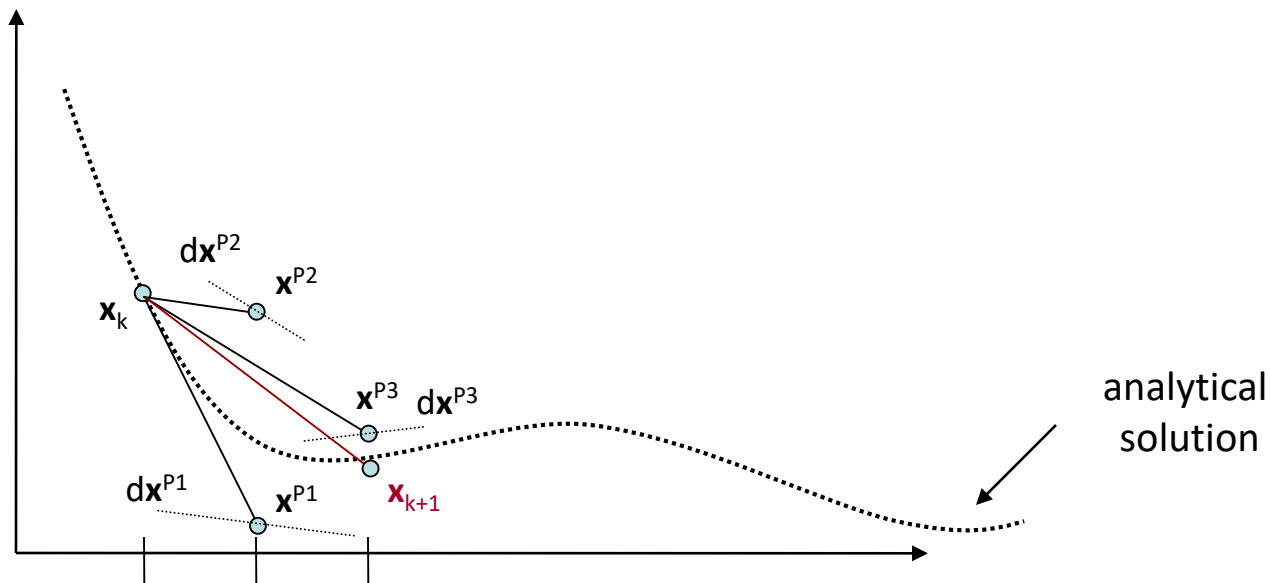# Virtual Physics
Equation-Based Modeling

TUM, January 10, 2023

Higher-Order Methods

analytical solution

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Heun

Let us look at an extension of Forward Euler:

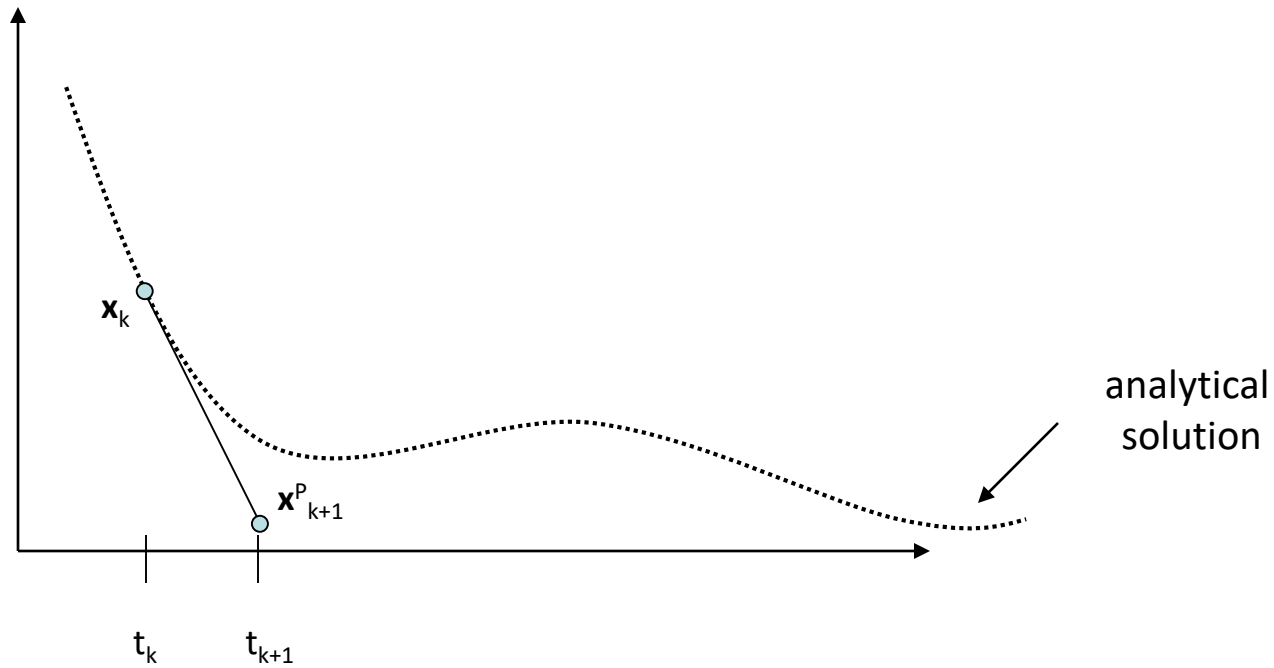- We start by making a prediction step using forward Euler:

  prediction: $d\mathbf{x}_k = f(\mathbf{x}_k, t_k)$ (We will now omit /dt in dx/dt)

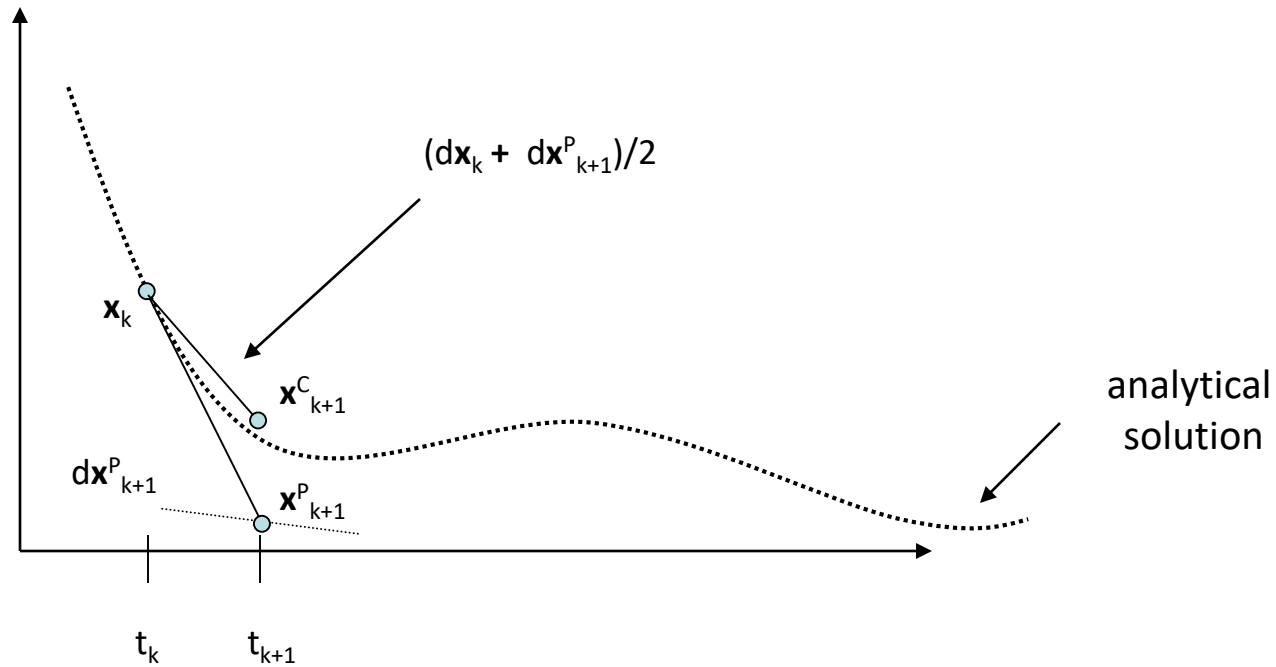 $\mathbf{x}^P_{k+1} = \mathbf{x}_k + h \cdot d\mathbf{x}_k$

- Using $\mathbf{x}^P$, we make a second guess of $d\mathbf{x}/dt$ and finally make a correction step, combining both guesses.

  correction: $d\mathbf{x}^P_{k+1} = f(\mathbf{x}^P_{k+1}, t_k + h)$

  $\mathbf{x}^C_{k+1} = \mathbf{x}_k + h/2 \cdot (d\mathbf{x}_k + d\mathbf{x}^P_{k+1})$

- This method is known as Heun's method.

- It involves two evaluations of f() but it is second order accurate.

analytical solution

$\mathbf{x}_k$

$\mathbf{x}^P_{k+1}$

t_k t_{k+1}

$(d\mathbf{x}_k + d\mathbf{x}^P_{k+1})/2$

$\mathbf{x}_k$

$\mathbf{x}^C_{k+1}$

analytical solution

$d\mathbf{x}^P_{k+1}$

$\mathbf{x}^P_{k+1}$

t_k

t_{k+1}

Why is this method second order accurate?

