Overcoming First Order

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Steven Roberts
Sidney Fernbach Postdoctoral Fellow
CASC
Center for Applied Scientific Computing

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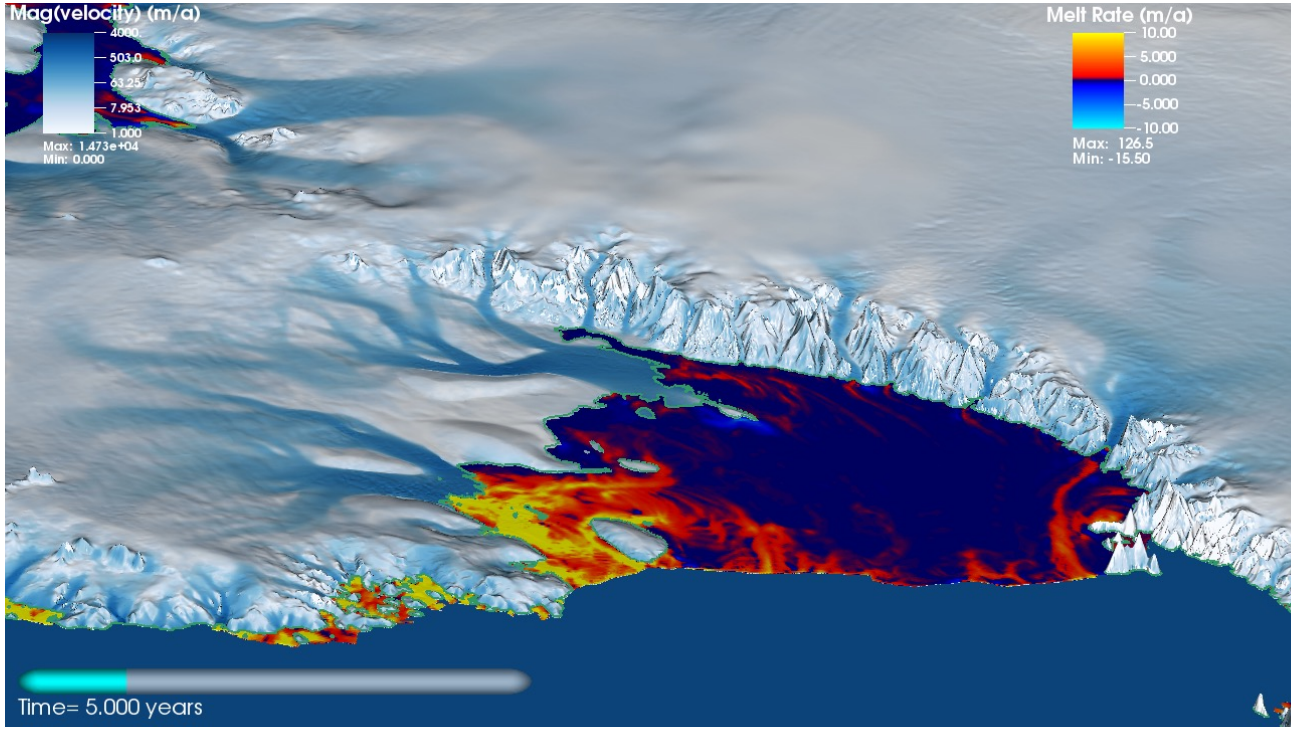
(Multi)physics Simulations Often use Low Temporal Order

- Sometimes this is fine
  - Non-smoothness
  - Low accuracy is acceptable
- Sometimes high order brings skepticism
  - Will the cost per step be too high?
  - Will the stability improve enough to offset the cost?
- Sometimes the numerical method is to blame
  - Low order splitting methods limit the overall order
  - Stiffness may cause order reduction
  - Constraints are not accurately enforced



This Talk will Focus on Runge-Kutta Methods

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

$$y' = f(y), \quad y(t_0) = y_0$$

with the numerical procedure

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

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

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

Part 1: Stiff Order Conditions and Runge-Kutta Methods for Semilinear ODEs

This work was done in collaboration with

David Shirokoff
New Jersey Institute of Technology

Abhijit Biswas
King Abdullah University of Science and Technology

David Ketcheson
King Abdullah University of Science and Technology

Benjamin Seibold
Temple University

Order Reduction Arises From Simple Problems

- Prothero and Robinson[1] proposed the simple problem

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

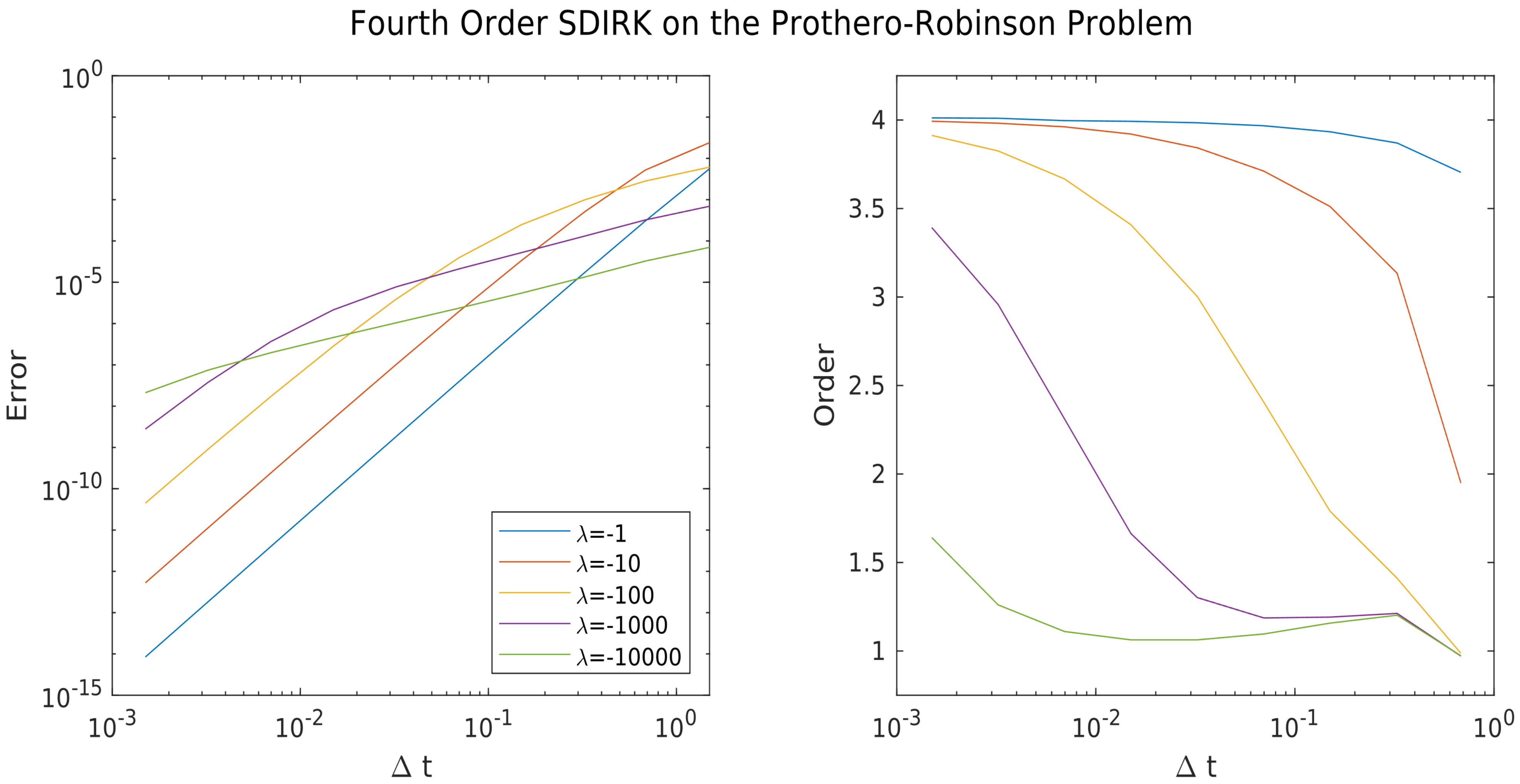
- When $|\lambda| \gg \Delta t^{-1}$, a Runge-Kutta method may converge at an order lower than the classical order.

- This phenomenon is called order reduction.

- Classical order condition theory makes unrealistic assumptions for stiff problems
  - The right-hand side has a moderate Lipschitz constant independent of Δt: $\|f(y) - f(z)\| \leq L\|y - z\|$
  - The time step is "sufficiently small"

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 Problem Reveals Order Reduction



My Problem Does Not Look Like This

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

What about PDEs?

Linear PDEs also Cause Order Reduction

- Much of the Prothero-Robinson convergence theory extends to linear PDEs

$$u_t = L(x, \partial)u + g(t)$$

- We often see fractional convergence orders depending on $L(x, \partial)$ and the norm used[1]
- Many authors have identified the additional stiff order conditions

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

- The largest q for which this holds is the *weak stage order*[2] or *pseudostage order*[3]
  - Explicit and diagonally implicit methods can have high weak stage order

1. 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.
2. Ketcheson, David I., et al. "DIRK schemes with high weak stage order." *Spectral and High Order Methods for Partial Differential Equations* (2020): 453.
3. 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.

What Happens on a Simple Advection PDE?

