The Order of Runge–Kutta Methods in Theory and Practice

Temple Seminar Talk

CASC
Center for Applied
Scientific Computing

12/6/23

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LLNL-PRES-857851

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

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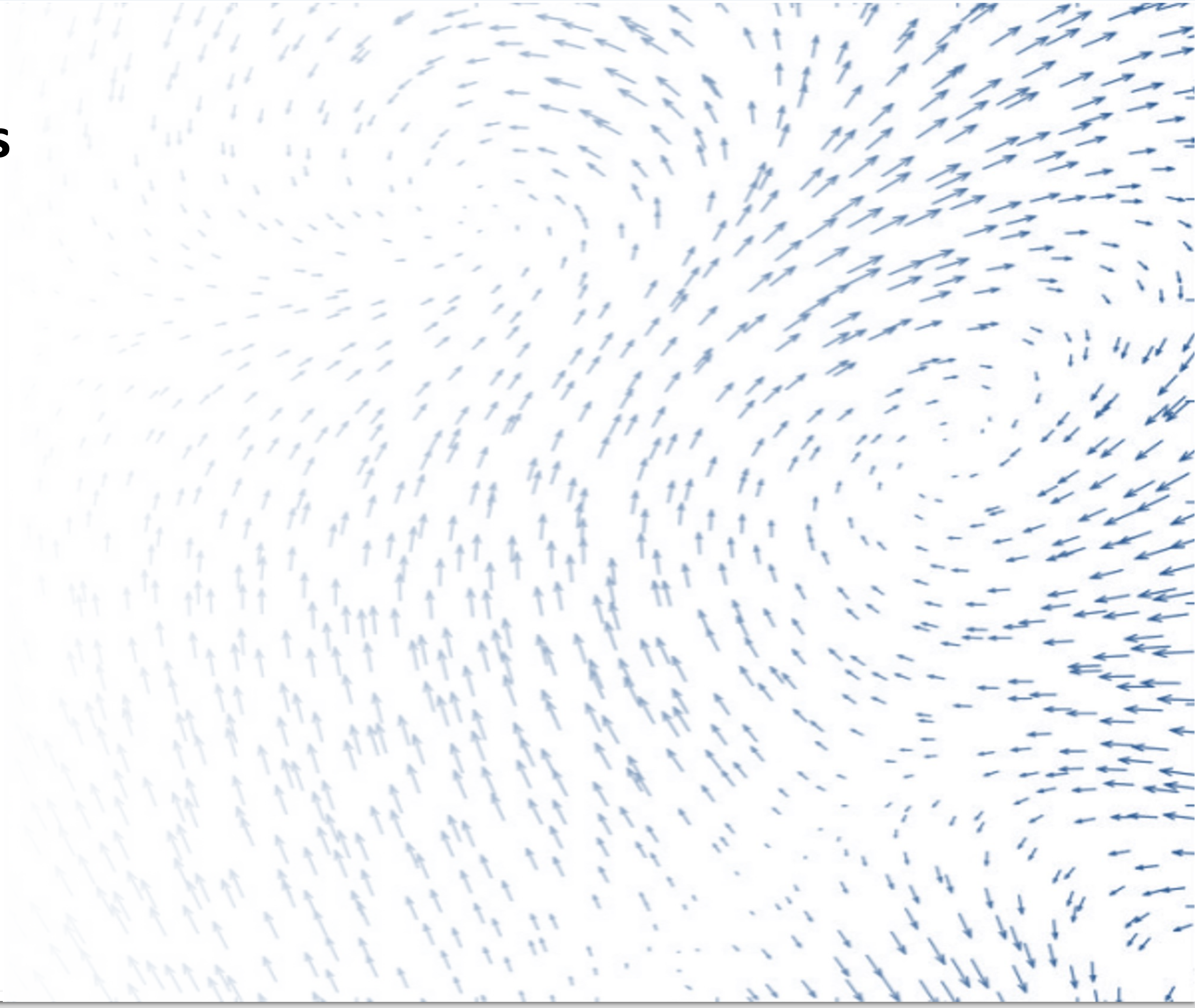
This work was supported by the Fernbach Fellowship through the LLNL-LDRD Program under Project No. 23-ERD-048

Outline

1. **Introduction to the Order Reduction Phenomenon for Runge–Kutta methods**
2. Explicit Runge–Kutta Methods that Alleviate Order Reduction
3. A New Theory for Semilinear ODEs
4. Conclusions



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

$$Y_i = y_n + \Delta t \sum_{j=1}^{s} a_{i,j} f\big(Y_j\big), \quad i = 1, \dots, s,$$
$$y_{n+1} = y_n + \Delta t \sum_{j=1}^{s} b_j f\big(Y_j\big)$$

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

Motivating Example: Let's Solve a Simple PDE

- Consider the following PDE[1] on $t, x \in [0,1]$:

$$
\begin{aligned}
u_t &= -u_x + \frac{t-x}{(1+t)^2}, \\
u(t,0) &= \frac{1}{1+t}, \\
u(0,x) &= 1+x
\end{aligned}
\quad \xrightarrow{\text{Semidiscretize}} \quad
y' = \begin{bmatrix}
-\frac{1}{\Delta x} & & & \\
\frac{1}{\Delta x} & -\frac{1}{\Delta x} & & \\
& \ddots & \ddots & \\
& & \frac{1}{\Delta x} & -\frac{1}{\Delta x}
\end{bmatrix} y + \begin{bmatrix}
\frac{t-x_1}{(1+t)^2} + \frac{1}{\Delta x(1+t)} \\
\frac{t-x_2}{(1+t)^2} \\
\vdots \\
\frac{t-x_N}{(1+t)^2}
\end{bmatrix}
$$

- The exact solution $u(t,x) = \frac{1+x}{1+t}$ is linear in space

- This finite difference discretization contributes no spatial error
  - Any numerical error will be entirely from the time discretization

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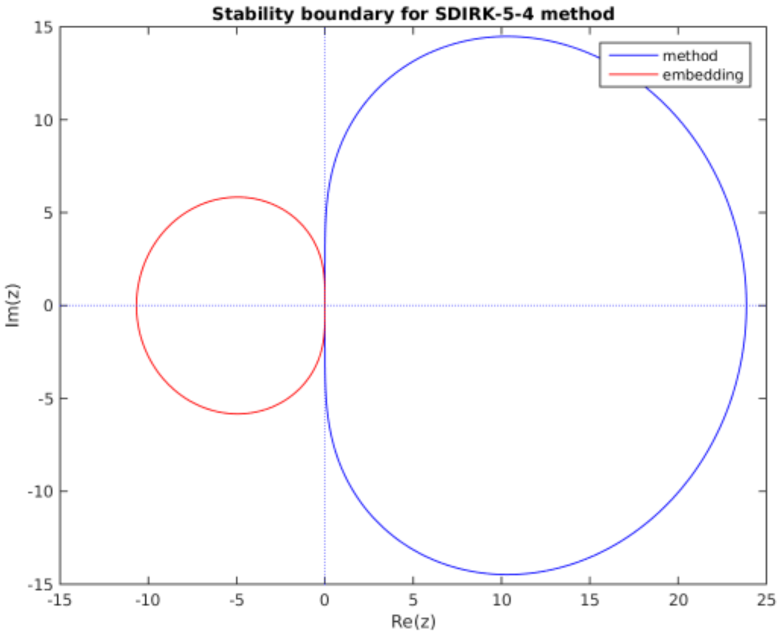
1. Sanz-Serna, Jesús María, Jan G. Verwer, and W. H. Hundsdorfer. "Convergence and order reduction of Runge-Kutta schemes applied to evolutionary problems in partial differential equations." *Numerische Mathematik* 50.4 (1986): 405-418.

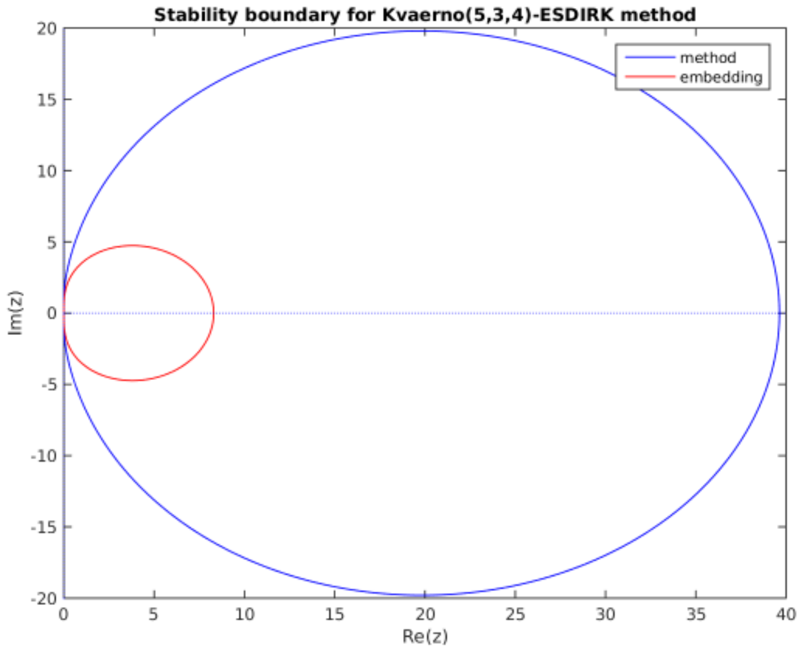
We Solve the Advection PDE with Two Fourth Order DIRK Methods from SUNDIALS

$$\begin{array}{c|ccccc}
\frac{1}{4} & \frac{1}{4} & 0 & 0 & 0 & 0 \\
\frac{3}{4} & \frac{1}{2} & \frac{1}{4} & 0 & 0 & 0 \\
\frac{11}{20} & \frac{17}{50} & -\frac{1}{25} & \frac{1}{4} & 0 & 0 \\
\frac{1}{2} & \frac{371}{1360} & -\frac{137}{2720} & \frac{15}{544} & \frac{1}{4} & 0 \\
1 & \frac{25}{24} & -\frac{49}{48} & \frac{125}{16} & -\frac{85}{12} & \frac{1}{4} \\
\hline
4 & \frac{25}{24} & -\frac{49}{48} & \frac{125}{16} & -\frac{85}{12} & \frac{1}{4} \\
3 & \frac{59}{48} & -\frac{17}{96} & \frac{225}{32} & -\frac{85}{12} & 0
\end{array}$$



