A Stiff Order Condition Theory for Runge–Kutta Methods: To Semilinearity and Beyond

ICERM Workshop on Innovative and Efficient Strategies for Stiff Differential Equations
July 25, 2025

Steven B. Roberts (Lawrence Livermore National Laboratory)
David Shirokoff (New Jersey Institute of Technology)
Abhijit Biswas (Indian Institute of Technology Kanpur)
Benjamin Seibold (Temple University)

Prepared by LLNL under Contract DE-AC52-07NA27344.

This Talk will Focus on Runge–Kutta Methods

- A Runge–Kutta method solves the ordinary differential equation (ODE)

$$y'(t) = f\big(y(t)\big), \quad y(t_0) = y_0$$

with the numerical procedure

$$Y_i = y_n + h \sum_{j=1}^{s} a_{i,j} f\left(Y_j\right), \quad i = 1, \dots, s,$$

$$y_{n+1} = y_n + h \sum_{j=1}^{s} b_j f\left(Y_j\right)$$

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$$

- We also use the notation $C = \mathrm{diag}(c)$.

Classical Runge–Kutta Convergence Requires Idealistic Assumptions

- Classical convergence assumes a moderate Lipschitz constant L for the RHS function f
- Δt must be "sufficiently small." Typically, we need $\Delta t \leq \mathrm{const}/L$ to reach the asymptotic regime
- When solving stiff problems, we use implicit method specifically to avoid an explicit-like time step restriction!
- Outside of the classical asymptotic regime, a method can experience degraded convergence called **order reduction**

There are Two Main Approaches to Eliminate Order Reduction

Modified Boundary Conditions	Enforce Additional Order Conditions
• Often intrusive to ODE/PDE solver implementations	• Compatible with any Runge–Kutta implementation
• Often require extra derivatives	• Often require additional stages
• No additional Runge–Kutta stages	• Deriving methods can be challenging
• See • Carpenter et al. "The theoretical accuracy of Runge–Kutta time discretizations for the IBVP." *SISC* (1995). • Pathria, D. "The Correct Formulation of Intermediate Boundary Conditions for Runge-Kutta Time Integration of IBVPs." *SISC* (1997). • …	• See • Skvortsov. "Model equations for accuracy investigation of Runge-Kutta methods." *Math. Models and Comp. Sims*. (2010). • Rang. "An analysis of the PR example for constructing new adaptive ESDIRK methods of order 3 and 4." *Appl. Numer. Math*. (2015). • Previous talks and more…

At the 2022 "Holistic Design of Time-Dependent PDE Discretizations" ICERM Workshop, I saw a few order reduction talks

Can we design practical Runge–Kutta methods without order reduction for **nonlinear** problems?

Order Reduction Remedies for Nonlinear Problems are Much Less Studied than Linear

Linear Problem	Nonlinear Problem
• Local error can be expressed in series involving only y derivatives: $e = c_1 h y' + c_2 h y'' + c_3 h y^{(3)} + \cdots$	• Local error typically involves derivatives of the RHS f: $e = c_1 h f + c_2 h^2 f' f + c_3 h^3 f'^2 f + \cdots$
• Derivative of y can be uniformly bounded away from transients	• Derivatives of f can grow disproportionally large from stiffness
• Scalar test problem sufficient, e.g., Prothero–Robinson	• Scalar test problem insufficient because terms commute & simplify

Let's Look Closer at a Standard Local Error Expansion for a Runge–Kutta Method

$$y(t_1) - y_1$$

$$= h(1 - b^T e)\underbrace{f(y_0)}_{= y'(t_0)} + h^2\left(\frac{1}{2} - b^T c\right)\underbrace{f'(y_0)f(y_0)}_{= y''(t_0)} + h^3\left(\frac{1}{6} + b^T A c\right)\underbrace{f'(y_0)^2 f(y_0)}_{= f'(y_0)y'(t_0)} + \cdots$$

Benign and bounded under typically assumptions

Benign and bounded under typically assumptions

This can't be bounded under typical assumptions!

We need an alternative expansion which can be uniformly bounded w.r.t stiffness

High Stage Order is a Well-Known Sufficient Condition for Nonlinear Problems

- The stage order of a method is the minimum of p, q satisfying

$$C(q): \quad Ac^{k-1} = \frac{c^k}{k}, \quad k = 1, \ldots, q,$$

$$B(p): \quad b^T c^{k-1} = \frac{1}{k}, \quad k = 1, \ldots, p$$

- This is very restrictive!
  - Explicit methods have max stage order of 1
  - Diagonally implicit methods have max of 2
- **But is high stage order necessary?**

Theorem 3.3: *Let $\alpha, \beta \in \mathbb{R}$ be given. Assume the Runge-Kutta method (1.3) is A-stable, AS-stable and ASI-stable. Then we have for the class of problems (1.5) satisfying (1.6) the (optimal) B-convergence result*

$$|\varepsilon_N| \leq C\tau^p \quad (0 < \tau \leq \bar{\tau})$$

with order

(a) $p = q$ if $B(q), C(q)$

(b) $p = q + 1$ if $B(q+1)$, $C(q)$ and ψ is uniformly bounded on $\mathbb{C}^-$.

Burrage, Kevin, W. H. Hundsdorfer, and Jan G. Verwer. "A study of B-convergence of Runge–Kutta methods." *Computing* 36.1-2 (1986): 17-34.

$$(3.3) \qquad p = \begin{cases} q & \text{if } B(q) \text{ and } C(q) \text{ hold,} \\ q+1 & \text{if } B(q+1) \text{ and } C(q) \text{ hold and } \psi(z) \text{ is uniformly bounded on } \mathbb{C}^-, \end{cases}$$

THEOREM 3.4.

i) *All Runge–Kutta methods of the family $\mathcal{M}_1$ are convergent on the class $\mathcal{F}_1$ with order p given by* (3.3)–(3.5).

ii) *All Runge–Kutta methods of the family $\mathcal{M}_2$ are convergent on the class $\mathcal{F}_2$ with order p given by* (3.3)–(3.5).

Calvo, M., S. González-Pinto, and J. I. Montijano. "Runge–Kutta methods for the numerical solution of stiff semilinear systems." *BIT Numerical Mathematics* 40 (2000): 611-639.

Singular Perturbation Theory is Also Relevant

- Consider the singular perturbation problem

$$y'(t) = f\big(y(t), z(t)\big)$$
$$\epsilon z'(t) = g\big(y(t), z(t)\big)$$

- We can expand the local error of a Runge–Kutta method as power series in both h and ϵ
- This gives order conditions for differential-algebraic equations of arbitrary index
- **These conditions are likely necessary but not sufficient**

ERROR OF RUNGE-KUTTA METHODS FOR STIFF PROBLEMS STUDIED VIA DIFFERENTIAL ALGEBRAIC EQUATIONS

E. HAIRER, CH. LUBICH and M. ROCHE

Université de Genève, Dept. de mathématiques, Rue du Lièvre 2-4, Case postale 240, CH-1211 Genève 24, Switzerland

Abstract.

