Implicit peer methods for large stiff ODEs

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INNOVATIVE INTEGRATORS
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Introduction

$$y'(t) = f(t, y)$$
$$y(t_0) = y_0 \in \mathbb{R}^n, \qquad t_0 \le t \le t_e$$

PDE $\Rightarrow$ MOL $\Rightarrow$ large stiff ODE

difficulty: linear systems of large dimensions have to be solved

possible solution: **Krylov-techniques**

- linear systems of dimension $\varkappa \ll n$
- f_y is only involved in $f_y v$, approx. per FD

AMF

- exploits special structure
- high implementation effort

PEER methods (2004-2010) are well suited for stiff problems (high stage-order)

Implicit Peer methods

$$Y_{m,i} = \sum_{j=1}^{s} b_{ij} Y_{m-1,j} + h_m \sum_{j=1}^{i} g_{ij} F_{m,j} \,, \qquad i = 1, \ldots, s$$

$$Y_{m,i} \approx y\left(t_m + c_i h_m\right), \quad F_{m,i} = f\left(t_m + c_i h_m, Y_{m,i}\right) \approx y'\left(t_m + c_i h_m\right)$$

coefficient matrices:

$$B_m = (b_{ij})_{i,j=1}^{s}, \quad G_m = (g_{ij})_{i,j=1}^{s} \quad \text{depend on} \quad \sigma_m = h_m / h_{m-1}$$

compact form: $Y_m = B_m Y_{m-1} + h_m G_m F_m$

- introduced by Schmitt,Weiner and Erdmann in APNUM 53 (2005)
  - small systems of ODEs
  - G_m diagonal matrix $\Rightarrow$ possibility of parallelization
- now
  - large systems
  - G_m lower triangular matrix

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Order conditions, consistency

Simplifying condition

$$B(p): \qquad 0 = c_i^k - \sum_{j=1}^{s} b_{ij} \left(\frac{c_j - 1}{\sigma_m} \right)^k - k \sum_{j=1}^{i} g_{ij} c_j^{k-1}$$

$$k = 0, \ldots, p\,, \quad i = 1, \ldots, s$$

Theorem (Consistency)

Let the peer method satisfy $B(p)$. Then, the method is consistent of order p.

$$B(s-1) \quad \Rightarrow \quad B_m = \left(V_0 - G_m V_0 D F_0^T \right) S_m P V_0^{-1} \quad \text{with}$$

$$V_0 = \left(c_i^{j-1} \right), S_m = \operatorname{diag}\left(\sigma^{i-1} \right), P = \binom{j-1}{i-1}, D = \operatorname{diag}(i), F_0 = \left(\delta_{i-1,j} \right)$$

Stability

Test equation: $y' = \lambda y$

Applying the method to the test equation yields:

$$Y_m = \underbrace{(\mathcal{I} - zG_m)^{-1} B_m}_{M(z)} Y_{m-1} , \qquad z = h\lambda$$

Definition (A- and L-Stability)

The method is *A-stable* if

$$\rho(M(z)) < 1 , \qquad z \in \mathbb{C}_- := \{z \in \mathbb{C} : \mathrm{Re}\, z < 0\}$$

and *L-stable* if, additionally $\rho(M(\infty)) = 0$.

Note: $M(\infty) = 0$ automatically satisfied, i.e. $A(\alpha) \Rightarrow L(\alpha)$

$M(0) = B_m$-matrix of zero stability

Definition (Zero-Stability)

The implicit peer method is *zero-stable*, if

$$\|B_{m+\ell} B_{m+\ell-1} \cdots B_{m+1} B_m\| \leq K$$

holds for some constant $K < \infty$ and for all m and $\ell \geq 0$.

Theorem (Convergency)

Zero-stability and order p of consistency guarantee convergence of order p.

optimal zero-stability: eigenvalues of B_m satisfy

$$\lambda_1 = 1 \quad \text{and} \quad \lambda_i = 0\,, \quad i = 2, \ldots, s$$

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Construction of methods of order $p = s$ and $s - 1$

We constructed optimally zero stable methods:

1. multi-implicit methods with $G(\sigma_m)$, (s3-,s4-,s5-sigma)
   - $G_m = \mathrm{diag}(\gamma_1, \ldots, \gamma_s) + G_0$
   - order of consistency $p = s$ also for variable step sizes
   - G_m has to be recomputed with the actual step size ratio σ_m.
2. superconvergent singly implicit methods, (s3-,s4-,s5-single)
   - $G = \gamma I + G_0$ ($\rightarrow$ suitable for AMF)
   - γ root of a special polynomial of degree s (superconvergence condition)
   - order $p = s - 1$ for general step sizes and order of convergence $p = s$ for constant ones.