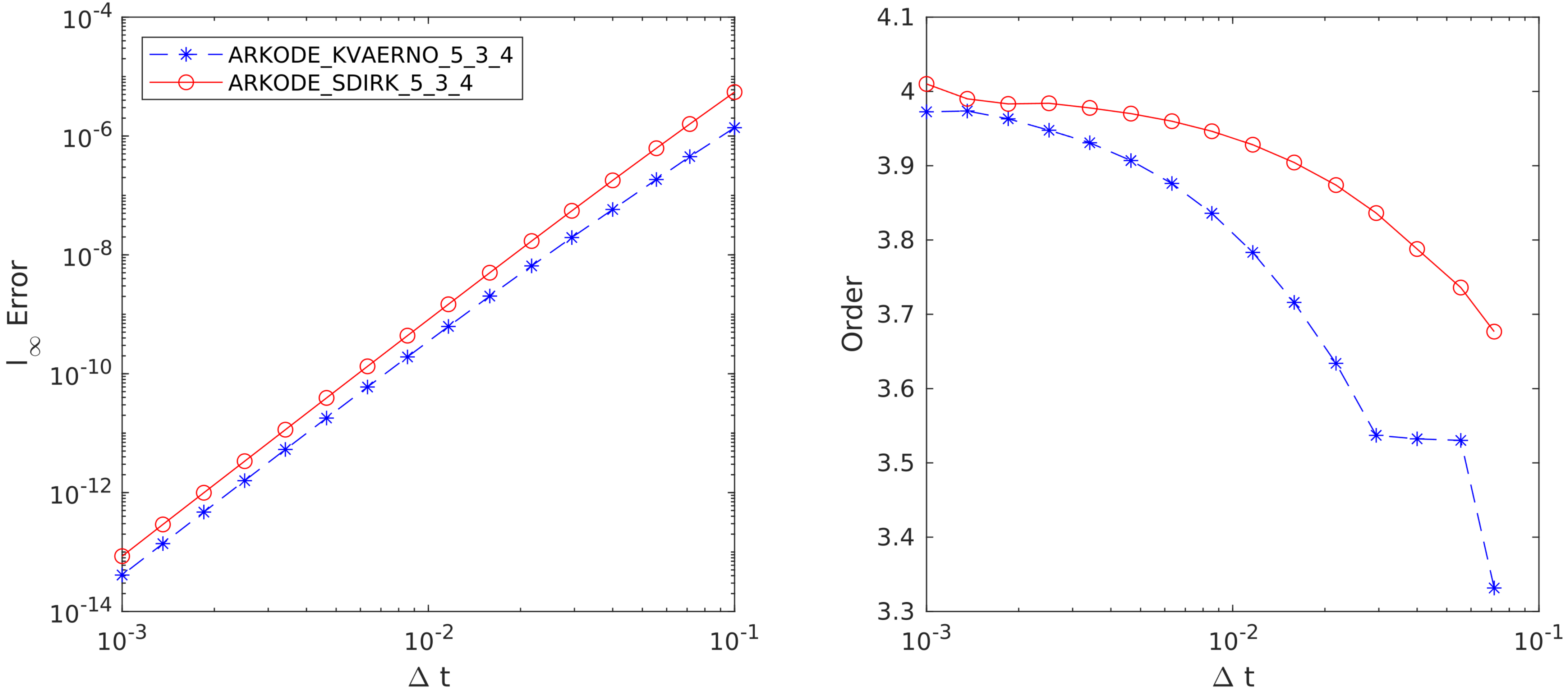
Stability boundary for SDIRK-5-4 method

$$\begin{array}{r|ccccc}
0 & 0 & 0 & 0 & 0 & 0 \\
0.871733043 & 0.4358665215 & 0.4358665215 & 0 & 0 & 0 \\
0.468238744853136 & 0.140737774731968 & -0.108365551378832 & 0.4358665215 & 0 & 0 \\
1 & 0.102399400616089 & -0.376878452267324 & 0.838612530151233 & 0.4358665215 & 0 \\
1 & 0.157024897860995 & 0.117330441357768 & 0.61667803039168 & -0.326899891110444 & 0.4358665215 \\
\hline
4 & 0.157024897860995 & 0.117330441357768 & 0.61667803039168 & -0.326899891110444 & 0.4358665215 \\
3 & 0.102399400616089 & -0.376878452267324 & 0.838612530151233 & 0.4358665215 & 0
\end{array}$$

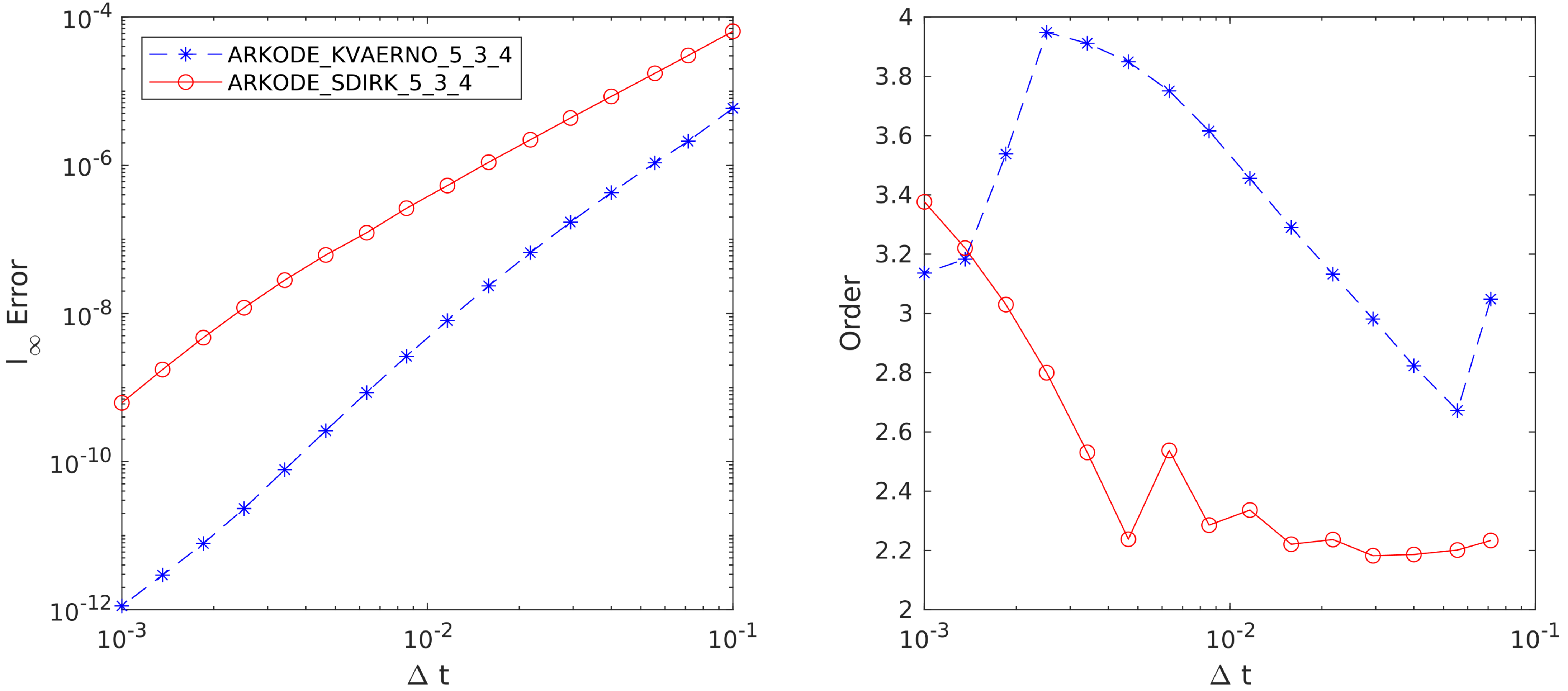


Stability boundary for Kvaerno(5,3,4)-ESDIRK method

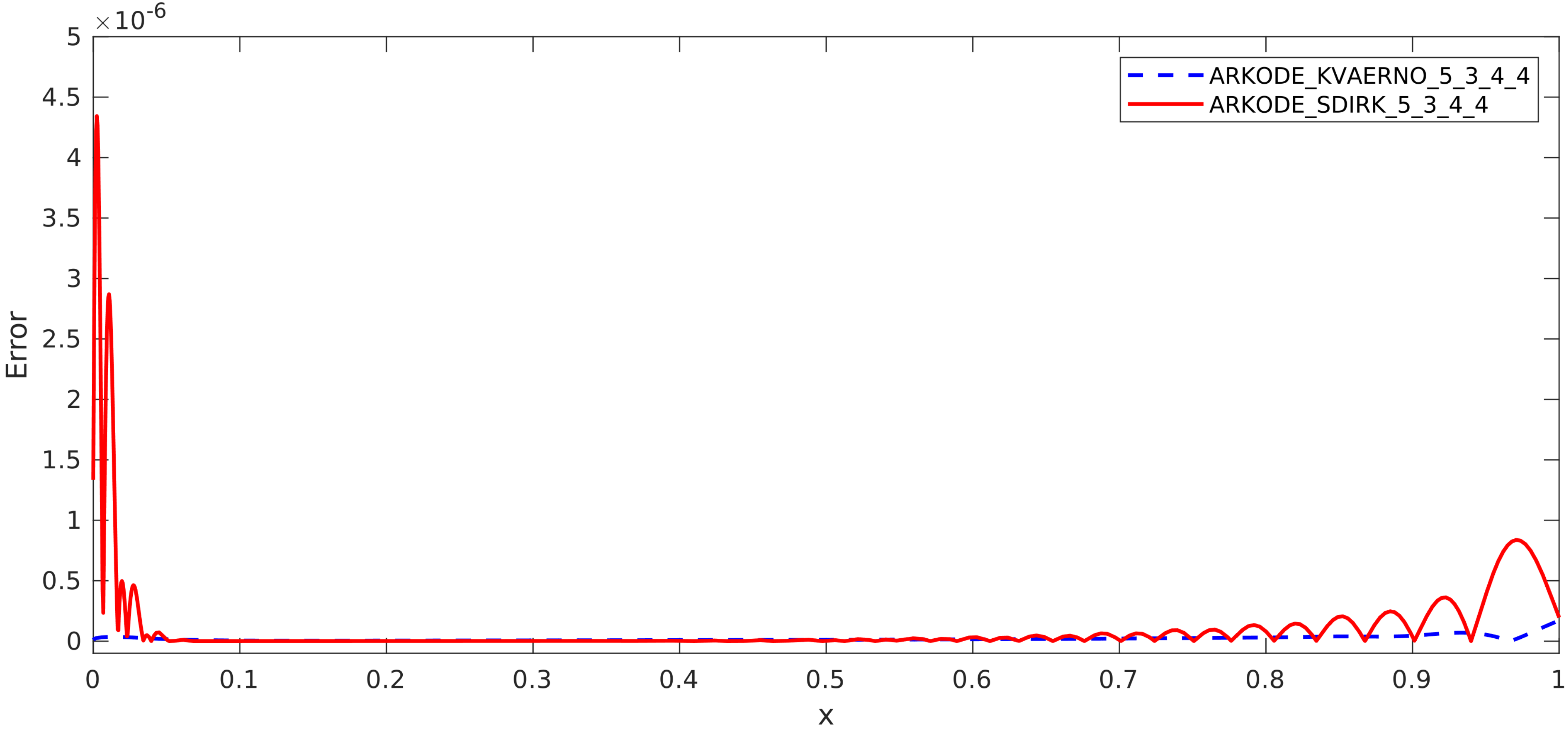
We See Asymptotic Convergence on a 16 Point Grid



