Stiff Order Barriers and Runge-Kutta Methods that Avoid Order Reduction with an Optimal Number of Stages

Innovative and Efficient Strategies
for Stiff Differential Equations
July 21 - 25, 2025
ICERM, Providence RI

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July 25, 2025

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- VIASM VIETNAM INSTITUTE FOR ADVANCED STUDY IN MATHEMATICS for hosting visit June 2025.

Outline of the Talk

1. Stiff order conditions (for linear problems).

2. Stiff order barriers.

3. Schemes that satisfy the stiff order conditions.

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1. ~~Stiff order conditions (for linear problems).~~
   The Polynomial Equations.

2. ~~Stiff order barriers.~~
   Solvability of the equations.

3. ~~Schemes with weak stage order.~~
   Parameterized families of solutions.

Part I

Stiff Order Conditions and Weak Stage Order

Runge-Kutta Methods for Linear Equations

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Runge-Kutta with s stages:

$$g_i = u_n + \Delta t \sum_{j=1}^{s} a_{ij} \Big(Lg_j + f(t_n + \Delta t c_j) \Big) \ , \quad i = 1, 2, \ldots, s$$

$$u_{n+1} = u_n + \Delta t \sum_{j=1}^{s} b_j \Big(Lg_j + f(t_n + \Delta t c_j) \Big) \ ,$$

Runge-Kutta Coefficients

$$A = \begin{pmatrix} a_{11} & \cdots & a_{1s} \\ \vdots & \ddots & \vdots \\ a_{s1} & \cdots & a_{ss} \end{pmatrix} \quad b = (b_1, \ldots, b_s)^T, \quad c = (c_1, \ldots, c_s)^T.$$

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Types of RK schemes:

Explicit (ERK) $\qquad A = \begin{pmatrix} 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \qquad$ "RK4" (1895, 1901)

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$$A = \begin{pmatrix} \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \end{pmatrix}$$

Fully implicit

$$A = \begin{pmatrix} \frac{1}{2} + \frac{\sqrt{3}}{6} & 0 \\ -\frac{\sqrt{3}}{3} & \frac{1}{2} + \frac{\sqrt{3}}{6} \end{pmatrix}$$

Diagonally implicit (DIRK)

4th order Gauss-Legendre (left); Crouzeix's 3rd order DIRK (right).

Order of a Method

Definition (From Hairer Norsett Wanner '96)

A Runge-Kutta method has *order p* if for sufficiently smooth problems if there is a constant K for which

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Order conditions ($C = \mathrm{diag}(c)$) by matching Taylor series:

$p = 1$	$b^T e = 1$
2	$b^T c = \frac{1}{2}$
3	$b^T c^2 = \frac{1}{3}$ $\quad b^T A^2 e = \frac{1}{3!}$
4	$b^T c^3 = \frac{1}{4}$ $\quad b^T A^3 e = \frac{1}{4!}$ $\quad b^T A c^2 = \frac{1}{2}$ $\quad ACAc = 1$

Classical Convergence

Theorem

For smooth enough problems, a Runge-Kutta method satisfying the classical order conditions admits the error

$$\|u(\Delta t) - u_1\| \leq K \Delta t^{p+1} \qquad when \;\; \Delta t \|L\| < \mathcal{O}(1)$$

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Semi-discretizations of PDEs admit no such error estimate.

Message: Classical order conditions are insufficient.

Some Historical Remarks

Earliest observations

1. Prothero, Robinson 1974, Error in linear ODEs.
2. Crouzeix 1975 (Thesis), linear PDEs,
   (i) Periodic domains: No order reduction.
   (ii) Non-periodic: Problem data unusual requirements.

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Generalizations to other PDEs:

1. Lubich, Ostermann 1995, quasilinear PDEs.
2. Ostermann, Thalhammer 2002, nonlinear elliptic PDEs.
3. Alonso-Mallo, Palencia 2002, C0 semigroups.

Why High Order?

