An intrinsically adaptive formulation of multistep methods

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To approximate the solution of an IVP

$$\frac{dx}{dt} = f(t,x), \quad x(t_0) = x_0, \quad t \in [t_0, t_f]$$

a *k-step* method uses k previous approximations $x_{n-i} \approx x(t_{n-i}), \quad i = 1:k,$

$$x_n = \alpha_{k-1}x_{n-1} + \cdots + \alpha_0 x_{n-k} + h_n(\beta_k f_n + \cdots + \beta_0 f_{n-k})$$
$$h_i = t_i - t_{i-1}, \qquad f_i = f(t_i, x_i)$$

Adaptivity: choose h_n to attain prescribed accuracy.

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Why do we need adaptivity?

- accuracy
- efficiency
- stability

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Adaptivity aims to control the error at each integration step

- estimate the local error
- choose h_n to keep the error at an assigned value (tolerance)

Order of a multistep method

Approximation: $x_n \approx x(t_n)$ and $x'_n \approx f(t_n, x(t_n))$

When is a method said to be of order q?

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Lower order methods $\rightarrow$ larger stability regions
Higher order methods $\rightarrow$ allow larger step-sizes

Polynomial of a method with k steps and order q

To advance a step of an order q method we construct a *method polynomial* $P_n \in \mathcal{P}_q$ using previously calculated values and define

$$x_n = P_n(t_n)$$

The polynomial of a k-step method will depend on the last k approximated solutions and their derivatives.

Maximal order multistep methods

Three types of high order k-step methods (Dahlquist 1st barrier):

type	max order
implicit	$k+1$
explicit	k

For **Nonstiff** problems:

- $\mathbf{E}_k$: *Explicit k-step*, order $q = k$, e.g. Adams–Bashforth
- $\mathbf{I}_k^+$: *Implicit k-step*, order $q = k + 1$, e.g. Adams–Moulton

For **Stiff** problems:

- $\mathbf{I}_k$: *Implicit k-step*, order $q = k$, e.g. BDF methods

Method polynomial for an E_k type method

Adams-Bashforth-3: explicit, $k = 3$, order $q = 3$, $P_n \in \mathcal{P}_3$

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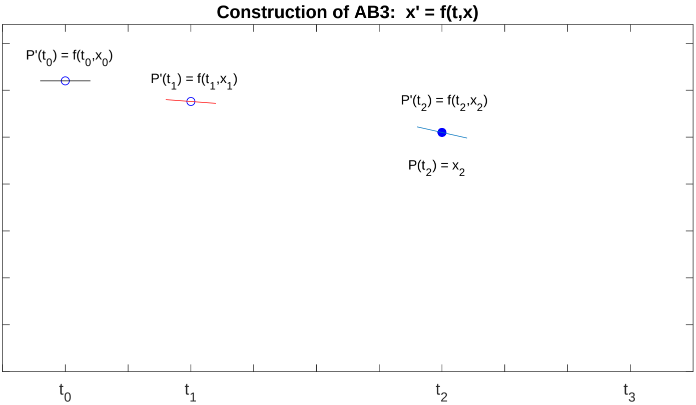

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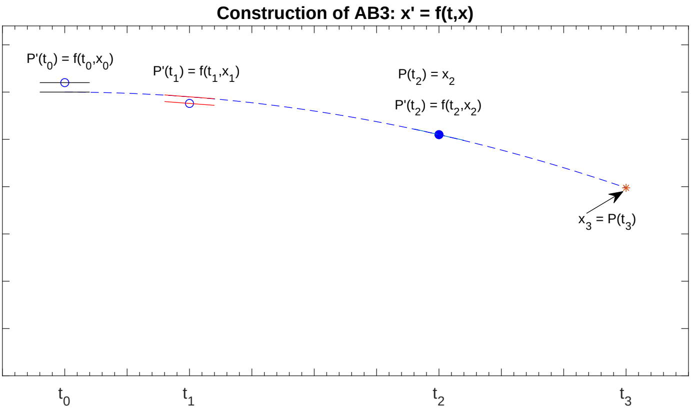