We See Order Reduction on a 2048 Point Grid



The Dominant Temporal Error is Located Near Boundary Cells



Classical Convergence Requires Unrealistic Assumptions

- Recall the semidiscretized PDE:

$$y' = \begin{bmatrix} -\frac{1}{\Delta x} & & & \\ \frac{1}{\Delta x} & -\frac{1}{\Delta x} & & \\ & \ddots & \ddots & \\ & & \frac{1}{\Delta x} & -\frac{1}{\Delta x} \end{bmatrix} y + \begin{bmatrix} \frac{t - x_1}{(1+t)^2} + \frac{1}{\Delta x(1+t)} \\ \frac{t - x_2}{(1+t)^2} \\ \vdots \\ \frac{t - x_N}{(1+t)^2} \end{bmatrix}$$

- The Lipschitz constant of the right-hand side function is $\frac{1}{\Delta x}$
  - As we refine in space, the problem becomes stiffer

- Classical convergence assumes a moderate Lipschitz constant and “sufficiently small” Δt

- We often do not see expected convergence order until $\Delta t \leq C\ \Delta \mathrm{x}$
  - This is a CFL-like condition present even though the method is implicit

The Error Contains Unbounded Terms

$y' = f(y)$

- A classical expansion of the local truncation error is based on Taylor series
- Let's examine a couple error terms

$$y(t_1) - y_1 = \cdots + \Delta t^2 \left(\frac{1}{2} - b^T c\right) \underbrace{f'(y_0) f(y_0)}_{\mathcal{O}(\Delta x^{-1})} + \Delta t^3 \left(\frac{1}{6} - b^T A c\right) \underbrace{f'(y_0)^2 f(y_0)}_{\mathcal{O}(\Delta x^{-2})} + \cdots$$

Bad interactions between spatial and temporal scales

The Order Reduction Phenomenon is Well-Known

- In 1974, Prothero and Robinson[1] proposed perhaps the simplest problem to cause order reduction

$$y' = \lambda\big(y - \phi(t)\big) + \phi'(t)$$

- Practical ways to avoid order reduction are still an area of active research

Modified Boundary Conditions

- Often intrusive to solve implementations
- Often require extra derivative information
- Difficult to generalize
- No additional stages

Enforce Additional Order Conditions

- Compatible with any Runge–Kutta implementation
- Deriving methods which satisfy the order conditions may be challenging
- Often require additional stages, and thus, are more expensive

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1. Prothero, A., and A. Robinson. "On the stability and accuracy of one-step methods for solving stiff systems of ordinary differential equations." *Mathematics of Computation* 28.125 (1974): 145-162.

The Prothero-Robinson and PDE Problem are Connected

- The ODE for the first grid point of the advection PDE behaves like the Prothero-Robinson problem

$$y' = \begin{bmatrix} -\frac{1}{\Delta x} & & & \\ \frac{1}{\Delta x} & -\frac{1}{\Delta x} & & \\ & \ddots & \ddots & \\ & & \frac{1}{\Delta x} & -\frac{1}{\Delta x} \end{bmatrix} y + \begin{bmatrix} \frac{t - x_1}{(1+t)^2} + \frac{1}{\Delta x(1+t)} \\ \frac{t - x_2}{(1+t)^2} \\ \vdots \\ \frac{t - x_N}{(1+t)^2} \end{bmatrix} \quad \Longrightarrow \quad y_1' = -\frac{1}{\Delta x}\left(y_1 - \frac{1}{1+t}\right) + \frac{t - x_1}{(1+t)^2}$$

$$\wr$$

$$y' = \lambda\ \left(y - \phi(t)\right) + \phi'(t)$$

- More refined approaches explain boundary layers and fractional orders of convergence before applying a spatial discretization[1,2]

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1. Rosales, Rodolfo Ruben, et al. "Spatial manifestations of order reduction in Runge–Kutta methods for initial boundary value problems." *arXiv preprint arXiv:1712.00897* (2017).
2. Ostermann, Alexander, and Michel Roche. "Runge–Kutta methods for partial differential equations and fractional orders of convergence." *Mathematics of Computation* 59.200 (1992): 403-420.

Weak Stage Order Conditions Guarantee High Order Convergence

- Many authors have identified the following order conditions to remove order reduction on **linear** problems:

$$0 = b^T (I - zA)^{-1} \left(A c^{k-1} - \frac{c^k}{k} \right), \quad \forall z \in \mathbb{C}^-, k = 1, \dots, q$$

- To remove the auxiliary variable z, we can take a Neumann series expansion

$$0 = b^T A^i \left(A c^{k-1} - \frac{c^k}{k} \right), \quad i = 0, \dots, s-1, \ \ k = 1, \dots, q$$

- The largest q for which this holds is the *weak stage order*[1] (WSO) or *pseudostage order*[2]

---

1. Ketcheson, David I., et al. "DIRK schemes with high weak stage order." *Spectral and High Order Methods for Partial Differential Equations* (2020): 453.
2. Skvortsov, LM. "How to avoid accuracy and order reduction in Runge–Kutta methods as applied to stiff problems." *Computational Mathematics and Mathematical Physics* 57 (2017): 1124-1139.

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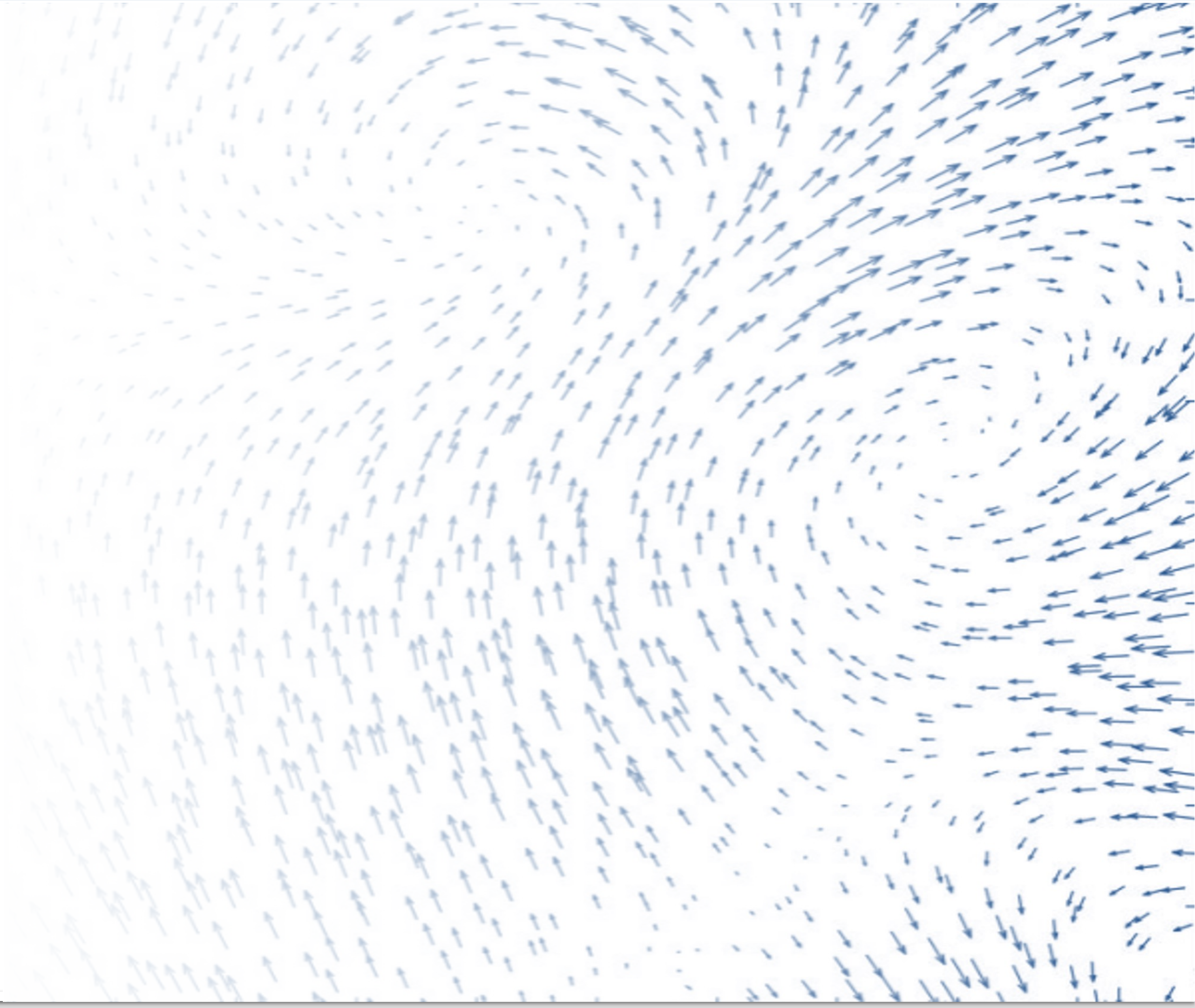
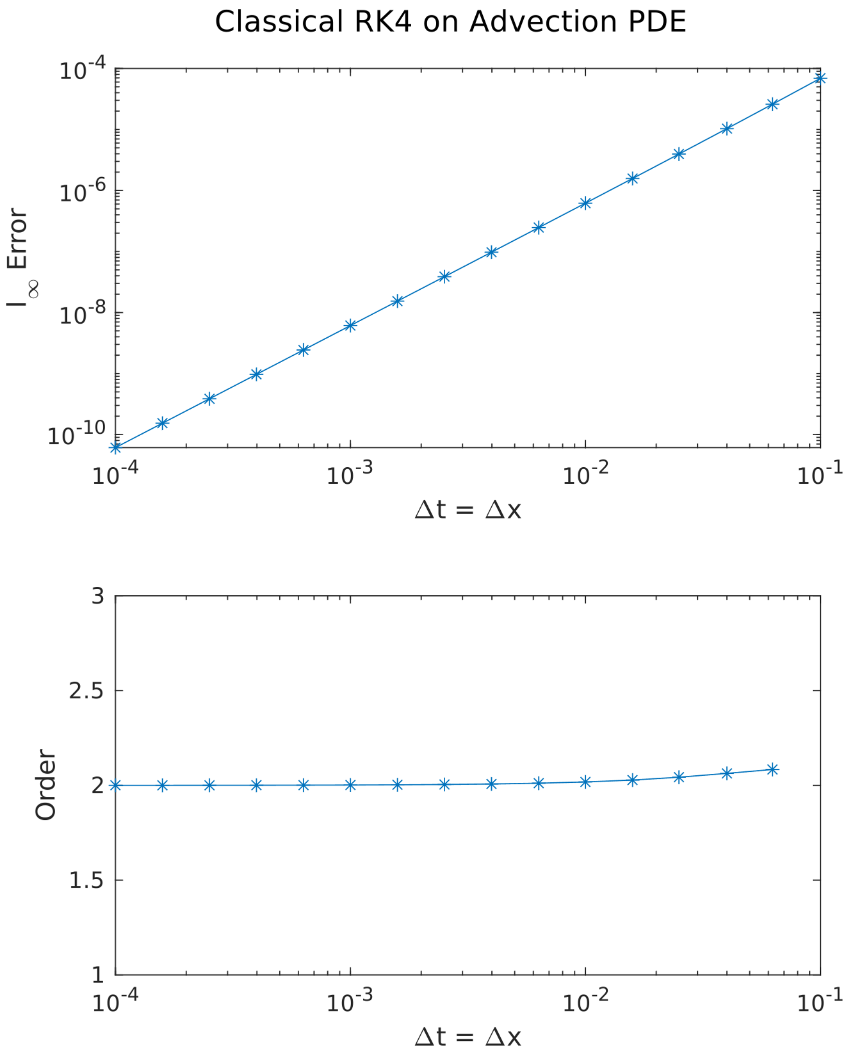


