Parallel implicit-explicit general linear methods

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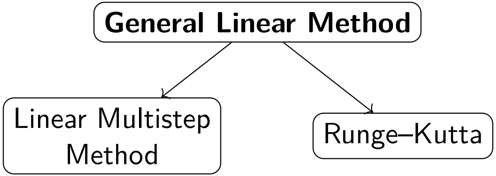
Methods for solving ordinary differential equations

- The initial value problem

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

  is a fundamental building block for time-dependent simulation of physical phenomena.
- General linear methods (GLMs) are a large family of methods that generalizes many popular time-stepping families.



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

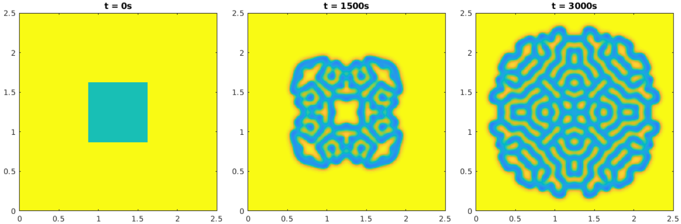
$$y_i^{[n]} = h \sum_{j=1}^{s} b_{i,j}\, f(Y_j) + \sum_{j=1}^{r} v_{i,j}\, y_j^{[n-1]}$$

Implicit-explicit methods

- Explicit methods are cheap but stability limits stepsize. Implicit methods have excellent stability but expensive (non)linear solves.
- Implicit-explicit (IMEX) methods offer a middle ground by combining both. They solve the system

$$y' = f(y) + g(y),$$

  where f is nonstiff and g is stiff.
- Examples include horizontally-explicit/vertically-implicit (HEVI) for atmospheric simulations, as well as advection-diffusion-reaction problems:



IMEX GLMs I

- One step of an implicit-explicit general linear method (IMEX GLM)[1] is given by

$$
\begin{aligned}
Y_i &= h \sum_{j=1}^{i-1} a_{i,j}\, f(Y_j) + \sum_{j=1}^{i} \widehat{a}_{i,j}\, g(Y_j) + \sum_{j=1}^{r} u_{i,j}\, y_j^{[n-1]}, && i = 1, \dots, s, \\
y_i^{[n]} &= h \sum_{j=1}^{s} \left(b_{i,j}\, f(Y_j) + \widehat{b}_{i,j}\, g(Y_j) \right) + \sum_{j=1}^{r} v_{i,j}\, y_j^{[n-1]}, && i = 1, \dots, r.
\end{aligned}
$$

- They are formed from an explicit GLM $(\mathbf{A}, \mathbf{B}, \mathbf{U}, \mathbf{V})$ and an implicit GLM $(\widehat{\mathbf{A}}, \widehat{\mathbf{B}}, \mathbf{U}, \mathbf{V})$.
- The coefficients of an IMEX GLM are represented by the Butcher tableau

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

IMEX GLMs II

- For high stage order methods, the order conditions are simple and elegant.
- High stage order makes them an excellent choice for very stiff problems, differential-algebraic equations, or whenever order reduction may be a concern.
- Ensuring IMEX GLMs have good stability at high orders is challenging.
  - Very sophisticated optimization procedures used to derive methods
  - Highest order achieved is six[2].
- Can we **systematically** construct stable, high order IMEX GLMs?

[1] Zhang, Sandu, and Blaise, "Partitioned and implicit-explicit general linear methods for ordinary differential equations".

[2] Jackiewicz and Mittelmann, "Construction of IMEX DIMSIMs of high order and stage order".

