Multirate stabilized explicit methods for deterministic and stochastic differential equations without clear-cut scale separation

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CECAM Workshop on: Multiscale Simulations of Soft Matter
October 2, 2020

Outline

1. Stabilized explicit schemes for stiff differential equations

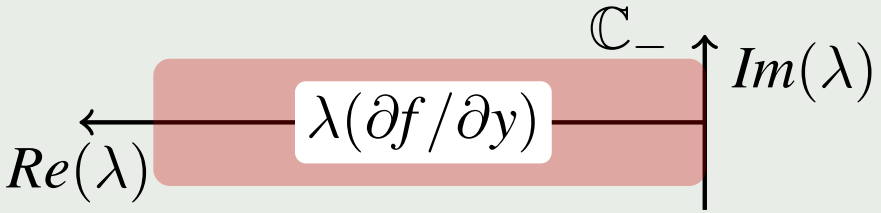
2. Multirate stabilized explicit schemes for *deterministic* differential equations

3. Multirate stabilized explicit schemes for *stochastic* differential equations

Motivating stabilized explicit methods

Stiff ordinary differential equation

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



Explicit Euler

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

- Straightforward to implement,
- cheap to evaluate.

Implicit Euler

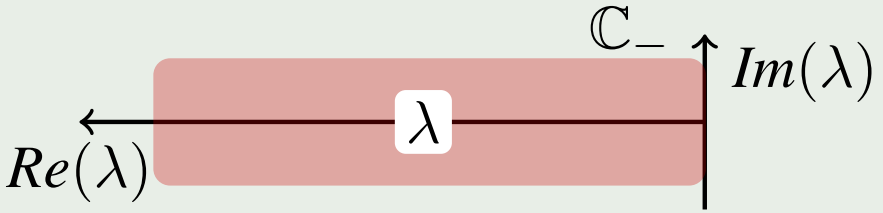
$$y_{n+1} = y_n + \tau f(y_{n+1})$$

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

Motivating stabilized explicit 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

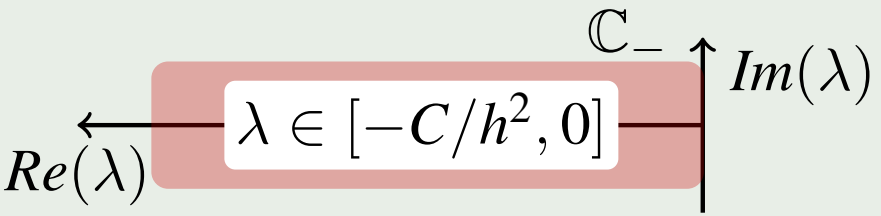
$$\begin{aligned} y_{n+1} &= (1 - \tau\lambda)^{-1} y_n \\ &= R(\tau\lambda) y_n \end{aligned}$$

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

Motivating stabilized explicit 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 stabilized explicit methods

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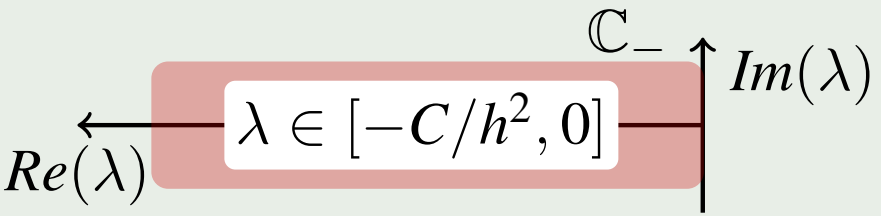

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Construction of stabilized explicit Runge–Kutta methods

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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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

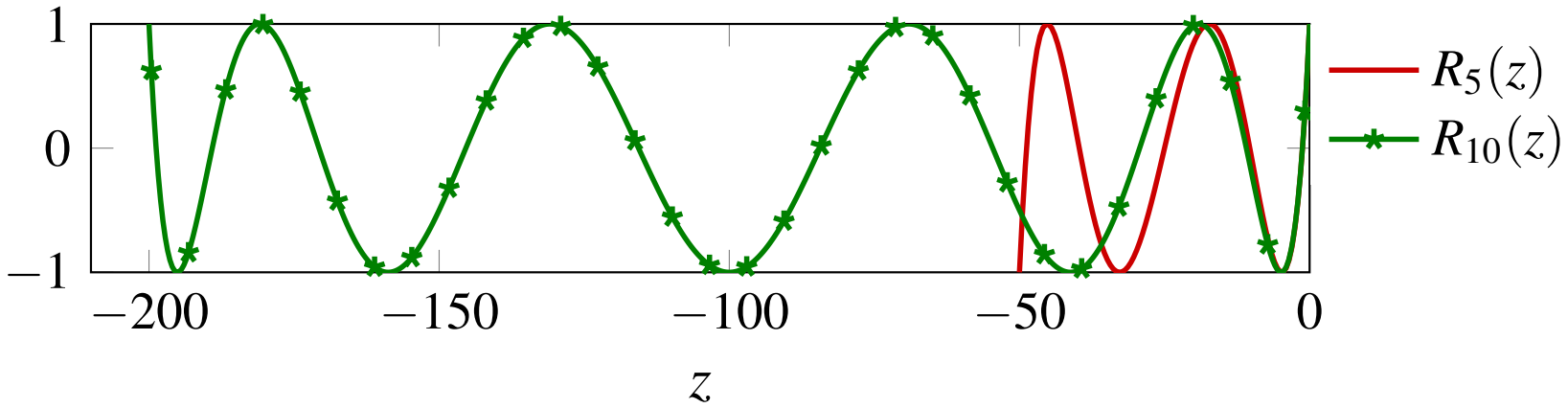
$$|R_s(z)| \leq 1 \text{ for } z \in [-\ell_s, 0] \text{ with } \ell_s \text{ maximal.}$$

Construction of stabilized explicit Runge–Kutta methods

The solution to the optimization problem is

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

where $T_s(x)$ is the Chebyshev polynomial of the first kind of degree s.



Consequences

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

$$\tau\rho \leq 2s^2, \qquad \rho = \rho\left(\frac{\partial f}{\partial y}\right).$$

- Instead of adapting the step size τ we can simply 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.

Runge–Kutta–Chebyshev method

From the recursive property

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

we can derive a Runge–Kutta scheme having $R_s(z)$ as stability polynomial (Van der Houwen and Sommeijer, 1980).

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: $y_{n+1} = T_s\left(1 + \frac{z}{s^2}\right) y_n = R_s(z) y_n$.

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 $\rho = C/h^2$:

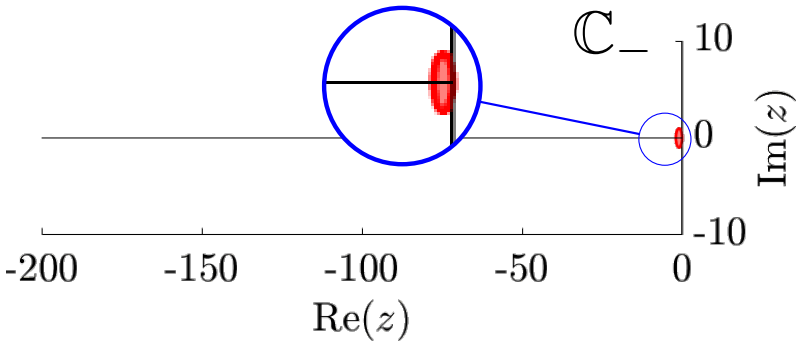
$$C_{RKC} = \sqrt{\frac{C}{2}}\frac{1}{h}, \qquad C_{EE} = \frac{C}{2}\frac{1}{h^2}.$$

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

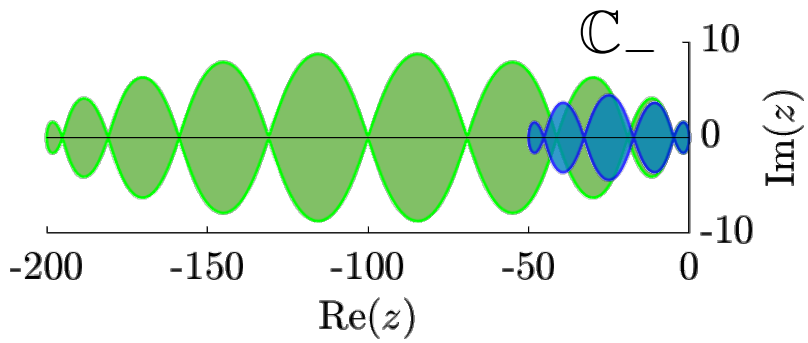
Stability domain

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

$\mathcal{S}$ for explicit Euler.



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



- Problem: unstable in imaginary direction.

