Multirate explicit stabilized integrators for stiff differential equations

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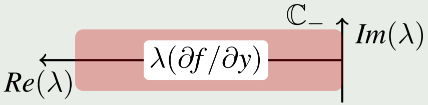
Explicit stabilized integrators for stiff differential equations

Motivating explicit stabilized methods

Stiff ordinary differential equation

$$y' = f(y), \quad t > 0,$$
$$y(0) = y_0.$$



Explicit Euler

$$y_{n+1} = y_n + \tau f(y_n)$$

- Straightforward to implement,
- cheap to evaluate.

Implicit Euler

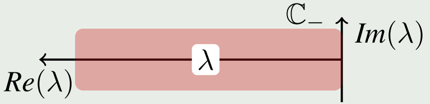
$$y_{n+1} = y_n + \tau f(y_{n+1})$$

- Needs non linear solver routine, preconditioners,
- expensive.

Motivating explicit stabilized methods

Dahlquist test equation

$$
\begin{aligned}
y' &= \lambda y, \quad t > 0, \\
y(0) &= y_0.
\end{aligned}
$$



Explicit Euler

$$
\begin{aligned}
y_{n+1} &= (1 + \tau\lambda) y_n \\
&= R(\tau\lambda) y_n
\end{aligned}
$$

- $R(z) = 1 + z$,
- $|R(z)| \leq 1$ for $z \in [-2, 0]$,
- stability condition $\tau \leq \frac{2}{|\lambda|}$.

Implicit Euler

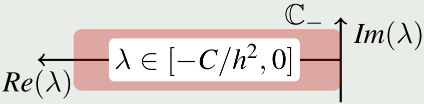
$$
\begin{aligned}
y_{n+1} &= (1 - \tau\lambda)^{-1} y_n \\
&= R(\tau\lambda) y_n
\end{aligned}
$$

- $R(z) = (1 - z)^{-1}$
- $|R(z)| \leq 1$ for all $Re(z) \leq 0$,
- unconditionally stable.

Motivating explicit stabilized methods

Space discretized parabolic equation

$$\begin{aligned} y' &= \Delta_h y, \quad t > 0, \\ y(0) &= y_0, \end{aligned}$$



where h is the smallest element size.

Explicit Euler

$$y_{n+1} = (I + \tau\Delta_h) y_n,$$

with

$$\tau \leq \frac{2}{|\lambda|} = \mathcal{O}\left(h^2\right).$$

Implicit Euler

$$y_{n+1} = (I - \tau\Delta_h)^{-1} y_n,$$

hence

large system to solve.

Motivating explicit stabilized methods

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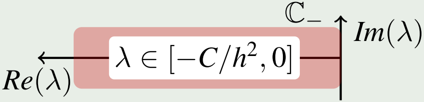

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Construction of explicit stabilized Runge–Kutta methods

Goal

Given a fixed number of stages s, find a first order explicit scheme with maximal stability domain along the negative real axis.

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Given a fixed number of stages s, find a first order explicit scheme with maximal stability domain along the negative real axis.

The stability polynomial of such a scheme solves the following

Optimization problem (Markoff, 1916; Guillou and Lago, 1960)

Find a polynomial $R_s(x)$ of degree s satisfying

$$R_s(0) = R_s'(0) = 1$$

and

$$|R_s(z)| \leq 1 \text{ for } z \in [-\ell_s, 0] \text{ with } \ell_s \text{ maximal.}$$

Solution to the optimization problem

Chebyshev polynomials of the first kind are defined recursively by

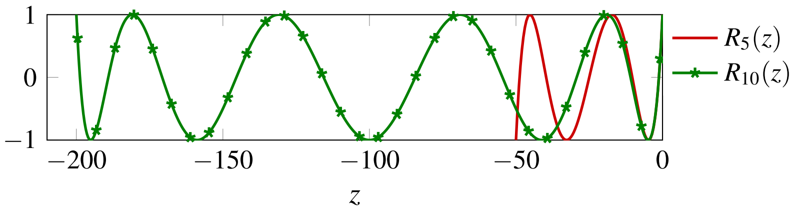
$$T_0(x) = 1, \qquad T_1(x) = x, \qquad T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$$

and satisfy

$$T_n(1) = 1, \qquad T_n'(1) = n^2, \qquad |T_s(x)| \leq 1 \text{ for all } x \in [-1, 1].$$