- Let us develop a 2nd order Taylor-Approximation for f().

$$\mathbf{x}_{k+1} = \mathbf{x}_k + h \cdot f(\mathbf{x}_k, t_k) + h^2/2 \cdot df(\mathbf{x}_k, t_k)/dt + O(h^3)$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + h \cdot f(\mathbf{x}_k, t_k) + h^2/2 \cdot (\partial f(\mathbf{x}_k, t_k)/\partial x \cdot d\mathbf{x}_k/dt + \partial f(\mathbf{x}_k, t_k)/\partial t) + O(h^3)$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + h \cdot f(\mathbf{x}_k, t_k) + h^2/2 \cdot (\partial f(\mathbf{x}_k, t_k)/\partial x \cdot f(\mathbf{x}_k, t_k) + \partial f(\mathbf{x}_k, t_k)/\partial t) + O(h^3)$$

Why is this method second order accurate?

- If we reformulate Heun just in terms of $\mathbf{x}_k$, $\mathbf{x}_{k+1}$ and f() we get:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + h/2 \cdot (\, f(\mathbf{x}_k + h \cdot f(\mathbf{x}_k,t_k)\,,t_k+h) + f(\mathbf{x}_k,t_k)\,)$$

- We now express $f(\mathbf{x}_k + h \cdot f(\mathbf{x}_k,t_k)\,,t_k+h)$ as linear 2D-Taylor Approximation of $f(\mathbf{x},t)$ around $f(\mathbf{x}_k,t_k)$:

$$f(\mathbf{x}_k+ h \cdot f(\mathbf{x}_k,t_k)\,,t_k+h) = f(\mathbf{x}_k,t_k) + h \cdot f(\mathbf{x}_k,t_k) \cdot \partial f(\mathbf{x}_k,t_k)/\partial x + h \cdot \partial f(\mathbf{x}_k,t_k)/\partial t$$

- Plugging into the original equation yields:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + h/2 \cdot (f(\mathbf{x}_k,t_k) + h \cdot f(\mathbf{x}_k,t_k) \cdot \partial f(\mathbf{x}_k,t_k)/\partial x + h \cdot \partial f(\mathbf{x}_k,t_k)/\partial t + f(\mathbf{x}_k,t_k)\,)$$

$$\mathbf{x}_{k+1} = \mathbf{x}_k + h \cdot f(\mathbf{x}_k,t_k) + h^2/2 \cdot (\partial f(\mathbf{x}_k,t_k)/\partial x \cdot f(\mathbf{x}_k,t_k) + \partial f(\mathbf{x}_k,t_k)/\partial t)$$

- This is identical to the 2nd order Taylor approximation!

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Is Heun the only 2nd order Method with two evaluations of f()?

- Let us generalize this procedure by introducing coefficients α and β:

  prediction:
  $$d\mathbf{x}_k = f(\mathbf{x}_k, t_k)$$
  $$\mathbf{x}^P = \mathbf{x}_k + h \cdot \beta_{11} \, d\mathbf{x}_k$$

  correction:
  $$d\mathbf{x}^P = f(\mathbf{x}^P, t_k + \alpha_1 h)$$
  $$\mathbf{x}_{k+1} = \mathbf{x}_k + h \cdot (\beta_{21} d\mathbf{x}_k + \beta_{22} d\mathbf{x}^P)$$

- The coefficients are typically arranged in the Butcher tableau

0	0	0
α_1	β_{11}	0
1	β_{21}	β_{22}

0	0	0
1	1	0
1	0.5	0.5

- On the right, you see the Butcher tableau of Heun.

- If we repeat the analysis for the Heun formula with the generalized coefficients, we get:

$$\mathbf{x}_{k+1} = \mathbf{x}_k$$

$$+ h \cdot (\beta_{21} + \beta_{22}) \cdot f(\mathbf{x}_k, t_k)$$

$$+ h^2/2 \cdot (2\,\beta_{11}\beta_{22}\partial f(\mathbf{x}_k, t_k)/\partial x \cdot f(\mathbf{x}_k, t_k) + 2\,\alpha_1\beta_{22}\,\partial f(\mathbf{x}_k, t_k)/\partial t)$$

- In order to be 2nd order accurate, the following equations must hold:

$$\beta_{21} + \beta_{22} = 1$$
$$2\beta_{11}\beta_{22} = 1$$
$$2\alpha_1\beta_{22} = 1$$

- This is evidently true for Heun, but there is a second solution. **The midpoint rule:**

0	0	0
0.5	0.5	0
1	0	1

Higher-Order RK Methods

Heun contains 2 sub-steps. If we allow *n* steps, we get more coefficients and can derive even higher-order methods:

step 0:
$$d\mathbf{x}^{P0} = f(\mathbf{x}_k, t_k)$$

...

step i:
$$\mathbf{x}^{Pi} = \mathbf{x}_k + h \cdot (\beta_{i1}d\mathbf{x}^{P0} + \beta_{i2}d\mathbf{x}^{P1} + ... + \beta_{ii}d\mathbf{x}^{P(i-1)})$$
$$d\mathbf{x}^{Pi} = f(\mathbf{x}^{Pi}, t_k + \alpha_i h)$$

...

final step n:
$$\mathbf{x}_{k+1} = \mathbf{x}_k + h \cdot (\beta_{n1}d\mathbf{x}^{P0} + \beta_{n2}d\mathbf{x}^{P1} + ... + \beta_{nn}d\mathbf{x}^{P(n-1)})$$
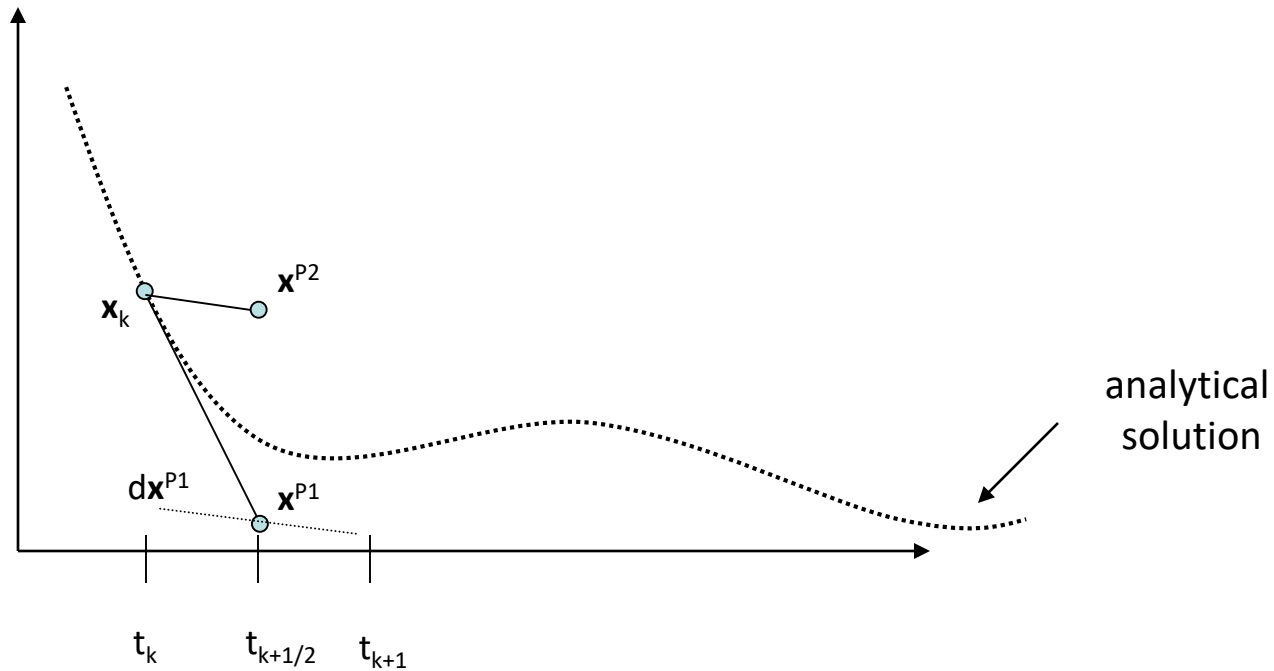
The best known algorithm from this class of numerical integration methods is the 4th-order accurate Runge-Kutta (RK4) algorithm characterized by the following Butcher tableau:

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

analytical solution

$\mathbf{x}_k$

$\mathbf{x}^{P1}$

t_k $t_{k+1/2}$ t_{k+1}

Various RK Methods
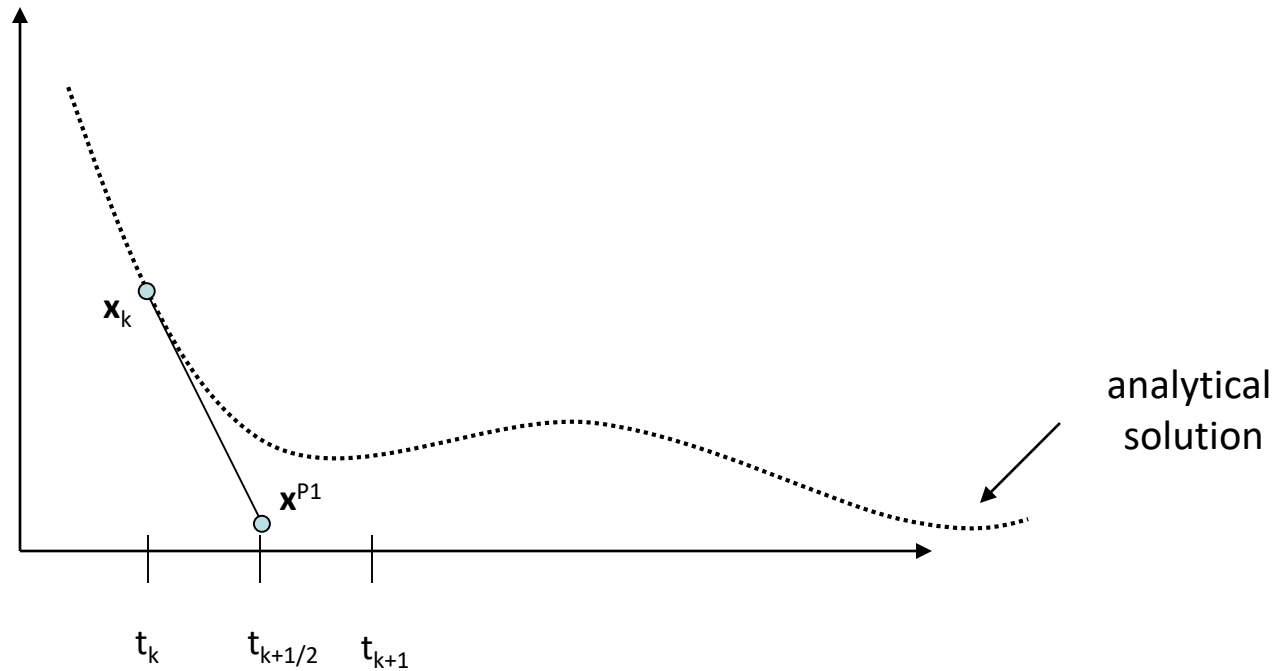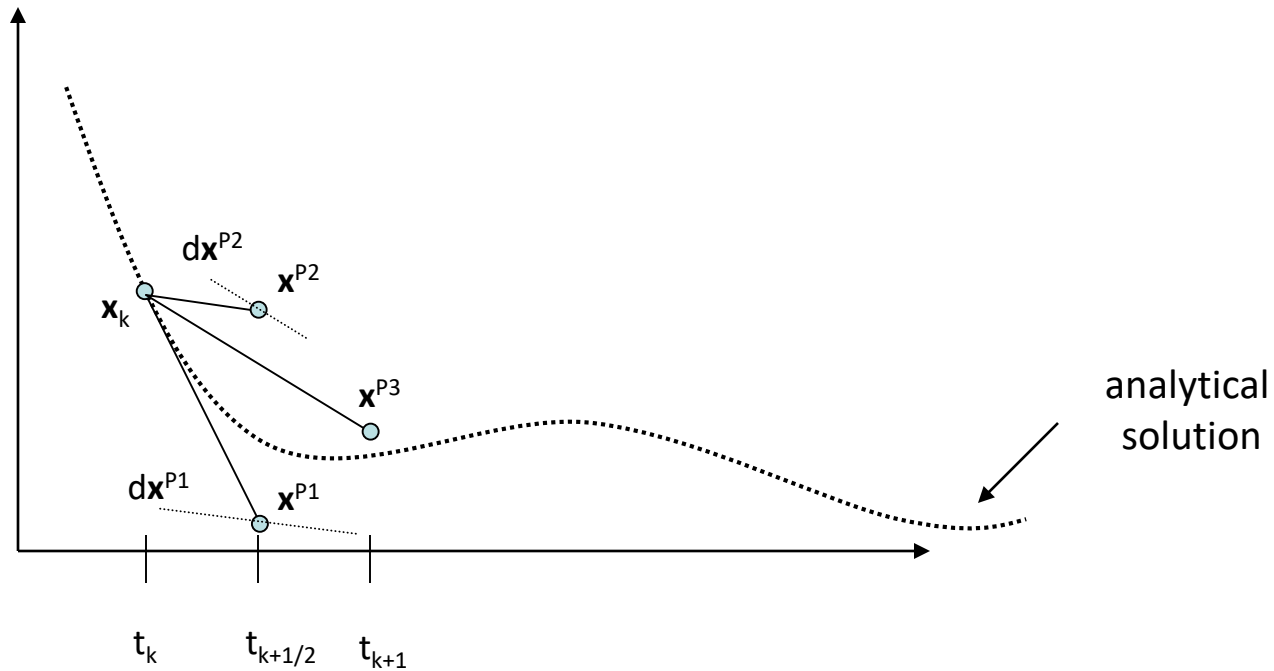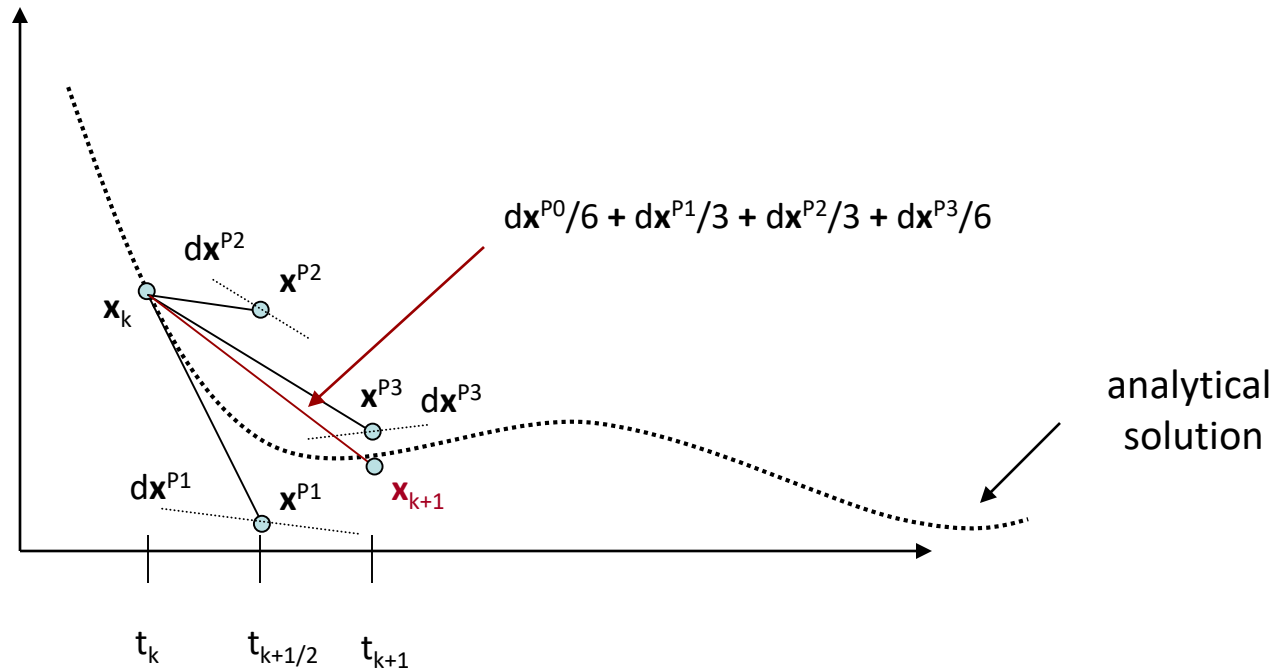
Over time, many RK methods have been developed:

Developer	Year	Order	# of Stages
Euler	1768	1	1
Runge	1895	4	4
Heun	1900	2	2
Kutta	1901	5	6
Huta	1956	6	8
Shanks	1966	7	9
Curtis	1970	8	11

- The number of non-linear equations grows rapidly with the order of the methods. Already for RK methods of order 5, there no longer exists a solution in 5 stages. More stages must be added in order to increase the number of parameters.

- In recent years, a sequence of yet higher-order RK methods were developed quite rapidly using computer algebra methods (Maple, Mathematica).
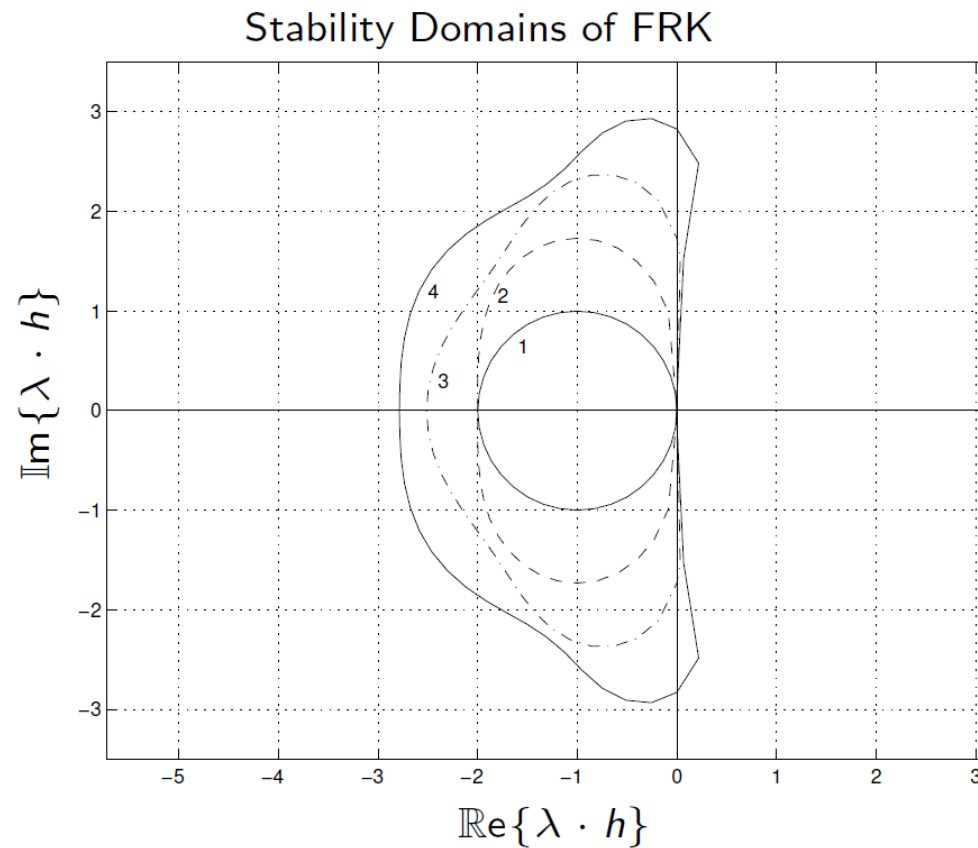
A nth-order method is more precise than a first-order method but it involves also more function evaluations per integration step. Is it worth its price?