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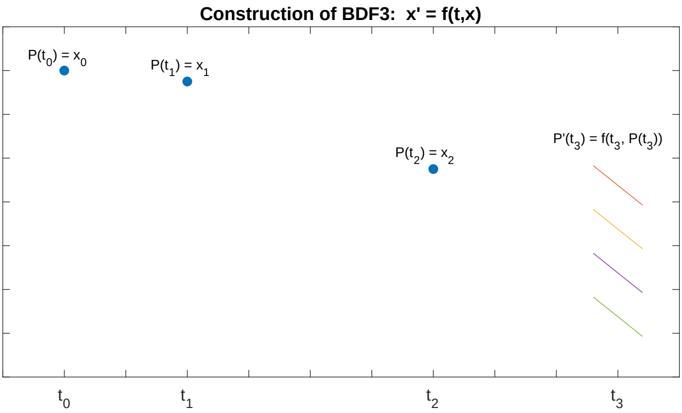

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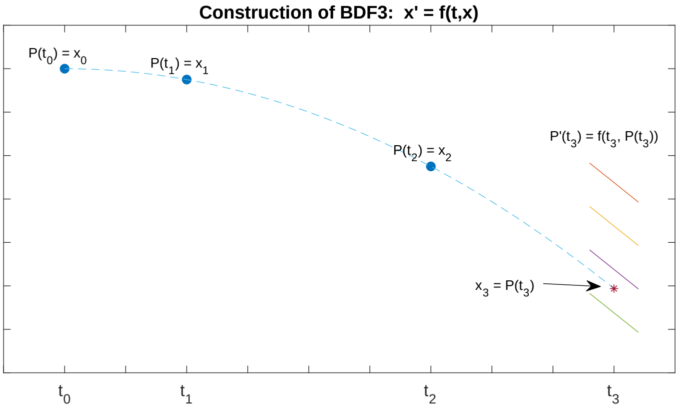

Construction of E_k method of order $q = k$

Interpolation conditions:

$$P(t_{n-i}) = x_{n-i}, \quad i = 1, \ldots, k$$

Collocation conditions:

$$\dot{P}(t_{n-i}) = x'_{n-i}, \quad i = 1, \ldots, k$$

$2k$ possible conditions to define $P \in \mathcal{P}_k$: choose $k+1$ conditions

$\binom{2k}{k+1} = \frac{(2k)!}{(k-1)!(k+1)!}$ $\quad$ *e.g.* $k = 3 \quad \Rightarrow \quad$ 15 possible methods

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But there are infinitely many explicit k-step, order k methods!

P_n for classical k-step formulas

ABk

$$\begin{aligned} P_n(t_{n-1}) &= x_{n-1} \\ \dot{P}_n(t_{n-i}) &= x'_{n-i}, \quad i = 1, \dots, k \end{aligned}$$

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AMk

$$\begin{aligned} P_n(t_{n-1}) &= x_{n-1} \\ \dot{P}_n(t_{n-i}) &= x'_{n-i}, \quad i = 1, \ldots, k \\ \dot{P}_n(t_n) &= f(t_n, P_n(t_n)) \end{aligned}$$

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Solution: slack conditions

Do not insist on interpolation/collocation conditions; allow a slack:

$$\begin{aligned} s_{n-i} &= P_n(t_{n-i}) - x_{n-i} \quad \text{(state slack)} \\ s'_{n-i} &= \dot{P}_n(t_{n-i}) - x'_{n-i} \quad \text{(derivative slack)} \end{aligned}$$

and combine each slack pair into a slack balance condition:

$$a\, s_{n-i} + b\, h_{n-i} s'_{n-i} = 0$$

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simplified to

$$\cos\theta\, s_{n-i} + \sin\theta\, h_{n-i} s'_{n-i} = 0, \quad \theta \in (-\pi/2, \pi/2]$$

