MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Generalizing Reduced Rank Extrapolation (RRE) to Low-Rank Matrix Sequences

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Joint work with **Pascal den Boef**[1] **Patrick Kürschner**[2] **Jos Maubach**[1] **Jens Saak**[3]
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1. Reduced Rank Extrapolation
2. Methodological Extensions
3. Numerical Experiments
4. Conclusions

Original sequence: x_1

Improved sequence:

Non-Cycling Mode

for $i \leftarrow 1, 2, \ldots$ **do**
  $x_{i+1} \leftarrow f(x_i)$
  if $i \geq n$ **then**
    $\hat{x}_i \leftarrow \text{extr.}(x_{i-n+1}, \ldots, x_i, x_{i+1})$
    if $\hat{x}_i$ converged **then** break
  end
end

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for $i \leftarrow 1, 2, \ldots$ **do**
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- Non-cycling mode generates new extrapolated sequence $\widehat{x}_n, \widehat{x}_{n+1}, \ldots$ (via window size n).
- Cycling mode restarts using the extrapolated iterate, to generate, e.g., $x_1, x_2, x_3, x_4, \ldots$.

Original sequence: x_1 x_2

Improved sequence:

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Original sequence: $x_1 \quad x_2 \quad x_3$

Improved sequence: $\hat{x}_3$

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Improved sequence: $\hat{x}_3$ $\hat{x}_4$

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Reduced Rank Extrapolation

Extrapolation Methods for Fixed-Point Processes

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Improved sequence: $\hat{x}_3 \quad \hat{x}_4 \quad \dots$

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- Objective: solve $Ax = b$.
- Iterative scheme: splitting $A = I - (I - A)$,

$$x_{i+1} := f(x_i) := (I - A)x_i + b.$$

- RRE Ansatz: find $\hat{x} := \sum_{i=1}^{n} \gamma_i x_i$ minimizing the **residual of the fix-point iteration**

$$\|f(\hat{x}) - \hat{x}\|,$$

where $\gamma_1 + \cdots + \gamma_n = 1$.
- Key observations:

$$f(x) - x = b - Ax$$
$$f(\hat{x}) - \hat{x} = \sum_{i=1}^{n} \gamma_i (f(x_i) - x_i) \quad \text{(linearity)}$$

Target properties

1. Nonstationary f
2. Low-rank x_i and x_{i+1}

Alert

1. Two notions of residual
2. One not suitable for nonstationary f

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Most derivations of reduced rank extrapolation (RRE) read off the iteration scheme from an underlying equation where both notions of the residual coincide:

$x = Ax + b$	[Mešina, '77], [Eddy, '79](not spelled out), [Sidi, '88], [Sidi, '91]
$Ax = b$	[Sidi & Shapira, '98]

or only consider the residual of the iteration:

$Ax = b$	[Kaniel & Stein, '74]
$x = f(x)$	[Sidi, '20]

Theorem (Sidi, '88), (Sidi, '17)

Let $\{x_m\}$ be the sequence generated by the fixed-point iteration

$$x_{m+1} = Fx_m + b, \quad m = 0, 1, 2, \ldots,$$

with initial guess x_0. The extrapolated solutions x_k^{RRE} (with window size $k+1$) obtained by applying non-cycling RRE to $\{x_m\}$ ***coincide*** *with the iterates x_k^{GMRES} obtained by applying GMRES (after k steps) to the linear system $(I - F)x = b$ with the same initial guess.*

Sketch proof: $x_{m+1} - x_m = b - (I - F)x_m = r_m \implies$ both RRE and GMRES minimize the residual over $\mathcal{K}_k(A, r_0) = \mathrm{span}\{r_0, Ar_0, \ldots, A^{k-1}r_0\}$, where $A = I - F$.

- No known mathematical equivalence between cycling RRE and restarted GMRES, though they are similar in *spirit* and *practical behavior*.