Runge-Kutta methods are studied when applied to stiff differential equations containing a small stiffness parameter ε. The coefficients in the expansion of the global error in powers of ε are the global errors of the Runge-Kutta method applied to a differential algebraic system. A study of these errors and of the remainder of the expansion yields sharp error bounds for the stiff problem. Numerical experiments confirm the results.

ON A CLASS OF UNIFORMLY ACCURATE IMEX RUNGE–KUTTA SCHEMES AND APPLICATIONS TO HYPERBOLIC SYSTEMS WITH RELAXATION*

SEBASTIANO BOSCARINO† AND GIOVANNI RUSSO†

Abstract. In this paper we consider hyperbolic systems with relaxation in which the relaxation time ε may vary from values of order one to very small values. When ε is very small, the relaxation term becomes very strong and highly stiff, and underresolved numerical schemes may produce spurious results. In such cases it is important to have schemes that work uniformly with respect to ε. IMplicit-EXplicit (IMEX) Runge–Kutta (R-K) schemes have been widely used for the time evolution of hyperbolic partial differential equations but the schemes existing in literature do not exhibit uniform accuracy with respect to the relaxation time. We develop new IMEX R-K schemes for hyperbolic systems with relaxation that present better uniform accuracy than the ones existing in the literature and in particular produce good behavior with high order accuracy in the asymptotic limit, i.e., when ε is very small. These schemes are obtained by imposing new additional order conditions to guarantee better accuracy over a wide range of the relaxation time. We propose the construction of new third-order IMEX R-K schemes of type CK [S. Boscarino, *SIAM J. Numer. Anal.*, 45 (2008), pp. 1600–1621]. In several test problems, these schemes, with a fixed spatial discretization, exhibit for all range of the relaxation time an almost uniform third-order accuracy.

New Theory for Stiff Semilinear ODEs

We Start by Considering Semilinear Problems

- In nonlinear problems, stiffness often arises from linear terms
- Let's consider semilinear problems

Nonpositive logarithmic norm ensures the eigenvalues of J reside in the left half-plane

$$y'(t) = Jy(t) + g\big(y(t)\big)$$

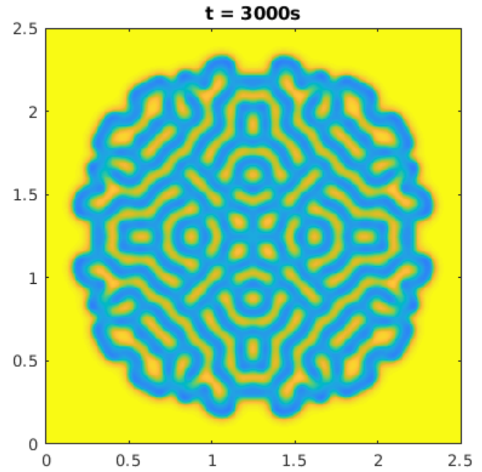
Stiff

$$\mathrm{Re}\langle y, Jy\rangle \leq 0$$

Nonstiff

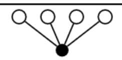
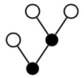
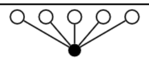
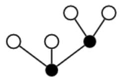
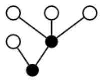
$$|g(y) - g(z)| \leq L|y - z|$$

- Examples include
  - Patten-forming diffusion reaction problems
  - Schrödinger equations
  - Air pollution transport models



Progress has been Made Outside of Runge–Kutta Methods

- Exponential Integrators
  - Hochbruck, and Ostermann. "Explicit exponential Runge-Kutta methods for semilinear parabolic problems." *SINUM* 43.3 (2005): 1069-1090.
  - **Luan, and Ostermann. "Exponential B-series: The stiff case."** ***SINUM*** **51.6 (2013).** →
  - Hochbruck, Leibold, and Ostermann. "On the convergence of Lawson methods for semilinear stiff problems." *Numerische Mathematik* 145 (2020).
- Splitting Methods
  - Hansen, and Ostermann. "High-order splitting schemes for semilinear evolution equations." *BIT Numerical Mathematics* (2016).
  - Einkemmer, and Ostermann. "Overcoming order reduction in diffusion-reaction splitting. Part 1: Dirichlet boundary conditions." *SISC* (2015).
  - Einkemmer, and Ostermann. "Overcoming order reduction in diffusion-reaction splitting. Part 2: Oblique boundary conditions." *SISC* (2016).
- Linear Multistep Methods
  - Wanner, and Hairer. Solving ordinary differential equations II. New York: Springer Berlin Heidelberg, 1996.
- Rosenbrock
  - Lubich, and Ostermann. "Linearly implicit time discretization of non-linear parabolic equations." *IMA Journal of Numerical Analysis* (1995).

Order	Tree	Stiff order conditions
3		$\sum_{i=2}^{s} b_i(Z)\frac{c_i^2}{2!} = \varphi_3(Z)$
4		$\sum_{i=2}^{s} b_i(Z)\frac{c_i^3}{3!} = \varphi_4(Z)$
5		$\sum_{i=2}^{s} b_i(Z)\frac{c_i^4}{4!} = \varphi_5(Z)$
5		$\sum_{i=2}^{s} b_i(Z)c_i K\psi_{3,i}(Z) = 0$
6		$\sum_{i=2}^{s} b_i(Z)\frac{c_i^5}{5!} = \varphi_6(Z)$
6		$\sum_{i=2}^{s} b_i(Z)c_i^2 M\psi_{3,i}(Z) = 0$
6		$\sum_{i=2}^{s} b_i(Z)c_i K\psi_{4,i}(Z) = 0$

For exponential methods, stiff order conditions can be mapped onto trees. The conditions must hold for all matrices Z, K, M

Our Semilinear Analysis Extends a Lesser-Known Classical Analysis

- Rooted trees and B-series are the standard tools for analyzing the local error of a Runge–Kutta scheme
- Albrecht proposed alternative order conditions based on recursive orthogonality conditions

SIAM J. NUMER. ANAL.
Vol. 33, No. 5, pp. 1712–1735, October 1996

THE RUNGE–KUTTA THEORY IN A NUTSHELL*

PETER ALBRECHT†

Abstract. In an earlier paper [Albrecht, *SIAM J. Numer. Anal.*, 24 (1987), pp. 391–406] Runge–Kutta methods were treated as (composite) linear methods. The resulting *linear* theory is elementary yielding the order conditions as orthogonal relations from a recursion. This paper further extends this approach and discusses its implications. It is extended to Fehlberg forms, and the global as well as the stage errors are given in great detail, including a new presentation of the principal error function that simplifies error minimization. The orthogonal structure of the order conditions has many advantages; it provides, in particular, a powerful strategy for existence proofs and facilitates the calculation of RK-methods. The recursion, which, originally, was designed to generate the order conditions, is considerably generalized by mappings and becomes a major tool also for the *classical* theory. It can be used for a *recursive* generation of rooted trees; also Butcher's elementary differentials and weights as well as his order conditions can be obtained recursively. To this purpose, the elementary weights are reformulated, and the rooted trees are complemented by "blossoms." The whole approach extends to Rosenbrock methods.

LEMMA 1.3. *$r_i(x_j)$, $w_i(x_j) \in \mathbb{R}^s$ are obtained from the following recursion.*
RECURSION 0.

