Peer two-step methods for parameter-dependent ODEs

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Scicade 2011

Outline

cooperation with E. Kostina

Peer two-step methods for ODEs

Peer methods originally introduced as multistage two-step methods for ODEs

$$y'(t) = f\big(t, y(t)\big),\ t \in [t_0, t_e], \quad y(t_0) = y_0 \in \mathbb{R}^n.$$

In time step $t_m \to t_m + h_m$ they compute stage solutions $Y_{mi} \cong y(t_m + h_m c_i)$ at s off-step points $t_{m,i} = t_m + h_m c_i$, e.g. by

$$Y_{m,i} - h_m \gamma_i F_{m,i} = \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{s} a_{ij} F_{m-1,j},\ i = 1, \dots, s,$$

$$\text{where} \qquad F_{m,j} = f(t_{m,j}, Y_{m,j}),\ 1 \le j \le s,\ m \ge 0.$$

- Essential: all stages $Y_{m,i}$ with same accuracy + stability ('peer')
- Introduced 2004 by S. and R. Weiner (SIAM J. Numer. Anal. 42)
- Published papers on for stiff and nonstiff ($\gamma_i = 0$) problems, parallel computation (shown here) and sequential (modified)
- Very competative, e.g. no order reduction for very stiff problems

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Parameter dependent ODEs

Parameter-dependent initial value problems

$$\begin{aligned} y'(t,p) &= f\big(t, y(t,p), p\big), \quad t \in [0, t_e], \\ y(0,p) &= u(p) \in \mathbb{R}^n, \quad p \in \mathbb{R}^q. \end{aligned} \tag{1}$$

Aim: Approximation of parameter derivatives (w.r. at $p = \hat{p} := 0$)

$$\varphi_i(t) = \frac{\partial y(t,p)}{\partial p_i}\Big|_{p=0}, \quad 1 \le i \le q.$$

Applications:

- Shooting with initial values: $f = f(t,y)$, $y(0,p) = y_0 + Lp$, $q \le n$
- Shooting with parameters (+ i.v.): periodic solutions
- parameter identification of observed trajectories

Standard approach:

- Solve q additional variational ODEs for $\varphi_k(t)$ with same scheme as (1).
- Overall: $q+1$ IVPs, with order k method means $\ge k \cdot (q+1)$ stages/data per time step

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Modification of peer methods for parameter ODEs ??

- Same scheme, only interpretation changes:

$$Y_{m,i} \cong y(t_{m,i}, \varrho r_i), \quad F_{m,i} := f(t_{m,i}, Y_{m,i}, \varrho r_i),$$

  with new offstep directions in parameter space

$$r_i = (r_{\nu i}) \in \mathbb{R}^q, \ i = 1, \ldots, s: \quad R := (r_1, \ldots, r_s) \in \mathbb{R}^{q \times s}.$$

  Fixed parameter stepsize $\varrho > 0$, R of full rank
- Compact method formulation with stacked vectors $Y_m = (Y_{m,i})_{i=1}^s$, and matrices $\Gamma = \mathrm{diag}(\gamma_i)$, $A = (a_{ij})$, $B = (b_{ij})$:

$$Y_m - h_m(\Gamma_m \otimes I)F_m = (B_m \otimes I)Y_{m-1} + h_m(A_m \otimes I)F_m.$$

  Index m on matrices: coefficients may depend on step
- 2 stepsizes now, smaller h: more effort
  smaller ϱ: same effort $\Rightarrow$ $\varrho \ll h$!?

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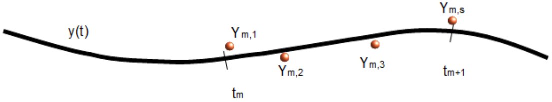
Peer methods for parameter ODEs/2

Interpretation:

- Ordinary DEs: Peer stages approximate solution trajectory $y(t)$:



- Parameter ODEs: Peer stages approximate solution manifold $y(t, p)$:

- Perspective:
  order k method + simple approximation of parameter derivatives
  with only $k + q$ stages instead of $k(q + 1)$ in standard approach!

