Runge-Kutta-Fehlberg 4/5 method: example





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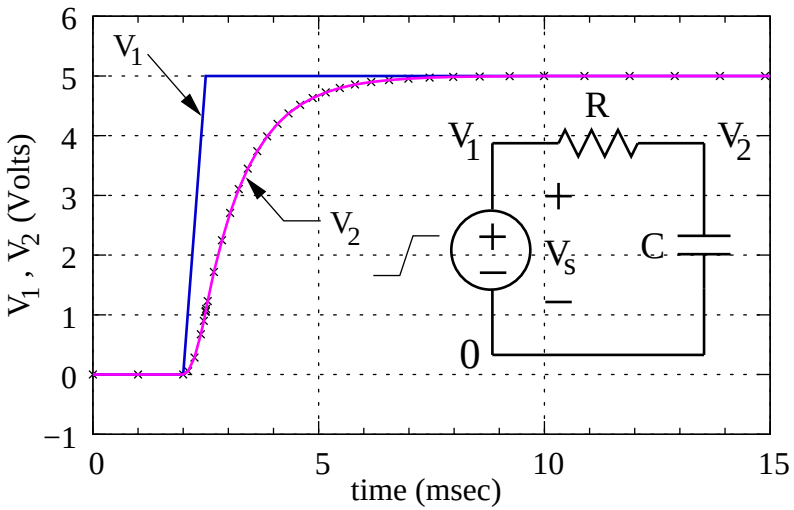

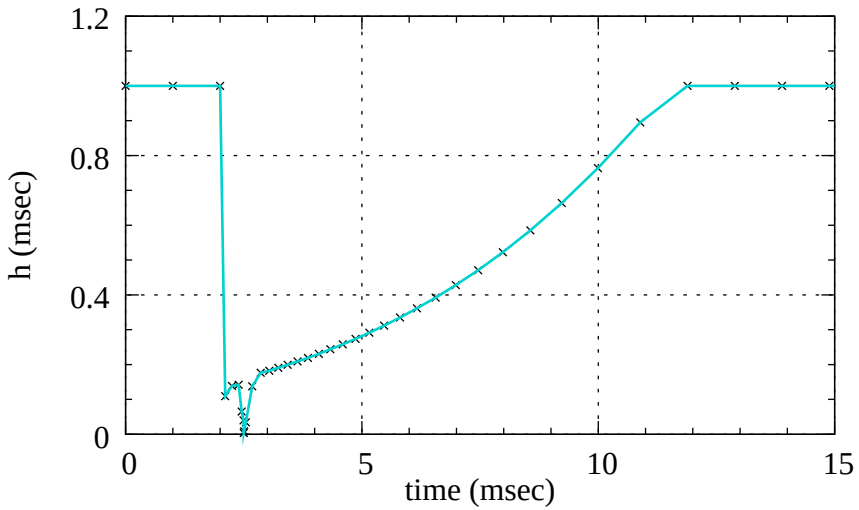

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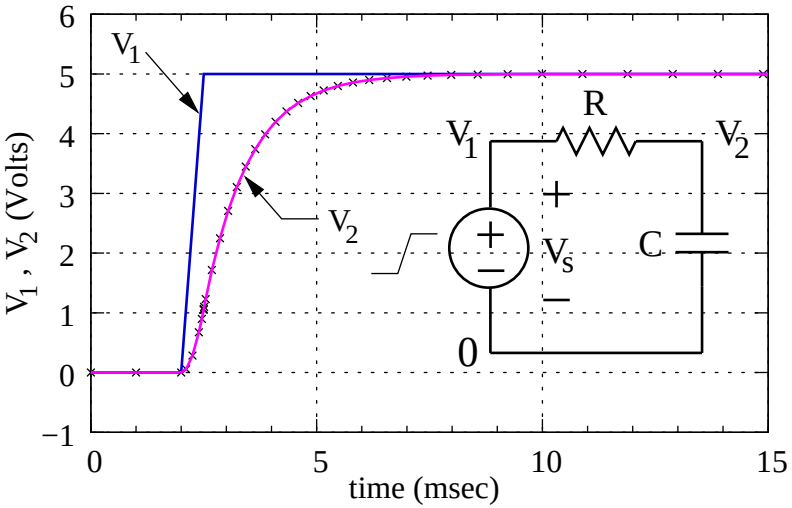

