

Low-rank Parareal: a low-rank parallel-in-time integrator

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Joint work with Martin J. Gander and Bart Vandereycken



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Schedule

- 1 Setup and motivation
- 2 Dynamical low-rank approximation
 - Definition and theory
 - Numerical integration
- 3 Low-rank Parareal
 - Description of the algorithm
 - Theoretical analysis
 - Numerical experiments
- 4 Conclusion



Matrix differential equations

$$\begin{aligned}\dot{X}(t) &= F(t, X(t)) \quad t \in [0, T] \\ X(0) &= X_0 \in \mathbb{R}^{m \times n}\end{aligned}$$

Examples

Lyapunov: $\dot{X}(t) = AX(t) + X(t)A^T + C,$

Sylvester: $\dot{X}(t) = AX(t) + X(t)B^T + C,$

Riccati: $\dot{X}(t) = AX(t) + X(t)A^T - X(t)BX(t) + C$

Suppose the solution has a good low-rank approximation:

$$X(t) \approx Y(t) \in \mathcal{M}_r = \{A \in \mathbb{R}^{m \times n} \mid \text{rank}(A) = r\}, \quad \text{for all } t \in [0, T].$$

Goal: for every t , find $Y(t) \in \mathcal{M}_r$ such that $\|X(t) - Y(t)\| \stackrel{!}{=} \min.$



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Low-rank approximation

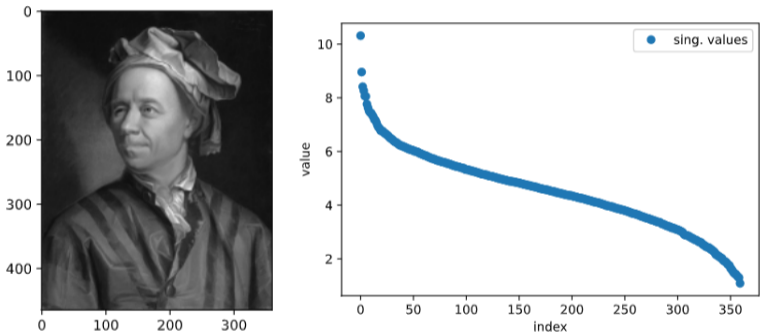
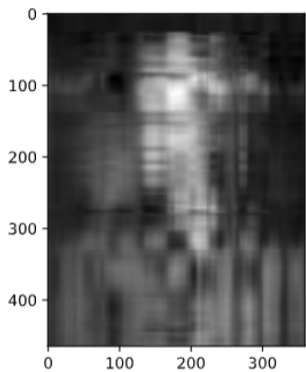
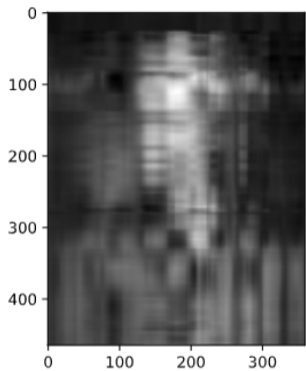


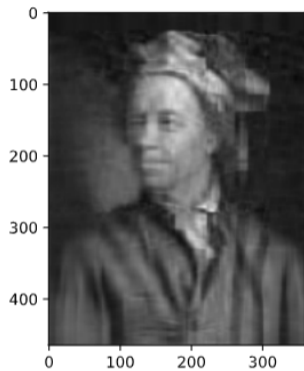
Figure: Leonhard Euler and its singular values.



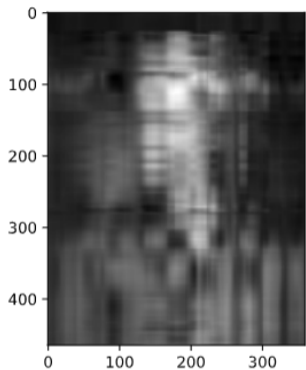
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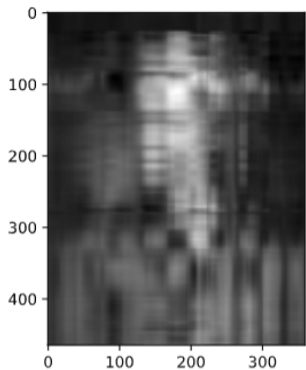
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→ Euler has a good low-rank approximation!!