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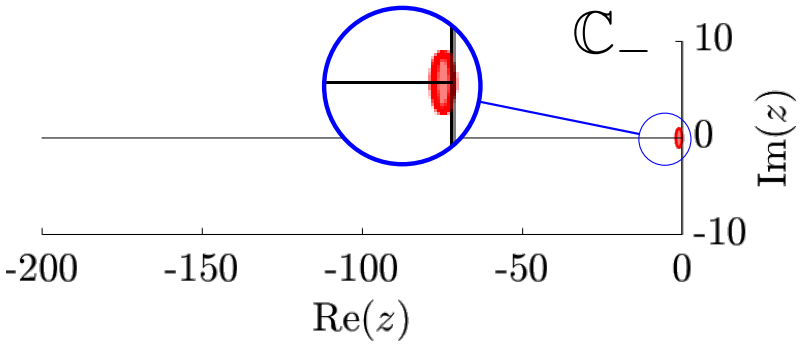
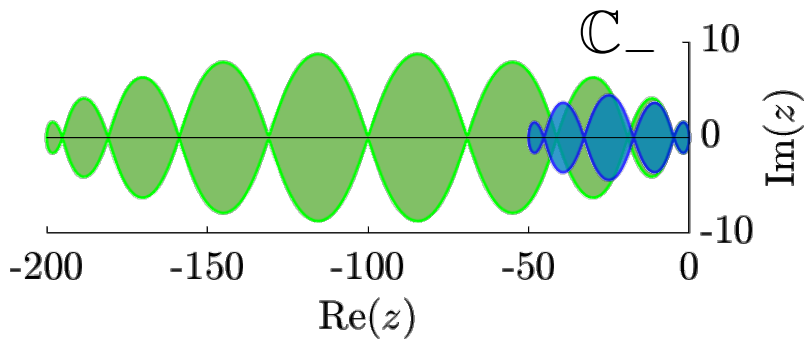


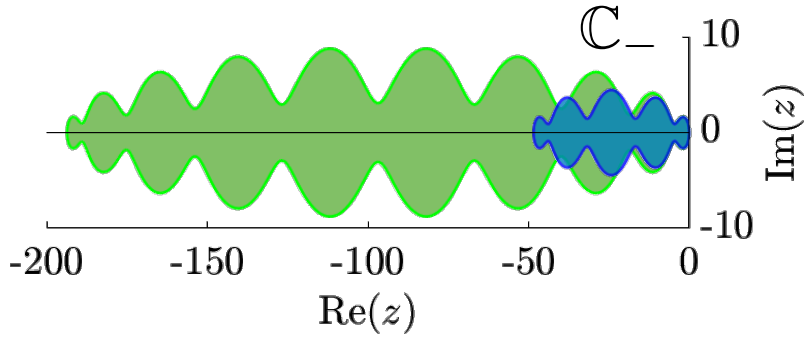
$\mathcal{S}$ for $s = 10$, $s = 5$.



- 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 $s = 10$, $s = 5$. 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

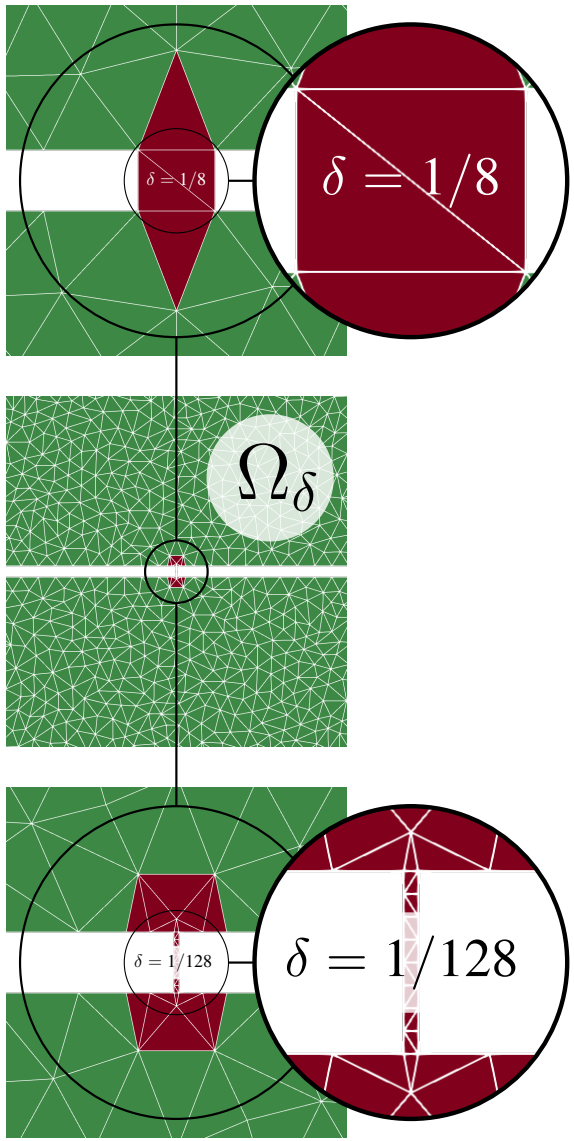
- with first order DG in space

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

- 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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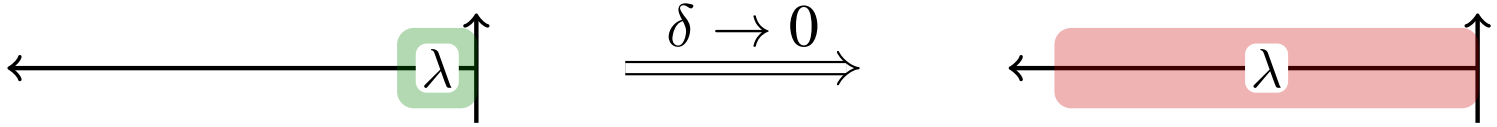

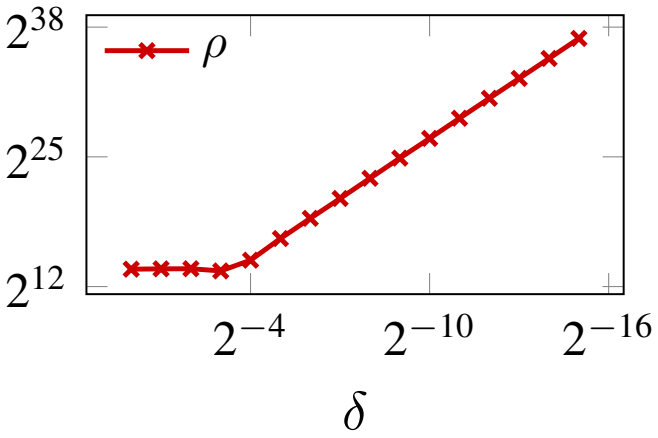

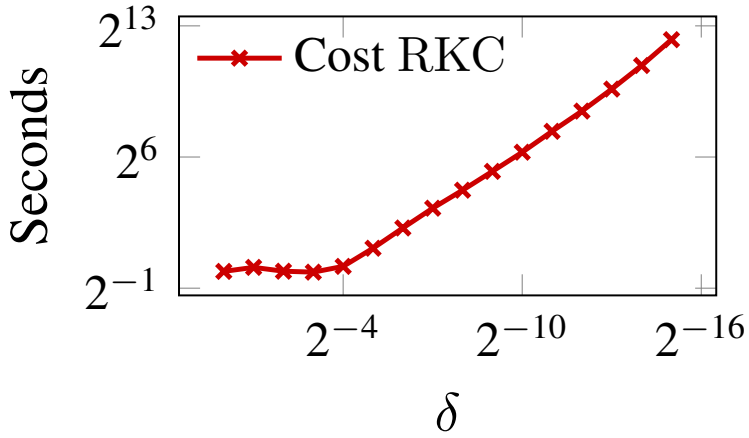

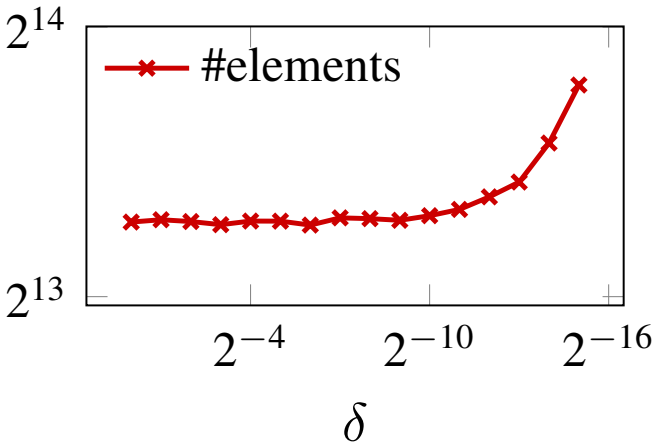

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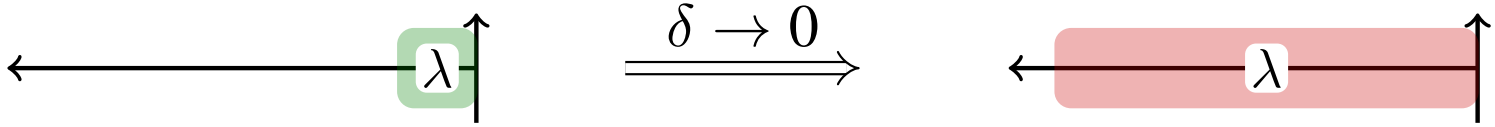
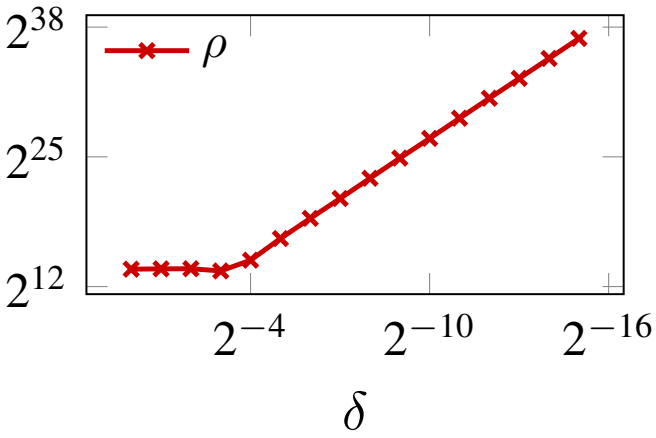
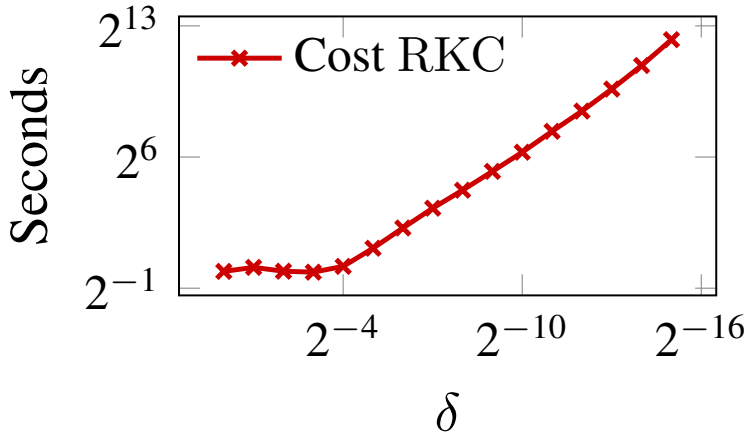
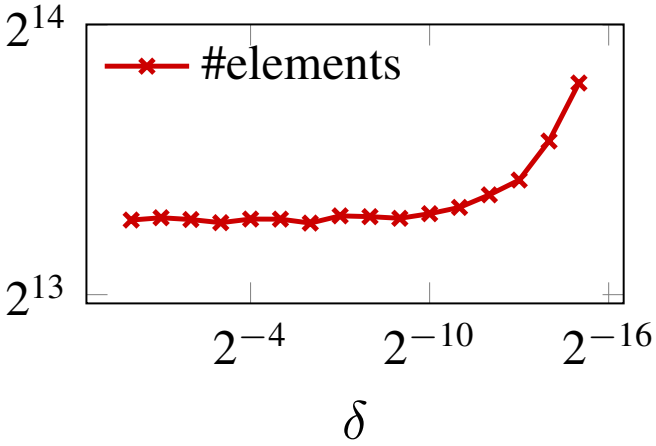








