

The Order of Runge–Kutta Methods in Theory and Practice

NJIT Department of Mathematical Sciences Fluid Mechanics and Waves Seminar



12/4/23

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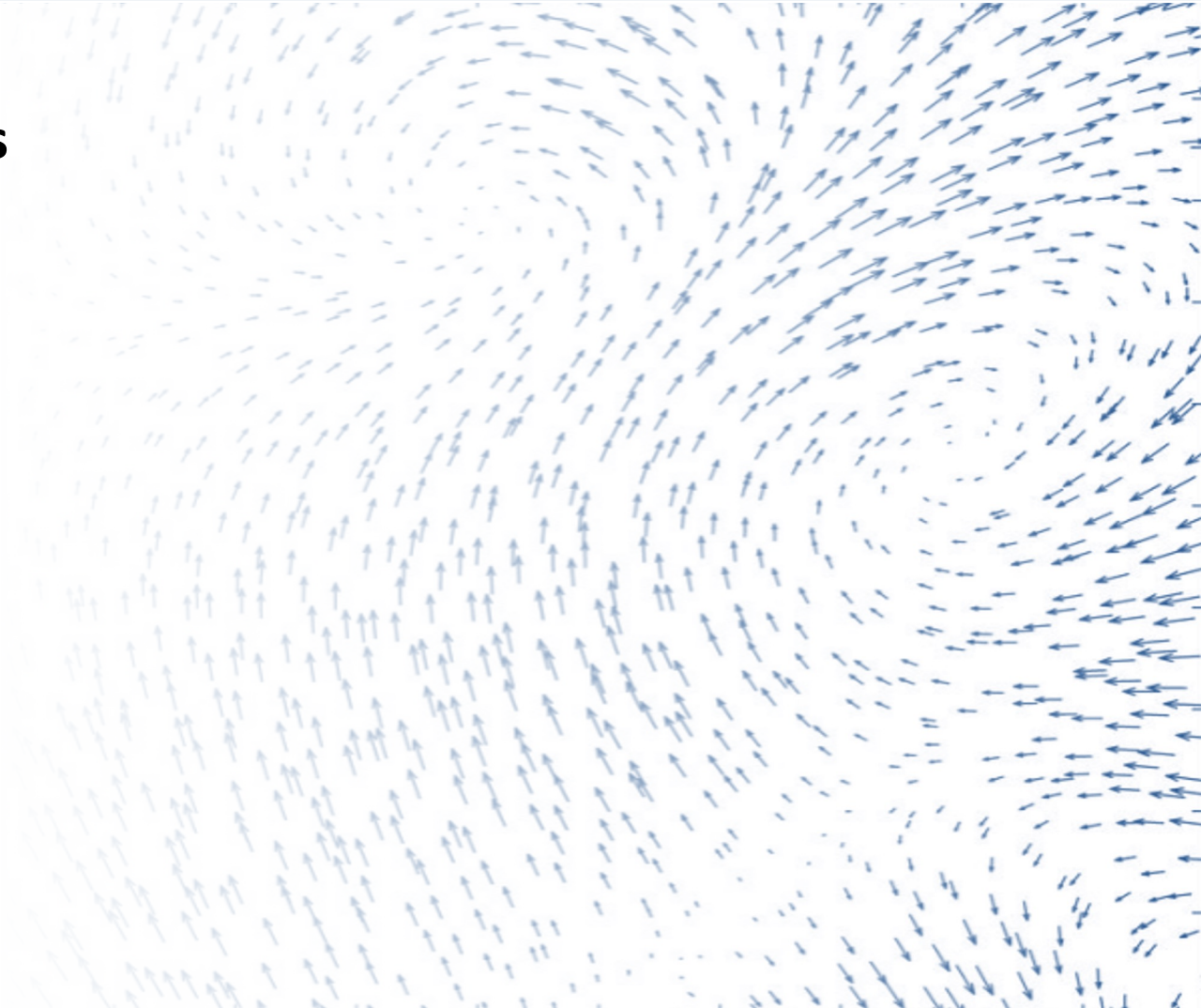


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This work was supported by the Fernbach Fellowship through the LLNL-LDRD Program under Project No. 23-ERD-048

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)

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

with the numerical procedure

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

$$y_{n+1} = y_n + \Delta t \sum_{j=1}^s b_j f(Y_j)$$

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

Motivating Example: Let's Solve a Simple PDE

- Consider the following PDE¹ on $t, x \in [0,1]$:

$$\begin{aligned}
 u_t &= -u_x + \frac{t-x}{(1+t)^2}, \\
 u(t, 0) &= \frac{1}{1+t}, \\
 u(0, x) &= 1+x
 \end{aligned}$$

Semidiscretize

→

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

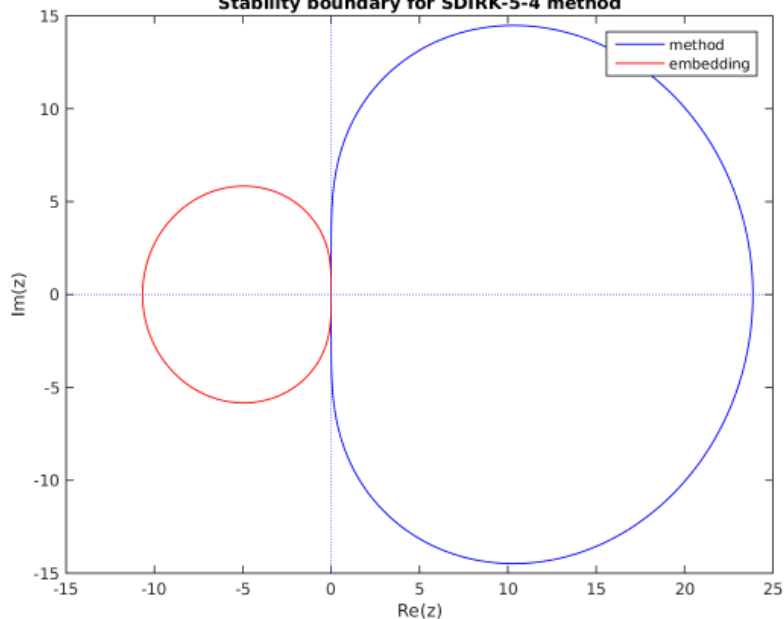
- The exact solution $u(t, x) = \frac{1+x}{1+t}$ is linear in space
- This finite difference discretization contributes no spatial error
 - Any numerical error will be entirely from the time discretization

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

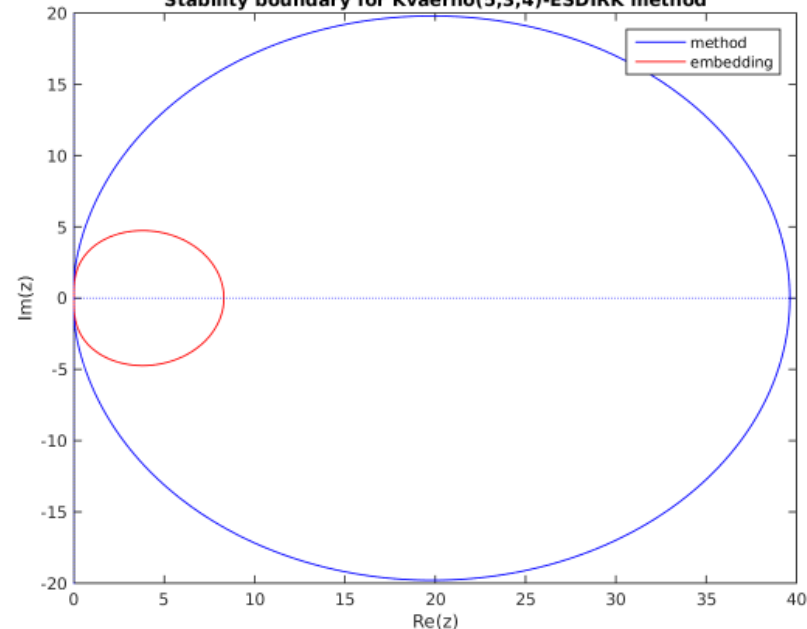
$\frac{1}{4}$	$\frac{1}{4}$	0	0	0	0
$\frac{3}{4}$	$\frac{1}{2}$	$\frac{1}{4}$	0	0	0
$\frac{11}{20}$	$\frac{17}{50}$	$-\frac{1}{25}$	$\frac{1}{4}$	0	0
$\frac{1}{2}$	$\frac{371}{1360}$	$-\frac{137}{2720}$	$\frac{15}{544}$	$\frac{1}{4}$	0
1	$\frac{25}{24}$	$-\frac{49}{48}$	$\frac{125}{16}$	$-\frac{85}{12}$	$\frac{1}{4}$
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

