The Many Faces of Stiffness, and how Runge-Kutta Methods can Overcome their Challenges

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Overview

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Overview

Charactizations/Definitions of "Stiffness"

"While the intuitive meaning of stiff is clear to all specialists, much controversy is going on about it's [sic] correct mathematical definition" [Hairer, Wanner: Solving ODE II]

Problem-driven

At least two time scales, and fast variables affect system dynamics but do not manifest (significantly) in solution.

Method-driven

"Stiff equations are equations where certain implicit methods [...] perform [...] tremendously better, than explicit ones." [Curtiss, Hirschfelder, 1952]

"Stiff equations are problems for which explicit methods don't work." [Hairer, Wanner: Solving ODE II]

"Stiffness occurs when stability requirements, rather than those of accuracy, constrain the step length." [Lambert: Numerical Methods for ODE]

This talk

- Stiffness is not just a stability issue; it is also an accuracy issue.
- Carefully understand manifestations in different ODE and PDE problems.
- Overcome order reduction uniformly; more than asymptotic preserving.

Runge-Kutta (RK) method

Butcher tableau

$$\begin{array}{c|c} \vec{c} & A \\ \hline & \vec{b}^T \end{array}\,, \qquad \vec{c} = A\vec{e}\,, \qquad \vec{e} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

for ODE $y' = f(y)$ encodes update rule

$$Y_i^n = y^n + \Delta t \sum_{j=1}^{s} a_{ij} f(Y_j^n)$$

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

Stability function

$R(\zeta) = 1 + \zeta \vec{b}^T (I - \zeta A)^{-1} \vec{e}$ is growth factor u^{n+1}/u^n per step of size Δt, where $\zeta = \lambda \Delta t$, when solving linear test problem

$$y' = \lambda y\,, \quad \lambda \in \mathbb{C}\,.$$

Region of absolute stability

$S = \{\zeta \in \mathbb{C} : |R(\zeta)| \leq 1\}$

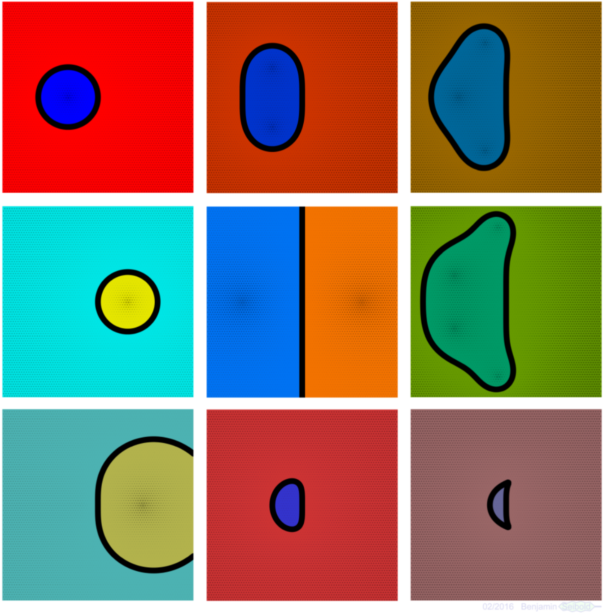
Stiffness as stability restriction

$y' = \lambda y$ with $|\lambda| \gg 1$

Explicit RK
$\Longrightarrow$ R polynomial
$\Longrightarrow$ S bounded

cannot "work"

"Absolutely Stable" [2016]



Fine, but

there is a lot more going on . . .

Overview

Initial-Boundary-Value Problem (IBVP)

$$\begin{cases} u_t = \mathcal{L}u + f & \text{for } x \in \Omega, t \in (0, T) \\ u = g & \text{for } x \in \partial\Omega, t \in [0, T] \\ u = u_0 & \text{for } x \in \Omega, t = 0 \end{cases}$$

where $\mathcal{L}$ differential operator.

Example: 1D Heat Equation

$$\begin{cases} u_t = u_{xx} + f(x,t) & \text{PDE} \\ u = g(x_{\text{b}}, t) & \text{b.c.} \\ u = u_0(x) & \text{i.c.} \end{cases}$$

where $x \in [0,1]$.

Implicit Time-Stepping of IBVP

Why? Avoid $\Delta t \leq O(\Delta x^2)$ time-step restriction of explicit schemes.

Semi-discretization in time (Rothe; justified if uncond. stable) yields BVP:

Backward Euler:
$$\begin{cases} \frac{1}{\Delta t}(u^{n+1} - u^n) = \mathcal{L}u^{n+1} + f^{n+1} & \text{in } \Omega \\ u^{n+1} = g^{n+1} & \text{on } \partial\Omega \end{cases}$$

Local (one time step) truncation error: $O(\Delta t^2)$

Global ($O(1/\Delta t)$ time steps) truncation error: $O(\Delta t)$

Incur order reduction, which is a temporal error phenomenon.

($\rightsquigarrow$ use super-fine spatial grids in examples)

Example: 1D Heat Equation

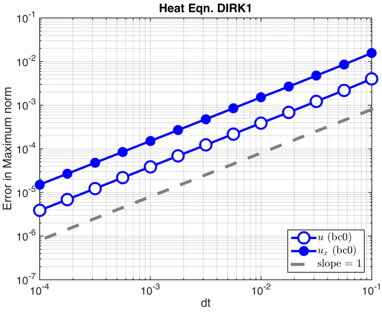
$$\begin{cases} u_t = u_{xx} + f(x,t) & \text{PDE} \\ u = g(x_b, t) & \text{b.c.} \\ u = u_0(x) & \text{i.c.} \end{cases}$$

Method of Manufactured Solutions

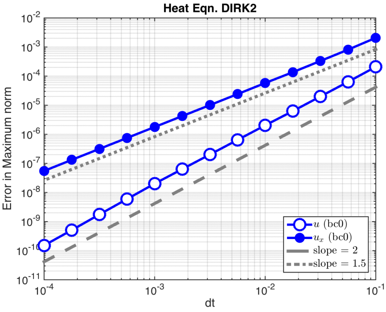
Choose $u(x,t)$. Calculate f, g, and u_0 s.t. IBVP has the chosen solution.