Each method type is characterized by its structural conditions

$$\mathbf{E}_k \quad \begin{cases} s_{n-1} = 0 & \text{(interpolation condition)} \\ s'_{n-1} = 0 & \text{(explicit collocation condition)} \end{cases}$$

$$\mathbf{I}_k^+ \quad \begin{cases} \dot{P}_n(t_n) = f(t_n, P_n(t_n)) & \text{(implicit collocation condition)} \\ s_{n-1} = 0 & \text{(interpolation condition)} \\ s'_{n-1} = 0 & \text{(explicit collocation condition)} \end{cases}$$

$$\mathbf{I}_k \quad \begin{cases} \dot{P}_n(t_n) = f(t_n, P_n(t_n)) & \text{(implicit collocation condition)} \\ \cos\theta_0\, s_{n-1} + \sin\theta_0\, h_{n-1}\, s'_{n-1} = 0 & \text{(slack balance condition)} \\ \quad \theta_0 \in (-\pi/2, \pi/2] \end{cases}$$

To complete the number of required conditions we impose $k-1$ additional *slack balance conditions*

$$\cos\theta_i \, s_{n-i-1} + \sin\theta_i \, h_{n-i-1} s'_{n-i-1} = 0$$

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Method parameters θ_i uniquely define a method.

The parameter set $\{\theta_i\}$ is grid independent.

Theorem: *Each linear multistep method of type* $\mathbf{E}_k$, $\mathbf{I}_k$, or $\mathbf{I}_k^+$ *can be represented by a single polynomial in* $[t_{n-1}, t_n]$, *with* $k-1$, k, *and* $k-1$ *parameters, respectively.*

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We can implement every maximal order method by constructing its *method polynomial,* P_n, advancing the integration at each step: $x_n = P_n(t_n)$.

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The solver (MODES) includes every possible multistep method of maximal order, stiff and non-stiff, implicit and explicit.

Parametric formulation of 0-stable multistep methods

Method	**Order**	I_k **method parameters** $\tan(\theta_j)$, $j = 0 : k-1$				
BDFk	$k \leq 6$	$\{0\}_{0:k-1}$				
Kregel	3	154/543	-11/78	0		
Rockswold	3	73/350	71/200	∞		

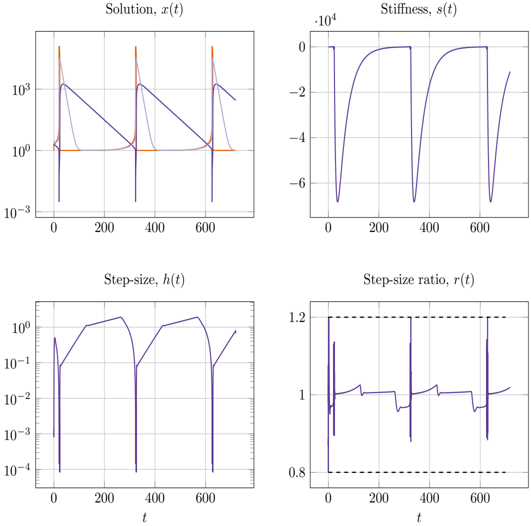
Method	**Order**	I_k^+ **method parameters** $\cot(\theta_j)$, $j = 1 : k-1$				
AMk	$k+1$	$\{0\}_{1:k-1}$				
dcBDFk	$k+1$	$\{(k+1)/(j+1)\}_{1:k-1}$				
Milne2	4	3				
Milne4	5	15/4	0	0		
IDC23	4	6/7	0			
IDC24	5	15/26	0	0		
IDC34	5	5/4	20/33	0		
IDC45	6	45/28	10/11	15/32	0	
IDC56	7	84/43	7/6	21/29	21/55	0

Method	**Order**	E_k **method parameters** $\cot(\theta_j)$, $j = 1 : k-1$				
ABk	k	$\{0\}_{1:k-1}$				
EDFk	k	$\{1/(j+1)\}_{1:k-1}$				
Explicit Euler	1					
Midpoint	2	∞				
Nyström3	3	-3/2	0			
Nyström4	4	-3/5	0	0		
Nyström5	5	-45/133	0	0	0	
EDC22	3	3/14	0			
EDC23	4	6/49	0	0		
EDC33	4	2/7	4/39	0		
EDC24	5	90/1121	0	0	0	
EDC34	5	10/53	10/219	0	0	
EDC45	6	45/193	10/121	15/692	0	0