Stage parallelism for IMEX GLMs I

- A parallel IMEX GLM is formed from GLMs of type 3 and 4:

$$Y_i = \lambda\, g(Y_i) + \sum_{j=1}^{r} u_{i,j}\, y_j^{[n-1]}, \qquad i = 1, \dots, s,$$

$$y_i^{[n]} = h \sum_{j=1}^{s} \left(b_{i,j}\, f(Y_j) + \widehat{b}_{i,j}\, g(Y_j) \right) + \sum_{j=1}^{r} v_{i,j}\, y_j^{[n-1]}, \qquad i = 1, \dots, r.$$

- The tableau has the form

$$\begin{array}{c|c|c|c} \mathbf{c} & \mathbf{0}_{s\times s} & \lambda\, \mathbf{I}_{s\times s} & \mathbf{U} \\ \hline & \mathbf{B} & \widehat{\mathbf{B}} & \mathbf{V} \end{array}.$$

Stage parallelism for IMEX GLMs II

- Our investigation considers parallel IMEX GLMs with $p = q = r = s$, where p and q are the order and stage order, respectively.
- Provided $\mathbf{U}$ is invertible and the $\mathbf{c}$'s are distinct, we proved a parallel IMEX GLM is fully determined once the implicit or explicit base is fixed.
- This allowed us to easily extends Butcher's type 4 (parallel, implicit) DIMSIMs[3] into IMEX GLMs. Here is a second order method, for example:

$$
\begin{array}{c|cc|cc|cc}
0 & 0 & 0 & \lambda & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & \lambda & 0 & 1 \\
\hline
 & \frac{4\lambda-3}{4} & \frac{4\lambda-3}{4} & \frac{(2\lambda+1)(4\lambda-3)}{4} & \frac{-8\lambda^2+10\lambda-3}{4} & \frac{4\lambda-3}{2} & \frac{5-4\lambda}{2} \\
 & \frac{4\lambda-5}{4} & \frac{4\lambda+3}{4} & \frac{8\lambda^2+2\lambda-5}{4} & \frac{-8\lambda^2+6\lambda+3}{4} & \frac{4\lambda-3}{2} & \frac{5-4\lambda}{2}
\end{array}, \qquad \lambda = \frac{3-\sqrt{3}}{2}.
$$

[3] Butcher, "Order and stability of parallel methods for stiff problems".

Parallel ensemble IMEX Euler I

- The simplest IMEX scheme is IMEX Euler

$$y_n = y_{n-1} + h\,f(y_{n-1}) + h\,g(y_n),$$

  which is only first order accurate.
- Suppose we start with an ensemble of states approximating $y(t_{n-1} + c_i\,h)$ for $i = 1, \ldots, s$.
- In parallel, IMEX Euler is applied to these states to propagate them one timestep forward.
- We take linear combinations of these first order accurate solutions to build a new high order ensemble $y(t_n + c_i\,h)$ for the text timestep.
- This timestepping strategy can be represented as an IMEX GLM.

Parallel ensemble IMEX Euler II

- We give a simple way to compute method coefficients using basic matrix operations:

$$\mathbf{A} = \mathbf{0}_{s\times s}, \quad \widehat{\mathbf{A}} = \mathbf{U} = \mathbf{V} = \mathbf{I}_{s\times s}, \quad \mathbf{B} = \mathbf{C}\,\mathbf{F}\,\mathbf{C}^{-1}, \quad \widehat{\mathbf{B}} = \mathbf{C}\,\mathbf{F}\,(\mathbf{I}_{s\times s} - \mathbf{K})\,\mathbf{C}^{-1},$$

  where

$$\mathbf{C} = \begin{bmatrix} \mathbb{1}_s & \mathbf{c} & \dots & \frac{\mathbf{c}^{s-1}}{(s-1)!} \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} 1 & \frac{1}{2} & \frac{1}{6} & \dots & \frac{1}{s!} \\ & 1 & \frac{1}{2} & \dots & \frac{1}{(s-1)!} \\ & & \ddots & \ddots & \vdots \\ & & & 1 & \frac{1}{2} \\ & & & & 1 \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & & 0 & 1 \\ & & & & 0 \end{bmatrix}.$$

- This is a systematic way to generate IMEX GLMs of arbitrary order!
- Stability is essentially identical to that of the IMEX Euler.
- Unfortunately coefficients become large at very high orders which can lead to an accumulation of finite precision cancellation errors.