Computation to accuracy ϵ over time $[0, T]$:

$$\|u(n\Delta t) - u_n\|_{L^\infty} \leq \epsilon = K\Delta t^p \quad \Longrightarrow \quad \#\,\text{steps} \sim T/\epsilon^{1/p}\ .$$

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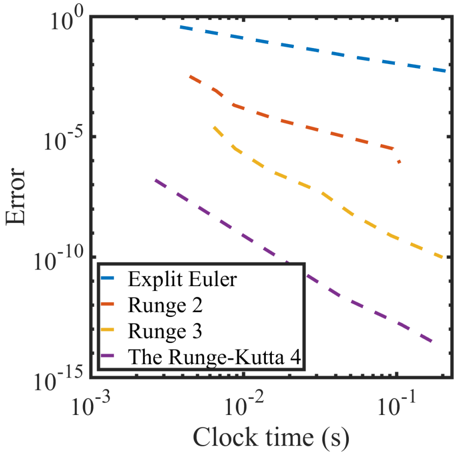

Figure: $y'' + y = 0,\ T = 10.$

Avoiding Order Reduction in RK Schemes

Approach # 1: Modifying Runge-Kutta Coefficients.

[1] Versions of this theorem are found: Burrage, Hundsdorfer, Verwer, '86 for ODEs and Ostermann, Roche '92, '93; Alonso-Mallo, Palencia '03 for PDEs.

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A big advance from the 1980's: theory of *stage order*.

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A Runge-Kutta method satisfies[1]

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Under mild assumptions, K is bounded uniform in L

$$K \sim b^T (I - \Delta t A \otimes L)^{-1} \left(Ac^k - \frac{1}{k}c^{k+1}\right) \otimes u^{(k)}$$

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Limitations of Stage Order

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Problem:

- DIRK have $q_s < 2$; at most 1st order.
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It turns out that while stage order is sufficient, it is not <u>necessary</u>!

There are in fact weaker necessary and sufficient stiff order conditions.

Stiff Order Conditions

The most general[2] stiff order conditions for linear problems:

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\begin{aligned}
b^T c^{k-1} &= \frac{1}{k} && k = 1, \dots, q \\
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We refer to as weak stage order.

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$$u^{(j)} = \left(g + \Delta t\, c_j \partial_t\, g + \Delta t^2 (Ac)_j\, \partial_t^2 g + \Delta t^3 (A^2 c)_j\, \partial_t^3 g\right)\Big|_{t=t_n+c_j\Delta t}$$

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Error estimates:

3. Alonso-Mallo 2002 (linear autonomous).
4. Alonso-Mallo, Cano 2004 (linear non-autonomous).

- Intrusive; Can require derivative information; DIRK Compatible.

Advances in Non-Runge-Kutta Schemes

1. Exponential Integrators
   (i) Hochbruck, Ostermann 2005, Explicit exponential RK for semilinear parabolic.
   (ii) Luan Vu Thai, Ostermann. 2013, Stiff order conditions.
   (iii) Hochbruck, Ostermann, 2018, Convergence Lawson methods on semilinear stiff problems.
   (iv) Cano, Moreta, 2022, Modified boundary conditions.

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   - (iv) Cano, Moreta, 2022, Modified boundary conditions.
2. Splitting Methods
   - (i) Hansen, Ostermann 2016, General stiff order conditions.
   - (ii) Einkemmer, Ostermann. 2015 & 2016, Modified boundary conditions.
3. Fractional step
   - (i) Alonso-Mallo, Cano, Jorge 2004, Modified boundary conditions.
4. Multistep Methods
   - (i) Lubich 1991, No order reduction, nonlinear stiff ODEs.

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$\Longrightarrow$ Runge-Kutta schemes are important for legacy codes.

$\Longrightarrow$ Motivates developing DIRK, ERK schemes that satisfy (weaker) stiff order conditions.

Avoiding Order Reduction in DIRKs via Coefficients

"To date, we are not aware of any efforts to remedy boundary order reduction by using Butcher coefficients for DIRK-type methods." —C. Kennedy and M. Carpenter 2016.

From: Diagonally Implicit Runge-Kutta Methods for Ordinary Differential Equations. A Review, NASA TM-2016-219173, 162 pg.