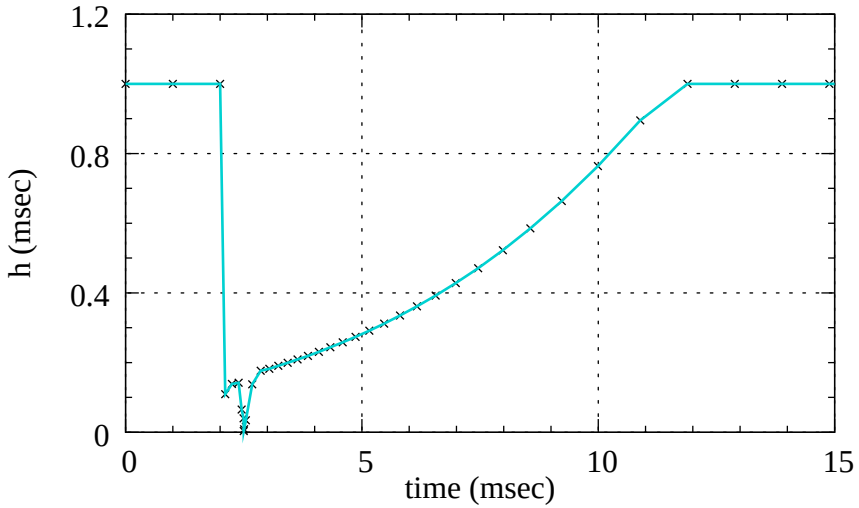

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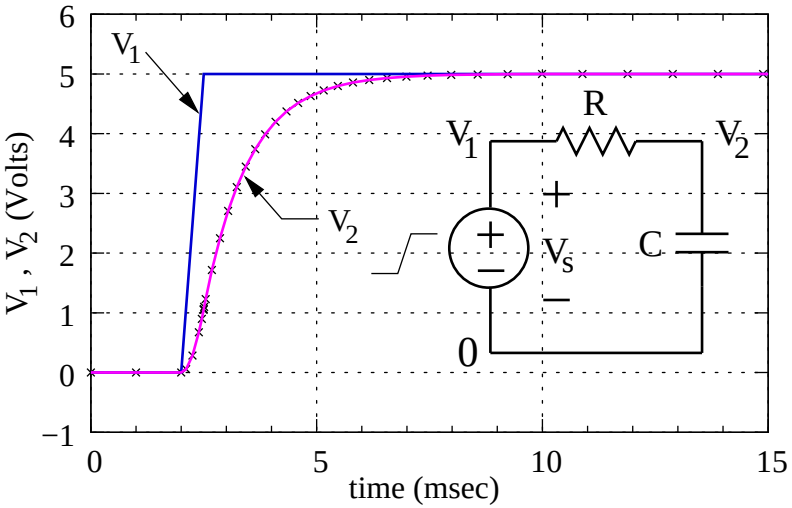

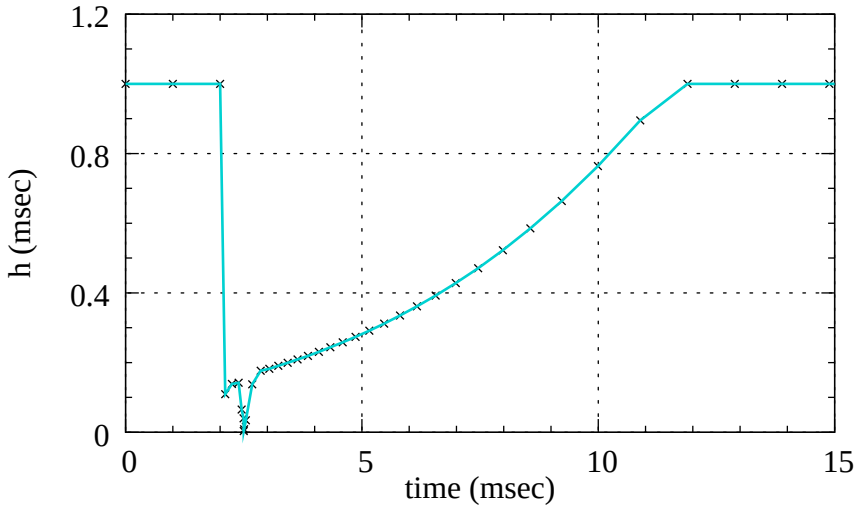

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* When the solution is changing rapidly, the time step is made small in order to meet the tolerance requirement.
* When the solution is changing slowly, the time step is made large (capped by a user-specified h_{max}).

