Second order explicit stabilized multirate method for stiff differential equations with error control

Mathieu Benninghoff

UNIVERSITÉ DE GENÈVE
FACULTÉ DES SCIENCES
Section de mathématiques

Based on joint work with Gilles Vilmart (University of Geneva)

Plan of the talk

Main Objective

Construct a **second-order** explicit stabilized multirate method for stiff differential equations.

Reference: M. B. and G. Vilmart, "Second order explicit stabilized multirate method for stiff differential equations with error control," submitted for publication (2025).

1. **Explicit Stabilized Methods:** Review of the Chebyshev methods [van der Houwen and Sommeijer, '80s] and ROCK2 schemes [Abdulle and Medovikov, 2002] for stiff ordinary differential equations.
2. **Local Stiffness & Multirate Integration:** Severe localized stiffness from spatial discretizations of PDEs is addressed via fast-slow system splitting, such as the first-order mRKC method [Abdulle, R. De Souza and Grote 2022].
3. **The New Second-Order Multirate Scheme:** New explicit stabilized **mROCK2** method, achieving second-order accuracy via a modified averaged force.

Explicit Stabilized methods for stiff problems

Diffusion PDE after spatial discretization

$$\dot{y}(t) = Ay(t) + g(y(t), t)$$

1. A has very large negative eigenvalues (**stiff system**)!
2. A is an $N \times N$ matrix, with $N \gg 1$.

- **Standard Explicit Methods:** Cheap per step, but suffer from **severe step-size restrictions** (for Euler explicit: $\tau < \frac{2}{\rho(A)}$).
- **Implicit Methods:** A-stable, but solving large linear systems at each step may incur **prohibitive computational and memory costs**.

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Efficient approach: Explicit Stabilized Methods

By using multiple stages, these methods quadratically increase the maximum allowed time step ($\tau < C \cdot s^2$), providing a fully explicit and efficient way to integrate stiff problems.

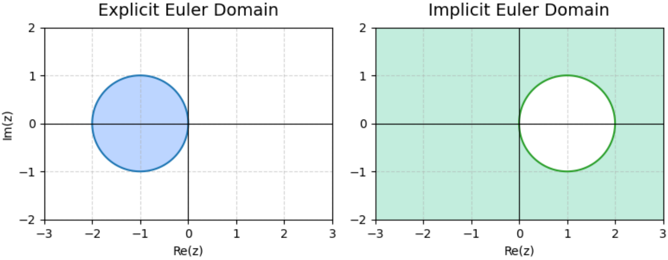
Explicit Stabilized (Chebyshev) Methods

The Stability Function

For Dahlquist's test equation $\dot{y} = \lambda y$ ($\lambda < 0$), a Runge-Kutta method with step-size τ yields:

$$y_{n+1} = R(\tau\lambda)y_n \implies y_n = [R(\tau\lambda)]^n y_0$$

Bounded solution if the stability function $R(z)$ satisfies $|R(z)| \leq 1$ for $z = \tau\lambda$. The stability domain is $\mathcal{S} := \{z \in \mathbb{C} \mid |R(z)| \leq 1\}$.



Stability domains for explicit Euler ($R(z) = 1 + z$) and implicit Euler ($R(z) = \frac{1}{1-z}$).

Explicit stabilized methods: first-order Chebyshev methods

For fixed integer s, and a first order stability function of degree at most s of the form

$$R_s(z) = 1 + z + a_2 z^2 + \cdots + a_s z^s,$$

find the coefficients $a_2, a_3, \ldots, a_s$ that maximize ℓ_s where $\ell_s := \sup l \geq 0$ such that $(-l, 0) \subset \mathcal{S} = \{z \in \mathbb{C} \mid |R(z)| \leq 1\}$.

Theorem (Markoff, 1892; ... Guillou, Lago, 1960)

For fixed integer s, the optimal solution that maximizes ℓ_s is unique and given by

$$R_s(z) = T_s\left(1 + \frac{z}{s^2}\right)$$

where $T_s(\cos x) = \cos(sx)$ are the Chebyshev polynomials.