Stability boundary for SDIRK-5-4 method

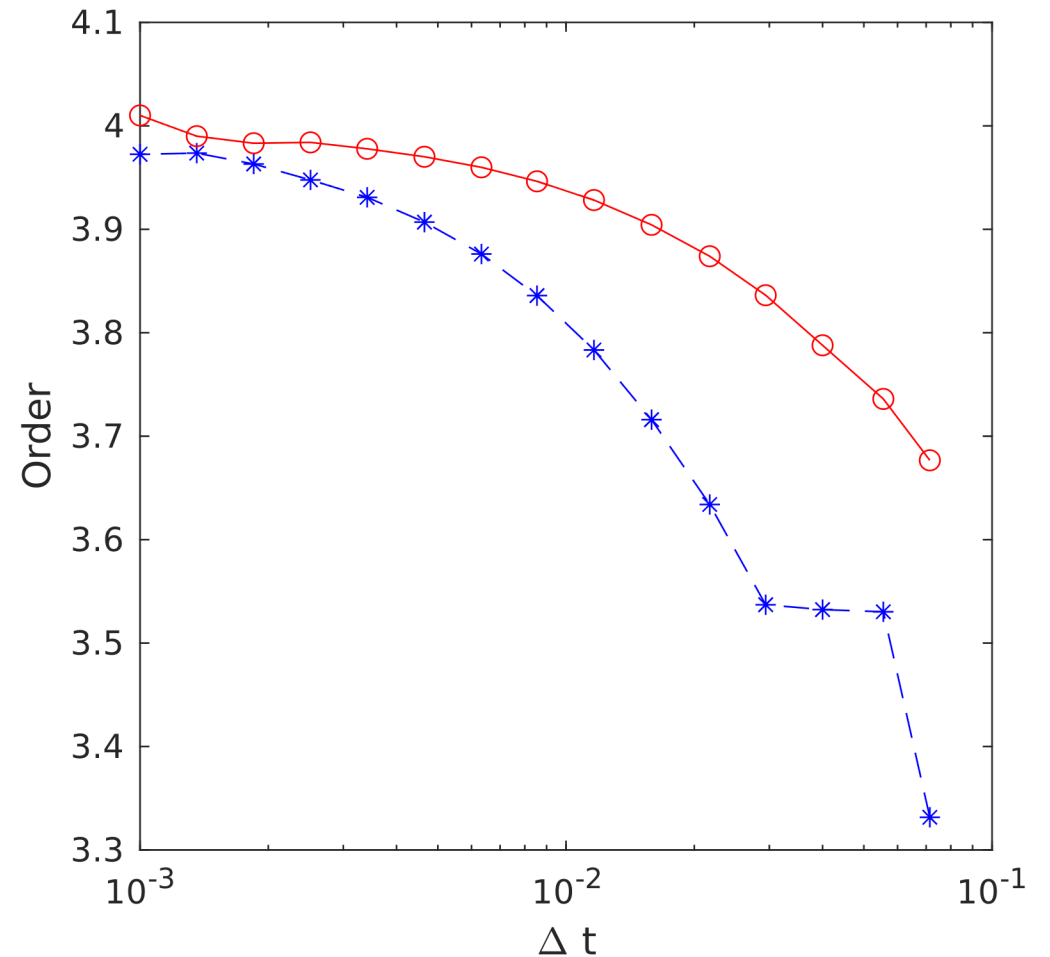
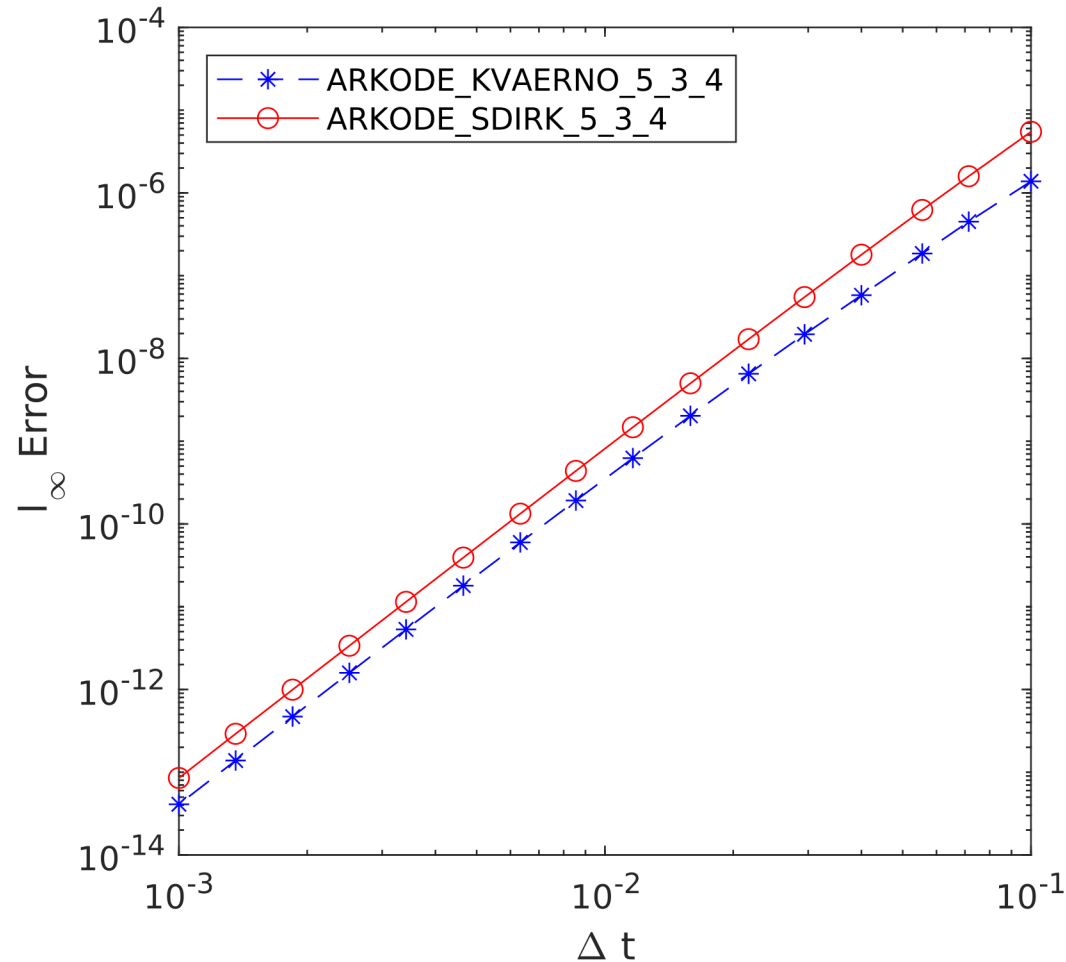


0	0	0	0	0	0
0.871733043	0.4358665215	0.4358665215	0	0	0
0.468238744853136	0.140737774731968	-0.108365551378832	0.4358665215	0	0
1	0.102399400616089	-0.376878452267324	0.838612530151233	0.4358665215	0
1	0.157024897860995	0.117330441357768	0.61667803039168	-0.326899891110444	0.4358665215
4	0.157024897860995	0.117330441357768	0.61667803039168	-0.326899891110444	0.4358665215
3	0.102399400616089	-0.376878452267324	0.838612530151233	0.4358665215	0

