# 3rd-order A-stable alternating implict RK schemes

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# An old breakthrough

- Alternating Direction Implicit (ADI) schemes [Peaceman & Rachford 55; Douglas & Rachford 56]
- Consider 2D parabolic problem

$$\partial_t u = \Delta u = L_0(u) + L_1(u), \quad L_0(u) := \partial_{xx} u, \quad L_1(u) := \partial_{yy} u$$

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$$\mathsf{U}^{n,1} = \mathsf{U}^n + \tfrac{1}{2}\tau \mathbb{L}_0(\mathsf{U}^{n,1}) + \tfrac{1}{2}\tau \mathbb{L}_1(\mathsf{U}^n)$$
$$\mathsf{U}^{n+1} := \mathsf{U}^{n,2} = \mathsf{U}^n + \tau \mathbb{L}_0(\mathsf{U}^{n,1}) + \tfrac{1}{2}\tau\big(\mathbb{L}_1(\mathsf{U}^n) + \mathbb{L}_1(\mathsf{U}^{n,2})\big)$$

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  Combination of midpoint and Crank–Nicolson schemes

- Second-order accurate and A-stable

- Highly efficient when using FD in space (tridiagonal solves)

- Quite popular in Russian literature [Yanenko 71; Marchuk 90]

# Runge–Kutta (RK) schemes

- $(s+1)$-stage scheme represented by Butcher tableau $\begin{array}{c|c} c & A \\ \hline & b \end{array}$
  - $A \in \mathbb{R}^{s+1,s+1}$ strictly lower triangular $\Longrightarrow$ explicit scheme
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  - Simplifying assumptions
    - $AU = c$ with $U := (1, \ldots, 1)^\mathsf{T}$ (Butcher's simplifying assumption)
    - $c_1 = A_{11} = 0$ (first stage trivial), $c_s = 1$ and $e_s^\mathsf{T} A = b$ (last stage trivial) $\Longrightarrow$ only $s$ nontrivial stages

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- Order conditions well understood
  - $bc = \frac{1}{2}$ (2nd-order), $bc^2 = \frac{1}{3}$, $bAc = \frac{1}{6}$ (third-order), $\cdots$

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- Linear stability studied through amplification function

$$R(z) := 1 + \frac{\rho(z)}{\det(I - zA)}, \qquad \rho(z) = \det(I - zA) z b (I - zA)^{-1} U$$

  - A($\alpha$)-stability whenever $|R(z)| \leq 1$ for all $z \in \mathbb{C}^-$, $\arg(-z) \leq \alpha$
  - L($\alpha$)-stability if also $\ell := \lim_{\Re(z) \to -\infty} R(z) = 0$
  - Dahlquist's test problem $\partial_t u = \lambda u$ (operator $\mathbb{L}$ with eigenvalue $\lambda \in \mathbb{C}^-$)

# Rewriting ADI as AIRK

- Two implicit Butcher arrays of size $s + 1 = 3$ (2 nontrivial stages)

$$\begin{array}{c|c} c & A_0 \\ \hline & b_0 \end{array} = \begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{2} & 0 & \frac{1}{2} & \\ 1 & 0 & 1 & 0 \\ \hline & 0 & 1 & 0 \end{array} \qquad \begin{array}{c|c} c & A_1 \\ \hline & b_1 \end{array} = \begin{array}{c|ccc} 0 & 0 & & \\ \frac{1}{2} & \frac{1}{2} & 0 & \\ 1 & \frac{1}{2} & 0 & \frac{1}{2} \\ \hline & \frac{1}{2} & 0 & \frac{1}{2} \end{array}$$

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  with $A_\theta := (1-\theta)A_0 + \theta A_1$, $b_\theta := (1-\theta)b_0 + \theta b_1$

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- For ADI, a simple calculation establishes A-stability

$$R_\theta(z) = \frac{1 + \frac{1}{2}\theta z}{1 - \frac{1}{2}\theta z} \times \frac{1 + \frac{1}{2}(1-\theta) z}{1 - \frac{1}{2}(1-\theta) z}$$

  Notice $\ell_\theta := \lim_{\Re(z)\to-\infty} R_\theta(z) = 1$, $\theta \notin \{0,1\}$, but $\ell_0 = \ell_1 = -1$

# Our goal

- Time-dependent (nonlinear) PDE (after space semi-discretization)

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- $\mathbb{L}_0, \mathbb{L}_1$ (diffusion/reaction) much stiffer than $\mathbb{L}_2$ (nonlinear transport)
- Use AIRK scheme for $\mathbb{L}_0, \mathbb{L}_1$ and explicit RK scheme for $\mathbb{L}_2$