Numerical search: $s = 3, 4, 5$

Search was done by a evolutionary algorithm

- for each type only the nodes c_i are free
- $0 < c_1 < c_2 < \cdots < c_s = 1$
- optimization criterions
  1. maximize the angle α of $L(\alpha)$-stability
  2. minimize the error constant (for $\sigma = 1$)

$$\text{err} = \| \frac{c^{p+1}}{(p+1)!} - B\frac{(c-1)^{p+1}}{(p+1)!} - G\frac{c^p}{p!} \|_2,$$

     $p =$ order of consistency
  3. minimize the γ_i or γ (best for Krylov)

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Methods with Krylov

- starting values are computed by ROWMAP with higher accuracy
- nonlinear systems are solved by Newton's method
  - maximum number of iterations is 10
  - the initial guess for Newton's method at stage i, polynomial extrapolation using

$$Y_{m-1,i}, \ldots, Y_{m-1,s}, Y_{m,1}, \ldots, Y_{m,i-1}$$

  $\Rightarrow$ works good for $0 < c_1 < c_2 < \cdots < c_s = 1$
  - in general, extrapolation by the s nearest points in time for any nodes $c_i \in [-1, 1), \quad i = 1, \ldots, s-1, \quad c_s = 1$

  $\Rightarrow$ works unsatisfactory
- linear systems are solved with the Krylov method FOM
  - maximum Krylov dimension 20

Approximate Matrix Factorization (AMF)

- proposed by Sommeijer, Rodríguez, Pinto for RADAU-IIA(2)
- The Jacobian matrix is split as $J = J_1 + \cdots + J_d$, J_i are band matrices
- The linear systems of type $(I - \gamma hJ)x = b$ which appear in the Newton iterations are solved by the process

$$\prod_{i=1}^{d}(I - \gamma hJ_i)x = b$$

$$(I - \gamma hJ_1)x_1 = b, \quad (I - \gamma hJ_2)x_2 = x_1, \quad \ldots \quad (I - \gamma hJ_d)x = x_{d-1}$$

- Interpretation: Newton's method with $\widetilde{J}$ is used, where

$$\prod_{i=1}^{d}(I - \gamma hJ_i) = (I - \gamma hJ + \mathcal{O}(h^2)) = (I - \gamma h\widetilde{J})$$

- Maximum number of 10 Newton iterations, initial guess: nearest vector Y_{nj}, $n \in \{m, m-1, ..., 1\}$, $j \in \{1, 2, \ldots, s\}$

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Test of Krylov codes in MATLAB

MATLAB codes:

- PEER-Krylov
  - s3-,s4-,s5-sigma
  - s3-,s4-,s5-single
- ROWMAP
  - (Weiner/Schmitt/Podhaisky 1997 FORTRAN)
  - (B. 2008 MATLAB)
- EXP4(Hochbruck/Lubich/Selhofer 1997)