(19a) $$r_i(x_j) = \gamma_i Y^{(i)}(x_j) + A w_{i-1}(x_j); \qquad w_1(x_j) := \mathbf{0};$$

$$w_i(x_j) = \sum_{l=0}^{i-2} D^l \frac{1}{l!} g_1^{(l)}(x_j) r_{i-l}(x_j)$$

$$+ \sum_{l=0}^{i-4} D^l \sum_{\substack{m,n\geq 2\\ m+n+l=i}} \frac{1}{l!} g_2^{(l)}(x_j) r_m(x_j)\cdot r_n(x_j)$$

$$+ \sum_{l=0}^{i-6} D^l \sum_{\substack{m,n,s\geq 2\\ m+n+s+l=i}} \frac{1}{l!} g_3^{(l)}(x_j) r_m(x_j)\cdot r_n(x_j)\cdot r_s(x_j)$$

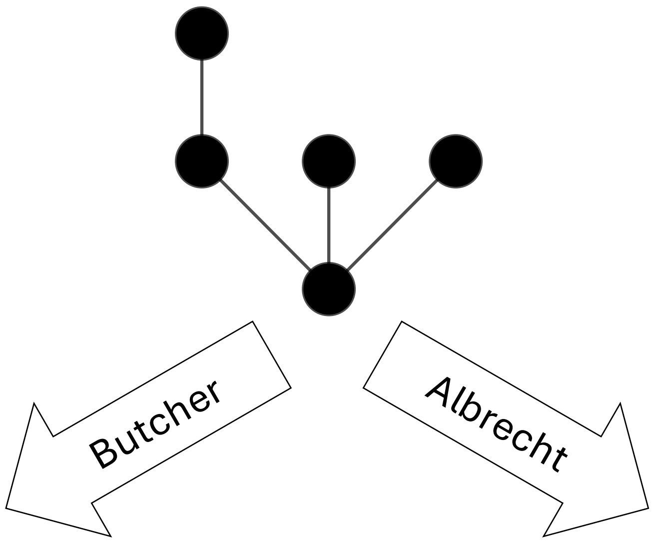
$$+ \quad \cdots$$

(19b) $$= \sum_{k=1}^{\infty} \sum_{l=0}^{i-2k} D^l \sum_{\substack{m_1,m_2,\ldots,m_k\geq 2\\ m_1+m_2+\ldots+m_k+l=i}} \frac{1}{l!} g_k^{(l)}(x_j) r_{m_1}(x_j)\cdot\cdots\cdot r_{m_k}(x_j),$$

$$i = 2, 3, \ldots, p-1.$$

Albrecht's Order Conditions are Equivalent to Butcher's, but…

- They use a different basis of elementary differentials
- Albrecht's initial derivation doesn't use trees, but he shows how to map order conditions to and from trees



Differential: $f'''(f, f, f'f)$

Order Condition: $\frac{1}{10} = b^T C^2 A c$

Differential: $\left(\frac{d^2 f'(y(t))}{dt^2}\right)_{t=t_0} y''(t_0)$

Order Condition: $0 = b^T C^2 \left(\frac{c^2}{2} - A c\right)$

The Primary Novelty is The Local Error Series for Stiff, Semilinear ODEs

We express the local error in the stages, step, and nonstiff function evaluation in the series

$$\Delta Y_0 = \sum_{i=1}^{r} \Delta Y_0^{\{i\}} h^i + \mathcal{O}(h^{r+1})$$

$$\Delta y_1 = \sum_{i=1}^{r} \Delta y_1^{\{i\}} h^i + \mathcal{O}(h^{r+1})$$

$$\Delta g_0 = \sum_{i=1}^{r-1} \Delta g_0^{\{i\}} h^i + \mathcal{O}(h^{r})$$

(Simplified) Theorem

Under mild ODE smoothness and Runge–Kutta stability assumptions, the series coefficients are

$$\Delta Y_0^{\{i\}} = (I - A \otimes Z)^{-1} \left(\left(\frac{c^i}{i!} - \frac{A c^{i-1}}{(i-1)!} \right) \otimes y^{(i)}(t_0) \right) + (A \otimes I)(I - A \otimes Z)^{-1} \Delta g_0^{\{i-1\}},$$

$$\Delta y_1^{\{i\}} = (b^T \otimes Z)(I - A \otimes Z)^{-1} \left(\left(\frac{c^i}{i!} - \frac{A c^{i-1}}{(i-1)!} \right) \otimes y^{(i)}(t_0) \right)$$
$$+ (b^T \otimes I)(I - A \otimes Z)^{-1} \Delta g_0^{\{i-1\}} + \left(\frac{1}{i!} - \frac{b^T c^{i-1}}{(i-1)!} \right) y^{(i)}(t_0),$$

$$\Delta g_0^{\{i\}} = \sum_{\ell=0}^{i-1} \sum_{\substack{m_1 + \dots \\ + m_k = i - \ell}} \frac{(-1)^{k+1}}{k! \ell!} (C^\ell \otimes I) \vec{g}^{(\ell;k)}(t_0) \left(\Delta Y_0^{\{m_1\}}, \dots, \Delta Y_0^{\{m_k\}} \right).$$

for h sufficiently small but independent of $Z = hJ$, i.e., stiffness.

Recall ODE is $y'(t) = Jy(t) + g(y(t))$

Let's Examine the 3rd Order Terms of the Local Error

$$\Delta y_1^{\{3\}} = \left(\frac{1}{6} - \frac{b^T c^2}{2}\right) y^{(3)}(t_0) + (b^T \otimes Z)(I - A \otimes Z)^{-1}\left(\left(\frac{c^3}{6} - \frac{Ac^2}{2}\right) \otimes y^{(3)}(t_0)\right)$$
$$+ (b^T \otimes Z)(I - A \otimes Z)^{-1}\big(I \otimes g'(y_0)\big)(I - A \otimes Z)^{-1}\left(\left(\frac{c^2}{2} - Ac\right) \otimes y^{(3)}(t_0)\right)$$

- Is everything bounded despite Z being unbounded? Yes!
- The derivatives $y^{(3)}(t_0)$ and $g'(y_0)$ are bounded by assumptions
- The matrices $(b^T \otimes Z)(I - A \otimes Z)^{-1}$ and $(I - A \otimes Z)^{-1}$ are bounded for most practical implicit Runge–Kutta methods

Recall ODE is $y'(t) = Jy(t) + g\big(y(t)\big)$ and $Z = hJ$

Here's Some Intuition

- Proof sketch
  - The local error in the stages, ΔY_0, is defined by an equation this is implicit in both J and g. We can remove the implicitness for J since it is linear:

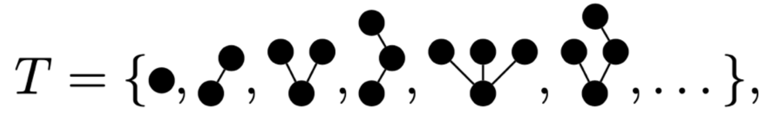
$$\Delta Y = h(A \otimes I)(I - A \otimes Z)^{-1}\Delta g_0 + (I - A \otimes Z)^{-1}\sum_{i=1}^{r} h^r \left(\frac{c^i}{i!} - \frac{Ac^{i-1}}{(i-1)!}\right) y^{(i)}(t_0)$$