- The answer is evident:

  YES!
  It is worth
  every penny!

Price per Accuracy for Different FRKs

RK: Stability

What about the stability?
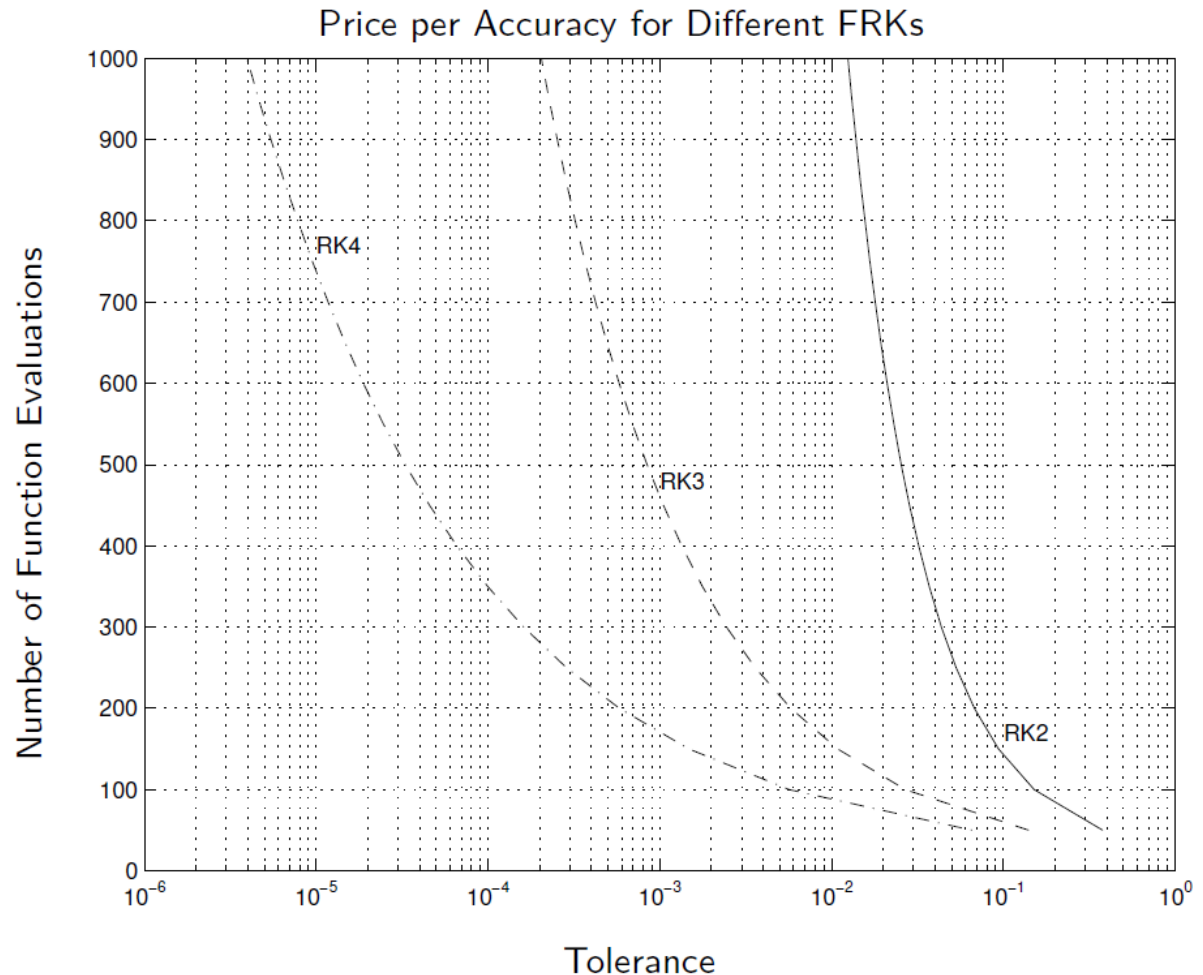
Stability Domains of FRK

What about the stability?

- n^{th}-order methods in n stages have the same stability domain. For orders higher than 5 the stability domain depends on the concrete Butcher tableau.

Stability Domains of FRK

- Although, higher order methods gain a lot in precision, the stability domain grows rather modestly.

- For stiff systems, all RK-methods are almost as bad as FE. We are still bound to use very small step-sizes.

- However, for oscillating systems (with eigenvalues near the imaginary axis), the situation improves significantly from RK2 on.

Local Integration Error Estimation
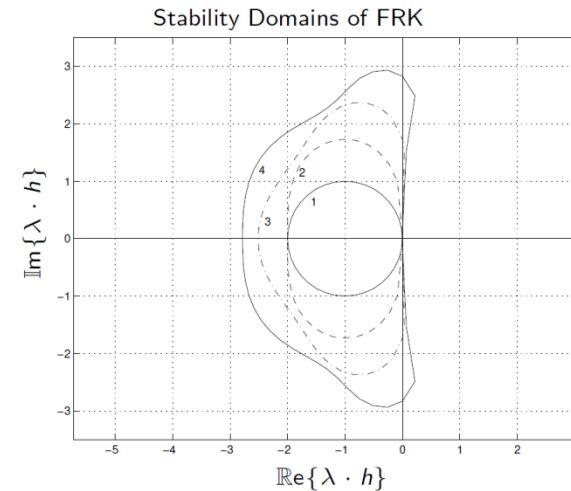
In order to control the step-size, we would like to have an estimate of the local integration error for each step.

- One way, is to perform the same step twice using two different integration methods.

- Using their results ($\mathbf{x}_1$ and $\mathbf{x}_2$) we may estimate the relative error ε_{rel}

$$\varepsilon_{rel} = |\mathbf{x}_1 - \mathbf{x}_2| \ / \ \max(|\mathbf{x}_1|, |\mathbf{x}_2|, \delta) \qquad \text{δ is a small fudge value > 0}$$

- We can now compare ε_{rel} with the desired tolerance tol_{rel} and control the step-size accordingly

It is not efficient to perform the same step twice. Hence, Fehlberg managed to integrate an RK4 method into an RK5 method.

- Here is the Butcher Tableau for Runge-Kutte-Fehlberg 4/5:

0	0	0	0	0	0	0
1/4	1/4	0	0	0	0	0
3/8	3/32	9/32	0	0	0	0
12/13	1932/2197	-7200/2197	7296/2197	0	0	0
1	439/216	-8	3680/513	-845/4104	0	0
1/2	-8/27	2	-3544/2565	1859/4104	-11/40	0
x_1	25/216	0	1408/2565	2197/4104	−1/5	0
x_2	16/135	0	6656/12825	28561/56430	−9/50	2/55

- Now the estimation of the local integration error is virtually for free.