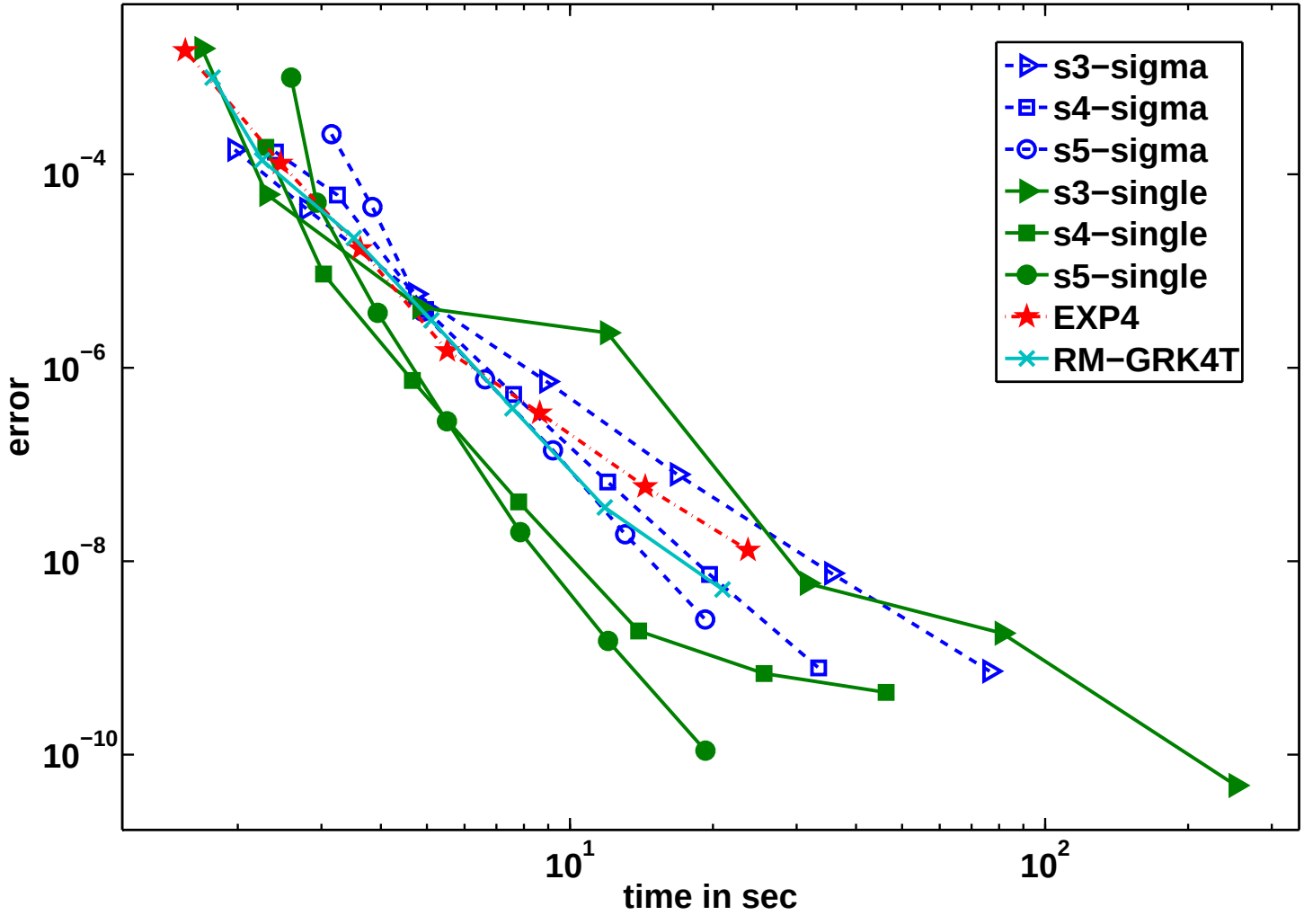
Examples: semidiscretized PDEs

- ROWMAP APNUM 25 (1997)

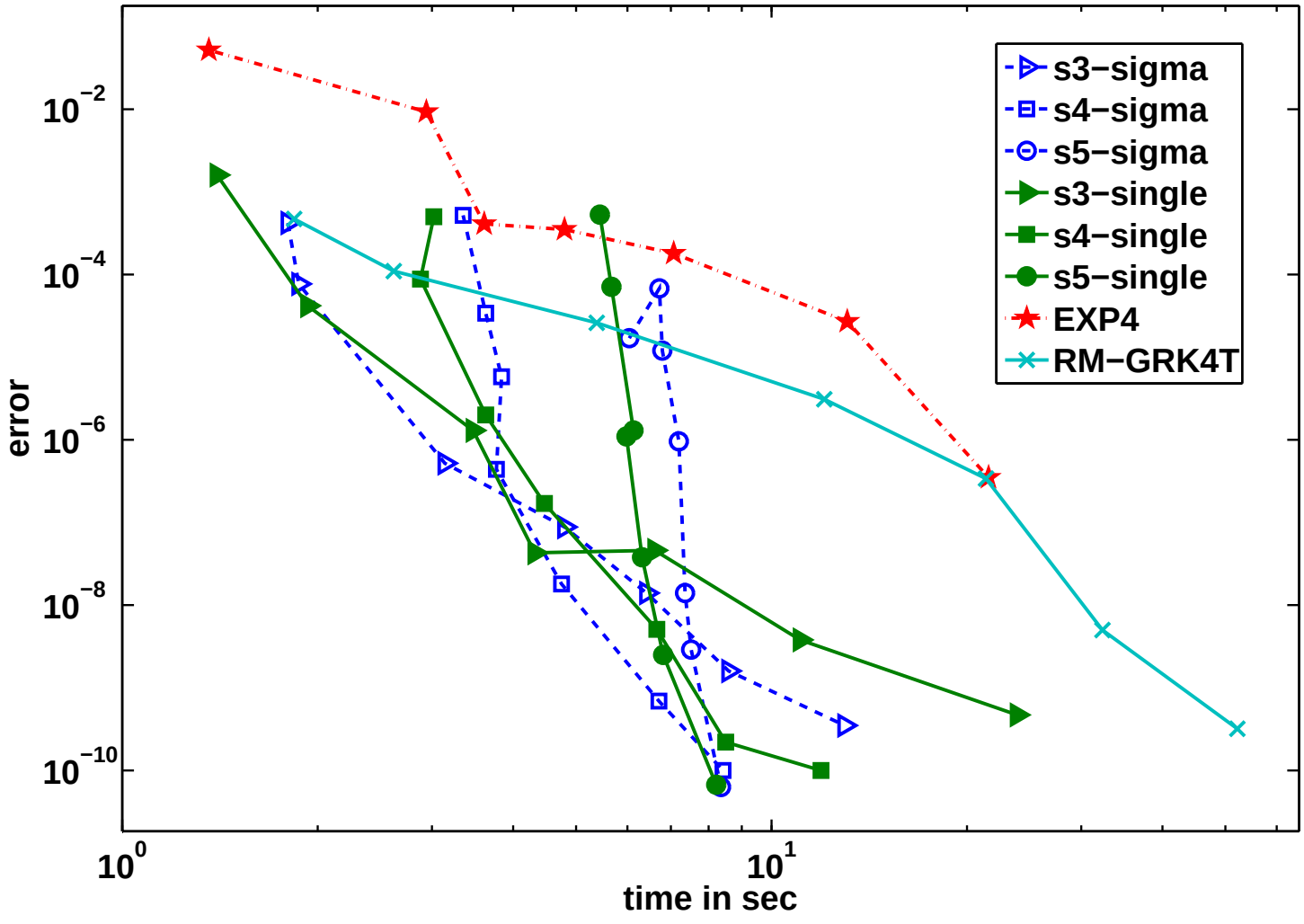
Remarks:

- Tolerances: $10^{-2}, \ldots, 10^{-8}$
- All matrix-vector products Jv are computed by finite differences

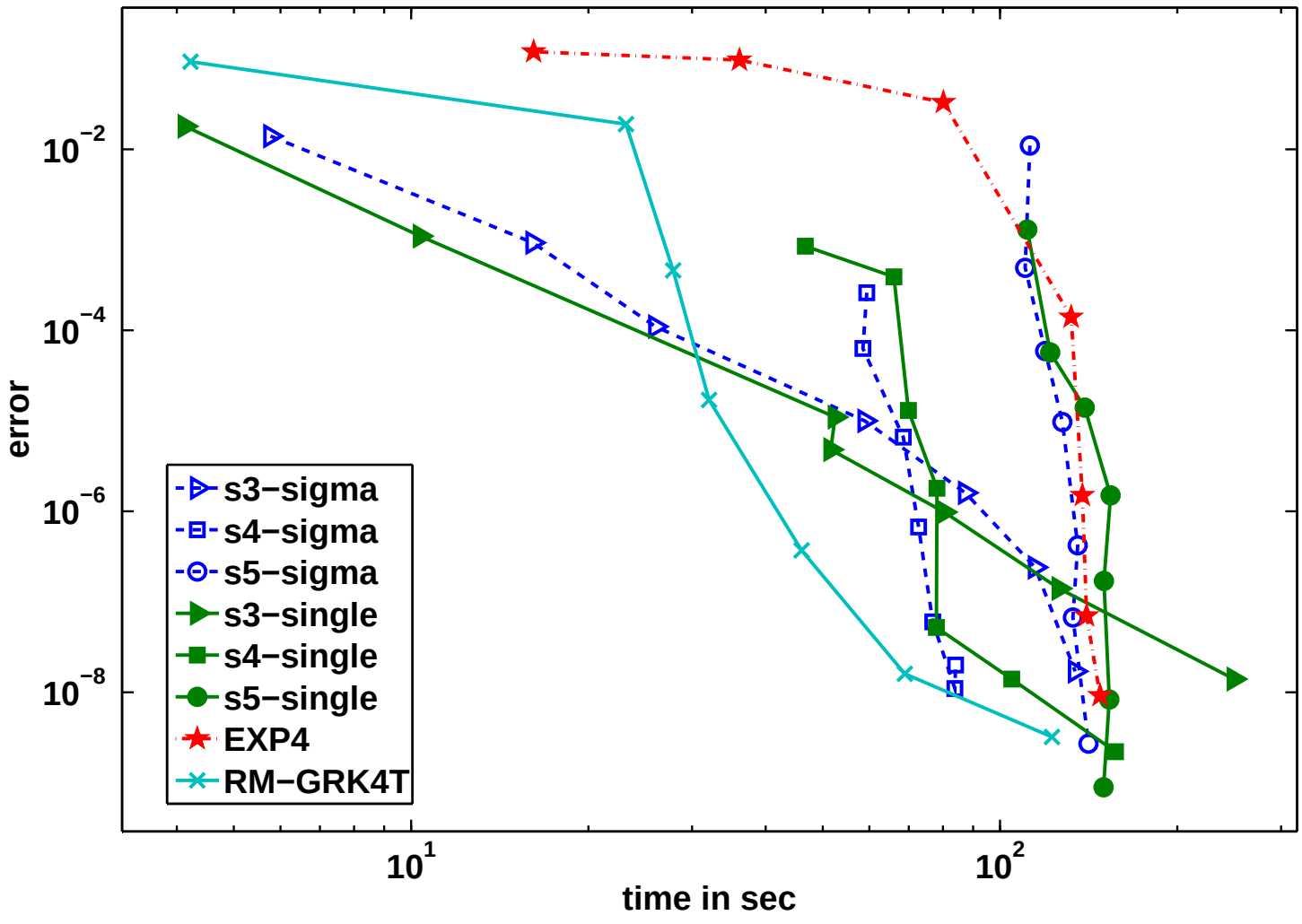
Bruss2D: The 2D Brusselator with diffusion, $N = 20000$



