Implicit-Explicit Generalized Additive Runge–Kutta Methods

Efficient high-order time discretization methods for PDEs

CASC
Center for Applied Scientific Computing

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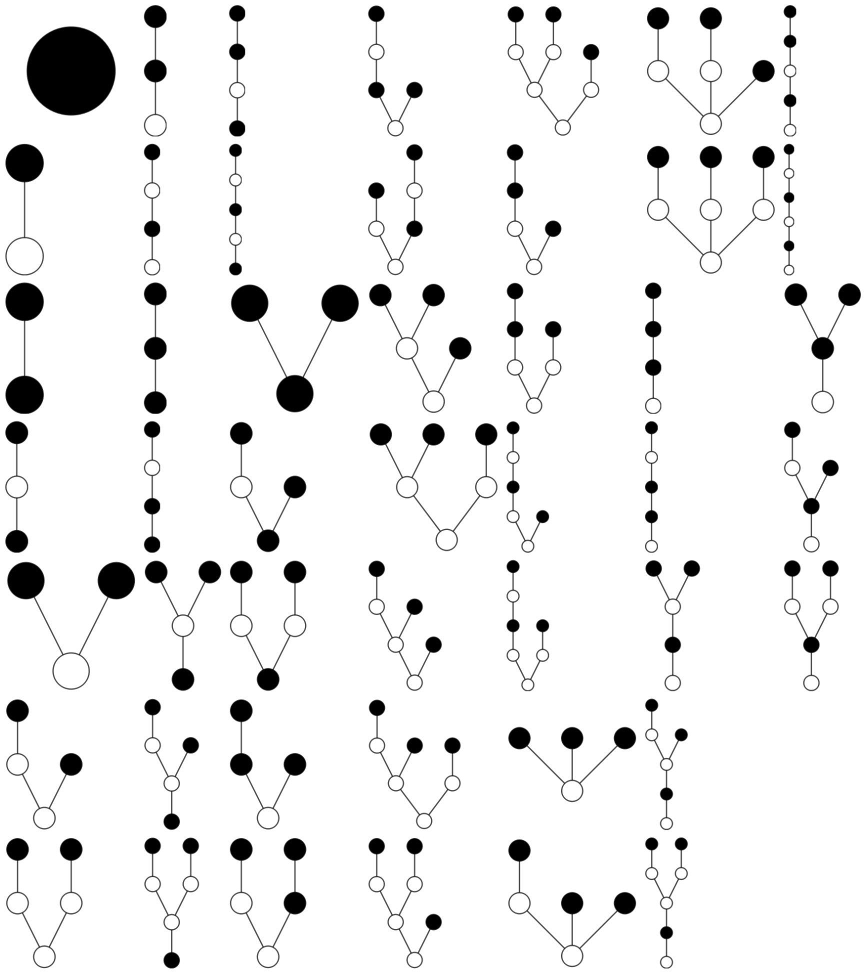
Outline

- Initial value problem and motivation
- Existing implicit-explicit Runge–Kutta frameworks
- Generalize additive Runge–Kutta
- Order conditions
- Numerical experiment
- Conclusions