Thus,

$$R_s(z) = T_s\left(1 + \frac{z}{s^2}\right) \quad \text{satisfies} \quad \begin{cases} R_s(0) = R_s'(0) = 1, \\ |R_s(z)| \leq 1 \qquad \forall\, z \in [-2s^2, 0]. \end{cases}$$



Consequences

- For each s, there is a first order accurate polynomial $R_s(z)$ satisfying $|R_s(z)| \leq 1$ for all $z \in [-2s^2, 0]$.
- If there exists a Runge–Kutta scheme having $R_s(z)$ as stability polynomial, the stability condition on that scheme would be

$$\tau\lambda \in [-2s^2, 0] \qquad \forall \lambda = \lambda\left(\frac{\partial f}{\partial y}\right) \qquad \iff$$
$$\tau\rho \leq 2s^2 \qquad \rho = \rho\left(\frac{\partial f}{\partial y}\right).$$

- If such a scheme exists for all s, instead of adapting the step size τ we can change scheme and take s larger.
- There is no step size restriction.
- The size of the stability domain of this *family* of Runge–Kutta schemes grows *quadratically* with the number of stages.

Does such a method exists?

First solution was given by Guillou and Lago (1960), the idea is to write

$$R_s(z) = \prod_{j=1}^{s} \left(1 - \frac{1}{z_i} z\right), \qquad \text{with} \qquad z_i \text{ roots of } R_s(z).$$

And represent the scheme as composition of Euler steps:

$$\begin{aligned} k_0 =& y_n, \\ k_j =& k_{j-1} - \frac{1}{z_i} \tau f(k_{j-1}) \quad \text{for } j = 1, \ldots, s, \\ y_{n+1} =& k_s. \end{aligned}$$

Disadvantage: when $|z_i|$ is small we do a large Euler step and the internal stages k_j become unstable.
Solution by Lebedev (1994): sort the roots, group them two-by-two and use quadratic factors. Becomes tricky to implement.

Does such a method exists?

A better solution was given by Van der Houwen and Sommeijer (1980), which uses the recursive property

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x).$$

Runge–Kutta–Chebyshev (RKC) method

Set $s \in \mathbb{N}$ such that $\tau\rho \leq 2s^2$. Iterate

$$\begin{aligned} k_0 &= y_n, \\ k_1 &= k_0 + \mu_1 \tau f(k_0), \\ k_j &= \nu_j k_{j-1} - \kappa_j k_{j-2} + \mu_j \tau f(k_{j-1}) \quad \text{for } j = 2, \ldots, s, \\ y_{n+1} &= k_s. \end{aligned}$$

For $y' = \lambda y$ and $z = \tau\lambda$ it holds

$$k_j = T_j\left(1 + \frac{z}{s^2}\right) y_n \quad \text{and thus} \quad y_{n+1} = T_s\left(1 + \frac{z}{s^2}\right) y_n = R_s(z) y_n.$$

Cost of the RKC method

We estimate the cost, in the number of function evaluations, when integrating from $t = 0$ to $t = 1$.

- For RKC: take $\tau = 1$, since $\tau\rho \leq 2s^2$ then $s = \sqrt{\rho/2}$:

$$C_{RKC} = s = \sqrt{\frac{\rho}{2}}.$$

- For explicit Euler: take $\tau = 2/\rho$ and $1/\tau$ time steps:

$$C_{EE} = \frac{1}{\tau} = \frac{\rho}{2}.$$

- For $\rho = C/h^2$:

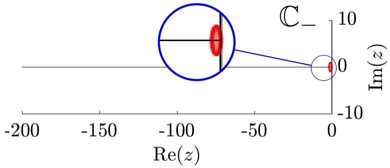
$$C_{RKC} = \sqrt{\frac{C}{2}}\frac{1}{h}, \qquad C_{EE} = \frac{C}{2}\frac{1}{h^2}.$$

- Comparison with implicit Euler depends on a multitude of factors: system size, non linearity, preconditioners, parallelism,...