Using $\varepsilon_{rel} = |\mathbf{x}_1 - \mathbf{x}_2| / \max(|\mathbf{x}_1|, |\mathbf{x}_2|, \delta)$, we can develop a step-size control for RKF 4/5

- $\mathbf{x}_1$ is a 4th order approximation whereas $\mathbf{x}_2$ is a 5th order approximation

- Hence the relative error ε_{rel} is proportional to h^5
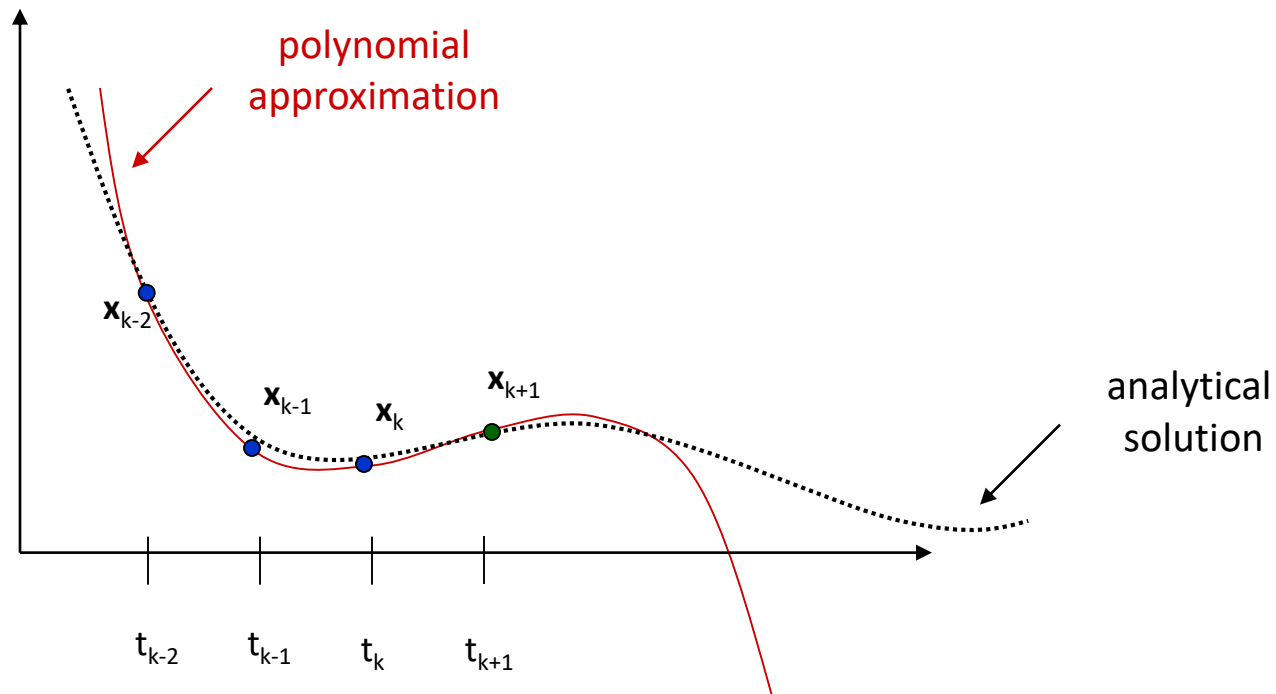
- It is therefore meaningful to state:

$$\varepsilon_{rel} / tol_{rel} = (h_{old} / h_{new})^5$$

➔ $$h_{new} = \sqrt[5]{tol_{rel}/\varepsilon_{rel}} \; h_{old}$$

- In this way, if the error is too large, the next step is reduced, and if the error is unnecessarily small, the next step is increased.
- This is an ***optimistic strategy*** since steps are never repeated, even if the error is excessively large

Single-Step

- So far, every integration step was independent from its preceding integrations steps.

- At each step, we have performed a single-step (with some sub-steps). The information contained in the previous integration steps has been discarded.

- Hence the RK methods are called *single-step methods*.

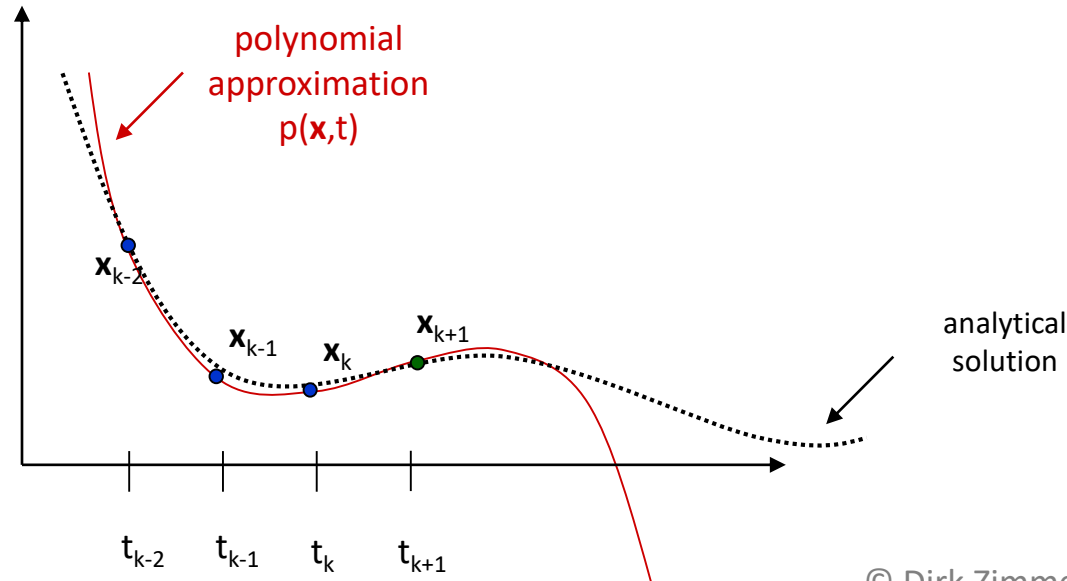- But there are also *multi-step methods*....

- The idea behind every multi-step method is to generate a higher-order method by a polynomial approximation of the previous steps.

- The figure below illustrates this principle:

- Let p() be the polynomial that approximates the last n-1 steps: $\mathbf{x}_{k+1}$, $\mathbf{x}_k$ ... $\mathbf{x}_{k-n+1}$

- We can then generate a nth-order method by solving the following equation for $\mathbf{x}_{k+1}$:

$$f(\mathbf{x}_{k+1}, t_{k+1}) = dp(\mathbf{x}_{k+1}, t_{k+1})/dt$$

- Hence this represents an implicit method (like BE).

polynomial
approximation
p(**x**,t)

$\mathbf{x}_{k-2}$

$\mathbf{x}_{k-1}$ $\mathbf{x}_k$ $\mathbf{x}_{k+1}$

analytical
solution

t_{k-2} t_{k-1} t_k t_{k+1}

Backwards Difference Formula

- Let p() be the polynomial that approximates the last n-1 steps: $\mathbf{x}_{k+1}$, $\mathbf{x}_k$ … $\mathbf{x}_{k-n+1}$

- We can then generate a nth-order method by solving the following equation for $\mathbf{x}_{k+1}$:

$$f(\mathbf{x}_{k+1}, t_{k+1}) = dp(\mathbf{x}_{k+1}, t_{k+1})/dt$$

- Hence this represents an implicit method (like BE).

- **Remark:** Since this is an implicit method, it can also be directly applied to the implicit DAE form $0 = F(d\mathbf{x}/dt, \mathbf{x}, \mathbf{u}, t)$:

$$0 = F(dp(\mathbf{x}_{k+1}, t_{k+1})/dt, \mathbf{x}_{k+1}, \mathbf{u}_{k+1} t_{k+1})$$

These kind of solvers can also be applied on systems that have not undergone index-reduction (but it is not necessarily an efficient way to do so..)

Backwards Difference Formula

- If we perform the integration with a fixed step-size, all points for the polynomial approximation are equally-distant spaced in time. This enables the usage of Newton-Gregory polynomials for p().

- $dp(\mathbf{x}_{k+1}, t_{k+1})/dt$ can be expressed as weighted sum of $\mathbf{x}_k$:

$$dp(\mathbf{x}_{k+1}, t_{k+1})/dt \cdot h = \alpha_1 \mathbf{x}_{k+1} + \alpha_2 \mathbf{x}_k + ... + \alpha_{n+1} \mathbf{x}_{k-n+1}$$

- This leads to the famous BDF methods:

	α_1	α_2	α_3	α_4	α_5	α_6
BDF 1	1	-1				
BDF 2	3/2	-2	1/2			
BDF 3	11/6	-3	3/2	-1/3		
BDF 4	25/12	-4	3	-4/3	1/4	
BDF 5	137/60	-5	5	-10/3	5/4	-1/5