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  - A($\alpha$)-stability for each constitutive implicit RK scheme, and possibly also L($\alpha$)-stability

# Literature

- Second-order barrier for exponential splitting methods (with only forward steps and positive coefficients) [Sheng 89; Suzuki 91; Goldman & Kaper 96; Blanes & Casas 05]

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- Interlacing two (or more) RK schemes
  - additive RK (ARK) methods [Rice 60; Cooper & Sayfy 83; Rentrop 85]
  - important example are IMEX methods [Zhong 96; Ascher, Ruuth & Spiteri 97; Pareschi & Russo 01; Kennedy & Carpenter 03]
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  - much less known about stability, even linear
- We prove that there is a stability barrier for $s = 4$ nontrivial stages
- Our goal can be achieved with $s = 6$ nontrivial stages

# Six-stage AIRK scheme(s)

- Butcher tableaux (we omit line vector $b$ for simplicity)

$$
\begin{array}{c|ccccccc}
0 & 0 & & & & & & \\
c_2 & \bullet & {\color{red}\bullet} & & & & & \\
c_3 & \bullet & \bullet & 0 & & & & \\
c_4 & \bullet & \bullet & \bullet & {\color{red}\bullet} & & & \\
c_5 & \bullet & \bullet & \bullet & \bullet & 0 & & \\
c_6 & \bullet & \bullet & \bullet & \bullet & \bullet & {\color{red}\bullet} & \\
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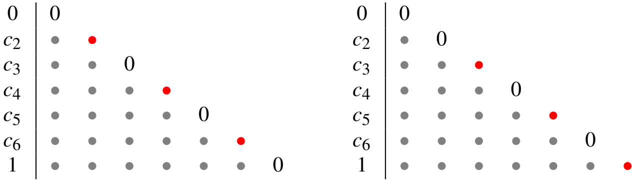


- We take equi-distributed substages, $c_m = \frac{m-1}{6}$, $m \in \{1{:}7\}$
  - optimizes CFL condition for ERK scheme [Shu & Osher 88; AE & JLG 23]

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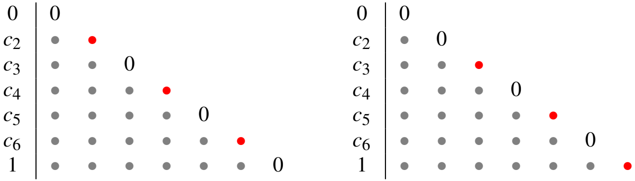


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- There are 48 unknown coefficients for AIRK (24 for each array)

- There are 24 (non)linear relations coming from
  - Butcher's simplifying assumption (12 linear relations)
  - third-order (single and coupled) conditions (8 (non)linear relations)
  - requiring singly diagonal schemes (4 linear relations)

- There are 15 additional nonlinear relations related to stability

# Our approach to stability

- Recall combined amplification function ($z \in \mathbb{C}^-$, $\theta \in [0,1]$)

$$R_\theta(z) = 1 + \frac{\rho_\theta(z)}{\det(I - zA_\theta)}, \qquad \rho_\theta(z) := \det(I - zA_\theta) z b_\theta (I - zA_\theta)^{-1} U$$

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- $\rho_\theta \in \mathbb{P}_6[z]$ (and not $\mathbb{P}_7[z]$ by Hamilton–Cayley)

$$\rho_\theta(z) = \sum_{k \in \{0:5\}} \omega_k(\theta) z^{k+1}$$

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  - $\omega_5(\theta) \in \mathbb{P}_5[\theta] \Longrightarrow$ 6 conditions
  - we also set $\omega_4'(0) = \omega_4'(1) = 0$ and $\omega_4(\frac{1}{2}) \approx 0 \Longrightarrow$ 3 conditions

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- A-stability of single RK schemes further requires 6 necessary conditions

$$\omega_4(0) = \omega_4(1) = \omega_3(0) = \omega_3(1) = 0$$

$$\omega_2(0) = (\ell_0 - 1)(\bullet_1)^3, \quad \omega_2(1) = (\ell_1 - 1)(\bullet_2)^3, \quad \ell_0, \ell_1 \in [-1, 1]$$

Two natural choices are $\ell_0 = \ell_1 = 0$ (L-stability) or $\ell_0 = \ell_1 = 1$

# Tidying up and ERK companion scheme

- 48 unknowns and 39 (non)linear relations
  - can be solved (with care) in quadruple precision with `julia`
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- Companion ERK scheme