Adaptive step size: convergence of N-R iterations

* The Newton-Raphson process is more likely to converge (in a given number of iterations) if the starting point, i.e., the "initial guess", is close to the solution.

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* The above observation is commonly used in circuit simulation for controlling the time step. (It works only for non-linear problems.)

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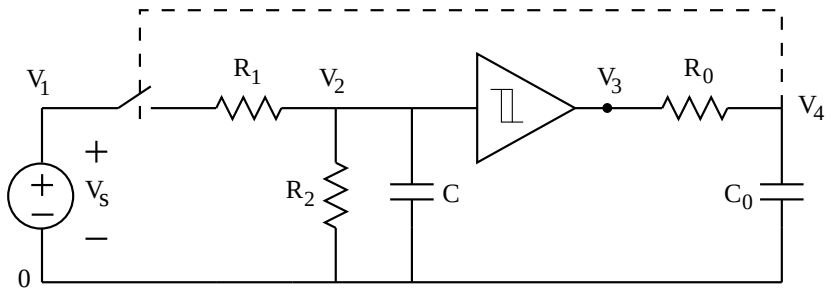

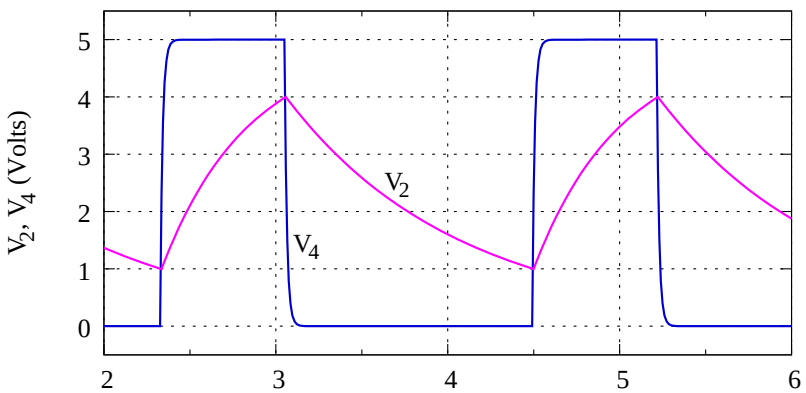

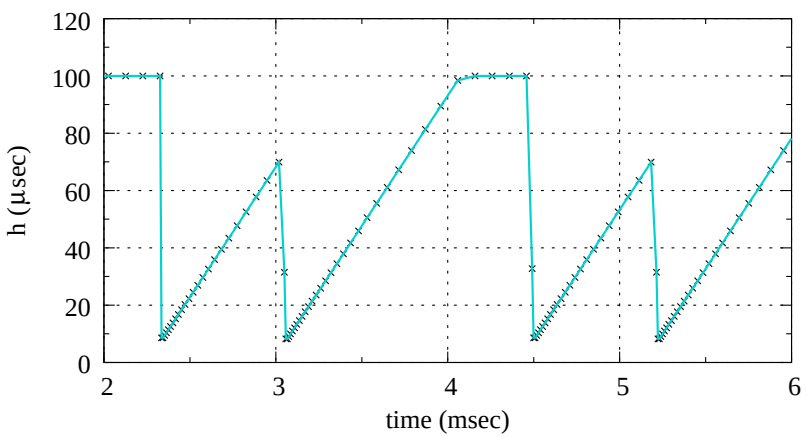

Circuit parameters:

$V_s = 10\ V$,

$R_1 = R_2 = 1\ \text{k}\Omega$,

$C = 1\ \mu F$,

$R_0 = 100\ \Omega$,

$C_0 = 0.1\ \mu F$,

$V_{IL} = 1\ V$,

$V_{IH} = 4\ V$,

$V_{OL} = 0\ V$,

$V_{OH} = 5\ V$.