It satisfies $|R_s(z)| \leq 1$ for all real $z \in (-\ell_s, 0)$, with:

$$\ell_s = 2s^2.$$

First-order Chebyshev methods

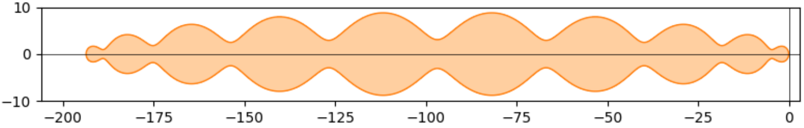
An s-stage Runge-Kutta method $y_0 \mapsto y_1$ implemented for the equation $\dot{y}(t) = f(y(t))$ using the Chebyshev recurrence relation $T_j(x) = 2xT_{j-1}(x) - T_{j-2}(x)$, $j \geq 2$ (v. der Houwen and Sommeijer, '80s):

$$\begin{aligned} K_0 &= y_0, \\ K_1 &= y_0 + \mu_1 hf(y_0), \\ K_i &= \mu_i hf(K_{i-1}) + \nu_i K_{i-1} + \kappa_i K_{i-2}, \quad i = 2, \dots, s, \\ y_1 &= K_s. \end{aligned}$$

Stability function:

$$R_s(z) = \frac{T_s(\omega_0 + \omega_1 z)}{T_s(\omega_0)} \qquad \text{where} \qquad \omega_0 = 1 + \frac{\varepsilon}{s^2}, \quad \omega_1 = \frac{T_s(\omega_0)}{T_s'(\omega_0)}.$$

It satisfies $|R_s(z)| \leq 1$ for all $z \in (-L_s, 0)$, with $L_s \approx (2 - \frac{4}{3}\varepsilon)s^2$.



Second-order explicit stabilized method: ROCK2 method

For a second-order stability function of degree at most s of the form

$$R_s(z) = 1 + z + \frac{1}{2}z^2 + a_3 z^3 + \cdots + a_s z^s,$$

find the coefficients $a_3, a_4, \ldots, a_s$ that maximize ℓ_s where $\ell_s := \sup l \geq 0$ such that $(-l, 0) \subset \mathcal{S}$.

ROCK2 method (Abdulle and Medovikov, 2002)

For a given number of stages s, the method provides second-order accuracy. It constructs a stability polynomial that converges to the optimal real stability interval using a three-term recurrence relation of orthogonal polynomials.
It satisfies stability $|R_s(z)| \leq 1$ for all real $z \in (-\ell_s, 0)$, with approximately:

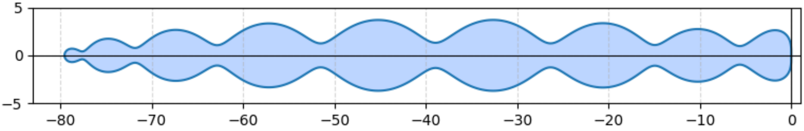
$$\ell_s \simeq 0.81 \cdot s^2.$$

ROCK2 method (Abdulle and Medovikov, 2002)

An s-stage ROCK2 $y_0 \mapsto y_1$ method is given by:

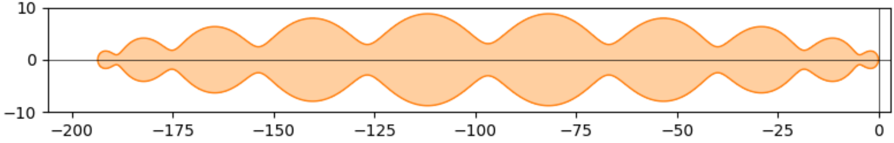
$$
\begin{aligned}
k_0 &= y_0 \\
k_1 &= k_0 + h\mu_1 f(k_0) \\
k_j &= h\mu_j f(k_{j-1}) - \nu_j k_{j-1} - \kappa_j k_{j-2}, \quad j = 2, \dots, s-2 \\
k_{s-1} &= k_{s-2} + h\sigma_1 f(k_{s-2}) \\
k_s^\star &= k_{s-1} + h\sigma_1 f(k_{s-1}) \\
k_s &= k_s^\star - h\sigma_1 (1 - \tfrac{\sigma_1}{\sigma_2^2})(f(k_{s-1}) - f(k_{s-2})),
\end{aligned}
$$

The stability function is $R_s(z) = \omega_2(z) P_{s-2}(z)$. Here, $\omega_2(z) = 1 + \sigma_1 z + \sigma_2 z^2$ is a polynomial chosen to guarantee the second-order convergence and P_{s-2} the orthogonal polynomial to construct the stability domain (with coefficients μ_i, ν_i and κ_i)