Biswas, Abhijit, et al. "Explicit Runge Kutta Methods that Alleviate Order Reduction." *arXiv preprint arXiv:2310.02817* (2023).

Order Reduction Occurs for Explicit Runge–Kutta Schemes Too

- Stiffness is a primary component of order reduction
- Nevertheless explicit methods are still susceptible to order reduction
- When solving a hyperbolic PDE, Δx and Δt often scale proportionally
  - Maintains a constant CFL number
  - Allows time and spatial errors to scale together
  - The stiffness grows as the time step shrinks so we are not in the classical asymptotic regime!



How Do We Construct Explicit Runge–Kutta Methods with High Weak Stage Order?

- Are weak stage order conditions compatible with classical order conditions?
- Are there order barriers?

$$\begin{array}{c|ccccc} 0 & & & & & \\ c_2 & a_{2,1} & & & & \\ c_3 & a_{3,1} & a_{3,2} & & & \\ \vdots & \vdots & & \ddots & & \\ c_s & a_{s,1} & a_{s,2} & \cdots & a_{s,s-1} & \\ \hline & b_1 & b_2 & \cdots & b_{s-1} & b_s \end{array}$$

$$0 = b^T A^i \left(A c^{k-1} - \frac{c^k}{k} \right), \quad i = 0, \dots, s-1, \;\; k = 1, \dots, q$$

$$\begin{aligned} 1 &= b^T e, \\ \frac{1}{2} &= b^T c, \\ \frac{1}{3} &= b^T c^2, \quad \frac{1}{6} = b^T A c, \\ \frac{1}{4} &= b^T c^3, \quad \frac{1}{8} = b^T \operatorname{diag}(c) A c, \quad \frac{1}{12} = b^T A c^2, \quad \frac{1}{24} = b^T A^2 c \\ &\vdots \end{aligned}$$

Weak Stage Order Necessitates Additional Stages

Theorem

For an explicit Runge–Kutta method

$$p + q \leq s + 1$$

p: classical order
q: weak stage order
s: # of stages

Minimum # of Stage Required

Classical Order p

Weak Stage Order q	**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

We found concrete methods which attain the theoretical bound sharply up to order 5 (except $p = 5, q = 1$ which is a classical order barrier)

Can we Systematically Build High Order Methods?

- Extrapolation and deferred correction are common techniques
  - Unfortunately, WSO generally does not increase

- A special case of deferred correction is parallel iteration

$$k_i^{(0)} = 0$$

$$k_i^{(\ell)} = f\left(y_n + \Delta t \sum_{j=1}^{s} \tilde{a}_{i,j} k_j^{(\ell-1)}\right), \quad \ell = 1, \ldots, \sigma$$

$$y_{n+1} = y_n + \Delta t \sum_{j=1}^{s} b_i k_i^{(\sigma)}$$

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array} = \begin{array}{c|ccccc} 0 & 0 & & & & \\ \tilde{c} & \tilde{A} & 0 & & & \\ \tilde{c} & 0 & \tilde{A} & 0 & & \\ \vdots & \vdots & & \ddots & \ddots & \\ \tilde{c} & 0 & \cdots & 0 & \tilde{A} & 0 \\ \hline & 0 & \cdots & 0 & 0 & \tilde{b}^T \end{array}$$

- This amounts to applying a fixed point iteration to the basic scheme $\left(\tilde{A}, \tilde{b}, \tilde{c}\right)$

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1. van der Houwen, Piet J., and Ben P. Sommeijer. "Iterated Runge–Kutta methods on parallel computers." *SIAM Journal on Scientific and Statistical Computing* 12.5 (1991): 1000-1028.

There Are Explicit Runge–Kutta Methods of Any Order Devoid of Order Reduction for Linear ODEs

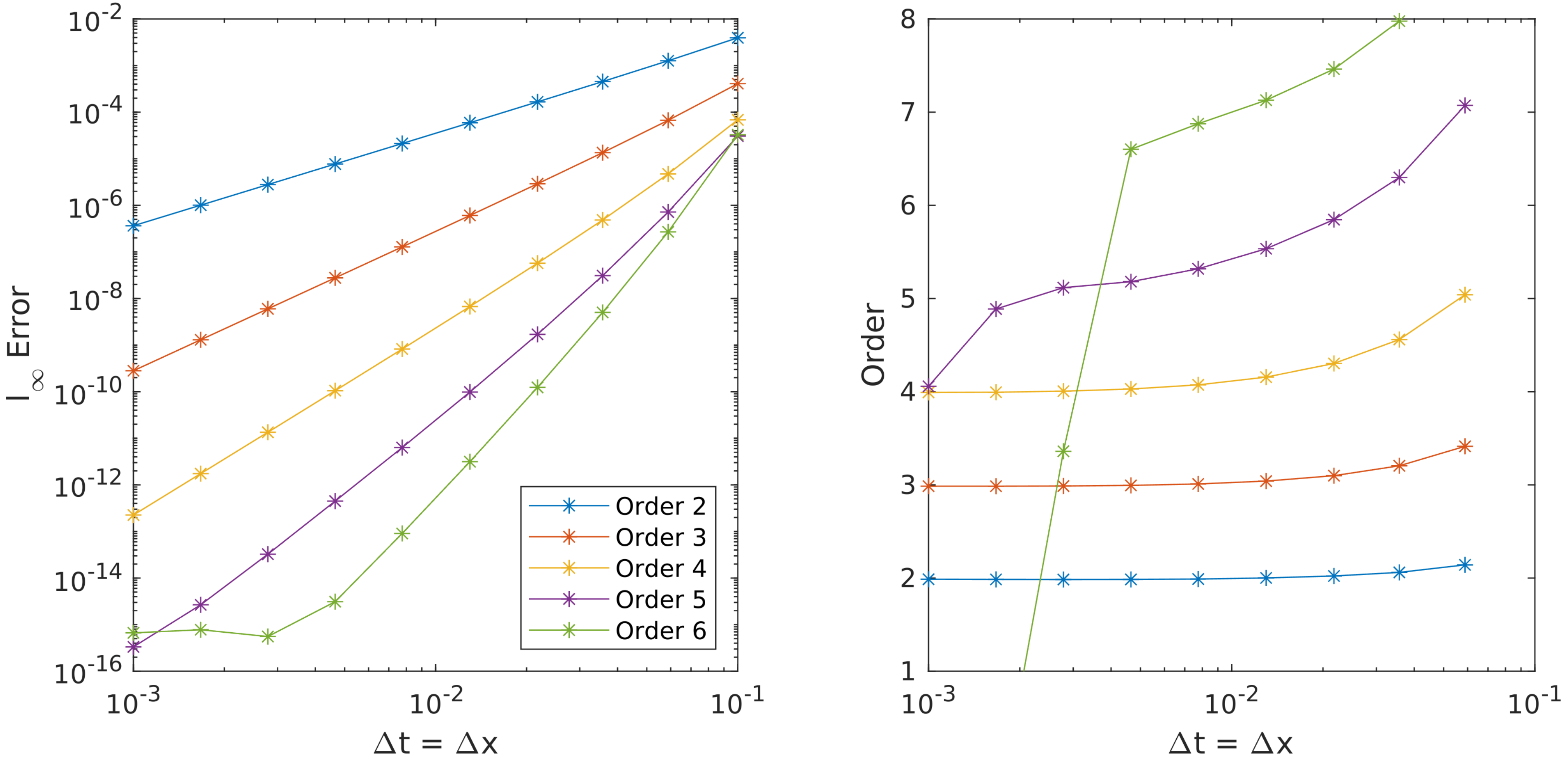
- Parallel iteration does not increase WSO unless we carefully chose the basic scheme

$$
\begin{aligned}
\widetilde{A} &= \widetilde{V}\widetilde{S}\widetilde{V}^{-1} \\
\widetilde{b}^T &= e^T\widetilde{S}\widetilde{V}^{-1} \\
\widetilde{V} &= \left[\; e \;\middle|\; \widetilde{c} \;\middle|\; \cdots \;\middle|\; \widetilde{c}^p \;\right]
\end{aligned}
\qquad
S = \begin{bmatrix} 0 & & & & \\ 1 & 0 & & & \\ & \frac{1}{2} & 0 & & \\ & & \ddots & \ddots & \\ & & & \frac{1}{p} & 0 \end{bmatrix}
$$