(Perhaps the closest is [Scholz 1989] for related ROW methods.)

Part II
Stiff Order Barriers

What can we say about the solvability?

Weak stage order (stiff order) conditions:

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\begin{aligned}
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Does a solution exist? (Over the reals)

Example: An $s = 2$ scheme

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \qquad b = \begin{pmatrix} b_1 & b_2 \end{pmatrix}^T \qquad c = Ae$$

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Equations for $q = 2$:

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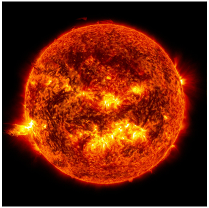

Photo credit: NASA (freely available).

In components:

$$b_1 + b_2 = 1$$
$$b_1 c_1 + b_2 c_2 = \tfrac{1}{2}$$
$$a_{11} b_1 c_1 - \tfrac{1}{2} b_2 c_2^2 - \tfrac{1}{2} b_1 c_1^2 + a_{12} b_1 c_2 + a_{21} b_2 c_1 + a_{22} b_2 c_2 = 0$$

$$\begin{aligned} a_{11}^2 b_1 c_1 - \tfrac{1}{2} a_{11} b_1 c_1^2 - \tfrac{1}{2} a_{12} b_1 c_2^2 - \tfrac{1}{2} a_{21} b_2 c_1^2 \\ -\tfrac{1}{2} a_{22} b_2 c_2^2 + a_{22}^2 b_2 c_2 + a_{11} a_{12} b_1 c_2 + a_{11} a_{21} b_2 c_1 \\ + a_{12} a_{21} b_1 c_1 + a_{12} a_{21} b_2 c_2 + a_{12} a_{22} b_1 c_2 + a_{21} a_{22} b_2 c_1 = 0 \end{aligned}$$

Equation and Variable Count

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Linear algebra guess for solvability?

Try:

$$\text{(Number variables)} \leq \text{(Number of equations)}.$$

Linear Algebra Guess

(Number variables) $\leq$ (Number of equations).

1. Actually gives a good estimate.
2. But (in some sense) for the wrong reason.

Historical Context: Classical Order Barriers

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Some classical order barriers:

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The barriers for ERK are still open.

$$\text{ERK}: \qquad p \leq s \qquad \text{(Linear theory)}$$

An improved (non-sharp) bound Butcher '75.

Historical Context: Stiff Order Barriers

Partial results exist but only when $q \leq 3$ for RK:

- Scholz '89: ROW methods, order barriers and schemes $q \leq 4$.
- Rang '16; Skvortsov '17: Schemes (including ERKs) $q \leq 3$.

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No systematic approach.

Order Barriers (Main Result)

$$b^T c^{k-1} = \frac{1}{k} \qquad b^T A^j \left(A c^{k-1} - \frac{1}{k} c^k \right) = 0 \qquad (k \le q, \forall j)$$

Theorem (Biswas Ketcheson Seibold Roberts DS '24-25)

An s stage Runge-Kutta method with stiff order $q \ge 2$ satisfies[3,4]

$$\begin{aligned} \text{Fully Implicit Schemes :} &\qquad q \le \frac{4}{3}s \\ \text{DIRK Schemes :} &\qquad q \le \frac{2}{3}s + 1 \\ \text{Explicit Schemes :} &\qquad q \le \frac{1}{2}s + \frac{1}{2}\ . \end{aligned}$$

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[3] A. Biswas, D. Ketcheson, B. Seibold, D.S., *Algebraic structure of the weak stage order conditions for Runge-Kutta methods* SIAM J. Numer. Anal., 62:1 (2024), pp. 48–72.

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- Sharper results for EDIRKs, confluent, stiffly accurate schemes.
- Generalize classical order barriers to include WSO.
- Significant for design of schemes (constructive information).

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Structure of Equations

Introduce

$$\tau^{(k)} = Ac^{k-1} - \frac{1}{k}c^k$$

The weak stage order equation is:

$$b^T A^j \tau^{(k)} = 0$$

How should we understand this equation?