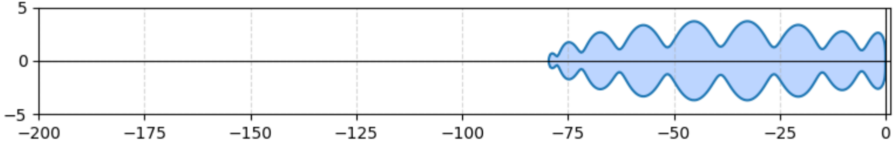


Stability comparison of the two methods

Case: $s = 10$, first-order Chebyshev method



Case: $s = 10$, ROCK2 method

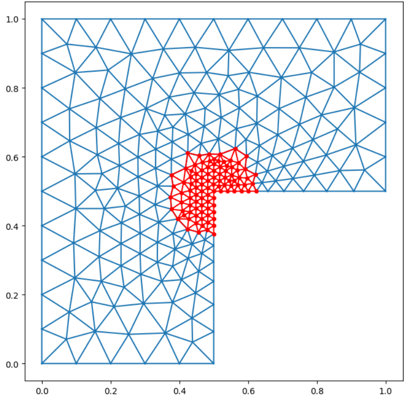


Applications of explicit stabilized methods

Explicit stabilized methods are highly efficient for very large systems of ODEs!

- **Simulations of the solar system:** Q. M. Wargnier, G. Vilmart, J. Martínez-Sykora, V. H. Hansteen, and B. De Pontieu, *Time-adaptive PIROCK method*, Astron. Astrophys. (2025), in collaboration with NASA.
- **Cardiology:** G. Rosilho de Souza, S. Pezzuto, and R. Krause, *High-order parallel-in-time method for the monodomain equation in cardiac electrophysiology*, arXiv preprint (2024).
- **Metal 3D Printing:** S. Essongue, B. Diarra, and E. Lacoste, *Runge-Kutta-Chebyshev Schemes to Accelerate Thermal Modelling of Additive Manufacturing Processes* (2025).
- etc...

Motivation: Stiff PDEs and Local Refinement



When solving PDEs (like the heat equation) with Finite Elements, local mesh refinement is highly efficient for singularities but creates **severe, localized stiffness**.

$$\frac{dy(t)}{dt} = \underbrace{A_F y(t)}_{f_F} + \underbrace{A_S y(t) + G(t)}_{f_S}.$$

- Coarse mesh: $\rho(A_S) = 10000$
- Fine mesh: $\rho(A_F) = 500000$

Multiscale Problem & mRKC Method

The Fast-Slow Splitting

We partition our stiff system into two distinct scales:

$$\dot{y}(t) = \underbrace{f_F(y)}_{\text{Fast/Stiff}} + \underbrace{f_S(y)}_{\text{Slow/Mild}}$$

- f_F **(Fast):** Severely stiff, but cheap to compute (e.g., highly localized).
- f_S **(Slow):** Mildly stiff, but expensive to compute (e.g., global domain).

2. The Multirate Solution: mRKC (Abdulle, de Souza, Grote, 2022)
mRKC solves the problem by splitting the work:

- **Micro-steps:** Takes many small steps of f_F to stabilize.
- **Macro-steps:** Evaluates f_S as few times as possible per large step.
- **Mechanism:** Uses an averaged vector field $f_{\eta,1}(y) = \frac{1}{\eta}(u(\eta) - y)$.

Only drawback: mRKC is only **first-order accurate**.

mRKC (Abdulle, de Souza, Grote, 2022)

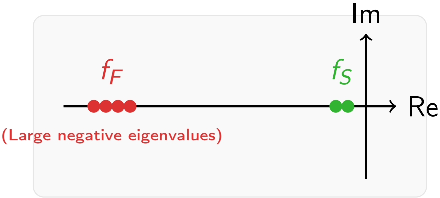
1. The Modified Equation & Averaged Force To isolate the severe stiffness, we freeze the slow dynamics and solve a **micro-problem** over a small window η:

$$\dot{u}(t) = \underbrace{f_F(u(t))}_{\text{Evolve fast}} + \underbrace{f_S(y)}_{\text{Freeze slow}}, \quad u(0) = y_0, \quad t \in [0, \eta]$$

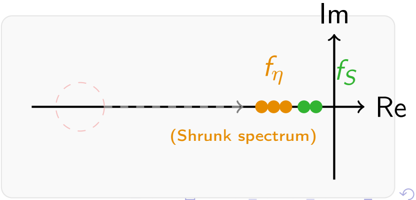
The **first-order averaged force** is defined as the effective finite difference:

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

1. Original Stiff System



2. Modified System



mRKC (Abdulle, de Souza, Grote, 2022)

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The **first-order averaged force** is defined as the effective finite difference:

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

2. The mRKC Method

Instead of solving the original differential equation $\dot{y} = f(y)$, the mRKC method applies RKC scheme to the **modified system**:

$$\dot{y}_{\eta,1} = f_{\eta,1}(y_{\eta,1})$$

and for the micro-problem $\dot{u}(t) = f_F(u(t)) + f_S(y)$ with a time step η This allows the method to bypass fine-mesh restrictions and take massive **macro-steps** $\tau \gg \eta$.