- Let's solve the following PDE[1] on $t, x \in [0,1]$:

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

Semidiscretize $\Rightarrow$

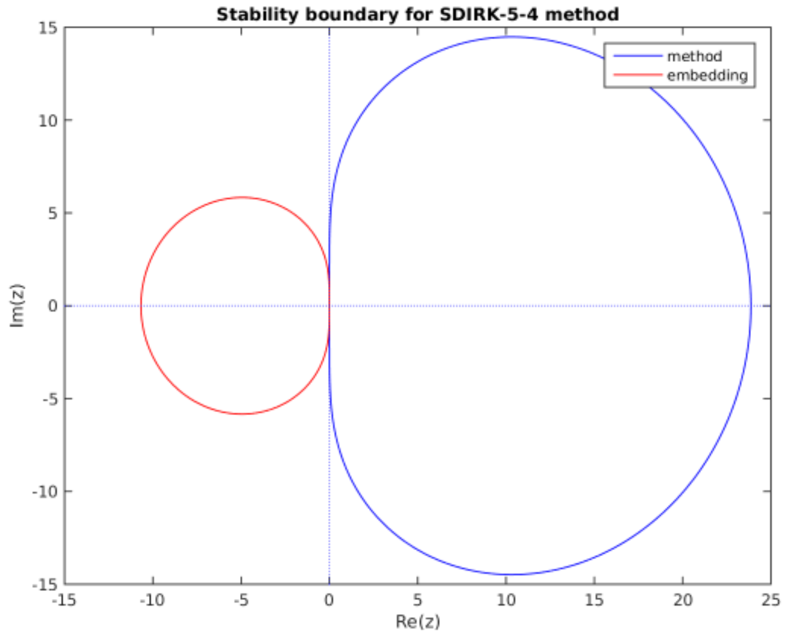
$$y' = \begin{bmatrix} -\frac{1}{\Delta x} & & & \\ \frac{1}{\Delta x} & -\frac{1}{\Delta x} & & \\ & \ddots & \ddots & \\ & & \frac{1}{\Delta x} & -\frac{1}{\Delta x} \end{bmatrix} y + \begin{bmatrix} \frac{t-x_1}{(1+t)^2} + \frac{1}{\Delta x(1+t)} \\ \frac{t-x_2}{(1+t)^2} \\ \vdots \\ \frac{t-x_N}{(1+t)^2}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

- This finite difference discretization contributes no spatial error.
- The Lipschitz constant is $L = \frac{1}{\Delta x}$, so we need $\Delta t < C\Delta x$ to be in the asymptotic regime.
  - This looks like a CFL condition even for implicit methods

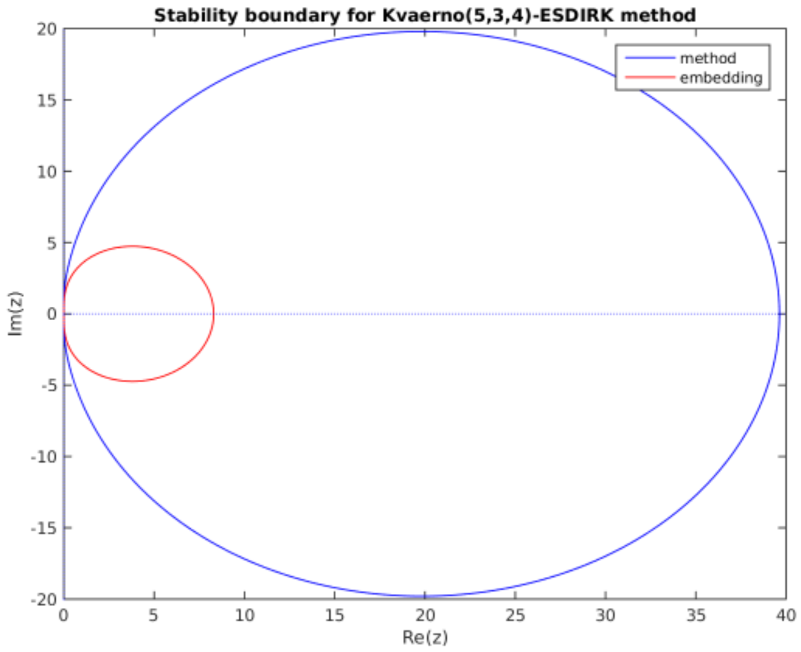
1. Sanz-Serna, Jesús María, Jan G. Verwer, and W. H. Hundsdorfer. "Convergence and order reduction of Runge-Kutta schemes applied to evolutionary problems in partial differential equations." *Numerische Mathematik* 50.4 (1986): 405-418.

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

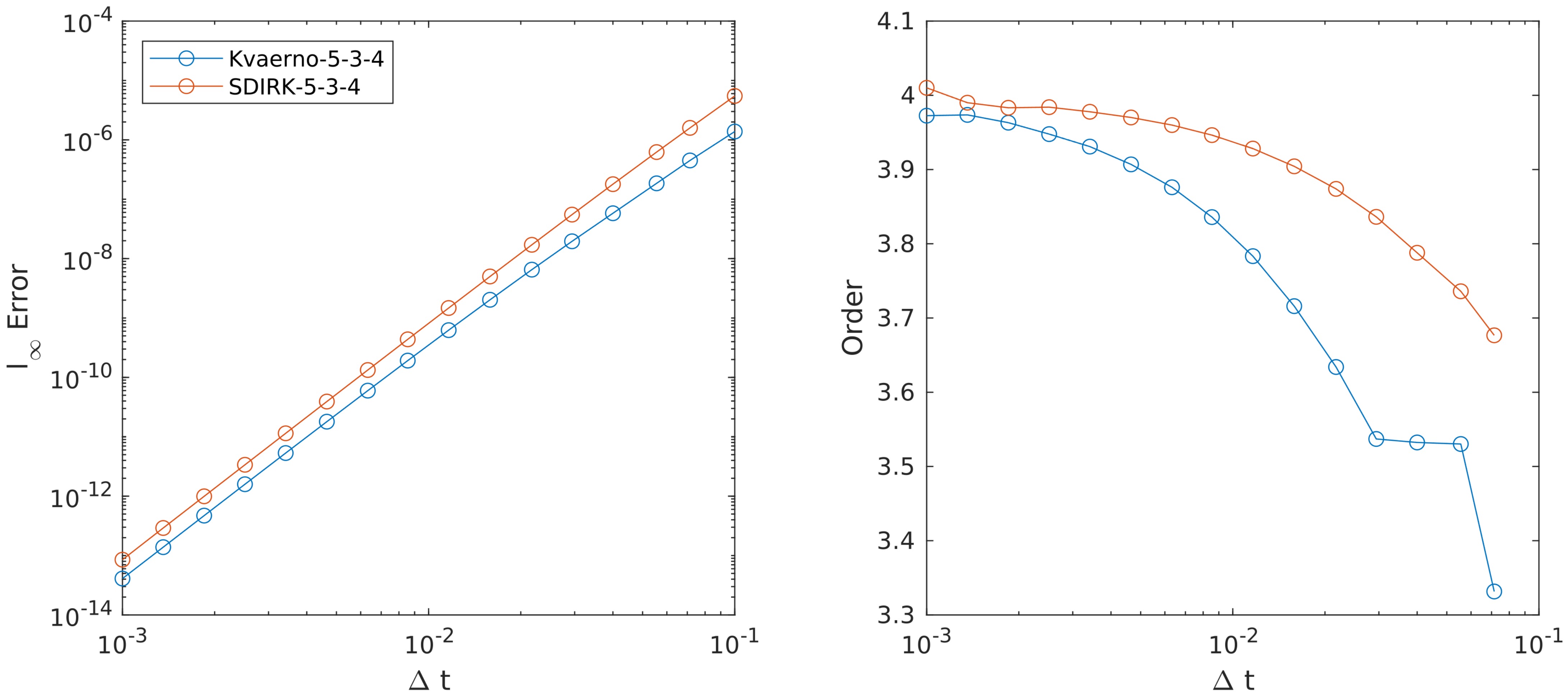
$\frac{1}{4}$	$\frac{1}{4}$	0	0	0	0
$\frac{3}{4}$	$\frac{1}{2}$	$\frac{1}{4}$	0	0	0
$\frac{11}{20}$	$\frac{17}{50}$	$-\frac{1}{25}$	$\frac{1}{4}$	0	0
$\frac{1}{2}$	$\frac{371}{1360}$	$-\frac{137}{2720}$	$\frac{15}{544}$	$\frac{1}{4}$	0
1	$\frac{25}{24}$	$-\frac{49}{48}$	$\frac{125}{16}$	$-\frac{85}{12}$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