Part 1: Dynamical low-rank approximation



DLRA: Definition

Original problem

$$\dot{X}(t) = F(X(t)), \quad t \in [0, T]$$

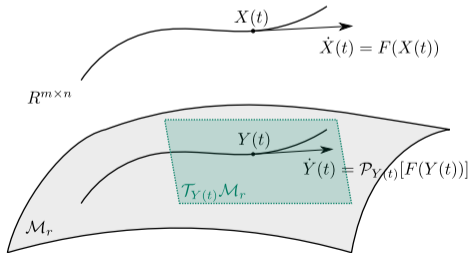
$$X(0) = X_0 \in \mathbb{R}^{m \times n}.$$

Dynamical low-rank approximation

([Koch and Lubich, 2007])

$$\dot{Y}(t) = \mathcal{P}_{Y(t)} [F(Y(t))], \quad t \in [0, T]$$

$$Y(0) = Y_0 \in \mathcal{M}_r.$$





DLRA: Theory

Standard DLRA assumptions:

- 1 F is Lipschitz: $\|F(X) - F(Y)\| \leq L \|X - Y\|$.
- 2 F is one-sided Lipschitz¹: $\langle X - Y, F(X) - F(Y) \rangle \leq \ell \|X - Y\|^2$.
- 3 F maps to a tangent bundle of \mathcal{M}_r : $\|F(Y) - \mathcal{P}_Y F(Y)\| \leq \varepsilon$.

Theorem (Accuracy of DLRA [Koch and Lubich, 2007])

Under the three assumptions above, the error made by DLRA verifies

$$\left\| \psi_r^h(Y_0) - \phi^h(X_0) \right\| \leq \underbrace{e^{\ell t} \|Y_0 - X_0\|}_{\text{initial error}} + \underbrace{\varepsilon \int_0^t e^{\ell s} ds}_{\text{modeling error}},$$

where ψ_r^h is the flow of the DLRA, and ϕ^h is the flow of the original problem.

¹If F is linear, ℓ is the largest eigenvalue, potentially negative.



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DLRA: Exponential Euler

$$\begin{aligned}\dot{X}(t) &= AX(t) + X(t)B^T + \mathcal{G}(X(t)) = \mathcal{L}(X(t)) + \mathcal{G}(X(t)), \quad t \in [0, T] \\ X(0) &= X_0 \in \mathbb{R}^{m \times n},\end{aligned}$$

Typically,

- \mathcal{L} is linear and stiff,
- \mathcal{G} is non-linear and non-stiff.

Closed form solution:
$$X(t) = e^{t\mathcal{L}}(X_0) + \int_0^t e^{(t-s)\mathcal{L}}(\mathcal{G}(X(s)))ds,$$

Exponential Euler:
$$X_1 = e^{h\mathcal{L}}(X_0) + h\varphi_1(h\mathcal{L})(\mathcal{G}(X_0)).$$

where $h\varphi_1(h\mathcal{L}) = \mathcal{L}^{-1}(e^{h\mathcal{L}} - Id)$. See [Hochbruck and Ostermann, 2010].



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DLRA: Projected exponential Euler (PERK1)

Now considering the DLRA problem,

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Definition (Projected exponential Euler [*C., Vandereycken*])

For a given stepsize h , the projected exponential Euler scheme is defined by

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DLRA: Lucky Krylov approximation

Question: Can we apply the scheme efficiently?

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Let us write the inner term differently,

$$Z(t) = e^{t\mathcal{L}}(Y_0) + t\varphi_1(t\mathcal{L})\mathcal{P}_{Y_0} [\mathcal{G}(Y_0)] \iff \begin{cases} \dot{Z}(t) = AZ(t) + Z(t)B + \mathcal{P}_{Y_0} [\mathcal{G}(Y_0)] \\ Z(0) = Y_0 \end{cases}$$

We are back to a Sylvester differential equation. Interesting because ...

$$Y_0 \text{ and } \mathcal{P}_{Y_0} [\mathcal{G}(Y_0)] \text{ are low-rank} \implies Y_0 = U_1 \Sigma V_1^T, \quad \mathcal{P}_{Y_0} [\mathcal{G}(Y_0)] = [U_1, U_2] \tilde{\Sigma} [V_1, V_2]^T$$

New idea: Use two rational Krylov² spaces to approximate the solution.

²See [Güttel, 2013] for overview.



