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Partitioned Methods for Multifield Problems

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Runge–Kutta methods

Consider

$$\dot{\mathbf{u}}(t) = \mathbf{f}(t, \mathbf{u}(t)), \quad \mathbf{u}(t_0) = \mathbf{u}_0$$

A Runge-Kutta method with s internal stages is given by

$$\mathbf{k}_i = \mathbf{f}\left(t_m + c_i\tau, \mathbf{u}_m + \tau \sum_{j=1}^{s} a_{ij}\mathbf{k}_j\right), \quad i = 1, \ldots, s,$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau \sum_{i=1}^{s} b_i \mathbf{k}_i.$$

The value s is called number of stages. The vector $\mathbf{c}$ includes the grid points of the time discretisation and $\mathbf{b}$ is vector with weights. The coefficients a_{ij}, b_i and c_i should be chosen in such a way that some order conditions are satisfied to obtain a sufficient consistency order.

Simplifying conditions

An s-stage Runge–Kutta method satisfies the simplifying conditions

$$B(p): \quad \sum_{i=1}^{s} b_i c_i^{k-1} = 1/k \qquad k = 1, \ldots, p,$$

$$C(q): \quad \sum_{j=1}^{s} a_{ij} c_j^{k-1} = c_i^k/k \qquad i = 1, \ldots, s, \; k = 1, \ldots, q,$$

$$D(r): \quad \sum_{i=1}^{s} b_i c_i^{k-1} a_{ij} = b_j(1 - c_j^k)/k \qquad j = 1, \ldots, s, \; k = 1, \ldots, r.$$

(see Butcher, 1964).

The simplifying conditions can be written in matrix-vector notation.

Remarks

- The condition $B(p)$ is equivalent to a quadrature rule with the nodes c_i and the weights b_i which integrates polynomials of degree $p-1$ exact.
- The conditions $C(q)$ have the following meaning. The intermediate values $\mathbf{k}_i$ are integrated exactly by a quadrature rule with the weights a_{ij} and the nodes c_i which integrates polynomials of degree q exactly.

Result

- An RK-method with s internal stages has the convergence order p, if the simplifying conditions $B(p)$, $C(l)$, and $D(m)$ with

$$p \leqslant \min\{l + m + 1, 2l + 2\}$$

  are satisfied.
- There exists only one RK-method with s stages and with $p = 2s$. This methods satisfies $B(2s)$, $C(s)$, and $D(s)$.

For the proof we refer to the book of Butcher.

Methods of order 2s

In the case of the Gauß quadrature rules the nodes c_i are choosen as the roots of the shifted Legendre polynomial of degree s, i.e.

$$P_s(2t-1) = \frac{1}{s!}\frac{d^s}{dt^s}[t^s(t-1)^s].$$

With respect to the $L_2(0,1)$-scalar product

$$\langle q, w\rangle := \int_0^1 q(t)w(t)dt$$

the polynomial $P_s(2t-1)$ is orthogonal to all polynomials of degree $< s$, i.e. $\langle P_s, w\rangle = 0$ for all polynomials w of degree less than s. The roots of the Legrendre polynomials P_s can be found in the book of Abramowitz and Stegun.

Methods of order 2s-2

nodes c_i are given by the roots of the polynomial

$$P_{s,\xi,\mu}(2x-1) = P_s(2x-1)+\xi P_{s-1}(2x-1)+\mu P_{s-2}(2x-1), \quad \xi, \mu \in \mathbb{R}.$$

Here the cases $\xi = 0$ and $\mu = 1$ are considered leading to the so-called Lobatto-III methods with $c_1 = 0$ and $c_s = 1$. The weights b_i are determined with $B(s)$ and the matrix A as follows:

- *Lobatto-IIIA* (see Ehle (1968)): with $C(s)$
- *Lobatto-IIIB* (see Ehle (1968)): with $D(s)$
- *Lobatto-IIIC* (see Chipman (1971)): with $C(s-1)$ and $a_{i1} = b_1$, $i = 1, \ldots, s$.

Lobatto-IIIA methods

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

0	0	0	0
$\frac{1}{2}$	$\frac{5}{24}$	$\frac{1}{3}$	$-\frac{1}{24}$
1	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$
	$\frac{1}{6}$	$\frac{2}{3}$	$\frac{1}{6}$

Lobatto-IIIB methods

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

$$
\begin{array}{c|ccc}
0 & \frac{1}{6} & -\frac{1}{6} & 0 \\
\frac{1}{2} & \frac{1}{6} & \frac{1}{3} & 0 \\
1 & \frac{1}{6} & \frac{5}{6} & 0 \\
\hline
 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6}
\end{array}
$$

Lobatto-IIIC methods

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

$$\begin{array}{c|ccc} 0 & \frac{1}{6} & -\frac{1}{3} & \frac{1}{6} \\ \frac{1}{2} & \frac{1}{6} & \frac{5}{12} & -\frac{1}{12} \\ 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

Prothero–Robinson example

Order results

method	local error	global error	
		τ const.	τ variable
Gauß (s odd)	τ^{s+1}	τ^{s+1}	τ^{s}
Gauß (s even)	τ^{s+1}	τ^{s}	τ^{s}
Radau IA	τ^{s}	τ^{s}	τ^{s}
Radau IIA	$z^{-1}\tau^{s+1}$	$z^{-1}\tau^{s+1}$	$z^{-1}\tau^{s+1}$
Lobatto IIIA (s odd)	$z^{-1}\tau^{s+1}$	$z^{-1}\tau^{s}$	$z^{-1}\tau^{s}$
Lobatto IIIA (s even)	$z^{-1}\tau^{s+1}$	$z^{-1}\tau^{s+1}$	$z^{-1}\tau^{s}$
Lobatto IIIB (s odd)	$z^{-1}\tau^{s-1}$	$z^{-1}\tau^{s-2}$	$z^{-1}\tau^{s-2}$
Lobatto IIIB (s even)	$z^{-1}\tau^{s-1}$	$z^{-1}\tau^{s-1}$	$z^{-1}\tau^{s-2}$
Lobatto IIIC	$z^{-1}\tau^{s}$	$z^{-1}\tau^{s}$	$z^{-1}\tau^{s}$