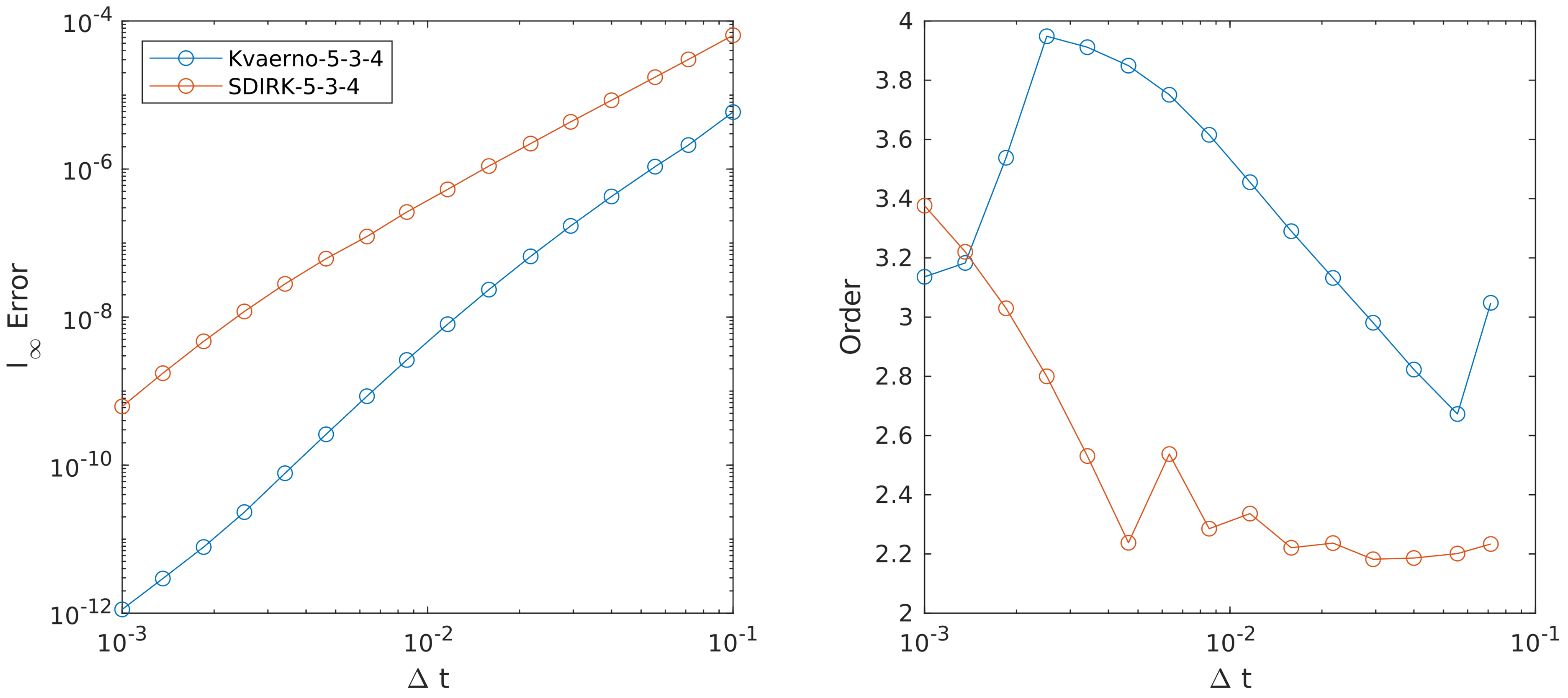
0	0	0	0	0	0
0.871733043	0.4358665215	0.4358665215	0	0	0
0.468238744853136	0.140737774731968	−0.108365551378832	0.4358665215	0	0
1	0.102399400616089	−0.376878452267324	0.838612530151233	0.4358665215	0
1	0.157024897860995	0.117330441357768	0.61667803039168	−0.326899891110444	0.4358665215
4	0.157024897860995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



We See Asymptotic Convergence on a 16 Point Grid



We See Order Reduction on a 2048 Point Grid



My Problem Does Not Look Like This

$$u_t = L(x, \partial)u + g(t)$$

What about nonlinear problems?

Nonlinear Problems Require Stringent Order Conditions

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

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

- 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

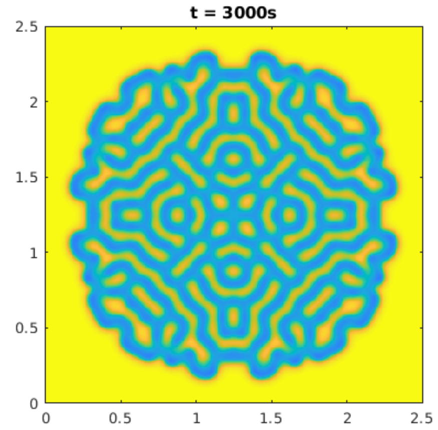
- In nonlinear problems, stiffness often arises from linear terms
- Let's consider semilinear problems

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

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



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.

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

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.

Sharper Order Conditions Do Exists for Stiff Semilinear Problems

- We propose conditions that ensure a convergence order uniformly with respect to stiffness

- Like classical order conditions, there is 1-to-1 correspondence with rooted trees

- The semilinear order conditions contain weak stage order condition
  - They coincide up to order 3

- The semilinear order conditions are sharper than stage order 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		$[[[\tau]]]$	$0 = b^T (I - z_1 A)^{-1} A (I - z_2 A)^{-1} (I - z_3 A)^{-1} \left(\frac{c^2}{2} - Ac \right.$

Our Error Expansion Uses Bounded Terms

- A classical expansion of the local truncation error looks like

$$y(t_1) - y_1 = \cdots + \Delta t^2 \left(\frac{1}{2} - b^T c\right)\left(J + g'(y_0)\right)y_0 + \Delta t^3 \left(\frac{1}{6} - b^T A c\right)\left(J + g'(y_0)\right)^2 y_0 + \cdots$$

Unbounded Terms

- Our new semilinear expansion looks like

$$y(t_1) - y_1$$
$$= \cdots + \Delta t^2 \left(\frac{1}{2} - b^T c + z b^T (I - zA)^{-1} \left(\frac{c^2}{2} - Ac\right)\right) y''(t_0) + \Delta t^3 b^T (I - zA)^{-2} \left(\frac{c^2}{2} - Ac\right) g'(y_0) y''(t_0)$$
$$+ \cdots$$

Bounded Terms

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

Our Semilinear Analysis Extends a Lesser-Known Classical Analysis

- Butcher trees and B-series are the typical tools for analyzing the local error of a Runge-Kutta scheme

- Albrecht[1] proposed alternative order conditions that do not (necessarily) use trees
  - Order 4 conditions, for example:
    - $0 = \frac{1}{24} - \frac{b^T c^3}{6}$
    - $0 = b^T C \left(\frac{c^2}{2} - Ac\right)$
    - $0 = b^T \left(\frac{c^3}{6} - \frac{Ac^2}{2}\right)$
    - $0 = b^T A \left(\frac{c^2}{2} - Ac\right)$

$$0 = \frac{1}{24} - \frac{b^T c^3}{6} + z_1 b^T (I - z_1 A)^{-1} \left(\frac{c^4}{24} - \frac{Ac^3}{6}\right)$$

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

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

$$0 = b^T (I - z_1 A)^{-1} A (I - z_2 A)^{-1} (I - z_3 A)^{-1} \left(\frac{c^2}{2} - Ac\right)$$

- We closely follow Albrecht's derivation, but the stiff, linear term introduces extra factors of $(I - hA \otimes J)^{-1}$.

1. Albrecht, Peter. "The Runge–Kutta theory in a nutshell." *SIAM Journal on Numerical Analysis* 33.5 (1996): 1712-1735.

Practical Methods with Semilinear Order 3 Exist

- Desired properties
  - Order 3
  - Singly diagonally implicit
  - L-stable

- Typically, this requires at least 3 stages

- With order 3 semilinear conditions, this requires at least 5 stages

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

Higher Order Methods are Challenging to Derive

- The first nonlinear order condition appears at order 4

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

Neumann Expansion →

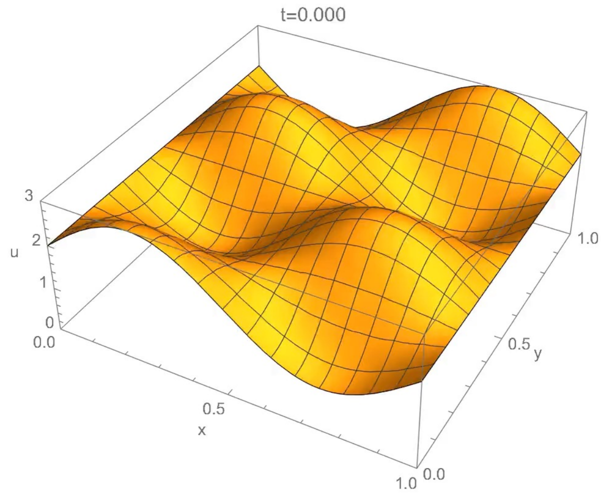
$$0 = b^T A^i C A^j \left(\frac{c^2}{2} - Ac \right), \quad i, j = 0, \dots, s - 1$$

- The number or order conditions increases with the order and the number of stages
- Explicit methods of semilinear order 4 exist
- Singly diagonally implicit method of classical order 4 and semilinear order 3 exist
  - This suffices for a global order of 4
  - Methods with semilinear order 4 almost certainly exist