Index-1 DAE trees up to order 3

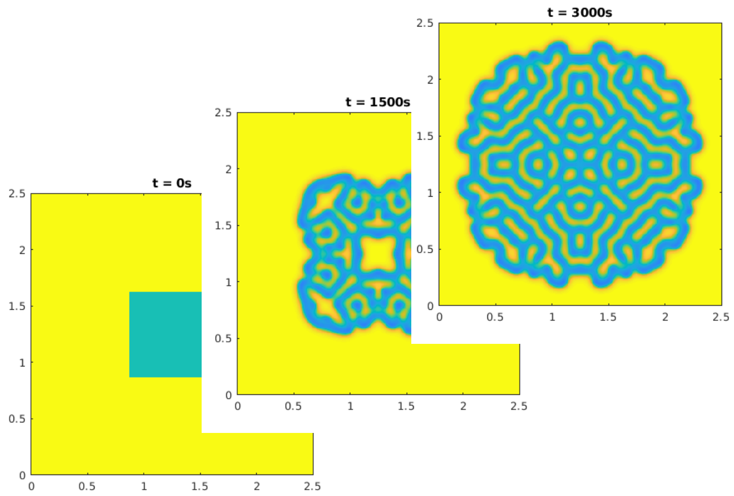
Problem Statement

- Goal: solve systems of ordinary differential equations of the form

$$y' = f^{\{E\}}(y) + f^{\{I\}}(y), \quad y(t_0) = y_0, \quad t \in [t_0, t_f]$$

  where $f^{\{E\}}(y)$ is nonstiff and $f^{\{I\}}(y)$ is stiff.

- Problems of this form arise in
  - Advection-diffusion-reaction systems
  - Atmospheric modeling[1]
  - Core-collapse supernova[2]
  - Cardiac electrical activity[3]



1. Gardner, David J., et al. "Implicit–explicit (IMEX) Runge–Kutta methods for non-hydrostatic atmospheric models." Geoscientific Model Development 11.4 (2018): 1497-1515.
2. Laiu, M. Paul, et al. "A DG-IMEX method for two-moment neutrino transport: Nonlinear solvers for neutrino–matter coupling." The Astrophysical Journal Supplement Series 253.2 (2021): 52.
3. Spiteri, Raymond J., and Ryan C. Dean. "On the performance of an implicit–explicit Runge--Kutta method in models of cardiac electrical activity." IEEE Transactions on Biomedical Engineering 55.5 (2008): 1488-1495.

Implicit-Explicit Runge–Kutta

- Implicit-explicit (IMEX) methods treat $f^{\{E\}}(y)$ explicitly and $f^{\{I\}}(y)$ implicitly.
- Limit costly implicit solves only to $f^{\{I\}}(y)$.
- Runge–Kutta-based IMEX methods combine an explicit and diagonally implicit method.

$$
\begin{array}{c|cccc}
c_1^{\{E\}} & 0 & & & \\
c_2^{\{E\}} & a_{2,1}^{\{E\}} & 0 & & \\
\vdots & \vdots & \ddots & \ddots & \\
c_s^{\{E\}} & a_{s,1}^{\{E\}} & \cdots & a_{s,s-1}^{\{E\}} & 0 \\
\hline
 & b_1^{\{E\}} & \cdots & b_{s-1}^{\{E\}} & b_s^{\{E\}}
\end{array}
\qquad
\begin{array}{c|cccc}
c_1^{\{I\}} & a_{1,1}^{\{I\}} & & & \\
c_2^{\{I\}} & a_{2,1}^{\{I\}} & a_{2,2}^{\{I\}} & & \\
\vdots & \vdots & \ddots & \ddots & \\
c_s^{\{I\}} & a_{s,1}^{\{I\}} & \cdots & a_{s,s-1}^{\{I\}} & a_{s,s}^{\{I\}} \\
\hline
 & b_1^{\{I\}} & \cdots & b_{s-1}^{\{I\}} & b_s^{\{I\}}
\end{array}
$$

Primary Frameworks for Implicit-Explicit Runge–Kutta Methods

Additive Runge–Kutta (ARK)[1]

$$Y_i = y_n + h \sum_{j=1}^{i-1} a_{i,j}^{\{E\}} f^{\{E\}}(Y_j) + h \sum_{j=1}^{i} a_{i,j}^{\{I\}} f^{\{I\}}(Y_j)$$

$$y_{n+1} = y_n + h \sum_{j=1}^{s} b_j^{\{E\}} f^{\{E\}}(Y_j) + h \sum_{j=1}^{s} b_j^{\{I\}} f^{\{I\}}(Y_j)$$