Coupled ODEs

Consider

$$\dot{\mathbf{u}} = \mathbf{f}(t, \mathbf{u}, \mathbf{v}), \quad \mathbf{u}(t_0) = \mathbf{u}_0,$$
$$\dot{\mathbf{v}} = \mathbf{g}(t, \mathbf{u}, \mathbf{v}), \quad \mathbf{v}(t_0) = \mathbf{v}_0$$

Examples:

- Second order systems such as mechanical systems
- coupled diffusion-reaction systems such as the Brussulator

A simplified model of a nuclear reactor

- Literature: Strehmel and Weiner, 1984
- $N(t)$ ... average density of neutrons
- $T_b(t)$ ... temperature of fuel
- $C_i(t)$ ... nuclear concentrations.
- system of ODEs:

$$\dot{N}(t) = \frac{1}{l}\left(\gamma(T_B(t) - T_B(0))N(t) + \sum_{i=1}^{6} \beta_i(C_i(t) - N(t))\right),$$

$$\dot{T}_B(t) = \frac{1}{C}(dN(t) - K(T_B(t) - T_M)),$$

$$\dot{C}_i(t) = \lambda_i(N(t) - C_i(t)), \quad i = 1, \ldots, 6.$$

- quantities γ, d, K, T_m, β_i, C, l and $\lambda_i \in [-3, 0)$ are given and independent from t.

Hamiltonian systems

Hamiltonian problems are ODEs of the form

$$\dot{\mathbf{p}} = -H_q(\mathbf{p}, \mathbf{q}) = -\frac{\partial H}{\partial \mathbf{q}}(\mathbf{p}, \mathbf{q}),$$

$$\dot{\mathbf{q}} = H_p(\mathbf{p}, \mathbf{q}) = \frac{\partial H}{\partial \mathbf{p}}(\mathbf{p}, \mathbf{q})$$

- $H(p_1, \ldots, p_d, q_1, \ldots, q_d)$ ... Hamiltonian (given function)
- The Hamiltonian represents the total energy.
- q_i ... position coordinates
- p_i ... momenta.
- $H(\mathbf{p}, \mathbf{q})$ is constant.

Movement of a pendulum

Pendulum of length 1: Consider

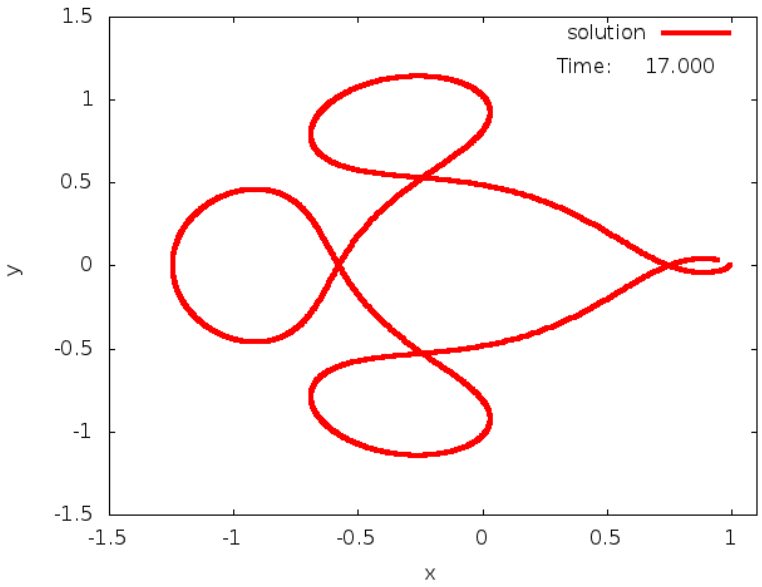
$$H(p, q) = \frac{1}{2}p^2 - \cos q.$$

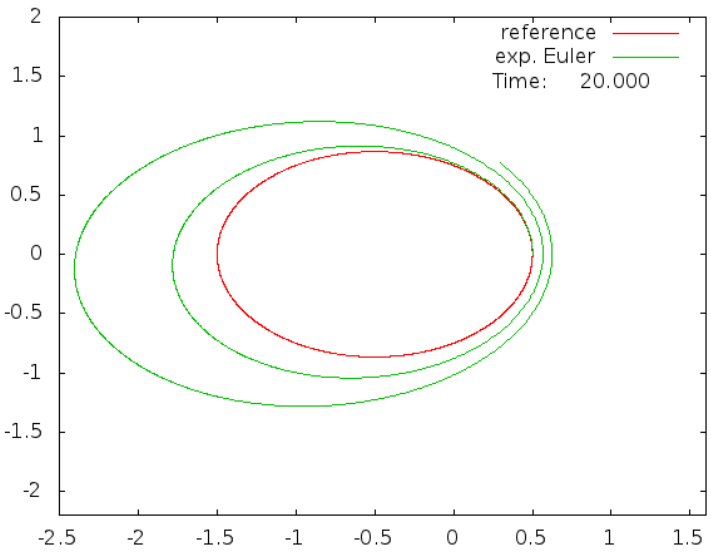
Then

$$\dot{p} = -\sin q,$$
$$\dot{q} = p$$

Further examples

- Keplers problem
- Arenstorf orbits
- movement of planets
- ...





Partitioned Runge–Kutta methods

$$\mathbf{k}_i = \mathbf{f}\left(t_m + c_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{s} a_{ij}\mathbf{k}_j, \mathbf{v}_m + \tau\sum_{j=1}^{s} \hat{a}_{ij}\mathbf{l}_j\right)$$

$$\mathbf{l}_i = \mathbf{g}\left(t_m + \hat{c}_i\tau, \mathbf{u}_m + \tau\sum_{j=1}^{s} a_{ij}\mathbf{k}_j, \mathbf{v}_m + \tau\sum_{j=1}^{s} \hat{a}_{ij}\mathbf{l}_j\right)$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau\sum_{i=1}^{s} b_i\mathbf{k}_i, \quad \mathbf{v}_{m+1} = \mathbf{v}_m + \tau\sum_{i=1}^{s} \hat{b}_i\mathbf{l}_i.$$

- Coefficients: a_{ij}, b_i, c_i, $\hat{a}_{ij}$, $\hat{b}_i$, $\hat{c}_i$
- Advantage: Each problem can be solved by a special Runge–Kutta method.