Simplest example: $u(x,t) = \cos(t)$; $x \in [0,1]$, $t \in [0,1]$.

DIRK1 (backward Euler)



Second-Order DIRK2



Expected orders in u. Loss of half an order in u_x for DIRK2.

Example: 1D Heat Equation

$$\begin{cases} u_t = u_{xx} + f(x,t) & \text{PDE} \\ u = g(x_\text{b}, t) & \text{b.c.} \\ u = u_0(x) & \text{i.c.} \end{cases}$$

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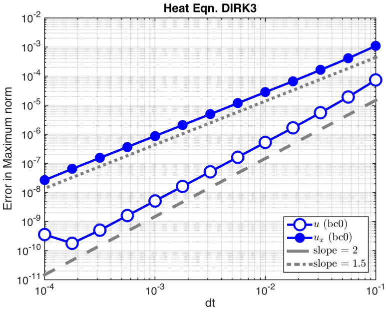
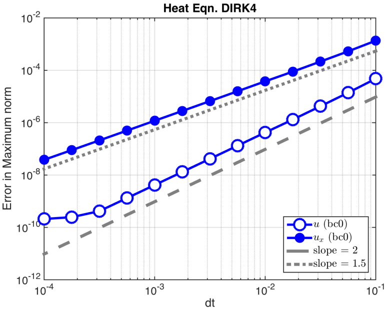
Third-Order DIRK3

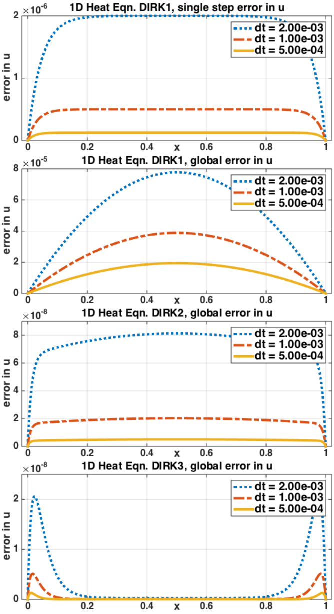


Fourth-Order DIRK4



DIRK3/4 only as accurate as DIRK2. Order-loss in u (and u_x).

Shape of Temporal Errors



Why are there Boundary Layers (BL) at all?

DIRK1 one-step error $\epsilon(x)$ solves BVP

$$\begin{cases} \epsilon - \Delta t\, \epsilon_{xx} = -\Delta t \sin(\Delta t) & \text{for } x \in (0,1) \\ \epsilon = 0 & \text{for } x \in \{0,1\} \end{cases}$$

Singularly perturbed problem:
$\epsilon = O(\Delta t^2)$ outside BL; BL thickness $O(\Delta t^{0.5})$.

Spatial boundary layers, caused by the temporal error.

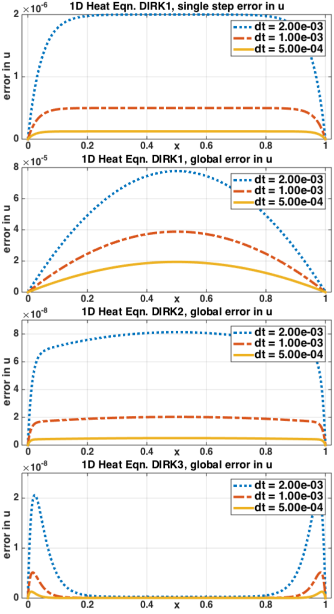
Why loss of 1/2 order in u_x?

Error away from BL: $O(\Delta t^p)$;
error on boundary: 0;
BL thickness: $O(\Delta t^{0.5})$.

Why DIRK 3 and DIRK 4 only second order?

Stages have different BL thickness. No order p Taylor series cancellation inside BLs. Error as accurate as each stage ($O(\Delta t^2)$).

Shape of Temporal Errors



Boundary Layer Error Theory

Spatial Manifestations of Order Reduction in Runge-Kutta Methods for IBVPs, Commun. Math. Sci. 2024

1. Modal analysis of semi-discretized (in space) system: $\vec{u}^n(x) = \vec{v}(x)e^{i\omega\Delta t\, n}$.
2. Yields BVP $\vec{v} = M \cdot \mathcal{L}\vec{v} + M \cdot \vec{\phi}$.
3. Spectrum of M:

$$M = \underbrace{\frac{\Delta t}{e^{i\omega\Delta t} - 1}\vec{e}\vec{b}^T}_{\text{O(1) rank 1 matrix}} + \underbrace{\Delta t A}_{O(\Delta t)\ \text{perturbation}}$$

4. One $O(1)$ eigenvalue, others $O(\Delta t)$.
5. Hence: Single-stage methods are devoid of OR. RK methods have BLs.
6. Avoiding OR means: BLs are present but are of the order of the method (or higher).

Note that OR does not always manifest, e.g., no time dependence in forcing or b.c.

Q: What is the simplest model problem that captures order reduction?

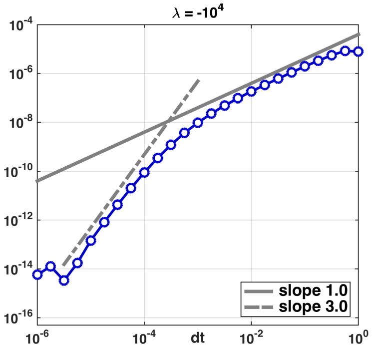
$y' = \lambda y$ does not (only one time scale).

A: Generalize via method of manufactured solutions [Prothero–Robinson]

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

with i.c. $y(0) = \phi(0)$ and $\operatorname{Re}\lambda \leq 0$.