Diffu2: The 2D diffusion equation, $N = 10000$



Nilidi: The nonlinear diffusion equation, $N = 40000$



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AMF vs. Krylov

MATLAB codes:

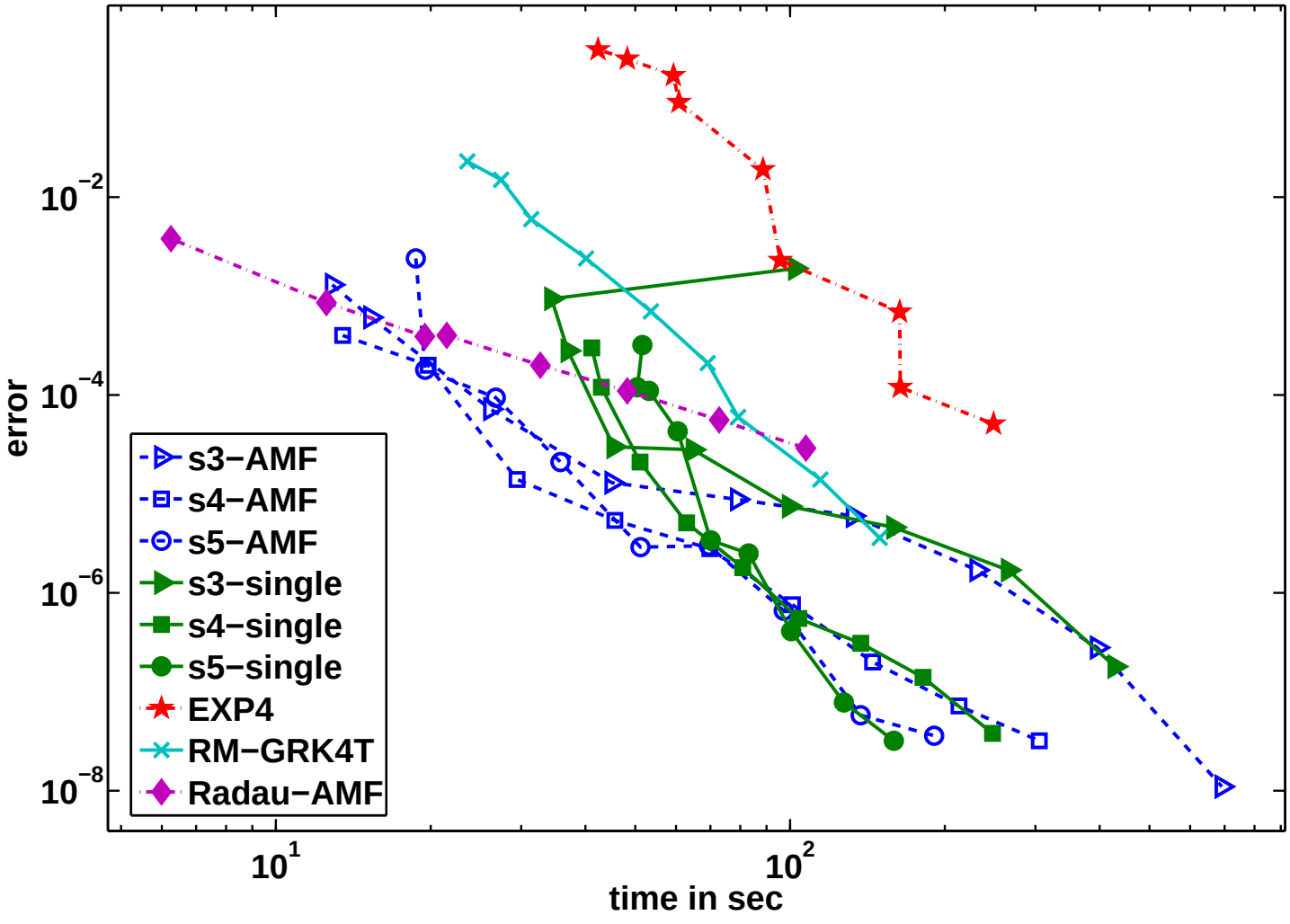
- EXP4, ROWMAP
- RADAU-IIA-SN-AMF (Rodríguez/Pinto)
- PEER-Krylov (s3-,s4-,s5-single)
- PEER-AMF (s3-,s4-,s5-AMF)