Application

Second order ODE written as first order:

$$\dot{\mathbf{u}} = \mathbf{v}, \quad \mathbf{v}(t_0) = \mathbf{v}_0,$$
$$\dot{\mathbf{v}} = \mathbf{f}(t, \mathbf{u}, \mathbf{v}), \quad \mathbf{u}(t_0) = \mathbf{u}_0$$

Apply partitioned Runge–Kutta method:

$$\mathbf{k}_i = \mathbf{v}_m + \tau \sum_{j=1}^{s} \hat{a}_{ij} \mathbf{l}_j$$

$$\mathbf{l}_i = \mathbf{f}\left(t_m + c_i\tau, \mathbf{u}_m + \tau \sum_{j=1}^{s} a_{ij} \mathbf{k}_j, \mathbf{v}_m + \tau \sum_{j=1}^{s} \hat{a}_{ij} \mathbf{l}_j \right)$$

$$= \mathbf{f}\left(t_m + c_i\tau, \mathbf{u}_m + \tau \sum_{j=1}^{s} a_{ij} \left(\mathbf{v}_m + \tau \sum_{k=1}^{s} \hat{a}_{jk} \mathbf{l}_k \right), \mathbf{v}_m + \tau \sum_{j=1}^{s} \hat{a}_{ij} \mathbf{l}_j \right)$$

Runge–Kutta–Nyström method

A Runge–Kutta–Nyström method can then we be written as

$$\mathbf{l}_i = \mathbf{f}\left(t_m + c_i\tau, \mathbf{u}_m + \tau c_i \mathbf{v}_m + \tau^2 \sum_{j=1}^{s} \bar{a}_{ij}\mathbf{l}_j, \mathbf{v}_m + \tau \sum_{j=1}^{s} \hat{a}_{ij}\mathbf{l}_j\right)$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau \mathbf{v}_m + \tau^2 \sum_{i=1}^{s} \bar{b}_i \mathbf{l}_i$$

$$\mathbf{v}_{m+1} = \mathbf{v}_m + \tau \sum_{i=1}^{s} \hat{b}_i \mathbf{l}_i.$$

where

$$\bar{a}_{ij} = \sum_{j=1}^{s} a_{ij}\hat{a}_{jk}, \qquad \bar{b}_i = b_i \sum_{j=1}^{s} \hat{a}_{ij}$$

Example

Nyström method of order 4:

	0			
c_i	1/2	1/8		$\bar{a}_{ij}$
	1	0	1/2	
$\hat{b}_i$		1/6	1/3	0
$\bar{b}_i$		1/6	4/6	1/6

Example

Advantage: ODE can be splitted into a stiff and into a non-stiff part.
Consider

$$\begin{pmatrix} \dot{u}_1 \\ \dot{u}_2 \end{pmatrix} = \begin{pmatrix} -81 & -34 \\ -38 & -24 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \qquad \begin{pmatrix} u_1(0) \\ u_2(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 3 \end{pmatrix}.$$

Exact solution:

$$\begin{pmatrix} u_1(t) \\ u_2(t) \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \end{pmatrix} \exp(-100t) + \begin{pmatrix} -1 \\ 2 \end{pmatrix} \exp(-5t).$$

Methods

- method of Heun:

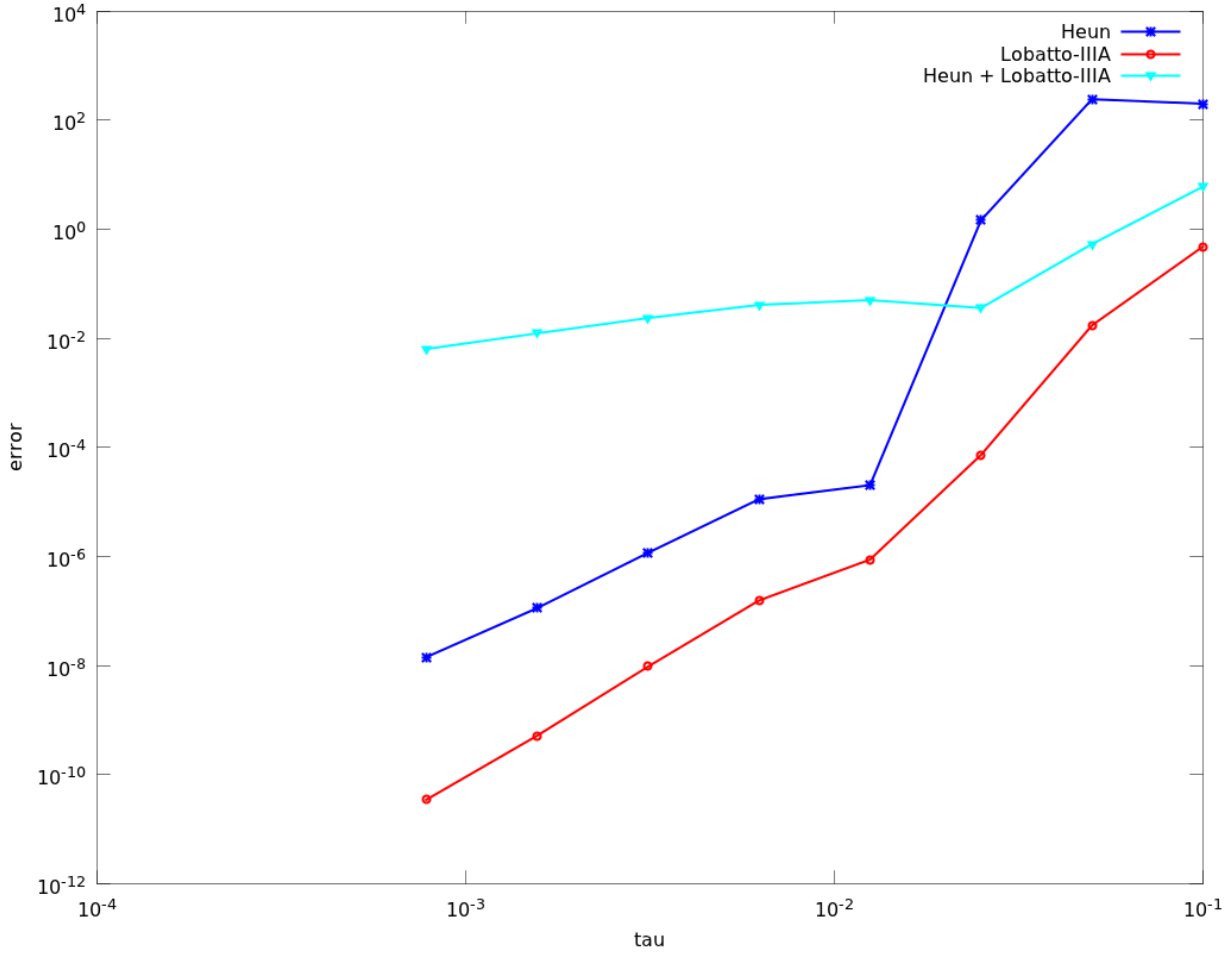
$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{3} & \frac{1}{3} & & \\ \frac{2}{3} & 0 & \frac{2}{3} & \\ \hline & \frac{1}{4} & 0 & \frac{3}{4} \end{array}$$

