A Parallel Ensemble Approach to Constructing Stable, High-Order Time-Steppers

CASC
Center for Applied Scientific Computing

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Steven Roberts, Arash Sarshar, and Adrian Sandu
Sidney Fernbach Postdoctoral Fellow

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Overview

- Introduction
- General Linear Methods and Parallel Ensemble Methods
- Implicit-Explicit and Other Extensions
- Numerical Experiments
- Conclusions

- Topics presented appear in
  - Roberts, Steven, Arash Sarshar, and Adrian Sandu. "Parallel implicit-explicit general linear methods." *Communications on Applied Mathematics and Computation* 3.4 (2021): 649-669.
  - Sarshar, Arash, Steven Roberts, and Adrian Sandu. "Alternating directions implicit integration in a general linear method framework." *Journal of Computational and Applied Mathematics* 387 (2021): 112619.
  - Roberts, Steven and Adrian Sandu. "Practical Multirate Time Integration Methods." Technical Report (2019)

Introduction

- Systems of ordinary differential equations (ODEs)

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

  are ubiquitous in modeling time-dependent phenomena.

- High-order time discretizations complement high-order spatial discretizations.

- Parallelism of function evaluations at method level
  - Challenging
  - Restrictive
  - Limited adoption and success

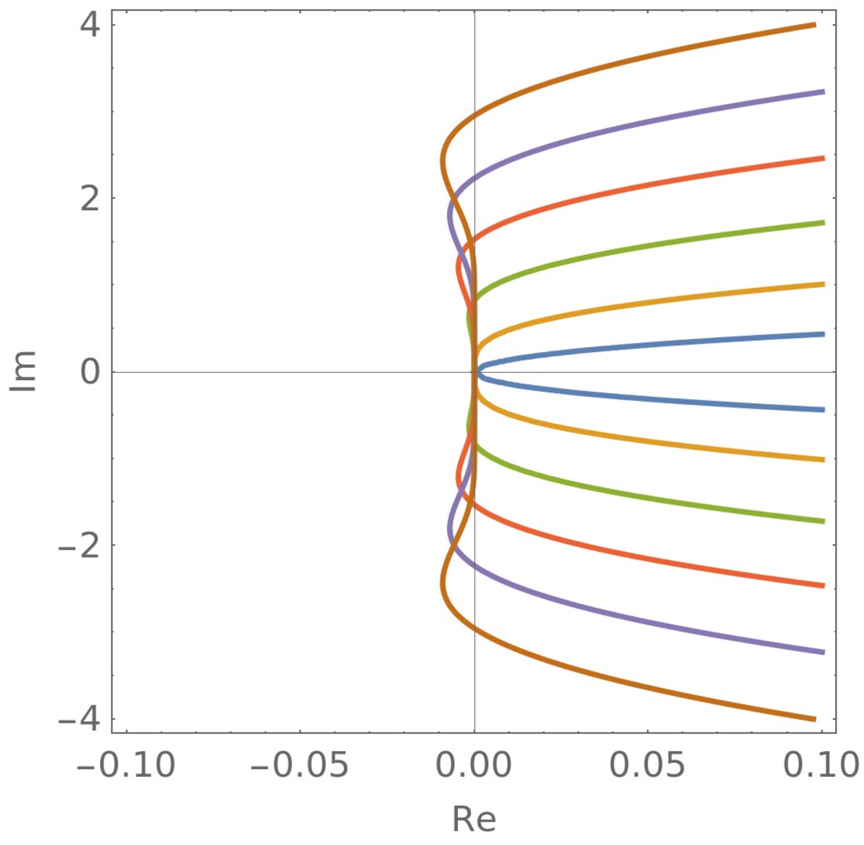
Systematically constructing integrators of order p

Method	Extrapolated Euler	Deferred Correction Euler	Backward Differentiation Formula & Adams Bashforth
Stages	$\frac{p^2 - p + 2}{2}$	$p(p-1)$	1
Minimum Parallel Processes for Maximum Speedup[1]	$\left\lceil \frac{p}{2} \right\rceil$	$p - 1$	1
Steps	1	1	p