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So far:

$$\hat{x} := \sum_{i=1}^{n} \gamma_i x_i, \quad \text{where}$$

Increment-Based RRE **(old)**

$$\gamma = \arg\min_{g \in \mathbb{R}^n} \left\| \sum_{i=1}^{n} g_i (x_{i+1} - x_i) \right\|,$$

$$\text{s.t.} \quad \sum_{i=1}^{n} g_i = 1.$$

Residual-Based RRE **(new)**

$$\gamma = \arg\min_{g \in \mathbb{R}^n} \left\| \sum_{i=1}^{n} g_i (A x_i - b) \right\|,$$

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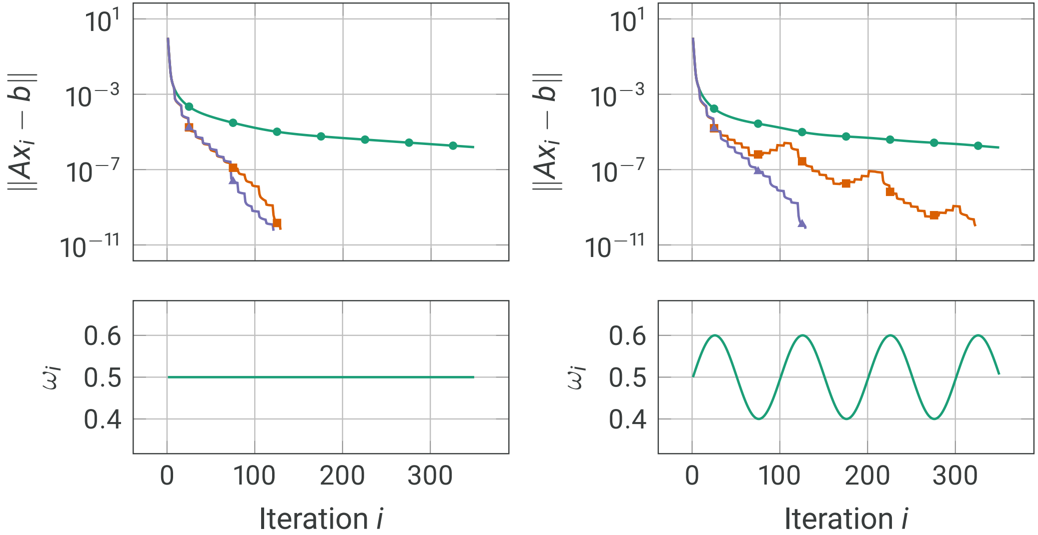

Figure: Comparison of increment-based (—■—) and residual-based (—▲—) RRE formulations applied to successive over-relaxation schemes (—●—).

- RRE for vector sequences $x_i \in \mathbb{R}^d$: via method of Lagrange multipliers

$$\gamma = \arg\min_{g \in \mathbb{R}^n} \left\| \sum_{i=1}^{n} g_i (Ax_i - b) \right\| \quad \text{s.t.} \quad \sum_{i=1}^{n} g_i = 1 \quad \Longleftrightarrow \quad U^{\mathsf{T}} U \alpha = 1 \in \mathbb{R}^n \text{ and } \gamma := \alpha / \|\alpha\|$$

$$\boxed{U} := \left[Ax_1 - b \middle| \dots \middle| Ax_n - b \right] \in \mathbb{R}^{d \times n}$$

- Low-rank matrix sequences $X_i =$ with residuals $\mathcal{R}(X_i) =$
- Assembling $X_i \in \mathbb{R}^{d \times d}$ is prohibitively expensive, despite inner factor having size r
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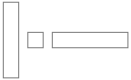
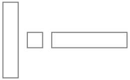
- Low-rank matrix sequences $X_i =$  with residuals $\mathcal{R}(X_i) =$ 

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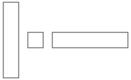
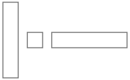
- Low-rank matrix sequences $X_i =$  with residuals $\mathcal{R}(X_i) =$ 
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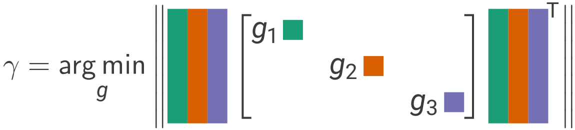
Main idea:

1. Move arithmetic onto inner factors of dimension $r \ll d$
2. Reduce dimension via QR decomposition of outer factors

Benefits:

Solution of $U^{\mathsf{T}} U \alpha = 1 \in \mathbb{R}^n$ now requires $U \in \mathbb{R}^{(nr)^2 \times n}$ where $(nr)^2 \ll d^2$.
Recall that $\gamma := \alpha / \|\alpha\|$, and that ■/■/■ may represent increments or residuals.

Main idea:



1. Move arithmetic onto inner factors of dimension $r \ll d$
2. Reduce dimension via QR decomposition of outer factors

Benefits:

Solution of $U^{\mathsf{T}}U\alpha = 1 \in \mathbb{R}^n$ now requires $U \in \mathbb{R}^{(nr)^2 \times n}$ where $(nr)^2 \ll d^2$.
Recall that $\gamma := \alpha / \|\alpha\|$, and that ■/■/■ may represent increments or residuals.

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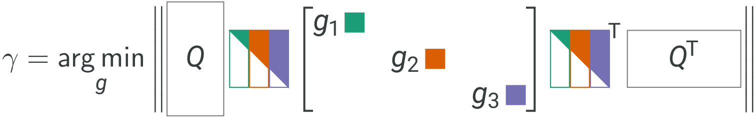

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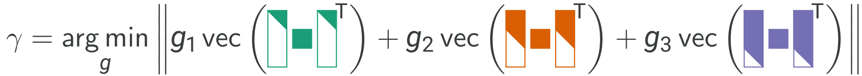

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Xiaobo Liu, xliu@mpi-magdeburg.mpg.de

Figure: Increment-based RRE for low-rank matrix sequences, where $\tau_i := \gamma_i + \cdots + \gamma_n$.

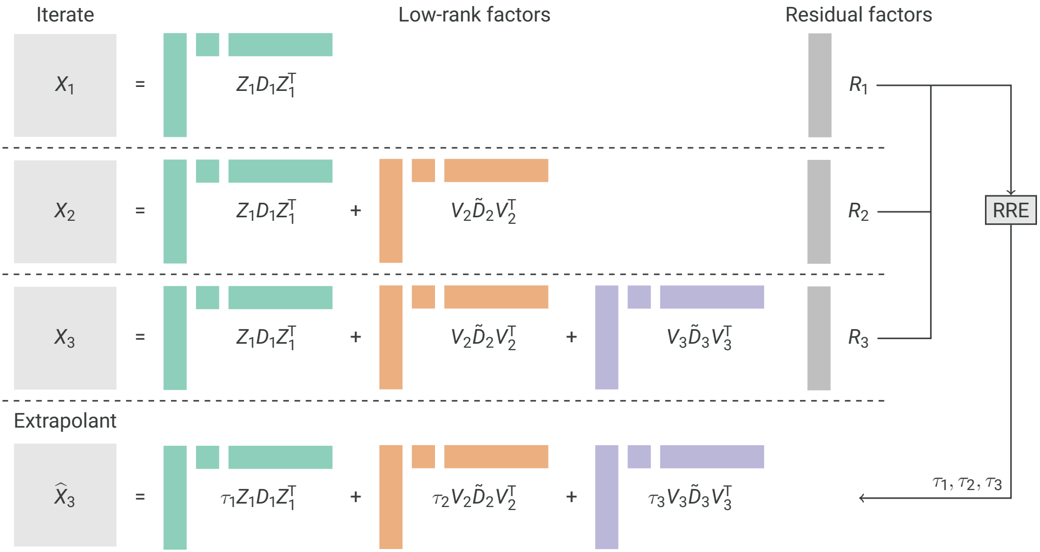


Figure: Residual-based RRE for low-rank matrix sequences, where $\tau_i := \gamma_i + \cdots + \gamma_n$.