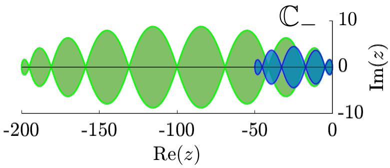
Stability domain

$$\mathcal{S} = \{z \in \mathbb{C}_- \; : \; |R_s(z)| \leq 1\}$$

$\mathcal{S}$ for explicit Euler.



$\mathcal{S}$ for $s = 10$, $s = 5$.



- Problem: unstable in imaginary direction.

Stability domain

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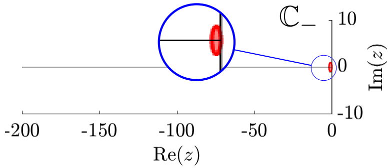
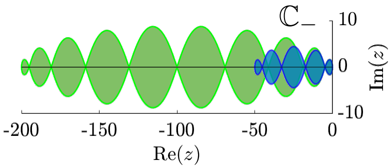
$\mathcal{S}$ for explicit Euler.



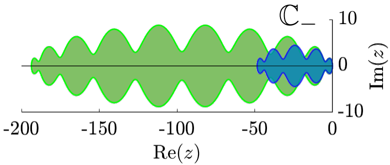
- Problem: unstable in imaginary direction.
- Replace $T_s\left(1+\frac{z}{s^2}\right)$ by

$$R_s(z) = \frac{T_s(\omega_0 + \omega_1 z)}{T_s(\omega_0)}$$

$\mathcal{S}$ for $s = 10$, $s = 5$.



$\mathcal{S}$ for $s = 10$, $s = 5$. Damped.



Numerical experiment

Solve

$$\begin{aligned} \partial_t u - \Delta u &= f && \text{in } \Omega_\delta \times [0,T], \\ \nabla u \cdot \boldsymbol{n} &= 0 && \text{in } \partial\Omega_\delta \times [0,T], \\ u &= 0 && \text{in } \Omega_\delta \times \{0\}, \end{aligned}$$

in a domain Ω_δ containing a narrow channel of width δ

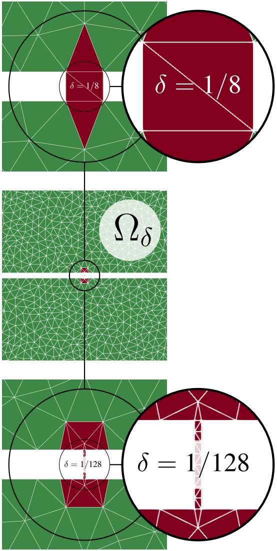
- with first order DG in space

$$\partial_t u_h = \Delta_h u_h + f_h$$

- and RKC in time

$$\tau \rho_h \leq 2s^2 \quad \Longrightarrow \quad s = \mathcal{O}\left(h^{-1}\right)$$

We fix $\tau = 0.01$ and monitor the performance of RKC as $\delta \to 0$.



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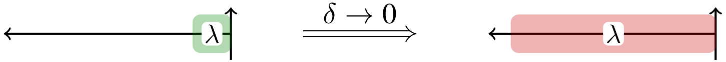

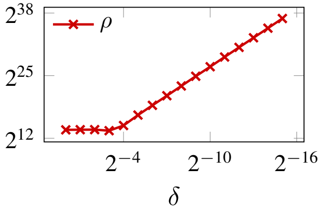

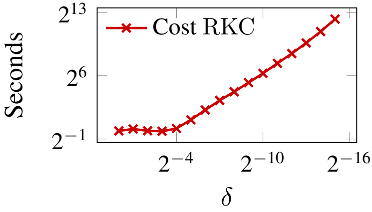

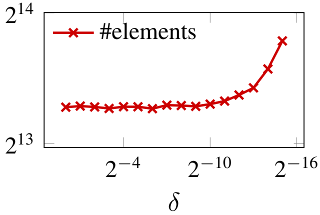

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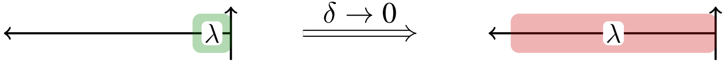
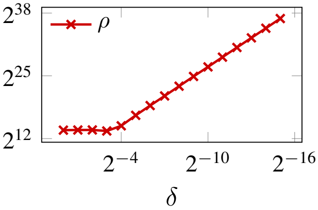
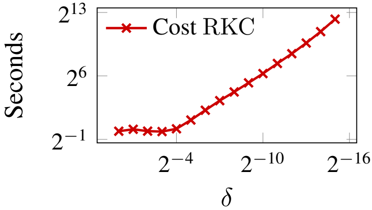
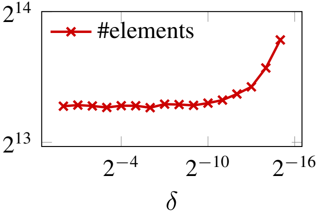








Conclusion
Stabilization of modes induced by a very few degrees of freedom comes at huge computational cost.