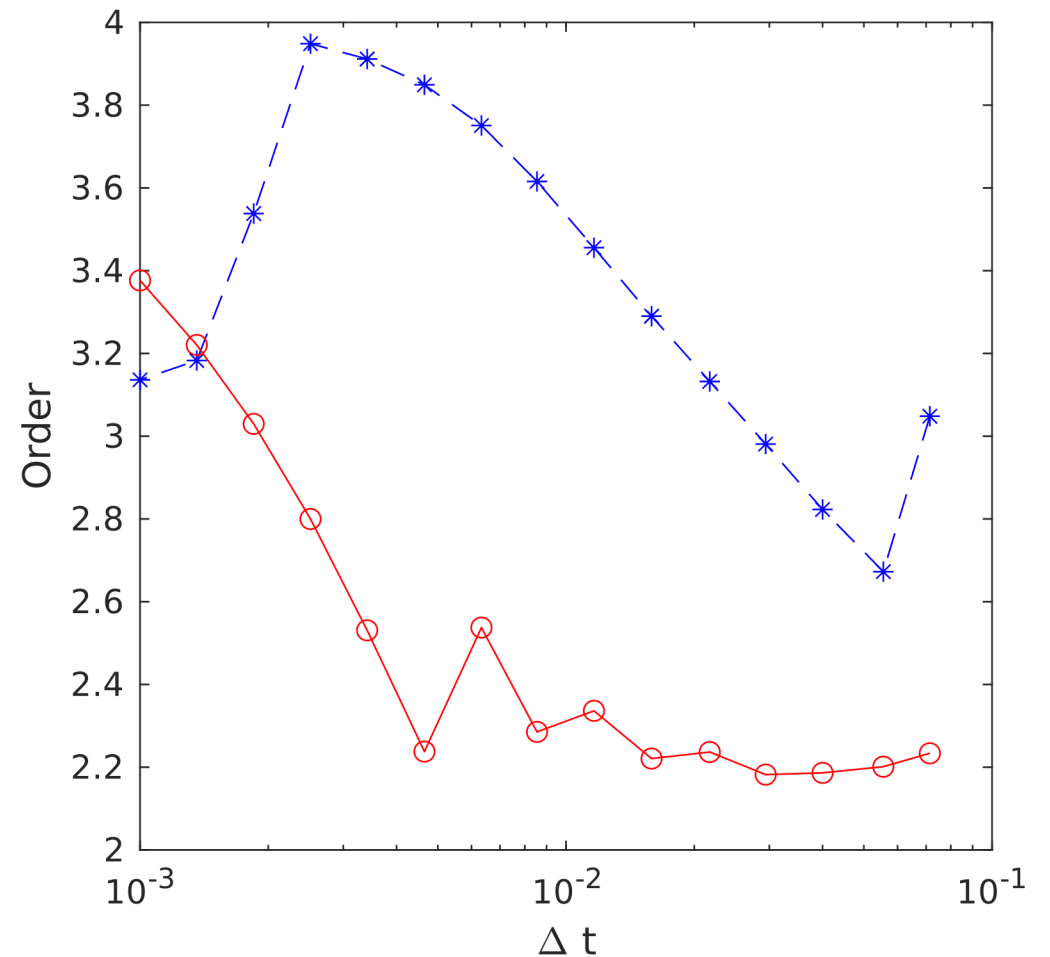
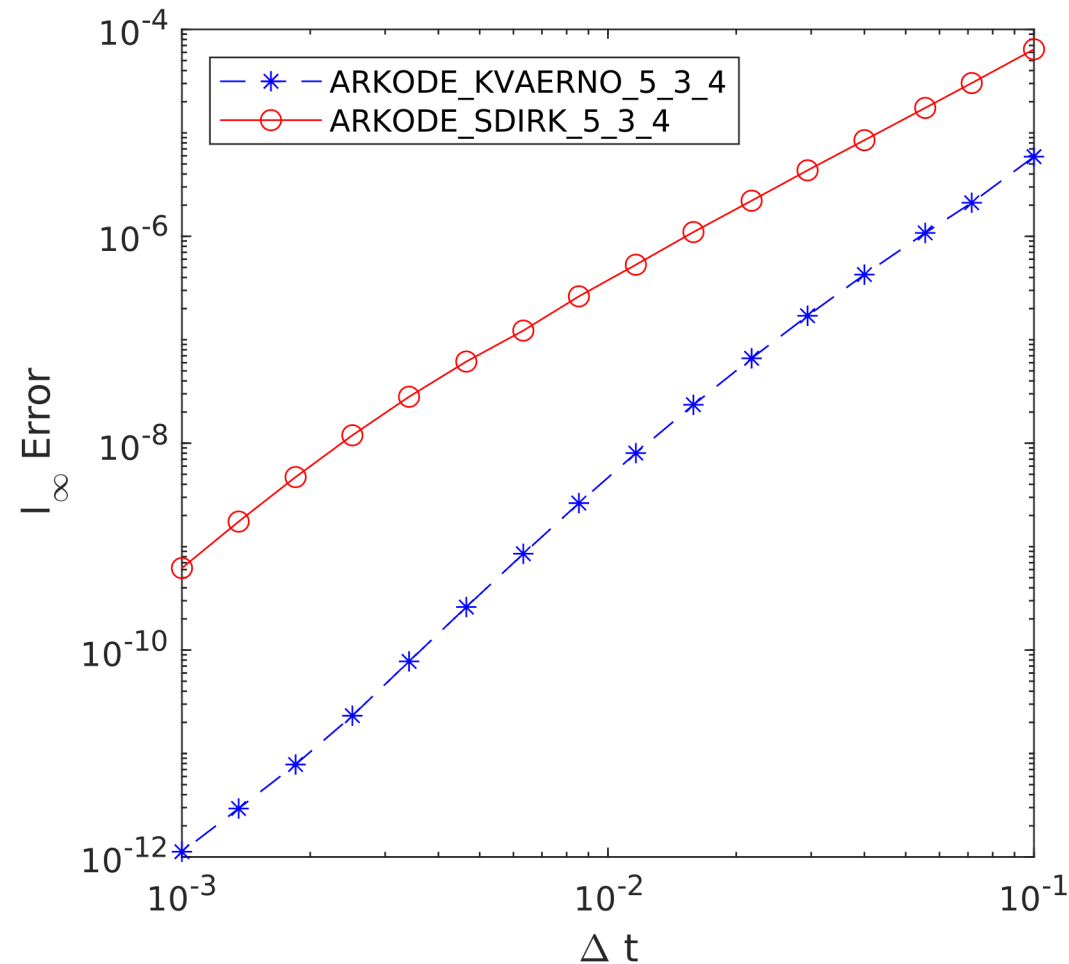
Stability boundary for Kvaerno(5,3,4)-ESDIRK method



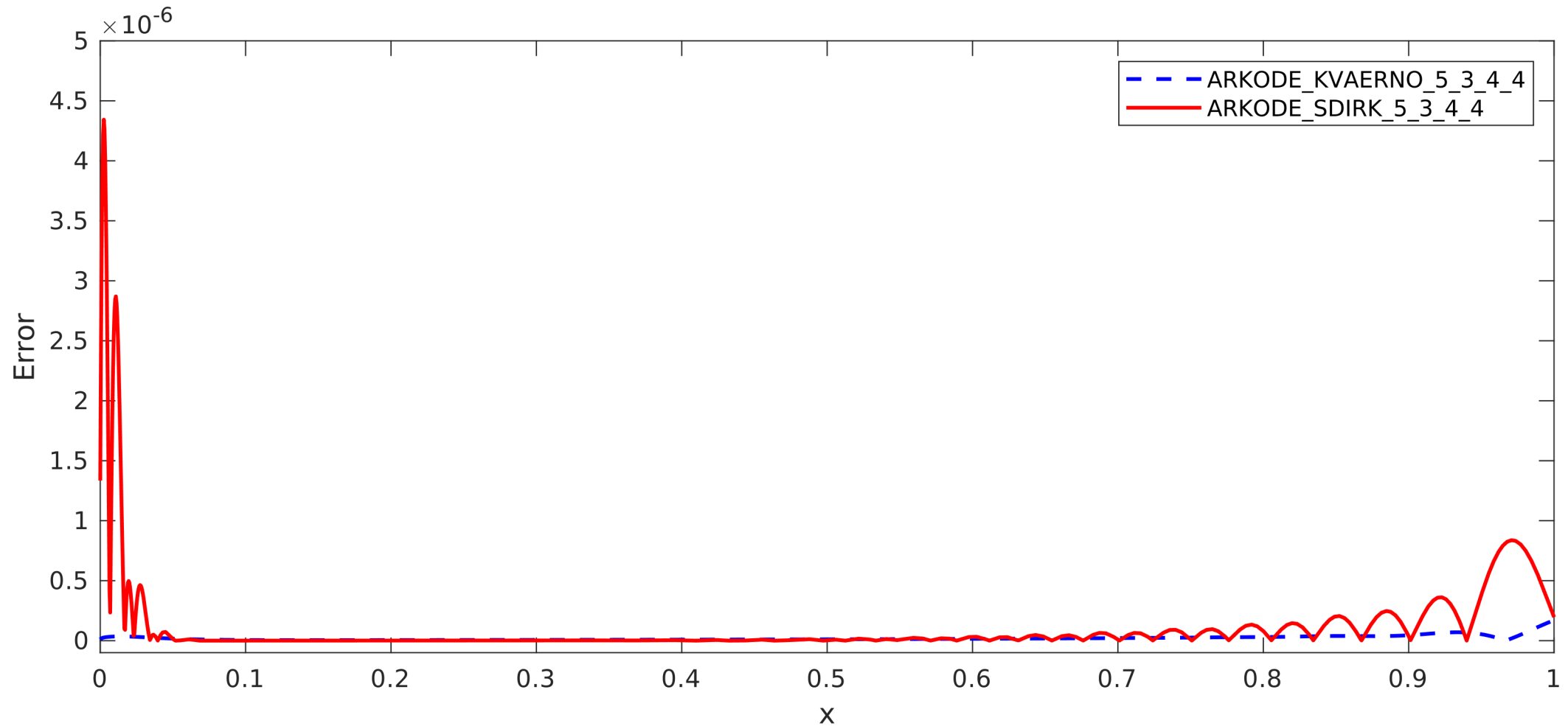
We See Asymptotic Convergence on a 16 Point Grid