- Without loss of generality

$$p(x) = at^2 + bt + c$$
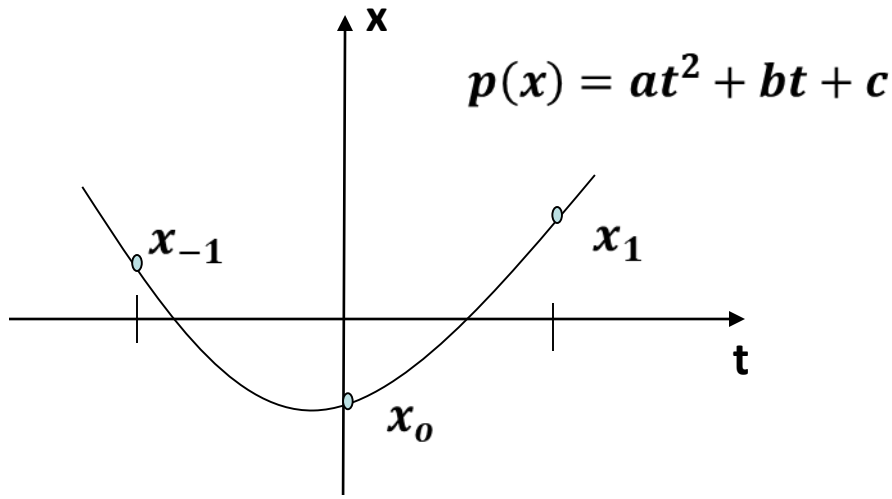
$$x_0 = c$$

$$x_{-1} = a - b + c$$
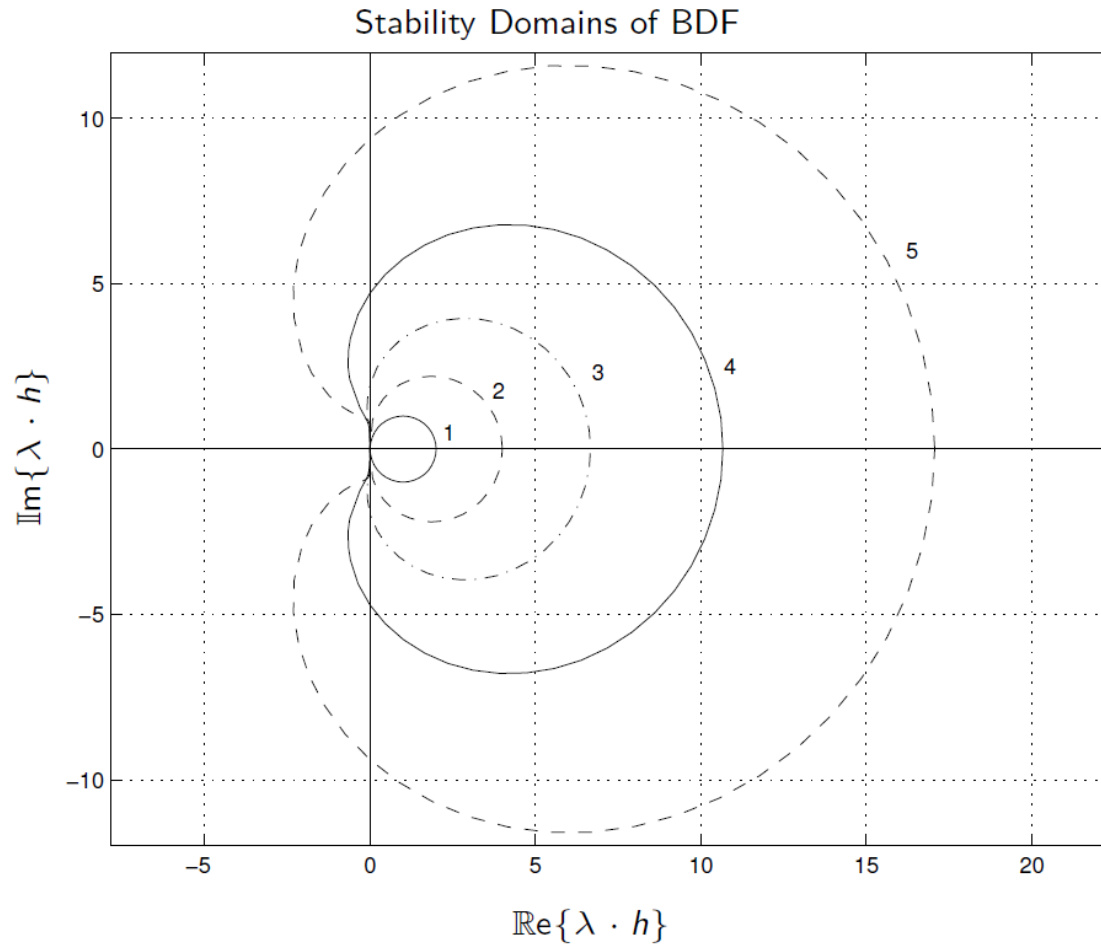
$$x_1 = a + b + c$$

$$a = \frac{x_1 + x_{-1}}{2} - x_0$$

$$b = \frac{x_1 - x_{-1}}{2} - x_0$$

$$\left.\frac{dp(t)}{dt}\right|_{t=1} = 2a + b = x_1 + x_{-1} - x_0 + \frac{x_1}{2} - \frac{x_{-1}}{2} - x_0$$

$$\left.\frac{dp(t)}{dt}\right|_{t=1} = \frac{3}{2}x_1 - 2x_0 + \frac{1}{2}x_{-1}$$

What about the stability?


Stability Domains of BDF

BDF: Stability

What about the stability?

- BDF 1 is Backward Euler
- BDF 2 is still maintains the analytical stability
- The region of unstability grows significantly with the number of the order.

Stability Domains of BDF

- From BDF 3 on, the unstable region overlaps the imaginary axis.

- Hence the higher order BDF methods (from 5 on) behave strangely for oscillatory systems.

- Thanks to their suitability for the simulation of stiff systems and due to their simplicity, the BDF algorithms are among the most widely used numerical ODE solvers for the simulation of dynamic systems.
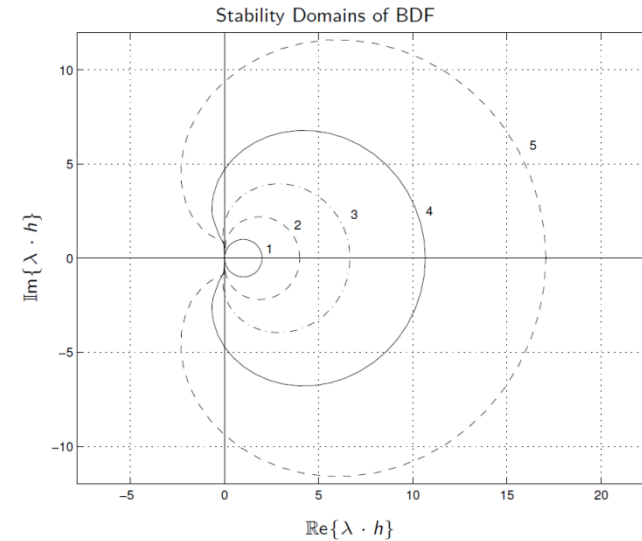
Multi-Step: Startup

- There are some extra problems involved with multi-step methods in general

- One of them is the startup problem.

- We simply assumed, that there for an nth-order method, there are n-1 past values available. At start, this assumption is obviously violated.

- Essentially, there are two solutions:

  - Work yourself up: Start with BDF 1, then continue with BDF 2, BDF 3 and so on... Unfortunately, the usage of BDF 1 may enforce small step-sizes initially.
  - Kick-start using a single-step method of the appropriate order.
    For instance use 3 steps of RK4 to start BDF 4. However, since RK4 cannot cope with stiff systems, small step-sizes might again be enforced.
  - Most probably the best choice is to use and implicit Runge-Kutta (see later on) method as Kick-start

- The other problem is step-size control.

- We have assumed a fixed step-size so far.

- If we want to adapt the step-size, we have to "relocate" our past integration values $\mathbf{x}_k$, $\mathbf{x}_{k-1}$, ... $\mathbf{x}_{k-n+1}$
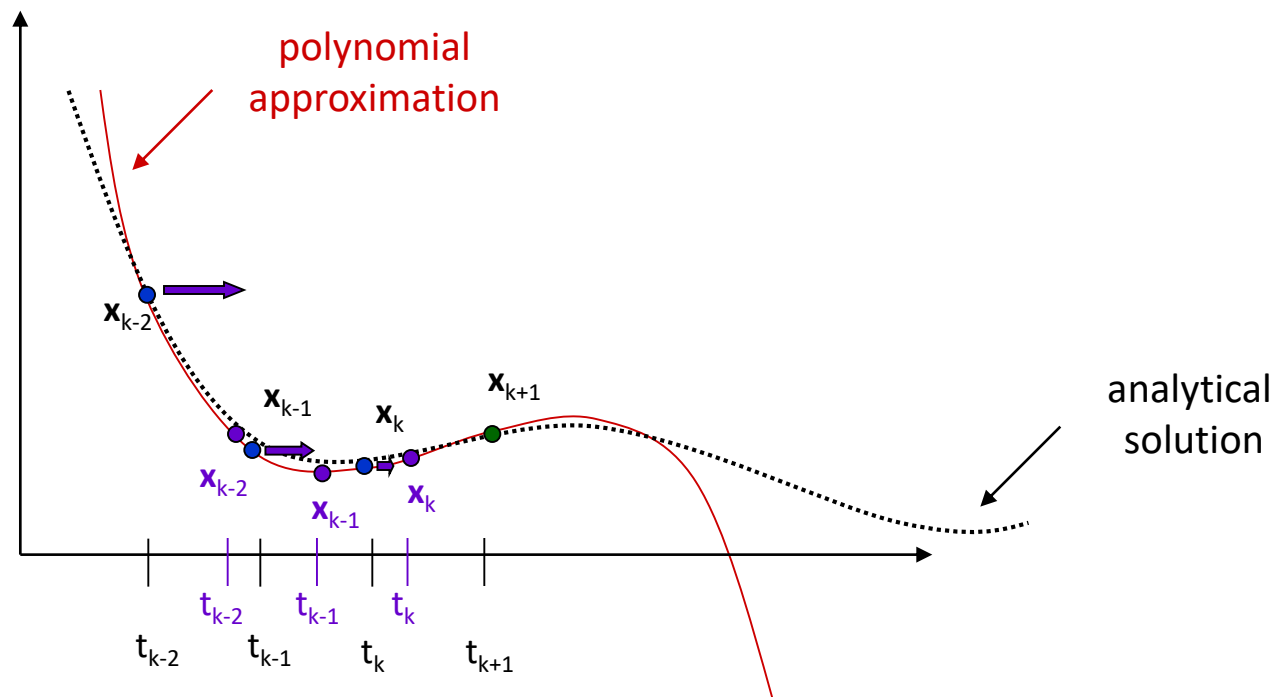
- This relocation of x_k, x_{k-1}, ... x_{k-n+1} can be performed with linear operations only and does not involve any loss of precision since the polynomial g() remains unchanged.