Orthogonality Relations

The weak stage order equation is:

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When $j = 0$:

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Orthogonality Relations

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When $j = 0$:

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When $j = 1$:

$$b^T A \tau^{(k)} = 0$$

implies

$$b \perp A\tau^{(k)} \qquad \text{and} \qquad A^T b \perp \tau^{(k)}$$

Orthogonality Relations

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For arbitrary powers:

$$(A^T)^i b \quad \perp \quad A^j \tau^{(k)} \qquad \forall\, i, j$$

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For arbitrary powers:

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Moreover,

(All linear combinations $(A^T)^i b$) $\perp$ (All linear combinations $A^j \tau^{(k)}$)

WSO as Orthogonal Subspaces

Define the spaces[5]:

$$K_m := \text{span}\left\{\tau^{(1)}, A\tau^{(1)}, \ldots, A^{s-1}\tau^{(1)}, \tau^{(2)}, A\tau^{(2)}, \ldots, A^{s-1}\tau^{(m)}\right\}.$$

$$Y := \text{span}\left\{b, A^T b, \ldots, (A^T)^{s-1} b\right\}.$$

Then K_m is A-invariant, Y is A^T-invariant.

[5] R. R. Rosales, B. Seibold, DS, D. Zhou *Spatial manifestations of order reduction in Runge-Kutta methods for initial boundary value problems*, Commun. Math. Sci., 22:3, (2024), pp 613-653.

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Lemma

Weak stage order of at least q iff $Y \perp K_q$, in which case

$$\dim(Y) + \dim(K_q) \leq s\ . \tag{1}$$

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[6] Algebraic conditions equivalent to $W_k(z) \equiv 0$ for $k \leq q$

Step 1: Lower bound on dim Y

$$\text{Fully Implicit Schemes:} \quad \dim Y \geq \left\lfloor \frac{q+1}{2} \right\rfloor ,$$

$$\text{DIRK Schemes:} \quad \dim Y \geq q - 1$$

$$\text{Explicit Schemes:} \quad \dim Y \geq q .$$

Step 1: Lower bound on dim Y

Stability function for pth order scheme

$$R(z) = 1 + zb^T(I - zA)^{-1}e = \frac{N(z)}{D(z)}$$

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3. Which bounds $q \leq \deg N + \deg D$ (fully implicit), $\leq \deg N + 1$ (DIRK) and $\leq \deg N$ (ERK) to e^z.

Step 2: Lower bound on dim K_q

- General schemes ($q \leq 2n_c$)

$$\dim K_q \geq q - n_c$$

- DIRK schemes

$$\dim K_q \geq \left\lfloor \frac{q}{2} \right\rfloor ,$$

- Explicit schemes

$$\dim K_q \geq q - 1 ,$$

where n_c is the number of distinct c values.

Intuition

We know that ($k \leq m$):

$$A^j \tau^{(k)} = A^j \left(Ac^{k-1} - \frac{1}{k} c^k \right) \in K_m$$

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What is $\operatorname{rank} V$?

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Observation that for large enough m:

$$\operatorname{col}(V) \subseteq K_m \qquad \text{then} \qquad \dim K_m \geq s$$

Lower Bound Using Matrix Lemma

- ERK/DIRK schemes A is lower triangular.
- ERK nilpotent.
- Lower triangular matrices form a sub-algebra in the matrix algebra, e.g.,

$$\begin{pmatrix} \star & & \\ \star & \star & \\ \star & \star & \star \end{pmatrix}^2 = \begin{pmatrix} \star & & \\ \star & \star & \\ \star & \star & \star \end{pmatrix}, \quad \begin{pmatrix} \star & \\ \star & \star \end{pmatrix} + \begin{pmatrix} \star & \\ \star & \star \end{pmatrix} = \begin{pmatrix} \star & \\ \star & \star \end{pmatrix}.$$

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Using this structure

$$\text{DIRKs:} \quad \dim K_m \geq \lfloor \tfrac{m}{2} \rfloor \qquad \text{ERKs:} \quad \dim K_m \geq m - 1\,.$$

Order Barriers: Putting the Pieces Together

Thus, we have:

- Bounds on $\dim Y$
- Bounds on $\dim K_q$
- along with $Y \oplus K_q \subseteq \mathbb{R}^s$

yields the order barriers.