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:

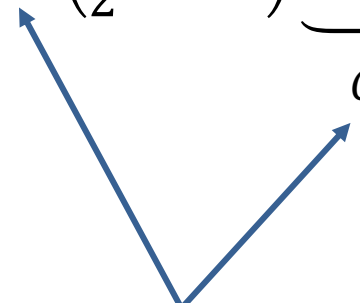
$$y' = \begin{bmatrix} -\frac{1}{\Delta x} & & & & \\ \frac{1}{\Delta x} & -\frac{1}{\Delta x} & & & \\ & \ddots & \ddots & & \\ & & \frac{1}{\Delta x} & -\frac{1}{\Delta x} & \\ & & & & \end{bmatrix} y + \begin{bmatrix} \frac{t - x_1}{(1+t)^2} + \frac{1}{\Delta x(1+t)} \\ \frac{t - x_2}{(1+t)^2} \\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

- 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 $\Delta t \leq C \Delta x$
 - 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

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


Bad interactions between spatial and temporal scales

The Order Reduction Phenomenon is Well-Known

- In 1974, Prothero and Robinson¹ proposed perhaps the simplest problem to cause order reduction

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

- 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

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

$$y' = \begin{bmatrix} -\frac{1}{\Delta x} & & & & \\ \frac{1}{\Delta x} & -\frac{1}{\Delta x} & & & \\ & \ddots & \ddots & & \\ & & \frac{1}{\Delta x} & -\frac{1}{\Delta x} & \\ & & & & \ddots & \ddots \end{bmatrix} y + \begin{bmatrix} \frac{t-x_1}{(1+t)^2} + \frac{1}{\Delta x(1+t)} \\ \frac{t-x_2}{(1+t)^2} \\ \vdots \\ \frac{t-x_N}{(1+t)^2} \end{bmatrix} \longrightarrow y'_1 = -\frac{1}{\Delta x} \left(y_1 - \frac{1}{1+t} \right) + \frac{t-x_1}{(1+t)^2}$$

\Downarrow

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

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

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:

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

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

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

- 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.

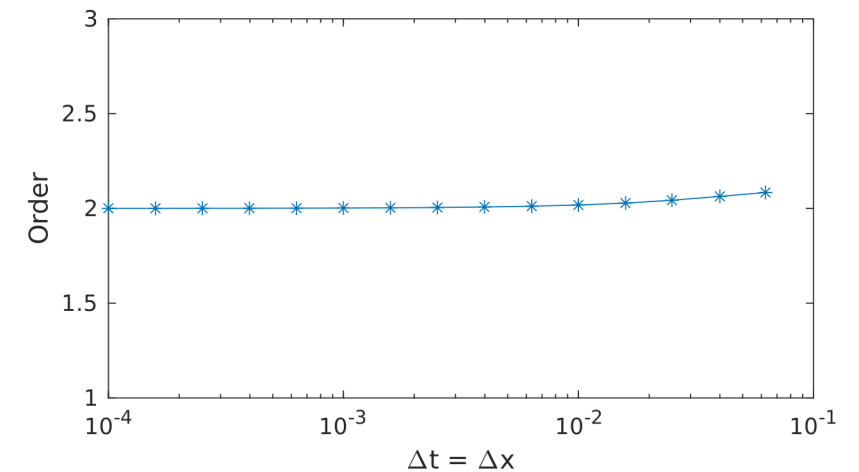
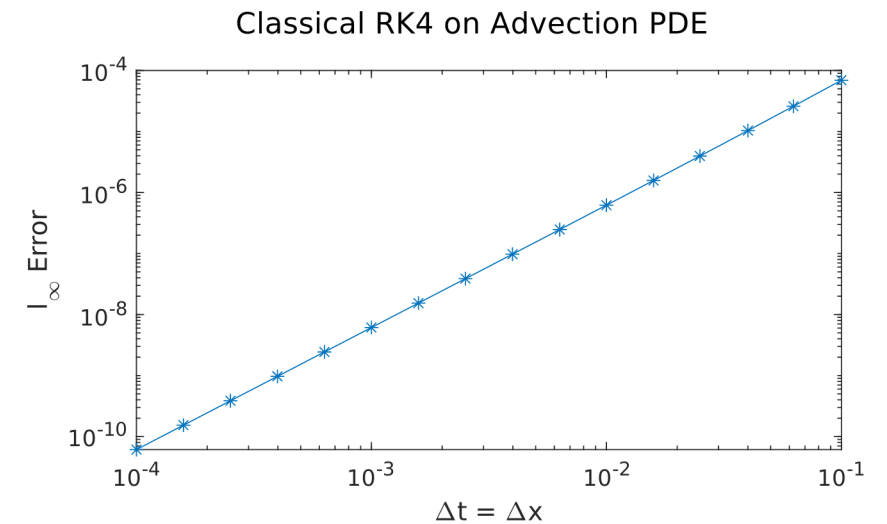
Outline

1. Introduction to the Order Reduction Phenomenon for Runge–Kutta methods
- 2. Explicit Runge–Kutta Methods that Alleviate Order Reduction**
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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?

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	$a_{s,s-1}$	
	b_1	b_2	\cdots	b_{s-1}	b_s

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

$$1 = b^T e,$$

$$\frac{1}{2} = b^T c,$$

$$\frac{1}{3} = b^T c^2, \quad \frac{1}{6} = b^T A c,$$

$$\frac{1}{4} = b^T c^3, \quad \frac{1}{8} = b^T \text{diag}(c) A c, \quad \frac{1}{12} = b^T A c^2, \quad \frac{1}{24} = b^T A^2 c$$

$$\vdots$$

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

	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

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

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

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

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

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

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.