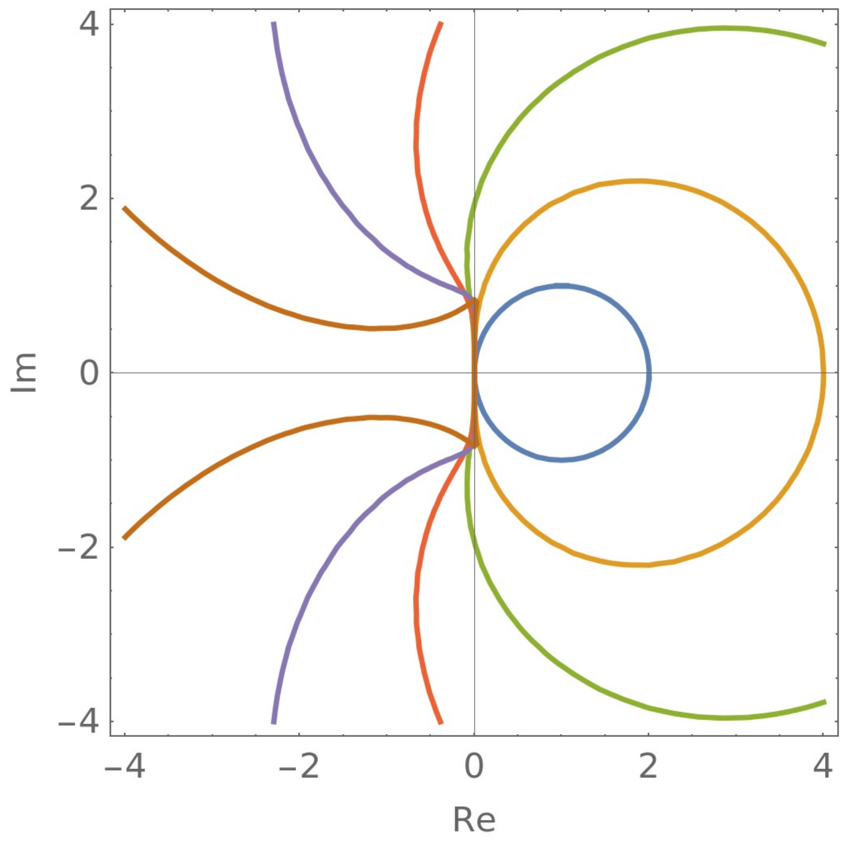
1. Ketcheson, David, and Umair bin Waheed. "A comparison of high-order explicit Runge–Kutta, extrapolation, and deferred correction methods in serial and parallel." *Communications in Applied Mathematics and Computational Science* 9.2 (2014): 175-200.

Linear stability can degrade as order increases

Stability regions for extrapolated backward Euler orders 1 to 8



Stability regions for BDF methods orders 1 to 6



General linear methods

- General linear methods (GLMs) are a broad class of integrators:

$$Y_i = h \sum_{j=1}^{s} a_{i,j} f(Y_j) + \sum_{j=1}^{r} u_{i,j} y_j^{[n-1]}, \quad i = 1, \ldots, s$$
$$y_i^{[n]} = h \sum_{j=1}^{s} b_{i,j} f(Y_j) + \sum_{j=1}^{r} v_{i,j} y_j^{[n-1]}, \quad i = 1, \ldots, r$$

$$\begin{array}{c|c|c} c & A & U \\ \hline & B & V \end{array}$$

- They contain s internal stages and r external stages.
- Internal stages can have a high order of accuracy, and external stages provide historical information

$$Y_i = y(t_n + c_i h) + O(h^{q+1})$$

$$y_i^{[n-1]} = \sum_{k=0}^{p} w_{i,k} h^k y^{(k)}(t_{n-1}) + O(h^{p+1})$$

Parallelism for general linear methods

- If $A = \lambda I$, then the stages of a GLM are independent[1].