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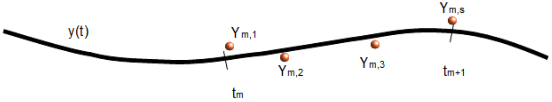

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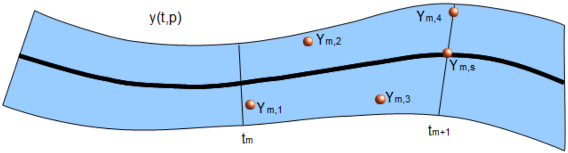

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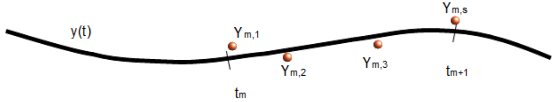

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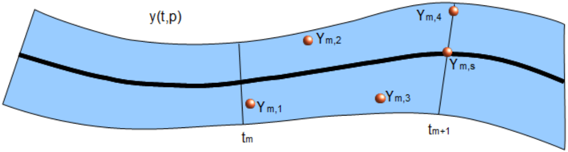

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Order conditions

Local error = residual with exact solution:

$$h_m\Delta_{m,i} = y(t_{m,i},\varrho r_i) - h_m\gamma_i y'(t_{m,i},\varrho r_i) - \sum_{j=1}^{s}\big(b_{ij}y(t_{m-1,j},\varrho r_j) + h_m a_{ij} y'(t_{m,j},\varrho r_j)\big)$$

Taylor expansion at $t = t_{m-1}$, $\hat{p} = 0$: order conditions for powers $h^i\varrho^j$:

- will depend on stepsize ratio $\sigma_m = h_m/h_{m-1}$.
- $h^0\varrho^0$: $\sum_{j=1}^{s} b_{ij} = 1 \iff B\mathbb{1} = \mathbb{1} = (1,\dots,1)^{\mathsf{T}}$ (preconsistency)
- $h^\ell\varrho^0$: $i = 1,\dots,s$

$$(1+\sigma_m c_i)^\ell - \sigma_m\ell\gamma_i(1+\sigma_m c_i)^{\ell-1} - \sum_{j=1}^{s}(b_{ij}c_j^\ell + \sigma_m\ell a_{ij}c_j^{\ell-1})$$

- $h^0\varrho^1$: $r_{\nu i} = \sum_{j=1}^{s} b_{ij} r_{\nu j}$, $i = 1,\dots,s$, $\nu = 1,\dots,q \iff BR^{\mathsf{T}} = R^{\mathsf{T}}$.
- new problem with zero stability: multiple eigenvalue one !

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- $h^0\varrho^0$: $\sum_{j=1}^{s} b_{ij} = 1 \iff B\mathbb{1} = \mathbb{1} = (1,\ldots,1)^{\mathsf{T}}$ (preconsistency)
- $h^\ell\varrho^0$: $i = 1,\ldots,s$

$$(1+\sigma_m c_i)^\ell - \sigma_m\ell\gamma_i(1+\sigma_m c_i)^{\ell-1} - \sum_{j=1}^{s}(b_{ij}c_j^\ell + \sigma_m\ell a_{ij}c_j^{\ell-1})$$

- $h^0\varrho^1$: $r_{\nu i} = \sum_{j=1}^{s} b_{ij}r_{\nu j}$, $i = 1,\ldots,s$, $\nu = 1,\ldots,q \iff BR^{\mathsf{T}} = R^{\mathsf{T}}$.
- new problem with zero stability: multiple eigenvalue one !

Order conditions

Local error = residual with exact solution:

$$h_m\Delta_{m,i} = y(t_{m,i},\varrho r_i) - h_m\gamma_i y'(t_{m,i},\varrho r_i) - \sum_{j=1}^{s}\left(b_{ij}y(t_{m-1,j},\varrho r_j) + h_m a_{ij}y'(t_{m,j},\varrho r_j)\right)$$

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Zero stability

Test equation $y' = \lambda y$: method step $Y_m = M_m(h_m\lambda)Y_{m-1}$ with stability matrix

$$M_m(z) = (I - z\Gamma_m)^{-1}(B_m + zA_m).$$

Special value at $\lambda = 0$: $M(0) = B_m$

- Zero stability: products $B_m B_{m-1} \cdots B_1$ uniformly bounded!
  E.g. $B_m \equiv B$ constant, $\|B^m\| \le K \forall m \in \mathbb{N}$
- But 1 is $q+1$-fold eigenvalue by $B\mathbb{1} = \mathbb{1}$, $Br^{(\nu)} = r^{(\nu)} = (r_{\nu j})_{j=1}^{s}$!?
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Let

$$B = X\tilde{B}X^{-1}, \quad \tilde{B} = \begin{pmatrix} I_{q+1} & \tilde{B}_2 \\ 0 & \tilde{B}_4 \end{pmatrix}$$