Theorem

An s stage Runge-Kutta method with stiff order q (≥ 2) satisfies

$$\begin{aligned}
\text{Fully Implicit Schemes :} \quad & q \leq \frac{4}{3}s \\
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Part III
Construction of Optimal Schemes

A Curious Observation

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$\frac{3}{11}$	$\frac{3}{11}$				
$\frac{15}{19}$	$\frac{285645}{493487}$	$\frac{103950}{493487}$			
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1	$\frac{196687}{177710}$	$-\frac{129383023}{426077496}$	$\frac{48013}{42120}$	$-\frac{2268}{2405}$	
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Notation for Main Result

Write

$$A = \begin{bmatrix} 0 & 0 & 0 \\ A_{21} & A_{22} & 0 \\ A_{31} & A_{32} & A_{33} \end{bmatrix}, \quad c = \begin{bmatrix} 0 \\ c_U \\ c_L \end{bmatrix}, \qquad (3)$$

Here $c_U \in \mathbb{R}^{q-1}$ and $c_L \in \mathbb{R}^{s-q}$.
Introduce the following (generalized) Vandermonde matrices:

$$V_U = \left[\; c_U \;\middle|\; c_U^2 \;\middle|\; \cdots \;\middle|\; c_U^{q-1} \; \right], \qquad W_U = \left[\; \tfrac{1}{2} c_U^2 \;\middle|\; \tfrac{1}{3} c_U^3 \;\middle|\; \cdots \;\middle|\; \tfrac{1}{q} c_U^q \; \right],$$

$$V_L = \left[\; c_L \;\middle|\; c_L^2 \;\middle|\; \cdots \;\middle|\; c_L^{q-1} \; \right], \qquad W_L = \left[\; \tfrac{1}{2} c_L^2 \;\middle|\; \tfrac{1}{3} c_L^3 \;\middle|\; \cdots \;\middle|\; \tfrac{1}{q} c_L^q \; \right].$$

ERK Schemes with Minimum s (Main Result)

- What structure do schemes with *smallest* $\dim K_q = q - 1$ have?
- Will be useful for constructing ERKs with WSO ($2q = s + 1$).

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$$A_{33}L - LW_U V_U^{-1} = (A_{33}V_L - W_L)\, V_U^{-1}\,, \tag{4}$$

$$LA_{22} - A_{33}L = A_{32}\,. \tag{5}$$

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(e) $R(z) = \sum_{j=0}^{p} \frac{1}{j!} z^j$ *is the q-th partial sum of e^z.*

Sketch of Proof

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- Necessary conditions are sufficient to construct schemes with WSO $\geq q$.

Construction of $(A, \mathbf{b})$ with WSO at least q:

Input: Parameters (A_{22}, A_{33}, c) where $0 = c_1, c_2, \ldots, c_{q+1}$ distinct.

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3. Set $\mathbf{b} = \begin{pmatrix} 1 & 0 \\ 0 & -L^T \\ 0 & I \end{pmatrix} \mathbf{d}$, $\quad A = \begin{pmatrix} 0 & 0 & 0 \\ \mathbf{a}_{21} & A_{22} & 0 \\ \mathbf{a}_{31} & A_{32} & A_{33} \end{pmatrix}$ and c.
4. Solve d to satisfy *bushy-tree* order conditions.

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1. Solve L via 2nd Sylvester equation (always possible).
2. Set $A_{32} := LA_{22} - A_{33}L$ and set $(\mathbf{a}_{21}, \mathbf{a}_{31})$ using $c = Ae$.
3. Set $\mathbf{b} = \begin{pmatrix} 1 & 0 \\ 0 & -L^T \\ 0 & I \end{pmatrix} \mathbf{d}, \qquad A = \begin{pmatrix} 0 & 0 & 0 \\ \mathbf{a}_{21} & A_{22} & 0 \\ \mathbf{a}_{31} & A_{32} & A_{33} \end{pmatrix}$ and c.
4. Solve d to satisfy *bushy-tree* order conditions.