Multirate explicit stabilized methods

Problem statement

Multirate equation

Solve the dissipative system

$$y' = f_F(y) + f_S(y), \quad t > 0,$$
$$y(0) = y_0.$$

Term	Stiff ?	Cost ?
f_F	stiff	cheap
f_S	not stiff	expensive
$f_F + f_S$	stiff	expensive

Examples:

- chemical systems with many slow reactions and a few fast reactions,
- highly integrated electrical circuits with latent and active components,
- parabolic problems on locally refined meshes,
- ...

Solve

$$\partial_t u - \Delta u + \boldsymbol{\beta} \cdot \nabla u + \mu u = 0.$$

Space discretization gives:

$$\begin{pmatrix} \partial_t u_h \\ \partial_t u_H \end{pmatrix} = \underbrace{\begin{pmatrix} \Delta_h u_h \\ 0 \end{pmatrix}}_{\text{Fast}} + \underbrace{\begin{pmatrix} \boldsymbol{\beta} \cdot \nabla_h u_h + \mu u_h \\ \Delta_H u_H + \boldsymbol{\beta} \cdot \nabla_H u_H + \mu u_H \end{pmatrix}}_{\text{Slow}}$$

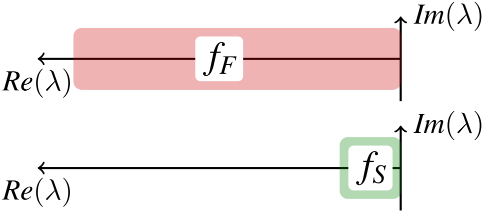
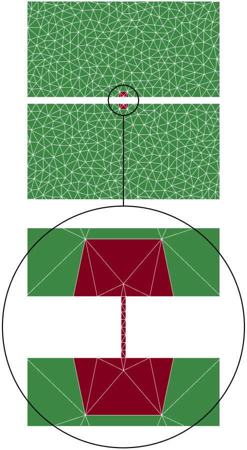


Figure. *Spectrum of* Δ_h *and* Δ_H.



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$f_F + f_S$	stiff	expensive

Integration with schemes for $y' = f(y)$:

~~explicit methods~~

stabilized/implicit methods

many function evaluations

very expensive

Literature review

Most of existing multirate methods

- have a spectrum clustering assumption, that is a clear partition between fast and slow variables (E, 2003),

- coupling of fast and slow variables done by *interpolation* or extrapolation $\Longrightarrow$ prone to *instabilities* and/or reduction of stability domain (Gear and Wells, 1984),
- when stable require solution of large and complex non linear systems (Ewing et al., 1990).

New explicit stabilized multirate method

Multirate RKC^2 method (Abdulle, Grote and Rosilho, 2019):

- no assumption on spectrum clustering,

- no interpolations,
- fully explicit,
- proven to be stable on a large region close to the negative real axis.

Modified multirate equation

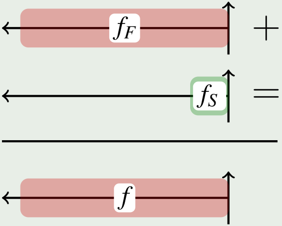
Idea

Shrink spectrum of f_F and integrate the modified system.