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Order conditions (continued)

Conditions in matrix/vector form

- $h^0\varrho^0$: $B\mathbb{1} = \mathbb{1}$
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Consequences:

- Each condition $h^\ell\varrho^j$, $j>0$ gives sq equations $\rightarrow$ needs q addit. stages
- effort independent of stepsize ϱ, choose $\varrho \ll h$!
- Minimal requirements, conditions $h^\ell\varrho^0$, $0 \le \ell \le k$, and $h^0\varrho^1$, $h^1\varrho^1$:

needs	$s = k + q$	stages,
local error	$h\Delta = O(h^{k+1} + \varrho h^2 + \varrho^2)$	
global error	$O(H^k + H\varrho + \varrho^2)$,	$\varrho \ll H = \max_j h_j$
		$\uparrow$ see later
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Low-rank representations

From now on only explicit methods!
Preconsistency and order conditions for h_ϱ and $h^1, \dots, h^{s-q}$ give relation

$$\sigma A = (I + \sigma C)(R^\mathsf{T}, \mathbb{1}, \frac{1}{2}(I + \sigma C)\mathbb{1}, \dots) - BC(R^\mathsf{T}, \mathbb{1}, \frac{1}{2}C\mathbb{1}, \dots) \qquad (2)$$

Recall basis matrix

$$X = (R^\mathsf{T}, \mathbb{1}, C\mathbb{1}, \dots, C^{s-q-1}\mathbb{1})$$

for B from Lemma:

- $B = I + W_0 Z^\mathsf{T}, \quad W_0, Z \in \mathbb{R}^{s \times (s-q-1)}$,
  where Z^T contains last $s - q - 1$ rows of X^{-1} and $I + Z^\mathsf{T} W_0 = \tilde{B}_4$ is small.
  Note: consider elements of W_0 not B as design parameters
- First columns in X and matrices in (2) identical
  $\Rightarrow$ low-rank structures also in A !
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Low-rank representations (cont.)

Peer step for parameter ODEs has structure

$$\begin{aligned} Y_m =& Y_{m-1} + h_{m-1}\big(I + \sigma_m C - C\big)F_{m-1} \\ &+ W_0 Z^{\mathsf{T}}\big(Y_{m-1} - h_{m-1}CF_{m-1}\big) + h_{m-1}W(\sigma)Z^{\mathsf{T}}F_{m-1}. \end{aligned}$$

Details:

- In first line only diagonal matrix C: decoupled Euler steps
- 2nd line: low rank correction terms, gathered only from subspace

$$Rg(Z) = ker(R)$$

- Choice of kernel of parameter-off-step matrix important

$$R = (r_1, \ldots, r_s) \in \mathbb{R}^{q \times s},\ s > q\ !$$

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A satellite configuration

- Good parameter derivatives: need $q+1$ stages distributed in parameter space at same time offstep (differences orthogonal to t axis)!
- 'Method center' with simple parameter offsteps: $r_j = 0$ for $s-q$ stages

Consider satellite configuration: final stage at $c_s = 1$ and

- last $s-q$ stages $Y_{m,q+1}, \ldots, Y_{ms}$ approximate central trajectory $y(t,0)$:

$$r_{q+1} = \ldots = r_s = 0.$$

- first q stages $Y_{m,1}, \ldots, Y_{m,q}$ off central trajectory:

$$c_1 = \ldots = c_q = 1 = c_s.$$

Consequences:

$$R^{\mathsf{T}} = E_q \hat{R}^{\mathsf{T}},\ E_q = \begin{pmatrix} I_q \\ 0 \end{pmatrix} \Rightarrow B = \begin{pmatrix} I_q & \square \\ & \square \end{pmatrix}, \quad A = \begin{pmatrix} \diagdown & \square \\ & \square \end{pmatrix}$$

Means: only central stages $Y_{m,q+1}, \ldots, Y_{ms}$ are fully coupled
first q stages are uncoupled satellites, with input from center only

A satellite configuration

- Good parameter derivatives: need $q+1$ stages distributed in parameter space at same time offstep (differences orthogonal to t axis)!
- 'Method center' with simple parameter offsteps: $r_j = 0$ for $s-q$ stages

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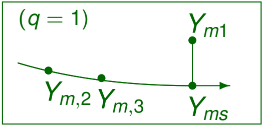