  - In this form, we can apply Albrecht's classical derivation which is involves a double Taylor series of $\Delta g_0 = g\big(y(t_0 + ch)\big) - g(Y_0)$
  - Care is needed to avoid commuting terms, hence the Kronecker products
- When $Z = 0$ for we recover Albrecht's classical, nonstiff results

Recall ODE is $y'(t) = Jy(t) + g\big(y(t)\big)$ and $Z = hJ$

Rooted Trees Offer a Graphical Representation

- The recursion and summation over integer partitions are complex and cumbersome but can be mapped to rooted trees



(rooted trees)

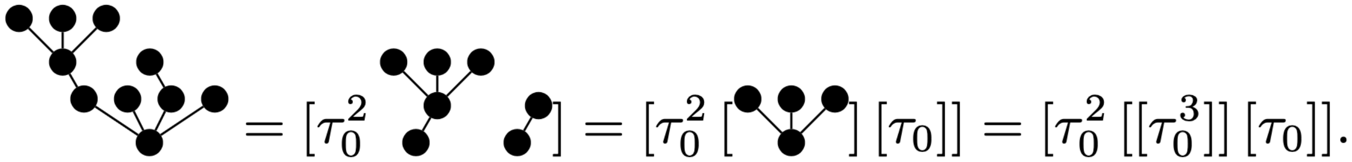
$$T_i = \{\tau \in T : |\tau| = i\}, \qquad \text{(rooted trees with } i \text{ vertices)}$$

- Following Albrecht, we use the *standardized form*

$$\tau = [\tau_0^\ell \tau_1 \ldots \tau_k], \qquad \ell \geq 0, \quad k \geq 0, \quad \tau_i \neq \tau_0 \quad (i = 1, \ldots, k),$$

with τ_0 the tree of order one.

- Example:



$$= [\tau_0^2 [[\tau_0^3]] [\tau_0]].$$

The Local Error Recursion Can Equivalently be Expressed As

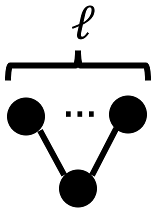
$$\Delta Y_0 = \sum_{\substack{\tau \in T \\ |\tau| \le r}} \underbrace{\zeta(\tau)}_{\text{Real Number}} \Psi(\tau; Z, t_0) h^{|\tau|} + \mathcal{O}(h^{r+1})$$

$$\Delta y_1 = \sum_{\substack{\tau \in T \\ |\tau| \le r}} \zeta(\tau) \psi(\tau; Z, t_0) h^{|\tau|} + \mathcal{O}(h^{r+1})$$

$$\Psi(\tau; Z, t) = (I - A \otimes Z)^{-1} \left(\left(\frac{c^{\ell+1}}{(\ell+1)!} - \frac{A c^{\ell}}{\ell!} \right) \otimes y^{(\ell+1)}(t) \right),$$

$$\psi(\tau; Z, t) = \left(\frac{1}{(\ell+1)!} - \frac{b^T c^{\ell}}{\ell!} \right) y^{(\ell+1)}(t) + (b^T \otimes Z) \Psi(\tau; Z, t).$$

when $\tau = [\tau_0^{\ell}] =$

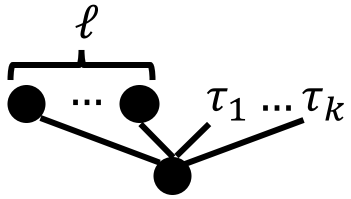


$$\Psi(\tau; Z, t) = (I - A \otimes Z)^{-1} ((AC^{\ell}) \otimes I)\ \vec{g}^{(\ell;k)}(t) \big(\Psi(\tau_1; Z, t), \ldots, \Psi(\tau_k; Z, t) \big),$$

$$\psi(\tau; Z, t) = (b^T \otimes I)(I - A \otimes Z)^{-1} (C^{\ell} \otimes I)\ \vec{g}^{(\ell;k)}(t) \big(\Psi(\tau_1; Z, t), \ldots, \Psi(\tau_k; Z, t) \big)$$

when $\tau = [\tau_0^{\ell}\ \tau_1 \ldots \tau_k]$

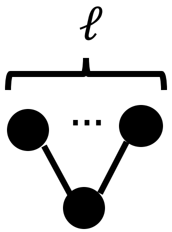
$=$



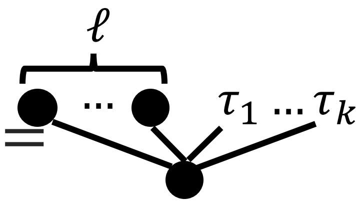
Ultimately, We Want Order Conditions In Terms of Coefficients

- The error interweaves differentials and coefficients because $(I - A \otimes Z)^{-1}$ lacks a Kronecker product structure.
- By Cayley–Hamilton, $(I - A \otimes Z)^{-1} = \sum_{i=0}^{s-1} A^i \otimes P_i(Z)$, with P_i polynomials.
- A vector space representation helps account for this summation.

$$V_\tau = \operatorname{span}\left\{A^j \left(\frac{c^{\ell+1}}{(\ell+1)!} - \frac{Ac^{\ell}}{\ell!}\right) \middle| j = 0, \dots, s-1\right\} \text{ when } \tau =$$

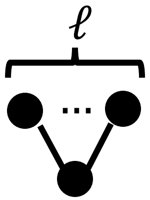


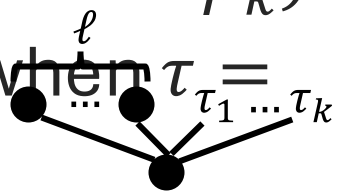
$$V_\tau = \operatorname{span}\left\{A^{j+1} C(\beta_1 \times \cdots \times \beta_k) \middle| j = 0, \dots, s-1,\ \ \beta_i \in V_{\tau_i}\right\} \text{ when } \tau =$$



Conditions to Attain Semilinear Order p_{sl}

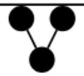
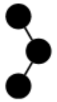
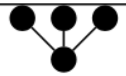
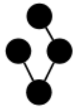
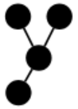
Under mild ODE smoothness and Runge–Kutta stability assumptions, if for all trees τ up to order p_{sl},

$b^T c^\ell = \frac{1}{\ell+1}$ and $b^T \beta = 0$ for all $\beta \in V_\tau$ when $\tau =$ 

$b^T A^j C^\ell (\beta_1 \times \cdots \times \beta_k) = 0$ for all $\beta_1 \in V_{\tau_1}, \ldots, \beta_k \in V_{\tau_k}$ and $j = 0, \ldots, s-1$ when $\tau =$ 

then there are constants $D, \tilde{h}$ independent of stiffness such that the local error satisfies $\|\Delta y_0\| \leq D h^{p_{sl}+1}$ for $h < \tilde{h}$.