Allen-Cahn is a Semilinear PDE Modeling Phase Separation

- We consider a 2D Allen-Cahn reaction-diffusion PDE

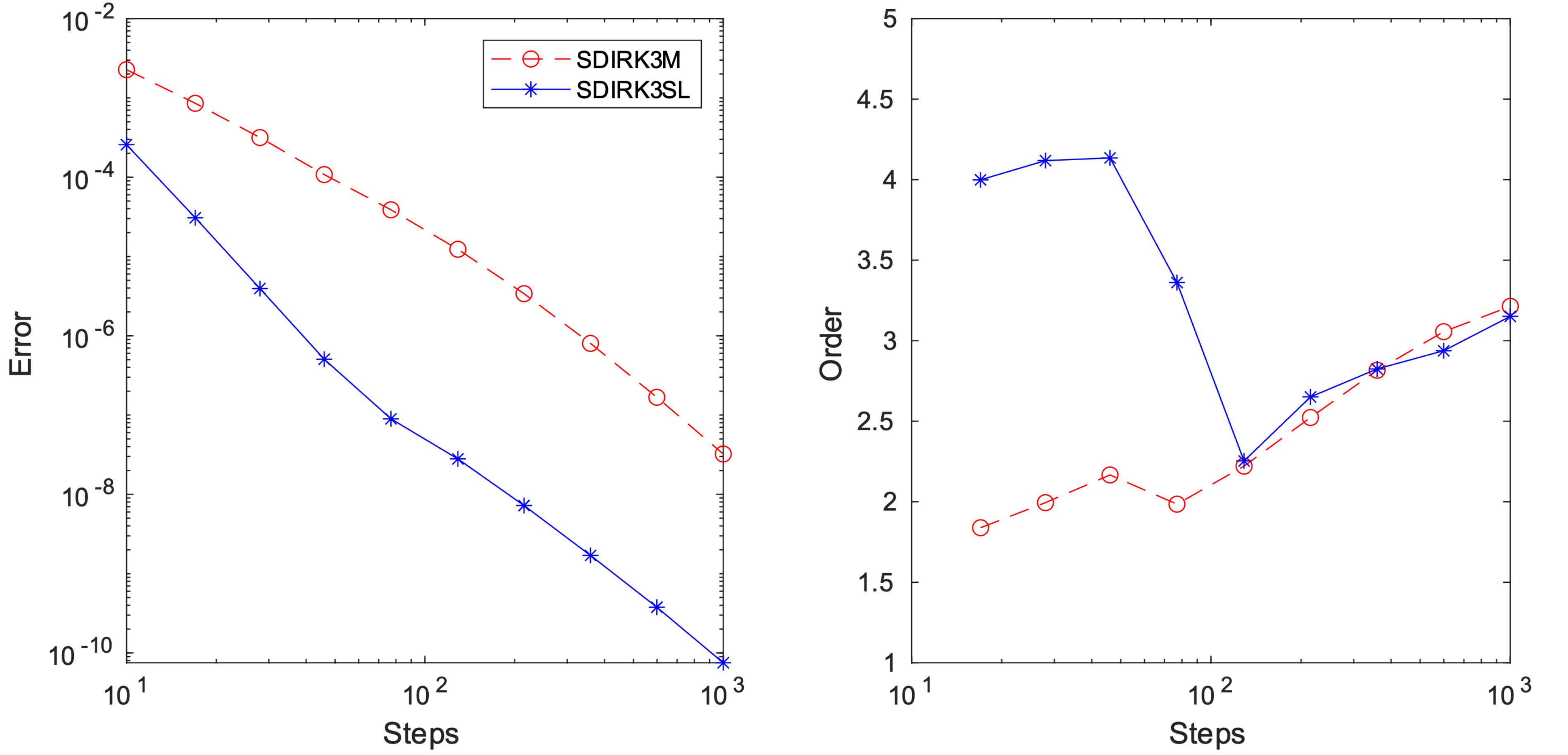
$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u + \beta(u - u^3) + s(t, x, y)$$



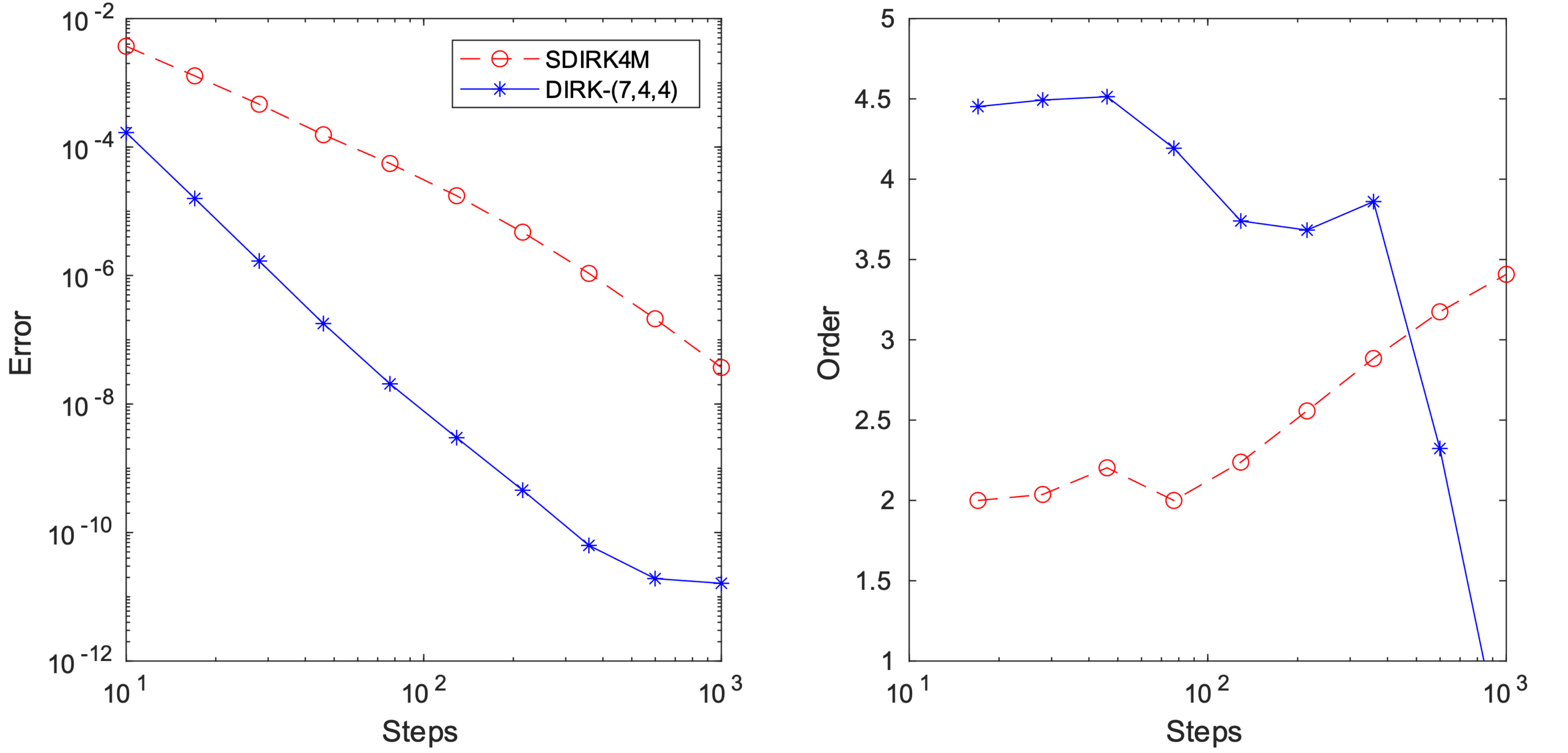
- We test methods of order 3 and 4 to validate the semilinear order conditions

Method	Source	Stages	Classical Order	Semilinear Order
SDIRK3SL	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
DIRK-(7,4,4)	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.	7	4	3
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 Avoid Order Reduction



The Existing DIRK-(7,4,4) Method Avoids Order Reduction



Conclusions

- Classical order conditions rely on assumptions that fail to hold for stiff problems
- The consequence is a reduction in order and accuracy for many integrators
- High stage order is not necessary to avoid order reduction on stiff, semilinear ODEs
- Weak stage order conditions for stiff, linear problems suffice up to order 4
- Order reduction and techniques to eliminate it are not limited to implicit Runge-Kutta methods
  - Implicit-explicit
  - Multirate
  - Explicit methods

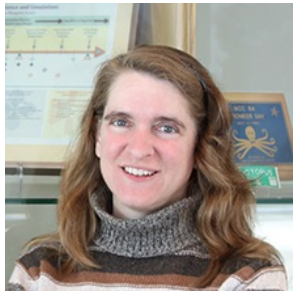
Part 2: Time-Stepping for the BISICLES Ice Sheet Model

This work was done in collaboration with

Daniel Martin
Lawrence Berkeley National Laboratory

David Gardner
Lawrence Livermore National Laboratory

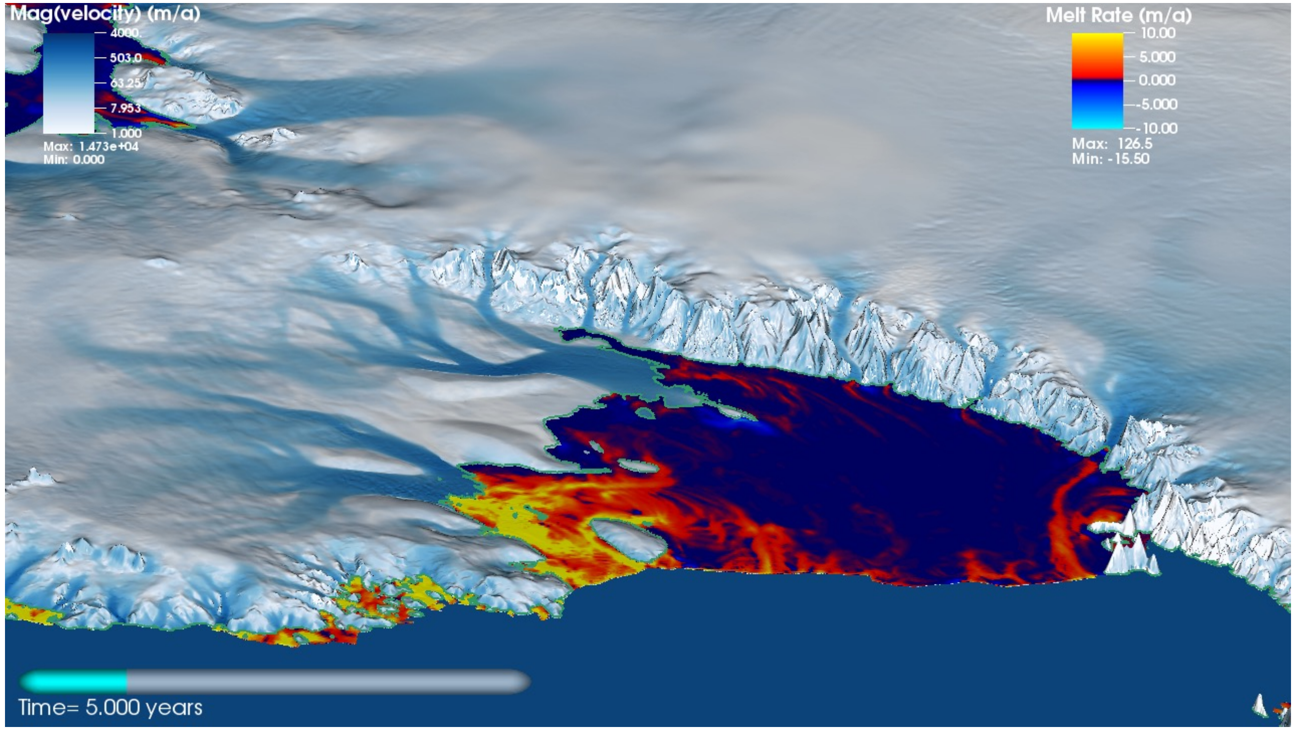
Hans Johansen
Lawrence Berkeley National Laboratory