Example: Radiation-Diffusion-Problem

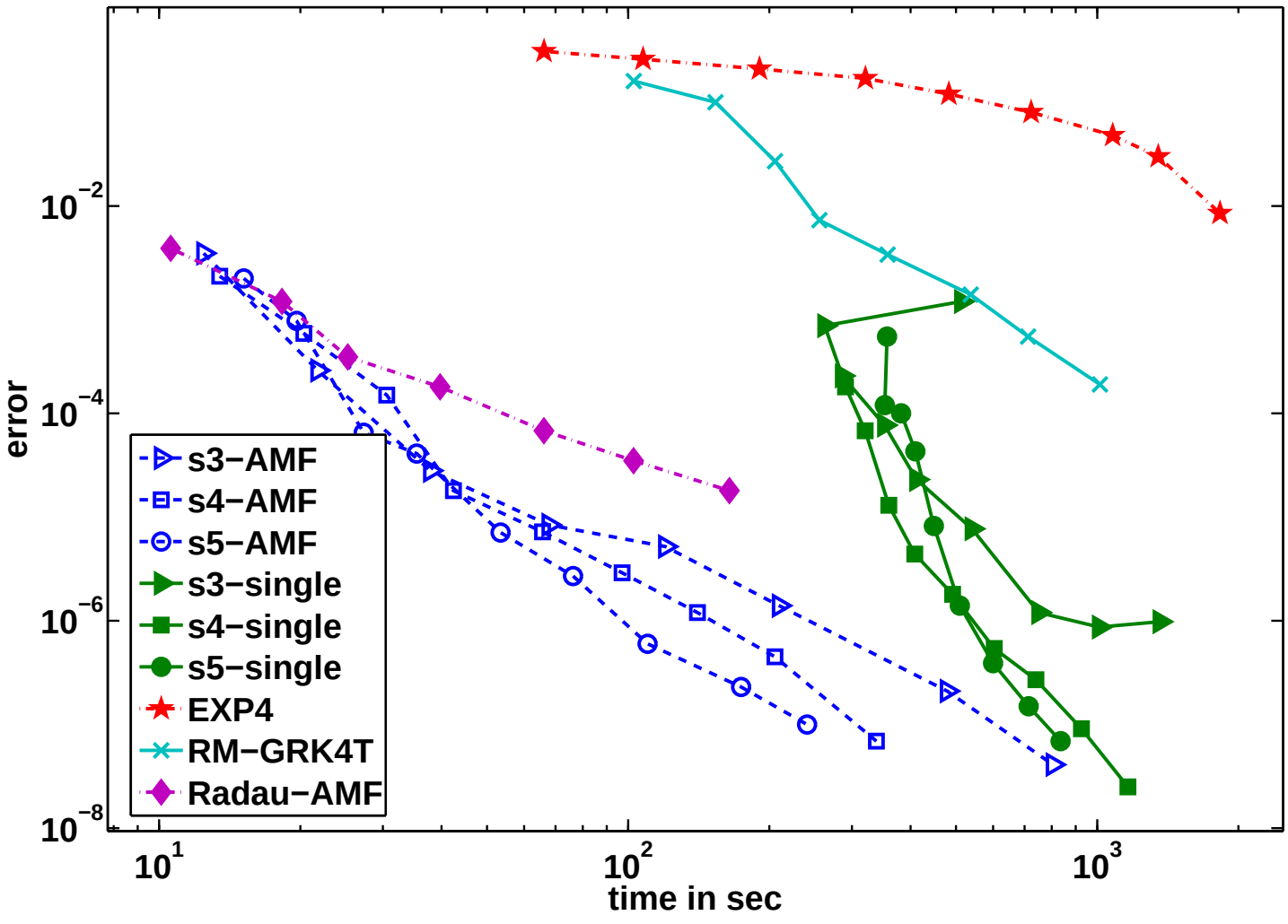
- from the book of Hundsdorfer/Verwer (2003)
  - two strongly coupled nonlinear diffusion equations
  - parameter Z_0: Difficulty of the problem increases with Z_0
- $J = J_x + J_y + J_r$
- J_x, J_y block-tridiagonal matrices(m x m-blocks), J_r block-diagonal matrix(2 x 2-blocks)
- $m = 100, 200\ , \qquad Z_0 = 1, 10$