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Left rational Krylov space:

$$\mathcal{RK}_k(A, U = [U_1, U_2]) = \text{span} \left\{ U, (A - \eta_2 I)^{-1} AU, \dots, \prod_{i=2}^k (A - \eta_i I)^{-1} A^{k-1} U \right\}$$

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Reduced differential equation (via Galerkin projection):

$$\begin{cases} \dot{Z}_k(t) = U_k^T A U_k Z_k(t) + Z_k(t) V_k^T B V_k + U_k^T \mathcal{P}_{Y_0} [\mathcal{G}(Y_0)] V_k \\ Z_k(0) = U_k^T Y_0 V_k \end{cases}$$

Final solution: $Z(t) \approx U_k Z_k(t) V_k^T$ where $Z_k(t) \in \mathbb{R}^{2kr \times 2kr}$



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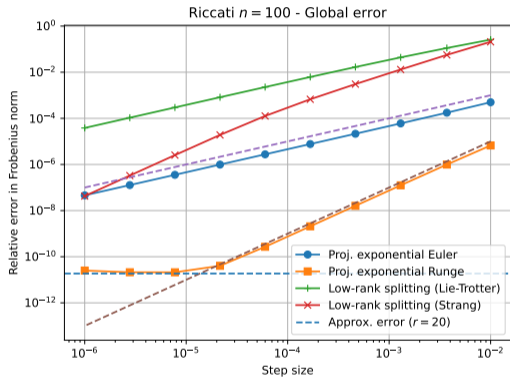
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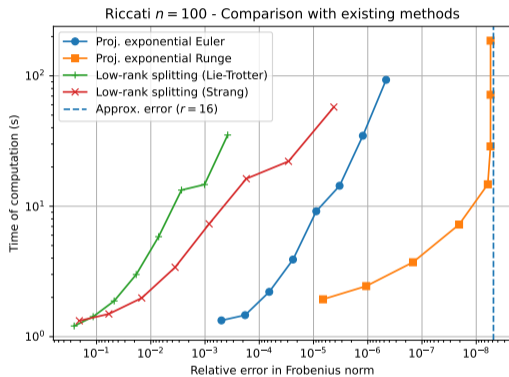
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Application to Riccati $\dot{X} = AX + XA + C^T C - XBB^T X$



(a) Global errors



(b) Performances

Figure: New methods applied to the Riccati equation, compared to [?]



DLRA: Conclusion

- Faster computations
- Low memory footprint
- Nice theoretical tools
- Active topic of research

Can we solve it in parallel in time?

Discretized DLRA

- Projector-splitting
[Lubich and Oseledets, 2014]
and [Kieri et al., 2016]
- Projection methods
[Kieri and Vandereycken, 2019]
- An unconventional
algorithm
[Ceruti and Lubich, 2022]
- A robust-to-stiffness
low-rank splitting
[Ostermann et al., 2019]

Continuous DLRA

- Application to
the Vlasov–poisson equation
[Einkemmer and Lubich, 2018]
- Stability (parabolic
problems)
[Kazashi et al., 2021]
- Stability (hyperbolic
problems)
[Kusch et al., 2023]

Rank-adaptive DLRA

- Rank-adaptive
unconventional
[Ceruti et al., 2022]
- Rank-adaptive DORK
[Charous and Lermusiaux, 2022]
- Rank-adaptive for
second-order MDEs
[Hochbruck et al., 2023]

Part 2: Low-rank Parareal



Low-rank Parareal: Motivation

Definition (Parareal [Lions et al., 2001])

The Parareal algorithm iterates

(Initial value) $X_0^k = X_0,$

(Initial approximation) $X_{n+1}^0 = \mathcal{G}^h(X_n^0),$

(Iteration) $X_{n+1}^{k+1} = \mathcal{F}^h(X_n^k) + \mathcal{G}^h(X_n^{k+1}) - \mathcal{G}^h(X_n^k),$

where \mathcal{F}^h and \mathcal{G}^h are the numerical integrators of the fine and coarse problems, respectively.

- Analysis [Gander and Vandewalle, 2007] and [Gander and Hairer, 2008].
- A link with multigrid [Gander et al., 2018].

- Task scheduling [Aubanel, 2011].
- A unified framework [Gander et al., 2022].