Conclusion

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

Outline

1. Stabilized explicit schemes for stiff differential equations

2. Multirate stabilized explicit schemes for *deterministic* differential equations

3. Multirate stabilized explicit schemes for *stochastic* differential equations

Problem statement

Multirate equation

Solve the dissipative system

$$y' = f_F(y) + f_S(y),$$
$$y(0) = y_0.$$

Term	Stiff ?	Cost ?
f_F	stiff	cheap
f_S	nonstiff	expensive
$f_F + f_S$	stiff	expensive

Examples:

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

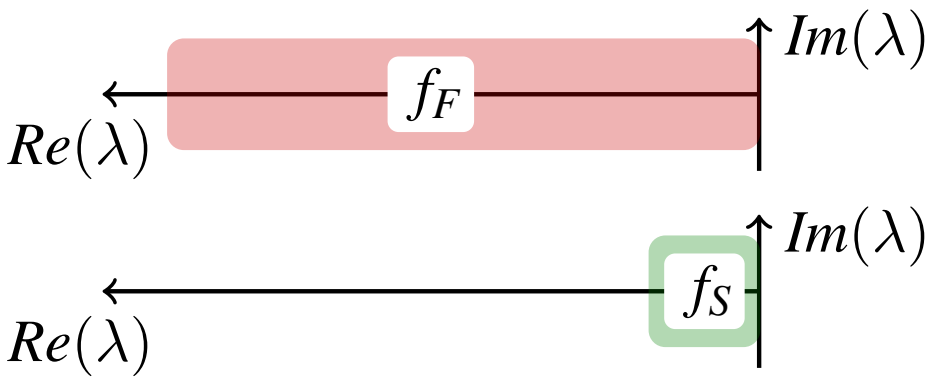
A parabolic problem on a locally refined mesh

Solve

$$\partial_t u - \Delta u = F.$$

Space discretization gives:

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



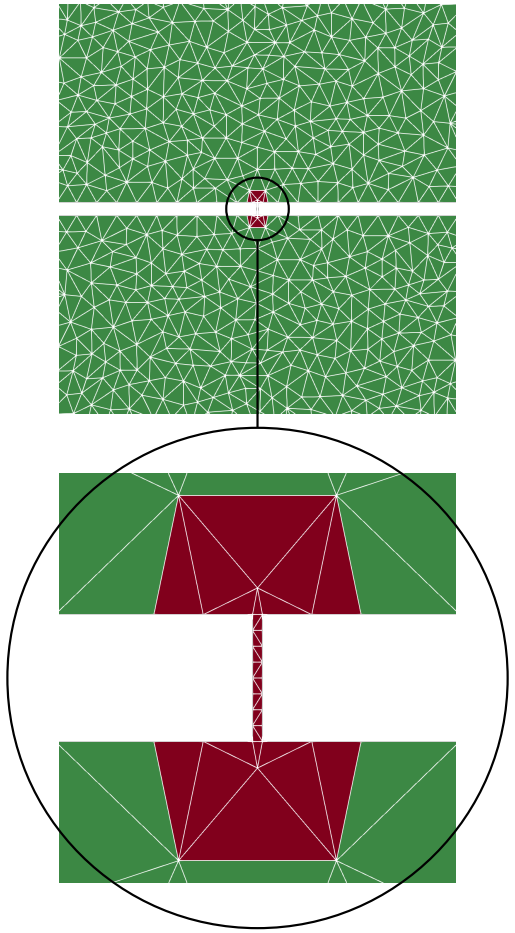


Figure. *Spectrum of* Δ_h *and* Δ_H.

A reaction rate equation with fast and slow reactions

$$\frac{\mathrm{d}y}{\mathrm{d}t} = \sum_{j=1}^{M} \boldsymbol{\nu}_j a_j(y) = \underbrace{\sum_{j=1}^{r} \boldsymbol{\nu}_j a_j(y)}_{f_F(y)} + \underbrace{\sum_{j=r+1}^{M} \boldsymbol{\nu}_j a_j(y)}_{f_S(y)}$$

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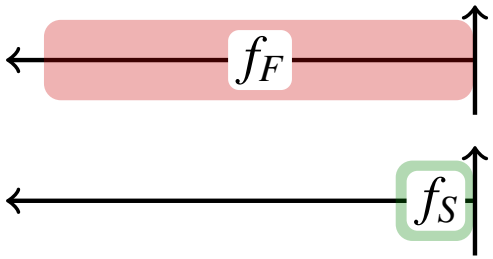
- f_F may contain slow reactions



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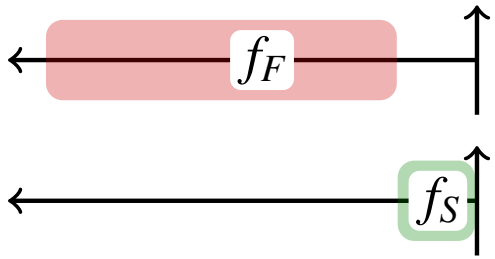
- f_F may contain slow reactions
- The fastest reaction in f_S may be almost as fast as the slowest reaction in f_F



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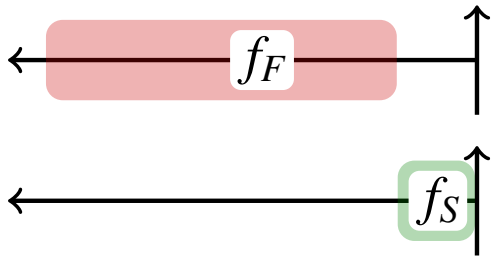
- f_F may contain slow reactions
- The fastest reaction in f_S may be almost as fast as the slowest reaction in f_F
- The system could be split in fast-slow species, instead of fast-slow reactions.



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

~~explicit methods~~

stabilized/implicit methods

very expensive

many function evaluations

Literature review on multirate methods

Most of existing multirate methods:

- are based on a spectrum clustering assumption, that is a clear-cut partition between fast and slow variables (E, 2003; Gear et al., 2003; Eriksson et al., 2003),

- perform the coupling of fast and slow variables by *interpolation* $\Longrightarrow$ prone to *instabilities* and/or shortening of the stability domain (Gear and Wells, 1984; Engstler and Lubich, 1997; Mirzakhanian, 2017),
- when are stable require the solution to large and complex nonlinear systems (Ewing et al., 1990; Shishkin and Vabishchevich, 2000).

New stabilized explicit multirate method

Multirate RKC (mRKC) method (Abdulle, Grote and Rosilho de Souza, 2020) based on modified equations:

- no need for scale separation,

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

Modified multirate equation

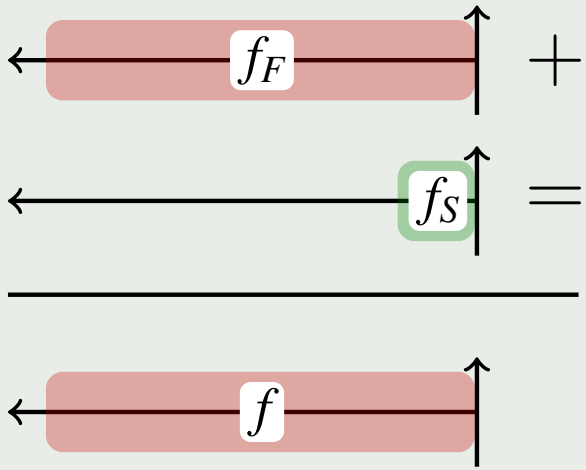
Idea

Shrink the spectrum of f_F and integrate a modified equation.

Original problem

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

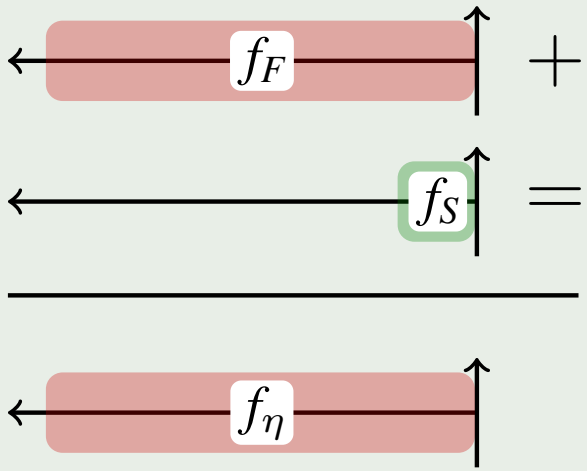
Spectral properties:



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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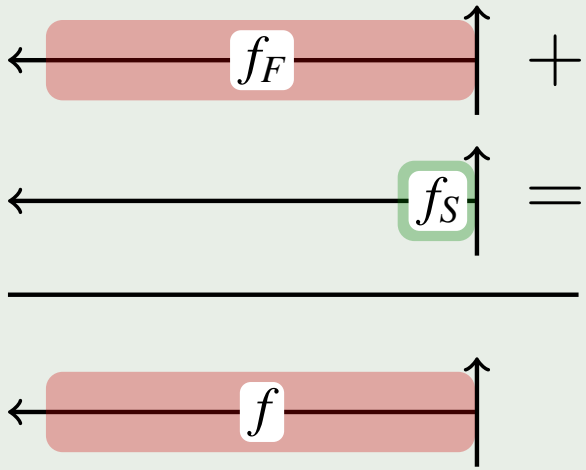