Original equation

$$y' = f(y) = f_F(y) + f_S(y).$$

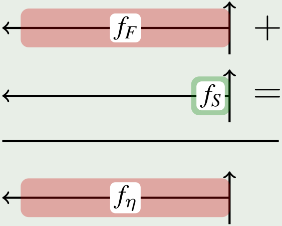
Spectral properties:



Modified equation

$$y_\eta' = f_\eta(y_\eta) \quad \text{with } \eta \geq 0.$$

For $\eta = 0$ it holds $f_\eta = f$ hence:



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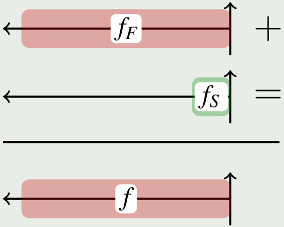

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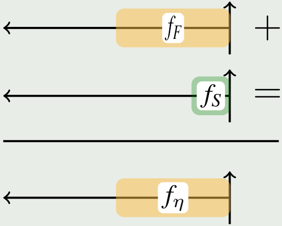
For $\eta > 0$ then $f_\eta = f + \mathcal{O}(\eta)$



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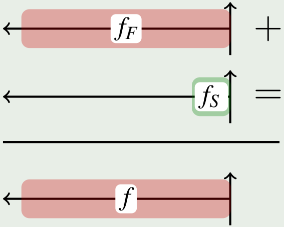

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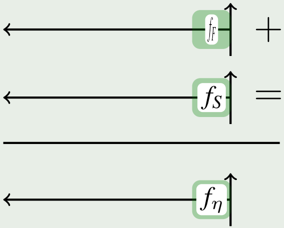

Motivating the definition of f_η

Properties of f_η

- $f_\eta = f + \mathcal{O}(\eta)$,
- $\rho_\eta \ll \rho$.

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- $f_\eta = f + \mathcal{O}(\eta)$, ✓
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Towards the definition of f_η

Let $u_0 \in \mathbb{R}^n$ and $u : [0, \eta] \to \mathbb{R}^n$ such that

$u(0) = u_0,$ and u is smooth.

Let

$$f_\eta(u_0) = \frac{1}{\eta} \int_0^\eta f(u(s))\, \mathrm{d}s.$$

Motivating the definition of f_η

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Definition of f_η

Properties of f_η

- $f_\eta = f + \mathcal{O}(\eta)$, ✓
- $\rho_\eta \ll \rho$. ✓

Definition of f_η

Let $u_0 \in \mathbb{R}^n$ and $u : [0, \eta] \to \mathbb{R}^n$ such that

$$u(0) = u_0, \qquad \text{and} \qquad u' = f_F(u) + f_S(u_0).$$

Let

$$f_\eta(u_0) = \frac{1}{\eta} \int_0^\eta f_F(u(s))\, \mathrm{d}s + f_S(u_0) = \frac{1}{\eta}(u(\eta) - u_0).$$

Advantages:

- Computations are cheap since the expensive term f_S is frozen.
- Stiffness is reduced since f_F is not frozen.

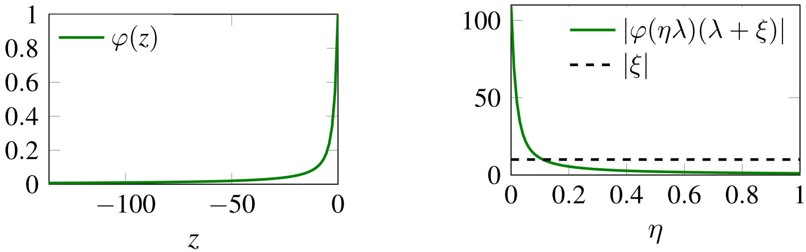
Stability analysis

Let the multirate Dahlquist equation be defined by

$$y' = f_F(y) + f_S(y) = \lambda y + \xi y, \quad \lambda, \xi \leq 0.$$

Then $u' = f_F(u) + f_S(u_0) = \lambda u + \xi u_0$ and it holds

$$f_\eta(u_0) = \varphi(\eta\lambda)(\lambda + \xi)u_0, \quad \text{with} \quad \varphi(z) = \frac{e^z - 1}{z}.$$

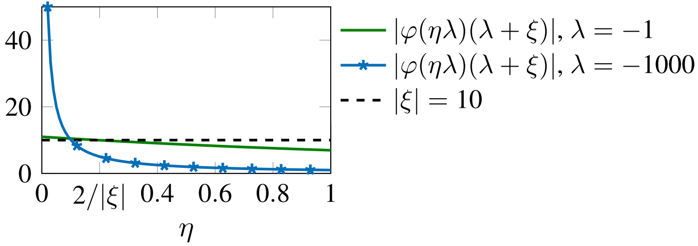


Goal: Choose η such that spectrum of f_η is similar to the one of f_S. Hence, we want $|\varphi(\eta\lambda)(\lambda + \xi)| \leq |\xi|$.