- However, the adaption of step-size is relatively costly. Controlling the step-size for each step is not recommendable. Consequently, a more conservative step-size has to be chosen so that overhasty changes can be avoided and the same step-size can be maintained over larger time-spans
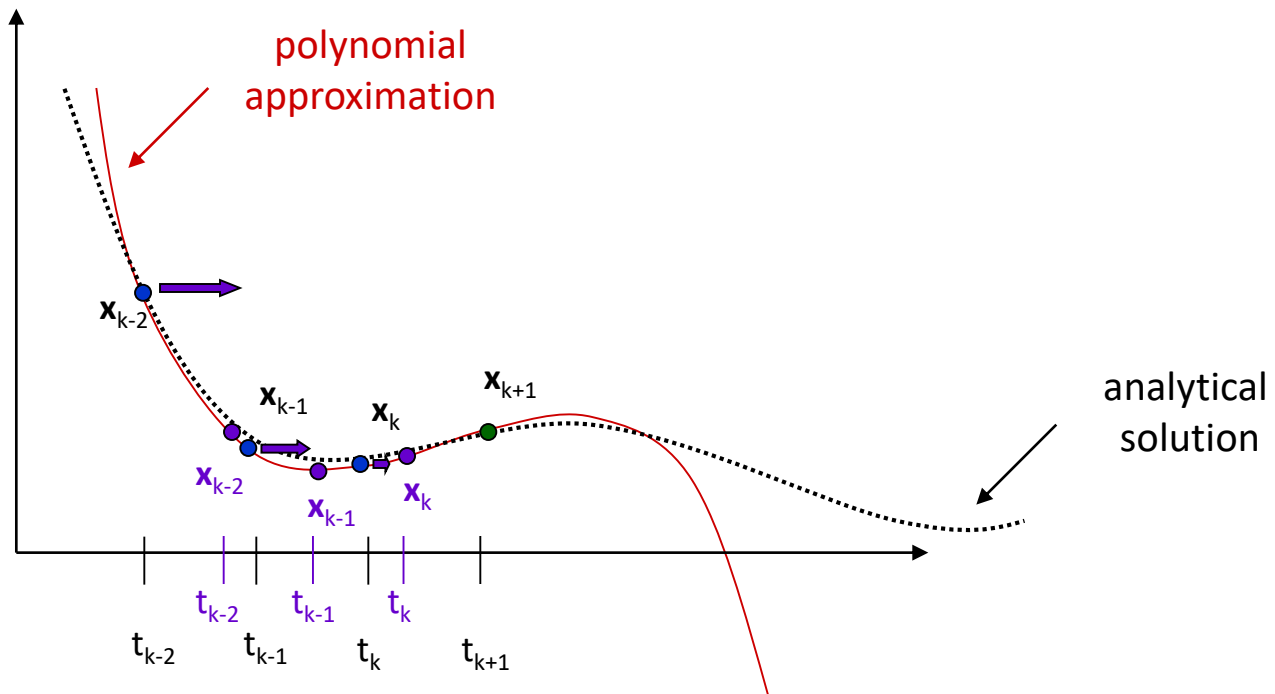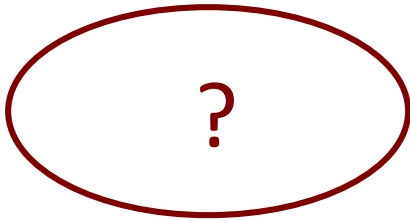
Multi-Step: On DASSL

- DASSL is a variable-order, variable step-size multistep method.

- Why variable-order? A high order reduces the convergence area of the implicit solution. You may have to take smaller step-sizes than needed for precision just to stay within the convergence intervall.

- Hence, order reduction helps robustness and DASSL is very robust.

- DASSL basically combines the BDF Formulas of different order

- The clue is the error estimation. Basic idea: In a normal situation you would expect the error estimate to decrease from order to order... When this is not the case, you may want to reduce your order and take smaller steps.

- There is no explicit method that is numerically stable for all analytical stable systems.

- There is no implicit multistep method of order > 2 that is numerically stable for all analytical stable systems.

Overview

So far, we have investigated two major classes of integration methods

	Explicit	Implicit
Single-Step	Runge-Kutta	
Multi-Step		BDF (DASSL)

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What about explicit multi-step methods. They would be great for real-time simulation or?
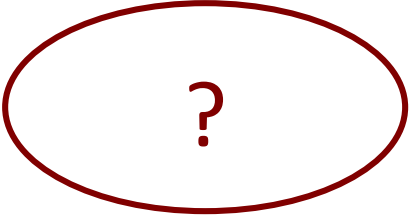
	Explicit	Implicit
Single-Step	Runge-Kutta	
Multi-Step	**?**	BDF (DASSL)

Adams-Bashforth

There are explicit multi-step methods available. There are called, for instance, Adams-Bashforth (AB).

- Whereas the implicit multi-step methods are based on polynomial interpolation, the explicit methods are based on polynomial extrapolation. This is potentially dangerous.

- It is therefore no surprise, that AB performs very poorly with respect to stability.

- Indeed, the numerical stable region shrinks for higher-order methods

- AB is practically **only** used for non-stiff, linear systems.

Stability Domains of AB

$\mathbb{Im}\{\lambda \cdot h\}$

$\mathbb{Re}\{\lambda \cdot h\}$
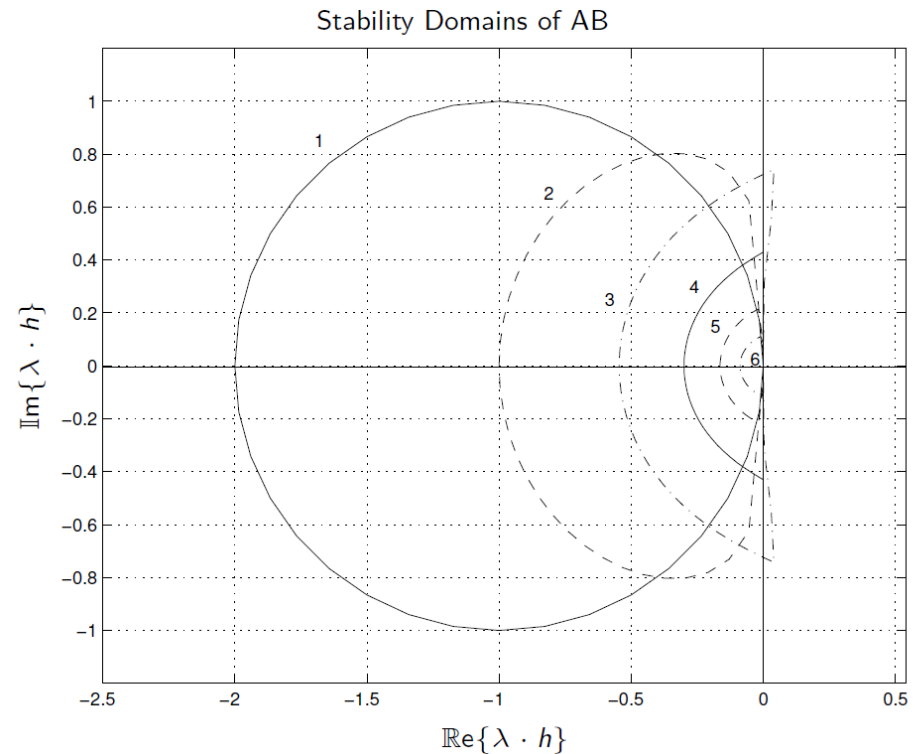
Wouldn't implicit single step methods be very suited for the simulation of stiff systems?

	Explicit	Implicit
Single-Step	Runge-Kutta	?
Multi-Step	Adams-Bashforth	BDF (DASSL)

The classic RK methods enabled an explicit computation since the Butcher Tableau does not contain entries at or above the diagonal.

- Here is the Butcher Tableau of 3rd order Radau IIa. It requires an implicit solver.

1/3	5/12	-1/12
1	3/4	1/4
1	3/4	1/4

$d\mathbf{x}^{P0} = f(\mathbf{x}_k + 5h/12 d\mathbf{x}^{P0} - h/12 d\mathbf{x}^{P1}, t_k + h/3)$

$d\mathbf{x}^{P1} = f(\mathbf{x}_k + 3h/4 d\mathbf{x}^{P0} + h/4 d\mathbf{x}^{P1}, t_k + h)$

➔ $\mathbf{x}_{k+1} = \mathbf{x}_k + 3h/4 d\mathbf{x}^{P0} + h/4 d\mathbf{x}^{P1}$

$d\mathbf{x}^{P0}$ and $d\mathbf{x}^{P1}$ need to be found by an iterative solver. Hence, Radau IIa (3rd order) requires twice as many iteration variables as BE and a single step is though (roughly) $2^3 = 8$ times more expensive as an BDF step of the same order.

Implicit RK

The classic RK methods enabled an explicit computation since the Butcher Tableau does not contain entries at or above the diagonal.