Low-rank Parareal: Definition

Definition (Low-rank Parareal [Carrel et al., 2023])

Choose a *coarse rank* q and a *fine rank* r such that $q < r$. The low-rank Parareal algorithm iterates

$$\text{(Initial value)} \quad Y_0^k = Y_0,$$

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where ψ_r^h is the solution of the DLRA of rank r at time h , and \mathcal{T}_r is the orthogonal projection onto \mathcal{M}_r . The notations ψ_q^h and \mathcal{T}_q are similar but apply to rank q .

Remark: The rank of each iteration is at most $r + 2q$.



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Low-rank Parareal: Analysis

The error verifies the **double recursion**

$$\left\| E_{n+1}^{k+1} \right\| \leq \alpha \left\| E_n^k \right\| + \beta \left\| E_n^{k+1} \right\| + \kappa, \quad n, k \geq 0,$$

with the positive constants

- Let C_q (resp. $C_{r,q}$) be the Lipschitz constant of \mathcal{T}_q (resp. $\mathcal{T}_r - \mathcal{T}_q$). Then,

$$\alpha = e^{\ell h} C_{r,q} \quad \text{and} \quad \beta = e^{\ell h} C_q.$$

By [Feppon and Lermusiaux, 2018],

$$C_q \lesssim \frac{1}{1 - \frac{\sigma_{q+1}}{\sigma_q}} \approx \frac{1}{1 - e^{-c}} \quad \text{when, for some } c > 0, \quad \sigma_k \approx e^{-ck}.$$

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Low-rank Parareal: Analysis

Theorem (Convergence of low-rank Parareal [Carrel et al., 2023])

Under the standard DLRA assumptions, and if $\alpha + \beta < 1$, the error satisfies

1st linear bound:
$$\max_{n \geq 0} \|E_n^k\| \leq \left(\frac{\alpha}{1 - \beta} \right)^k \max_{n \geq 0} \|E_n^0\| + \frac{\kappa}{1 - \alpha - \beta},$$

2nd linear bound:
$$\|E_n^k\| \leq \alpha^k (1 + \beta)^{n-1} \max_{n \geq 0} \|E_n^0\| + \frac{\kappa}{1 - \alpha - \beta},$$

Superlinear bound:
$$\|E_n^k\| \leq \frac{\alpha^k}{(k-1)!} \frac{\prod_{j=2}^k (n-j)}{1 - \beta} \max_{n \geq 0} \|E_n^0\| + \frac{\kappa}{1 - \alpha - \beta}.$$



Low-rank Parareal: Analysis

Theorem (Convergence of low-rank Parareal [Carrel et al., 2023])

Under the standard DLRA assumptions, and if $\alpha + \beta < 1$, the error satisfies

1st linear bound:
$$\max_{n \geq 0} \|E_n^k\| \leq \left(\frac{\alpha}{1 - \beta} \right)^k \max_{n \geq 0} \|E_n^0\| + \frac{\kappa}{1 - \alpha - \beta},$$

2nd linear bound:
$$\|E_n^k\| \leq \alpha^k (1 + \beta)^{n-1} \max_{n \geq 0} \|E_n^0\| + \frac{\kappa}{1 - \alpha - \beta},$$

Superlinear bound:
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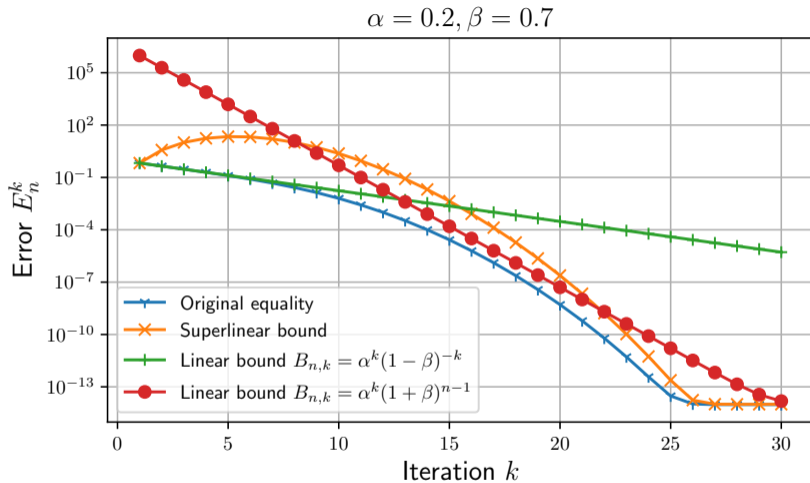


Figure: Comparison of the bounds

Lyapunov equation

$$\dot{X}(t) = AX(t) + X(t)A^T + CC^T,$$

where

- $t \in [0, 2]$
- $X(0) = X_0$ is low-rank.
- $A \in \mathbb{R}^{100 \times 100}$ is sparse.
- $C \in \mathbb{R}^{100 \times 5}$ is a tall matrix.