- Lobatto-IIIA method with 3 internal stages

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\ 1 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}$$

- partitioned Runge–Kutta method with the Heun and Lobatto-IIIA method.

Numerical result



Remarks

- Partitioned Runge–Kutta methods may have order reduction.
- Higher order PRK methods must satisfy further order conditions
- A partitioned Runge–Kutta method is of order 2, if and only if both Runge–Kutta methods have at least order 2 and if the coupling condition

$$\sum_{i,j=1}^{s} b_i \hat{a}_{ij} = \sum_{i,j=1}^{s} \hat{b}_i a_{ij} = \frac{1}{2}$$

  is satisfied.
- This condition is valid, if $c_i = \hat{c}_i$, $b_i = \hat{b}_i$, and both methods satisfy the condition

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

New method

Aim: Find an explicit Runge–Kutta method of order 3 with

$$c_1 = 0, \quad c_2 = 1/2, \quad c_3 = 1$$
$$b_1 = 1/6, \quad b_2 = 2/3, \quad b_3 = 1/6.$$

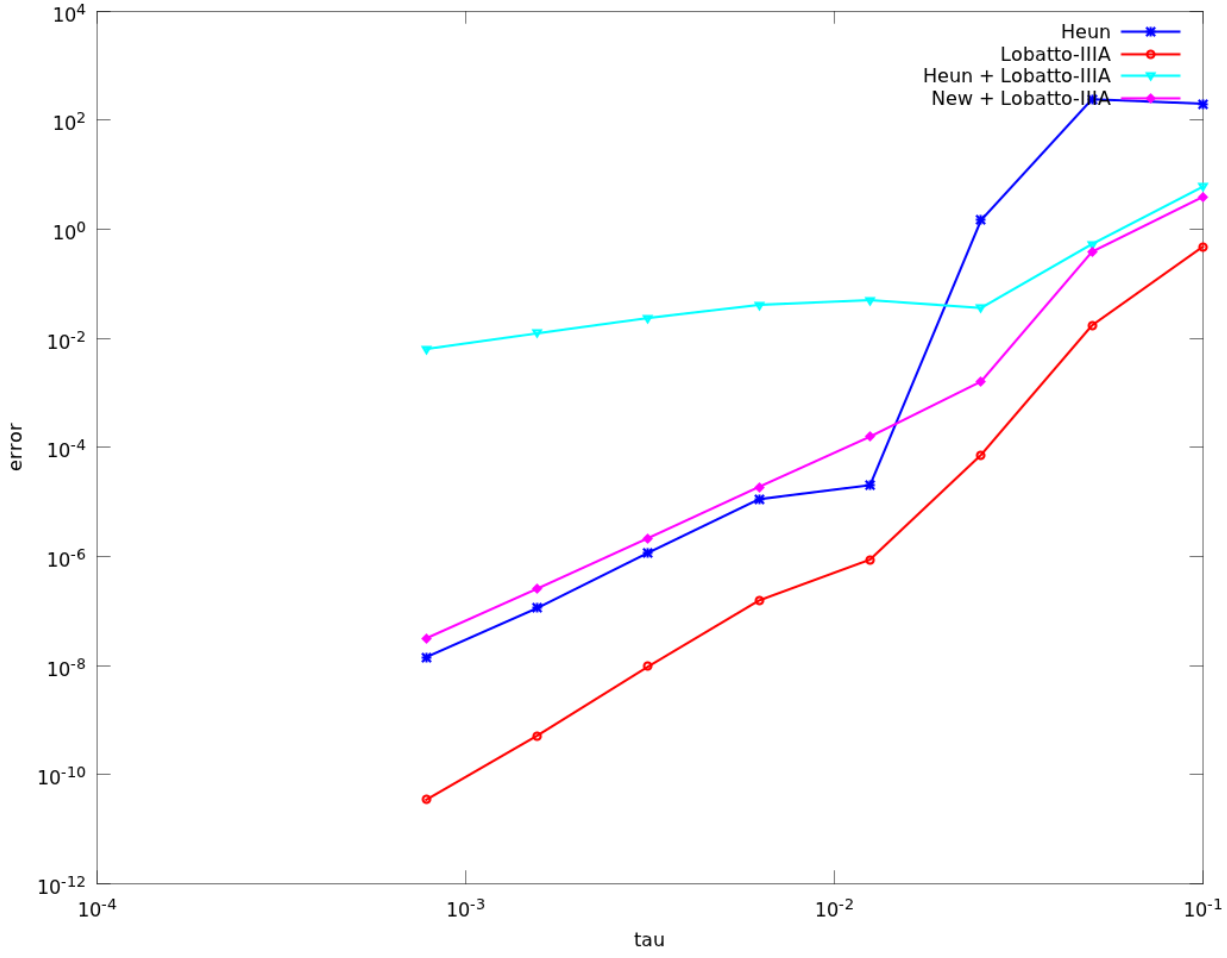
remaining order condition

$$\sum_{i=1}^{s} b_i a_{ij} c_j = 1/6$$

is valid, if we choose $\alpha_{32} = 2$. Finally we have $\alpha_{31} = -1$.