- Here is the Butcher Tableau of 3rd order Radau IIa. It requires an implicit solver.

$$
\begin{array}{c|cc}
1/3 & 5/12 & -1/12 \\
1 & 3/4 & 1/4 \\
\hline
1 & 3/4 & 1/4
\end{array}
$$

- Implicit RK methods behave excellently w.r.t. stability
- However, a step of IRK is significantly more expensive than a step of BDF of the same order.
- However, IRK feature a more flexible step-size control and can compensate for this in highly non-linear or discontinuous systems


Stability Domains of IRK
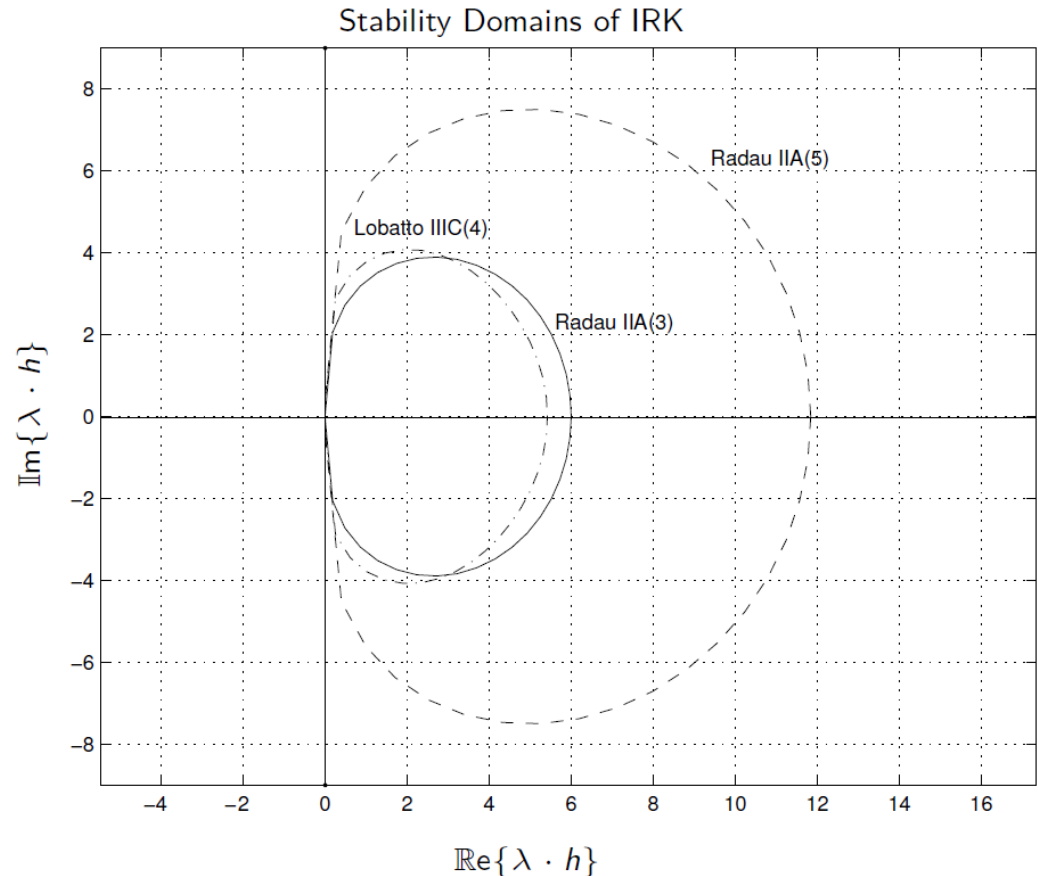
So.. this is what we have learned today:

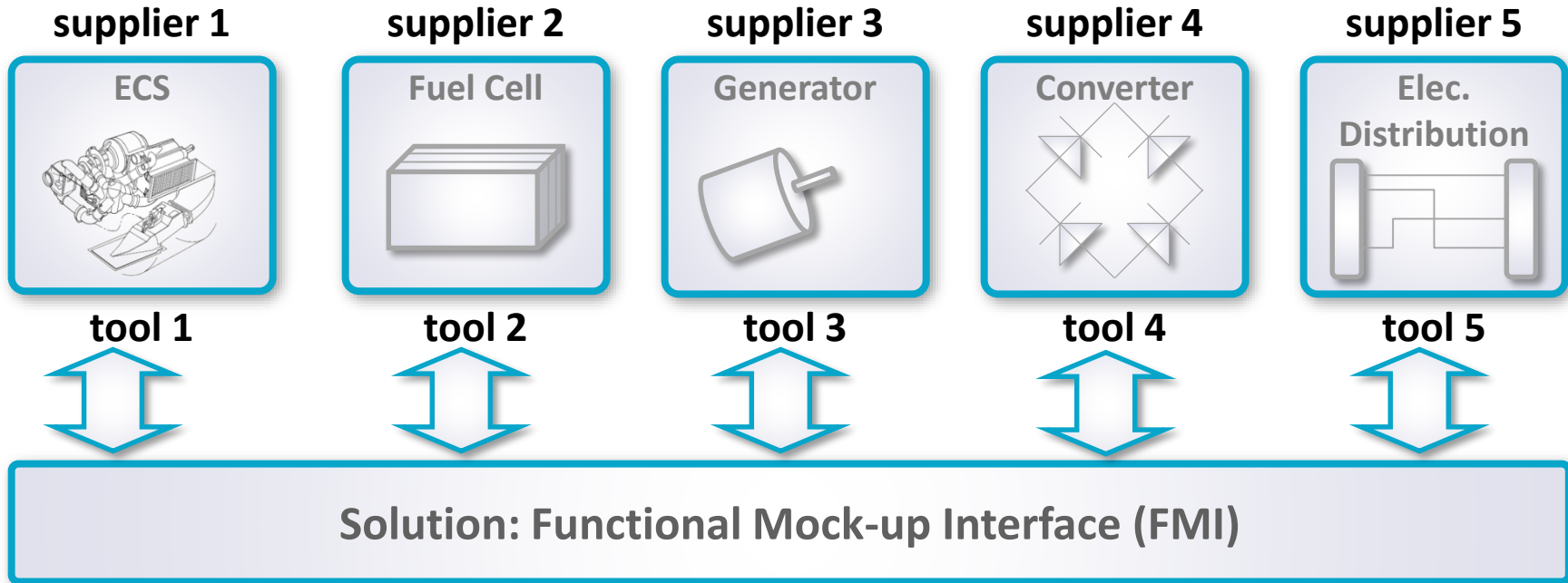|	**Explicit**	**Implicit**
Single-Step	Runge-Kutta	Implicit Runge-Kutta (Radau IIa)
Multi-Step	Adams-Bashforth	BDF (DASSL)

Convergence

We haven't spoken about convergence yet.

- For any implicit solver we do simply assume that our iterative numerical solver finds the solution but this only happens when the initial guess value is in the convergence area.

- The initial guess value stems from the last integration step. If this is outside the convergence area, we have to lower step-size.

- With higher orders the size of convergence area, typically shrinks. Hence lowering the order might enable larger steps to be taken.

- Even for explicit solvers, the model-evaluation function still may contain non-linear parts to be iteratively solved. In this case, many of the above also holds true.

- Stepsize control works good for precision but is hardly optimized for convergence. Hence it can happen that by lowering precision, your simulation becomes slower... (or fails at all)...

Depending on your model, your simulation performance might be limited by either stability constraints, convergence constraints or precision requirements.

Stability

Convergence
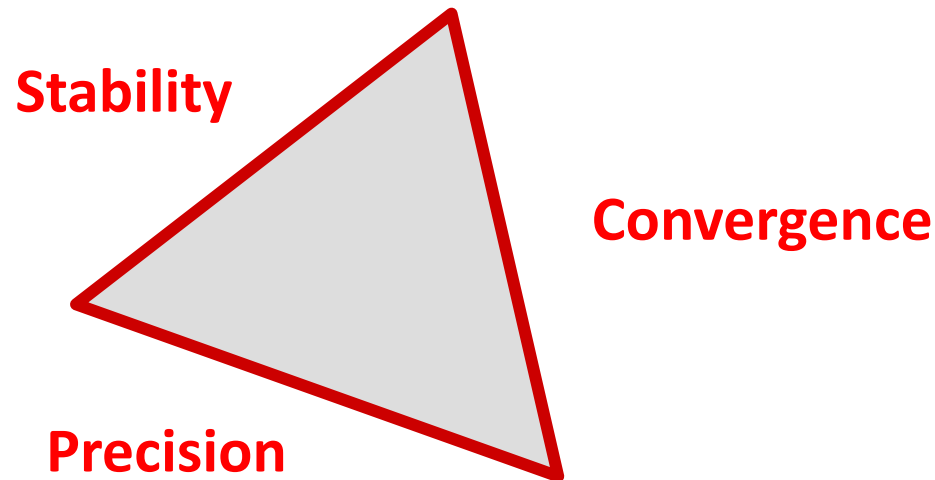
Precision

For many, many practical applications, stability and convergence are the greater source of trouble than sheer precision.

FMI Standard

supplier 1	supplier 2	supplier 3	supplier 4	supplier 5
ECS	Fuel Cell	Generator	Converter	Elec. Distribution
tool 1	tool 2	tool 3	tool 4	tool 5

Solution: Functional Mock-up Interface (FMI)

- Couple different tools for system simulation
- www.fmi-standard.org

FMI Standard

FMI for Model Exchange	**FMI for Co-Simulation**
• $dx/dt = f(x,u,t)$ • does not include ODE-solver	• $x_{t+h} = f(x_t,u,t)$ • includes ODE solver

- Both version of FMI support hybrid systems with discrete events.
- Standard takes into account many solutions for large, stiff systems

Questions ?