Algorithm parameters:

$\tau = 10^{-12}$,

$h_{\text{min}} = 10^{-9}$ s,

$h_{\text{max}} = 10^{-4}$ s,

$k_{\text{up}} = 1.1$,

$k_{\text{down}} = 0.8$,

$N_{\text{NR}}^{\text{max}} = 10$.

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* Application of the MNA method to circuits would generally yield a set of equations of the following type [7]:

$$\mathbf{F}(\mathbf{x}', \mathbf{x}, \mathbf{y}, t) = 0\,, \tag{37}$$

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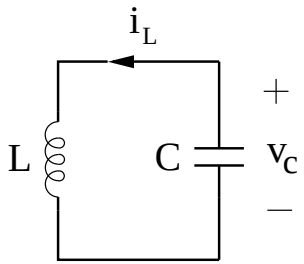
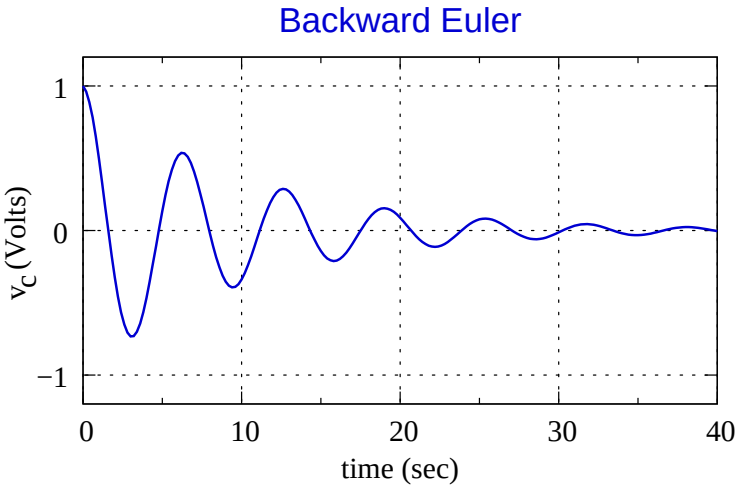
* Runge-Kutta methods are not suitable for DAEs. $\Rightarrow$ The choice is further reduced to BE, TRZ, BDF2.