Exact solution: $y(t) = \phi(t)$.



+ Can analyze error as bi-variate function of Δt and λ.
+ Different convergence notions explain order reduction behavior in ODE, in PDE, stiff limits, semi-stiffness in ERK, etc.
+ Explicit expressions for error (instead of just error estimates).
+ Simplest analysis for IRK or ERK, but extension to ImEx also natural.
− Does not cover conditions specific to nonlinear problems ($p \geq 4$).

Overview

Error for Prothero–Robinson model problem $y' = \lambda(y - \phi(t)) + \phi'(t)$

Apply RK scheme. Error at t_{n+1} (with $\zeta = \lambda \Delta t$):

$$\epsilon^{n+1} = R(\zeta)\,\epsilon^n + \zeta \vec{b}^{\,T}(I - \zeta A)^{-1}\vec{\delta}_s^{\,n+1} + \delta^{n+1}\,.$$

Truncation errors at intermediate stages and end of step:

$$\vec{\delta}_s^{\,n+1} = \sum_{j\geq 2} \tfrac{\Delta t^j}{(j-1)!}\,\vec{\tau}^{\,(j)}\phi^{(j)}(t_n)\,,\quad \delta^{n+1} = \sum_{j\geq 1} \tfrac{\Delta t^j}{(j-1)!}\left(\vec{b}^{\,T}\vec{c}^{\,j-1} - \tfrac{1}{j}\right)\phi^{(j)}(t_n)$$

with *stage order residuals* $\vec{\tau}^{\,(j)} = A\vec{c}^{\,j-1} - \frac{1}{j}\vec{c}^{\,j}\,,\quad j = 1, 2, \ldots$

- Order conditions render δ^{n+1} always high order.
- Stability $|R(\zeta)| < 1$ for $\zeta \neq 0$ ensures error is governed by $\vec{\delta}_s^{\,n+1}$ term:

$$e(\Delta t, \zeta) = \sum_{j\geq 2} \Delta t^j\,\tfrac{\phi^{(j)}(t_n)}{(j-1)!}\,\zeta\vec{b}^{\,T}(I - \zeta A)^{-1}\vec{\tau}^{\,(j)}$$

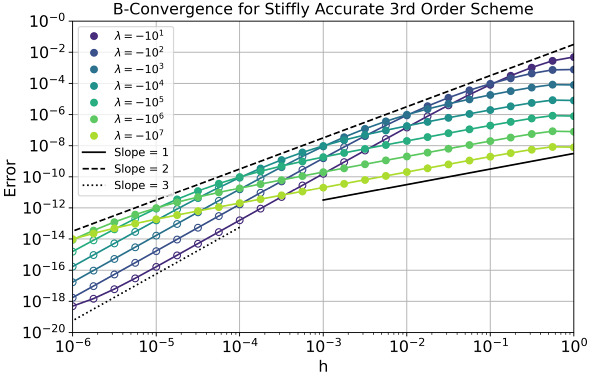
Error of p-th order RK scheme for Prothero–Robinson model problem

$$e(\Delta t, \zeta) = \sum_{j\geq 2} \Delta t^j \, \tfrac{\phi^{(j)}(t_n)}{(j-1)!} \, \zeta \vec{b}^T (I - \zeta A)^{-1} \vec{\tau}^{(j)}$$

Convergence notions:

- Classical limit $\Delta t \to 0$ and $\zeta \to 0$: Order conditions ($\vec{b}^T A^\ell \, \vec{c}^k = \frac{1}{(\ell+k+1)\cdots(k+1)}$ for $0 \leq j+k \leq p-1$) imply full order p ($\zeta(I-\zeta A)^{-1} = \zeta+\zeta^2 A+\zeta^3 A^2+\dots$ and $\vec{b}^T \vec{\tau}^{(j)} = 0$ for $j \leq p-1$) .
- Stiff limit $\Delta t \to 0$ and $\zeta \to -\infty$: Conditions $\vec{b}^T A^{-1} \vec{\tau}^{(j)} = 0$ due to expansion $(\zeta(I-\zeta A)^{-1} = -A^{-1} - \zeta^{-1} A^{-2} - \zeta^{-2} A^{-3} - \dots)$
  [Stiff accuracy and A invertible imply $\vec{b}^T A^{-1} \vec{\tau}^{(j)} = 0$ due to order conditions.]
- Semi-stiff limit $\Delta t \to 0$ and $\zeta = -\mu$: (e.g.: ERK for advective PDE) Middle range $\vec{b}^T (I-\mu A)^{-1} \vec{\tau}^{(j)} = 0$ for μ fixed.
- B-convergence: Convergence $\Delta t \to 0$ of $\max_\zeta |e(\Delta t, \zeta)|$
  (The natural convergence for PDE due to unbounded spectrum)
- DAE-limit = AP: Is $\lim_{\zeta \to -\infty} e(\Delta t, \zeta) = 0$ for Δt fixed?
- Weak uniform: B-convergence of order p (yes/no?)
- Strong uniform: For any λ have $e(\Delta t, \lambda \Delta t) = C \Delta t^p$ (yes/no?)