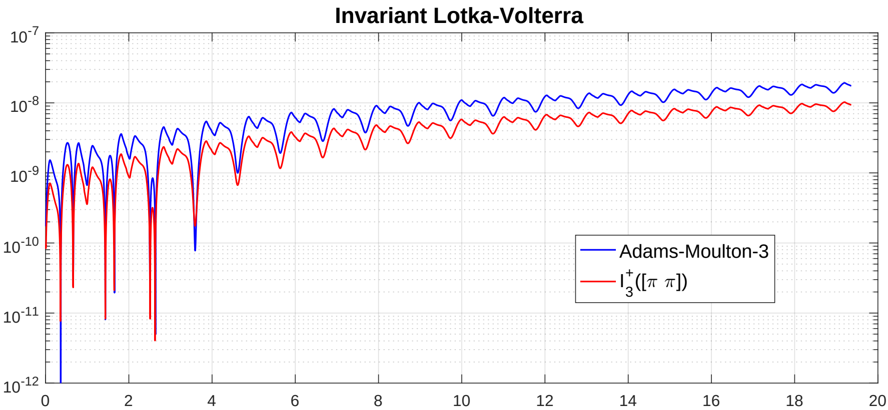
Experimental software platform, **MODES** offers:

- Any multistep method of type E_k, I_k or I_k^+
- Constant or variable step-sizes
- Constant or variable order
- Initial step-size and starters (classical Gear, Runge-Kutta)
- Error per step or error per unit step
- Step-size controllers (several PI and low pass digital filters)
- Upper and lower bounds for step-size ratios

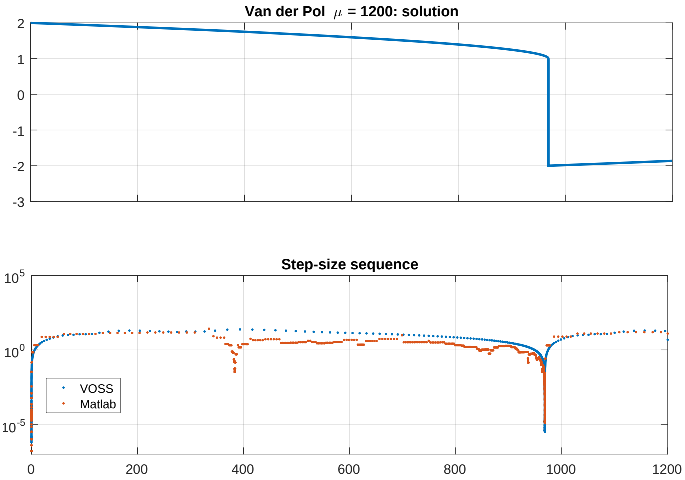
Results for the Oregonator problem solved with MODES-BDF5



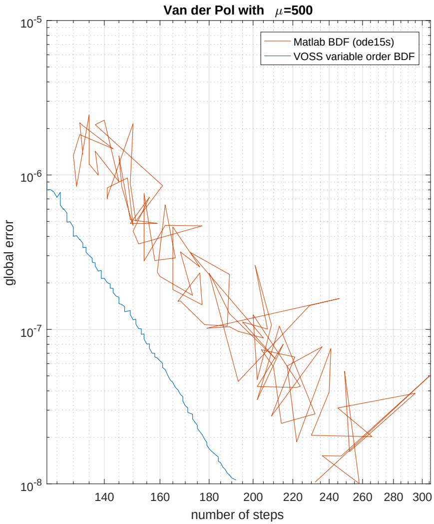
Compare different methods under exact same conditions: AM3 vs. another I_3^+ method. The second method is twice as accurate.



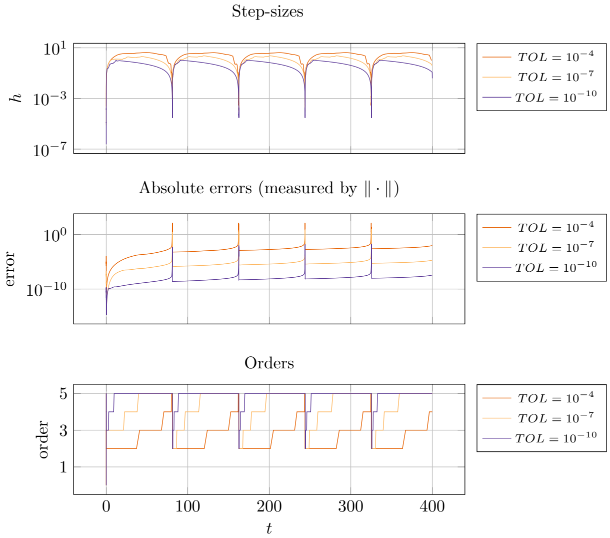
State-of-the-art error control: Matlab BDF1-5 vs. MODES BDF1-5 implementation



Accuracy/Work proportionality for MODES and Matlab's ode15s.