$$Y_i = h\lambda f(Y_j) + \sum_{j=1}^{r} u_{i,j} y_j^{[n-1]}$$

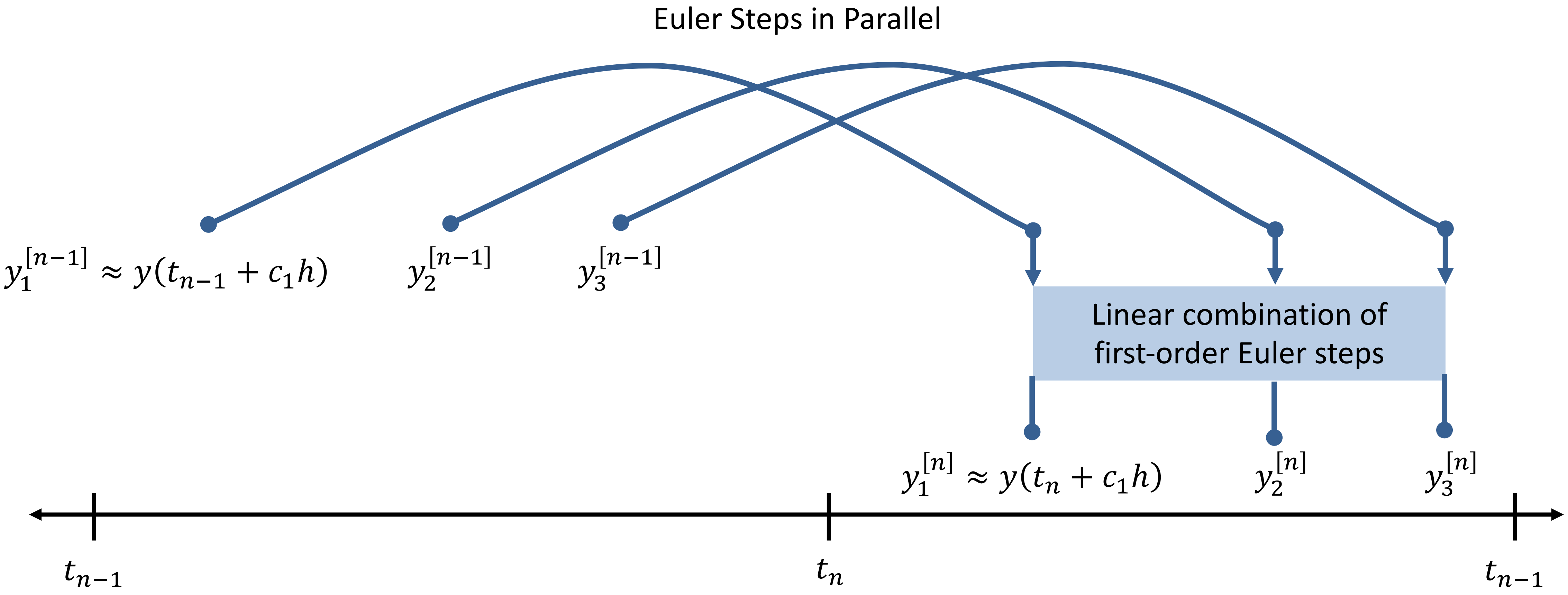
$$y_i^{[n]} = h \sum_{j=1}^{s} b_{i,j} f(Y_j) + \sum_{j=1}^{r} v_{i,j} y_j^{[n-1]}$$

c	λI	U
	B	V

- All s stages can be evaluated in parallel.
- Explicit methods have $\lambda = 0$.
- Implicit methods have $\lambda > 0$.

1. Jackiewicz, Zdzislaw. *General linear methods for ordinary differential equations*. John Wiley & Sons, 2009.

Parallel ensemble idea



Parallel ensemble general linear methods

- This idea can be cast as a GLM with tableau

$$
\begin{array}{c|c|c}
c & \lambda I_{s\times s} & I_{s\times s} \\
\hline
 & CF(I_{s\times s} - \lambda K)C^{-1} & I_{s\times s}
\end{array}
$$

where

$$
C = \left[\mathbb{1}, c, \frac{c^2}{2}, \ldots, \frac{c^{s-1}}{(s-1)!}\right] \qquad
F = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{6} & \cdots & \frac{1}{n!} \\ & 1 & \frac{1}{2} & \cdots & \frac{1}{(n-1)!} \\ & & \ddots & \ddots & \vdots \\ & & & 1 & \frac{1}{2} \\ & & & & 1 \end{bmatrix} \qquad
K = \begin{bmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & & 0 & 1 \\ & & & & 0 \end{bmatrix}
$$