Stiffly accurate L-stable 3rd order DIRK3



$$
\begin{array}{c|ccc}
x & x & & \\
\frac{1+x}{2} & \frac{1-x}{2} & x & \\
1 & -\frac{3}{2}x^2+4x-\frac{1}{4} & \frac{3}{2}x^2-5x+\frac{5}{4} & x \\
\hline
 & -\frac{3}{2}x^2+4x-\frac{1}{4} & \frac{3}{2}x^2-5x+\frac{5}{4} & x
\end{array}
$$

where $x = 0.4358665215$

Convergence notions

- Classical limit: For $\zeta \ll 1$: $e = O(\Delta t^3)$
- Stiff limit: For $\zeta \gg 1$: $e = O(\Delta t^1)$
- DAE limit: $\vec{b}^{\,T}A^{-1}\vec{\tau}^{(2)} = 0$, hence $e = O(\zeta^{-1})$ and thus AP.
- B-convergence: $O(\Delta t^2)$
- Weak uniform: no
- Strong uniform:no

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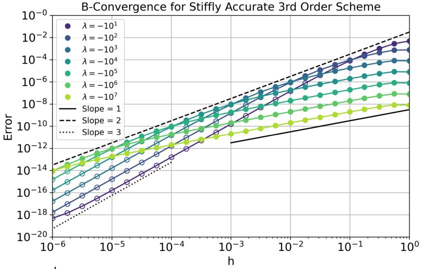
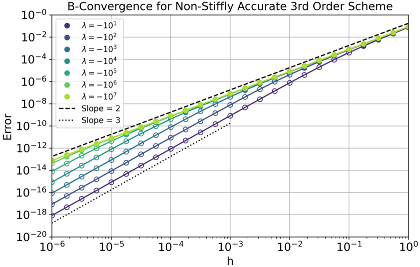
3rd order DIRK with $\vec{b}^T A^{-1} \vec{\tau}^{(2)} = 0$



$$
\begin{array}{c|ccc}
x & x & & \\
\frac{1+x}{2} & \frac{1-x}{2} & x & \\
1 & -\frac{3}{2}x^2+4x-\frac{1}{4} & \frac{3}{2}x^2-5x+\frac{5}{4} & x \\
\hline
 & -\frac{3}{2}x^2+4x-\frac{1}{4} & \frac{3}{2}x^2-5x+\frac{5}{4} & x
\end{array}
$$

where $x = 0.4358665215$

3rd order DIRK with $\vec{b}^T A^{-1} \vec{\tau}^{(2)} \neq 0$



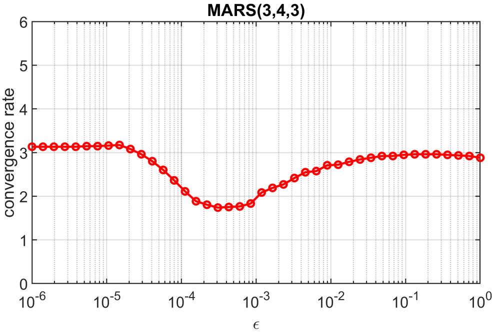
Crouzeix's 3rd order DIRK method

$$
\begin{array}{c|cc}
\frac{1}{2}+\frac{1}{6}\sqrt{3} & \frac{1}{2}+\frac{1}{6}\sqrt{3} & \\
\frac{1}{2}-\frac{1}{6}\sqrt{3} & -\frac{1}{3}\sqrt{3} & \frac{1}{2}+\frac{1}{6}\sqrt{3} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

- Identical classical ($O(\Delta t^3)$) and B-convergence ($O(\Delta t^2)$).
- $\vec{b}^T A^{-1} \vec{\tau}^{(2)} = 0$ generates $O(\Delta t^1)$ behavior in stiff triangle ($\zeta \gg 1$), which is superior to $O(\Delta t^2)$ behavior incurred with $\vec{b}^T A^{-1} \vec{\tau}^{(2)} \neq 0$ $\rightsquigarrow$ asymptotic preserving (AP).

"Pothole phenomenon" in AP ImEx Runge-Kutta schemes

[Boscarino, Russo, SISC 2009]



Broadwell model

$$\partial_t \rho + \partial_x m = 0$$
$$\partial_t m + \partial_x z = 0$$
$$\partial_t z + \partial_x m = \frac{1}{\varepsilon}(\rho^2 + m^2 - 2\rho z)$$

"lack of accuracy of the schemes for intermediate values of the stiffness parameter" [Boscarino, Russo, SISC 2009]

Note: ImEx framework, but same story because order reduction is solely due to $\frac{1}{\varepsilon}$-stiffness (periodic domain and smooth solutions).

Overview

Recall: error of RK scheme for RP problem dominated by

$$e(\Delta t,\zeta) = \sum_{j\geq 2} \Delta t^j \tfrac{\phi^{(j)}(t_n)}{(j-1)!}\, \zeta \underbrace{\vec{b}^T(I-\zeta A)^{-1}\vec{\tau}^{(j)}}_{\textbf{goal: }\text{make } = 0 \text{ for many } j} \quad \text{with} \quad \vec{\tau}^{(j)} = A\vec{c}^{\,j-1} - \tfrac{1}{j}\vec{c}^{\,j}$$

Def.: Scheme has *stage order* q if $p \geq q$ and $\vec{\tau}^{(j)} = 0$ for $1 \leq j \leq q$.

Thm.: Irreducible DIRK schemes have $q \leq 2$; & if A non-singular: $q = 1$.

Def.: Scheme has *weak stage order* (WSO) q if an A-invariant subspace $\mathcal{V}$ exists that is orthogonal to $\vec{b}$ and $\vec{\tau}^{(j)} \in \mathcal{V}$ for $1 \leq j \leq q$.

Thm.: WSO achieves the **goal** as well:

$$\vec{\tau}^{(j)} \in \mathcal{V} \overset{\mathcal{V}\ A\text{-inv.}}{\Longrightarrow} (I-\zeta A)^{-1}\vec{\tau}^{(j)} \in \mathcal{V} \overset{\mathcal{V}\perp\vec{b}}{\Longrightarrow} \vec{b}^T(I-\zeta A)^{-1}\vec{\tau}^{(j)} = 0 \quad \square$$

Thm.: WSO $q \iff \vec{b}^T A^\ell \vec{\tau}^{(j)} = 0$ for $1 \leq j \leq q$ and $0 \leq \ell \leq s-1$.