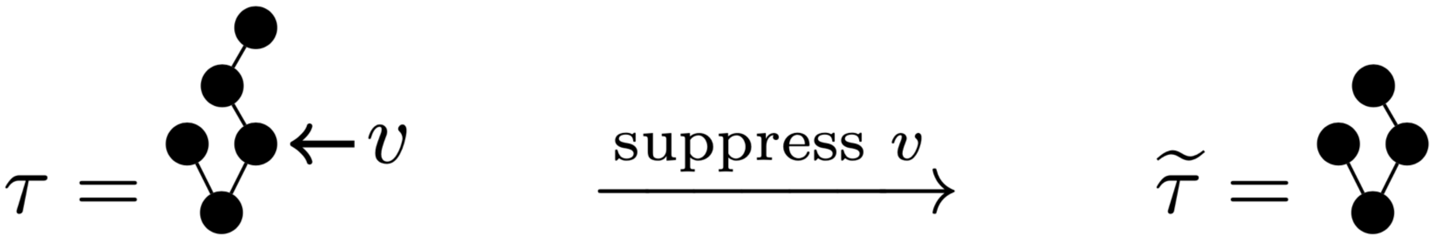
Here are the Semilinear Order Conditions which Eliminate Order Reduction

Label	Tree τ	Order Condition ($\forall i_1, i_2, i_3, i_4 \in \{0, \dots, s-1\}$)	Implied By
1a		$0 = 1 - b^T e$	$B(1)$
2a		$0 = \frac{1}{2} - b^T c = b^T A^{i_1} \left(\frac{c^2}{2} - Ac \right)$	$B(2), C(2)$
3a		$0 = \frac{1}{6} - \frac{b^T c^2}{2} = b^T A^{i_1} \left(\frac{c^3}{6} - \frac{Ac^2}{2} \right)$	$B(3), C(3)$
3b		$0 = b^T A^{i_1+i_2} \left(\frac{c^2}{2} - Ac \right)$	2a
4a		$0 = \frac{1}{24} - \frac{b^T c^3}{6} = b^T A^{i_1} \left(\frac{c^4}{24} - \frac{Ac^3}{6} \right)$	$B(4), C(4)$
4b		$0 = b^T A^{i_1} C A^{i_2} \left(\frac{c^2}{2} - Ac \right)$	$C(2)$
4c		$0 = b^T A^{i_1+i_2} \left(\frac{c^3}{6} - \frac{Ac^2}{2} \right)$	3a
4d		$0 = b^T A^{i_1+i_2+i_3+1} \left(\frac{c^2}{2} - Ac \right)$	2a

- The "bushy trees" give weak stage order conditions
- Some order conditions are redundant
- The first uniquely nonlinear condition is 4b

It Suffices to Consider a Subset of Trees

- We found that when a tree has a singly-branched vertex with a non-leaf child, we get an order condition implied by suppressing that vertex:



- If we suppress these vertices from all rooted trees, we're left with the *semi-lone-child-avoiding* trees

Order	1	2	3	4	5	6	7	8	9	10
Number of trees	1	1	2	4	9	20	48	115	286	719
Number of semi-lone-child-avoiding trees	1	1	1	2	4	7	15	29	62	129

https://oeis.org/A331934

Global Error and Superconvergence

- Textbook convergence theory implies $\mathcal{O}(h^{p_{sl}+1})$ local errors accumulate to a $\mathcal{O}(h^{p_{sl}})$ global error
- For fixed steps, this may not be sharp
- We showed that if the semilinear order is p_{sl}, the classical order is $p_{sl}+1$, and the linear stability function satisfies

$$\lim_{z\to\infty} R(z) \neq 1 \qquad \text{and} \qquad \frac{1}{z}(1-R(z)) \;\; \text{has no zeros in} \;\; \mathbb{C}^-$$

  then we have "superconvergence" with a $\mathcal{O}(h^{p_{sl}+1})$ global error.
- The results hold uniformly w.r.t stiffness which is called *B-convergence*

Deriving New Methods

We Want to Design DIRK Methods Satisfying the Semilinear Order Conditions

- The order conditions appear quite demanding
  - The number of conditions can increase as more stages are added
  - Not immediately obvious they can be enforced without resorting to high stage order
- We'll focus on methods with the "wishlist"
  - Diagonally implicit
  - Order >3
  - L-stable
- We used a combination of symbolic and optimization methods to derive schemes

EDIRK-(7,4,4) has 7 stages, Classical Order 4, and Semilinear Order 4

- We wanted to see if a method that uses no simplifying assumptions, i.e., has stage order 1, exists. Yes!

$a_{1,1}$	0	$a_{2,1}$	$\frac{66719178356146069}{104971894986575178}$	$a_{2,2}$	$\frac{66719178356146069}{104971894986575178}$
$a_{3,1}$	$\frac{1157487899475829 1}{117719113355115783}$	$a_{3,2}$	$-\frac{18581975408986 96}{70529361366069153}$	$a_{3,3}$	$\frac{11617133062216757}{43245479316548780}$
$a_{4,1}$	$\frac{312078294212599530}{408234247007768 21}$	$a_{4,2}$	$\frac{155312269009595199}{86710391005988198}$	$a_{4,3}$	$-\frac{743789150637775609}{1133522186312213 11}$
$a_{4,4}$	$\frac{98271968880200657}{179019545289054999}$	$a_{5,1}$	$\frac{1246868775297421168}{137070970121741807}$	$a_{5,2}$	$\frac{114921713922407255}{52367417556902641}$
$a_{5,3}$	$-\frac{2059475023054192 61}{24454220481972685}$	$a_{5,4}$	$\frac{18936671640200689}{104159855867653343}$	$a_{5,5}$	$\frac{47397311839212708}{127463680130367391}$
$a_{6,1}$	$-\frac{1517405090960743 88}{196613682401464609}$	$a_{6,2}$	$\frac{254369392774793867}{44087509892864172}$	$a_{6,3}$	$-\frac{73864359103986538}{65744654972066205}$
$a_{6,4}$	$-\frac{37706375961306427}{179802732674457709}$	$a_{6,5}$	$\frac{7953265906419399}{38933344132172515}$	$a_{6,6}$	$\frac{48325866641079469}{46020097947328612}$
$a_{7,1}$	$\frac{3312403043354842}{33496693975407517}$	$a_{7,2}$	$-\frac{77452645449945 59}{74509708869668763}$	$a_{7,3}$	$\frac{75463258779378077}{134382831179297809}$
$a_{7,4}$	$-\frac{116967648762176 91}{132584149662964151}$	$a_{7,5}$	$\frac{9114026243344448}{106054923174086269}$	$a_{7,6}$	$\frac{5594692490207 6}{75756035623695139}$
$a_{7,7}$	$\frac{34834932759942553}{78271243704016222}$				

We Recommend Two Optimized ESDIRK Methods

- The previous method is mostly of theoretical interest
- We found using the $C(2)$ simplifying assumption to be beneficial
- We propose ESDIRK-(8,4,3) which has classical order 4 but semilinear order 3
  - With superconvergence, we should see 4^{th} order B-convergence
  - It is indeed L-stable
- We also propose ESDIRK-(10,5,4) which is L-stable and 5^{th} order B-convergent