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c_6 & \bullet & \bullet & \bullet & \bullet & \bullet & 0 & \\
1 & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & 0
\end{array}$$

# Tidying up and ERK companion scheme

- 48 unknowns and 39 (non)linear relations
  - can be solved (with care) in quadruple precision with `julia`
  - for both choices, $\ell_0 = \ell_1 = 0$ (L-stability) or $\ell_0 = \ell_1 = 1$
  - A(0)-stability is indeed achieved for all $\theta \in [0, 1]$

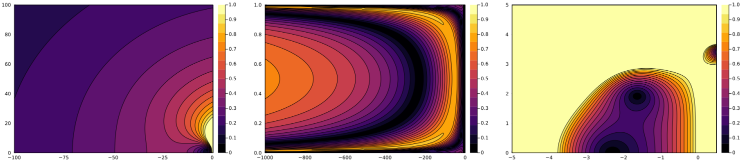
- Companion ERK scheme

$$\begin{array}{c|ccccccc} 0 & 0 & & & & & & \\ c_2 & \bullet & 0 & & & & & \\ c_3 & \bullet & \bullet & 0 & & & & \\ c_4 & \bullet & \bullet & \bullet & 0 & & & \\ c_5 & \bullet & \bullet & \bullet & \bullet & 0 & & \\ c_6 & \bullet & \bullet & \bullet & \bullet & \bullet & 0 & \\ 1 & \bullet & \bullet & \bullet & \bullet & \bullet & \bullet & 0 \end{array}$$

  - 21 unknowns
  - Butcher's simplifying assumption and third-order (single and coupled) conditions $\Longrightarrow$ 13 (non)linear relations
  - one can also prescribe 3 additional conditions to achieve linear order 4
  - solved using `julia`

# Numerical illustrations

- L-stable AIRK. Left: modulus of amplification function $R_0(z)$ in $\mathbb{C}^-$ ($\alpha \approx 75°$). Center: absolute value of amplification function $R_\theta(x)$ along negative real axis and $\theta \in [0, 1]$. Right: modulus of amplification function for ERK companion scheme



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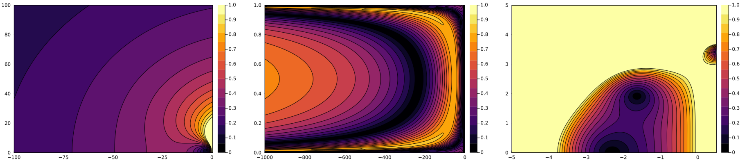

- 2D diffusion with nonlinear transport: $\partial_t u = \mu(\partial_{xx}u + \partial_{yy}u) - \boldsymbol{v}\cdot\nabla(\frac{1}{2}u^2)$, space semi-discretization using FEM

| $\mathbb{P}_1$ | | | $\mathbb{P}_2$ | | | $\mathbb{P}_3$ | | |
|---|---|---|---|---|---|---|---|---|
| $I$ | $L^2$-err | rate | $I$ | $L^2$-err | rate | $I$ | $L^2$-err | rate |
| 121 | 1.80E-02 | – | 441 | 4.95E-04 | – | 961 | 4.44E-05 | – |
| 441 | 5.08E-03 | 1.96 | 1681 | 3.39E-05 | 4.01 | 3721 | 2.76E-06 | 4.10 |
| 1681 | 1.31E-03 | 2.03 | 6561 | 2.17E-06 | 4.04 | 14641 | 1.76E-07 | 4.02 |
| 6561 | 3.29E-04 | 2.03 | 25921 | 1.37E-07 | 4.03 | 58081 | 1.25E-08 | 3.85 |
| 25921 | 8.24E-05 | 2.02 | 103041 | 8.60E-09 | 4.01 | 231361 | 1.49E-09 | 3.07 |
| 103041 | 2.06E-05 | 2.01 | 410881 | 5.90E-10 | 3.87 | 923521 | 2.86E-10 | 2.39 |

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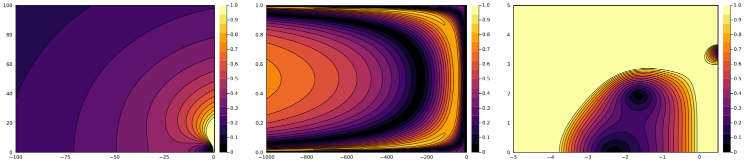

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| 121 | 1.80E-02 | – | 441 | 4.95E-04 | – | 961 | 4.44E-05 | – |
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Thank you for your attention!