Additive Semi-Implicit Runge–Kutta (ASIRK)[2]

$$Y_i^{\{E\}} = y_n + h \sum_{j=1}^{i-1} a_{i,j}^{\{E\}} f^{\{E\}}\left(Y_j^{\{E\}}\right) + h \sum_{j=1}^{i-1} a_{i,j}^{\{E\}} f^{\{I\}}\left(Y_j^{\{I\}}\right)$$

$$Y_i^{\{I\}} = y_n + h \sum_{j=1}^{i} a_{i,j}^{\{I\}} f^{\{E\}}\left(Y_j^{\{E\}}\right) + h \sum_{j=1}^{i} a_{i,j}^{\{I\}} f^{\{I\}}\left(Y_j^{\{I\}}\right)$$

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

1. Cooper, G. J., and Ali Sayfy. "Additive methods for the numerical solution of ordinary differential equations." *Mathematics of Computation* 35.152 (1980): 1159-1172.
2. Zhong, Xiaolin. "Additive semi-implicit Runge–Kutta methods for computing high-speed nonequilibrium reactive flows." *Journal of Computational Physics* 128.1 (1996): 19-31.

Primary Frameworks for Implicit-Explicit Runge–Kutta Methods

Additive Runge–Kutta (ARK)

$$k_i^E = h\, f^{\{E\}}\left(y_n + \sum_{j=1}^{i-1} a_{i,j}^{\{E\}} k_j^{\{E\}} + \sum_{j=1}^{i} a_{i,j}^{\{I\}} k_j^{\{I\}}\right)$$

$$k_i^I = h\, f^{\{I\}}\left(y_n + \sum_{j=1}^{i-1} a_{i,j}^{\{E\}} k_j^{\{E\}} + \sum_{j=1}^{i} a_{i,j}^{\{I\}} k_j^{\{I\}}\right)$$

$$y_{n+1} = y_n + \sum_{j=1}^{s} b_j^{\{E\}} k_j^{\{E\}} + h \sum_{j=1}^{s} b_j^{\{I\}} k_j^{\{I\}}$$

Additive Semi-Implicit Runge–Kutta (ASIRK)

$$k_i^E = h\, f^{\{E\}}\left(y_n + \sum_{j=1}^{i-1} a_{i,j}^{\{E\}} k_j^{\{E\}} + \sum_{j=1}^{i-1} a_{i,j}^{\{E\}} k_j^{\{I\}}\right)$$

$$k_i^I = h\, f^{\{I\}}\left(y_n + \sum_{j=1}^{i} a_{i,j}^{\{I\}} k_j^{\{E\}} + \sum_{j=1}^{i} a_{i,j}^{\{I\}} k_j^{\{I\}}\right)$$

$$y_{n+1} = y_n + \sum_{j=1}^{s} b_j k_j^{\{E\}} + h \sum_{j=1}^{s} b_j k_j^{\{I\}}$$

Certain coefficients are duplicated. Why not utilize all four “A” coefficients?

Limitations of Current IMEX Frameworks

- The implicit and explicit methods must have equal number of stages.
- Simplifying assumptions and order conditions such as

$$b^{\{E\}} = b^{\{I\}}, \qquad c^{\{E\}} = c^{\{I\}}, \qquad b^{\{I\}} A^{\{I\}} A^{\{E\}} c^{\{E\}} = \frac{1}{24}$$

  tightly couple base methods.
- Rarely can ”optimal” base methods be combined to form a high-order IMEX scheme.
- Existing IMEX methods are reaching limits for optimizations.
  - “it is unclear how these two methods could be substantially improved.” — Kennedy and Carptenter[1]

1. Kennedy, Christopher A., and Mark H. Carpenter. "Higher-order additive Runge–Kutta schemes for ordinary differential equations." *Applied numerical mathematics* 136 (2019): 183-205.