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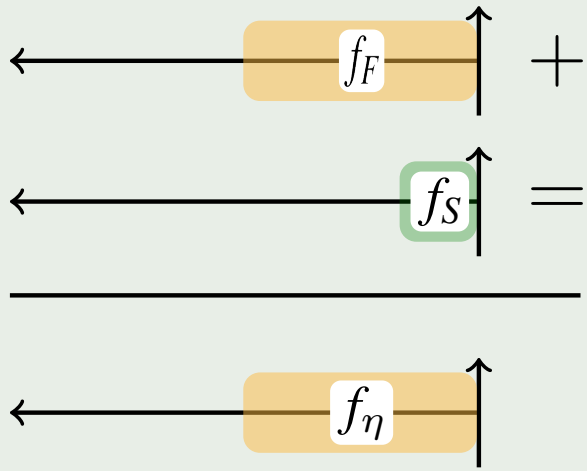

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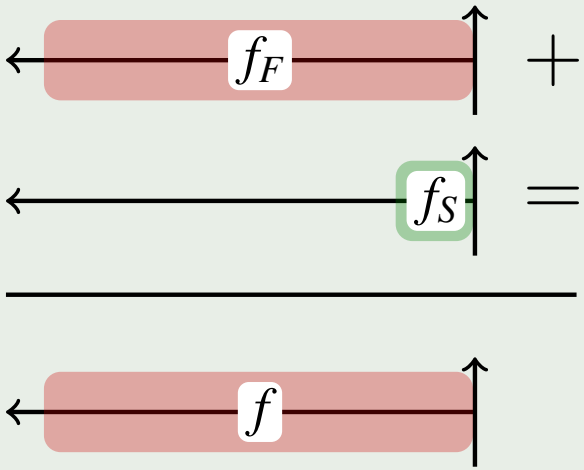

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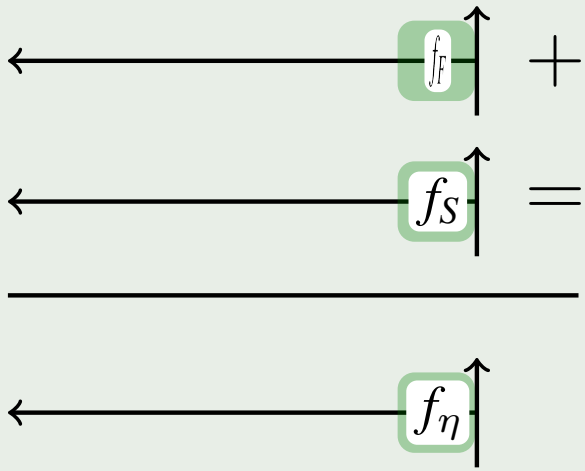


The averaged force f_η

Properties of f_η

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

The averaged force f_η

Properties of f_η

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

Definition of f_η

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

$$u' = f_F(u) + f_S(u_0), \qquad u(0) = u_0.$$

Let

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

The averaged force f_η

Properties of f_η

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

Definition of f_η

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

$$u' = f_F(u) + f_S(u_0), \qquad u(0) = u_0.$$

Let

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

Advantages:

- Evaluation cost of f_η is comparable to $f_F + f_S$, as f_S is frozen.
- Stiffness is reduced thanks to the smoothing effect of f_F.

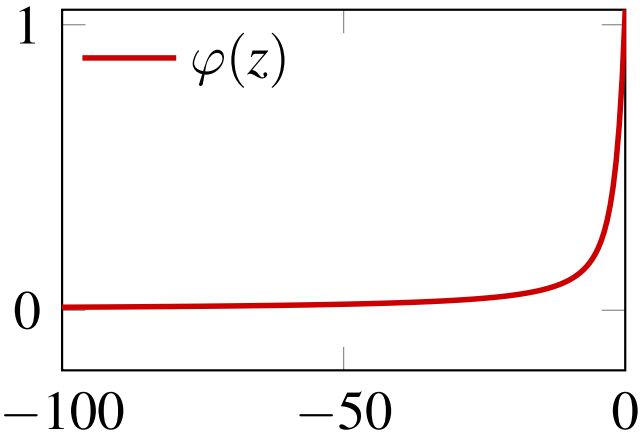
The smoothing effect

Theorem

Let $f_F(y) = A_F\, y$ with $A_F \in \mathbb{R}^{n\times n}$ negative definite. Then

$$f_\eta(y) = \varphi(\eta A_F) f(y), \qquad \text{with} \qquad \varphi(z) = \frac{e^z - 1}{z}.$$

- $A_F < 0$ and $\varphi(z) \in (0, 1)$ for $z < 0$: $\varphi(\eta A_F)$ has a smoothing effect on $f(y)$,
- $\eta \geq 0$ is a free parameter: enhances or tames the smoothing effect as needed.



Accuracy of the modified equation

Theorem

Let A_F be symmetric and such that commutes with $\partial f_S/\partial y$. Then, if f is contractive also f_η is contractive. Furthermore,

$$\|y(t) - y_\eta(t)\| \leq \max_{\lambda \in \lambda(A_F)} |1 - \varphi(\eta\lambda)| \int_0^t e^{\mu_\eta (t-s)} \|f(y(s))\| \, \mathrm{d}s,$$

with $\mu_\eta \leq 0$ and $\lambda(A_F)$ the spectrum of A_F.

- The error is bounded independently of the stiffness.
- Since $1 - \varphi(\eta\lambda) = \mathcal{O}(\eta)$ as $\eta \to 0$, then

$$\|y(t) - y_\eta(t)\| = \mathcal{O}(\eta) \qquad \text{as} \qquad \eta \to 0.$$

Stiffness of the modified equation

Let the *multirate test equation* be defined by

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

Then

$$f_\eta(y) = \varphi(\eta\lambda)(\lambda + \zeta)y.$$

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

Stiffness of the modified equation

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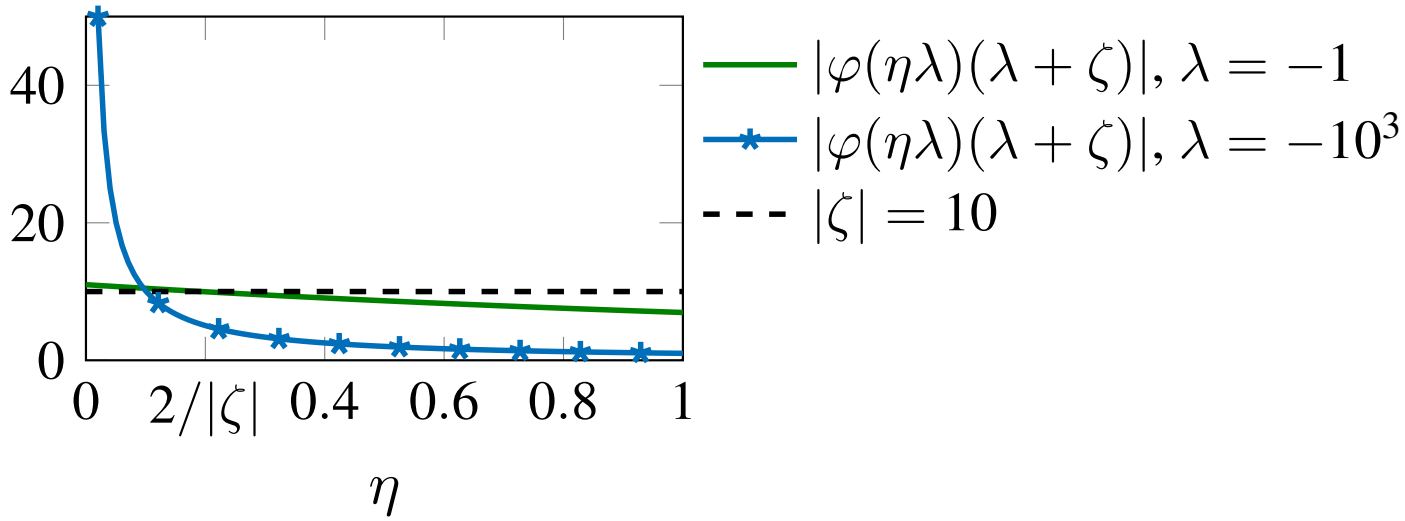

Stiffness of the modified equation

Lemma

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

- The result holds for all $\lambda \leq 0$, i.e. no scale separation is needed.
- The parameter η depends only on ζ.
- For $\eta \geq 2/|\zeta|$ the stiffness of f_η depends only on f_S.

Stiffness of the modified equation

Lemma

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- The parameter η depends only on ζ.
- For $\eta \geq 2/|\zeta|$ the stiffness of f_η depends only on f_S.

Back to the examples:

- For a parabolic equation, λ and ζ 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 $\lambda \leq 0$.
- For a chemical reaction system, λ and ζ represent the speed of different reactions or species. As $\lambda \approx \zeta$ is allowed, there's no need for a clear gap between reactions speed.

Modified multirate equation

Modified multirate equation

Solve

$$y'_\eta = f_\eta(y_\eta), \qquad y_\eta(0) = y_0$$

with

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

where u is defined by

$$u' = f_F(u) + f_S(u_0), \qquad u(0) = u_0, \qquad \eta = 2/\rho_S$$

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

Modified multirate equation

Modified multirate equation

Solve

$$y'_\eta = f_\eta(y_\eta), \qquad y_\eta(0) = y_0$$

with

Integrated numerically $\Longrightarrow$ different spectral properties

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

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$$u' = f_F(u) + f_S(u_0), \qquad u(0) = u_0, \qquad \eta = 2/\rho_S$$

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

Multirate RKC scheme

Definition of the mRKC scheme

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

$$y'_\eta = \overline{f_\eta}(y_\eta), \qquad y_\eta(0) = y_0,$$

using an s-stage RKC scheme, where $\tau\rho_S \leq 2s^2$. The right-hand side $\overline{f_\eta}$ is defined by

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

where u_η is an approximation of $u(\eta)$, solution of

$$u' = f_F(u) + f_S(u_0), \qquad u(0) = u_0, \qquad \eta = ?,$$

obtained by one step of an m-stage RKC scheme, where $\eta\rho_F \leq 2m^2$.