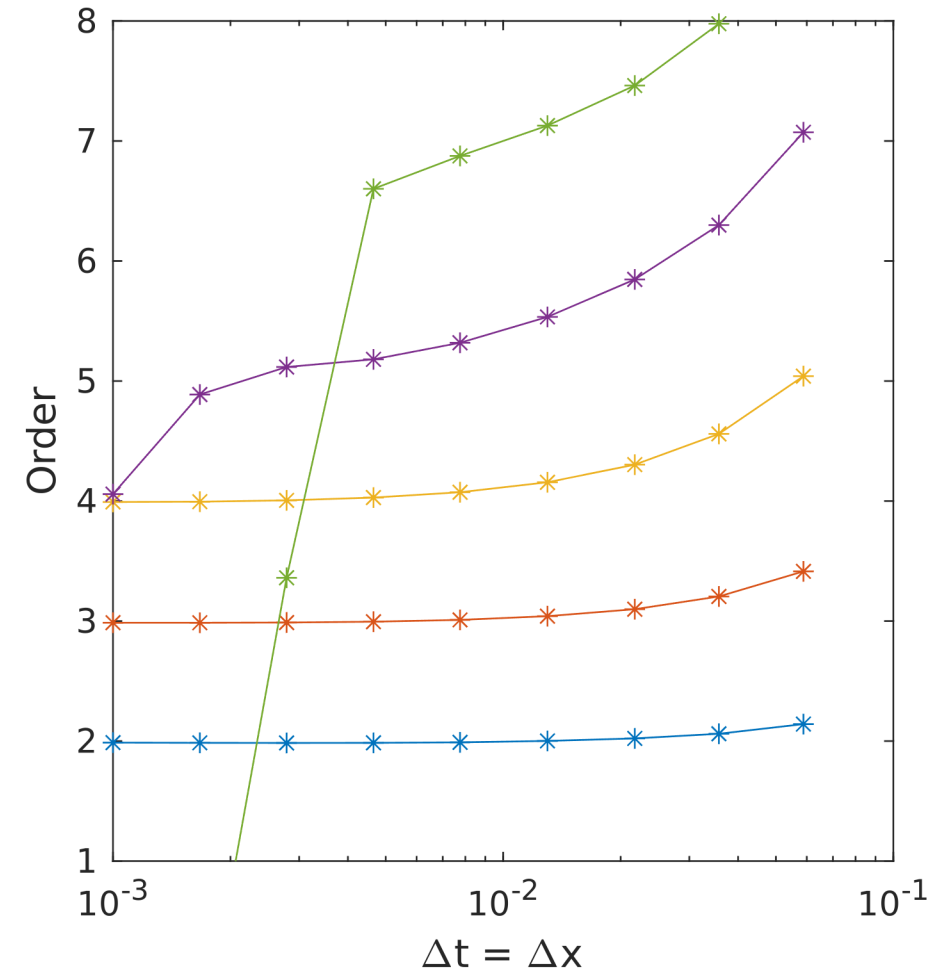
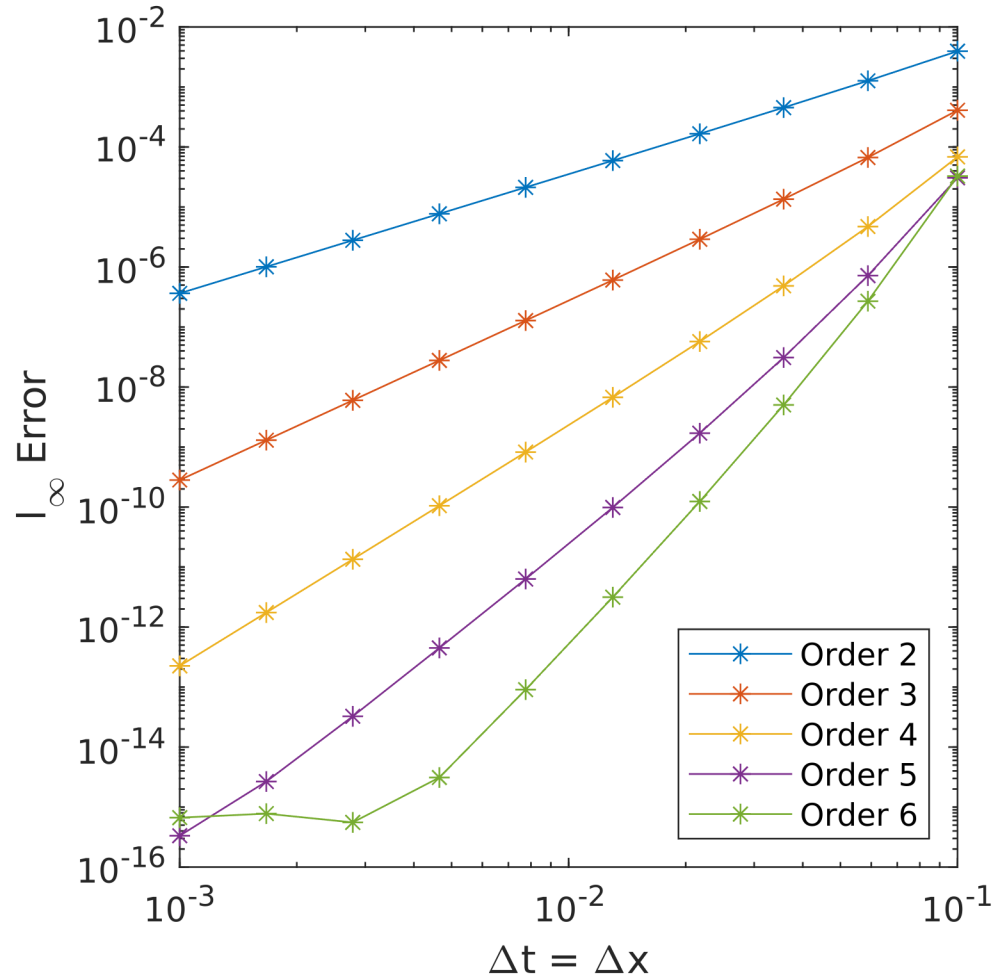
There Are Explicit Runge–Kutta Methods of Any Order Devoid of Order Reduction for Linear ODEs

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

$$\begin{aligned}\tilde{A} &= \tilde{V} \tilde{S} \tilde{V}^{-1} \\ \tilde{b}^T &= e^T \tilde{S} \tilde{V}^{-1} \\ \tilde{V} &= [e \mid \tilde{c} \mid \cdots \mid \tilde{c}^p]\end{aligned}\quad S = \begin{bmatrix} 0 & & & & & \\ 1 & 0 & & & & \\ & \frac{1}{2} & 0 & & & \\ & & \ddots & \ddots & & \\ & & & \ddots & \ddots & \\ & & & & \frac{1}{p} & 0 \end{bmatrix}$$

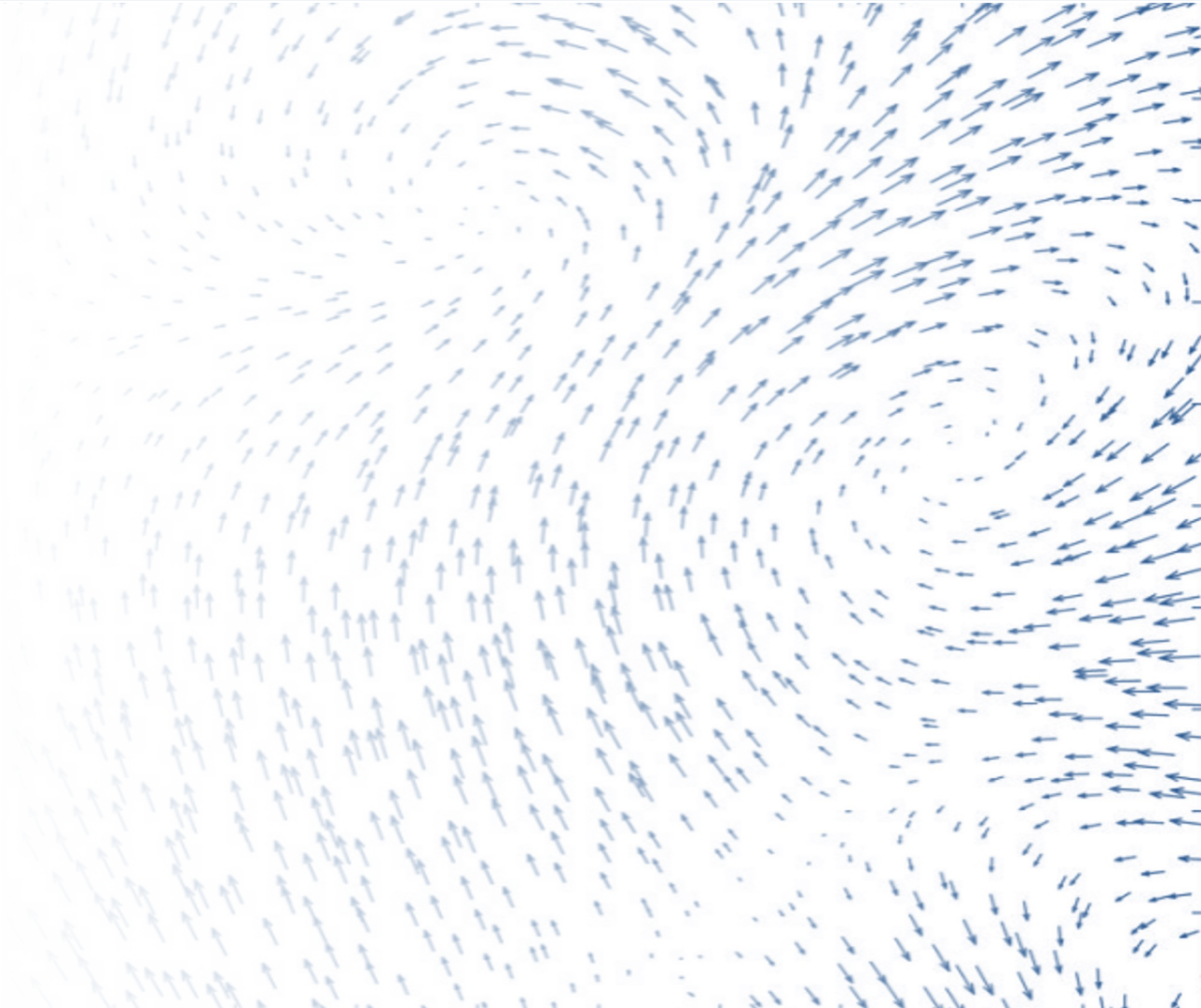
- The basic method is fully implicit, but all eigenvalues of \tilde{A} are zero
- We achieve order p and WSO p after p parallel iterations
 - The total number of stages is p^2
 - Expensive if implemented serially, but competitive if parallelism is exploited