- By construction, $p = q = r = s$

Third order parallel ensemble methods

Explicit

$$
\begin{array}{c|ccc|ccc}
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
1/2 & 0 & 0 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 1 \\
\hline
 & 1/6 & 2/3 & 1/6 & 1 & 0 & 0 \\
 & 1/6 & -1/3 & 7/6 & 0 & 1 & 0 \\
 & 7/6 & -10/3 & 19/6 & 0 & 0 & 1
\end{array}
$$

Implicit

$$
\begin{array}{c|ccc|ccc}
0 & 1 & 0 & 0 & 1 & 0 & 0 \\
1/2 & 0 & 1 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 1 \\
\hline
 & 7/6 & 2/3 & -5/6 & 1 & 0 & 0 \\
 & -5/6 & -11/3 & -11/6 & 0 & 1 & 0 \\
 & -11/6 & -14/3 & -11/6 & 0 & 0 & 1
\end{array}
$$

Linear stability of parallel ensemble methods

- When a generic GLM is applied to the Dahlquist test problem

$$y' = \xi y$$

we get the linear stability matrix

$$M(z) = V + B(I - zA)^{-1}U$$

- For stability at $z = h\xi$, $M(z)$ must be power bounded.
- The A, B, U, and V coefficients of parallel ensemble methods simultaneously triangularize to reveal the eigenvalues of $M(z)$:

$$\operatorname{eigs} M(z) = \left\{\frac{1 + z - \lambda z}{1 - \lambda z}, \dots, \frac{1 + z + \lambda z}{1 - \lambda z}\right\}$$

- This is stability of a one stage Runge-Kutta method!

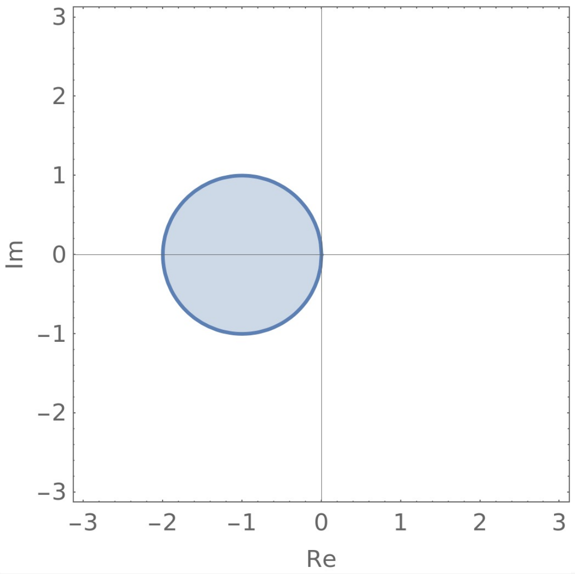
Third order parallel ensemble methods

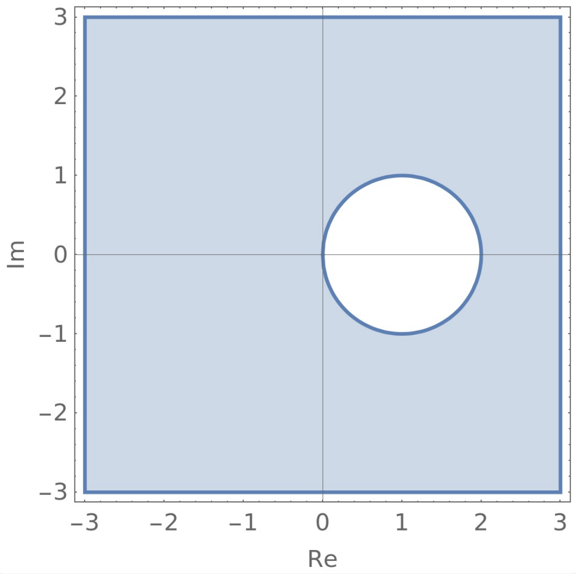
Explicit

0	0	0	0	1	0	0
1/2	0	0	0	0	1	0
1	0	0	0	0	0	1
	1/6	2/3	1/6	1	0	0
	1/6	−1/3	7/6	0	1	0
	7/6	−10/3	19/6	0	0	1