Stability analysis of numerical $\overline{f_\eta}$

We apply the scheme to the *multirate test equation*

$$y' = f_F(y) + f_S(y) = \lambda y + \zeta y.$$

Thus $u' = \lambda u + \zeta u_0$, which yields

$$u_\eta = (P_m(\eta\lambda) + \Phi_m(\eta\lambda)\eta\zeta)u_0, \qquad u(\eta) = (e^{\eta\lambda} + \varphi(\eta\lambda)\eta\zeta)u_0$$

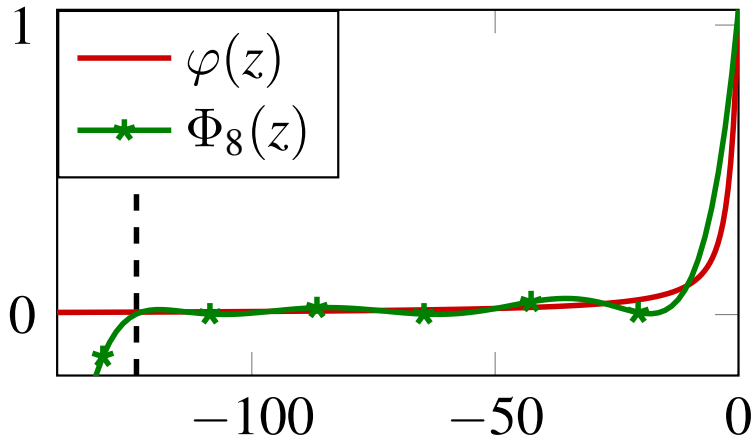
with

$$P_m(z) = a_m T_m(\upsilon_0 + \upsilon_1 z), \quad \Phi_m(z) = \frac{P_m(z) - 1}{z}. \quad \varphi(z) = \frac{e^z - 1}{z}$$

stability polynomial

Theorem

$$\overline{f_\eta}(u_0) = \Phi_m(\eta\lambda)(\lambda + \zeta)u_0.$$
$$f_\eta(u_0) = \varphi(\eta\lambda)(\lambda + \zeta)u_0$$



Stability analysis of numerical $\overline{f_\eta}$

The modified equation

$$y'_\eta = \overline{f_\eta}(y_\eta) = \Phi_m(\eta\lambda)(\lambda+\zeta)y_\eta$$

is integrated with an s-stage RKC scheme, with $\tau\rho_S \leq 2s^2$.

Goal: choose η such that $\tau\Phi_m(\eta\lambda)(\lambda+\zeta)$ fits into the stability domain of the s-stage RKC scheme, i.e. $\tau|\Phi_m(\eta\lambda)(\lambda+\zeta)| \leq 2s^2$.

Stability analysis of numerical $\overline{f_\eta}$

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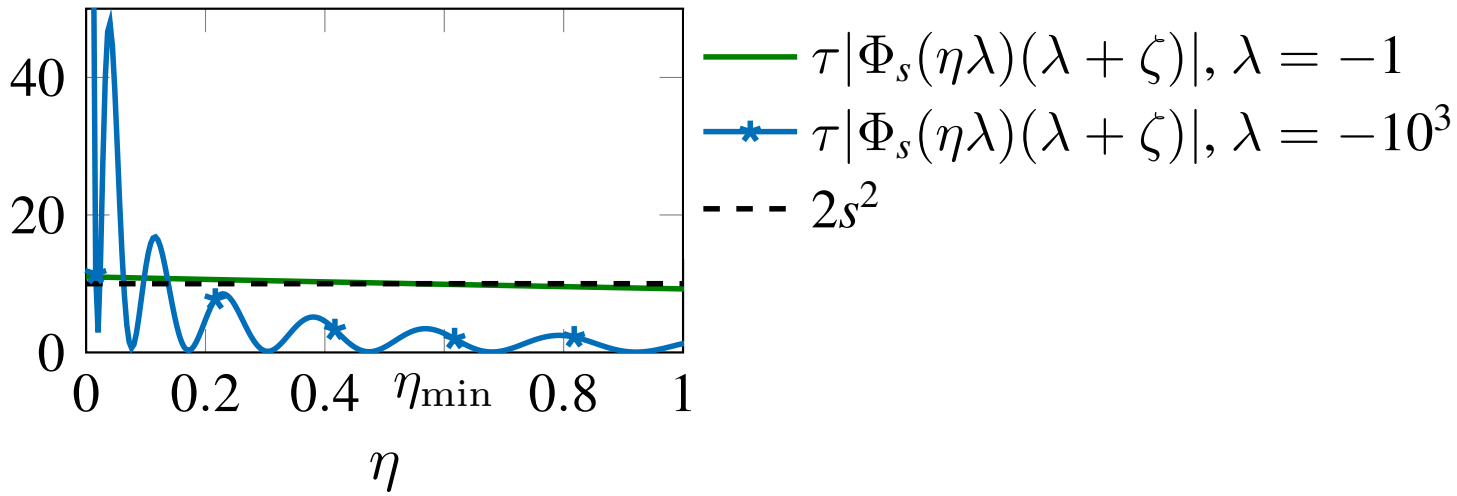


Stability analysis of numerical $\overline{f_\eta}$

Remember: s is the number of stages needed to stabilize the slow terms f_S.

Lemma

It holds $\tau|\Phi_m(\eta\lambda)(\lambda+\zeta)| \leq 2s^2$ *for* $\eta\lambda \in [-2m^2, 0]$ *if, and only if,* $\eta \geq 3\tau/s^2$.

- In practice, $\eta = 3\tau/s^2$,
- $\eta = \mathcal{O}(\tau)$.
- Usually $s > 1$, thus $\eta \ll \tau$ and the averaging error is negligible.

Multirate RKC scheme

Definition of the mRKC scheme

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

$$y'_\eta = \overline{f_\eta}(y_\eta), \qquad y_\eta(0) = y_0,$$

using an s-stage RKC scheme, where $\tau\rho_S \leq 2s^2$. The right-hand side $\overline{f_\eta}$ is defined by

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

where u_η is an approximation of $u(\eta)$, solution of

$$u' = f_F(u) + f_S(u_0), \qquad u(0) = u_0, \qquad \eta = 3\tau/s^2,$$

obtained by one step of an m-stage RKC scheme, where $\eta\rho_F \leq 2m^2$.

Theorem

The scheme is stable and is first-order accurate.

Numerical experiment: diffusion through a narrow channel

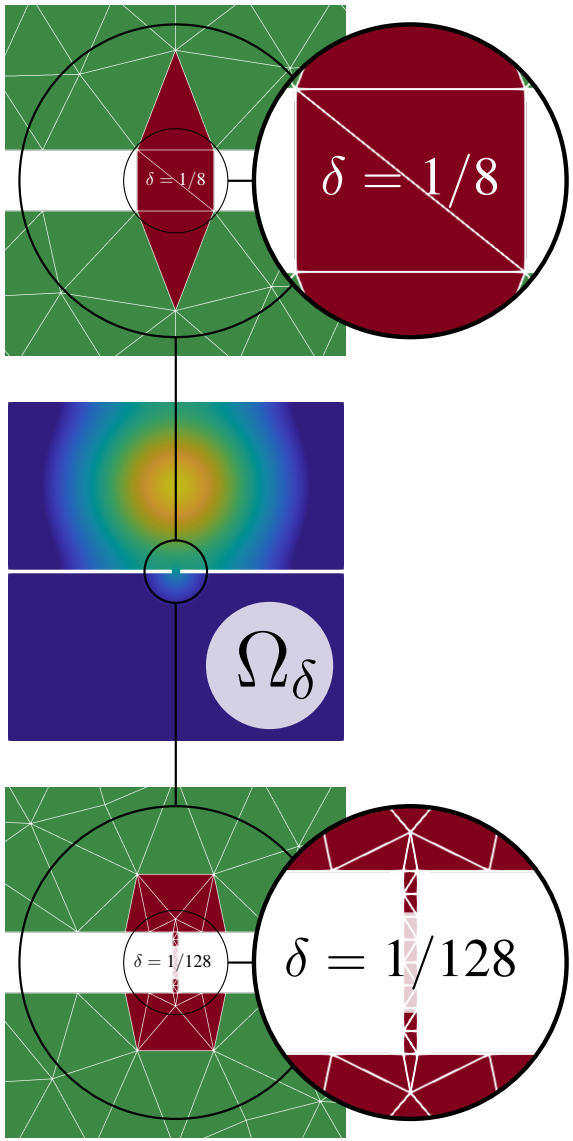
Solve

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

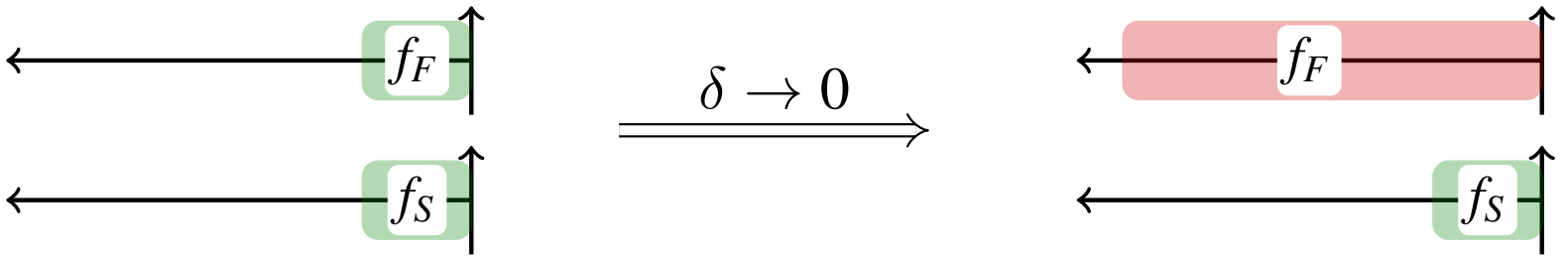
using first-order DG in space:

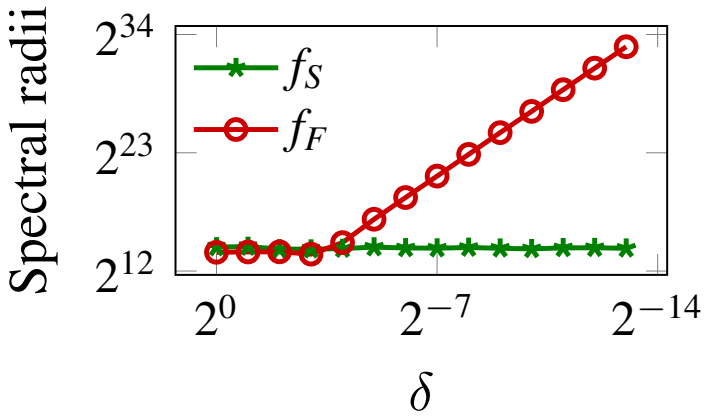
$$\begin{pmatrix} \partial_t u_h \\ \partial_t u_H \end{pmatrix} = \underbrace{\begin{pmatrix} \Delta_h u_h \\ 0 \end{pmatrix}}_{\text{Fast}} + \underbrace{\begin{pmatrix} F_h \\ \Delta_H u_H + F_H \end{pmatrix}}_{\text{Slow}}.$$

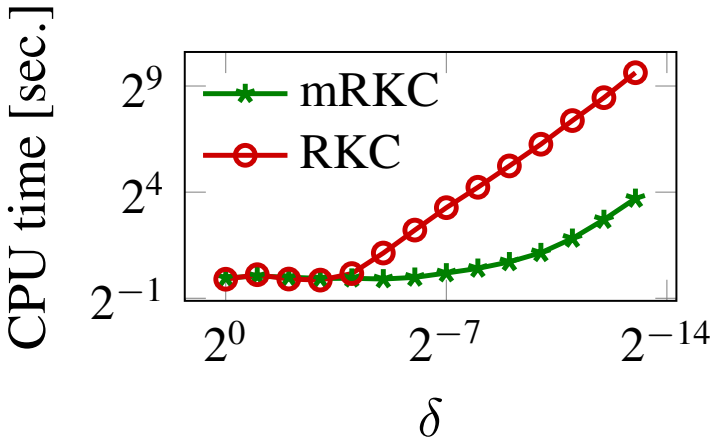
- As $\delta \to 0$ the elements in the channel get smaller.
- For varying channel width δ, compare the efficiencies of mRKC and RKC.

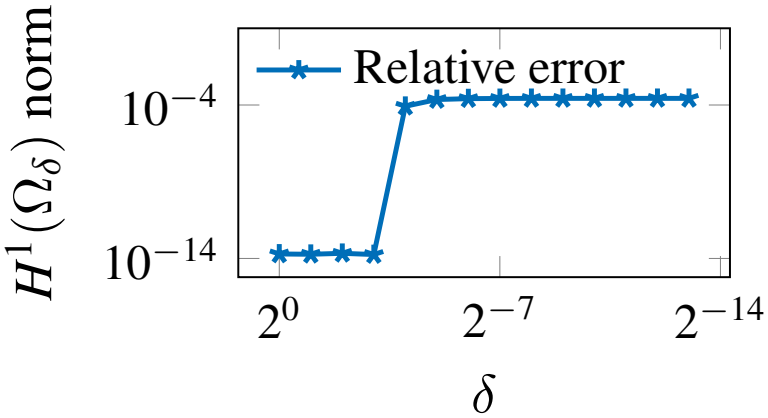


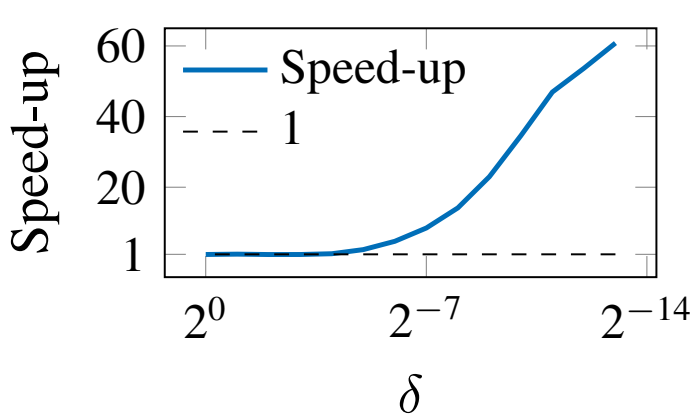
Numerical experiment: diffusion through a narrow channel











Outline

1. Stabilized explicit schemes for stiff differential equations

2. Multirate stabilized explicit schemes for *deterministic* differential equations

3. Multirate stabilized explicit schemes for *stochastic* differential equations

Problem statement

Stochastic multirate equation

Solve the SDE

$$\mathrm{d}X = f_F(X)\,\mathrm{d}t + f_S(X)\,\mathrm{d}t + g(X)\,\mathrm{d}W, \qquad X(0) = X_0,$$

with $g : \mathbb{R}^n \to \mathbb{R}^{n\times r}$ the diffusion term and $W(t)$ an r-dimensional Wiener process.

- Very scarce literature: only multiscale-like methods exist (Vanden-Eijnden, 2003; Abdulle et al., 2017), i.e. assuming scale separation.

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- Very scarce literature: only multiscale-like methods exist (Vanden-Eijnden, 2003; Abdulle et al., 2017), i.e. assuming scale separation.

Our strategy (Abdulle and Rosilho de Souza, 2020):

- Replace $f_F + f_S$ by f_η to decrease stiffness. ✓
- Replace g by a damped diffusion g_η. Why? How?
- Integrate the resulting modified equation and the auxiliary problems with stabilized explicit methods. Which ones?

Why must g be replaced by some g_η?

Consider the *stochastic multirate test equation*

$$\mathrm{d}X = (\lambda + \zeta)X\,\mathrm{d}t + \mu X\,\mathrm{d}W,$$

with $\lambda, \zeta \leq 0$, $\mu \in \mathbb{R}$.
The equation is mean-square stable if, and only if,

$$\lambda + \zeta + \frac{1}{2}\mu^2 < 0.$$

Replace $\lambda + \zeta$ by the averaged force $\varphi(\eta\lambda)(\lambda + \zeta)$, yielding

$$\mathrm{d}X_\eta = \varphi(\eta\lambda)(\lambda + \zeta)X_\eta\,\mathrm{d}t + \mu X_\eta\,\mathrm{d}W$$

and keep μ as is.
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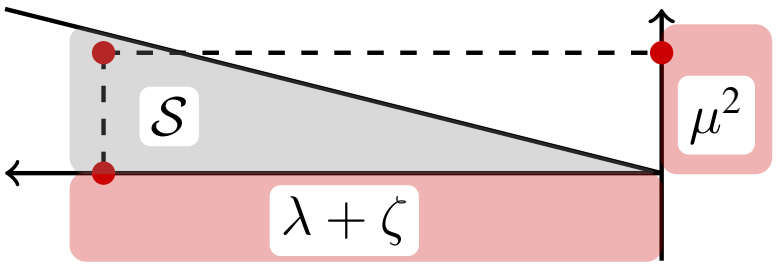

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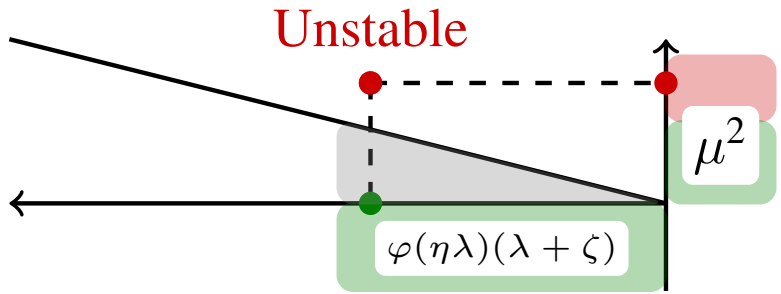

The damped diffusion g_η

Properties of g_η

- $g_\eta = g + \mathcal{O}(\eta)$.
- Modified equation inherits the mean-square stability of the original problem.

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- Modified equation inherits the mean-square stability of the original problem.

Definition of g_η

Let $v_0 \in \mathbb{R}^n$ and $v, \bar{v} : [0, \eta] \to \mathbb{R}^n$ such that

$$v' = \frac{1}{2} f_F(v) + g(v_0), \qquad \bar{v}' = \frac{1}{2} f_F(\bar{v}), \qquad v(0) = \bar{v}(0) = v_0.$$

Let

$$g_\eta(v_0) := \frac{1}{\eta}(v(\eta) - \bar{v}(\eta)) = g(v_0) + \frac{1}{2\eta} \int_0^\eta (f_F(v(s)) - f_F(\bar{v}(s)))\, \mathrm{d}s.$$

For linear $f_F(y) = A_F\, y$ then $g_\eta(y) = \varphi\left(\frac{1}{2}\eta A_F\right) g(y)$.