→ Model for 2D heat diffusion (stiff).

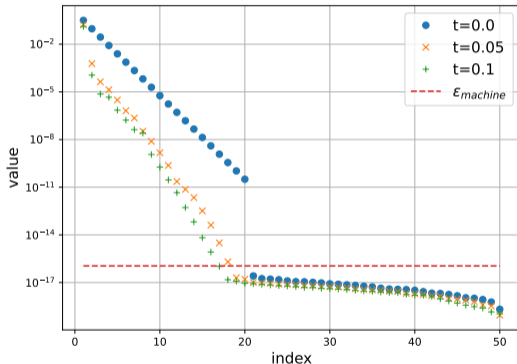
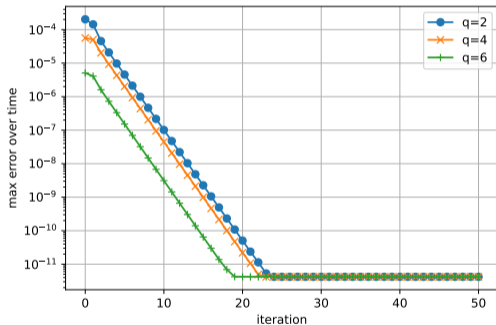
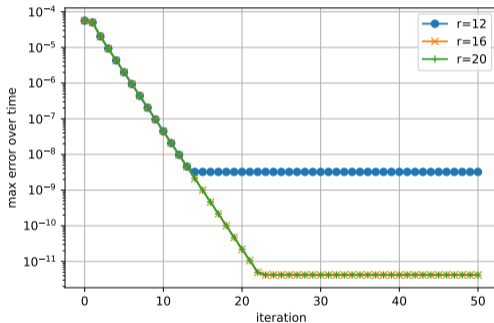


Figure: Singular values of the reference solution.

$$\text{Lyapunov: } \dot{X}(t) = AX(t) + X(t)A^T + C$$



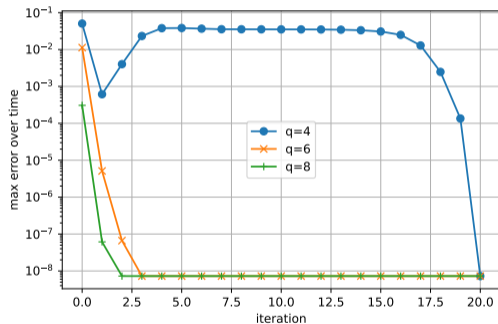
(a) Several coarse ranks q with fine rank $r = 16$.



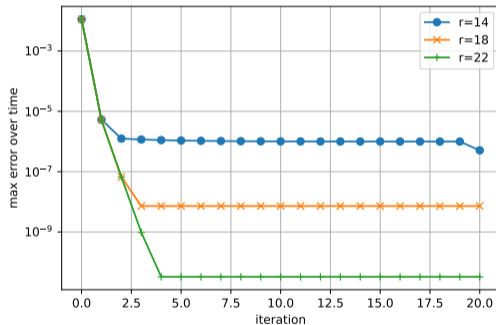
(b) Several fine ranks r with coarse rank $q = 4$.

Figure: Low-rank Parareal applied to Lyapunov ODE with $n = 100$ and $T = 2.0$.

$$\text{Riccati: } \dot{X}(t) = AX(t) + X(t)A^T - X(t)BX(t) + C$$



(a) Several coarse ranks with fine rank $r = 18$.



(b) Several fine ranks with coarse rank $q = 6$.

Figure: Low-rank Parareal applied to Riccati ODE with $n = 200$ and $T = 0.1$.



Conclusion:

- Low-rank Parareal is the first parallel-in-time integrator for DLRA
- A priori linear and superlinear bounds
- Good behavior on the heat equation

Links:

- Published in BIT Numerical Mathematics:
<https://link.springer.com/article/10.1007/s10543-023-00953-3>
- Code on GitHub: <https://github.com/BenjaminCarrel/Low-rank-Parareal>

Merci pour votre attention! Questions?



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