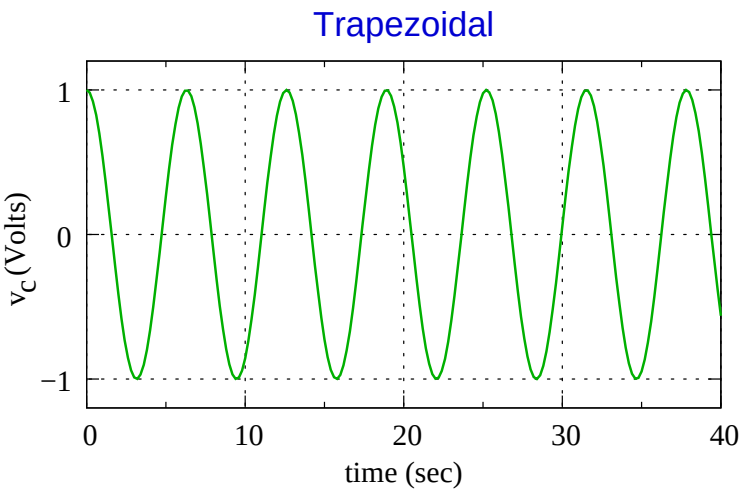
Outline

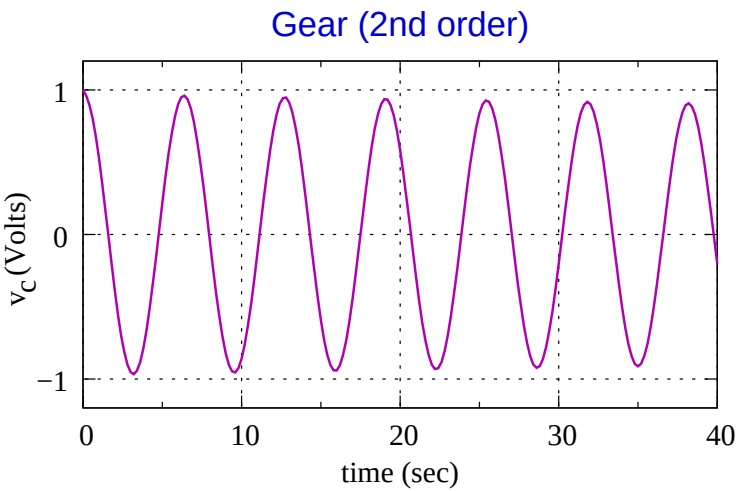
* Introduction and problem definition
* Taylor series methods
* Runge-Kutta methods
* Specific multi-step methods
* Generalized multi-step methods
* Predictor-corrector methods
* Numerical results
* Stability of numerical methods
* Regions of stability
* Stiff equations
* Adaptive step size
* Miscellaneous topics

Undamped oscillations









($L = 1$ H, $C = 1$ F, and h (time step)=0.2 sec in all cases.)