Carol Woodward
Lawrence Livermore National Laboratory

BISICLES Models Ice Sheet Dynamics

- Accurate modeling of ice-sheets is critical to understanding and predicting
  - Future see level rise
  - Potential regional collapses in the West Antarctic ice sheet
- BISICLES is a simulation tool developed at LBNL, LANL, and the University of Bristol[1]
- Long-term time evolution of these models requires accurate, conservative, and stable numerical methods



1. Cornford, Stephen L., et al. "Adaptive mesh, finite volume modeling of marine ice sheets." *JCP* 232.1 (2013): 529-549.

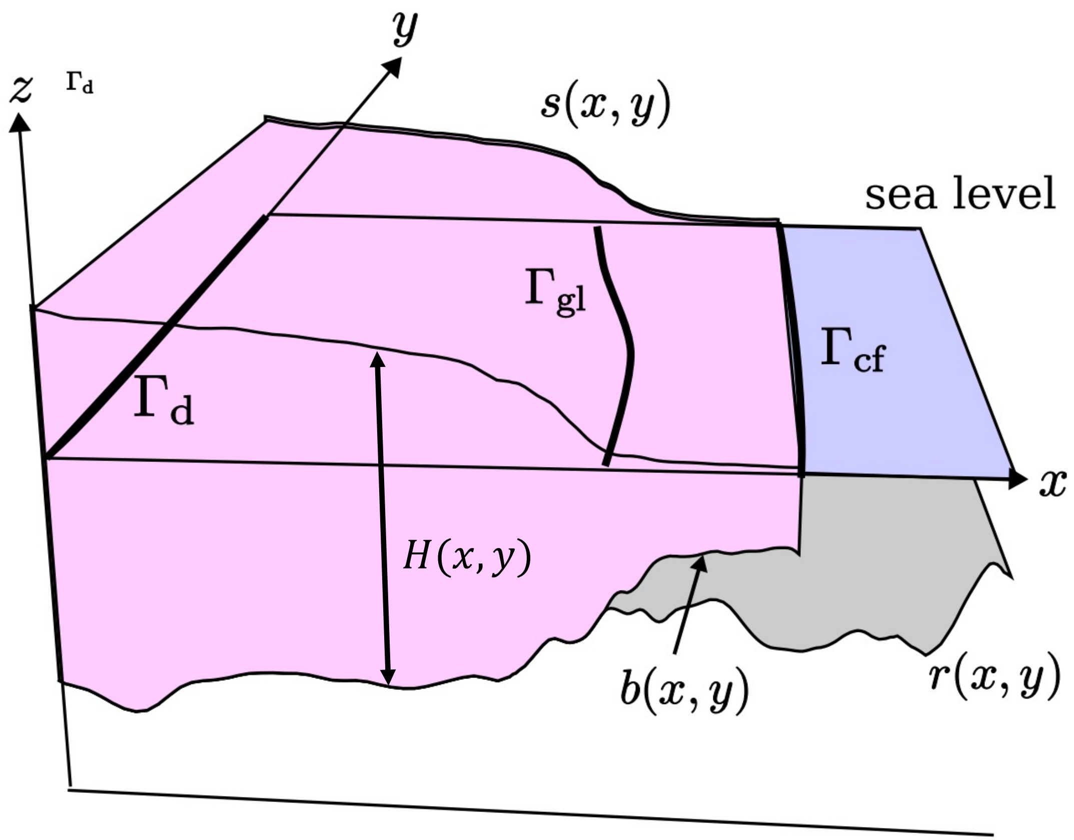
The Ice Model Combines Hyperbolic and Elliptic Partial Differential Equations

- In the simplest case, the two primary variables are
  - Ice thickness $H(t,x,y)$
  - Ice velocity $v(t,x,y)$
- An asymptotically-derived approximation to Stokes Flow is used[1]

$$\frac{\partial H}{\partial t} = \frac{\partial}{\partial x}(v_x H) + \frac{\partial}{\partial y}(v_y H)$$

$$\beta^2 v - \nabla \cdot (H\mu(v)\,\nabla v) = -\rho_i g H\,\nabla \cdot s$$

- The Chombo library is used for the spatial discretization with adaptive mesh refinement (AMR)
  - Second order finite volume method



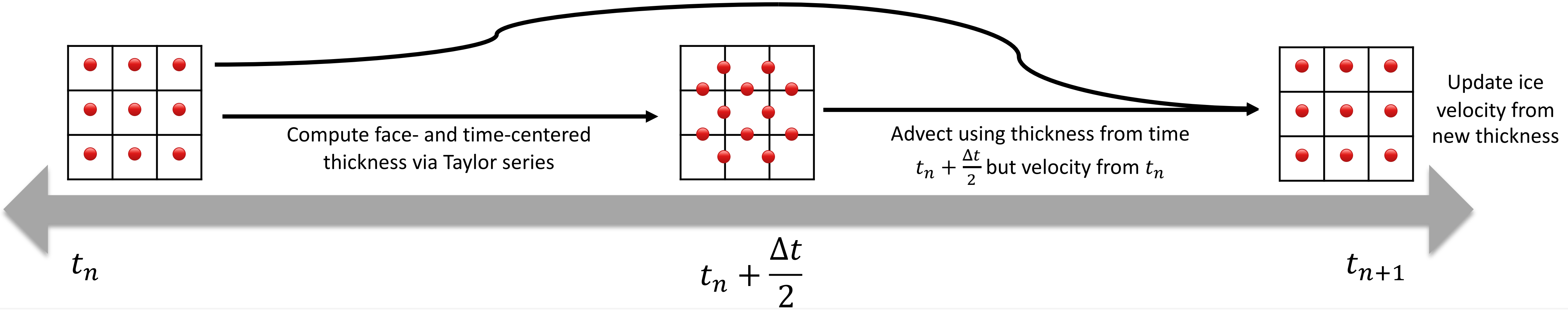
From Cornford, Stephen L., et al. "Adaptive mesh, finite volume modeling of marine ice sheets." *JCP* 232.1 (2013): 529-549.

1. Schoof, Christian, and Richard CA Hindmarsh. "Thin-film flows with wall slip: an asymptotic analysis of higher order glacier flow models." *QJMAM* 63.1 (2010): 73-114.

BISICLES was Limited by the Time Discretization

- BISICLES uses an unsplit Godunov piecewise parabolic method
  - First order accurate in time
  - Explicit
  - Not method of lines
  - Limited maximum stable time step
  - No error estimation
  - Time step chosen by CFL condition

- Project Goals
  - Introduce high order time-stepping methods for improved accuracy and stability
  - Introduce adaptive methods
  - Determine which class of integrators is best-suited to the problem



We can Solve an Ordinary or Differential-Algebraic Equation

- The time evolution problem is an index-1 differential-algebraic equation (DAE)

$$\frac{dH}{dt} = f(H, v)$$
$$0 = g(H, v)$$

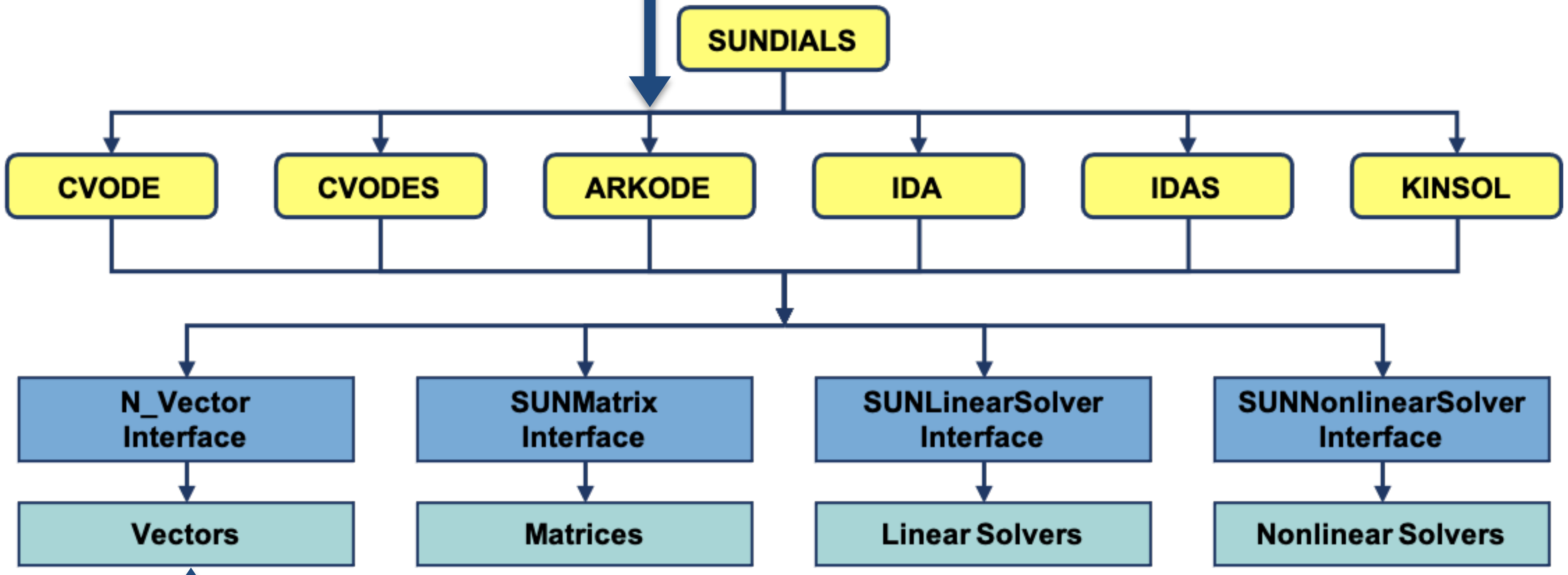
- Over 90% of the runtime is spent solving the nonlinear system $0 = g(H, v)$!
- Or we can view this as an ordinary differential equation (ODE) where $v = \mathcal{G}(H)$ is a derived quantity computed via a nonlinear solve. This is the "state space form"

