Multirate explicit stabilized integrators for stiff differential equations

Assyr Abdulle, Marcus Grote,
Giacomo Rosilho de Souza

EPFL

École Polytechnique Fédérale de Lausanne (EPFL), SB-MATH-ANMC, Station 8, 1015 Lausanne, Switzerland

SciCADE 2019, Innsbruck

Problem statement

Multirate equation

Solve the dissipative system

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

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,
- ...

Parabolic problem on locally refined mesh

Solve

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

Space discretization gives:

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

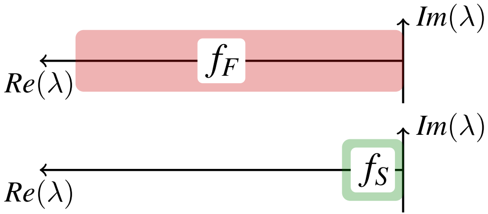
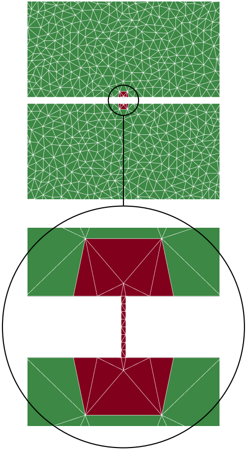


Figure. *Spectrum of* Δ_h *and* Δ_H.



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

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

~~explicit methods~~

stabilized/implicit methods

very expensive

many function evaluations

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

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

~~explicit methods~~

stabilized/implicit methods

very expensive

many function evaluations

Use multirate schemes!
Exploit special structure $f_F + f_S$

Literature review

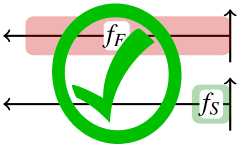
Most of existing multirate methods

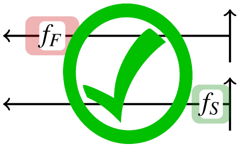
- have a spectrum clustering assumption, that is a clear partition between fast and slow variables (E, 2003),

- 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).

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

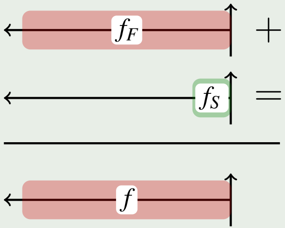
Idea

Shrink spectrum of f_F and integrate the modified system.

Original equation

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

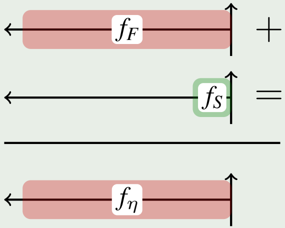
Spectral properties:



Modified equation

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

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



Modified multirate equation

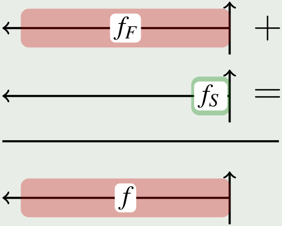
Idea

Shrink spectrum of f_F and integrate the modified system.

Original equation

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

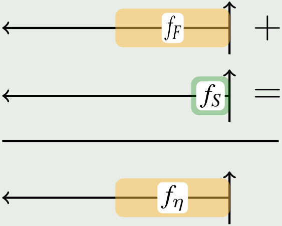
Spectral properties:



Modified equation

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

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



Modified multirate equation

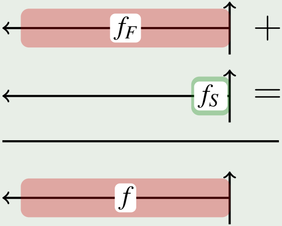
Idea

Shrink spectrum of f_F and integrate the modified system.

Original equation

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

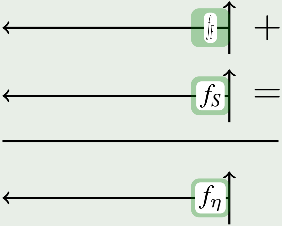
Spectral properties:



Modified equation

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

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



Motivating the definition of f_η

Properties of f_η

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

Motivating the definition of f_η

Properties of f_η

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

Towards the definition of f_η

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

$$u(0) = u_0, \qquad \text{and} \qquad u \text{ is smooth.}$$

Let

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

Motivating the definition of f_η

Properties of f_η

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

Towards the definition of f_η

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

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

Let

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

Motivating the definition of f_η

Properties of f_η

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

Towards the definition of f_η

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

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

Let

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

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.