A third order parallel ensemble IMEX Euler method

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

Numerical experiment: Allen–Cahn

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

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

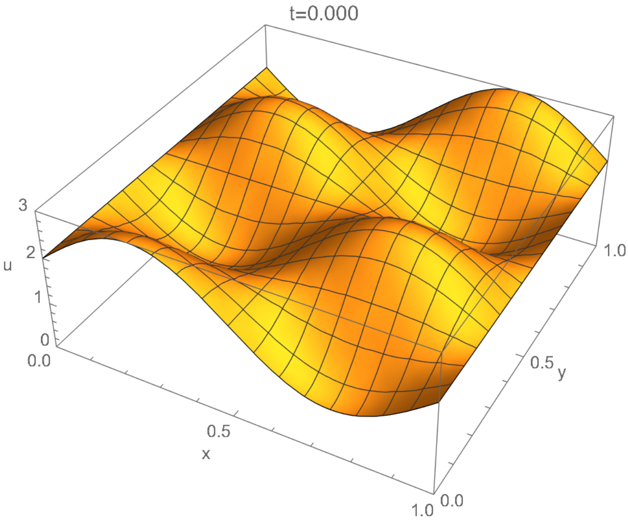
- We discretize in space with degree two, continuous finite elements on uniform, triangular mesh.
- The timing experiments use FEniCS[4] with both OpenMP and MPI parallelism.
- The fourth and fifth order the serial methods we tested against are IMEX-DIMSIM4 and IMEX-DIMSIM5 from Zhang, Sandu, and Blaise[5], as well as ARK4(3)7L[2]SA$_1$ and ARK5(4)8L[2]SA$_2$ from Kennedy and Carpenter[6].

[4] Alnæs et al., "The FEniCS Project Version 1.5".

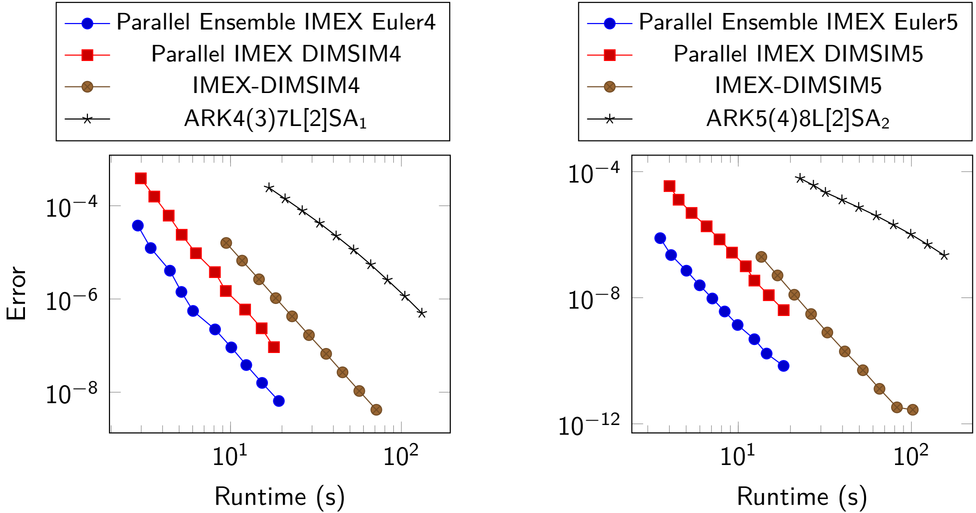
[5] Zhang, Sandu, and Blaise, "High order implicit–explicit general linear methods with optimized stability regions".

[6] Kennedy and Carpenter, "Higher-order additive Runge–Kutta schemes for ordinary differential equations".

Allen–Cahn animation



IMEX timing results for Allen–Cahn



Conclusion

- We propose a systematic approach to develop stable, high order IMEX methods.
- They are suitable for ordinary differential euqations, differential algebraic equations, and singular perturbation problems.
- Numerical experiments show parallel IMEX GLMs can outperform traditional, serial IMEX methods.

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Questions?

- Paper is avilable at `https://arxiv.org/pdf/2002.00868.pdf`
- Links to the paper and presentation are also available at `https://steven-roberts.github.io/`