$$\frac{dH}{dt} = f\big(H, \mathcal{G}(H)\big)$$

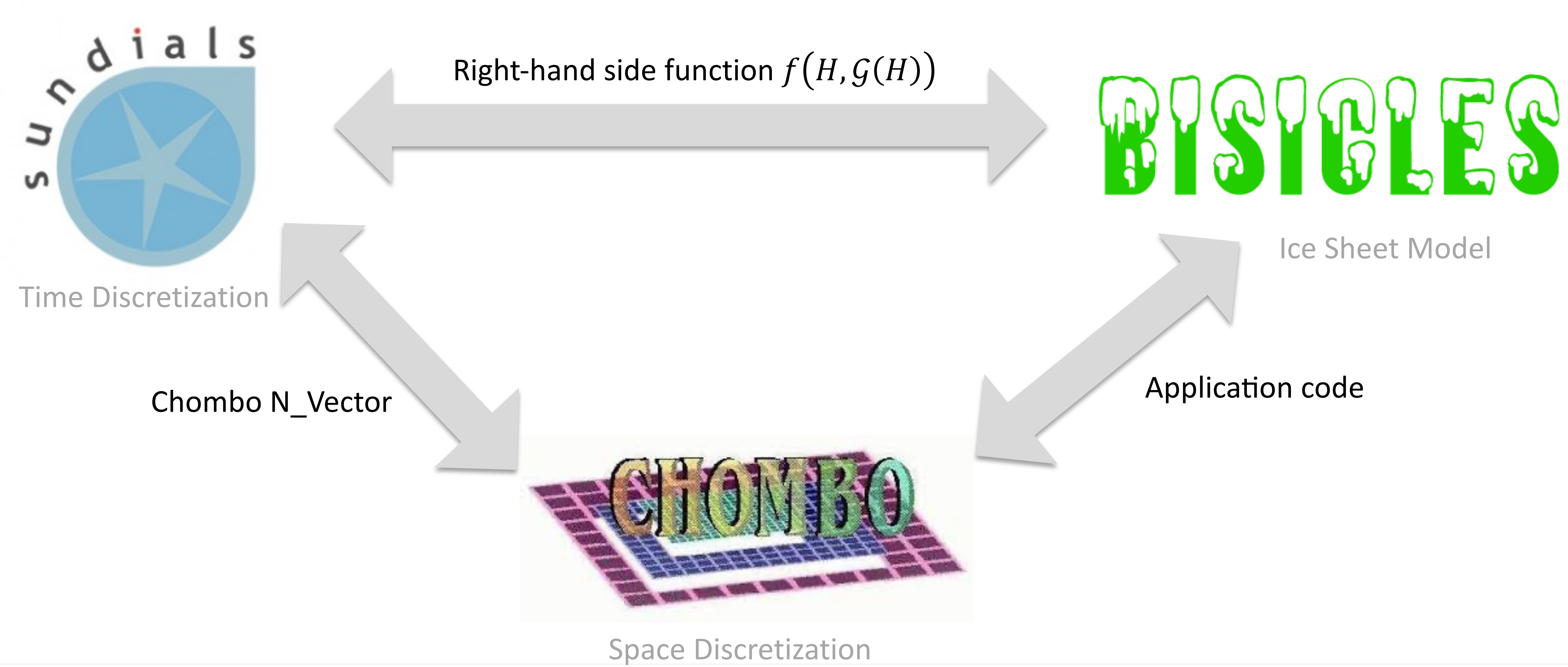
SUNDIALS Provides Efficient ODE, DAE, and Nonlinear Solvers

- ARKODE provides (additive) Runge-Kutta methods
- Adaptive or fixed step size
- We use explicit Runge-Kutta methods to solve the state space form $\frac{dH}{dt} = f\big(H, \mathcal{G}(H)\big)$

- N_Vectors decouple integrators from application data structures
- Includes norms, dot product, axpy, and other generic operations
- **We developed a Chombo N_Vector to operate on AMR grids**



Our New Chombo N_Vector Enables Package Interoperability



Second Order is Feasible at the Cost of Order One

$$\frac{dH}{dt} = f(H, v)$$
$$0 = g(H, v)$$

- BISICLES' first order integrator does **1** expensive algebraic solve for ice velocity each time step
- A second order, explicit Runge-Kutta applied to the state space form requires at least **2** algebraic solves per time step
- We proposed to use a second order "half-explicit Heun's method" with **1** algebraic solve per step

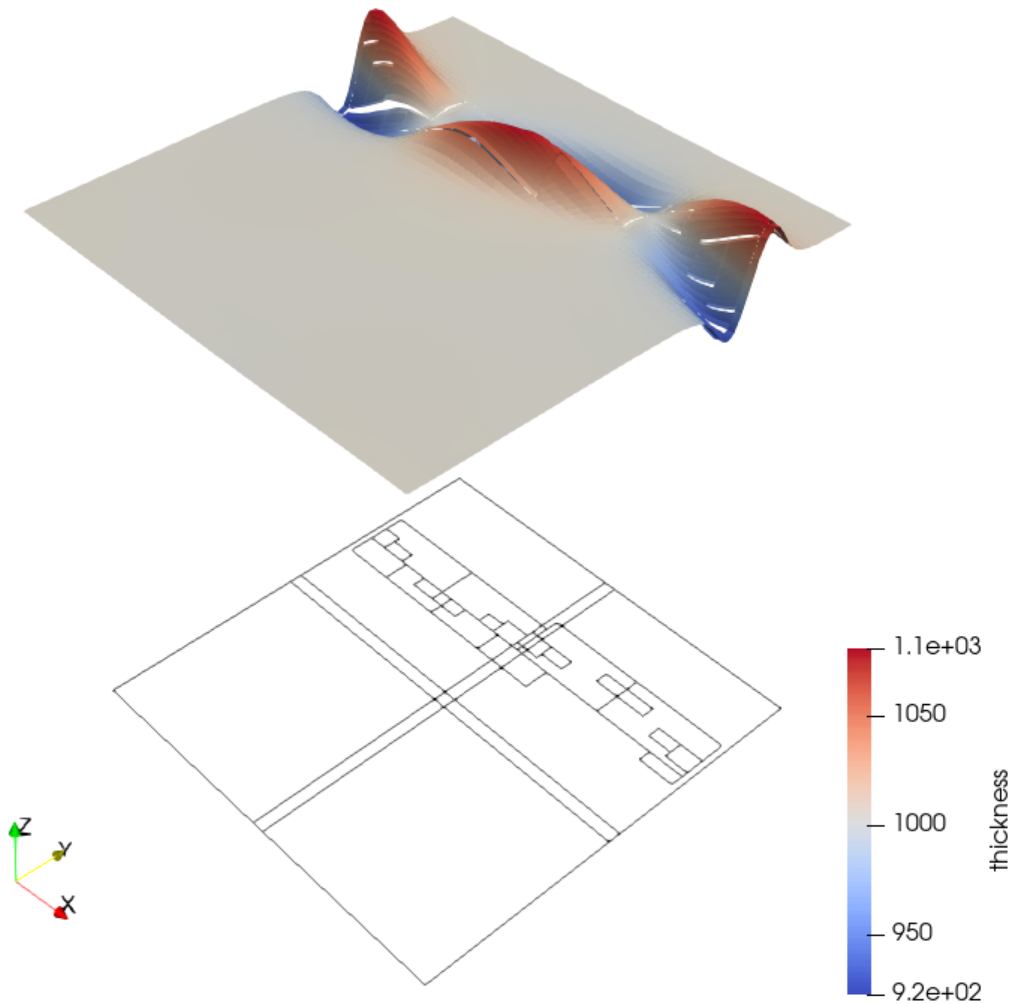
$$\begin{aligned} K_1 &= f(H_n, v_n) \\ K_2 &= f(H_n + \Delta t\, K_1, v_{n+1}) \\ 0 &= g(H_n + \Delta t\, K_1, v_{n+1}) \\ H_{n+1} &= H_n + \frac{\Delta t}{2}(K_1 + K_2) \end{aligned}$$

$$\begin{array}{cc|c} 0 & 0 & 0 \\ 1 & 0 & 1 \\ \hline 1 & 0 & 1 \\ \hline \frac{1}{2} & \frac{1}{2} & 1 \end{array}$$

- It is not a traditional Runge-Kutta method but a generalized additive Runge-Kutta.