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & -1 & 2 & \\ \hline & \frac{1}{6} & \frac{4}{6} & \frac{1}{6} \end{array}$$

Numerical result



Literature

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Dynamic iteration methods

- Let us start with the coupled system of ODEs given by

$$\dot{\mathbf{u}} = \mathbf{f}(t, \mathbf{u}, \mathbf{v}), \qquad \mathbf{u}(0) = \mathbf{u}_0$$
$$\dot{\mathbf{v}} = \mathbf{g}(t, \mathbf{u}, \mathbf{v}), \qquad \mathbf{v}(0) = \mathbf{v}_0.$$

- As in the case of stationary problems a splitting can be introduced.
- In the case of dynamic problem this approach is called waveform relaxation (WR).
- We have the same partitioned methods as in the case of linear/non-linear systems, i.e. Jacobi, Gauß–Seidel, and SOR.

Jacobi WR method

- Jacobi WR method:

$$\dot{\mathbf{u}}^{(k+1)} = \mathbf{f}(t, \mathbf{u}^{(k+1)}, \mathbf{v}^{(k)})$$
$$\dot{\mathbf{v}}^{(k+1)} = \mathbf{g}(t, \mathbf{u}^{(k)}, \mathbf{v}^{(k+1)})$$

- As in the case of stationary problems both ODEs can be solved in parallel independently from each other.
- The communication of the two solvers is needed only at the end of each timestep.

SOR WR method

SOR WR method:

$$
\begin{aligned}
\dot{\tilde{\mathbf{u}}}^{(k+1)} &= \mathbf{f}(t, \tilde{\mathbf{u}}^{(k+1)}, \mathbf{v}^{(k)}), \qquad \tilde{\mathbf{u}}^{(k+1)}(0) = \mathbf{u}_0 \\
\dot{\tilde{\mathbf{v}}}^{(k+1)} &= \mathbf{g}(t, \tilde{\mathbf{u}}^{(k+1)}, \tilde{\mathbf{v}}^{(k+1)}), \qquad \tilde{\mathbf{v}}^{(k+1)}(0) = \mathbf{v}_0 \\
\mathbf{u}^{(k+1)} &= \omega \tilde{\mathbf{u}}^{(k+1)} + (1-\omega)\mathbf{u}^{(k)} \\
\mathbf{v}^{(k+1)} &= \omega \tilde{\mathbf{v}}^{(k+1)} + (1-\omega)\mathbf{v}^{(k)}.
\end{aligned}
$$

For $\omega = 1$ we get the Gauß–Seidel WR method.

Convergence in the linear case

$$\dot{\mathbf{u}} + A\mathbf{u} = \mathbf{f}(t), \qquad \mathbf{u}(0) = \mathbf{u}_0 \tag{1}$$

Splitting $A = M - N$:

$$\dot{\mathbf{u}}^{(k+1)} + M\mathbf{u}^{(k+1)} = N\mathbf{u}^{(k)} + \mathbf{f}(t), \qquad \mathbf{u}^{(k)}(0) = \mathbf{u}_0 \tag{2}$$

Let $\mathcal{K} : \mathbf{v} \mapsto \mathbf{u}$ be a linear integral operator given by

$$\mathcal{K}\mathbf{u}(t) = \int_0^t e^{(s-t)M} N\mathbf{u}(s)ds.$$

Then the solution of (**??**) can be written as

$$\mathbf{u}^{(k+1)} = \mathcal{K}\mathbf{u}^{(k)} + \varphi$$

with

$$\varphi(t) = e^{-tM}\mathbf{u}_0 + \int_0^t e^{(s-t)M}\mathbf{f}(s)ds. \tag{3}$$

Convergence in the linear case

Let X be a Banach space and assume that $\mathcal{K}$ is a bounded operator in X. For the convergence we need that spectral radius of $\mathcal{K}$

$$\rho(\mathcal{K}) := \lim_{k\to\infty} \|\mathcal{K}^k\|^{1/k}$$

satisfies $\rho(\mathcal{K}) < 1$, since $\mathbf{f} \in X$ implies $\varphi \in X$. In the following we are interested in the uniform convergency on a long but bounded time interval.

Convergence in the linear case

First we want to show that $\rho(\mathcal{K}) = 0$ in the space of uniform convergence in $[0, T]$. We have

$$|\mathcal{K}\varphi(t)| \leqslant C \int_0^t |\varphi(s)| ds \leqslant Ct \|\varphi\|_\infty$$

with $C = \exp(T\|M\|)\|N\|$, where $\|\cdot\|$ denotes a norm in $\mathbb{C}^n$. It follows

$$|\mathcal{K}^j\varphi(t)| \leqslant C^j \frac{t^j}{j!} \|\varphi\|_\infty$$

and

$$\left\| \left(1 - \frac{1}{\lambda}\mathcal{K}\right)^{-1} \right\| = \left\| \sum_{j=0}^{\infty} \left(\frac{1}{\lambda}\mathcal{K}\right)^j \right\| \leqslant \sum_{j=0}^{\infty} \left(\frac{CT}{\lambda}\right)^j \frac{1}{j!} = \exp\left(\frac{CT}{\lambda}\right)$$

for all $\lambda \neq 0$.

Convergence in the linear case

- If $\rho(\mathcal{K}) = 0$ then no effect of the splitting on the actual rate of convergence can be observed.
- Therefore use the weighted norm

$$\|\mathbf{u}\| := \sup_{t \in [0,T]} \|\exp(-\alpha t)\mathbf{u}(t)\|$$

  in which $\mathcal{K}$ becomes a contraction.
- A similar estimate as above holds for the weighted space.
- Find estimates, which are independent of the length of the interval.
- Consider Banach spaces on $[0, \infty)$. Let X denote any usual L^p-space of $\mathbb{C}^n$-valued functions defined on $[0, \infty)$.

Theorem

Let $X = L^p(\mathbb{R}_+, \mathbb{C}^n)$ with $1 \leqslant p \leqslant \infty$.