Generalized Additive Runge-Kutta

- A generalized additive Runge–Kutta (GARK)[1] method applied to our ODE reads

$$Y_i^{\{E\}} = y_n + h \sum_{j=1}^{s^{\{E\}}} a_{i,j}^{\{E,E\}} f^{\{E\}}\left(Y_j^{\{E\}}\right) + h \sum_{j=1}^{s^{\{I\}}} a_{i,j}^{\{E,I\}} f^{\{I\}}\left(Y_j^{\{I\}}\right)$$

$$Y_i^{\{I\}} = y_n + h \sum_{j=1}^{s^{\{E\}}} a_{i,j}^{\{I,E\}} f^{\{E\}}\left(Y_j^{\{E\}}\right) + h \sum_{j=1}^{s^{\{I\}}} a_{i,j}^{\{I,I\}} f^{\{I\}}\left(Y_j^{\{I\}}\right)$$

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

$A^{\{E,E\}}$	$A^{\{E,I\}}$
$A^{\{I,E\}}$	$A^{\{I,I\}}$
${b^{\{E\}}}^T$	${b^{\{I\}}}^T$

- There are 4 "A" coefficient matrices defining the method.
  - Implicit and explicit methods can have a different number of stages.
  - Diagonal matrices specify base method and off-diagonal specify coupling.

1. Sandu, Adrian, and Michael Günther. "A generalized-structure approach to additive Runge-Kutta methods." *SIAM Journal on Numerical Analysis* 53.1 (2015): 17-42.

Primary Frameworks for Implicit-Explicit Runge–Kutta Methods

Additive Runge–Kutta (ARK)

$$Y_i = y_n + h\sum_{j=1}^{i-1} a_{i,j}^{\{E\}} f^{\{E\}}(Y_j) + h\sum_{j=1}^{i} a_{i,j}^{\{I\}} f^{\{I\}}(Y_j)$$

$$y_{n+1} = y_n + h\sum_{j=1}^{s} b_j^{\{E\}} f^{\{E\}}(Y_j) + h\sum_{j=1}^{s} b_j^{\{I\}} f^{\{I\}}(Y_j)$$

$A^{\{E\}}$	$A^{\{I\}}$
$A^{\{E\}}$	$A^{\{I\}}$
${b^{\{E\}}}^T$	${b^{\{I\}}}^T$

Additive Semi-Implicit Runge–Kutta (ASIRK)

$$Y_i^{\{E\}} = y_n + h\sum_{j=1}^{i-1} a_{i,j}^{\{E\}} f^{\{E\}}\left(Y_j^{\{E\}}\right) + h\sum_{j=1}^{i-1} a_{i,j}^{\{E\}} f^{\{I\}}\left(Y_j^{\{I\}}\right)$$

$$Y_i^{\{I\}} = y_n + h\sum_{j=1}^{i} a_{i,j}^{\{I\}} f^{\{E\}}\left(Y_j^{\{E\}}\right) + h\sum_{j=1}^{i} a_{i,j}^{\{I\}} f^{\{I\}}\left(Y_j^{\{I\}}\right)$$

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

$A^{\{E\}}$	$A^{\{E\}}$
$A^{\{I\}}$	$A^{\{I\}}$
b^T	b^T

Example IMEX GARK Method

- Third order accurate
- 3 stage explicit method
- 2 stage SDIRK method
- No padding required
- Simple but not very optimized

$$
\begin{array}{ccc|cc}
0 & 0 & 0 & 0 & 0 \\
\frac{1}{2} & 0 & 0 & \frac{1}{2} & 0 \\
0 & \frac{3}{4} & 0 & -\frac{3}{16}\left(-1+\sqrt{3}\right) & \frac{3}{16}\left(3+\sqrt{3}\right) \\
\hline
\frac{1}{6}\left(3+\sqrt{3}\right) & 0 & 0 & \frac{1}{6}\left(3+\sqrt{3}\right) & 0 \\
\frac{1}{6}\left(-1-\sqrt{3}\right) & \frac{2}{3} & 0 & -\frac{1}{\sqrt{3}} & \frac{1}{6}\left(3+\sqrt{3}\right) \\
\hline
\frac{2}{9} & \frac{1}{3} & \frac{4}{9} & \frac{1}{2} & \frac{1}{2}
\end{array}
$$