Def.: Scheme satisfies *WSO eigenvector criterion* if $A\vec{\tau}^{(j)} = \mu_j \vec{\tau}^{(j)}$ and $\vec{b}^T\vec{\tau}^{(j)} = 0$ for $1 \leq j \leq q$.

Thm.: WSO EC limited to $q \leq 3$ for DIRK schemes with non-singular A.

No limitation on WSO q (other than needing more stages).
WSO yields polynomial conditions for Butcher coefficients a_{ij}, b_i.

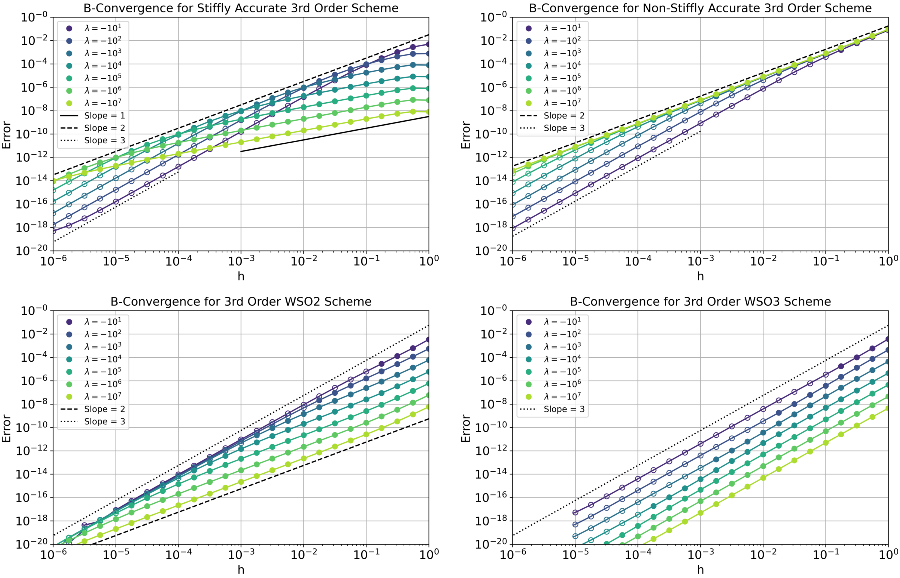
Two simple stiffly accurate and L-stable DIRK schemes

Order $p = 3$ and WSO $q = 2$:

c_1	0.019000729223994			
c_2	0.404346056373926	0.384357175127182		
c_3	0.064879089771843	−0.163896403659870	0.51545231222	
1	0.023435499759592	−0.412078784899592	0.96661161281	0.42203167233
	0.023435499759592	−0.412078784899592	0.96661161281	0.42203167233

Order $p = 3$ and WSO $q = 3$:

c_1	0.137565435510819			
c_2	0.566951227943062	0.234838887815719		
c_3	−1.083540728288038	2.966182238854014	0.44915521951	
1	0.597612915006364	−0.434209975846364	−0.05305815322	0.88965521406
	0.597612915006364	−0.434209975846364	−0.05305815322	0.88965521406



Both WSO 2 and 3 achieves B-convergence 3 and thus weak uniform convergence. But only WSO 3 exhibits strong uniform convergence.

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Application example: existing ImEx method [Boscarino, Russo, SISC 2009]

0	0	0	0	0	0	0	0	0	0	0
c_2	c_2	0	0	0	0	$c_2-\gamma$	γ	0	0	0
c_3	$c_3-\tilde{a}_{32}$	$\tilde{a}_{32}$	0	0	0	$c_3-a_{32}-\gamma$	a_{32}	γ	0	0
c_4	$c_4-\tilde{a}_{42}-\tilde{a}_{43}$	$\tilde{a}_{42}$	$\tilde{a}_{43}$	0	0	$c_4-a_{42}-a_{43}-\gamma$	$a_{42}-\gamma$	a_{43}	γ	0
1	b_1	0	b_3	b_4	γ	b_1	0	b_3	b_4	γ
1	b_1	0	b_3	b_4	γ	b_1	0	b_3	b_4	γ

with coefficients to satisfy (non-stiff) order conditions and moreover:

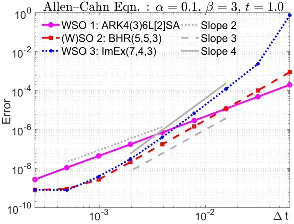
$$\tau_{\text{Im}}^{(2)} = 0 \quad \text{and} \quad \tau_{\text{Ex}}^{(2)} = Ac - \tfrac{1}{2}c^2 = \beta e_2 \;\;,\;\; A\tau_{\text{Ex}}^{(2)} = \mu e_2 \;\;,\;\; b^T e_2 = 0\;.$$

This is in fact a special case of the WSO eigenvector criterion. Thus the implicit part is WSO2. But while this specific approach cannot be (easily) extended to higher orders, general WSO *can*.

New scheme with WSO3, yielding 4th order

7-stage ImEx scheme

$\longrightarrow$ talk to A. Biswas



Construct error-optimal L-stable schemes with high order and WSO

$(s,p,q) = (4,3,2)$

0.01900072890	0.01900072890			
0.78870323114	0.40434605601	0.38435717512		
0.41643499339	0.06487908412	-0.16389640295	0.51545231222	
1	0.02343549374	-0.41207877888	0.96661161281	0.42203167233
	0.02343549374	-0.41207877888	0.96661161281	0.42203167233

$(s,p,q) = (4,3,3)$

0.13756543551	0.13756543551			
0.80179011576	0.56695122794	0.23483888782		
2.33179673002	-1.08354072813	2.96618223864	0.44915521951	
1	0.59761291500	-0.43420997584	-0.05305815322	0.88965521406
	0.59761291500	-0.43420997584	-0.05305815322	0.88965521406