1. Then $\varphi \in X$ is implied by $\mathbf{f} \in X$, if and only if all eigenvalues of M have positive real part.
2. If all eigenvalues of A have positive real parts then $\mathcal{K}$ is a bounded operator in X if and only if the eigenvalues of M have positive real parts.

Proof

We want to show, that

$$\left(\int_0^\infty |\varphi(s)|^p ds \right)^{1/p} < \infty$$

holds. From equation

$$\varphi(t) = e^{-tM}\mathbf{u}_0 + \int_0^t e^{(s-t)M}\mathbf{f}(s)ds.$$

we have

$$\left(\int_0^\infty \left| e^{-sM}\mathbf{u}_0 + \int_0^s e^{(\tau-s)M}\mathbf{f}(\tau)d\tau \right|^p ds \right)^{1/p} < \infty$$

Theorem

- Let $X = L^p(\mathbb{R}_+, \mathbb{C}^n)$ with $1 \leqslant p \leqslant \infty$.
- Assume that all eigenvalues of M have positive real part.
- Then

$$\rho(\mathcal{K}) = \max_{\xi \in \mathbb{R}} \rho((i\xi I + M)^{-1} N).$$

- Note, that ρ in the left-hand side is the spectral radius of the operator
- Note, that ρ in the right-hand side is the spectral radius of the matrix.

Jacobi overrelaxation (JOR) WR method

- decomposition: $A = D - L - U$
- Splitting:

$$A = M - N = \frac{1}{\omega} D - \left(\frac{1-\omega}{\omega} D + L + U \right).$$

- For $\omega = 1$ we have the usual Jacobi WR method.
- Let $J(0) = D^{-1}(L+U)$ be the Jacobi matrix.
- Theorem: For any H-matrix A with $D > 0$ and $M(A)$ a nonsingular M-matrix the dynamic JOR WR method converges whenever

$$0 < \omega < \frac{2}{1 + \rho(|J(0)|)}.$$

SOR WR method

- Splitting:

$$A = M - N = \left(\frac{1}{\omega}D - L\right) - \left(\frac{1-\omega}{\omega}D + U\right).$$

- Theorem: For any H-matrix A with $D > 0$ and $M(A)$ a nonsingular M-matrix the SOR WR method converges whenever

$$0 < \omega < \frac{2}{1 + \rho(|J(0)|)}.$$

Symmetric SOR (SSOR) WR method

Consider methods that involve two different phases. Therefore let

$$\begin{aligned} \dot{\mathbf{u}}^{(k+1/2)} + M_1 \mathbf{u}^{(k+1/2)} &= N_1 \mathbf{u}^{(k)} + \mathbf{g}_1 \\ \dot{\mathbf{u}}^{(k+1)} + M_2 \mathbf{u}^{(k+1)} &= N_2 \mathbf{u}^{(k+1/2)} + \mathbf{g}_2 \\ \mathbf{u}^{(k+1)}(0) &= \mathbf{u}^{(k+1/2)}(0) = \mathbf{u}_0. \end{aligned}$$

For the symmetric SOR (SSOR) WR method we have

$$\begin{aligned} M_1 &= \frac{1}{\omega} D - L, & N_1 &= \frac{1-\omega}{\omega} D + U, \\ M_2 &= \frac{1}{\omega} D - U, & N_2 &= \frac{1-\omega}{\omega} D + L. \end{aligned}$$

Symmetric SOR (SSOR) WR method

For any H-matrix A with $D > 0$ and $M(A)$ a nonsingular M-matrix the symmetric SOR WR method converges whenever

$$0 < \omega < \frac{2}{1 + \rho(|J(0)|)}.$$

Example

Let

$$A = \begin{pmatrix} 1 & -\lambda \\ \lambda & 1 \end{pmatrix}, \quad \lambda \in (0,1).$$

Let us now check the assumptions from the Theorems.

- We have $D = I > 0$.
- A is an H-matrix, i.e. $M(A)$ is a M-matrix, since

$$M(A) = \begin{pmatrix} 1 & -\lambda \\ -\lambda & 1 \end{pmatrix}.$$

It follows

$$[M(A)]^{-1} = \frac{1}{1-\lambda^2} \begin{pmatrix} 1 & \lambda \\ \lambda & 1 \end{pmatrix}.$$

Example

- Moreover we have

$$J(0) = D^{-1}(L+U) = L+U = \begin{pmatrix} 0 & \lambda \\ -\lambda & 0 \end{pmatrix}$$

- $\rho(|J(0)|) = \lambda < 1$.
- The condition

$$0 < \omega < \frac{2}{1+\lambda}$$

  is satisfied for all $\lambda \in (0,1)$.

Example

Let

$$A = (n+1)^2 \begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix} \in \mathbb{R}^{n,n}.$$

Then A is a H-matrix with $D > 0$.

A model problem

Let us consider the ODE

$$\dot{\mathbf{u}} + Q\mathbf{u} = 0, \quad \mathbf{u}(0) = \mathbf{u}_0$$

with

$$Q = \begin{pmatrix} 1 & -\lambda \\ \lambda & 1 \end{pmatrix}.$$

First we solve this ODE with explicit Euler method. In this case we get

$$\mathbf{u}_{m+1} = \mathbf{u}_m - \tau Q\mathbf{u}_m = (I - \tau Q)\mathbf{u}_m.$$

Our numerical solution is stable, if the spectral radius $\rho(I - \tau Q) < 1$. The eigenvalues of $I - \tau Q$ are given by

$$\lambda_{1,2} = 1 - \tau \pm i\tau\lambda$$

and this implies $\tau < 2/(1 + \lambda^2)$, i. e. we get a stepsize restriction.