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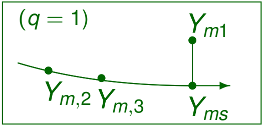

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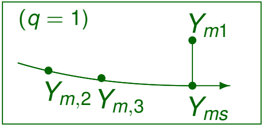

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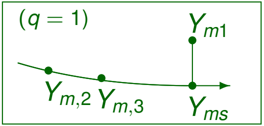

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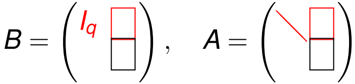

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- conditions $h^1\varrho^0$, $h^2\varrho^0$, $h^0\varrho^1$, $h^1\varrho^1$,
- stages: $s = q + 2$
- Low-rank representation: $B = I + W_0 Z^\mathsf{T}$, here

$$Z^\mathsf{T} = \frac{1}{1 - c_{s-1}}(0, \dots, 0, -1, 1), \quad 1 + Z^\mathsf{T} W_0 = \tilde{B}_4 \stackrel{!}{=} 0$$

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Observation carries over to other satellite methods with

$$c_1 = \ldots = c_q = 1 = c_s,\ R = (I_q, 0) = E_q^\mathsf{T}. \tag{3}$$

Theorem

For peer methods with satellite configuration (3) *satisfying the order conditions* $\varrho, h\varrho, h^1, \ldots, h^{s-q}$, *and* $E_q^\mathsf{T} B = E_q^\mathsf{T}$, $E_q^\mathsf{T} W_0 = 0$, *all coefficients of the satellite stages are essentially identical, i.e.*

$$\begin{aligned} a_{ij} = &\quad \delta_{ij}, \quad 1 \le i \le n,\ 1 \le j \le q, \\ a_{ij} = &\quad a_{1j} \quad 1 \le i \le q,\ q < j \le s. \end{aligned}$$

Practical consequences:

- choose any explicit peer method for central stages (no parameters)
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The global error

Local error for order k method:

$$h\Delta_m = O(h^{k+1} + h^2\rho + \rho^2)$$

Do $O(\varrho^2)$-errors accumulate to $O(\varrho^2/h)$?

- No!
- Satellite configuration: no $O(\varrho^2)$ in local error
- General methods: $O(\varrho^2)$ has left factor $I - B$
  $\Rightarrow$ is either multiplied by h or B in time steps:

$$\sum_{m\geq 0} \|B^m(I-B)\| < \infty \text{ by Lemma.}$$

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Simple choice $\tilde{B}_4 = 0$: $B(I-B) = 0$

Global error:

$$O(H^k + H\varrho + \varrho^2).$$

The global error

Local error for order k method:

$$h\Delta_m = O(h^{k+1} + h^2\rho + \rho^2)$$

Do $O(\varrho^2)$-errors accumulate to $O(\varrho^2/h)$?

- No!
- Satellite configuration: no $O(\varrho^2)$ in local error
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Parameter derivatives

Approximation of parameter derivatives by differences of stages.

- Approximates

$$\frac{1}{\varrho}\big(y(t_{m,i},\varrho r_i)-y(t_{m+1},0)\big)=\frac{\partial y}{\partial p}\Big|_{(t_{m+1},0)} r_i+\underbrace{\frac{h_m}{\varrho}(c_i-c_s)}+O(\varrho+\dots)$$

  where $t_{m,s}=t_{m+1}$, with $c_s=1$, $r_s=0$.

- No h/ϱ terms! Need $c_i=1$ if $r_i\neq 0$, as in satellite configuration
- Difference quotient with satellite stages $\hat{Y}_m\in\mathbb{R}^{q\times s}$:

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- Accuracy parameter derivatives $O(H)$ only, good enough for Newton?!
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Confirm by application to following problem types:

problem type	param.kind	dim n, q

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Computations:
Order-3 method, $s = 3 + q$-stages,
with stepsize control+ different *tol*,
Fortran90

Shooting with Newton's method

- Shooting with initial values for BVPs with boundary conditions

$$g\big(y(t_0,p),y(t_e,p)\big)=0$$

or parameters for special solutions (e.g. periodic)

- Compute starting values $Y_{m,0}$ in first interval $[t_0,t_0+h_0]$

$$Y_{0,i}\cong y(t_{0,i},\varrho r_i),\ i=1,\dots,s,$$

from $y(t_0,\varrho r_i)$ by Runge-Kutta method.