Implicit

0	1	0	0	1	0	0
1/2	0	1	0	0	1	0
1	0	0	1	0	0	1
	7/6	2/3	−5/6	1	0	0
	−5/6	−11/3	−11/6	0	1	0
	−11/6	−14/3	−11/6	0	0	1





Systematically constructing integrators of order p

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Minimum Parallel Processes for Maximum Speedup[1]	$\left\lceil \frac{p}{2} \right\rceil$	$p-1$	p	1
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Implicit-explicit general linear methods

- Consider the partitioned ODE

$$y' = \boldsymbol{f}(\boldsymbol{y}) + \boldsymbol{g}(\boldsymbol{y})$$

  with f nonstiff and g stiff.

- Implicit-explicit (IMEX) GLMs were proposed[1] to treat f explicitly and g implicitly:

$$Y_i = h \sum_{j=1}^{i-1} a_{i,j} \boldsymbol{f}(\boldsymbol{Y}_j) + h \sum_{j=1}^{i} \hat{a}_{i,j} \boldsymbol{g}(\boldsymbol{Y}_j) + \sum_{j=1}^{r} u_{i,j} y_j^{[n-1]}$$

$$y_i^{[n]} = h \sum_{j=1}^{s} b_{i,j} \boldsymbol{f}(\boldsymbol{Y}_j) + h \sum_{j=1}^{s} \hat{b}_{i,j} \boldsymbol{g}(\boldsymbol{Y}_j) + \sum_{j=1}^{r} v_{i,j} y_j^{[n-1]}$$

$$\begin{array}{c|c|c|c} c & A & \hat{A} & U \\ \hline & B & \hat{B} & V \end{array}$$

1. Zhang, Hong, Adrian Sandu, and Sebastien Blaise. "Partitioned and implicit–explicit general linear methods for ordinary differential equations." *Journal of Scientific Computing* 61.1 (2014): 119-144.

Implicit-explicit parallel ensemble methods

- Idea: combine an explicit and implicit parallel ensemble method

$$
\begin{array}{c|ccc|ccc}
0 & 0 & 0 & 0 & 1 & 0 & 0 \\
1/2 & 0 & 0 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 1 \\
\hline
 & 1/6 & 2/3 & 1/6 & 1 & 0 & 0 \\
 & 1/6 & -1/3 & 7/6 & 0 & 1 & 0 \\
 & 7/6 & -10/3 & 19/6 & 0 & 0 & 1
\end{array}
\qquad
\begin{array}{c|ccc|ccc}
0 & 1 & 0 & 0 & 1 & 0 & 0 \\
1/2 & 0 & 1 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 1 \\
\hline
 & 7/6 & 2/3 & -5/6 & 1 & 0 & 0 \\
 & -5/6 & -11/3 & -11/6 & 0 & 1 & 0 \\
 & -11/6 & -14/3 & -11/6 & 0 & 0 & 1
\end{array}
$$

$$
\begin{array}{c|ccc|ccc|ccc}
0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\
1/2 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\
\hline
 & 1/6 & 2/3 & 1/6 & 7/6 & 2/3 & -5/6 & 1 & 0 & 0 \\
 & 1/6 & -1/3 & 7/6 & -5/6 & -11/3 & -11/6 & 0 & 1 & 0 \\
 & 7/6 & -10/3 & 19/6 & -11/6 & -14/3 & -11/6 & 0 & 0 & 1
\end{array}
$$

Implicit-explicit parallel ensemble methods

- Maintains properties of base methods
  - Arbitrary order
  - Stage Parallelism
  - Stability independent of order
- The linear stability region matches that of IMEX Euler!