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 $\eta \geq 2/|\xi|$.

Hence, for $\eta \geq 2/|\xi|$ the stiffness of f_η depends only on f_S!
Observe that η depends only on ξ.

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.

Runge–Kutta–Chebyshev schemes

Explicit stabilized schemes have a stability region that grows quadratically with the number of stages.

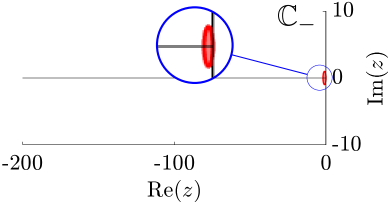
Explicit Euler

- Applied to $y' = \lambda y$ gives $y_1 = R(\tau\lambda)y_0$ with
- $R(z) = 1 + z$,
- $|R(z)| \leq 1$ for $z \in [-2, 0]$.

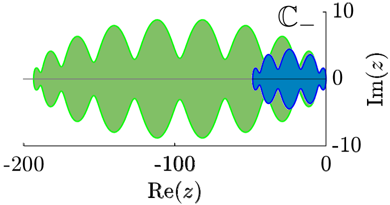
Runge–Kutta–Chebyshev (RKC)

- Applied to $y' = \lambda y$ gives $y_1 = R_s(\tau\lambda)y_0$ with
- $R_s(z) = 1 + z + \sum_{i=2}^{s} \alpha_i z^i$,
- $|R_s(z)| \leq 1$ for $z \in [-2s^2, 0]$.

Stability domain explicit Euler.



Stability domain for $s = 10$, $s = 5$.



Runge–Kutta–Chebyshev schemes

The stability polynomial $R_s(z)$ is a shifted Chebyshev polynomial of the first kind of degree s. It satisfies a recurrence relation

- $k_0 = 1, \quad k_1 = 1 + \mu_1 z,$
- $k_j = \nu_j k_{j-1} + \kappa_j k_{j-2} + \mu_j z k_{j-1}$ for $j = 2, ..., s,$
- $R_s(z) = k_s.$

From which follows the RKC scheme.

RKC scheme for $y' = f(y)$

- Let $\tau > 0$ be the time step and ρ spectral radius of $\partial f / \partial y$.
- Let $s \in \mathbb{N}$ such that $\tau\rho \leq 2s^2$. (stability condition)
- $k_0 = y_0, \quad k_1 = k_0 + \mu_1 \tau f(k_0),$
- $k_j = \nu_j k_{j-1} + \kappa_j k_{j-2} + \mu_j \tau f(k_{j-1})$ for $j = 2, ..., s,$
- $y_1 = k_s.$

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.

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 $\tau\overline{\rho}_\eta \leq 2m^2$.
The right hand side $\bar{f}_\eta$ is defined by

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

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

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

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 chosen such that $\eta|\lambda| \leq 2s^2$. We obtain (shown by recursion)

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

with

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

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. Then,

$$\bar{f}_\eta(u_0) = \frac{1}{\eta}(\bar{u}_\eta - u_0) = \frac{1}{\eta}(R_s(\eta\lambda) + \Phi_s(\eta\lambda)\eta\xi - 1)u_0$$

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 chosen such that $\eta|\lambda| \leq 2s^2$. We obtain (shown by recursion)

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

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. Then,

$$\bar{f}_\eta(u_0) = \frac{1}{\eta}(\bar{u}_\eta - u_0) = \frac{1}{\eta}(R_s(\eta\lambda) + \Phi_s(\eta\lambda)\eta\xi - 1)u_0$$

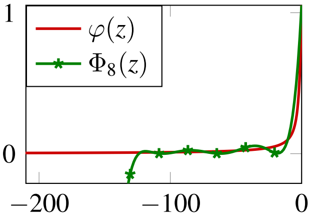
$$f_\eta(u_0) = \varphi(\eta\lambda)(\lambda + \xi)u_0$$

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

Lemma

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

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



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 $|\Phi_s(\eta\lambda)(\lambda + \xi)| \leq |\xi|$.