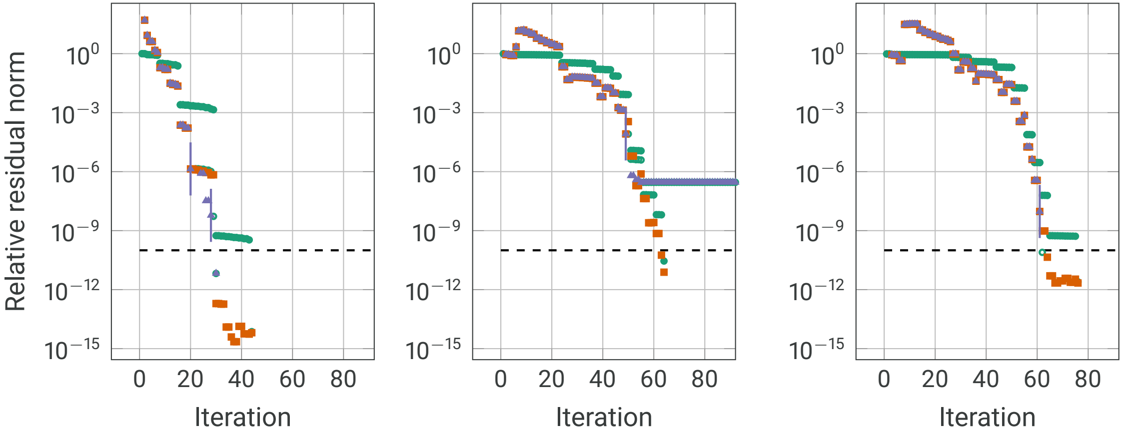
1. Reduced Rank Extrapolation
2. Methodological Extensions
3. Numerical Experiments
4. Conclusions

Numerical Experiments

- Underlying equation: algebraic Riccati equation (ARE)

$$C^{\mathsf{T}} C + A^{\mathsf{T}} X E + E^{\mathsf{T}} X A - E^{\mathsf{T}} X B H^{-1} B^{\mathsf{T}} X E = 0 \in \mathbb{R}^{d\times d}$$

- $X \approx Z\, D\, Z^{\mathsf{T}}$ and $\mathcal{R}(X) \approx R\, T\, R^{\mathsf{T}}$ **[Benner & Bujanović, ’16]**
- Iterative process: RIccati Alternating Directions Implicit (RADI) **[Benner et al., ’18]**
- Implementation derived from M-M.E.S.S (The Matrix Equation Sparse Solvers library) **[Saak, Köhler, & Benner, ’25]**



(a) $q = 1$. (b) $q = 20$. (c) $q = 40$.

Figure: RADI (●○), non-cycling RRE (■), and cycling RRE (▲) applied to nonlinear *Toeplitz* example **[Benner et al., '20]**, $d = 100\,000$, for varying numbers of outputs; $C \in \mathbb{R}^{q \times d}$.

- Stagnation of cycling mode is likely due to non-PSD res. of the extrapolant (as initializer).