$$y_{n+1} = y_n + h\boldsymbol{f}(\boldsymbol{y}_n) + h\boldsymbol{g}(\boldsymbol{y}_{n+1})$$

Apply to
$y' = \xi_1 y + \xi_2 y$

$$R(\boldsymbol{z}_1, \boldsymbol{z}_2) = \frac{1 + \boldsymbol{z}_1}{1 - \boldsymbol{z}_2}$$

Other partitioned methods

- An alternating direction implicit (ADI) method solves

$$y' = f_1(y) + f_2(y) + f_3(y)$$

in a decoupled manner. Consider ADI Euler:

$$\begin{aligned} Y_1 &= y_n + h\boldsymbol{f_1}(\boldsymbol{Y_1}) + hf_2(y_n) + hf_3(y_n) \\ Y_2 &= y_n + hf_1(Y_1) + h\boldsymbol{f_2}(\boldsymbol{Y_2}) + hf_3(y_n) \\ Y_3 &= y_n + hf_1(Y_1) + hf_2(Y_2) + h\boldsymbol{f_3}(\boldsymbol{Y_3}) \\ y_{n+1} &= Y_3 \end{aligned}$$

- ADI GLMs[1] based on parallel ensemble methods have same linear stability region as ADI Euler.
- Similar results hold for multirate methods.

1. Sarshar, Arash, Steven Roberts, and Adrian Sandu. "Alternating directions implicit integration in a general linear method framework." *Journal of Computational and Applied Mathematics* 387 (2021): 112619.

Numerical experiment: Allen-Cahn

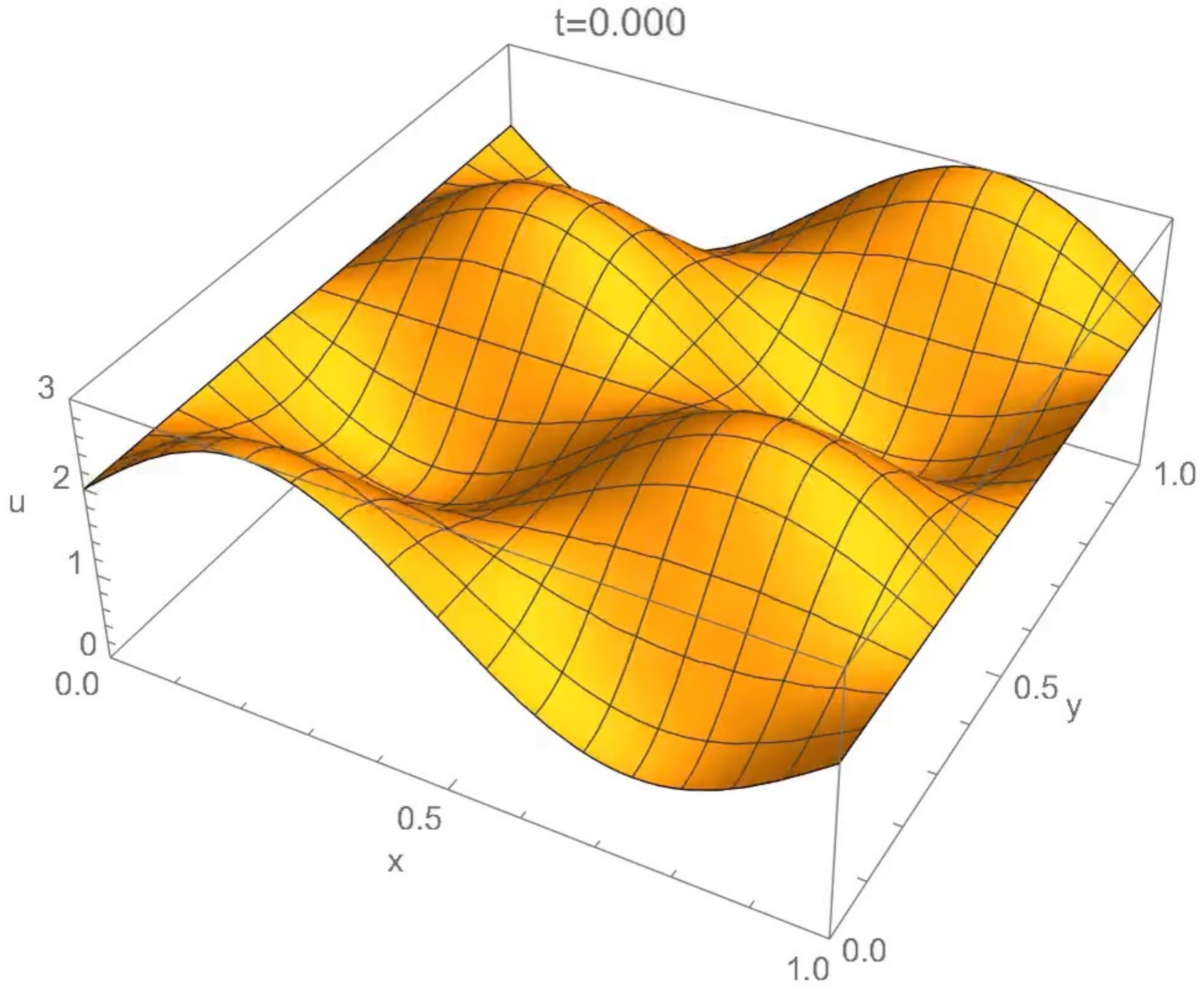
- We consider a 2D Allen-Cahn reaction-diffusion PDE:

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

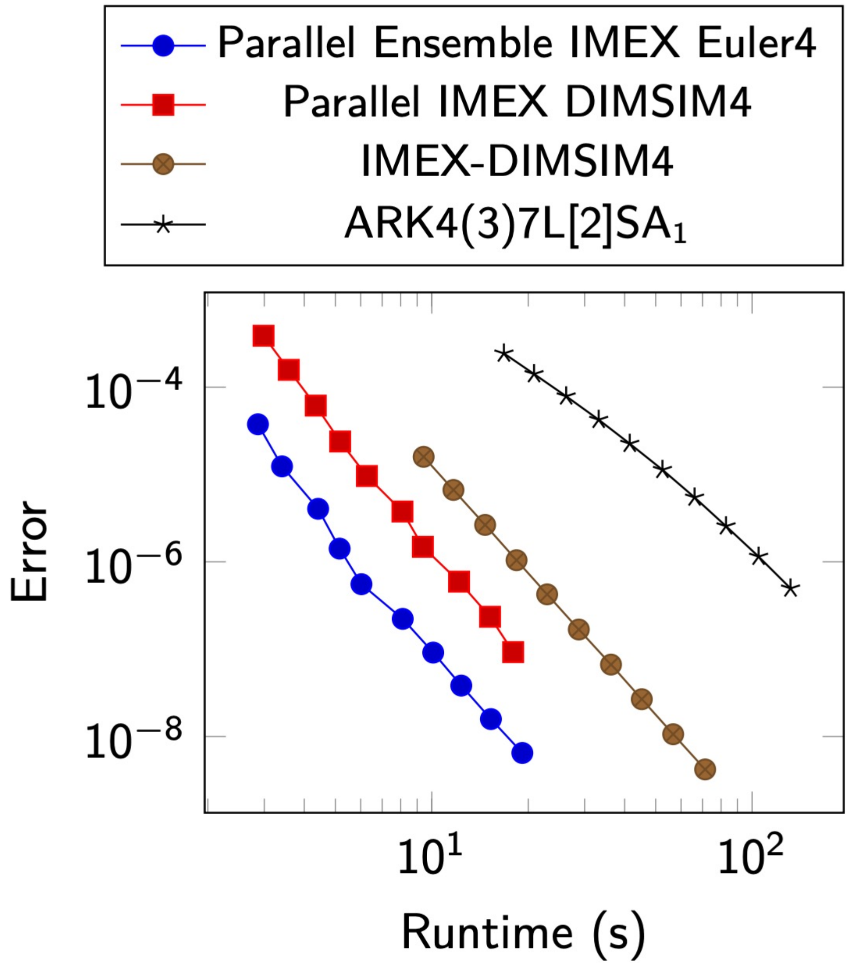
- FEniCS[1] was used for a continuous finite element spatial discretization.
- MPI was used for stage parallelism.
- The fourth and fifth order serial methods we tested against are IMEX-DIMSIM4 and IMEX-DIMSIM5 from Zhang, Sandu, and Blaise[2], as well as ARK4(3)7L[2]SA$_1$ and ARK5(4)8L[2]SA$_2$ from Kennedy and Carpenter[3] .