Deriving IMEX GARK Methods

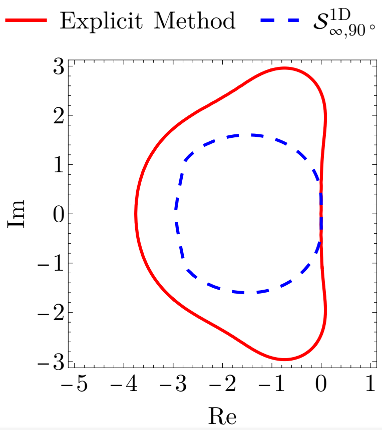
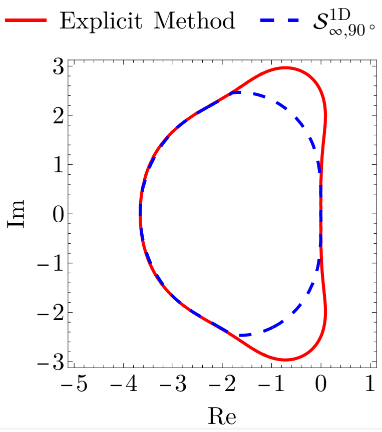
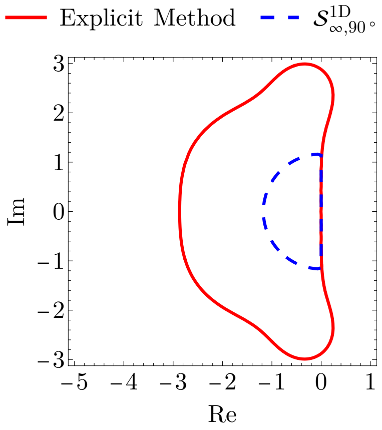
- Pick optimized base methods and solve for coupling coefficients.
- Order conditions for ODEs and index-1 DAEs come from tree-based theory.
  - Same number of trees as ARK or ASIRK methods.
  - Use simplifying assumptions like internal consistency.
  - Stiffly accurate methods are well-suited to DAEs.
- Free parameters were used to optimize stability and principal error.
- Over 30 method properties considered!

Order	ODE	Index-1 DAE
1	$b^{\{E\}}\mathbb{1} = 1$ $b^{\{I\}}\mathbb{1} = 1$	$b^{\{E\}}\mathbb{1} = 1$ $b^{\{I\}}{A^{\{I,I\}}}^{-1}A^{\{I,E\}}\mathbb{1} = 1$
2	$b^{\{E\}}A^{\{E,I\}}\mathbb{1} = 1$ $\vdots$	$b^{\{I\}}{A^{\{I,I\}}}^{-1}\left(A^{\{I,E\}}\mathbb{1}\right)^2 = 1$ $\vdots$
3	14 Conditions	38 Conditions
4	52 Conditions	242 Conditions
5	214 Conditions	1698 Conditions