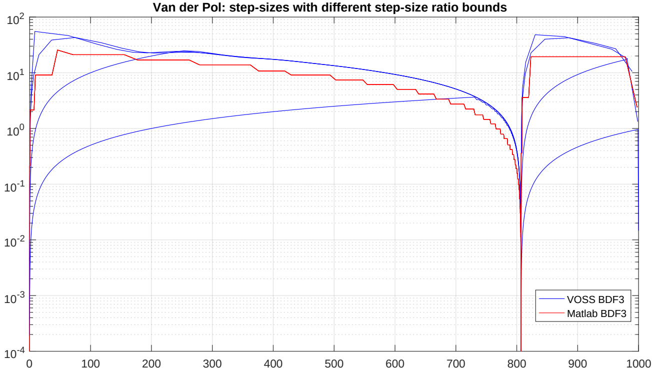


Van der Pol with variable order BDF



Various step-size ratio bounds: none, 160%, 10% and 0.05%.

The controller in MODES keeps the step-size ratios in check to maintain stability.



An application to SSP multistep methods

Strong stability preserving methods avoid instabilities when solving ODEs arising from the semi-discretization of hyperbolic PDEs.

$$\dot{y} = F(y), \quad y(t_0) = y_0, \quad t \in [t_0, t_f]$$

with the property

$$\|y + hF(y)\| \leq \|y\| \quad \text{for all } y \text{ and } h \leq h^*$$

solved by explicit multistep method

$$y_n = \sum_{i=1}^{k} (\alpha_i y_{n-i} + h\beta_i F(y_{n-i})), \quad \text{with } \alpha_i, \beta_i \geq 0$$

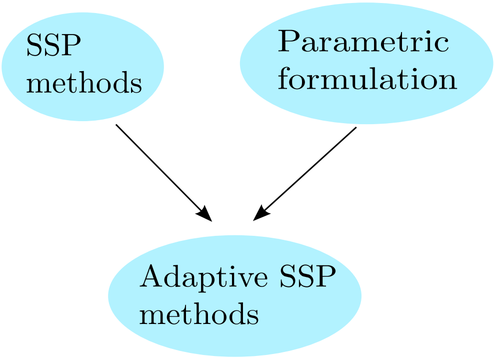
SSP if $\|y_n\| \leq \max\{\|y_{n-1}\|, \ldots, \|y_{n-k}\|\}$ for $0 < h \leq Ch^*$

Explicit SSP multistep methods

- $\alpha_i, \beta_i \geq 0$
- $0 < h \leq Ch^*$
- SSP constant: $C = \min_i \{\alpha_i / \beta_i\}$
- $q < k$
- Zero coefficients of fixed step-size formula should be preserved by variable step-size extension

Adaptive explicit SSP multistep methods: formulation for lower order methods that preserves pattern of zero coefficients

Hadjimichael et al. (2016): first variable step-size optimal SSP methods of orders 2 and 3



Formulation of optimal SSP methods

Procedure to construct optimal SSP(k, q) method

- Take $s_{n-1} = 0$ and $s'_{n-1} = 0$
- Take $s_{n-i} + h_{n-i}\frac{\beta_i}{\alpha_i}s'_{n-i} = 0$ whenever $\alpha_i \neq 0$, $1 < i < k$
- Take $s_{n-k} = 0$
- If q is odd, also add $s'_{n-k} = 0$