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



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Nonlinear Problems Require Stringent Order Conditions

- Nonlinearity often worsens order reduction
- The typical remedy is high stage order

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

- 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

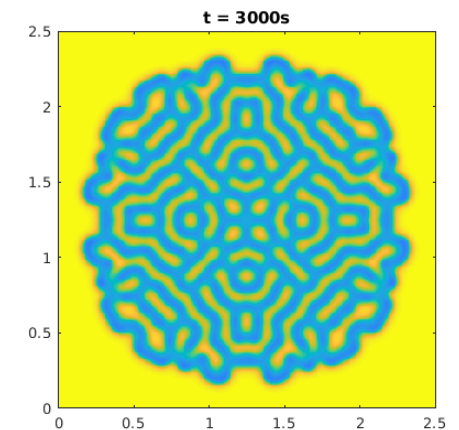
- In nonlinear problems, stiffness often arises from linear terms
- Let's consider semilinear problems

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

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

Stiff $\text{Re}\langle y, Jy \rangle \leq 0$ Nonstiff $|g(y) - g(z)| \leq L|y - z|$

- Examples include
 - Pattern-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

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

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.

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

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

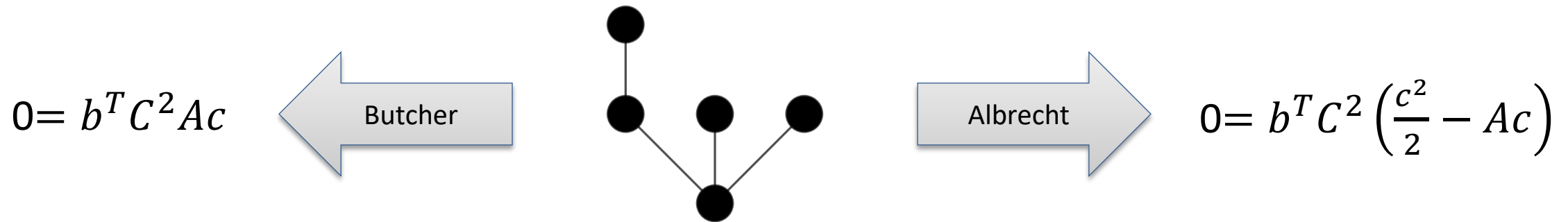
- Wanner, Gerhard, and Ernst Hairer. *Solving ordinary differential equations II*. Vol. 375. New York: Springer Berlin Heidelberg, 1996.

■ 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-series¹ are the standard tools for analyzing the local error of a Runge–Kutta scheme
- Albrecht² 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



Example Condition of Order 5

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

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

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

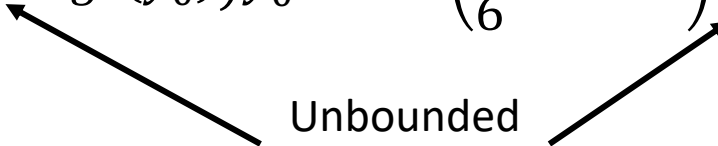
- The stiff term $Z = \Delta t J$ is confined to bounded terms
- All differential are bounded
 - $- G^{(\ell,k)}(x) = \frac{d^\ell}{dx^\ell} g^{(k)}(y(x)) \Big|_{x=x_0}$
- When $Z = 0$, we recover Albrecht's classical, nonstiff order conditions

Our Error Expansion Uses Bounded Terms II

- A classical expansion of the local truncation error looks like

$$y(x_1) - y_1 = \dots + \Delta t^2 \left(\frac{1}{2} - b^T c \right) (J + g'(y_0)) y'_0 + \Delta t^3 \left(\frac{1}{6} - b^T A c \right) (J + g'(y_0))^2 y'_0 + \dots$$

Unbounded Terms











- Our new semilinear expansion looks like

$$y(x_1) - y_1 = \dots + \Delta t^2 \left(\frac{1}{2} - b^T c + z b^T (I - zA)^{-1} \left(\frac{c^2}{2} - Ac \right) \right) y''_0 + \Delta t^3 b^T (I - zA)^{-2} \left(\frac{c^2}{2} - Ac \right) g'(y_0) y''_0 + \dots$$

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

We Found that Sharper Order Conditions Do Exist 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		$[\tau]$	$0 = \frac{1}{2} - b^T c + z_1 b^T (I - z_1 A)^{-1} \left(\frac{c^2}{2} - Ac \right)$
3a		$[\tau^2]$	$0 = \frac{1}{6} - \frac{b^T c^2}{2} + z_1 b^T (I - z_1 A)^{-1} \left(\frac{c^3}{6} - \frac{Ac^2}{2} \right)$
3b		$[[\tau]]$	$0 = b^T (I - z_1 A)^{-1} (I - z_2 A)^{-1} \left(\frac{c^2}{2} - Ac \right)$
4a		$[\tau^3]$	$0 = \frac{1}{24} - \frac{b^T c^3}{6} + z_1 b^T (I - z_1 A)^{-1} \left(\frac{c^4}{24} - \frac{Ac^3}{6} \right)$
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

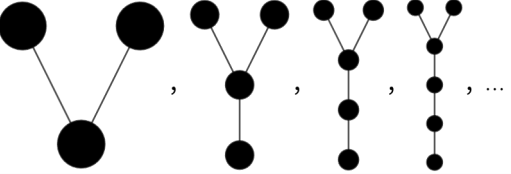
$$0 = b^T (I - z_1 A)^{-1} (I - z_2 A)^{-1} \left(\frac{c^3}{6} - \frac{Ac^2}{2} \right), \quad \forall z_1, z_2 \in \mathbb{C}^-$$



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



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

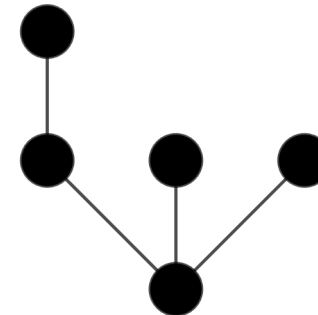
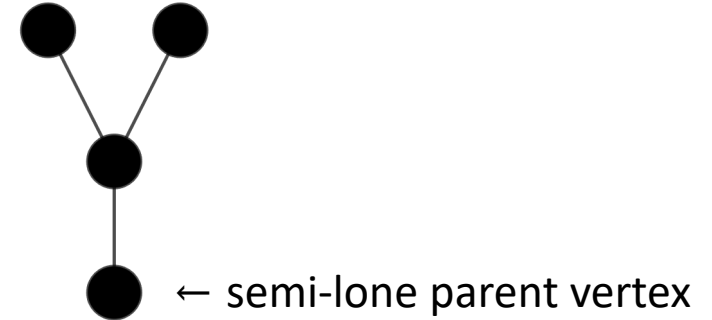
Classical Albrecht order conditions associated with $t \in$ 

We Need to Define a Special Vertex Type

Definition¹

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**.



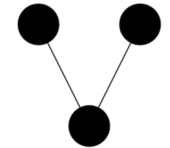
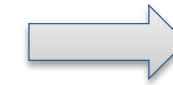
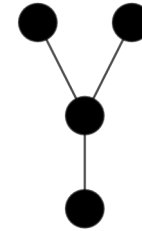
semi-lone-child-avoiding

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.