Lemma

It holds $|\varphi(\eta\lambda)(\lambda+\xi)| \leq |\xi|$ *for all* $\lambda \leq 0$ *if and only if* $\eta \geq 2/|\xi|$.

- For $\eta \geq 2/|\xi|$ the stiffness of f_η depends only on f_S.
- η depends only on ξ.
- True for all $\lambda \leq 0$, so there is no scale separation assumption.
- For a parabolic equation, λ and ξ represent the eigenvalues of the laplacians Δ_h and Δ_H. Since Δ_h has large and small eigenvalues it is important that the result holds for all $\lambda \leq 0$.



Modified multirate equation

Modified multirate equation

Solve

$$y_\eta' = f_\eta(y_\eta),\ t > 0, \qquad y_\eta(0) = y_0$$

with

$$f_\eta(u_0) = \frac{1}{\eta}(u(\eta) - u_0),$$

where u is defined by

$$u' = f_F(u) + f_S(u_0),\ t \in]0, \eta], \qquad u(0) = u_0, \qquad \eta = 2/\rho_S$$

and ρ_S is the spectral radius of the Jacobian of f_S.

Modified multirate equation

Modified multirate equation

Solve

$$y'_\eta = f_\eta(y_\eta), \quad t > 0, \qquad y_\eta(0) = y_0$$

with

Integrated numerically $\Longrightarrow$ different stability properties

$$f_\eta(u_0) = \frac{1}{\eta}(u(\eta) - u_0),$$

where u is defined by

$$u' = f_F(u) + f_S(u_0), \quad t \in]0, \eta], \qquad u(0) = u_0, \qquad \eta = 2/\rho_S$$

and ρ_S is the spectral radius of the Jacobian of f_S.

Multirate RKC^2 scheme

Multirate RKC^2 scheme

Let $\tau > 0$ be the time step, integrate

$$y_\eta' = \bar{f}_\eta(y_\eta),\ t > 0, \qquad y_\eta(0) = y_0,$$

using an RKC scheme with m stages, where $\tau\rho_S \leq 2m^2$.
The right hand side $\bar{f}_\eta$ is defined by

$$\bar{f}_\eta(u_0) = \frac{1}{\eta}(\bar{u}_\eta - u_0),$$

where $\bar{u}_\eta$ is an approximation of $u(\eta)$, solution of

$$u' = f_F(u) + f_S(u_0),\ t \in]0,\eta], \qquad u(0) = u_0, \qquad \eta = ?,$$

obtained by one step of RKC with s stages, where $\eta\rho_F \leq 2s^2$.

Stability analysis of numerical $\bar{f}_\eta$

We apply the scheme to the multi rate Dahlquist equation

$$y' = f_F(y) + f_S(y) = \lambda y + \xi y$$

Hence $u' = \lambda u + \xi u_0$ and $s \in \mathbb{N}$ is such that $\eta|\lambda| \leq 2s^2$. For $\bar{u}_\eta$:

$$\begin{aligned} k_0 &= u_0, \\ k_1 &= k_0 + \mu_1 \eta(\lambda k_0 + \xi u_0), \\ k_j &= \nu_j k_{j-1} + \kappa_j k_{j-2} + \mu_j \eta(\lambda k_{j-1} + \xi u_0) \quad \text{for } j = 2, \dots s, \\ \bar{u}_\eta &= k_s. \end{aligned}$$

It can be shown by recursion that

$$\bar{u}_\eta = (R_s(\eta\lambda) + \Phi_s(\eta\lambda)\eta\xi)u_0,$$

with

$$\Phi_s(z) = \sum_{k=1}^{s} \beta_k U_k(\omega_0 + \omega_1 z)$$

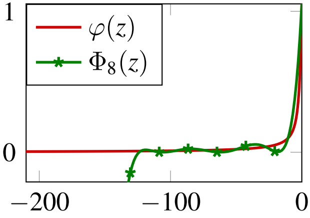
where $U_k(z)$ is a Chebyshev polynomial of the second kind of degree k and $\beta_k, \omega_0, \omega_1$ are parameters of the scheme.