Constructing a Second-Order Averaged Force

In the mRKC method, Taylor expansion of the modified equation reveals:

$$f_{\eta,1}(y_0) = f(y_0) + \frac{\eta}{2} f_F'(y_0) f(y_0) + \mathcal{O}(\eta^2)$$

Because the modified force $f_{\eta,1}$ only matches the true force $f(y)$ up to $\mathcal{O}(\eta)$, the overall method is restricted to first-order accuracy.

New modified averaged force for high-order multirate method

We introduce a newly modified averaged force $f_{\eta,2}$ which satisfies:

$$f_{\eta,2}(y) = f(y) + \mathcal{O}(\eta^2)$$

This allows the macro-step integrator to achieve genuine second-order accuracy.

mROCK2: The New Averaged Force (B., Vilmart, 2025)

Definition of the Second-Order Averaged Force

Introduce the modified differential equation $\dot{y}_{\eta,2} = f_{\eta,2}(y_{\eta,2})$ where:

$$f_{\eta,2}(y) = \frac{1}{\eta}(v(\eta) - y)$$

and $v(t)$ is the solution to the modified micro-problem:

$$\dot{v} = f_F\left(v - \frac{\eta}{2} f_{\eta,1}(y)\right) + f_S(y), \quad v(0) = y.$$

(Here, $f_{\eta,1}(y)$ is the classical first-order averaged force from mRKC).

By shifting the evaluation of the fast field f_F, we cancel the first-order error term entirely.

Second-order mROCK2 multirate algorithm (B., Vilmart, 2025)

Micro-macro method combining RKC and ROCK2

1. Micro-step (New Averaged Force): Compute averaged force using two steps of RKC.

function AVERAGED_FORCE$(t, y, \eta, f_F, f_S, m)$
    $f_u(u) \leftarrow f_F(u) + f_S(y)$ ▷ Freeze slow dynamics
    $u_\eta \leftarrow \text{RKC}(t, y, \eta, f_u, m, \epsilon)$ ▷ First RKC step
    $\overline{f}_{\eta,1} \leftarrow \frac{1}{\eta}(u_\eta - y)$ ▷ Classical averaged force
    $f_v(v) \leftarrow f_F(v - \frac{\alpha_m \eta}{2}\overline{f}_{\eta,1}) + f_S(y)$ ▷ Modified fast field
    $v_\eta \leftarrow \text{RKC}(t, y, \eta, f_v, m, \epsilon)$ ▷ Second RKC step
    return $\overline{f}_{\eta,2} = \frac{1}{\eta}(v_\eta - y)$ ▷ New second-order averaged force
end function

2. Macro-step: Advance y_n using ROCK2 with the new averaged force.

function MROCK2_STEP$(t_n, y_n, \tau, f_F, f_S, \rho_F, \rho_S)$
    $s, m, \eta \leftarrow \text{Get\_Stages}(\tau, \rho_S, \rho_F, \epsilon)$ ▷ Optimal parameters
    $\overline{f}_{\eta,2}(t, y) \leftarrow \text{Averaged\_Force}(t, y, \eta, f_F, f_S, m)$
    $y_{n+1} \leftarrow \text{ROCK2}(t_n, y_n, \tau, \overline{f}_{\eta,2}, s)$ ▷ Macro-step with ROCK2
    return y_{n+1}
end function

Theoretical Properties of mROCK2

Theorem (Stability of mROCK2, B. & Vilmart, 2025)

Let $\lambda \leq 0$ and $\zeta < 0$ for the multirate linear test equation:

$$\dot{y}(t) = \lambda y(t) + \zeta y(t).$$

We define $\alpha_m = P_m''(0)$ (the second derivative of the RKC stability function at the origin), β_s the stability coefficient of the ROCK2 method. Then, for all $\tau > 0, s, m$ and η such that

$$(1+\alpha_m)\tau|\zeta| \leq \tilde{\beta}_s s^2, \qquad \eta|\lambda| \leq 1.92 m^2 \qquad \textit{with} \qquad \eta \geq \frac{2\tau(1+\alpha_m)}{\alpha_m \tilde{\beta}_s s^2},$$

$|R_{s,m}(\lambda, \zeta, \tau, \eta)| \leq 1$, i.e. the mROCK2 scheme is stable.