Stochastic modified equation and mean-square stability

Stochastic modified equation

$$\mathrm{d}X_\eta = f_\eta(X_\eta)\,\mathrm{d}t + g_\eta(X_\eta)\,\mathrm{d}W, \qquad X_\eta(0) = X_0.$$

Stochastic modified equation and mean-square stability

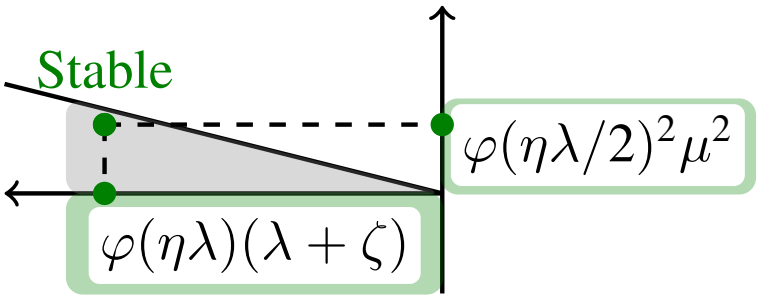
Stochastic modified equation

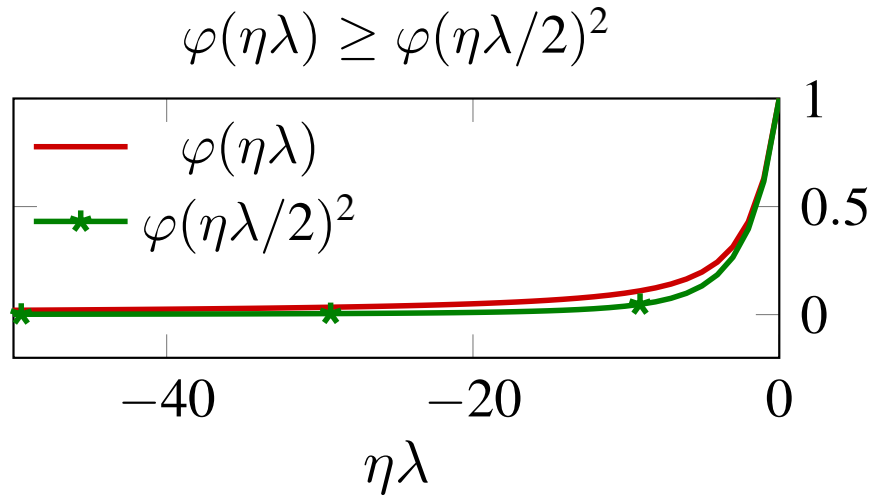
$$\mathrm{d}X_\eta = f_\eta(X_\eta)\,\mathrm{d}t + g_\eta(X_\eta)\,\mathrm{d}W, \qquad X_\eta(0) = X_0.$$

For the stochastic multirate test equation it holds

$$\mathrm{d}X_\eta = \varphi(\eta\lambda)(\lambda+\zeta)X_\eta\,\mathrm{d}t + \varphi\left(\frac{1}{2}\eta\lambda\right)\mu X_\eta\,\mathrm{d}W,$$

which is mean-square stable.





Integrating the stochastic modified equation

Stochastic modified equation

$$\mathrm{d}X_\eta = f_\eta(X_\eta)\,\mathrm{d}t + g_\eta(X_\eta)\,\mathrm{d}W, \qquad X_\eta(0) = X_0.$$

applied to the stochastic multirate test equation

$$\mathrm{d}X = (\lambda + \zeta)X\,\mathrm{d}t + \mu X\,\mathrm{d}W.$$

yields

$$\mathrm{d}X_\eta = \varphi(\eta\lambda)(\lambda + \zeta)X_\eta\,\mathrm{d}t + \varphi\left(\frac{1}{2}\eta\lambda\right)\mu X_\eta\,\mathrm{d}W,$$

which is stable due to $\varphi(z) \geq \varphi(z/2)^2$.

And numerically?

Integrating the stochastic modified equation

Stochastic modified equation

$$\mathrm{d}X_\eta = \overline{f_\eta}(X_\eta)\,\mathrm{d}t + \overline{g_\eta}(X_\eta)\,\mathrm{d}W, \qquad X_\eta(0) = X_0.$$

applied to the stochastic multirate test equation

$$\mathrm{d}X = (\lambda + \zeta)X\,\mathrm{d}t + \mu X\,\mathrm{d}W.$$

yields

$$\mathrm{d}X_\eta = \Phi_m(\eta\lambda)(\lambda + \zeta)X_\eta\,\mathrm{d}t + \Psi_r\left(\frac{1}{2}\eta\lambda\right)\mu X_\eta\,\mathrm{d}W,$$

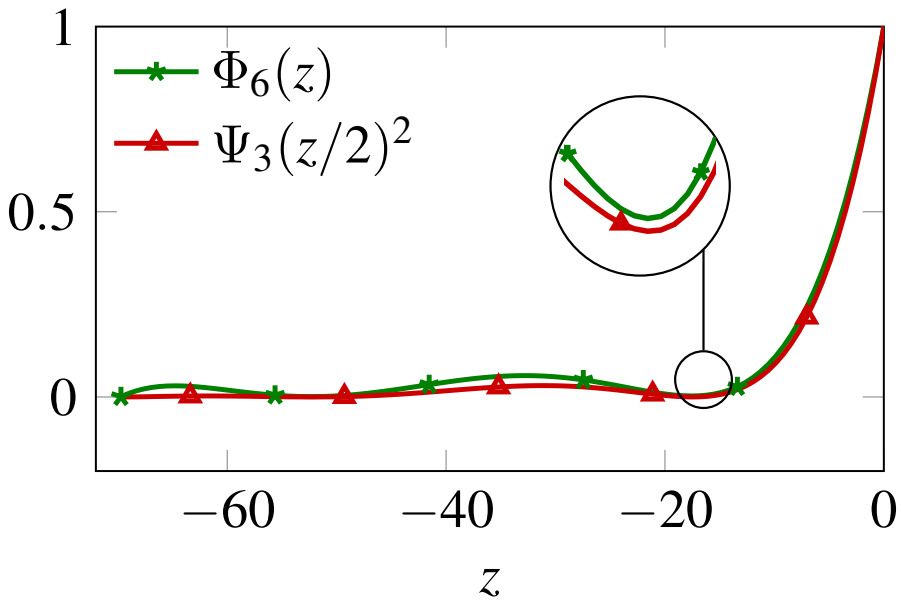
for some polynomial $\Psi_r(z)$. It would be stable if

$$\Phi_m(z) \geq \Psi_r(z/2)^2.$$

Approximation of g_η

Solution: approximate g_η with an $m/2$-stage *modified* RKC scheme.

$$\underbrace{\Phi_m(z)}_{\text{associated to RKC}} \geq \underbrace{\Psi_{m/2}(z/2)^2}_{\text{modified RKC}}.$$



Warning: employing a *standard* RKC scheme for the approximation of g_η would *not* yield in a stable equation.

Multirate SK-ROCK scheme

Definition of the mSK-ROCK scheme

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

$$\mathrm{d}X_\eta = \overline{f_\eta}(X_\eta)\,\mathrm{d}t + \overline{g_\eta}(X_\eta)\,\mathrm{d}W, \qquad X_\eta(0) = X_0$$

using an s-stage SK-ROCK scheme (Abdulle et al., 2018), where $\tau\rho_S \leq 2s^2$,

$$\overline{f_\eta}(u_0) = \tfrac{1}{\eta}(u_\eta - u_0), \qquad \overline{g_\eta}(v_0) = \tfrac{1}{\eta}(v_\eta - \overline{v_\eta})$$

and $u_\eta, v_\eta, \overline{v_\eta}$ are approximations to $u(\eta), v(\eta), \bar{v}(\eta)$ computed by RKC schemes. With η as for the mRKC scheme,

- u_η is computed with an m-stage RKC scheme, $\eta\rho_F \leq 2m^2$.
- $v_\eta, \overline{v_\eta}$ are computed with an r-stage RKC scheme, with $r = m/2$.

Theorem

The scheme is stable, has strong order $1/2$ *and weak order* 1.

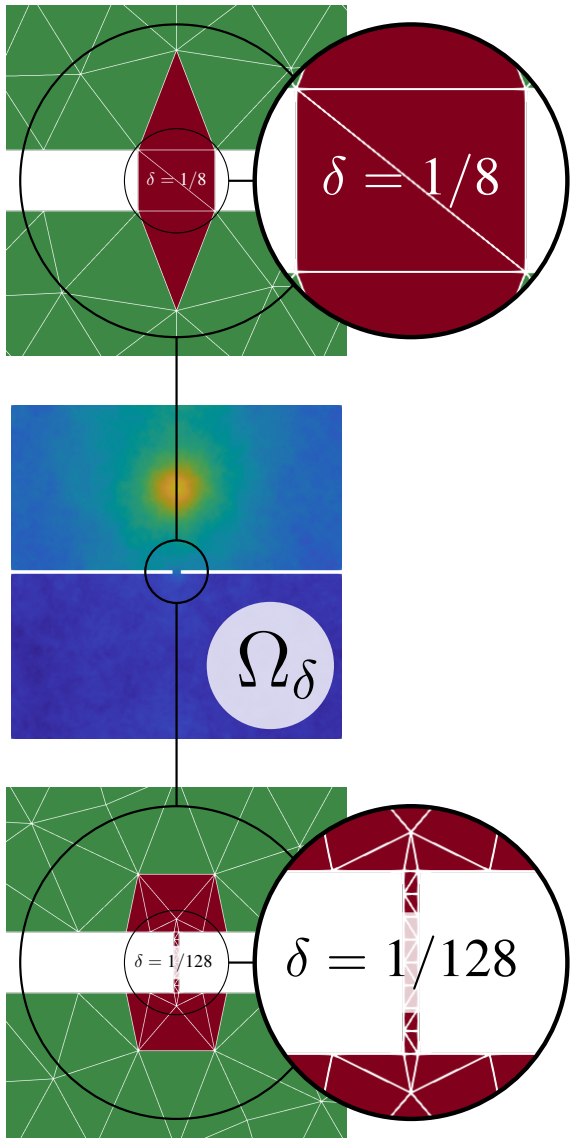
Numerical experiment: diffusion through a narrow channel