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

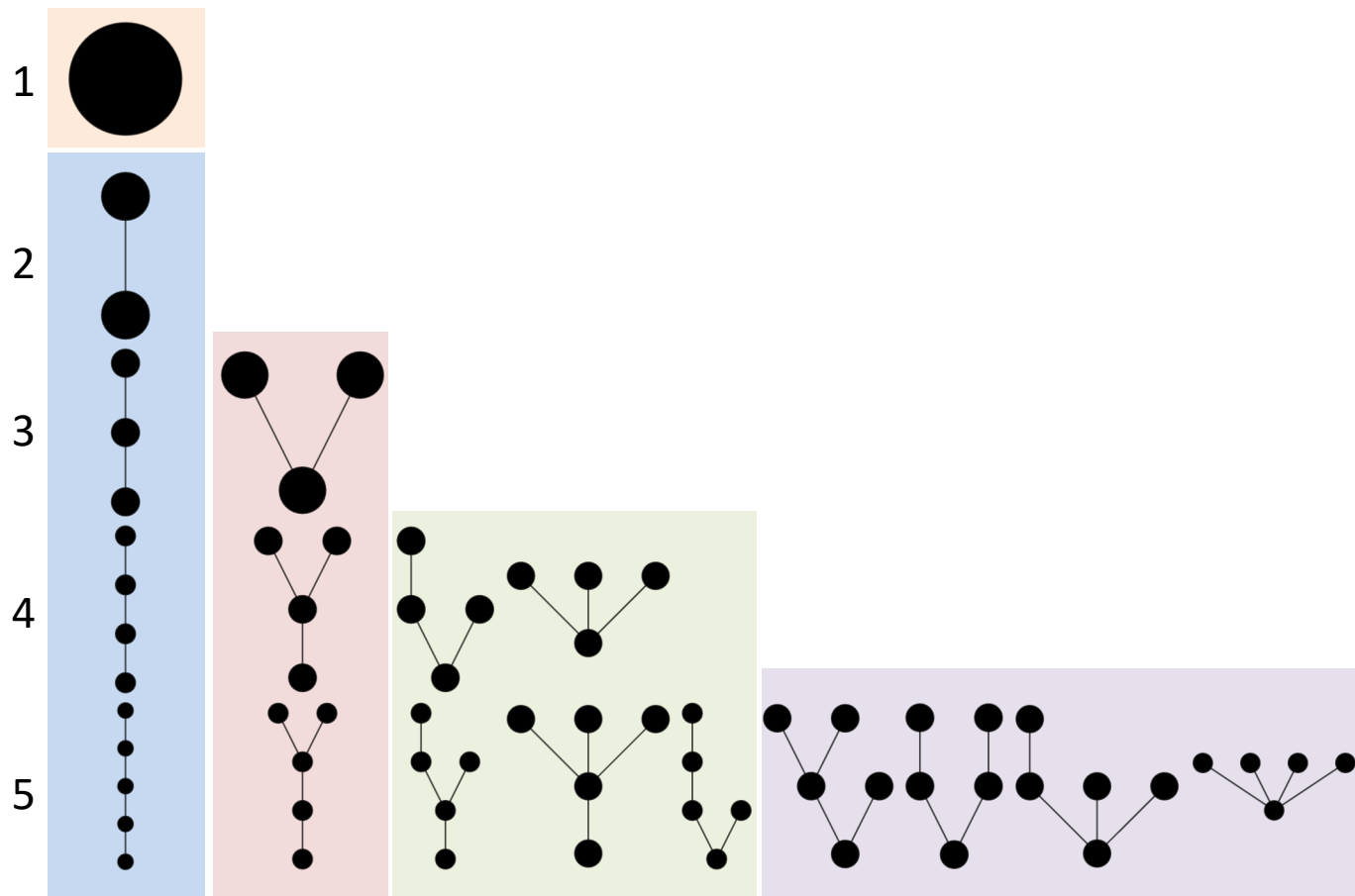
$$0 = b^T (I - z_1 A)^{-1} \left(\frac{c^3}{6} - \frac{Ac^2}{2} \right)$$

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 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 of 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

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

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

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

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

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

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

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

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

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

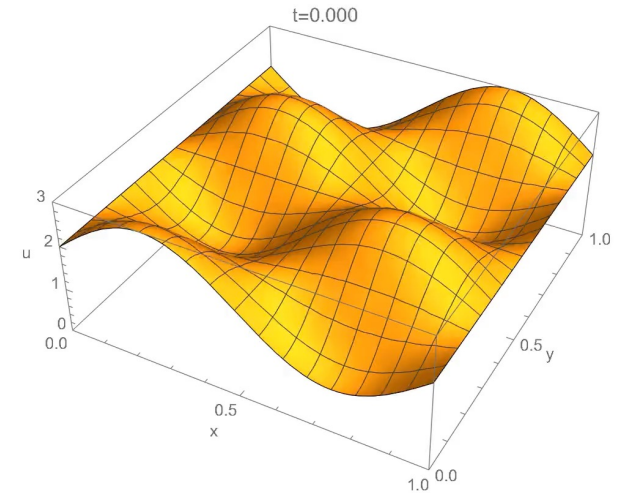
6.78237×10^{-8}	6.78237×10^{-8}	0	0	0	0	0	0
1.27118	0.635591	0.635591	0	0	0	0	0
0.340612	0.0983263	-0.0263464	0.268632	0	0	0	0
3.42294	7.64459	1.79116	-6.56175	0.548945	0	0	0
3.42294	9.09652	2.19453	-8.42176	0.181804	0.371850	0	0
4.91905	-0.771770	5.76965	-1.12350	-0.209710	0.204279	1.05010	0
1.00000	0.0988876	-0.103950	0.561554	-0.0882214	0.0859368	0.000738514	0.445054
	0.0988876	-0.103950	0.561554	-0.0882214	0.0859368	0.000738514	0.445054

Allen-Cahn is a Semilinear PDE Modeling Phase Separation

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

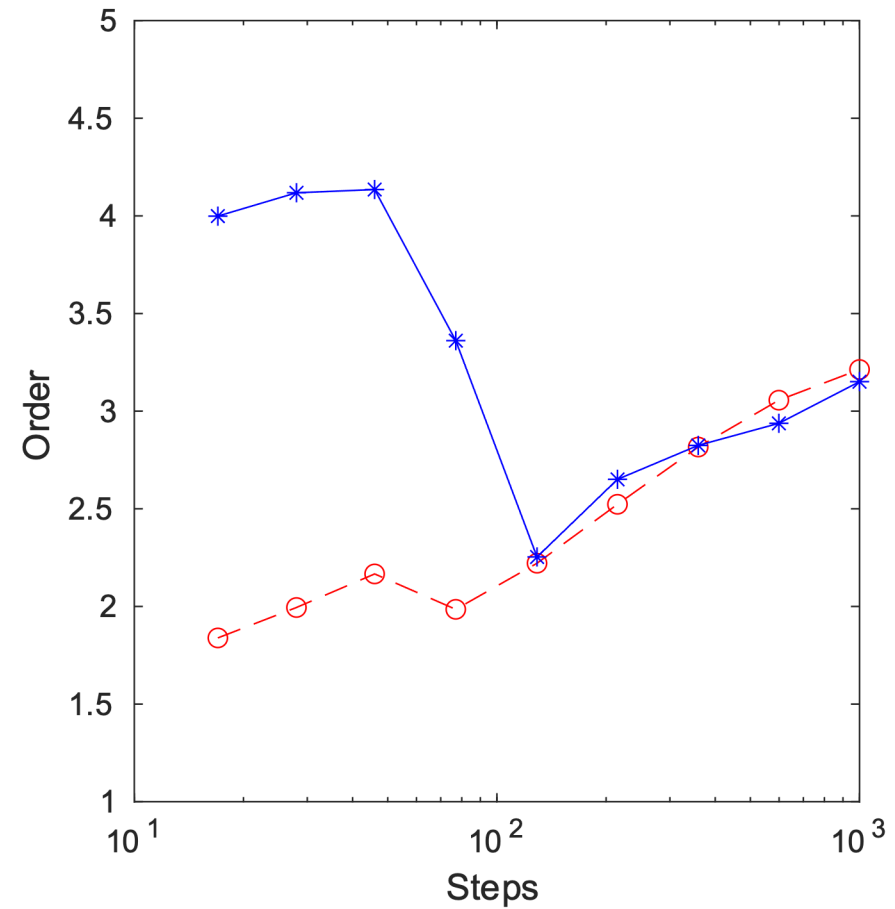
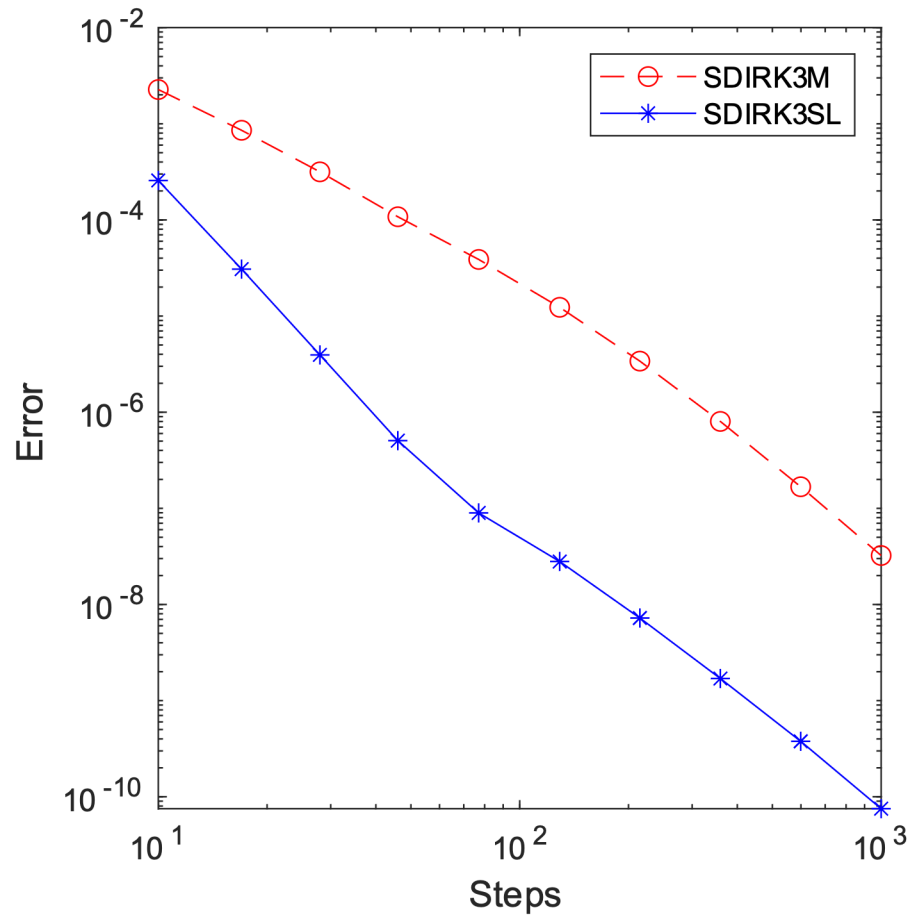
$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u + \beta(u - u^3) + s(t, x, y)$$