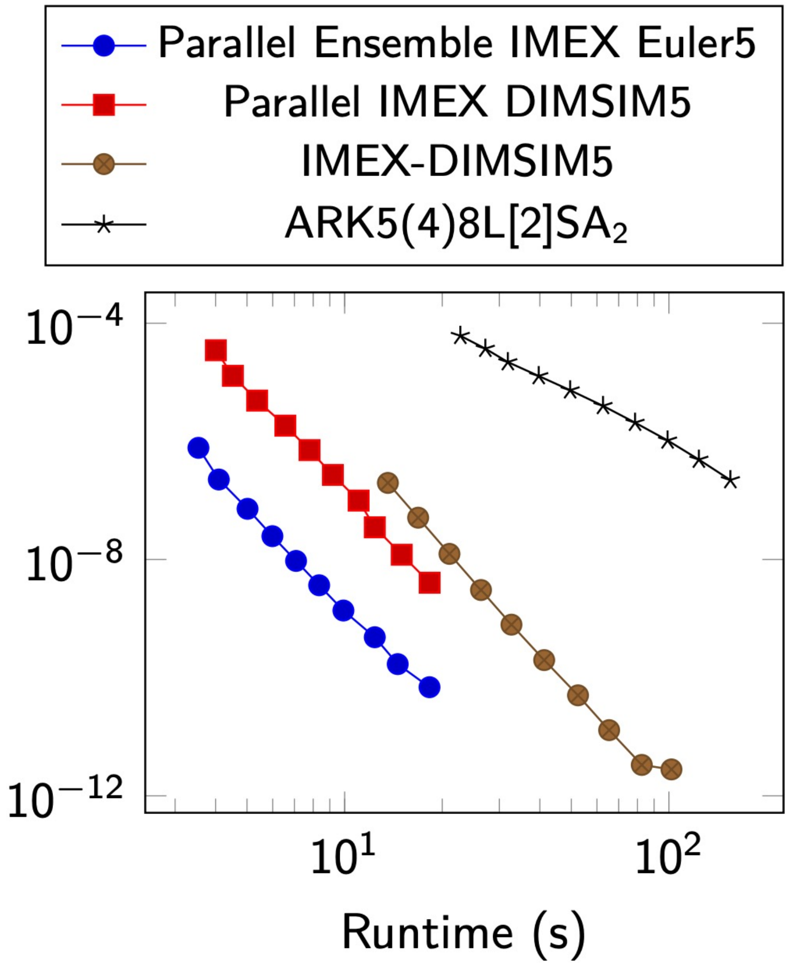
1. Alnæs, Martin, et al. "The FEniCS project version 1.5." *Archive of Numerical Software* 3.100 (2015).
2. Zhang, Hong, Adrian Sandu, and Sebastien Blaise. "High order implicit-explicit general linear methods with optimized stability regions." *SIAM Journal on Scientific Computing* 38.3 (2016): A1430-A1453.
3. Kennedy, Christopher A., and Mark H. Carpenter. "Higher-order additive Runge–Kutta schemes for ordinary differential equations." *Applied numerical mathematics* 136 (2019): 183-205.

Allen-Cahn solution



Work precision plots for 4th and 5th order IMEX methods





Conclusions

- Parallel ensemble methods provide a systematic approach to derive high-order GLMs.
- A unique simultaneous triangularization property provides a stability region that is independent of order.
- Potentially large coefficients can lead to cancelation error.
- **Parallel ensemble methods are perfect building blocks for partitioned methods.**

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Questions?

Additional info at people.llnl.gov/roberts115