Solve the heat equation with multiplicative colored noise

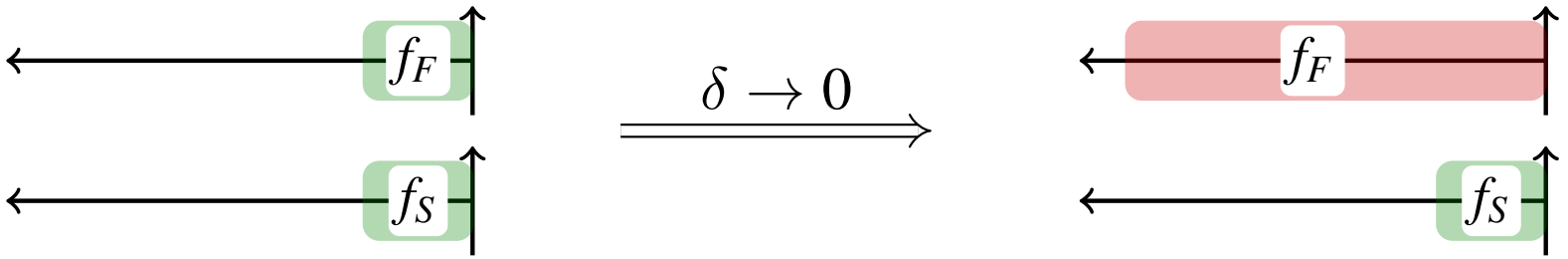
$$
\begin{aligned}
\mathrm{d}u - \Delta u \,\mathrm{d}t &= F \,\mathrm{d}t + G(u)\,\mathrm{d}W && \text{in } \Omega_\delta \times [0,T], \\
\nabla u \cdot \boldsymbol{n} &= 0 && \text{in } \partial\Omega_\delta \times [0,T], \\
u &= 0 && \text{in } \Omega_\delta \times \{0\},
\end{aligned}
$$

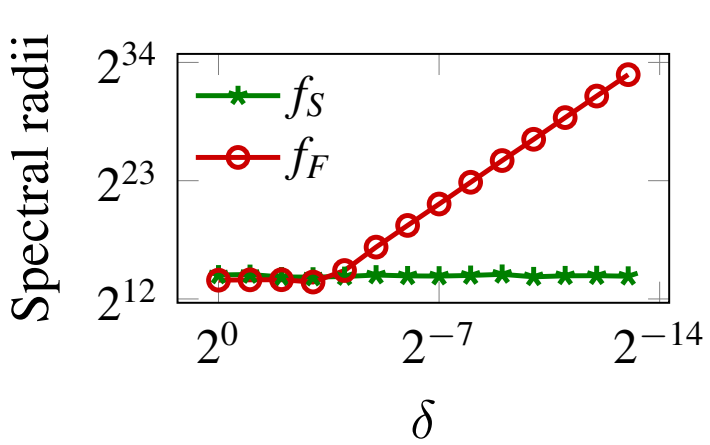
using first-order DG in space.

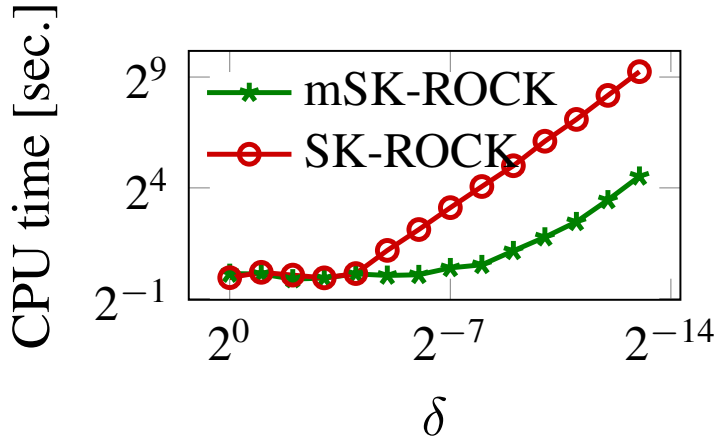
We let $\delta \to 0$ and compare the efficiency of mSK-ROCK against SK-ROCK.

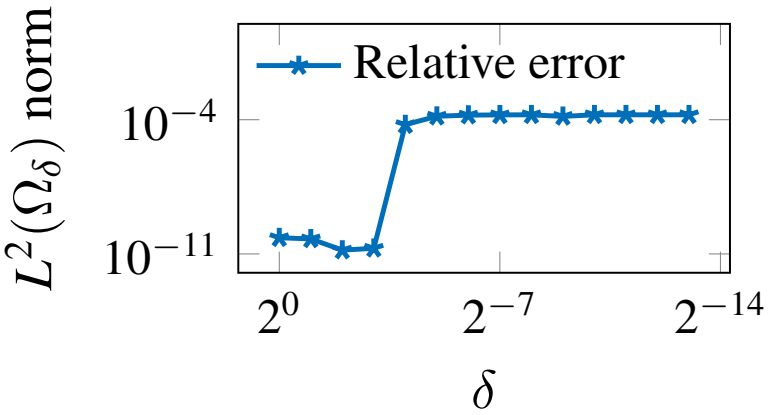


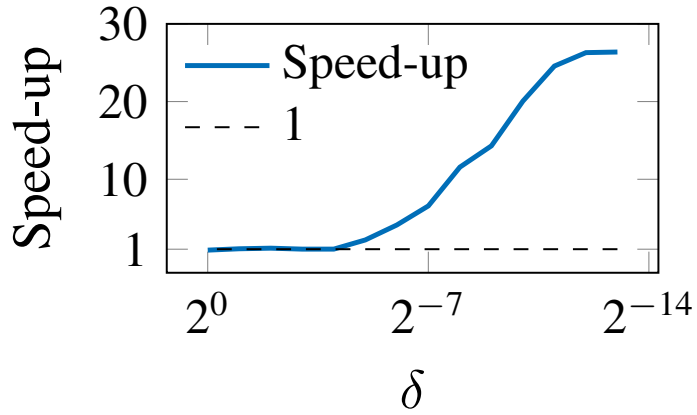
Numerical experiment











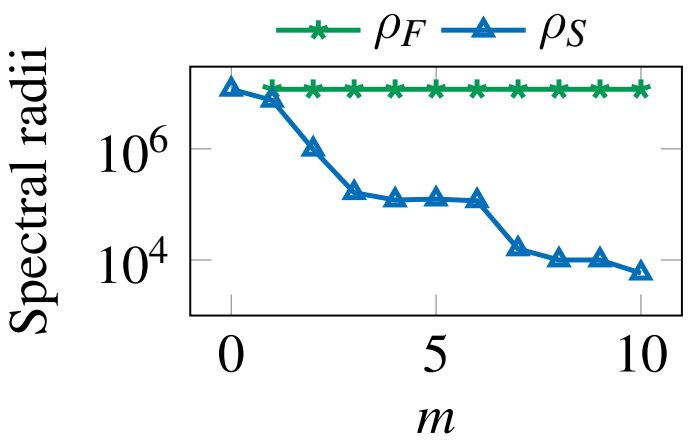
E. Coli bacteria heat shock response

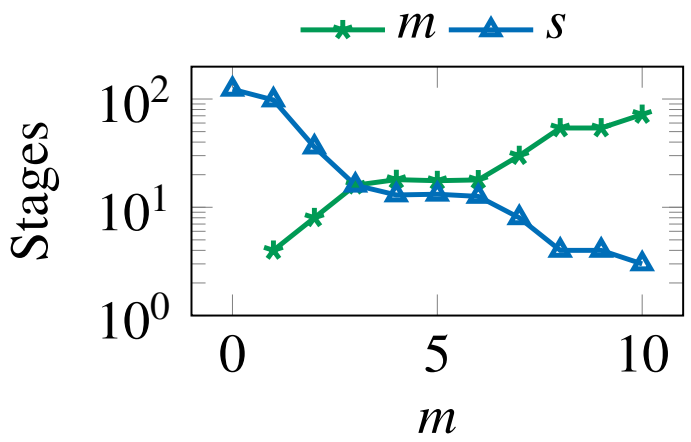
Consider a chemical Langevin equation modeling E. Coli bacteria's protein denaturation under heat shocks. The model consists in 28 species and 61 reactions.

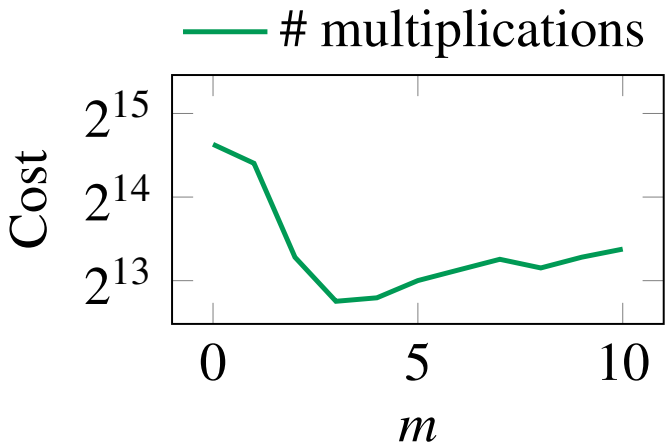
$$\mathrm{d}X = \underbrace{\sum_{j=1}^{m} \boldsymbol{\nu}_j a_j(X)\,\mathrm{d}t}_{f_F(X)} + \underbrace{\sum_{j=m+1}^{61} \boldsymbol{\nu}_j a_j(X)\,\mathrm{d}t}_{f_S(X)} + \underbrace{\sum_{j=1}^{61} \boldsymbol{\nu}_j \sqrt{a_j(X)}\,\mathrm{d}W_j(t)}_{g(X)}$$

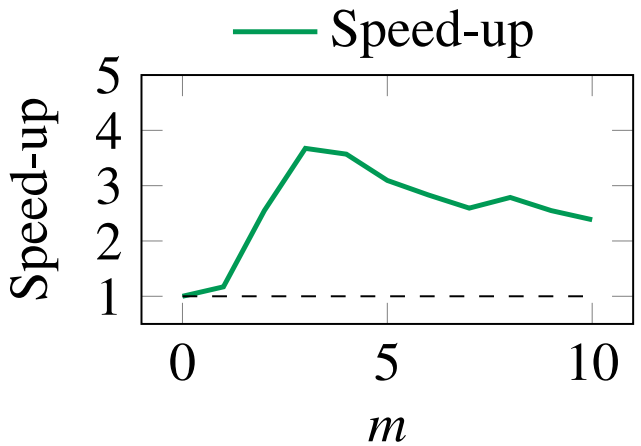
- f_F contains the m fastest reactions.
- We compare the efficiency of the scheme for different values of $m = 0, 1, \ldots, 10$.

E. Coli bacteria heat shock response









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Thank you for your attention!

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