Stability analysis of numerical $\bar{f}_\eta$

Lemma

It holds $\Phi_s(0) = 1$ *and for* $z < 0$

$$\Phi_s(z) = \frac{R_s(z) - 1}{z}. \quad \varphi(z) = \frac{e^z - 1}{z}$$



Stability analysis of numerical $\bar{f}_\eta$

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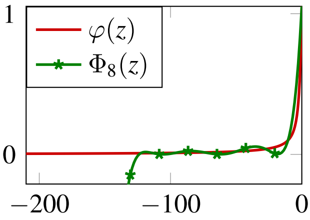


Which leads to

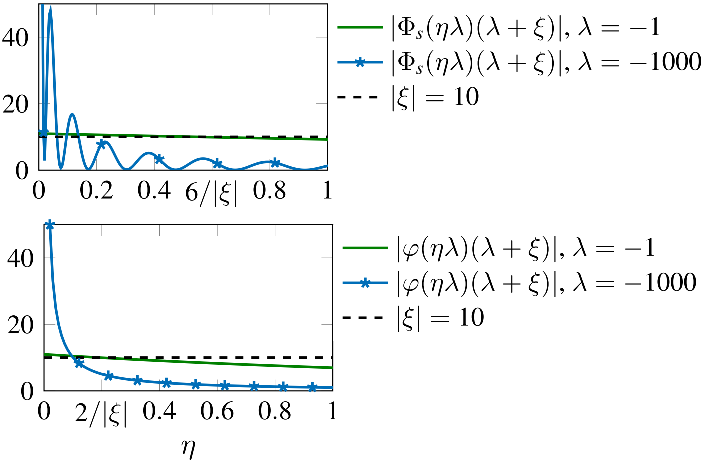
$$\bar{f}_\eta(u_0) = \Phi_s(\eta\lambda)(\lambda + \xi)u_0 \quad f_\eta(u_0) = \varphi(\eta\lambda)(\lambda + \xi)u_0$$

Goal: as before, we want the spectrum of $\bar{f}_\eta$ to be similar to the one of f_S. Hence, we want $|\Phi_s(\eta\lambda)(\lambda + \xi)| \leq |\xi|$.

Stability analysis of numerical $\bar{f}_\eta$

Lemma

It holds $|\Phi_s(\eta\lambda)(\lambda+\xi)| \leq |\xi|$ *for* $\eta\lambda \in [-2s^2, 0]$ *if and only if* $\eta \geq 6/|\xi|$. *(we had* $\eta \geq 2/|\xi|$*)*



Integration of $y' = \bar{f}_\eta$

We apply an RKC scheme to

$$y' = \bar{f}_\eta(y) = \Phi_s(\eta\lambda)(\lambda + \xi)y.$$

Let $m \in \mathbb{N}$ be such that $\tau|\xi| \leq 2m^2$, iterate

$$\begin{aligned} k_0 &= y_n, \\ k_1 &= k_0 + \mu_1 \tau \Phi_s(\eta\lambda)(\lambda + \xi)k_0, \\ k_j &= \nu_j k_{j-1} + \kappa_j k_{j-2} + \mu_j \tau \Phi_s(\eta\lambda)(\lambda + \xi)k_{j-1} \quad \text{for } j = 2, \ldots, m, \\ y_{n+1} &= k_m. \end{aligned}$$

Hence,

$$y_{n+1} = R_m(\tau \Phi_s(\eta\lambda)(\lambda + \xi))y_n.$$

Since $|\Phi_s(\eta\lambda)(\lambda + \xi)| \leq |\xi|$ then $|R_m(\tau\Phi_s(\eta\lambda)(\lambda + \xi))| \leq 1$.

Weakening the condition $\eta \geq 6/|\xi|$

- Problem: For $|\xi| \to 0$ then $\eta \to \infty$.
- But,
$$|R_m(\tau\Phi_s(\eta\lambda)(\lambda+\xi))| \leq 1$$
already for
$$\tau|\Phi_s(\eta\lambda)(\lambda+\xi)| \leq 2m^2,$$
$|\Phi_s(\eta\lambda)(\lambda+\xi)| \leq |\xi|$ is too strong.
- $\eta \geq 3\tau/m^2$ is enough for stability.
- The parameter η depends on the stabilization procedure for $|\xi|$, not on $|\xi|$ itself.
- In practice
$$\eta = 3\frac{\tau}{m^2} = \mathcal{O}(\tau) \quad \text{and generally} \quad \eta \ll \tau.$$
- It follows that the multirate scheme is first order accurate.