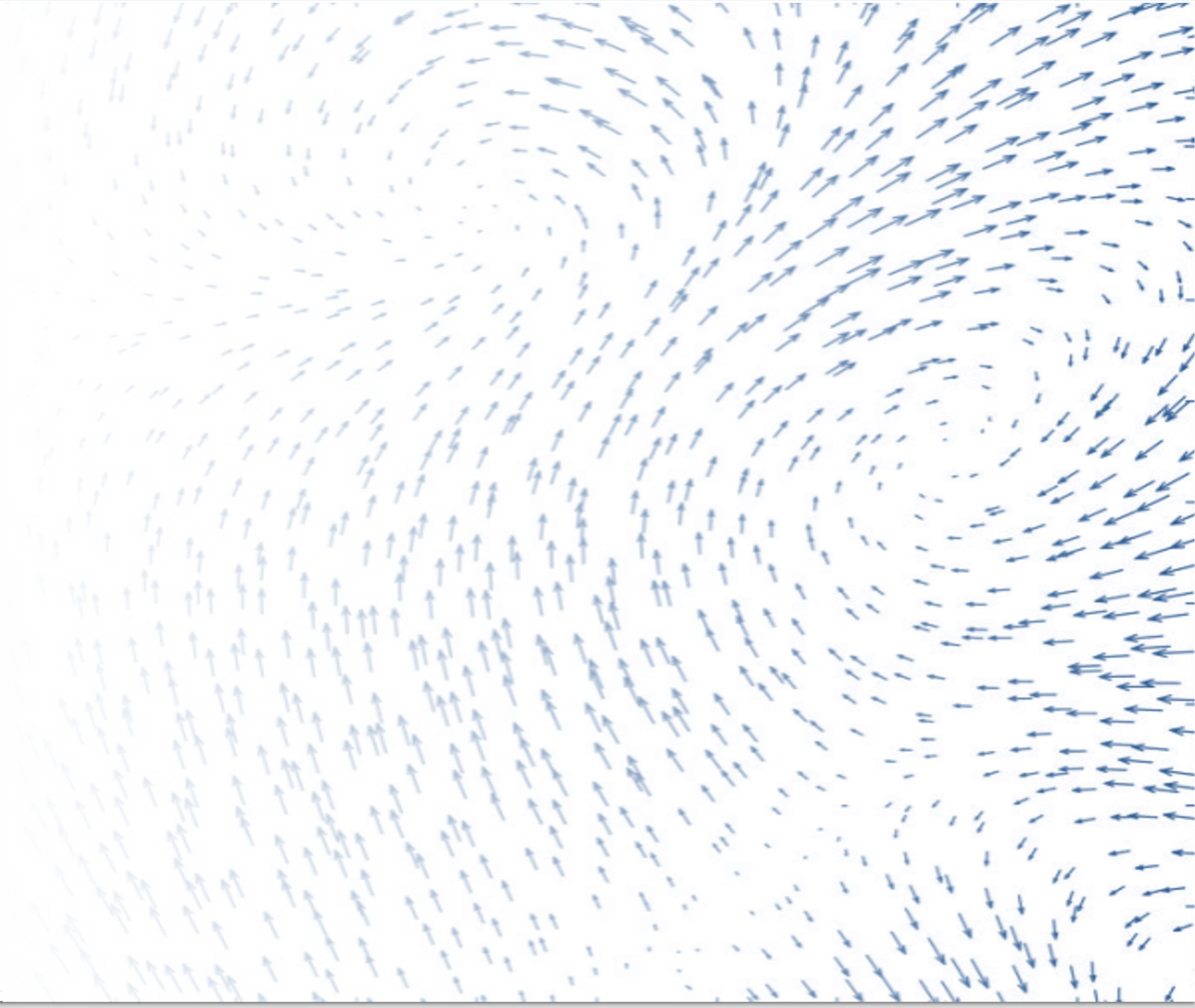
- The basic method is fully implicitly, but all eigenvalues of $\tilde{A}$ are zero

- We achieve order p and WSO p after p parallel iterations
  - The total number of stages is p^2
  - Expensive if implemented serially, but competitive if parallelism is exploited

The Parallel Iterated Runge–Kutta Methods Attain High Order on the Advection PDE



Outline



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Nonlinear Problems Require Stringent Order Conditions

- Nonlinearity often worsens order reduction

- The typical remedy is high stage order

$$\begin{aligned} C(q)&: \quad Ac^{k-1} = \frac{c^k}{k}, \quad k = 1, \dots, q, \\ B(p)&: \quad b^T c^{k-1} = \frac{1}{k}, \quad k = 1, \dots, p \end{aligned}$$

- This is very restrictive!
  - Explicit methods have max stage order of 1
  - Diagonally implicit methods have max stage order of 2

- Within the Runge–Kutta family, fully implicit schemes are seemingly the only ones that can achieve high orders outside the classical regime.

We Consider 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

$$y' = Jy + g(y)$$

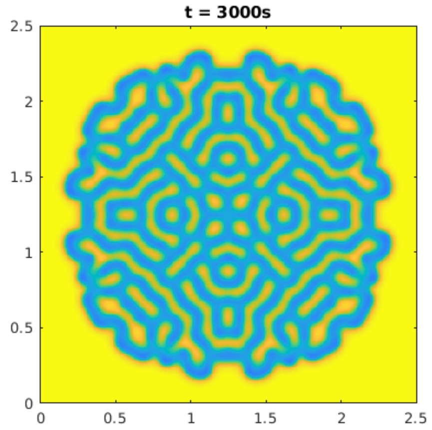
Stiff

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

Nonstiff

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

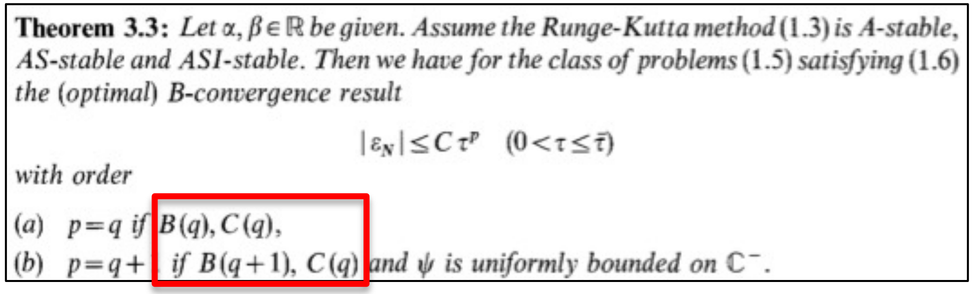
- Examples include
  - Patten-forming diffusion reaction problems
  - Schrödinger equations
  - Air pollution transport models



The Situation for Semilinear Problems is Unclear

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

- Do we need the restrictive condition of high stage order for semilinear problems?
  - The literature suggests yes
- Are there sharper order conditions for semilinear problems?
- Can we find methods devoid of order reduction with practical structures?
  - We will focus on diagonally implicit methods



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*

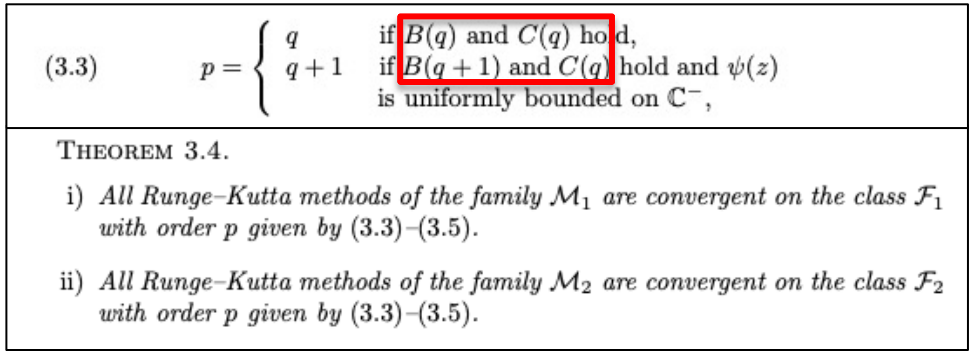
$$|\varepsilon_N| \le C\tau^p \quad (0 < \tau \le \bar{\tau})$$

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.

Progress has been Made Outside of Runge–Kutta Methods

- Exponential Integrators
  - Hochbruck, Marlis, and Alexander Ostermann. "Explicit exponential Runge--Kutta methods for semilinear parabolic problems." *SINUM* 43.3 (2005): 1069-1090.
  - Luan, Vu Thai, and Alexander Ostermann. "Exponential B-series: The stiff case." *SINUM* 51.6 (2013): 3431-3445.
  - Hochbruck, Marlis, Jan Leibold, and Alexander Ostermann. "On the convergence of Lawson methods for semilinear stiff problems." *Numerische Mathematik* 145 (2020): 553-580.

- Splitting Methods
  - Hansen, Eskil, and Alexander Ostermann. "High-order splitting schemes for semilinear evolution equations." *BIT Numerical Mathematics* 56 (2016): 1303-1316.
  - Einkemmer, Lukas, and Alexander Ostermann. "Overcoming order reduction in diffusion-reaction splitting. Part 1: Dirichlet boundary conditions." *SISC* 37.3 (2015): A1577-A1592.
  - Einkemmer, Lukas, and Alexander Ostermann. "Overcoming order reduction in diffusion-reaction splitting. Part 2: Oblique boundary conditions." *SISC* 38.6 (2016): A3741-A3757.

- Linear Multistep Methods
  - Wanner, Gerhard, and Ernst Hairer. Solving ordinary differential equations II. Vol. 375. New York: Springer Berlin Heidelberg, 1996.

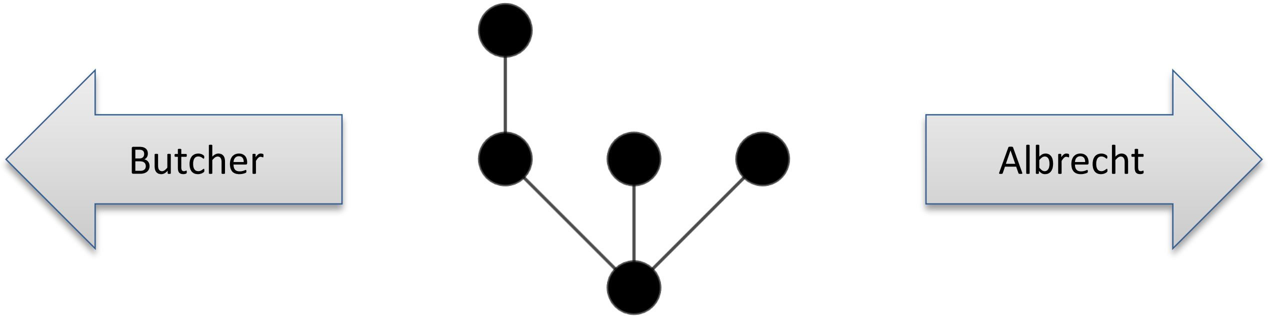
- Rosenbrock
  - Lubich, Ch, and Alexander Ostermann. "Linearly implicit time discretization of non-linear parabolic equations." *IMA Journal of Numerical Analysis* 15.4 (1995): 555-583.