$(s,p,q) = (6,4,3)$

0.0796724	0.0796724					
0.4643647	0.3283554	0.1360093				
1.3485592	-0.6507728	1.7428591	0.2564730			
1.3126642	-0.7145806	1.7937458	-0.0782548	0.3117538		
0.9894693	-1.1200928	1.9834523	3.1173939	-3.7619302	0.7706460	
1	0.2148237	0.5363674	0.1544881	-0.2177486	0.0722264	0.2398430
	0.2148237	0.5363674	0.1544881	-0.2177486	0.0722264	0.2398430

$(s,p,q) = (7,4,4)$

1.290066345260422e-01	1.290066345260422e-01						
4.492833135308985e-01	3.315354455306989e-01	1.177478680001996e-01					
9.919659086525534e-03	-8.009819642882672e-02	-2.408450965101765e-03	9.242630648045402e-02				
1.230475897454758e+00	-1.730636616639455e+00	1.513225984674677e+00	1.221258626309848e+00	2.266279031096887e-01			
2.978701803613543e+00	1.475353790517696e-01	3.618481772236499e-01	-5.603544220240282e-01	2.455453653222619e+00	5.742190161395324e-01		
1.247908693583052e+00	2.099717815888321e-01	7.120237463672882e-01	-2.012023940726332e-02	-1.913828539529156e-02	-5.556044541810300e-03	3.707277349712966e-01	
1.000000000000000e+00	2.387938238483883e-01	4.762495400483653e-01	1.233935151213300e-02	6.011995982693821e-02	6.553618225489034e-05	-1.270730910442124e-01	3.395048796261326e-01
	2.387938238483883e-01	4.762495400483653e-01	1.233935151213300e-02	6.011995982693821e-02	6.553618225489034e-05	-1.270730910442124e-01	3.395048796261326e-01

$(s,p,q) = (12,5,4)$

2.345371908646273e-01	2.345371908646273e-01											
7.425871511958302e-01	6.874344413888787e-01	5.515270980695153e-02										
3.296674204078279e-02	-1.183552669539587e-01	5.463563002913454e-03	1.458584459918280e-01									
7.379564717201322e-01	-1.832235204042292e-01	5.269029412008775e-02	8.203685085133529e-01	4.812118949092085e-02								
2.376643917109970e-01	9.941572060659400e-02	4.977904930055774e-03	5.414758174284321e-02	-1.666571741820749e-03	8.078975617332473e-02							
1.750238160341377e+00	-9.896614721582678e-01	2.860682690577833e+00	-1.236119341063179e+00	2.130219523351530e+00	-1.260655031676537e+00	2.457717913099987e-01						
2.990308150015702e+00	-5.656238413439102e-02	1.661985685769353e-01	6.464600922362508e-01	6.608854962269927e-01	3.736054198873429e-01	6.294456964407685e-01	5.702752607818027e-01					
2.882138003112822e+00	8.048962104724392e-01	-6.232034990249100e-02	5.737234603323347e-01	-9.613723511489970e-02	5.524106361737929e-01	5.961002486833255e-01	1.978411600659203e-01	3.156238724024008e-01				
2.914399924907188e+00	-1.606381759216300e-01	6.833397073337708e-01	4.734578665308685e-01	8.037708984872738e-01	-1.094498069459834e-02	6.151263362711297e-01	3.908946848682723e-01	8.966103265353116e-02	2.973255537857041e-02			
2.573507348677332e+00	7.074283235644631e-01	4.392037300952482e-01	-3.623592480237268e-02	7.189990308645932e-04	5.820968279166545e-01	3.302003177175218e-01	-2.394564021215881e-01	-7.540283547997615e-03	1.702137469523672e-01	6.268780138721711e-01		
3.567266961364713e+00	1.361197981133694e-01	-7.486549901902831e-01	1.893908350024949e+00	3.940485196730028e-01	6.240233526545023e-02	7.511983862200027e-01	-5.283465265730526e-01	-1.661625677872943e+00	9.998723833190827e-01	1.377776742457387e+00	8.905676409277480e-01	
1.000000000000000e+00	-7.433675378768276e-01	1.490594423766965e-01	-2.042884056742363e-02	8.565329438087443e-04	1.357261590983184e+00	2.067512027776675e-03	9.836884265759428e-02	-1.357936974507222e-02	-5.428992174996300e-02	-3.803299038293005e-02	-9.150525836295019e-03	2.712352651694511e-01
	-7.433675378768276e-01	1.490594423766965e-01	-2.042884056742363e-02	8.565329438087443e-04	1.357261590983184e+00	2.067512027776675e-03	9.836884265759428e-02	-1.357936974507222e-02	-5.428992174996300e-02	-3.803299038293005e-02	-9.150525836295019e-03	2.712352651694511e-01