Multirate RKC^2 scheme

Multirate RKC^2 scheme

Let $\tau > 0$ be the time step, integrate

$$y_\eta' = \bar{f}_\eta(y_\eta),\ t > 0, \qquad y_\eta(0) = y_0$$

using an RKC scheme with m stages, where $\tau\rho_S \leq 2m^2$.
The right hand side $\bar{f}_\eta$ is defined by

$$\bar{f}_\eta(u_0) = \frac{1}{\eta}(\bar{u}_\eta - u_0),$$

where $\bar{u}_\eta$ is an approximation of $u(\eta)$, solution of

$$u' = f_F(u) + f_S(u_0),\ t \in]0,\eta] \qquad u(0) = u_0, \quad \eta = 3\tau/m^2,$$

obtained by one step of RKC with s stages, where $\eta\rho_F \leq 2s^2$.

Theorem

The multirate RKC^2 *scheme has first order of accuracy and is stable.*

Numerical experiment

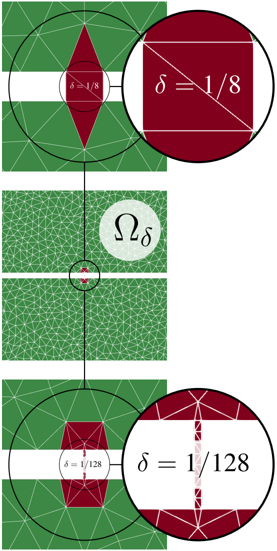
Solve

$$\begin{aligned} \partial_t u - \Delta u &= f && \text{in } \Omega_\delta \times [0,T], \\ \nabla u \cdot \boldsymbol{n} &= 0 && \text{in } \partial\Omega_\delta \times [0,T], \\ u &= 0 && \text{in } \Omega_\delta \times \{0\}, \end{aligned}$$

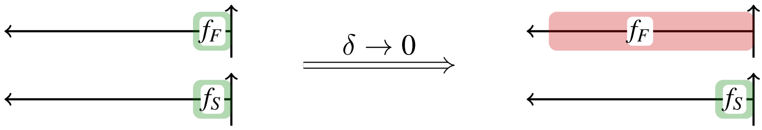
- first order DG in space,
- RKC^2 and RKC in time.

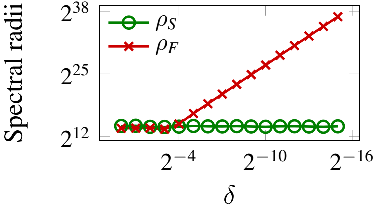
We let $\delta \to 0$ and compare the performance of RKC^2 against the one of standard RKC.

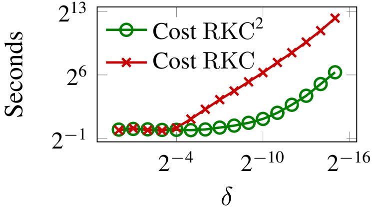
$$\begin{pmatrix} \partial_t u_h \\ \partial_t u_H \end{pmatrix} = \underbrace{\begin{pmatrix} \Delta_h u_h \\ 0 \end{pmatrix}}_{\text{Fast}} + \underbrace{\begin{pmatrix} f_h \\ \Delta_H u_H + f_H \end{pmatrix}}_{\text{Slow}}$$

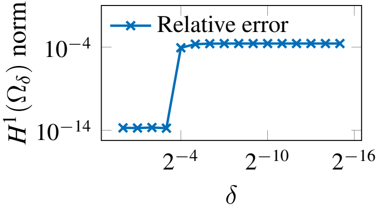


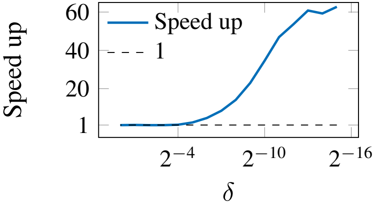
Numerical experiment











Thank you for your attention!

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