Theorem (Accuracy, B. & Vilmart, 2025)

The mROCK2 scheme is second-order accurate.

Comparison of RKC, mRKC, ROCK2, mROCK2

Method	Order	$\#f_S$	$\#f_F$	ℓ_s	ℓ_m
RKC (1960s)	1	m	m	$\approx 2m^2$	$\approx 2m^2$
ROCK2 (Abdulle & Medovikov 2001)	2	m	m	$\approx 0.81m^2$	$\approx 0.81m^2$
mRKC (Abdulle, R. De Souza and Grote 2022)	1	s	ms	$\approx 2s^2$	$\approx 0.66s^2m^2$
New mROCK2 (B., Vilmart 2025)	2	s	$2ms$	$\approx 0.6s^2$	$\approx 0.27s^2m^2$

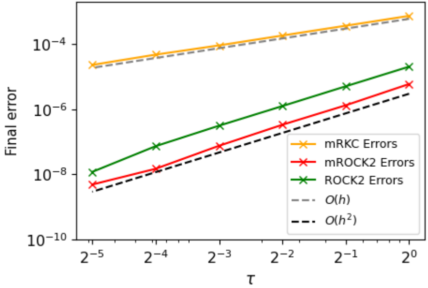
Table: Number of function evaluations per time step and stability domain sizes.

Numerical Results: Robertson's stiff non-linear problem

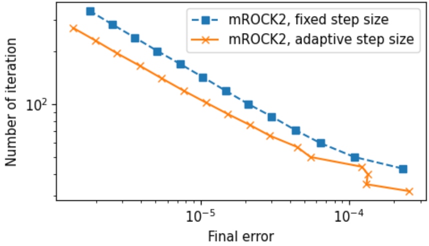
We consider Robertson's non-linear chemical reaction model ($t \in [0, 100]$):

$$y_1' = -0.04 y_1 + 10^4 y_2 y_3,$$
$$y_2' = 0.04 y_1 - 10^4 y_2 y_3 - 3 \cdot 10^7 y_2^2,$$
$$y_3' = 3 \cdot 10^7 y_2^2.$$

Initial conditions: $y(0) = (1,\ 2 \cdot 10^{-5},\ 10^{-1})^T$.

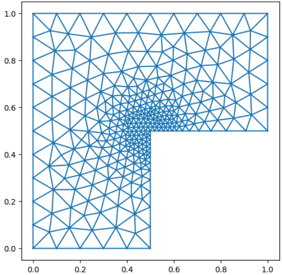


(a) Convergence: mROCK2 successfully achieves $\mathcal{O}(\tau^2)$.

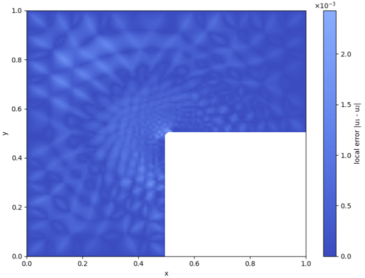


(b) Efficiency: Error vs. Function Evaluations. Adaptive mROCK2 wins.

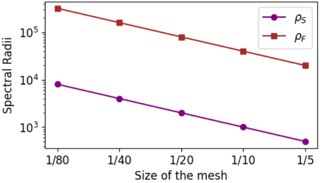
Efficiency of mROCK2 on the L-shape problem



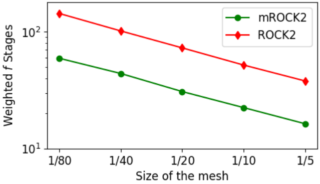
The refined mesh



The precision of the solution



Spectral radius of A_F and A_S vs refinement.



Theoretical stages: mROCK2 vs ROCK2 ($\#f = 0.95\#f_S + 0.05\#f_F$).

Conclusion and Future Work

Summary

- Developed **mROCK2**, a second-order explicit stabilized multirate method.
- Constructed a novel averaged force $\overline{f}_{\eta,2}$ that eliminates the first-order error constraint.
- Proved stability bounds and second-order convergence.

Ongoing & Future Work

- Adapting mROCK2 to large-scale, high-dimensional stochastich S(P)DE's .
- Developing explicit stabilized preconditioning techniques for invariant measure sampling (joint work with G. Vilmart and A. Busnot Laurent).

Thank you for your attention!