- Complete parameterization of all schemes $2q = s + 1$.
- We use free parameters to solve non-linear order conditions, optimize error constants!

Example: $(3,2,2)$ schemes

All $(3,2,2)$ schemes have $a_{3,2}=0$. Complete parameterization:

$$\begin{array}{c|ccc} 0 & & & \\ c_2 & c_2 & & \\ c_3 & c_3 & & \\ \hline & -1-\frac{1}{2c_2}-\frac{1}{2c_3} & \frac{c_3}{2c_2(c_3-c_2)} & \frac{c_2}{2c_3(c_2-c_3)} \end{array}.$$

Example scheme (with smallest magnitude coefficients):

$$\begin{array}{c|ccc} 0 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ 1 & 1 & & \\ \hline & -\frac{1}{2} & 2 & -\frac{1}{2} \end{array}.$$

An Optimized $(5, 3, 3)$ scheme

There is a 6-parameter family of $(5, 3, 3)$ schemes (2 parameters from A_{22}, A_{33}, 4 from c).
An optimal scheme is:

$$
\begin{array}{c|ccccc}
0 & & & & & \\
\frac{3}{11} & \frac{3}{11} & & & & \\
\frac{15}{19} & \frac{285645}{493487} & \frac{103950}{493487} & & & \\
\frac{5}{6} & \frac{3075805}{5314896} & \frac{1353275}{5314896} & & & \\
1 & \frac{196687}{177710} & -\frac{129383023}{426077496} & \frac{48013}{42120} & -\frac{2268}{2405} & \\
\hline
 & \frac{5626}{4725} & -\frac{25289}{13608} & \frac{569297}{340200} & \frac{324}{175} & -\frac{13}{7}
\end{array}
$$

Above scheme first minimizes the principle error:

$$
\sum_{t \in T_{p+1}} \left(\frac{1}{\sigma(t)} \left(\frac{1}{\gamma(t)} - \sum_{j=1}^{s} b_j \Phi_j(t) \right) \right)^2
$$

Among minimizers of principle error, then minimizes $\max\{|a_{i,j}|, |b_i|, |c_i|\}$.

Constructed Schemes: Number of Stages

$q \diagdown p$	2	3	4	5
1	2	3	4	6
2	3	4	5	6
3	4	5	6	7
4	5	6	7	8
5	6	7	8	9

Table: # stages for constructed RK schemes with order p and WSO q.

- $q = 1$ row $\Longrightarrow$ well-known bounds for ERK up to $p \leq 5$.
- All other schemes are sharp: $s = p + q - 1$.
- $p = 1$ is omitted; explicit Euler has $q = \infty$.
- Solid and dashed boxes represent practically relevant schemes.
- Note: scheme coefficients $\in \mathbb{Q}$, exactly satisfy order conditions; minimal principle errors.

A Flavour of Other Results

1. Efficient implementations for explicit WSO schemes as GARKS
   - p evaluations of Lu
   - s evaluations of $f(t)$.

---

2. Parallel iterated schemes: p parallel schemes with p stages:

Theorem

For all $p \geq 2$, $\exists$ explicit RK schemes with $(s, p, q) = (p^2, p, p)$.

---

3. Theoretical compatibility of WSO with a strong stability preserving property for linear problems — but not nonlinear conditions.

Example: Implicit Schemes with WSO

Ex. DIRK $(s, q) = (3, 3)$: $\dim Y = 2$, $\dim K_q = 1$

$$A = \begin{pmatrix} (1 \mp \frac{\sqrt{2}}{2})a & 0 & 0 \\ (\frac{1}{2} \pm \frac{\sqrt{2}}{2})a & \frac{1}{2}a & 0 \\ a_{31} & a_{32} & \frac{3a-2}{6(a-1)} \end{pmatrix}, \quad a \in \mathbb{R}.$$

Ex. (Infinite family) Gauss-Legendre satisfy a version of the fully implicit bounds sharply ($q = s$, $p = 2s$ implies $\dim K_q = 0$, $\dim Y = s$).