A model problem

Apply implicit Euler method:

$$\mathbf{u}_{m+1} = (I + \tau Q)^{-1} \mathbf{u}_m.$$

The numerical solution is stable, if the absolute values of the eigenvalues of the matrix $(I + \tau Q)^{-1}$ are bounded by one. The eigenvalues are given by

$$\frac{1 + \tau \pm i\tau\lambda}{(1 + \tau)^2 + (\tau\lambda)^2}.$$

A model problem

Apply Gauß–Seidel WR method:

$$\dot{\mathbf{u}}^{(k+1)} + M\mathbf{u}^{(k+1)} = N\mathbf{u}^{(k)},$$

where

$$M = D - L = \begin{pmatrix} 1 & -\lambda \\ 0 & 1 \end{pmatrix}, \qquad N = U = \begin{pmatrix} 0 & 0 \\ -\lambda & 0 \end{pmatrix}.$$

If we use the explicit Euler method, we obtain

$$\mathbf{u}_{m+1}^{(k+1)} = \mathbf{u}_m^{(k+1)} + \tau \left[N\mathbf{u}_m^{(k)} - M\mathbf{u}_m^{(k+1)} \right].$$

A model problem

In each timestep we iterate w. r. t. k until convergence. Then

$$\mathbf{u}_m^{(k+1)} = \mathbf{u}_m^{(k)} = \mathbf{u}_m.$$

Then it follows

$$\mathbf{u}_{m+1}^{(k+1)} = \mathbf{u}_m + \tau\left[N\mathbf{u}_m - M\mathbf{u}_m\right] = (I - \tau Q)\mathbf{u}_m,$$

which is the same approximation as in the monolythical approach.

A model problem

Apply Gauß–Seidel WR method and the implicit Euler method:

$$\mathbf{u}_{m+1}^{(k+1)} = \mathbf{u}_m + \tau \left[N\mathbf{u}_{m+1}^{(k)} - M\mathbf{u}_{m+1}^{(k+1)} \right].$$

It follows

$$\mathbf{u}_{m+1}^{(k+1)} = (I + \tau M)^{-1}\mathbf{u}_m + \tau(I + \tau M)^{-1} N\mathbf{u}_{m+1}^{(k)}.$$

For the matrix $\tau(I + \tau M)^{-1} N$ we have

$$\tau(I + \tau M)^{-1} N = \begin{pmatrix} \dfrac{-(\tau\lambda)^2}{(1-\tau)^2} & 0 \\ \dfrac{\tau\lambda}{1-\tau} & 0 \end{pmatrix},$$

which has the eigenvalues 0 and $\dfrac{-(\tau\lambda)^2}{(1-\tau)^2}$. The Gauß–Seidel WR method converges, if $\tau < 1/(1+\lambda)$.

A model problem

Apply Runge–Kutta method on model problem:

$$\mathbf{k}_i^{(k+1)} = N\left(\mathbf{u}_m^{(k)} + \tau \sum_{j=1}^{s} a_{ij}\mathbf{k}_j^{(k)}\right) - M\left(\mathbf{u}_m^{(k)} + \tau \sum_{j=1}^{s} a_{ij}\mathbf{k}_j^{(k+1)}\right).$$

With $Q = M - N$ it follows

$$\begin{pmatrix} I + \tau M a_{11} & \dots & \tau M a_{1s} \\ \vdots & \ddots & \vdots \\ \tau M a_{s1} & \dots & I + \tau M a_{ss} \end{pmatrix} \begin{pmatrix} \mathbf{k}_1^{(k+1)} \\ \vdots \\ \mathbf{k}_s^{(k+1)} \end{pmatrix} =$$

$$\begin{pmatrix} -Q\mathbf{u_m} \\ \vdots \\ -Q\mathbf{u_m} \end{pmatrix} + \tau N \begin{pmatrix} \sum_{j=1}^{s} a_{1j}\mathbf{k}_j^{(k)} \\ \vdots \\ \sum_{j=1}^{s} a_{sj}\mathbf{k}_j^{(k)} \end{pmatrix}$$

A model problem

Next we introduce the setting $\mathbf{k} := (\mathbf{k}_1, \ldots, \mathbf{k}_s)^\top$ and $A = (a_{ij})_{i,j=1}^s$ and get with the Kronecker product

$$(I + \tau(A \otimes M))\, \mathbf{k}_i^{(k+1)} = -(Q \otimes \mathbf{e})\mathbf{u_m} + \tau(A \otimes N)\mathbf{k}_j^{(k)}.$$

Next we need the eigenvalues of the matrix

$$\tau\,(I + \tau(A \otimes M))^{-1}\,(A \otimes N),$$

Implementation

We start our considerations with the PDE

$$\dot{u} - u'' = -e^{-t}(x^2 + 2), \qquad \text{in } (0, \bar{t}] \times (0, 1). \tag{4}$$

The Dirichlet boundary and the initial conditions are taken from the exact solution, which is given by

$$u(t, x) = 1 + e^{-t}x^2.$$

The space discretisation is done with central differences, i. e. we have

$$u''(t, x) \approx \frac{1}{h^2}\left[u(t, x + h) + u(t, x - h) - 2u(t, x)\right].$$

Implementation

Finally we get the MOL-ODE

$$\dot{\mathbf{u}} + A\mathbf{u} = \mathbf{f} \tag{5}$$

with

$$A = \frac{1}{h^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix},$$

$$\mathbf{f}(t) = -e^{-t}\begin{pmatrix} x_1^2 + 2 \\ x_2^2 + 2 \\ \vdots \\ x_{n-1}^2 + 2 \\ x_n^2 + 2 \end{pmatrix} + \frac{1}{h^2}\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 1 + e^{-t} \end{pmatrix}.$$

Splitting

Next we apply the splitting $A = M - N$ and get

$$\dot{\mathbf{u}}^{(k+1)} + M\mathbf{u}^{(k+1)} = N\mathbf{u}^{(k)} + \mathbf{f}. \tag{6}$$

For the time discretisation of the MOL-ODE we use diagonally implicit Runge–Kutta methods. We choose the L-stable implicit Euler method, the trapezoidual rule (order 2, implict, A-stable) and the method DIRK2 given by the Butcher table

$$\begin{array}{c|cc} \gamma & \gamma & 0 \\ 1 & 1-\gamma & \gamma \\ \hline & 1-\gamma & \gamma \end{array}, \quad \gamma = 1 - \sqrt{1/2} \approx 0,29.$$

The method is implicit, of second order and L-stable.