Our Semilinear Analysis Extends a Lesser-Known Classical Analysis

- Rooted trees and B-series[1] are the standard tools for analyzing the local error of a Runge–Kutta scheme

- Albrecht[2] proposed alternative order conditions based on recursive orthogonality conditions
  - These conditions are in 1-to-1 correspondence with rooted trees too
  - We adapt this analysis approach for stiff, semilinear ODEs

$$0= b^T C^2 A c$$



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

Example Condition of Order 5

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1. Butcher, J.C. (2021). B-series and Algebraic Analysis. In: B-Series. Springer Series in Computational Mathematics, vol 55. Springer, Cham.
2. Albrecht, Peter. "The Runge–Kutta theory in a nutshell." *SIAM Journal on Numerical Analysis* 33.5 (1996): 1712-1735.

Our Error Expansion Uses Bounded Terms I

- The local truncation error satisfies $y(x_1) - y_1 = \sum_{t \in T} \Psi(t)$, where T is the set of rooted trees and

$$\Psi(t) = \begin{cases} \boxed{(I - A \otimes Z)^{-1}} \left(\left(\frac{c^j}{j!} - \frac{Ac^{j-1}}{(j-1)!} \right) \otimes \boxed{y^{(i)}(x_0)} \right), & t = [\tau^\ell], \\ \zeta(t) \boxed{(I - A \otimes Z)^{-1}} ((AC^\ell) \otimes I) \boxed{G^{(\ell,k)}(x_0)} (\Psi(t_1), \ldots, \Psi(t_k)), & t = [\tau^\ell t_1 \ldots t_k], k \geq 1, \end{cases}$$

$$\psi(t) = \begin{cases} \left(\frac{1}{k!} - \frac{b^T c^{k-1}}{(k-1)!} \right) y^{(i)}(x_0) + (b^T \otimes Z)\Psi(t), & t = [\tau^\ell], \\ \zeta(t) \boxed{(b^T \otimes I)(I - A \otimes Z)^{-1}} (C^\ell \otimes I) \boxed{G^{(\ell,k)}(x_0)} (\Psi(t_1), \ldots, \Psi(t_k)), & t = [\tau^\ell t_1 \ldots t_k], k \geq 1. \end{cases}$$

- The stiff term $Z = \Delta t\, J$ is confined to bounded terms

- All differential are bounded
  - $G^{(\ell,k)}(x) = \frac{d^\ell}{dx^\ell} g^{(k)}(y(x))\Big|_{x=x_0}$

- When $Z = 0$, we recover Albrecht's classical, nonstiff order conditions

Our Error Expansion Uses Bounded Terms II

- A classical expansion of the local truncation error looks like

$$y(x_1) - y_1 = \cdots + \Delta t^2 \left(\frac{1}{2} - b^T c\right)\left(J + g'(y_0)\right) y_0' + \Delta t^3 \left(\frac{1}{6} - b^T A c\right)\left(J + g'(y_0)\right)^2 y_0' + \cdots$$

Unbounded Terms

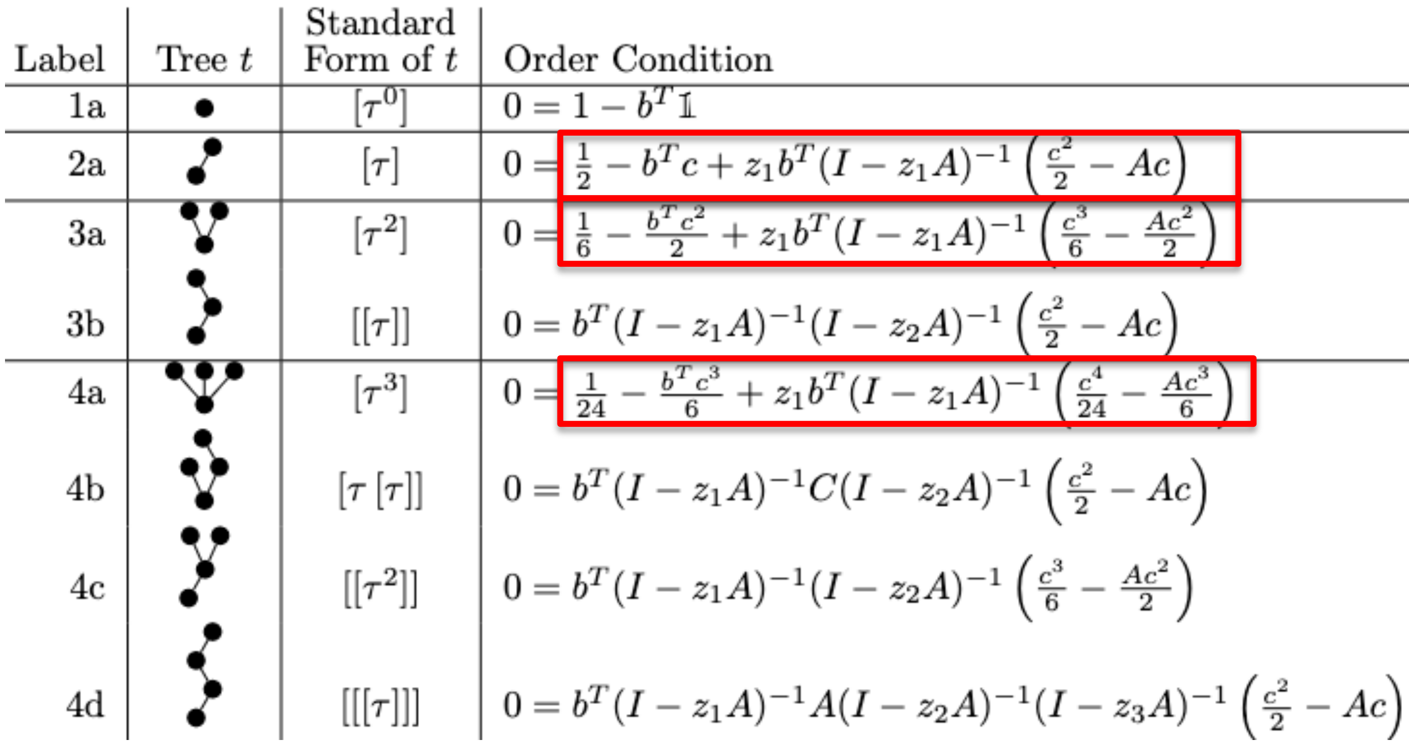
- Our new semilinear expansion looks like

$$\begin{aligned} & y(x_1) - y_1 \\ & = \cdots + \Delta t^2 \left(\frac{1}{2} - b^T c + z b^T (I - zA)^{-1} \left(\frac{c^2}{2} - Ac\right)\right) y_0'' + \Delta t^3 b^T (I - zA)^{-2} \left(\frac{c^2}{2} - Ac\right) g'(y_0) y_0'' + \cdots \end{aligned}$$

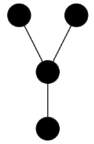
where $z = \Delta t\, J$ (scalar here for simplicity).

We Found that Sharper Order Conditions Do Exists for Stiff Semilinear Problems

- From our new error expansion we can extract order conditions
- Like classical order conditions, there is 1-to-1 correspondence with rooted trees
- The semilinear order conditions are sharper than stage order conditions
- “Bushy trees” (trees with height 2) give WSO conditions

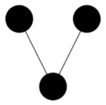


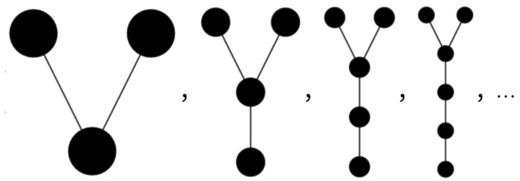
Label	Tree t	Standard Form of t	Order Condition
1a		$[\tau^0]$	$0 = 1 - b^T \mathbb{1}$
2a		$[\tau]$	$0 = \boxed{\frac{1}{2} - b^T c + z_1 b^T (I - z_1 A)^{-1} \left(\frac{c^2}{2} - Ac \right)}$
3a		$[\tau^2]$	$0 = \boxed{\frac{1}{6} - \frac{b^T c^2}{2} + z_1 b^T (I - z_1 A)^{-1} \left(\frac{c^3}{6} - \frac{Ac^2}{2} \right)}$
3b		$[[\tau]]$	$0 = b^T (I - z_1 A)^{-1} (I - z_2 A)^{-1} \left(\frac{c^2}{2} - Ac \right)$
4a		$[\tau^3]$	$0 = \boxed{\frac{1}{24} - \frac{b^T c^3}{6} + z_1 b^T (I - z_1 A)^{-1} \left(\frac{c^4}{24} - \frac{Ac^3}{6} \right)}$
4b		$[\tau\,[\tau]]$	$0 = b^T (I - z_1 A)^{-1} C (I - z_2 A)^{-1} \left(\frac{c^2}{2} - Ac \right)$
4c		$[[\tau^2]]$	$0 = b^T (I - z_1 A)^{-1} (I - z_2 A)^{-1} \left(\frac{c^3}{6} - \frac{Ac^2}{2} \right)$
4d		$[[[\tau]]]$	$0 = b^T (I - z_1 A)^{-1} A (I - z_2 A)^{-1} (I - z_3 A)^{-1} \left(\frac{c^2}{2} - Ac \right)$

The Conditions for $t =$  Reveals Redundancies and Patterns

$$0 = b^T (I - z_1 A)^{-1} (I - z_2 A)^{-1} \left(\frac{c^3}{6} - \frac{Ac^2}{2} \right), \quad \forall z_1, z_2 \in \mathbb{C}^-$$

$$0 = b^T A^i \left(\frac{c^3}{6} - \frac{Ac^2}{2} \right), \quad i = 0,1,2 \ldots$$

Semilinear order condition associated with with $t =$  (One order lower)

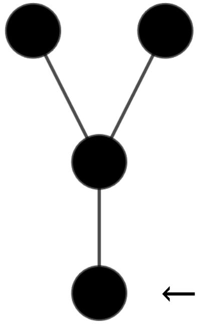
Classical Albrecht order conditions associated with with $t \in$ 

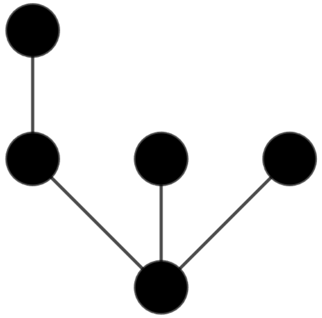
We Need to Define a Special Vertex Type

Definition[1]

A vertex of a tree is called a **semi-lone-parent** if it has a single child which is not a leaf.