GARK3(2)55L[2]DAE: A Third Order IMEX GARK Method

$$
\begin{array}{ccccc|ccccc}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{3} & 0 & 0 & 0 & 0 & \frac{1}{6} & \frac{1}{6} & 0 & 0 & 0 \\
0 & \frac{2}{3} & 0 & 0 & 0 & \frac{8-3\sqrt{2}}{15} & \frac{8-3\sqrt{2}}{15} & \frac{2(\sqrt{2}-1)}{5} & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & \frac{743-131\sqrt{2}}{1890} & \frac{743-131\sqrt{2}}{1890} & \frac{131(\sqrt{2}-1)}{945} & \frac{37}{105} & 0 \\
\frac{1}{8} & \frac{3}{8} & \frac{3}{8} & \frac{1}{8} & 0 & \frac{1187\sqrt{2}-1181}{2835} & \frac{1187\sqrt{2}-1181}{2835} & \frac{2374(1-\sqrt{2})}{2835} & \frac{5827}{7560} & \frac{9}{40} \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{9}{20} & 0 & 0 & 0 & 0 & \frac{9}{40} & \frac{9}{40} & 0 & 0 & 0 \\
\frac{9(52-271\sqrt{2})}{12920} & \frac{2673(\sqrt{2}+1)}{6460} & 0 & 0 & 0 & \frac{9(\sqrt{2}+1)}{80} & \frac{9(\sqrt{2}+1)}{80} & \frac{9}{40} & 0 & 0 \\
-\frac{881835}{7528484} & \frac{7282818}{9410605} & -\frac{1323}{23308} & 0 & 0 & \frac{7\sqrt{2}+8}{80} & \frac{7\sqrt{2}+8}{80} & \frac{7(1-\sqrt{2})}{40} & \frac{9}{40} & 0 \\
\frac{1}{8} & \frac{3}{8} & \frac{3}{8} & \frac{1}{8} & 0 & \frac{1187\sqrt{2}-1181}{2835} & \frac{1187\sqrt{2}-1181}{2835} & \frac{2374(1-\sqrt{2})}{2835} & \frac{5827}{7560} & \frac{9}{40} \\
\hline
\frac{1}{8} & \frac{3}{8} & \frac{3}{8} & \frac{1}{8} & 0 & \frac{1187\sqrt{2}-1181}{2835} & \frac{1187\sqrt{2}-1181}{2835} & \frac{2374(1-\sqrt{2})}{2835} & \frac{5827}{7560} & \frac{9}{40} \\
\hline
-\frac{391709805}{8420574392} & \frac{5377304043}{8420574392} & \frac{98431707}{271631432} & \frac{5507}{46616} & -\frac{9}{124} & \frac{5547709\sqrt{2}-4800247}{16519545} & \frac{5547709\sqrt{2}-4800247}{16519545} & \frac{11095418(1-\sqrt{2})}{16519545} & \frac{30698249}{44052120} & \frac{49563}{233080}
\end{array}
$$

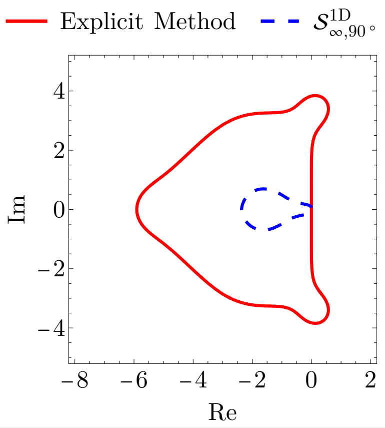
Comparison of 3rd Order IMEX Methods

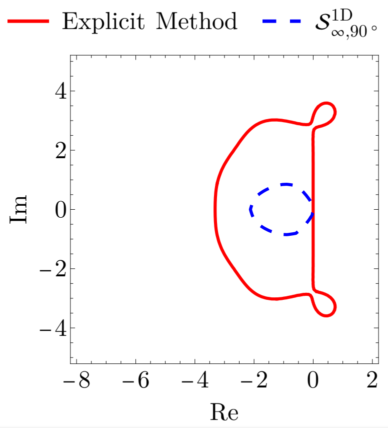
Method	**GARK3(2)55L[2]SA**	ARK3(2)4L[2]SA	BHR(5,5,3)
Info	Method from previous slide	Kennedy, Christopher A., and Mark H. Carpenter. "Additive Runge–Kutta schemes for convection–diffusion–reaction equations." *Applied numerical mathematics* 44.1-2 (2003): 139-181.	Boscarino, Sebastiano. "On an accurate third order implicit-explicit Runge–Kutta method for stiff problems." *Applied Numerical Mathematics* 59.7 (2009): 1515-1528.
Stages	5 (but with FSAL)	4	5
ODE Order	3	3	3
DAE Order	3	2	3
Principal Error	**0.051**	0.166	0.200
Stability Region			