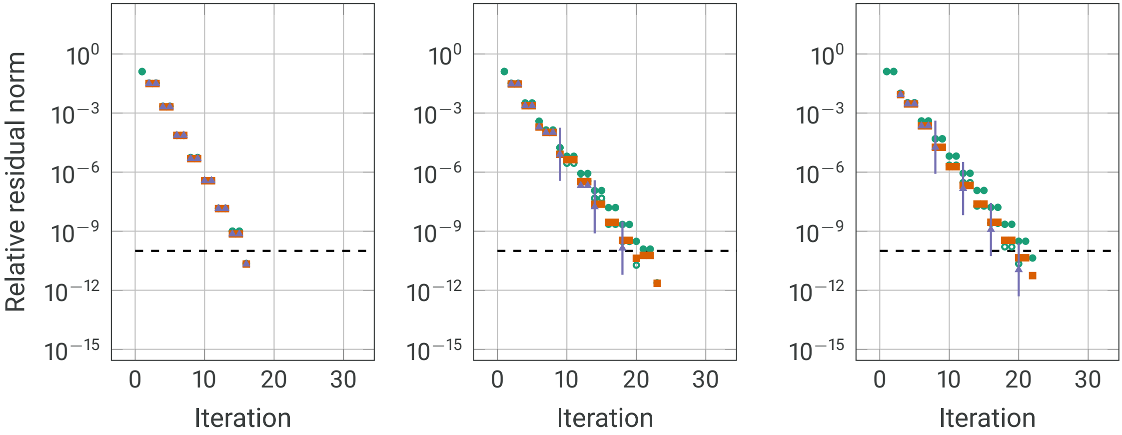


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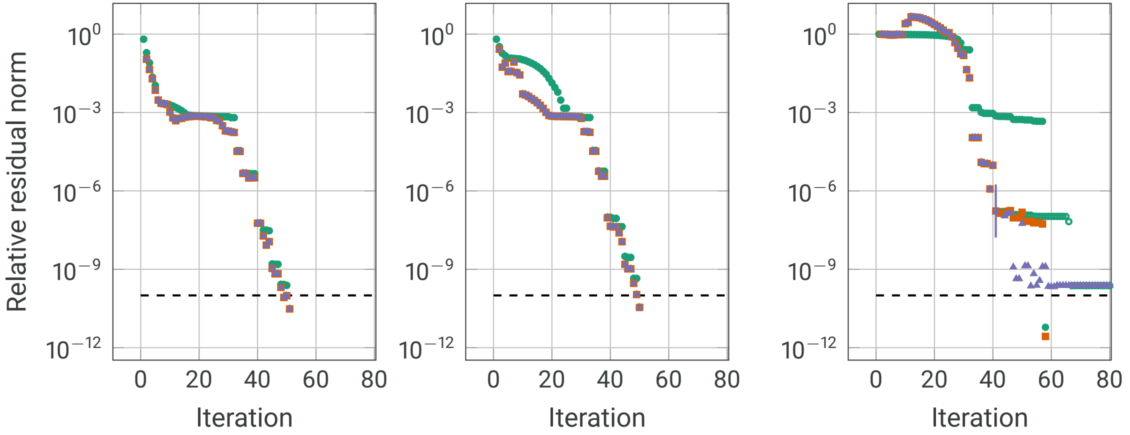
Figure: ADI (●○), non-cycling RRE (■), and cycling RRE (▲) applied to *Toeplitz* example **[Benner et al., '20]**, $d = 10^5$ and **B=0** ($\Rightarrow$ Algebraic Lyapunov Equation (ALE)), for varying outputs q; $C \in \mathbb{R}^{q \times d}$.

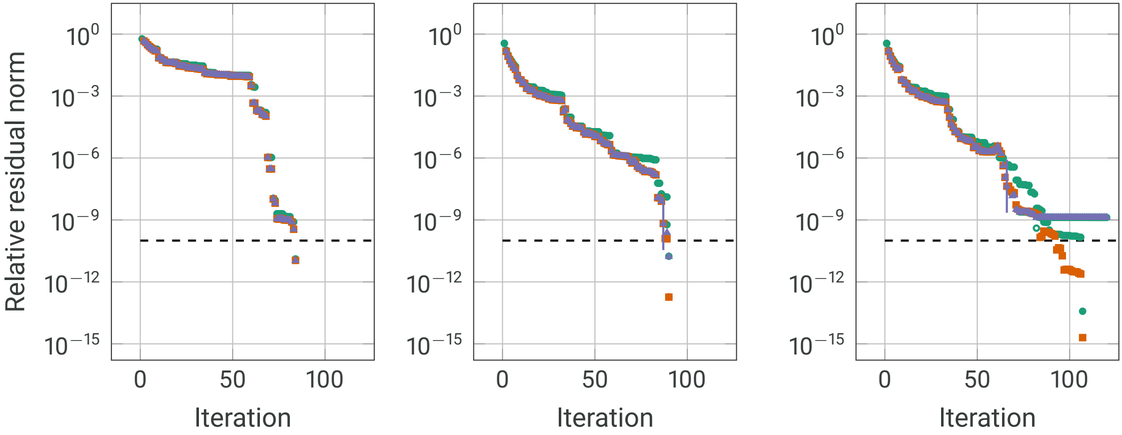
- No stagnation observed in this linear case. More benefits of RRE with larger q.