Tolerances: $10^{-2}, 10^{-2.5}, \ldots, 10^{-6}$

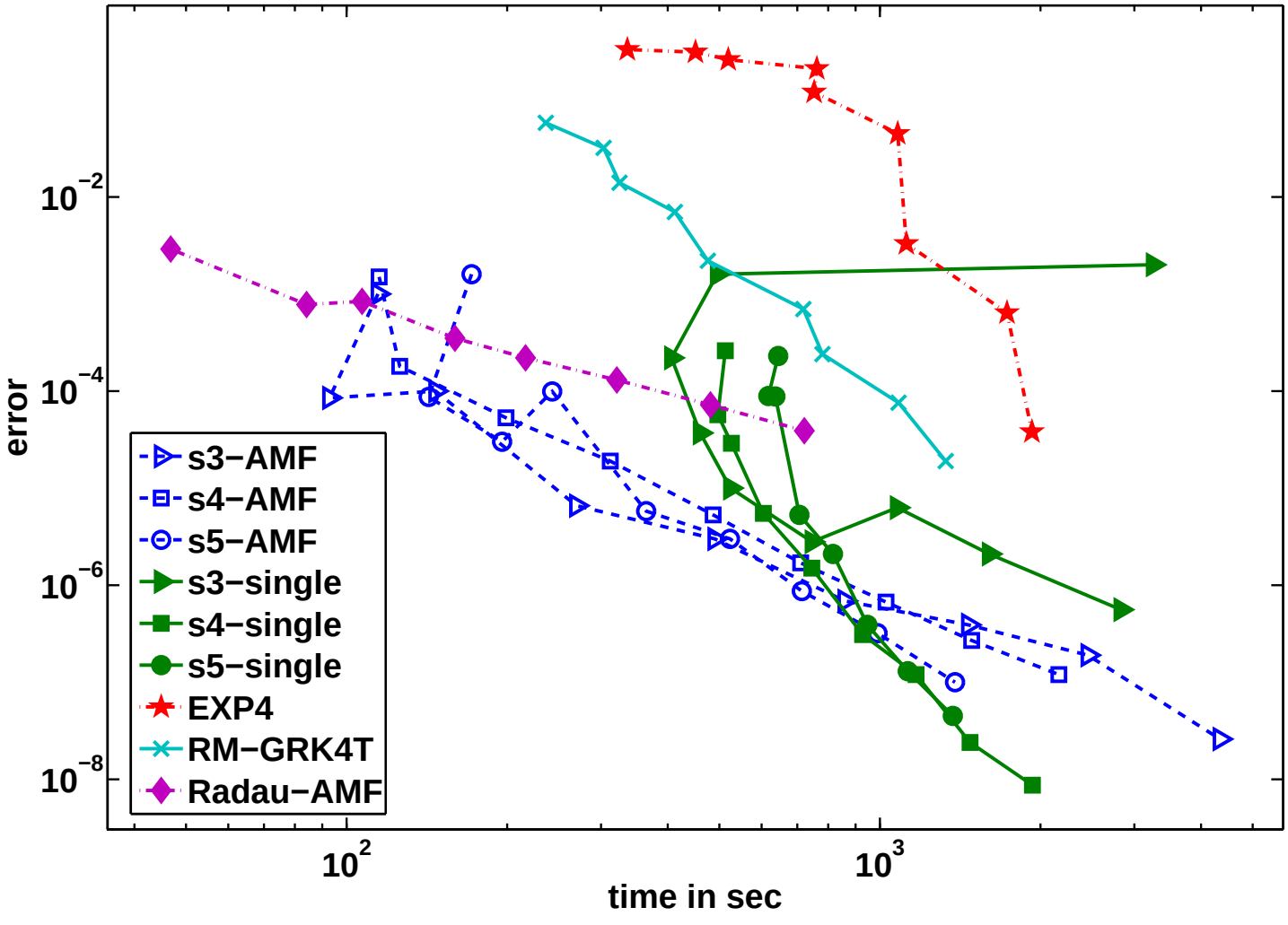
Radiation: $N = 20000,\ Z_0 = 1$



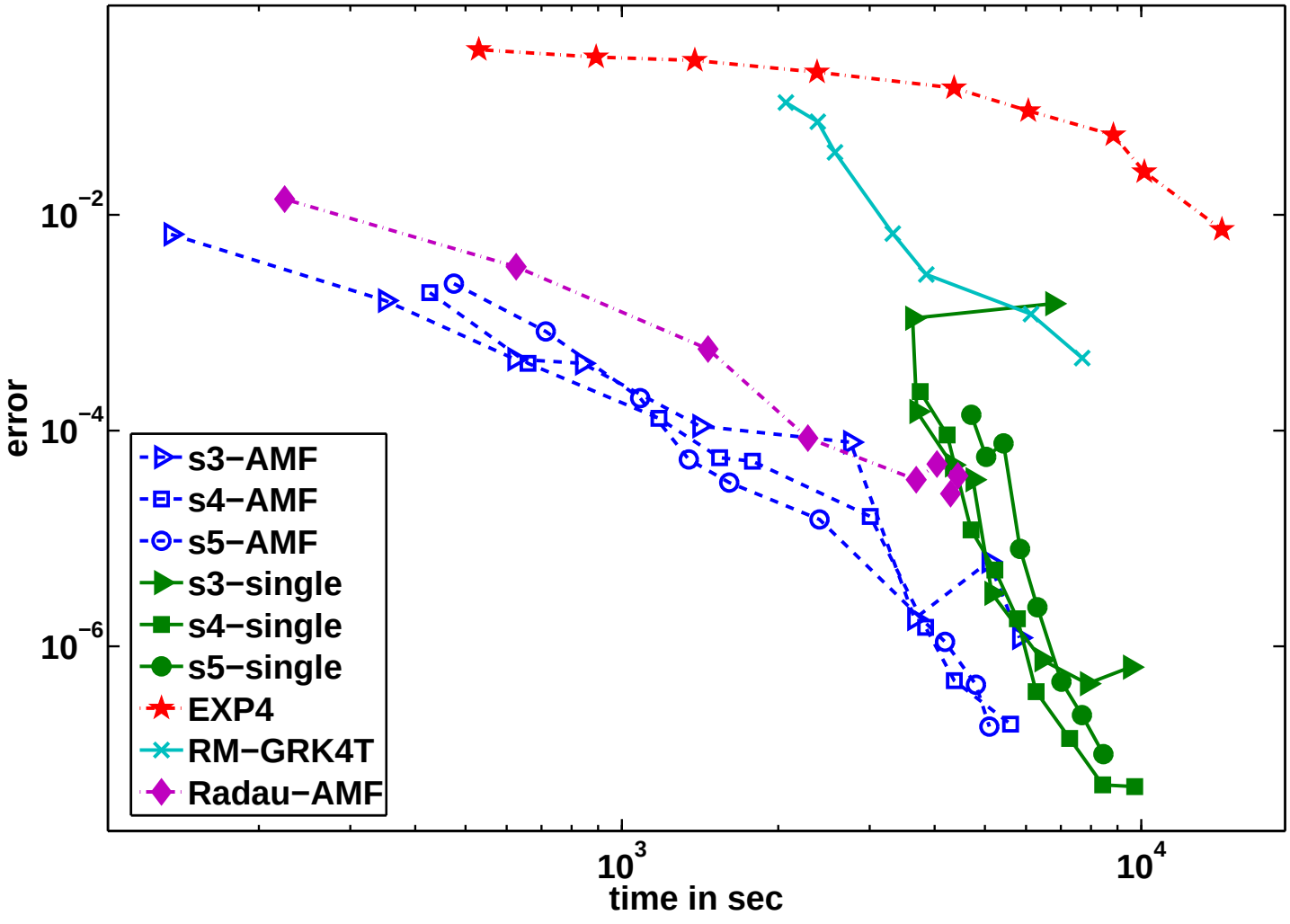
Radiation: $N = 20000,\ Z_0 = 10$



Radiation: $N = 80000,\ Z_0 = 1$



Radiation: $N = 80000,\ Z_0 = 10$



Conclusions:

- Implicit peer methods with Krylov and AMF efficient and reliable
- $M(\infty) = 0$, L-stability possible
- No order reduction observed
- Krylov: robust and requires no special implementation
- AMF: implementation is very time consuming, but is faster especially for crude tolerances

Outlook:

- Application to DAEs/PDAEs
- parallel methods

MATLAB codes: ROWMAP, PEER-Krylov, Radiation-AMF available

Thank you for your

attention!