$(s,p,q) = (12,5,5)$

4.113473525867655e-02	4.113473525867655e-02											
2.269850660400232e-01	1.603459327727949e-01	6.663913326722831e-02										
6.222969192243949e-01	-3.424389044264752e-01	8.658006324816373e-01	9.893519116923277e-02									
1.377989449231234e+00	9.437182028870806e+00	-1.088783359642350e+01	2.644025436733866e+00	1.846155800500574e-01								
1.259841986970257e+00	-3.425409029430815e-01	5.172239272544332e-01	9.163589909678043e-01	5.225142808845742e-02	1.165485436026433e-01							
1.228350442796143e+00	-2.094441177460360e+00	2.577655753533404e+00	5.704405293326313e-01	1.213637180023516e-01	-4.752289775376601e-01	5.285605969257756e-01						
1.269855051265635e+00	3.391631788320480e-01	-2.797427027028997e-01	1.039483063369094e+00	5.978770926212172e-02	-2.132900327070380e-01	8.344318363436753e-02	2.410106515779412e-01					
2.496200652601413e+00	5.904282488642163e+00	3.171195765985073e+00	-1.236822836316587e+01	-4.989519066913001e-01	2.160529620826442e+00	1.916104322021480e+00	1.988059486291180e+00	2.232092386922440e-01				
2.783820705331141e+00	4.616443509508975e-01	-1.933433560549238e-01	-1.212541486279519e-01	6.662362039716674e-02	4.254912950625259e-01	7.856131647013712e-01	8.369551389357689e-01	1.604780447895926e-01	3.616125951766939e-01			
3.337101417632813e+00	-7.087669749878204e-01	6.466527094491541e-01	4.758821526542215e-01	-2.570518451375722e-01	1.123185062554392e+00	5.546921612875290e-01	3.192424333237050e-01	3.612077612576969e-01	5.866779836068974e-01	2.353799736246102e-01		
4.173423133876636e+00	4.264162484855930e-01	1.322816663477840e+00	4.245673729758231e-01	-2.530402764527700e+00	-7.822016897497742e-02	1.054463080605071e+00	4.645590541391895e-01	1.145097379521439e+00	4.301337846893282e-01	1.499513057076809e+00	1.447942640822165e-02	
1.000000000000000e+00	1.207394392845339e-02	5.187080074649261e-01	1.121304244847239e-01	-4.959806334780896e-03	-1.345031364651444e+00	3.398828703760807e-01	8.159251531671077e-01	-2.640104266439604e-03	1.439060901763520e-02	-6.556567796749947e-03	6.548135446843367e-04	5.454220210658036e-01
	1.207394392845339e-02	5.187080074649261e-01	1.121304244847239e-01	-4.959806334780896e-03	-1.345031364651444e+00	3.398828703760807e-01	8.159251531671077e-01	-2.640104266439604e-03	1.439060901763520e-02	-6.556567796749947e-03	6.548135446843367e-04	5.454220210658036e-01

Explicit RK schemes

Order reduction can also happen in the stability regime of ERK schemes.
Semi-stiff limit, e.g., for advective PDE.

⊕ Pleasing algebraic structure.
⊖ Must choose: high WSO or nonlinear SSP.

Structure & construction ⟶ talk by D. Shirokoff

(3,2,2) method

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

$R(z) = 1 + z + z^2/2$
Linear SSP coeff. 1

(4,3,2) method

$$\begin{array}{c|cccc} 0 & & & & \\ \frac{3}{10} & \frac{3}{10} & & & \\ \frac{2}{3} & \frac{2}{3} & & & \\ \frac{3}{4} & -\frac{21}{320} & \frac{45}{44} & -\frac{729}{3520} & \\ \hline & \frac{7}{108} & \frac{500}{891} & -\frac{27}{44} & \frac{80}{81} \end{array}$$

$R(z) = 1 + z + z^2/2 + z^3/6$
Linear SSP coeff. 1

(5,3,3) method

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

$R(z) = 1 + z + z^2/2 + z^3/6, \quad \text{LSSP}=1$

Towards Nonlinearity

Weak stage order, as presented thus far, is a linear concept.

To reliably overcome order reduction beyond order 3, extension to nonlinear *stiff order conditions* is needed.

Key step: semilinear problems

$$y'(t) = Jy(t) + g(y(t)),$$

where $g(y(t))$ is non-stiff but can be nonlinear, while Jy is linear but can be arbitrarily stiff.

`arxiv.org/abs/2505.15099` provides up to ESDIRK-(10,5,4) with embedding.

$\longrightarrow$ talk by S. Roberts

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Overview

Schrödinger Equation

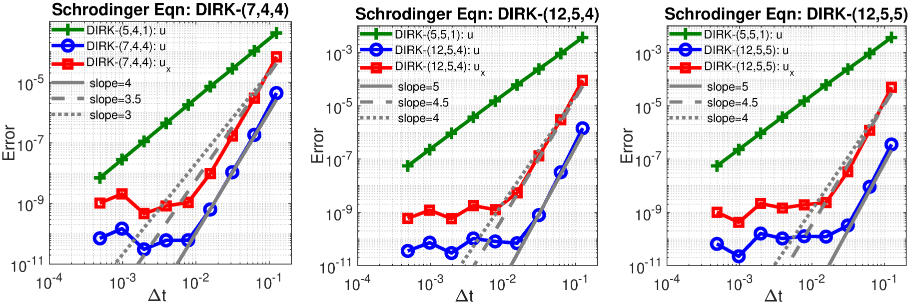
$$u_t = \frac{i\omega}{\xi^2} u_{xx} + f$$

Manufactured Solution

$$u(x,t) = \exp(-(x-t)^2)\cos(10x)\sin(t)$$

with $\omega = 2\pi$, $\xi = 20$, and $T = 1.2$.

DIRK Methods



WSO $q = 1$ clearly incurs order reduction (order 2).
WSO $q = p-1$ recovers full order in u, but loses half order in u_x.
WSO $q = p$ yields full order in u and u_x.

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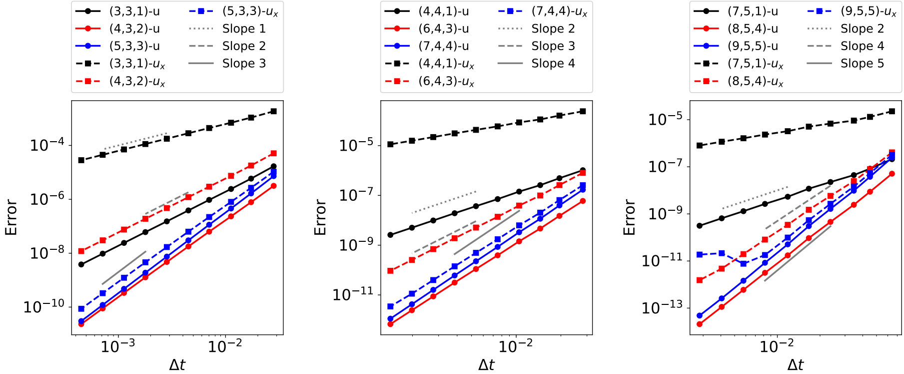
Linear Advection Equation

$$u_t = -u_x + f \;, \quad u(x,0) = u_0(x) \;, \;\; u(0,t) = g_0(t)$$

Manufactured Solution

$$u(x,t) = \frac{1+x}{1+t}$$

ERK Methods



Order reduction for WSO 1 reference schemes.
WSO recovers full order (linear PDE).