- Same peer scheme for shooting with ($L\neq I$ for separated BCs)
  - initial values: $y(t_0,p)=y_0+Lp,\quad f=f(t,y),$
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$\Rightarrow$ problem coding in two subroutines only

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Single shooting for BVP

Simple boundary value problem for pendulum (no trivial solutions)

$$y''(t) + \sin(y(t)) = 0, \quad y(0) - y'(0) = 1, \ y(T) + y'(T) = 0.$$

Q: choice of ϱ?

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Q: choice of ϱ?

- Newton convergence, integration with stepsize control for tolerances $tol = 1E-2 \ldots 1E-8$, fixed ϱ:
  $\varrho = 10^{-1}$ $\quad$ $\varrho = 10^{-2}$ $\quad$ $\varrho = 10^{-4}$
- rule of thumb: $\varrho \geq tol$, not too small:
  set $\varrho = a \cdot tol + \varrho_0$, $\varrho_0 = 10^{-4} \ldots 10^{-3}$

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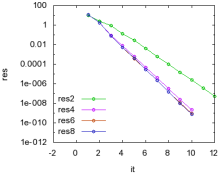
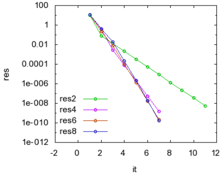
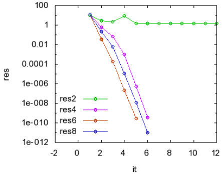


$\varrho = 10^{-2}$



$\varrho = 10^{-4}$



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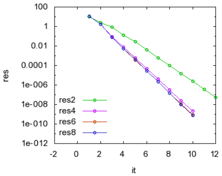

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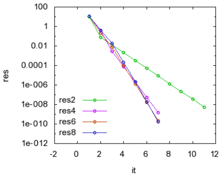

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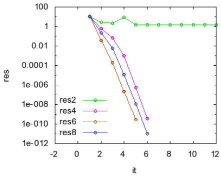

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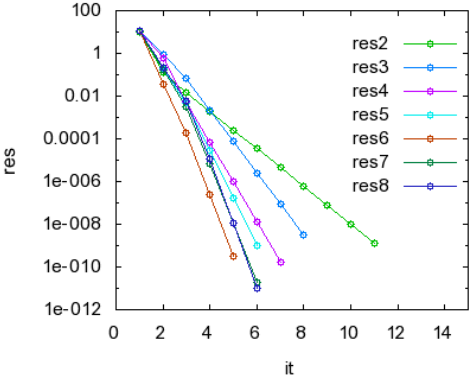
- Now, Newton convergence with adapted $\varrho = 2 \cdot tol + 10^{-4}$:



Time-periodic solutions for Brusselator ODE

Brusselator - ODE for $n = 2, q = 2$:

$$y_1' = \alpha - (\beta + 1)y_1 + y_1^2 y_2,$$
$$y_2' = \beta y_1 - y_1^2 y_2.$$

- Has two parameters $p_1 = \alpha$ and $p_2 = \beta$ and limit cycle for $\beta > 1 + \alpha^2$
- Computation of periodic orbits:
  1. fix initial values shoot with parameters
  2. fix parameters shoot with initial values
- Undamped Newton convergence for time periodic solution for $T = 7.16$, parameters unknown, start with $p = (1, 3)^T$.
  4 BCs: $y(0) = (1.8, 1.8)^T$,
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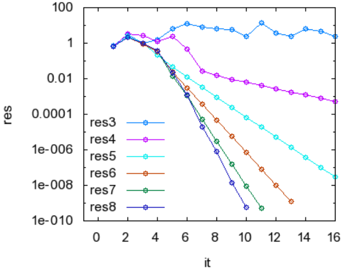

Time-periodic solutions for 1D-Brusselator

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- Lust/Roose/Spence/Champneys'98: space grid 31 points, D_1 =8E-3, D_2 =4E-3 (non-stiff ODE), stable periodic solution with $T \cong 3.44$.
- Shooting with initial values: $p = y(0)$, dim $q = n = 62$
- Difficulty: for BCs $y(T) - y(0) = 0$ singular Jacobian, has kernel $f(y(0))$! Regularized Newton step:

$$\begin{pmatrix} J - I & f_0 \\ f_0^T & 0 \end{pmatrix} \begin{pmatrix} u \\ \tau \end{pmatrix} = \begin{pmatrix} y(0) - y(T) \\ 0 \end{pmatrix}, \quad J = \frac{\partial y(T)}{\partial y(0)}.$$