A tree without semi-lone-parents is **semi-lone-child-avoiding**.




semi-lone-child-avoiding

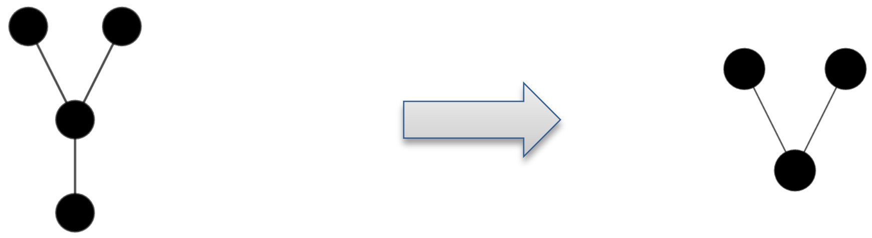
---

1. https://oeis.org/A331934

Semilinear Conditions for Trees with a Semi-Lone-Parent are Redundant

Theorem

If a tree has a semi-lone-parent vertex, the corresponding semilinear order condition is implied by the tree with that vertex removed.



$$0 = b^T(I - z_1 A)^{-1}(I - z_2 A)^{-1}\left(\frac{c^3}{6} - \frac{Ac^2}{2}\right)$$

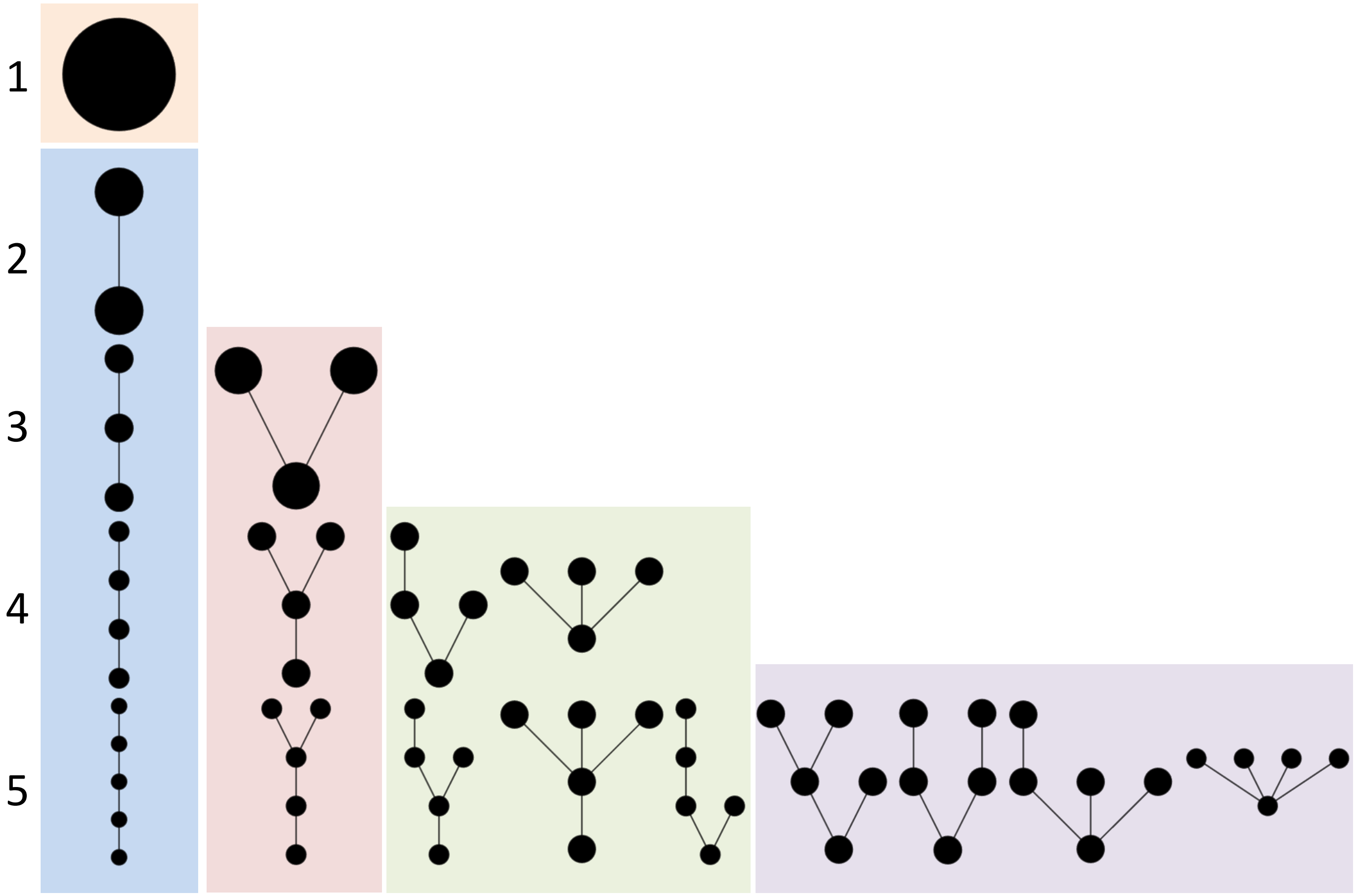
$$0 = b^T(I - z_1 A)^{-1}\left(\frac{c^3}{6} - \frac{Ac^2}{2}\right)$$

We only need to consider the set of 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

Let's Express Semilinear Order Conditions in Terms of Classical Order Conditions

- Classical order p conditions map to trees with p vertices
- Semilinear order conditions map to trees with with p vertices that are not a semi-lone-parent
  - The subsets are infinite!
- **Semilinear order conditions can be viewed as a regrouping of classical order conditions in Albrecht's form**



Can we Derive Diagonally Implicit Runge–Kutta (DIRK) Methods with the Semilinear Order Conditions?

- Desired properties
  - Order >2
  - (Singly) diagonally implicit
  - L-stable

- The semilinear conditions coincide with WSO up to order 3
  - We can leverage existing DIRK methods designed for linear problems[1,2]
  - Explains better-than-expected convergence in tests

- Order conditions are challenging to solve
  - The number or order conditions increases with the order and the number of stages
  - We use both symbolic and constrained optimization techniques

---

1. Ketcheson, David I., et al. "DIRK schemes with high weak stage order." *Spectral and High Order Methods for Partial Differential Equations* (2020): 453.
2. Biswas, Abhijit, et al. "Design of DIRK schemes with high weak stage order." *Communications in Applied Mathematics and Computational Science* 18.1 (2023): 1-28.

SDIRK3SL is a New 3rd Order Method for Stiff, Semilinear ODEs

- We minimize the principal error with the order condition constraints

$$\frac{1}{k} = b^T c^{k-1}, \quad k = 1,2,3$$

$$0 = b^T A^i \left(\frac{c^j}{j} - A c^{j-1} \right), \quad i = 0, \ldots, s-1, \;\; j = 2,3$$

- While methods exist with 5 stages, an additional stage significantly improves accuracy

$$\begin{array}{c|cccccc}
\frac{13}{58} & \frac{13}{58} & 0 & 0 & 0 & 0 & 0 \\
\frac{26}{29} & \frac{39}{58} & \frac{13}{58} & 0 & 0 & 0 & 0 \\
0 & -\frac{13}{58} & 0 & \frac{13}{58} & 0 & 0 & 0 \\
\frac{13}{29} & \frac{65}{174} & -\frac{13}{348} & -\frac{13}{116} & \frac{13}{58} & 0 & 0 \\
\frac{12\,971}{17\,611} & \frac{2\,015\,824\,758\,301\,938\,982\,625}{11\,720\,872\,553\,456\,507\,801\,646} & -\frac{554\,819\,849\,934\,875}{11\,076\,945\,065\,425\,668} & \frac{68\,790\,302\,177\,688\,571\,375}{269\,445\,346\,056\,471\,443\,716} & \frac{7\,705\,505\,568\,680\,430\,000}{56\,998\,053\,973\,484\,343\,863} & \frac{13}{58} & 0 \\
1 & \frac{3\,455\,277\,656}{28\,312\,464\,375} & -\frac{1\,061\,001\,132\,073}{3\,749\,092\,092\,720} & \frac{780\,513\,524\,467}{5\,751\,892\,408\,080} & \frac{342\,906\,676\,217}{1\,125\,548\,760\,960} & \frac{77\,214\,825\,271\,310\,213\,828\,561}{155\,527\,924\,398\,245\,799\,120\,000} & \frac{13}{58} \\
\hline
 & \frac{3\,455\,277\,656}{28\,312\,464\,375} & -\frac{1\,061\,001\,132\,073}{3\,749\,092\,092\,720} & \frac{780\,513\,524\,467}{5\,751\,892\,408\,080} & \frac{342\,906\,676\,217}{1\,125\,548\,760\,960} & \frac{77\,214\,825\,271\,310\,213\,828\,561}{155\,527\,924\,398\,245\,799\,120\,000} & \frac{13}{58} \\
\hline
 & \frac{83\,396\,117\,862\,679\,251\,596\,686}{543\,808\,069\,678\,473\,491\,279\,817} & -\frac{51\,873\,391\,680\,781\,295\,917\,121}{197\,748\,388\,973\,990\,360\,465\,388} & \frac{91\,834\,777\,272\,491\,463\,252\,761}{725\,077\,426\,237\,964\,655\,039\,756} & \frac{5\,676\,271\,777\,638\,433\,424\,524}{20\,141\,039\,617\,721\,240\,417\,771} & \frac{11}{23} & \frac{2}{9}
\end{array}$$

DIRK4SL is a New 4th Order Method for Stiff, Semilinear ODEs

- Now there are 74 conditions for a 4th order method in 7 stages!

$$\frac{1}{k} = b^T c^{k-1}, \quad k = 1,2,3,4$$

$$0 = b^T A^i \left(\frac{c^j}{j} - A c^{j-1} \right), \quad i = 0, \dots, 6, \;\; j = 2,3,4$$

$$0 = b^T A^i C A^j \left(\frac{c^2}{2} - A c \right), \quad i, j = 0, \dots, 6$$