The method parameters are $\tau_i = \beta_i/\alpha_i$

Example of optimal explicit 8-step SSP method of order 5

Its nonzero coefficients:

$$\alpha_1 = \frac{1360}{4363}, \quad \alpha_4 = \frac{233}{2112}, \quad \alpha_5 = \frac{2323}{10831}, \quad \alpha_8 = \frac{896}{2465}$$

$$\beta_1 = \frac{275}{128}, \quad \beta_4 = \frac{1044}{1373}, \quad \beta_5 = \frac{6661}{4506}, \quad \beta_8 = \frac{1781}{5144}$$

$$\begin{aligned} s_{n-1} &= 0 \\ s'_{n-1} &= 0 \\ s_{n-4} + h_{n-4}\tau_4 s'_{n-4} &= 0 \\ s_{n-5} + h_{n-5}\tau_5 s'_{n-5} &= 0 \\ s_{n-8} &= 0 \\ s'_{n-8} &= 0 \end{aligned}$$

$$\tau_4 = \beta_4/\alpha_4, \quad \tau_5 = \beta_5/\alpha_5$$

An application to differential-algebraic systems

DAEs are differential equations coupled with algebraic constraints

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\begin{aligned}
\dot{x} &= f(x, \lambda) \\
0 &= g(x, \lambda)
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λ is called the algebraic variable

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The *index* characterizes the difficulty of a DAE.

Index 2 Euler-Lagrange DAE in multibody dynamics:

$$\begin{aligned} \dot{x} &= f(x) - G(x)^{\mathrm{T}}\lambda \\ 0 &= g(x) \end{aligned}$$

with $G(x) = \partial g/\partial x$, $G(x)G(x)^{\mathrm{T}}$ invertible

Generating polynomials of a multistep method: ρ, σ

$$\sum_{j=0}^{k} \alpha_{k-j} x_{n-j} = h \sum_{j=0}^{k} \beta_{k-j} f_{n-j}$$

As difference operators

$$\rho x_n = \sum_{i=0}^{k} \alpha_{k-i} x_{n-i}, \quad \sigma f_n = \sum_{i=0}^{k} \beta_{k-i} f_{n-i}$$

As generating polynomials:

$$\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j, \quad \sigma(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j$$

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Requirement for convergence:

- ODE methods: roots of $\rho(\zeta)$ on or within the unit circle; those on the unit circle are simple
- methods for index 2 DAEs: roots of $\sigma(\zeta)$ inside the unit circle

Consequence of σ not satisfying the strict root condition?

Instability in algebraic variables

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Instability in algebraic variables

Implicit methods with roots of $\sigma(\zeta)$ inside the unit circle

- e.g. BDF (k-step, order k)
- no implicit k-step method of order $k+1$ (e.g. Adams-Moulton)

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Instability in algebraic variables

Implicit methods with roots of $\sigma(\zeta)$ inside the unit circle

- e.g. BDF (k-step, order k)
- no implicit k-step method of order $k+1$ (e.g. Adams-Moulton)

Solution: β-blocking

- Modify σ to move roots into unit circle
- New operator $\sigma + \tau$, with roots inside unit circle, should only affect algebraic variables
- τ should disturb order as little as possible

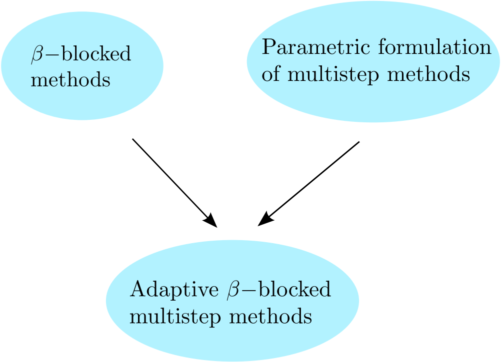
Construction of β-blocker operator

- Reduce order as little as possible by taking $\tau = c\nabla^k$
- Keep σ for differential variables
- $\sigma + \tau$ for algebraic variables

Order:

$k + 1$ for differential variable, k for algebraic variable

β-blocking published 1997–2000 as fixed step-size technique



Standard formulation of index-2 Euler-Lagrange DAE

$P_n \in \mathcal{P}_{k+1}$

$$
\begin{aligned}
&P_n'(t_n) = f(P_n(t_n)) - G(P_n(t_n))^{\mathrm{T}}\lambda_n \\
&P_n(t_{n-1}) = x_{n-1} \\
&P_n'(t_{n-1}) = f(x_{n-1}) - G(x_{n-1})^{\mathrm{T}}\lambda_{n-1} \\
&\cos\theta_{j-1}s_{n-j} + h_{n-j}\sin\theta_{j-1}(s_{n-j}' + G(x_{n-j})^{\mathrm{T}}\lambda_{n-j}) = 0 \\
&g(P_n(t_n)) = 0
\end{aligned}
$$

for $j = 2 : k$.