Discrete WR method

The discrete WR method is given by

$$\mathbf{k}_i^{(k+1)} = \mathbf{f}(t_m + c_i\tau) - (M-N)\mathbf{u}_m - \tau \sum_{j=1}^{s} a_{ij}\left(M\mathbf{k}_j^{(k+1)} - N\mathbf{k}_j^{(k)}\right), \quad k$$

$$\mathbf{u}_{m+1}^{(k+1)} = \mathbf{u}_m + \tau \sum_{i=1}^{s} b_i \mathbf{k}_i^{(k+1)}.$$

The symmetric SOR WR method is then given by

$$\dot{\mathbf{u}}^{(k+1/2)} + M_1\mathbf{u}^{(k+1/2)} = N_1\mathbf{u}^{(k)} + \mathbf{g}_1$$
$$\dot{\mathbf{u}}^{(k+1)} + M_2\mathbf{u}^{(k+1)} = N_2\mathbf{u}^{(k+1/2)} + \mathbf{g}_2.$$

Application

Applying the RK method on the symmetric SOR WR method gives us

$$\mathbf{k}_i^{(k+1/2)} = \mathbf{g}_1(t_m + c_i\tau) - (M_1 - N_1)\mathbf{u}_m - \tau \sum_{j=1}^{s} a_{ij} \left(M_1 \mathbf{k}_j^{(k+1/2)} - N_1 \mathbf{k}_j^{(k)} \right),$$

$$\mathbf{k}_i^{(k+1)} = \mathbf{g}_2(t_m + c_i\tau) - (M_2 - N_2)\mathbf{u}_m - \tau \sum_{j=1}^{s} a_{ij} \left(M_2 \mathbf{k}_j^{(k+1)} - N_2 \mathbf{k}_j^{(k+1/2)} \right),$$

$$\mathbf{u}_{m+1}^{(k+1)} = \mathbf{u}_m + \tau \sum_{i=1}^{s} b_i \mathbf{k}_i^{(k+1)}.$$

Results

First we apply the SOR WR method with $\omega = 1$. The central differences are applied with $h = 1/10$. Then we get the following numerical results:

	impl. Euler	trap. rule	DIRK2
$\tau = 0.100$	6.99e-04 (70)	1.62e-05 (50)	8.59e-05 (42)
$\tau = 0.050$	3.89e-04 (47)	3.72e-06 (32)	2.11e-05 (26)
$\tau = 0.025$	2.07e-04 (30)	9.13e-07 (20)	5.63e-06 (17)
$\tau = 0.013$	1.13e-04 (19)	2.31e-07 (13)	1.49e-06 (12)

Results

For $h = 1/100$ the following results are obtained

	impl. Euler	trap. rule	DIRK2
$\tau = 0.100$	1.98e-03 (1500)	2.94e-04 (1500)	1.45e-04 (1500)
$\tau = 0.050$	6.18e-04 (1500)	9.18e-06 (1500)	1.98e-05 (1450)
$\tau = 0.025$	2.10e-04 (1500)	2.35e-06 (978)	4.87e-06 (778)
$\tau = 0.013$	1.15e-04 (899)	3.13e-06 (518)	1.83e-06 (406)

Results

Next we compute the optimal ω_{opt}, which is given by $\omega_{opt} = 4/(4 - \mu^2)$, where $\mu = \rho(J(0)) = \rho(D^{-1}(L + U)) \approx 0.99951$. Then $\omega_{opt} \approx 1.3329$. Then we have for the SOR WR method

	impl. Euler	trap. rule	DIRK2
$\tau = 0.100$	7.39e-04 (1500)	1.25e-05 (1500)	8.39e-05 (1380)
$\tau = 0.050$	3.77e-04 (1500)	2.20e-06 (964)	2.04e-05 (780)
$\tau = 0.025$	2.02e-04 (894)	8.10e-07 (534)	5.24e-06 (420)
$\tau = 0.013$	1.12e-04 (495)	1.44e-06 (285)	1.34e-06 (222)

Results

symmetric SOR method

	impl. Euler	trap. rule	DIRK2
$\tau = 0.100$	6.74e-04 (1252)	1.49e-05 (870)	8.42e-05 (729)
$\tau = 0.050$	3.76e-04 (810)	2.85e-06 (514)	2.06e-05 (412)
$\tau = 0.025$	2.01e-04 (478)	2.79e-07 (283)	5.39e-06 (221)
$\tau = 0.013$	1.10e-04 (264)	5.74e-07 (151)	1.28e-06 (116)

Convergence analysis

For the ”monolythical” Runge–Kutta method we have

$$\mathbf{k}_i = \mathbf{f}(t_m + c_i\tau) - (M - N)\mathbf{u}_m - \tau \sum_{j=1}^{s} a_{ij}(M - N)\mathbf{k}_j)$$

and for the discrete WR method we have

$$\mathbf{k}_i^{(k+1)} = \mathbf{f}(t_m + c_i\tau) - (M - N)\mathbf{u}_m - \tau \sum_{j=1}^{s} a_{ij} \left(M\mathbf{k}_j^{(k+1)} - N\mathbf{k}_j^{(k)} \right).$$

Local error

The local error of the internal stages can be computed via

$$\begin{aligned}\epsilon_i^{(k+1)} &:= \mathbf{k}_i^{(k+1)} - \mathbf{k}_i \\ &= \tau \sum_{j=1}^{s} a_{ij} N \epsilon_j^{(k)} - \tau \sum_{j=1}^{s} a_{ij} M \epsilon_j^{(k+1)}.\end{aligned}$$

With the help of the Kronecker product we obtain

$$\epsilon^{(k+1)} = \tau(A \otimes N)\epsilon^{(k)} - \tau(A \otimes M)\epsilon^{(k+1)}.$$

It follows

$$\epsilon^{(k+1)} = \tau(I + \tau(A \otimes M))^{-1}(A \otimes N)\epsilon^{(k)}$$

Convergence analysis

- By C we denote we matrix $C := (I + \tau(A \otimes M))^{-1}(A \otimes N)$.
- numerical method converges, if $\tau < 1/\rho(C)$.
- implicit Euler method: $C := (I + \tau M)^{-1} N$
- trapezoidual rule: $C := \frac{1}{2}(I + \tau/2M)^{-1} N$.
- trapezoidual rule converges faster than the implicit Euler method.

Literature

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