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

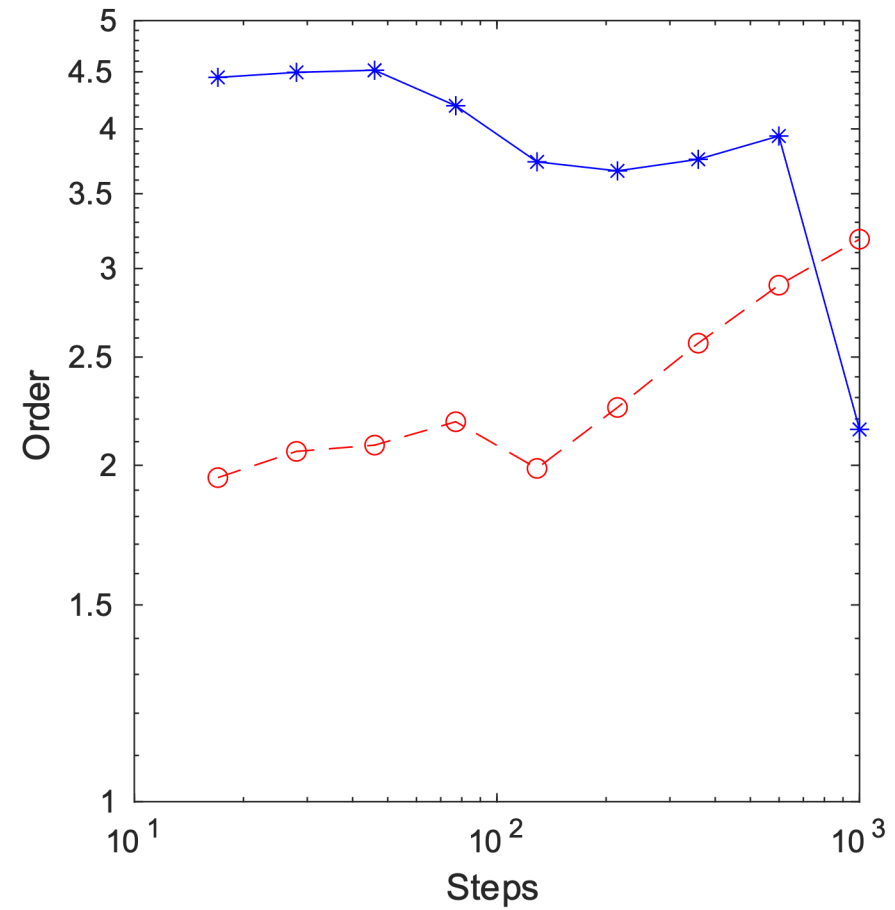
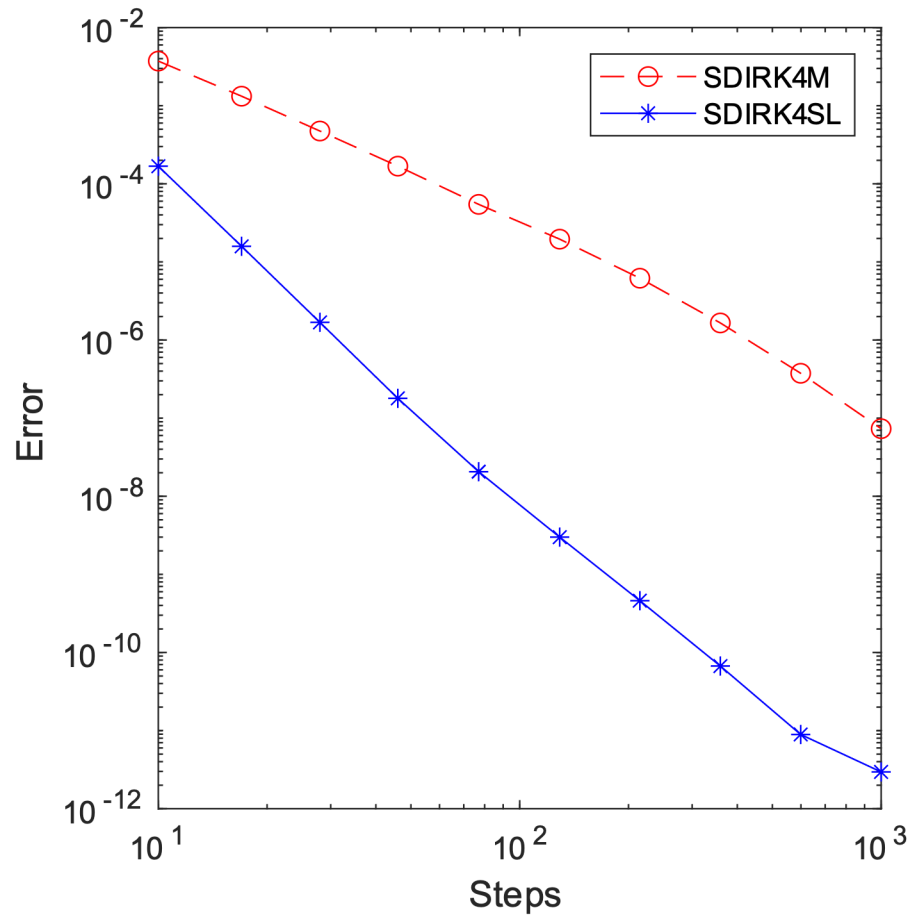


Method	Source	Stages	Classical Order	Semilinear Order
SDIRK3SL	New method from this work	6	3	3
SDIRK3M	Kennedy, Christopher A., and Mark H. Carpenter. Diagonally implicit Runge–Kutta methods for ordinary differential equations. A review. 2016.	4	3	1
DIRK4SL	New method from this work	7	4	4
SDIRK4M	Kennedy,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