(a) $\lambda = 10^0$. (b) $\lambda = 10^{-2}$. (c) $\lambda = 10^{-4}$.

Figure: RADI (●○), non-cycling RRE (■), and cycling RRE (▲) applied to *Chip* example **[Moosmann et al., '04]**, $d = 20\,082$, for varying contributions of the quadratic factor matrix $H^{-1} = \lambda^{-1} I_p$.

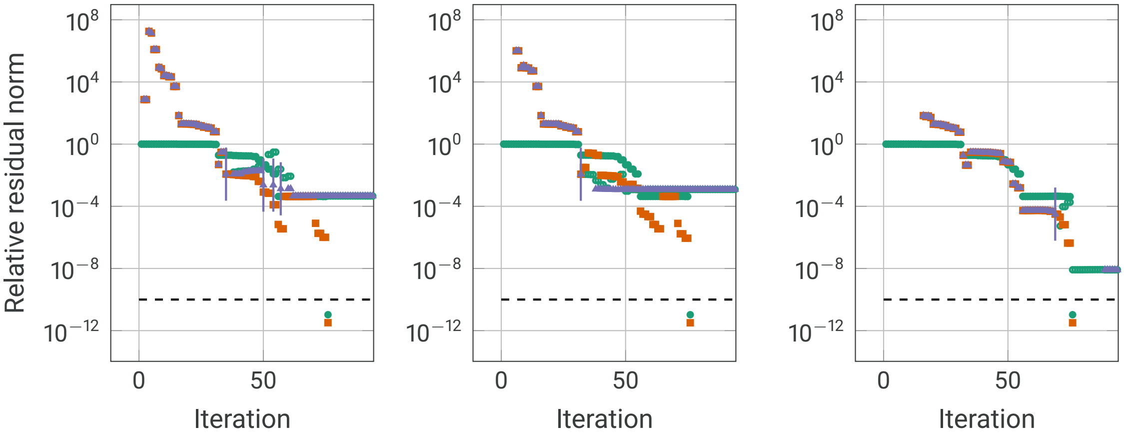
- ARE more nonlinear with smaller λ, greater benefits of RRE observed.



(a) ADI for Controllability ALE (b) ADI for Observability ALE (c) RADI for ARE

Figure: (R)ADI (●○), non-cycling RRE (■), and cycling RRE (▲) applied to *Steel Profile* example **[Benner & Saak, '05]**, $d = 317\,377$.

- Little acceleration of RRE for ALEs (the ADI iterates near optimal?); clear benefits for ARE.



(a) $n = 3$.

(b) $n = 6$.

(c) $n = 12$.

Figure: RADI (●○), non-cycling RRE (■), and cycling RRE (▲) applied to *Triple Chain* mass-spring-damper example [Truhar & Veselić, '09], $d = 60\,002$, with varying RRE window size $n \in \mathbb{N}^+$.

- Residual of non-cycling mode RRE decreases faster for larger n.

Conclusions

- Proposed two extensions to RRE, applicable to any sequence of low-rank matrices:
  1. Nonstationary fixed-point iterations
  2. Low-rank matrix sequences
- Demonstrated feasibility of RADI + non-cycling RRE for ARE
  under a simple condition on RRE coefficients γ
  for various system behaviors, parameters, and equation types
- Problem: non-PSD residuals
  which leads to stagnation for RADI + cycling RRE for nonlinear equations

Outlook:

- Convergence analysis
- Other equation types: multi-term Sylvester, Lyapunov-plus-positive, etc.

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