Construction of Implicit Schemes with WSO

Developed[7] optimized diagonally implicit schemes:

- 7 stage, 4th order, WSO 4 scheme DIRK-$(7, 4, 4)$
- 12 stage, 5th order, WSO 4 scheme DIRK-$(12, 5, 4)$
- 12 stage, 5th order, WSO 5 scheme DIRK-$(7, 5, 5)$

They satisfy other desirable properties:

- A-stability with rigorous certificates[8];
- Stiff accuracy;
- Positive abscissas.

---

[7] A. Biswas, D. Ketecheson, B. Seibold, DS, *Design of DIRK schemes with high weak stage order*, CAMCOS 18(1):1-28, 2023.

[8] A. Juhl, DS, *Algebraic conditions for stability in Runge-Kutta methods and their certification via semidefinite programming*, Appl. Numer. Math., 207 (2025), pp 136-155.

Conclusions

For stiff order conditions:

1. New necessary solvability conditions.
2. New solution approaches: highly optimized schemes.
3. Open: SSP + Stiff order still open for implicit schemes.

Thank You!

Alternative Version Matrix Lemma

Given

$$K_m := \text{span}\left\{\tau^{(1)}, A\tau^{(1)}, \ldots, A^{s-1}\tau^{(1)}, \tau^{(2)}, A\tau^{(2)}, \ldots, A^{s-1}\tau^{(m)}\right\}.$$

Lemma (Bound on dim K_m)

The space K_m has the bound, $n_c = \#$ distinct c_j (abscissa):

$$\dim K_m \geq m - n_c \;, \quad \textit{if } m < 2n_c$$

and

$$K_m = \mathcal{K}(V) \;, \quad \textit{if } m \geq 2n_c \;.$$

Here $\mathcal{K}(V)$ is the smallest A-invariant space containing V where

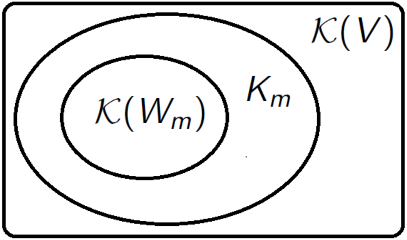
$$V = [e, c, \ldots, c^{n_c - 1}] \;, \quad \textit{if no } c_j = 0 \;,$$
$$V = [c, \ldots, c^{n_c - 1}] \;, \quad \textit{if a } c_j = 0 \;.$$

Intuition for proof — K_m "sandwich"

We establish

$$\mathcal{K}(W_m) \subseteq K_m \subseteq \mathcal{K}(V) \ ,$$

where $\mathcal{K}(X)$ is the smallest A-invariant space containing X.



- V is the Vandermonde matrix

$$V = \left(e \mid c \mid \ldots \mid c^{n_c - 1}\right) \ , \quad (\text{no } c_j = 0 \ ) \ .$$

- W_j are nested subspaces that converge

$$W_j \subset W_{j+1} \subset \ldots \subset V \ .$$

Lower bound on dim K_m: General Case

Denoting a polynomial $w(x)$ as

$$w(x) = w_{m-1}x^{m-1} + \ldots + w_0, \quad \text{and} \quad W(x) := \int_0^x w(s)\,\mathrm{ds}\ ,$$

The space K_m contains lin. combinations of $\tau^{(j)} = A\mathbf{c}^{j-1} - \frac{1}{j}\mathbf{c}^j$:

$$\sum_{j=1}^{m} w_{j-1}\tau^{(j)} = \big(Aw(C) - W(C)\big)\mathbf{e} \in K_m\ .$$

- Set $w(x) = \alpha(x)P_C(x)$, (allowed when m large enough)
- $P_C(x)$ is minimum polynomial of C, e.g., $P_C(C) = 0$

$$\big(\underbrace{Aw(C)}_{=0} - W(C)\big)\mathbf{e} = W(C)\mathbf{e} = W(\mathbf{c}) \in K_m\ .$$