Numerical Experiments

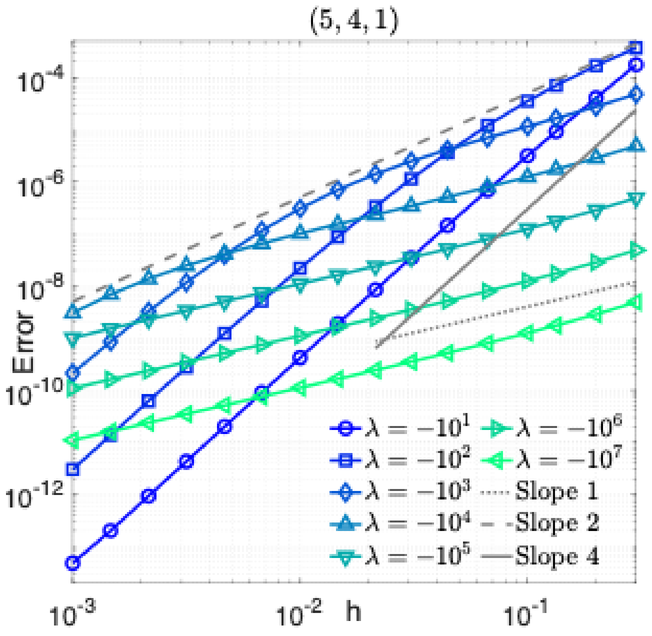
We Start with a Semilinear Variant of the Prothero–Robinson Problem

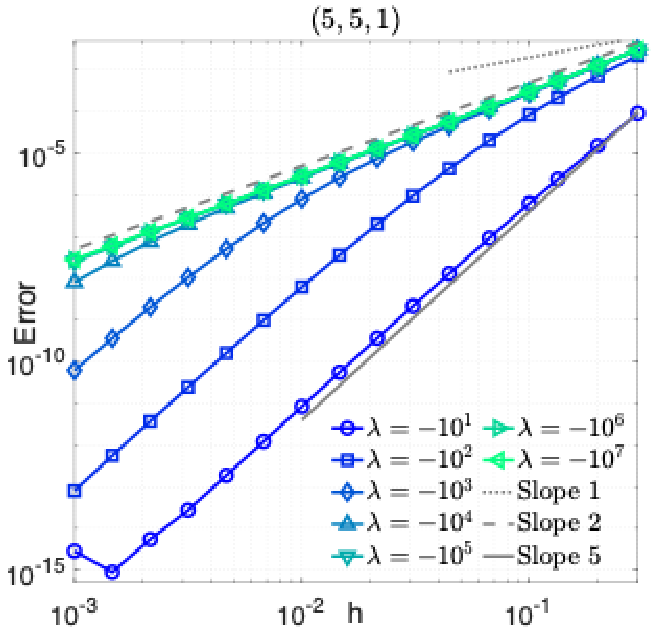
- The solution to this ODE is independent of the stiffness (λ):

$$y'(t) = \lambda\left(y(t) - \sqrt{1+t^2} + t\right) - 2y(t)^2/(1 + y(t)^2)$$

- Baseline 4$^{\text{th}}$ and 5$^{\text{th}}$ order methods have semilinear order 1

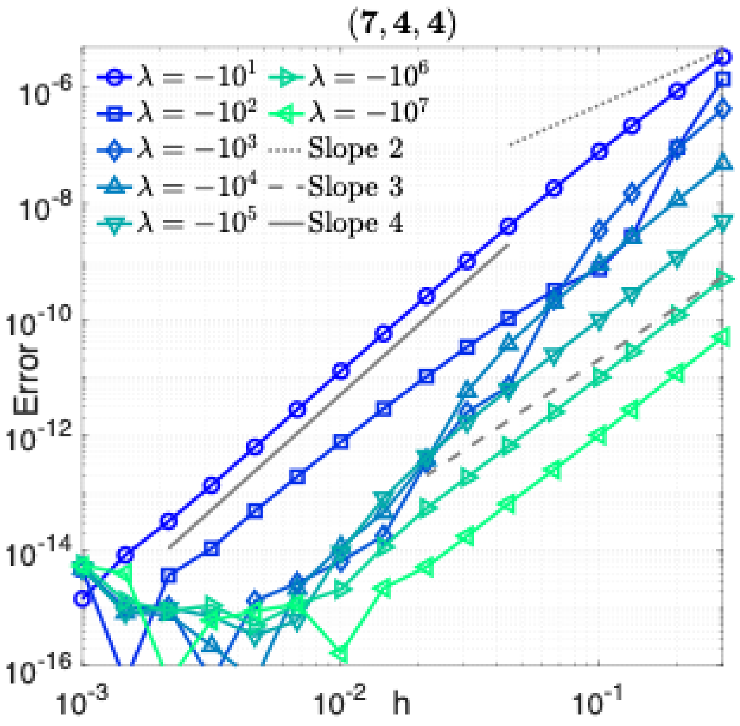
SDIRK4 from Hairer, Wanner. Solving ordinary differential equations II. New York: Springer Berlin Heidelberg, 1996.



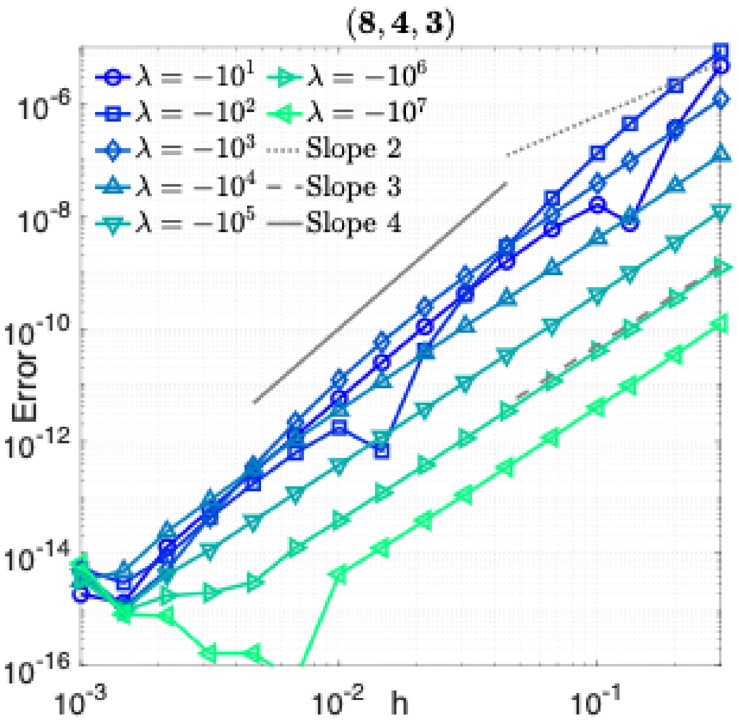


SDIRK5()5L[1] from Kennedy, Carpenter. Diagonally implicit Runge-Kutta methods for ordinary differential equations. A review.