Then $x_n := P_n(t_n)$.

β-blocked formulation of index-2 Euler-Lagrange DAE

$P_n \in \mathcal{P}_{k+1}$ and $Q_n \in \mathcal{P}_k$

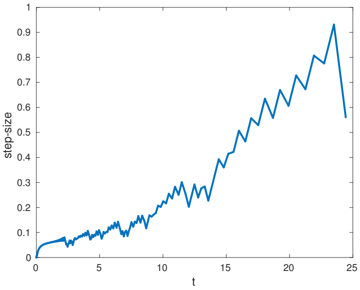
$$
\begin{aligned}
&P_n'(t_n) = f(P_n(t_n)) - G(P_n(t_n))^{\mathrm{T}}(Q_n(t_n) + \hat{c}\; h_{n-1}^k Q_n^{(k)}(t_n)) \\
&P_n(t_{n-1}) = x_{n-1} \\
&P_n'(t_{n-1}) = f(x_{n-1}) - G(x_{n-1})^{\mathrm{T}} Q_n(t_{n-1}) \\
&Q_n(t_{n-j}) = \lambda_{n-j} \\
&\cos\theta_{j-1} s_{n-j} + h_{n-j} \sin\theta_{j-1}(s_{n-j}') + G(x_{n-j})^{\mathrm{T}}\lambda_{n-j}) = 0 \\
&g(P_n(t_n)) = 0
\end{aligned}
$$

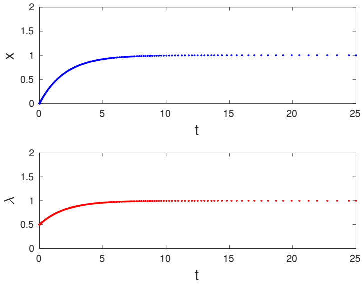
for $j = 2 : k, \quad \hat{c} = c\; \beta_k^{-1}.$

Set $x_n := P_n(t_n)$ and $\lambda_n := Q_n(t_n)$.

$\beta-$blocked AM2

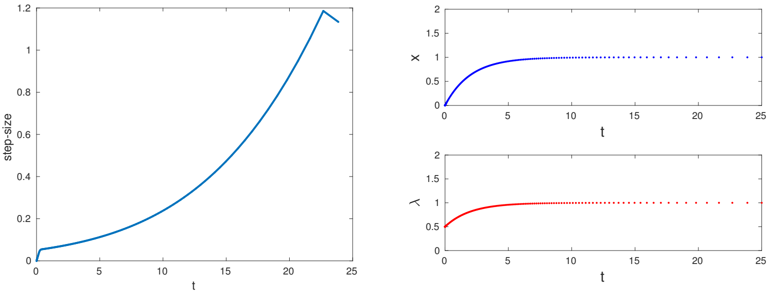
Effect of standard PI controller





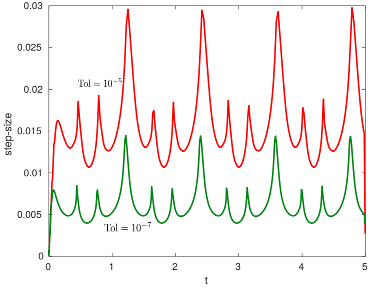
$\beta-$blocked AM2

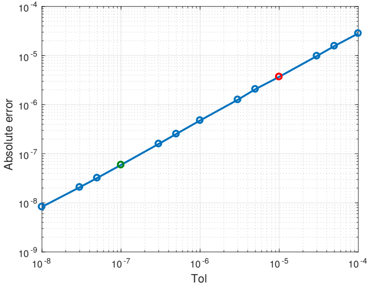
Effect of low-pass digital filter controller



4−step β−blocked Adams-Moulton for nonlinear pendulum

Low-pass filter controller: error-tolerance proportionality





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MODES: a comprehensive multistep solver that uses these new formulations; this allows experimentation with adaptive multistep methods.


Köszönöm