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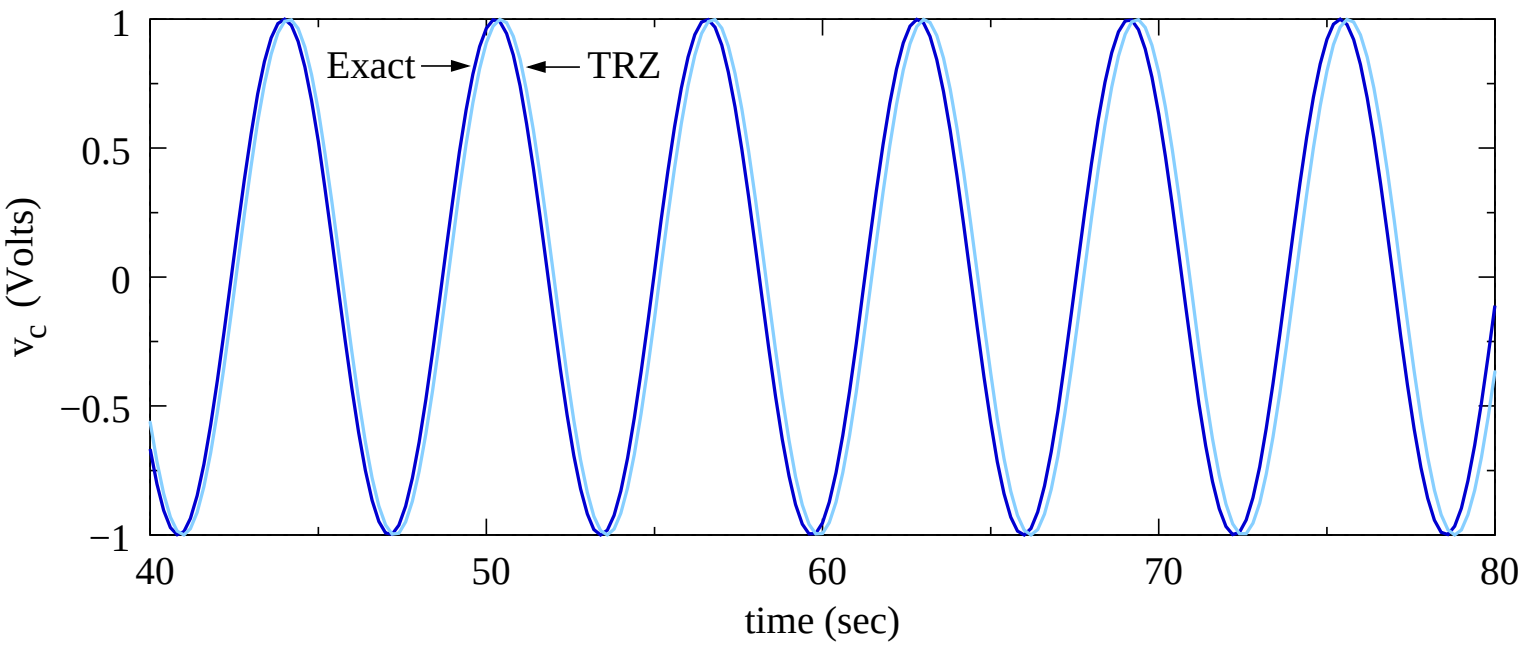