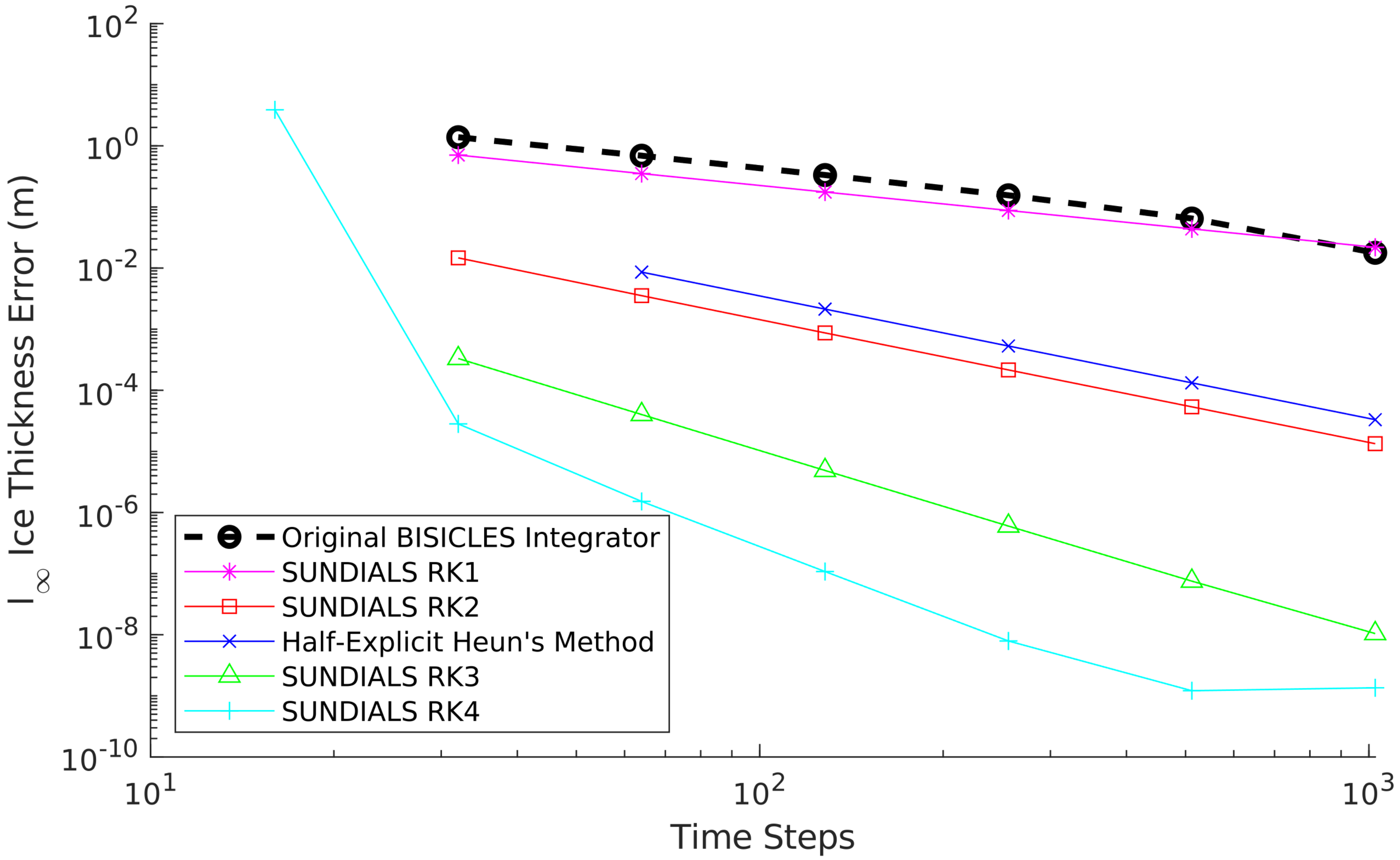
Twisty Steam is a Benchmark Test Problem

- Ice streams are fast-flowing regions within a sheet
- Ice streams account for about 90% of ice mass lost from the Antarctic ice sheet[1]
- We compare the temporal accuracy of
  - The original unsplit Godunov piecewise parabolic method in BISICLES
  - Explicit Runge-Kutta methods from ARKODE of order 1-4
  - The half-explicit Heun's method from the previous slide

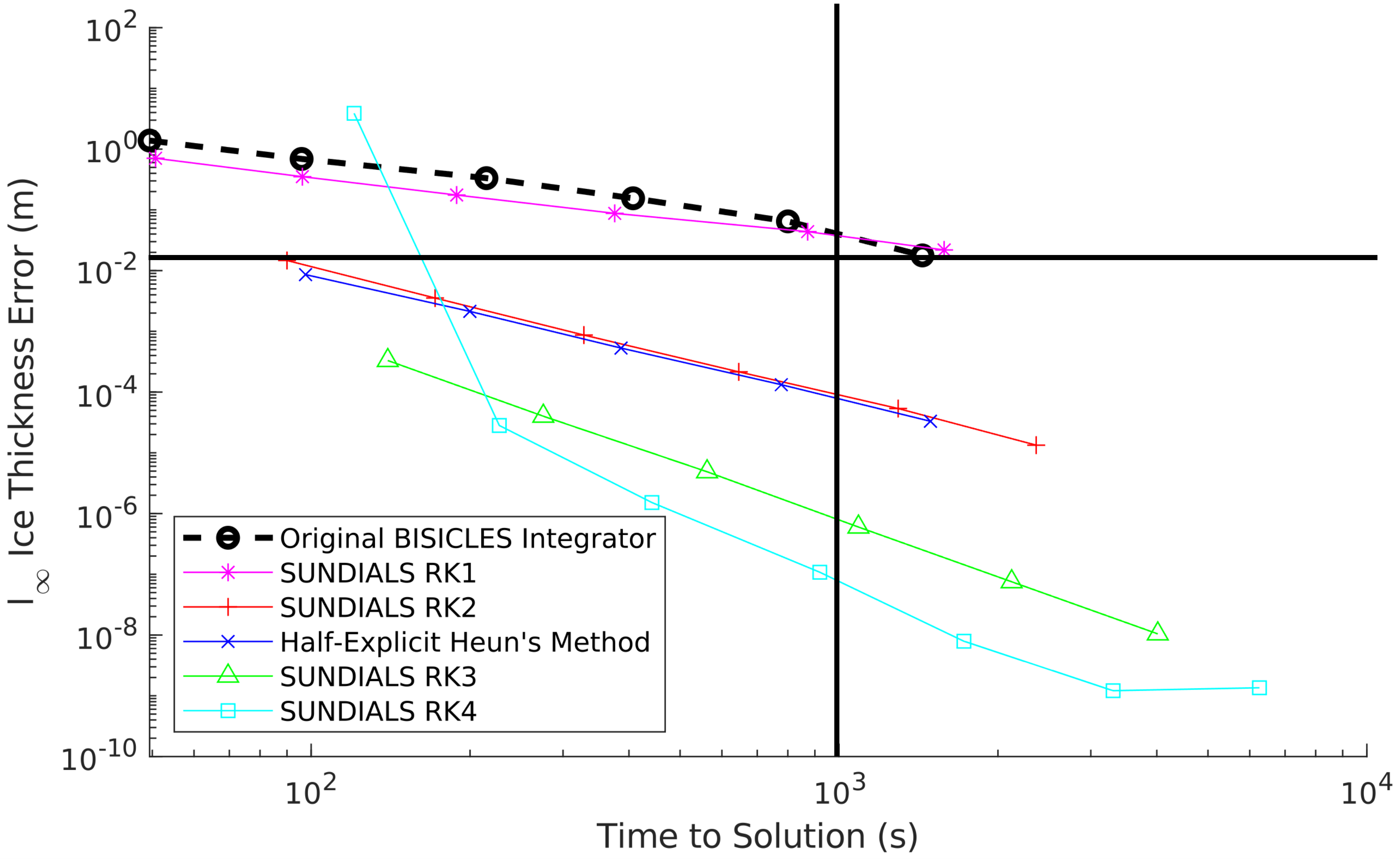


1. https://www.antarcticglaciers.org/glacier-processes/glacier-types/ice-streams/

The Integrators Converge



The New Integrators Are Significantly More Efficient



BISICLES is Often Stability-Limited

$$\frac{\partial H}{\partial t} = \frac{\partial}{\partial x}(v_x H) + \frac{\partial}{\partial y}(v_y H)$$
$$\beta^2 v - \nabla \cdot (H\mu(v)\,\nabla v) = -\rho_i g H\,\nabla \cdot s$$