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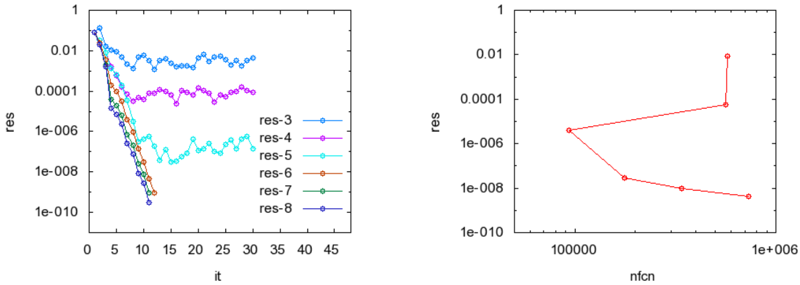
Series of integration tolerances, parameter stepsize $\varrho = 10 \cdot tol + 10^{-3}$.

- left: Convergence of undamped Newton's method
- right: efficiency, number of f-evaluations needed; Newton stopped at $0.1 \cdot tol$



Time-periodic solutions for 1D-Brusselator

Series of integration tolerances, parameter stepsize $\varrho = 10 \cdot tol + 10^{-3}$.

- left: Convergence of undamped Newton's method
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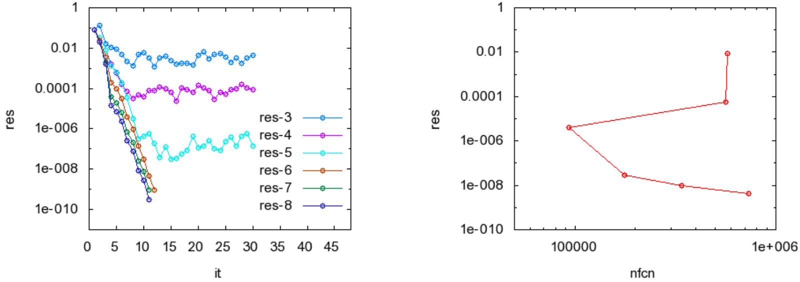

convergence good for $tol \leq 10^{-5}$, slow for $tol > 10^{-5}$

effort proportional to tol for $tol \leq 10^{-5}$

Parameter identification for Brusselator ODE

Problem: Identify parameters $(p_1, p_2) = (\alpha, \beta)$ and initial values $y(0)$ from observed Brusselator trajectory ($q = 4$)

Details:

- highly accurate trajectory with $p = (1, 3)^\mathsf{T}$, $y(0) = (1.8, 1.8)^\mathsf{T}$, $t \in [0, 7.16]$ (Dopri, tol=1E-11)
- only first component saved $y_1(jt_e/10)$ at 10 points, $j = 1, \ldots, 10$.
- time integration with fixed stepsize to hit points (no dense output yet), several runs with $h = 0.0716 \cdot 4^{-m}$ (labels 'res-m')
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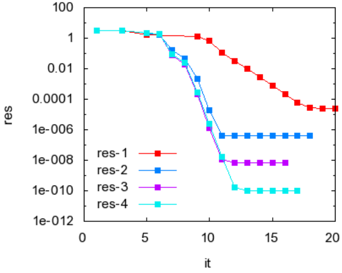

residuals level off at error of time integration = perturbation level of measurements

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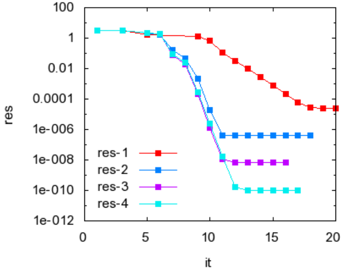
Note: In line searches where no derivatives are needed, satellite stages can be switched off!



residuals level off at error of time integration = perturbation level of measurements

Summary & perspectives

- Peer methods get approximate solution + q parameter derivatives with only q additional stages instead of $k \cdot q$ for order k methods
- Special satellite configuration flexible + efficient: approximates central trajectory+ arbitrary number of satellites
- Satellites not required in Newton line search
- Low accuracy of derivatives: still good convergence in several simple applications
- Mainly *proof of concept* intended, no comparison with other methods yet

To do:

- Good choice of parameter stepsize ϱ needs further investigation
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Thank you !

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