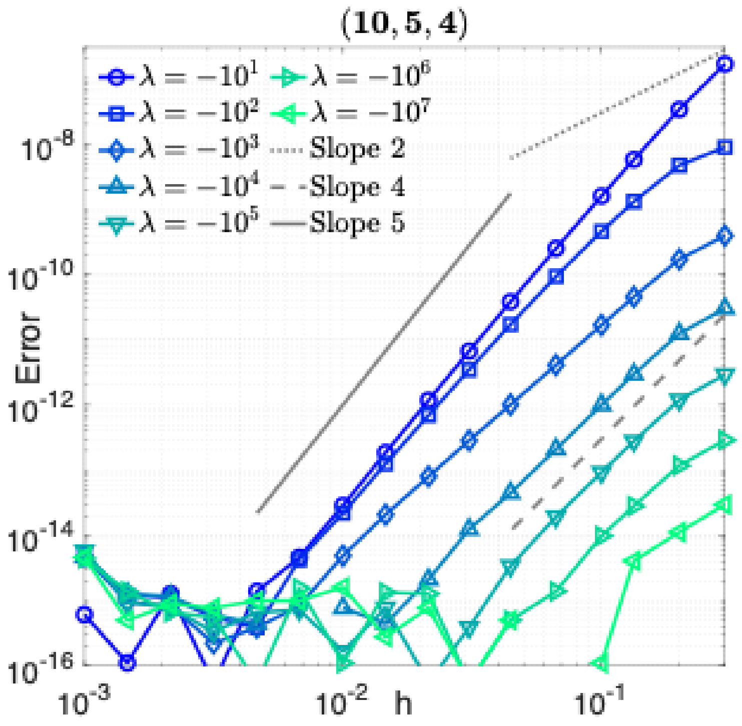
Our New Methods Avoid Order Reduction



✓ B-Convergent of Order 4



✓ B-Convergent of Order 4



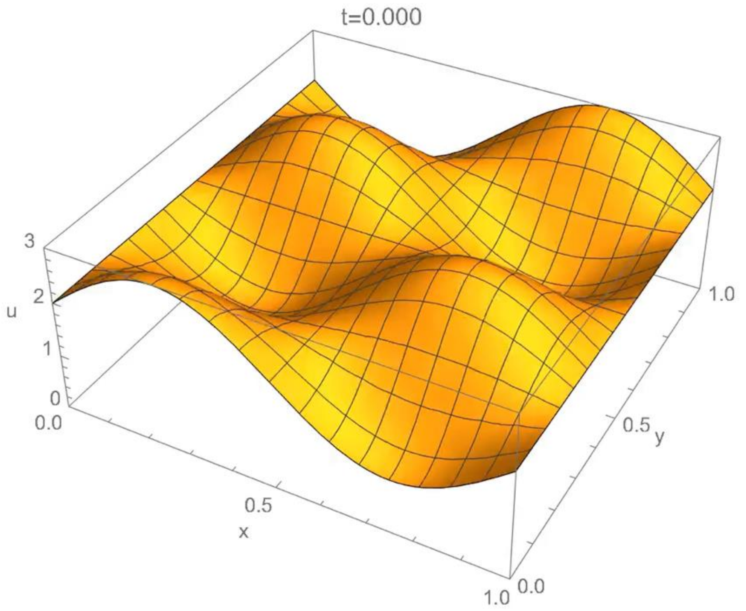
✓ B-Convergent of Order 5

Next We Test with the Allen–Cahn Problem

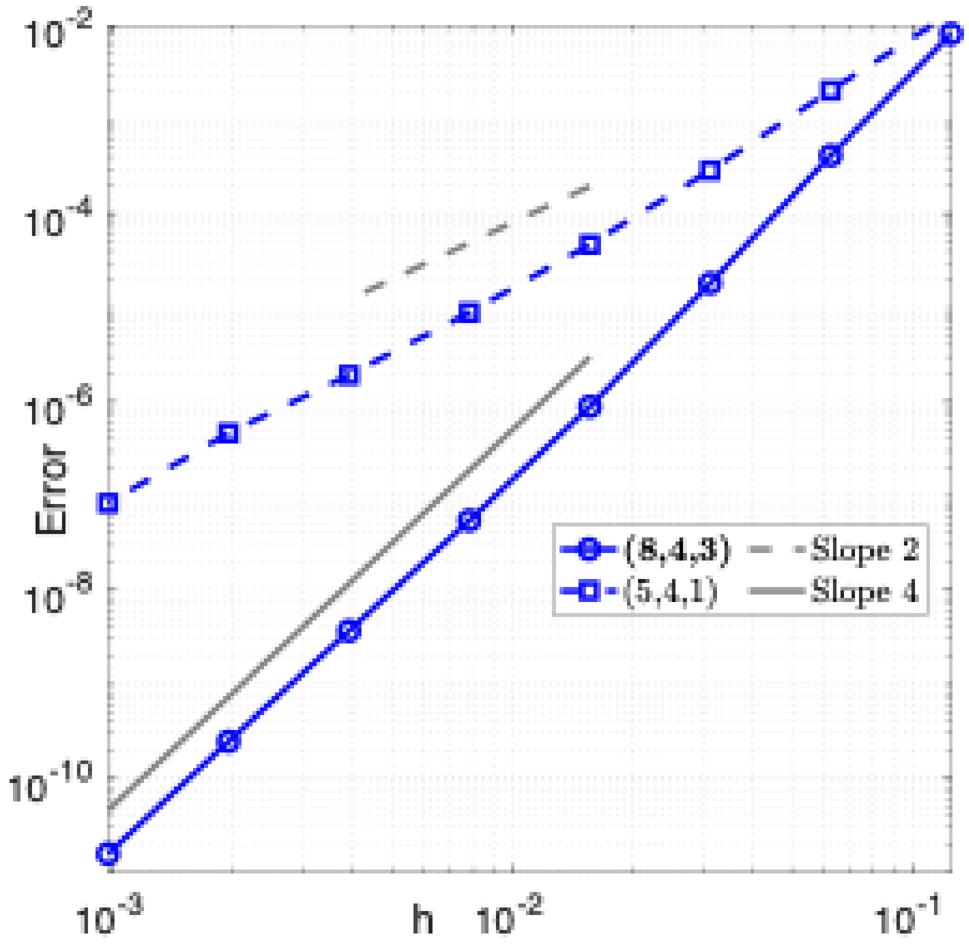
- We construct an Allen–Cahn problem using the method of manufactured solutions