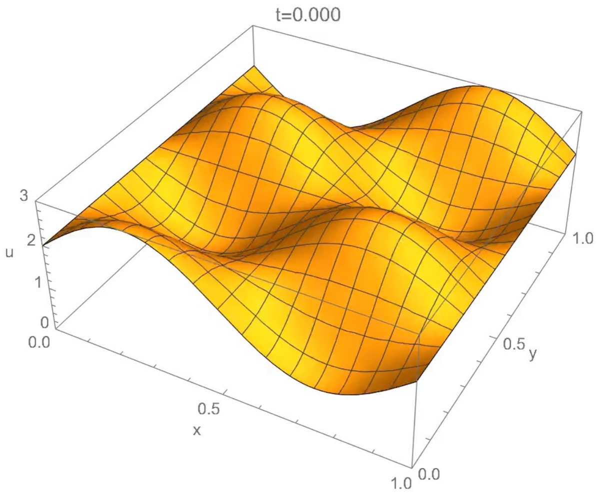
$$\begin{array}{c|ccccccc}
6.78237 \times 10^{-8} & 6.78237 \times 10^{-8} & 0 & 0 & 0 & 0 & 0 & 0 \\
1.27118 & 0.635591 & 0.635591 & 0 & 0 & 0 & 0 & 0 \\
0.340612 & 0.0983263 & -0.0263464 & 0.268632 & 0 & 0 & 0 & 0 \\
3.42294 & 7.64459 & 1.79116 & -6.56175 & 0.548945 & 0 & 0 & 0 \\
3.42294 & 9.09652 & 2.19453 & -8.42176 & 0.181804 & 0.371850 & 0 & 0 \\
4.91905 & -0.771770 & 5.76965 & -1.12350 & -0.209710 & 0.204279 & 1.05010 & 0 \\
1.00000 & 0.0988876 & -0.103950 & 0.561554 & -0.0882214 & 0.0859368 & 0.000738514 & 0.445054 \\
\hline
 & 0.0988876 & -0.103950 & 0.561554 & -0.0882214 & 0.0859368 & 0.000738514 & 0.445054
\end{array}$$

Allen-Cahn is a Semilinear PDE Modeling Phase Separation

- Consider the 2D Allen-Cahn reaction-diffusion PDE

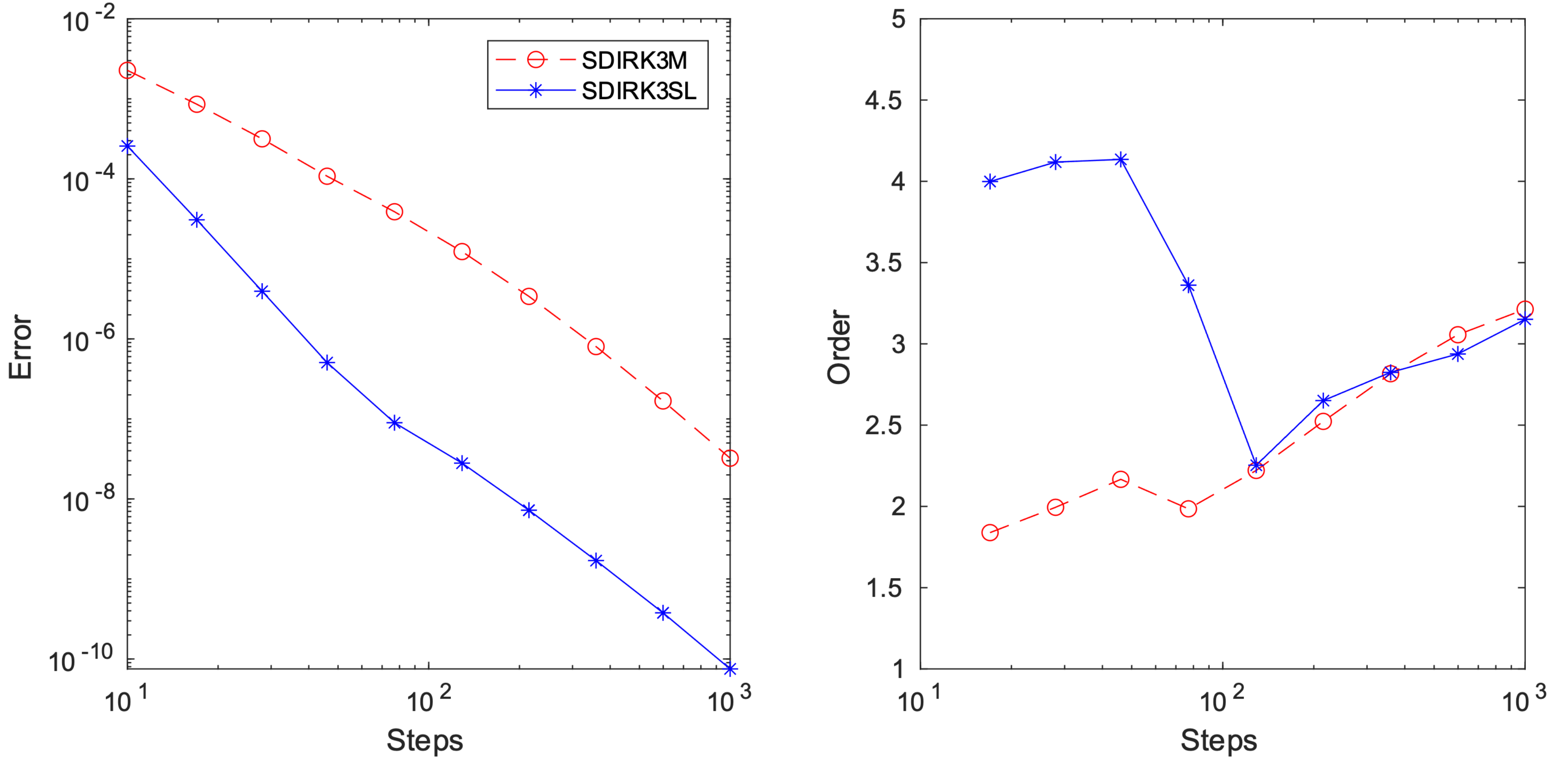
$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u + \beta(u - u^3) + s(t, x, y)$$

- I tested methods of order 3 and 4 to validate the semilinear order conditions

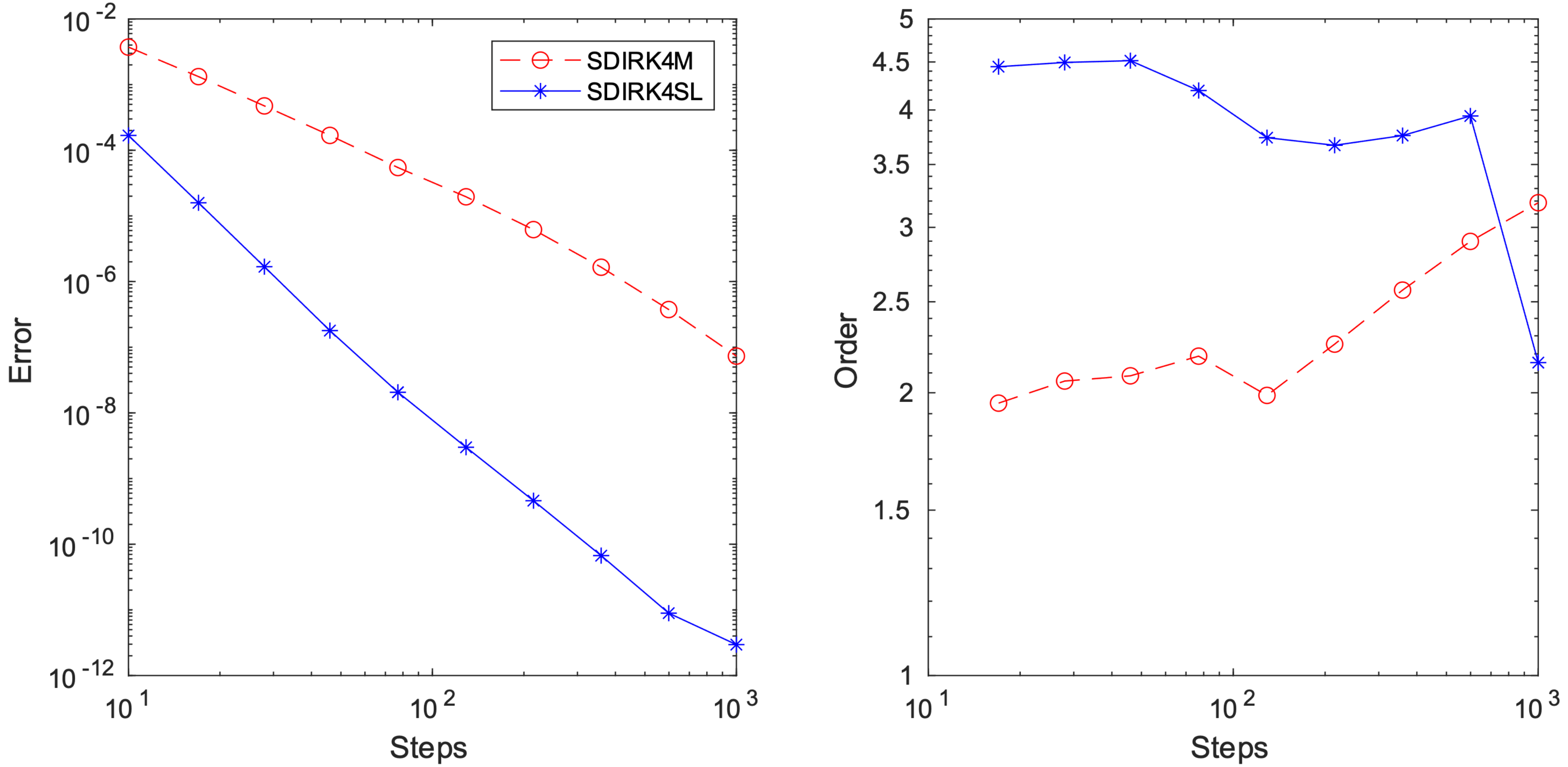


Method	Source	Stages	Classical Order	Semilinear Order
SDIRK3SL	New method from this work	6	3	3
SDIRK3M	Kennedy, Christopher A., and Mark H. Carpenter. Diagonally implicit Runge–Kutta methods for ordinary differential equations. A review. 2016.	4	3	1
DIRK4SL	New method from this work	7	4	4
SDIRK4M	Kennedy, Christopher A., and Mark H. Carpenter. Diagonally implicit Runge–Kutta methods for ordinary differential equations. A review. 2016.	5	4	1

The New Method SDIRK3SL Avoids Order Reduction



SDIRK4SL Also Avoids Order Reduction



Conclusions

- Classical order conditions rely on assumptions that often fail to hold for stiff problems
- The consequence is a reduction in order and efficiency for most Runge–Kutta methods
- We proposed a new error analysis and order condition theory resilient to stiffness
- High stage order is not necessary to avoid order reduction on stiff, semilinear ODEs
- Future work
  - Fully nonlinear problems
  - Other classes of integrators

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Questions?

> To create greater convergence, we need more integration.
>
> —Emmanuel Macron