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 $\eta \geq 2/|\xi|$)

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

$$u' = f_F(u) + f_S(u_0),\ t \in]0,\eta] \qquad u(0) = u_0, \quad \eta = 6/\rho_S,$$

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

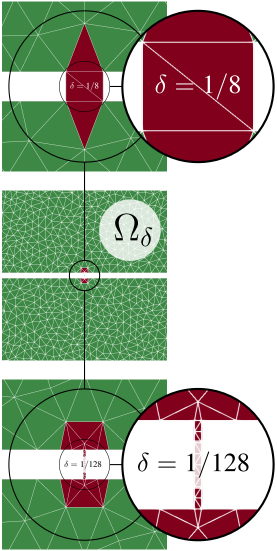
Solve

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

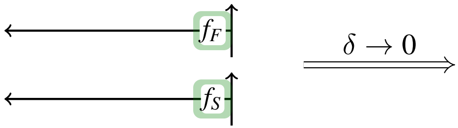
- first order DG in space,
- RKC^2 and RKC in time.

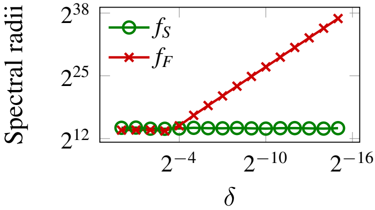
We let $\delta \to 0$ and compare the performance of RKC^2 against the one of standard RKC.

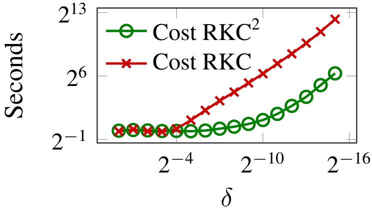
$$\begin{pmatrix} \partial_t u_h \\ \partial_t u_H \end{pmatrix} = \underbrace{\begin{pmatrix} \Delta_h u_h \\ 0 \end{pmatrix}}_{\text{Fast}} + \underbrace{\begin{pmatrix} f_h \\ \Delta_H u_H + f_H \end{pmatrix}}_{\text{Slow}}$$

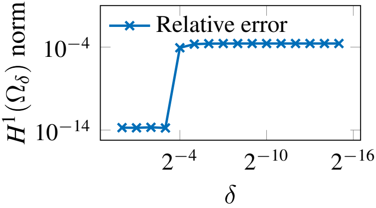


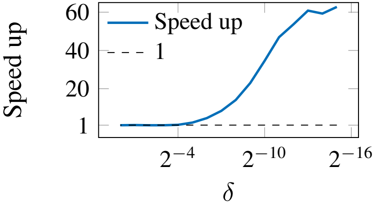
Numerical experiment











Future work

Natural directions to follow:

- When $f_F(y) = Ay$, replace "inner" RKC scheme by exponential Euler.
  - Gives same stability as continuous modified equation,
  - computation of $e^{\eta A}$ is faster than $e^{\tau A}$ since $\eta \ll \tau$.
- Generalize to

$$\mathrm{d}X(t) = f_F(X(t))\,\mathrm{d}t + f_S(X(t))\,\mathrm{d}t + \sum_{r=1}^{m} g_r(X(t))\,\mathrm{d}W_r(t)$$

replacing by

$$\mathrm{d}X_\eta(t) = f_\eta(X(t))\,\mathrm{d}t + ???$$

Thank you for your attention!

Abdulle, A., Grote, M. J., and Rosilho de Souza, G. (2019). Multirate explicit stabilized integrators for stiff differential equations. *Manuscript*.

E, W. (2003). Analysis of the heterogeneous multiscale method for ordinary differential equations. *Commun. Math. Sci.*, 1(3):423–436.

Ewing, R. E., Lazarov, R. D., and Vassilevski, P. S. (1990). Finite difference schemes on grids with local refinement in time and space for parabolic problems I. Derivation, stability, and error analysis. *Computing*, 45(3):193–215.

Gear, C. W. and Wells, D. R. (1984). Multirate linear multistep methods. *Bit*, 24(4):484–502.