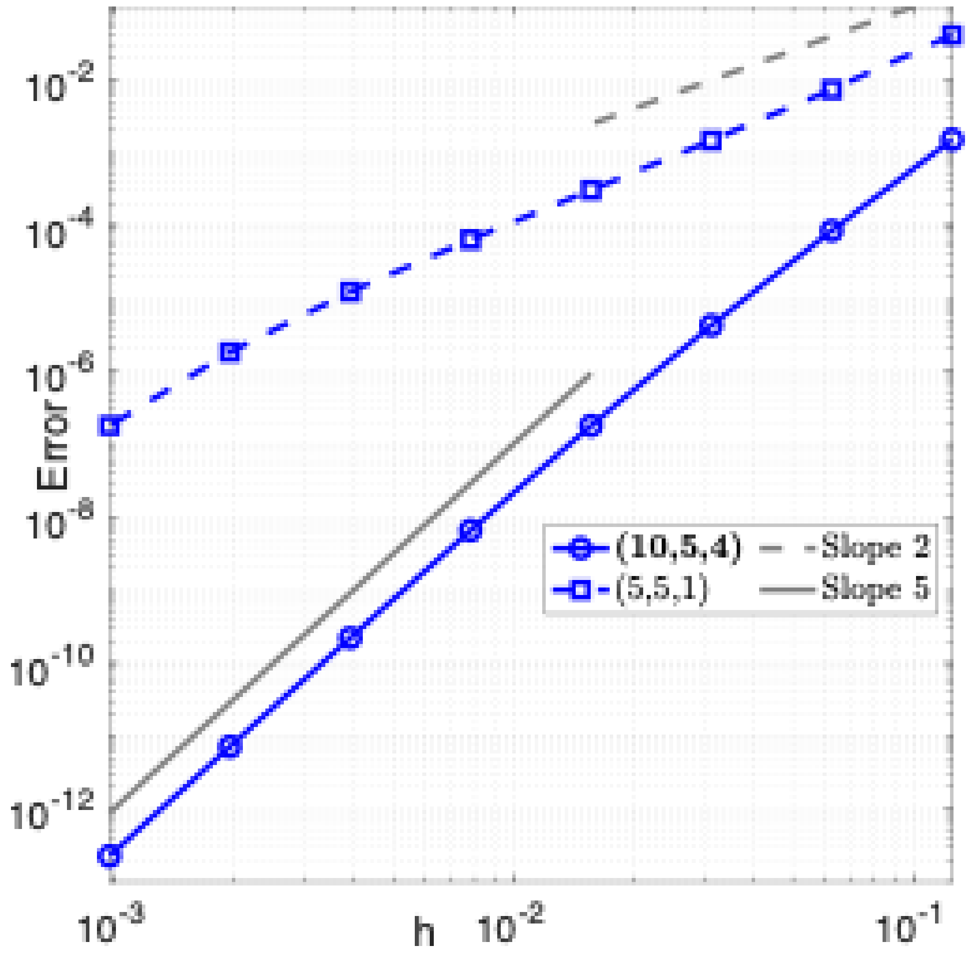
$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u + \beta(u - u^3) + s(t, x, y)$$

- Time-dependent boundary conditions are a typical recipe for order reduction
- A pseudo-spectral method is used to discretize space



Our New Methods Avoid Order Reduction





Can We Move Beyond Semilinear Problems to Fully Nonlinear?

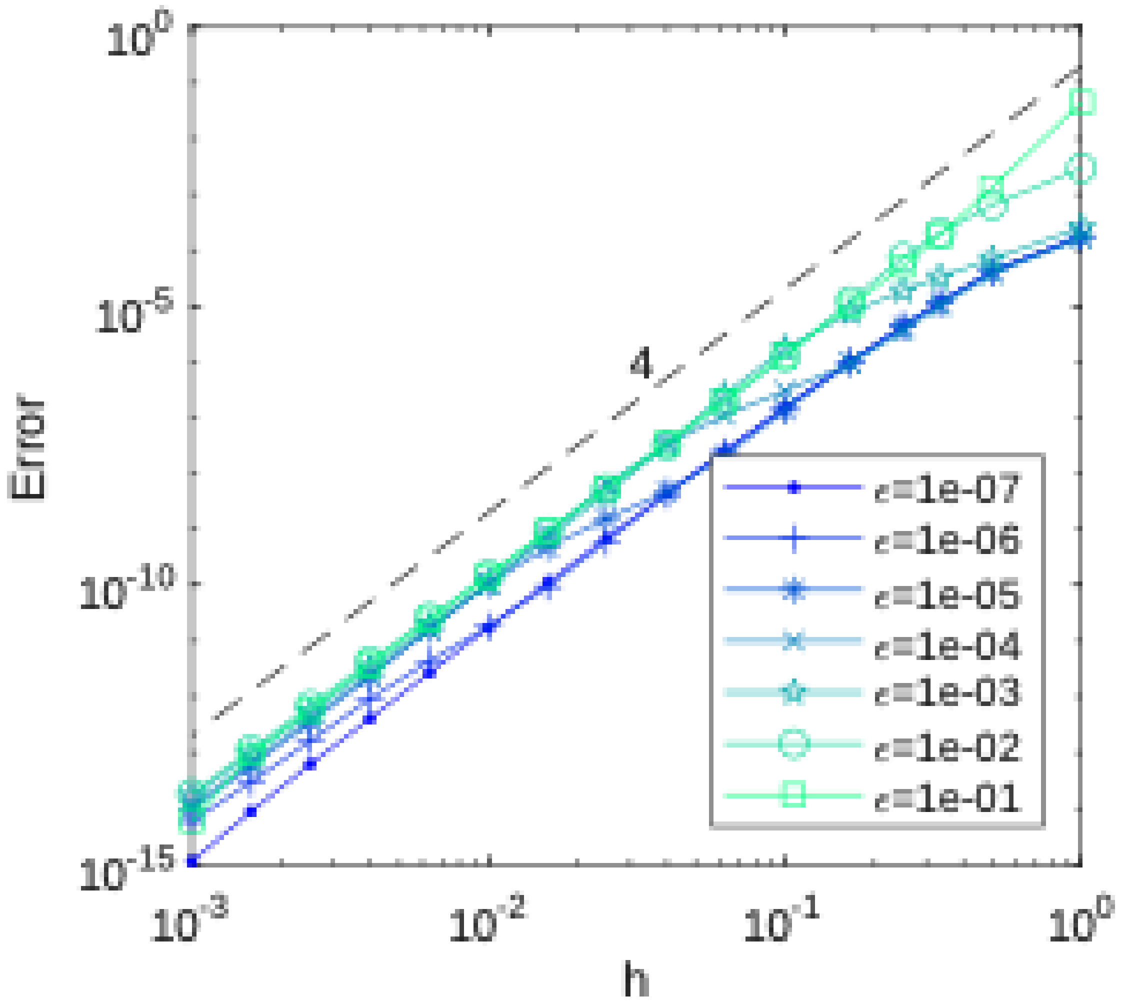
Conjecture
High stage order is not necessary to eliminate order reduction for Runge–Kutta methods applied to singular perturbation problems. That is, weaker conditions to attain B-convergence exist.

Promising Evidence Supports the Conjecture

- The Kaps' problem is a nonlinear singular perturbation problem:

$$\epsilon y_1' = -(1+2\epsilon)y_1 + y_2^2$$
$$y_2' = y_1 - y_2 - y_2^2$$

- Our EDIRK-(7,4,4) method designed for semilinear ODEs has order 4 B-convergence here!
- Other stiff nonlinear problems show similar results



Conclusions

- Stiff semilinear ODEs can cause Runge–Kutta methods to experience order reduction
- We developed a sharp order condition theory to explain this and provided order conditions to eliminate order reduction
- Our new DIRK methods validate the theory and appear to work for even broader classes of nonlinear problems
- Next steps
  - IMEX
  - Fully nonlinear singular perturbation problems

Preprint available at
https://arxiv.org/abs/2505.15099

Acknowledgements: The authors would like to thank David I. Ketcheson for many helpful discussions.