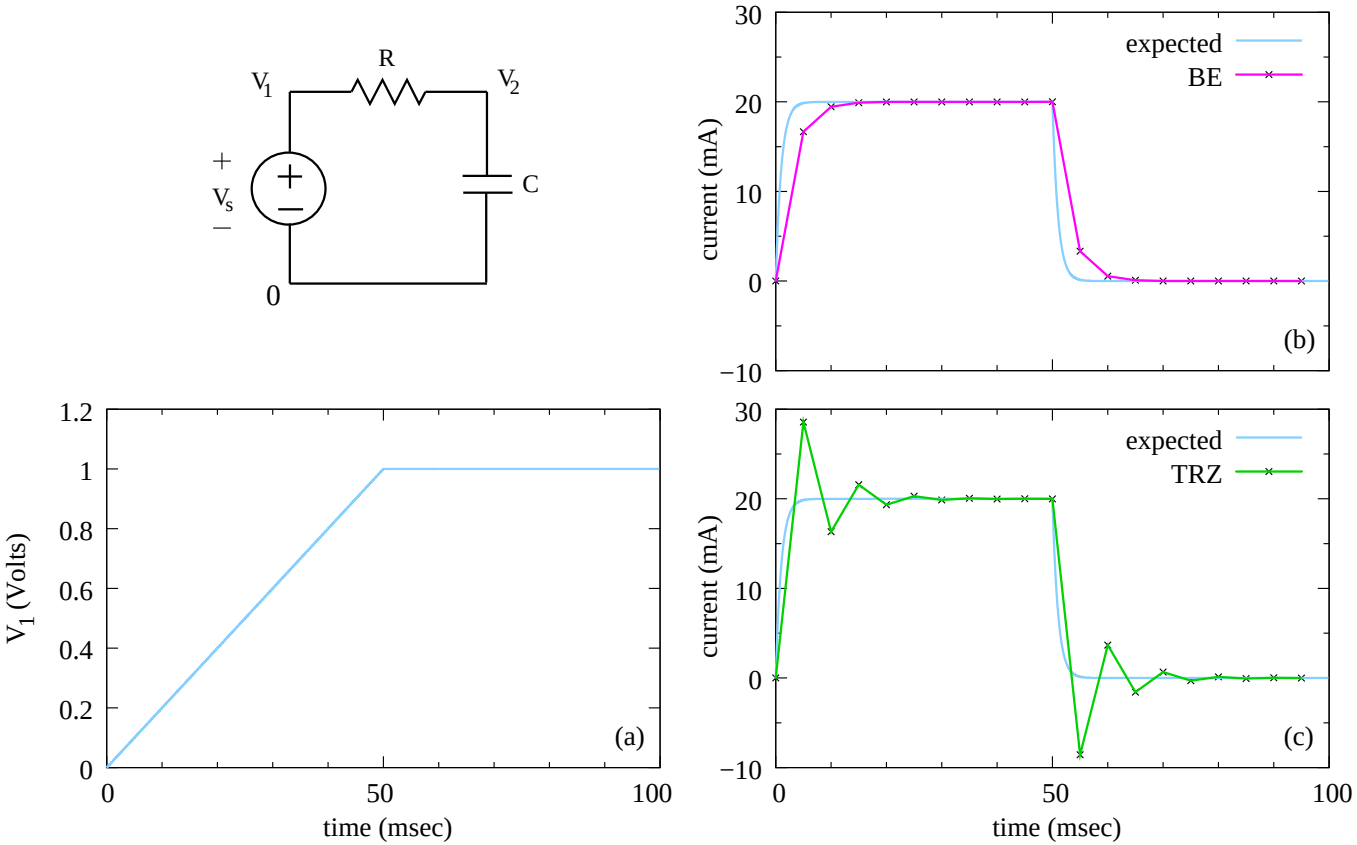
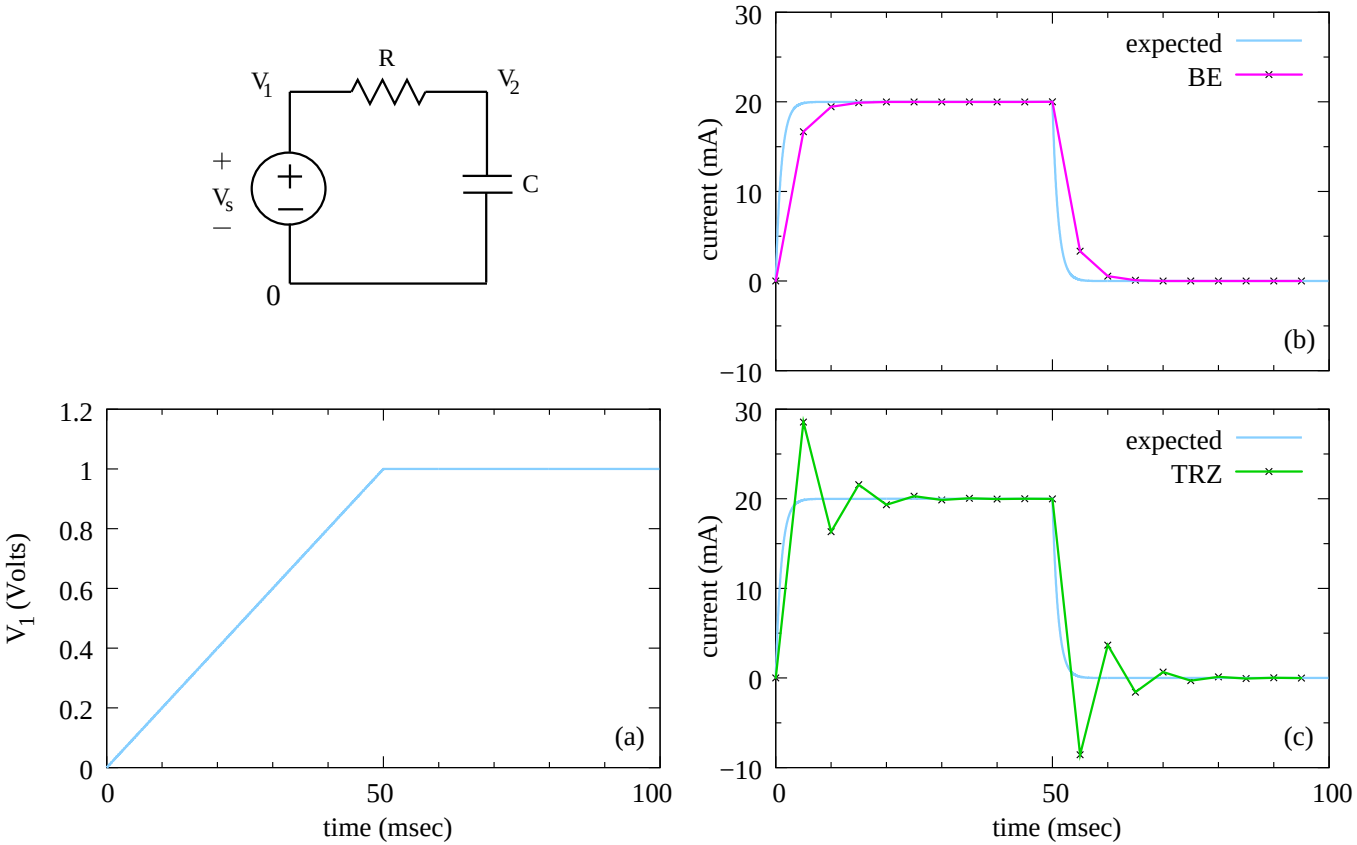