Lower bound on dim K_m: General Case

Can then define:

$$W_m := \left\{ W(\mathbf{c}) \mid W \in \mathrm{range}\, \mathcal{I}[\alpha]\, , \alpha \in \Pi_{m-1-n_c} \right\}$$

where Π_d is the space of degree d polynomials and

$$\mathcal{I}[\alpha] := \left(\int_0^x \alpha(x) P_{\mathrm{C}}(x)\, \mathrm{dx} \right) \mod P_{\mathrm{C}}(x)\ .$$

We have shown that:

$$W_m \subseteq K_m \quad (\text{provided } m \geq n_c + 1)\ . \tag{7}$$

We can then compute the dimension of W_m to show that

$$\dim K_m \geq m - n_c\ .$$

Reason: $\mathcal{I}$ has a trivial null space (whenever $m < 2n_c$).
(Use the fact that $P_C(x)$ and $P'_C(x)$ are relatively prime.)

Lower bound on dim K_m

Part 2. $\dim \mathbf{W}_m$ bounds $\dim K_m$ from below.

- We can uniquely identify vectors $W(C)\mathbf{e}$ in $\mathbf{W}_m$ with the polynomial $W(x)$ mod $P_C(x)$.
- $\mathbf{W}_m$ has the same dimension as the range of $I : \mathbf{V}_{m-1-n_c} \to \mathbf{V}_{n_c-1}$ ($\mathbf{V}_d$ polynomials of deg $\leq$ d) defined by

$$I[\alpha] := \left(\int_0^x \alpha(x) P_{\mathrm{C}}(x) \, \mathrm{dx} \right) \quad \mathrm{mod} \ P_{\mathrm{C}}(x) \, ,$$

- We now claim that $I[\cdot]$ has a trivial null space whenever $m \leq 2n_c - 1$.
- Suppose not, $\exists \ \alpha(x)$ ($\deg \alpha \leq n_c - 2$) and $\beta(x)$ ($\deg \beta \leq n_c - 1$) such that

$$\int_0^x \alpha(x) P_{\mathrm{C}}(x) \mathrm{dx} = \beta(x) P_{\mathrm{C}}(x) \, .$$

- Differentiating both sides:
  $(\alpha(x) - \beta'(x)) \, P_{\mathrm{C}}(x) = \beta(x) P'_{\mathrm{C}}(x) \, .$
- Impossible since P_C and P'_C have no common root.

Lower bound on dim K_m: For DIRKs

For DIRKs: the top j components of τ_k depend only on the top $j \times j$ entries of A, e.g., let

$$[A]_j := \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1j} \\ a_{21} & \ddots & & \vdots \\ \vdots & & & \\ a_{j1} & a_{j2} & \cdots & a_{jj} \end{pmatrix} \quad \text{and} \quad [\mathbf{c}]_j := \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_j \end{pmatrix}.$$

Then

$$[A^n]_j = \left([A]_j\right)^n, \quad \text{and} \quad [\mathbf{c}^n]_j = \left([\mathbf{c}]_j\right)^n.$$

$$\tau^{(k)}([A]_j) := [A]_j \left[\mathbf{c}^{k-1}\right]_j - \frac{1}{k}\left[\mathbf{c}^k\right]_j$$

- $[A]_j$ and vectors $\tau^{(k)}([A]_j)$, define an $[A]_j$-invariant space.
- Apply the lower bound theorem to each $[A]_j$ $1 \le j \le s$, where n_c replaced with the # of distinct values in $\{c_1, \ldots, c_j\}$.
- We then pick the "worst case" j ($\sim q/2$ for non-confluent schemes) yields the tightest bound.

Lower bound on dim K_m: For DIRKs

Lemma (Dimension of K_m for a DIRK scheme)

Consider a DIRK scheme with n_c distinct abscissas, and the corresponding space K_m. Then

$$\dim K_m \geq \min\left\{\left\lfloor \frac{m+\kappa}{2} \right\rfloor, n_c\right\} - \kappa\ , \tag{8}$$

where $\kappa = 1$ if A is a GEDIRK scheme, and $\kappa = 0$ otherwise.

Combining the

- lower bound on $\dim(Y)$
- lower bound on $\dim(K_m)$
- orthogonal subspaces $\dim(Y) + \dim(K_m) \leq s$

We obtain the main result.