- Despite the hyperbolic PDE for ice thickness, the problem is sometimes diffusive
- Spatial error often dominates temporal error, even when using the native, first order method
- In this regime, we achieve the best efficiency by taking Δt near the CFL limit
- The following metric is key

$$\frac{\text{max stable } \Delta t}{\text{cost per step}}$$

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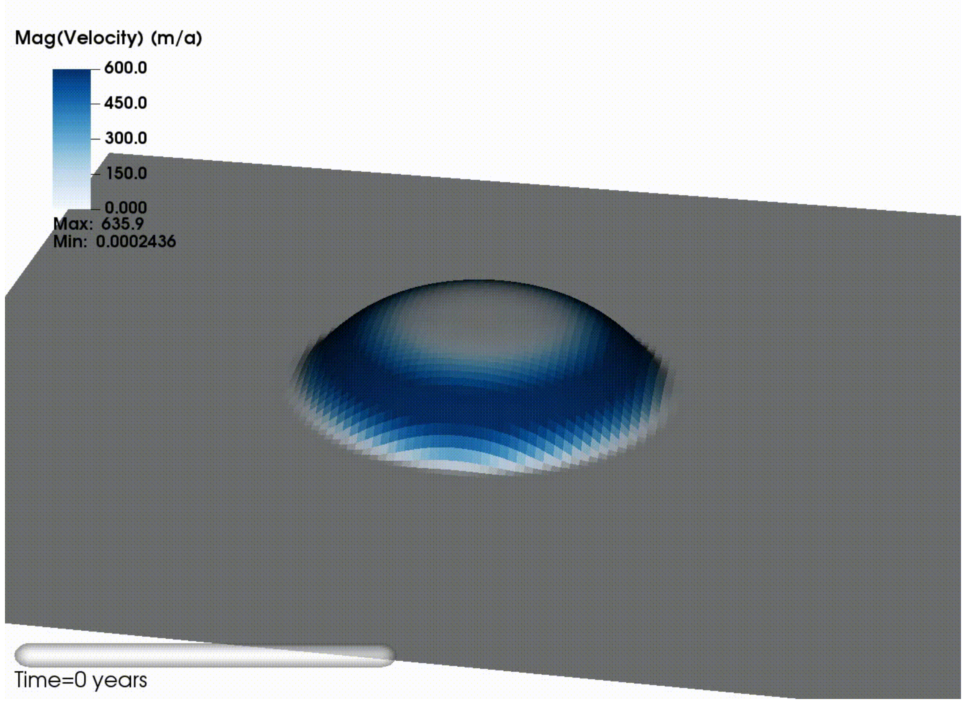
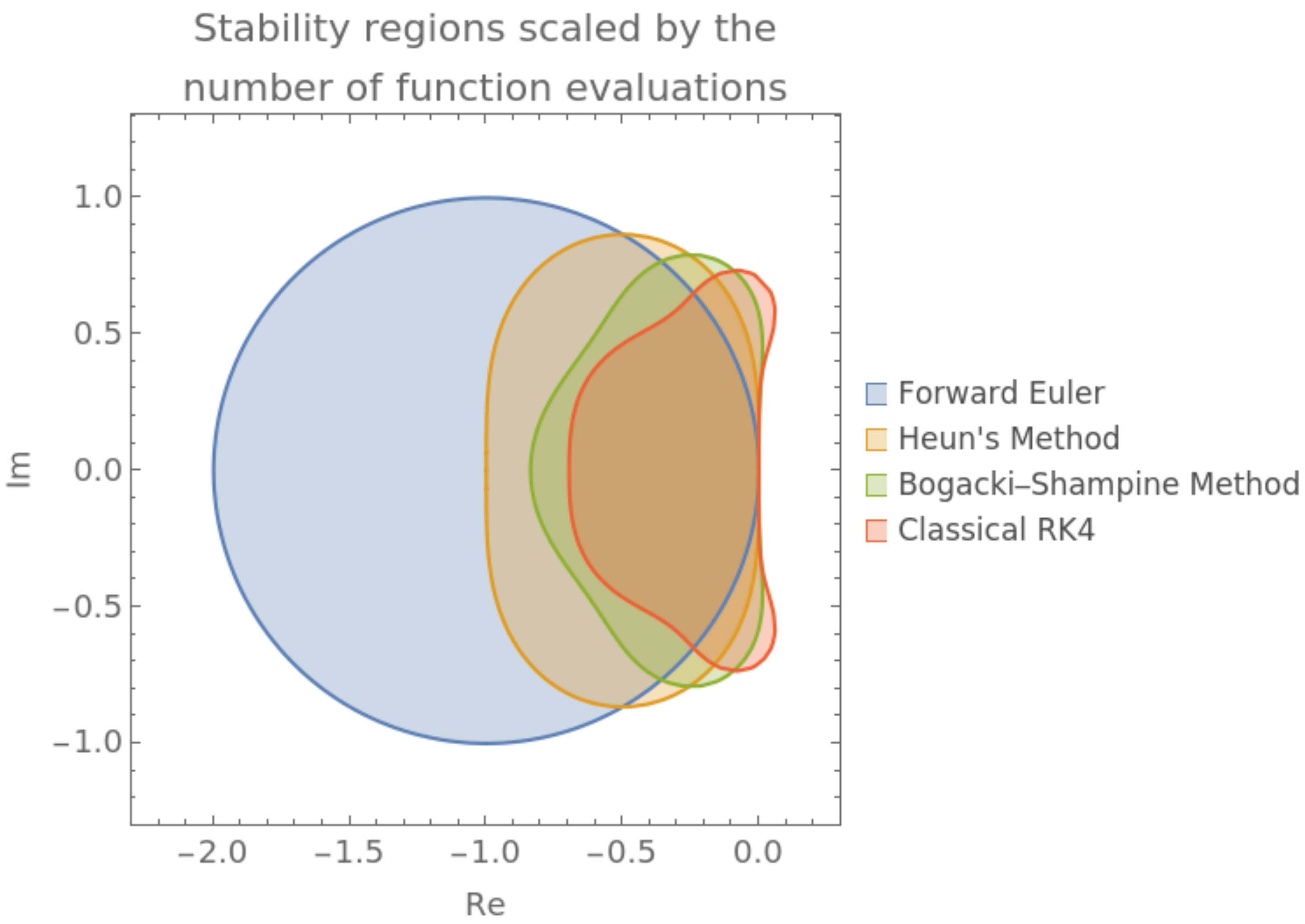


High Order is Not Always Advantageous for Linear Stability



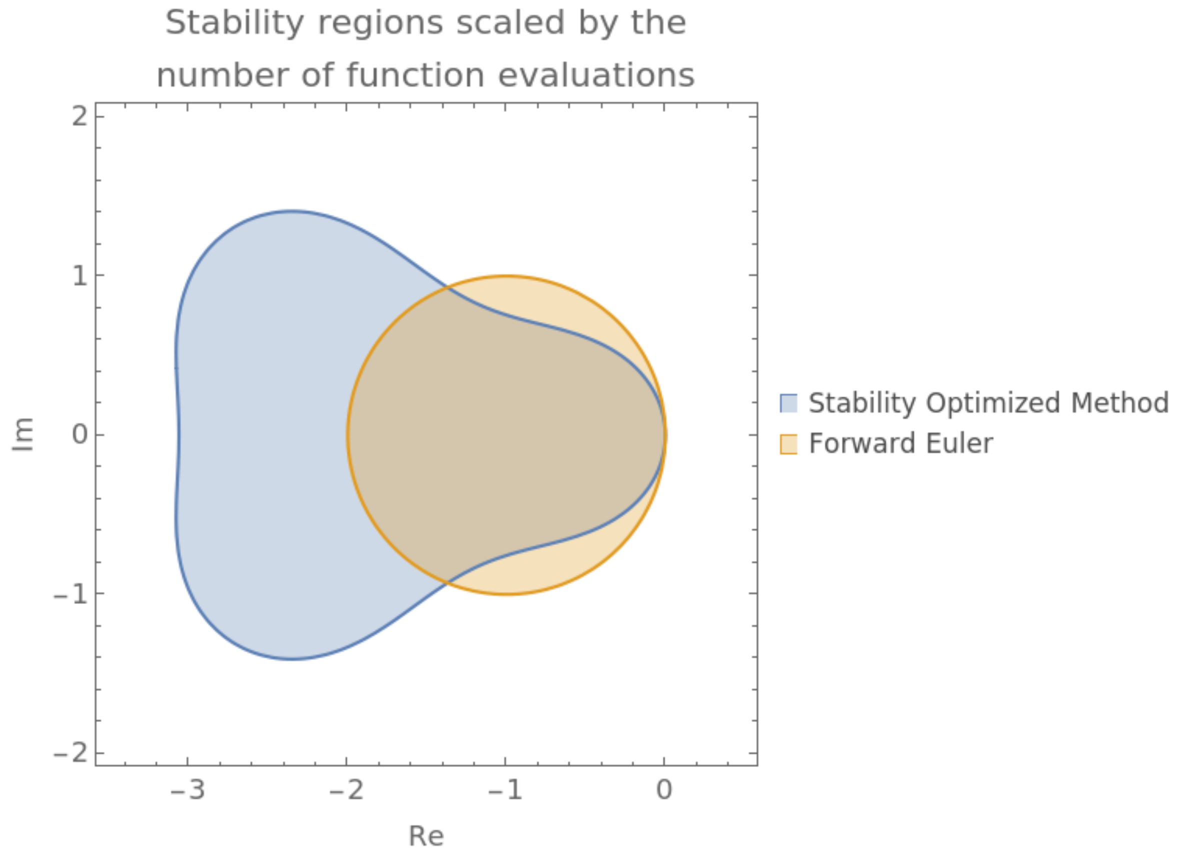
We Can Optimize The Stability with Additional Stages

- We derived a first order method in 3 stages with a large stability region

$$
\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
\frac{1}{3} & \frac{1}{3} & 0 & 0 \\
\frac{2}{3} & \frac{11}{21} & \frac{1}{7} & 0 \\
\hline
 & \frac{53}{80} & \frac{3}{40} & \frac{21}{80}
\end{array}
$$

- For the twisty stream problem, we can take a time step roughly 5x bigger

- The minimum time to a stable solution is reduced by about 35% for the twisty stream problem



Conclusions

- New Runge-Kutta integrators from SUNDIALS facilitate faster and more accurate modeling of ice sheets
- Embedded error estimation offers a simpler and effective alternative to CFL based time step selection
- Chombo N_Vector is now available in Chombo 3.2 patch 8
- Future and ongoing work
  - Testing multirate methods
  - Exploring other stabilized methods
  - Parallel-in-time leveraging SUNDIALS' wrappers for XBraid
  - Exploring more-complex (realistic) ice sheet configurations (grounding-line retreat, realistic Greenland and Antarctic geometries, etc).

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computing.llnl.gov/sundials

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