Ringing



(Parameters: $R = 1\ \Omega$, $C = 1$ mF, and h (time step) $= 5$ msec.)

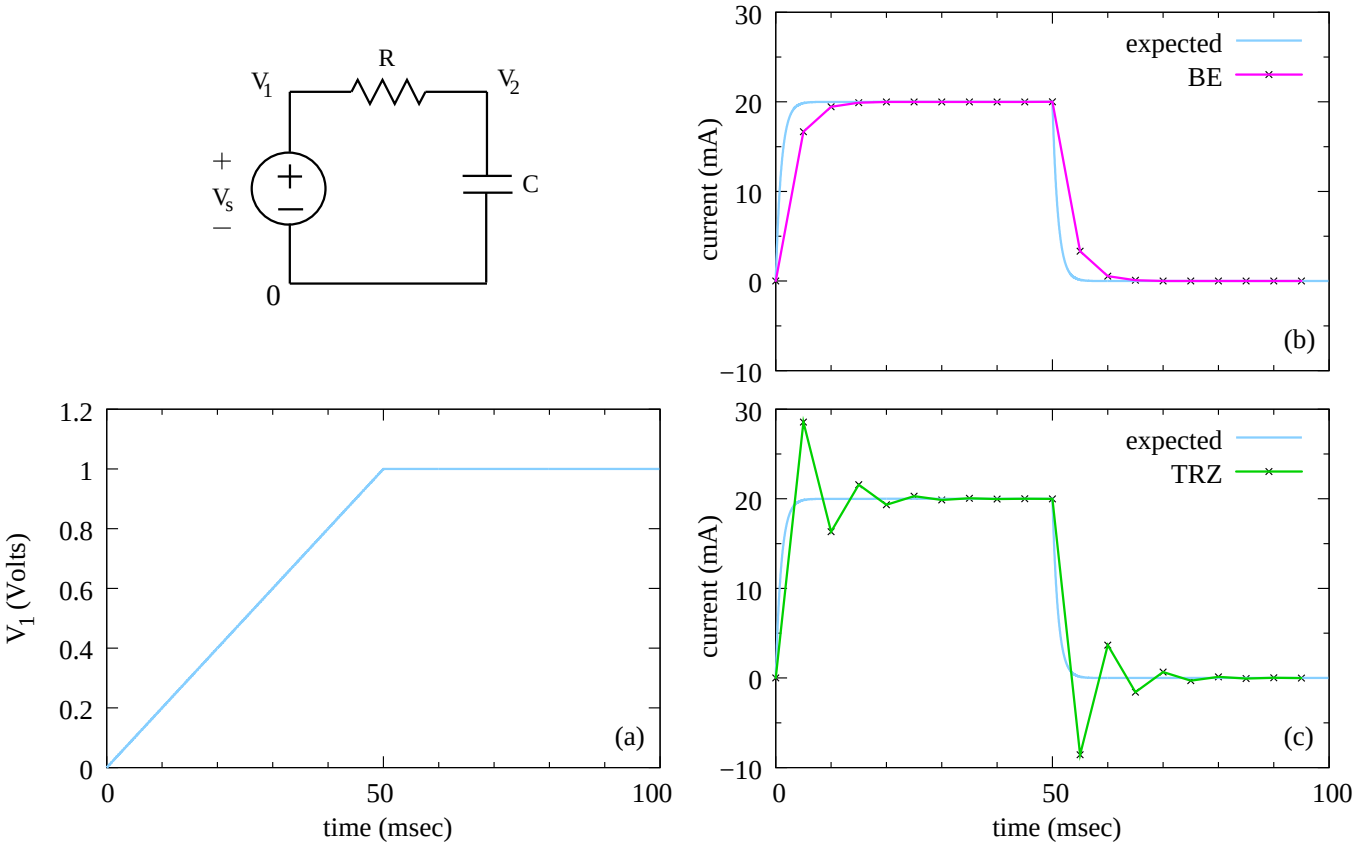
Ringing



(Parameters: $R = 1\ \Omega$, $C = 1$ mF, and h (time step) $= 5$ msec.)

* If h is large, TRZ results in ringing.

Ringing



(Parameters: $R = 1\ \Omega$, $C = 1$ mF, and h (time step) $= 5$ msec.)

* If h is large, TRZ results in ringing.
* Ringing can be reduced by using a smaller time step.

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