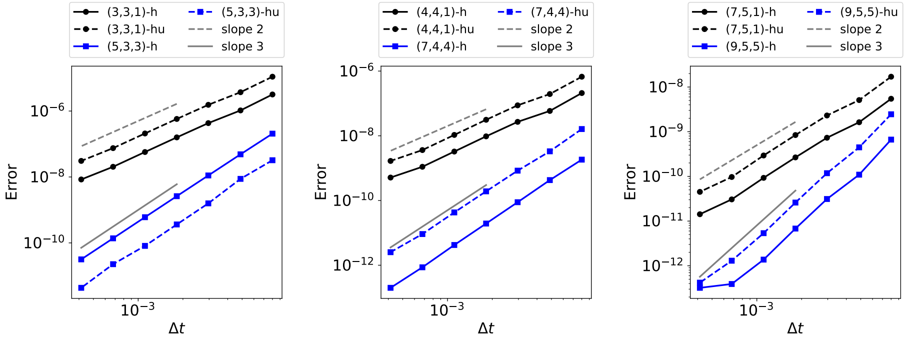
1D Shallow Water Equation

$$h_t + (hu)_x = f^h$$
$$(hu)_t + \left(hu^2 + \tfrac{1}{2}gh^2\right)_x = f^{hu}$$

Manufactured Solution

$$h(x,t) = \frac{1+x}{1+t}\,, \quad u(x,t) = \frac{1+x^2}{0.5+t}$$

ERK Methods



For this nonlinear problem, high WSO does *not* recover the full order; but yields clear improvement over WSO 1 (observed order 3 vs. 2).

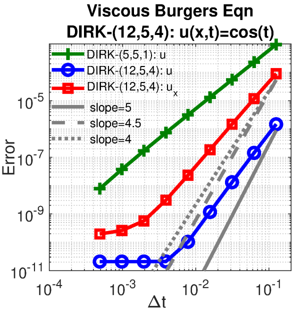
Viscous Burgers' Equation

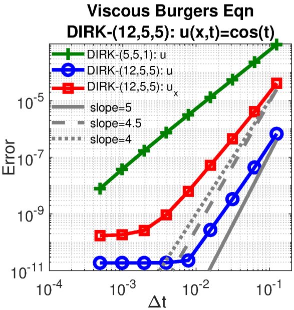
$$u_t + uu_x = \nu u_{xx} + f \ , \quad \nu = 0.1$$

Manufactured Solution

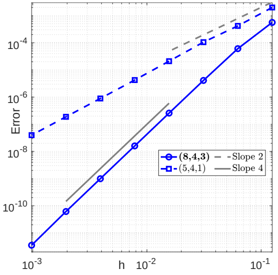
$$u(x,t) = \cos(t)$$

DIRK Methods with linear WSO





Semilinear conditions



WSO 1 schemes converge at order 2.

Linear WSO does not recover full order, but raises observed order to 3.

Semilinear order conditions yield observed order 4.

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Van der Pol Oscillator ver 1

$x' = y$ and $y' = \mu(1 - x^2)y - x$

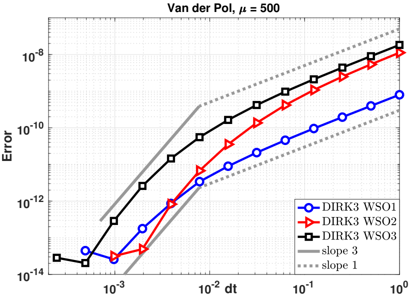
$(x(0), y(0)) = (2, 0) \qquad \mu = 500$

Van der Pol Oscillator ver 2

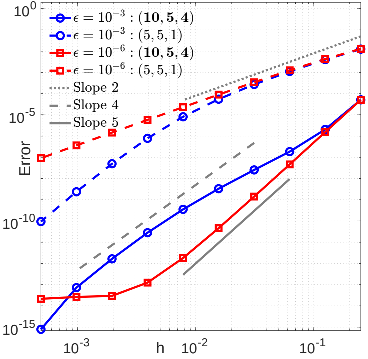
$x' = y$ and $\epsilon y' = (1 - x^2)y - x$

$(x(0), y(0)) = (2, -\frac{2}{3} + \frac{10}{81}\epsilon - \frac{292}{2187}\epsilon^2 - \frac{1814}{19683}\epsilon^3).$

DIRK with linear WSO



Semilinear order conditions



Fully nonlinear problem.

Linear WSO has clear order reduction.

Semilinear order yields convergence order 4–5, depending on stiffness.

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Overview

Take-home messages

- Stiffness is not only a stability challenge, but also an accuracy issue.
- Order reduction is generic for ODE and PDE, even if it often goes unnoticed.
- A simple scalar model problem incurs a huge richness of insight and prediction power of the error behavior for more complicated problems.
- Many desirable convergence concepts, including uniform convergence, are generated by weak stage order, respectively stiff order conditions.
- Novel ERK, DIRK (done), and ImEx (in progress) schemes constructed with high WSO.
- Excellent accuracy in a variety of relevant test problems.

WSO concept: `arxiv.org/abs/1811.01285`
Constructing DIRK schemes: `arxiv.org/abs/2204.11264`
Algebraic structure: `arxiv.org/abs/2204.03603`
Spatial manifestations: `arxiv.org/abs/1712.00897`
ERK schemes: `arxiv.org/abs/2310.02817`
Semilinear: `arxiv.org/abs/2505.15099`

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