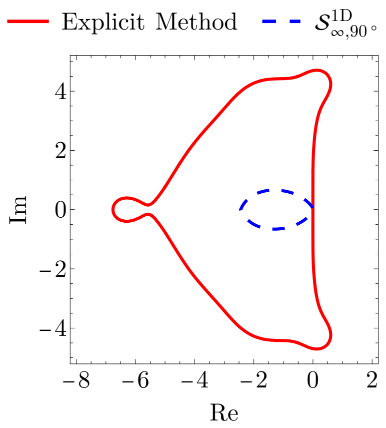
Comparison of 4^{th} Order IMEX Methods

Method	**GARK4(3)77L[2]SA**	**ARK4(3)8L[2]DAE**	ARK4(3)7L[2]SA$_1$
Info	New GARK Method	New ARK for DAEs	Kennedy, Christopher A., and Mark H. Carpenter. "Higher-order additive Runge–Kutta schemes for ordinary differential equations." *Applied numerical mathematics* 136 (2019): 183-205.
Stages	7 (but with FSAL)	4 (but with FSAL)	7
ODE Order	4	4	4
DAE Order	2	**4**	3
Principal Error	0.00792	**0.00641**	0.01112

Stability Region





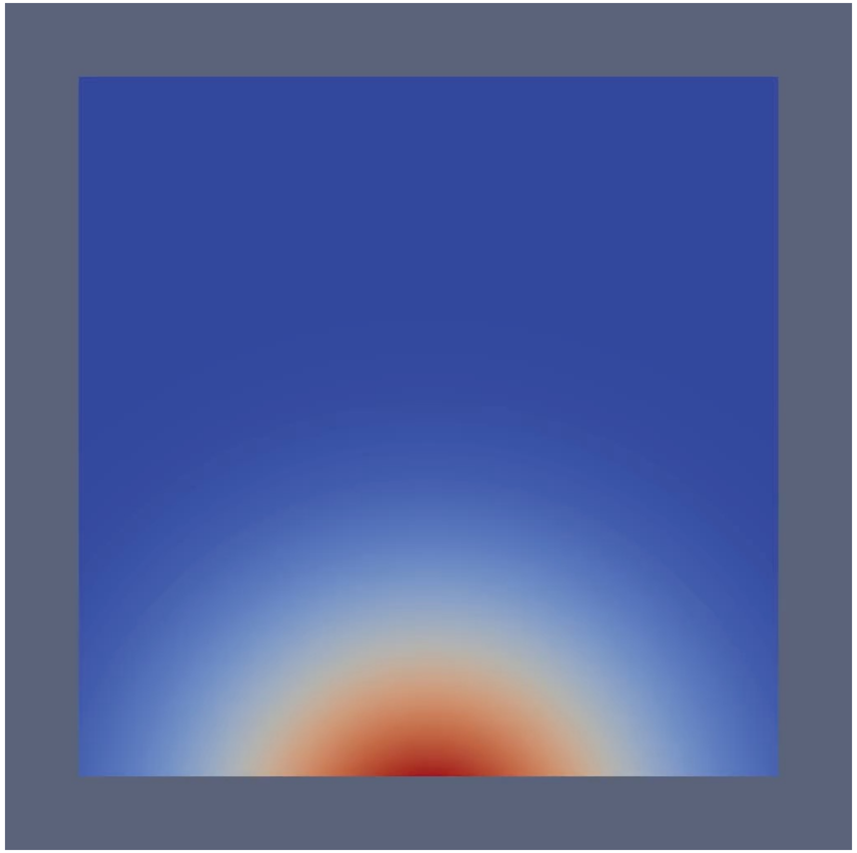


Numerical Experiment: BSVD

- We will test IMEX methods on the BSVD reaction-diffusion PDE[1]

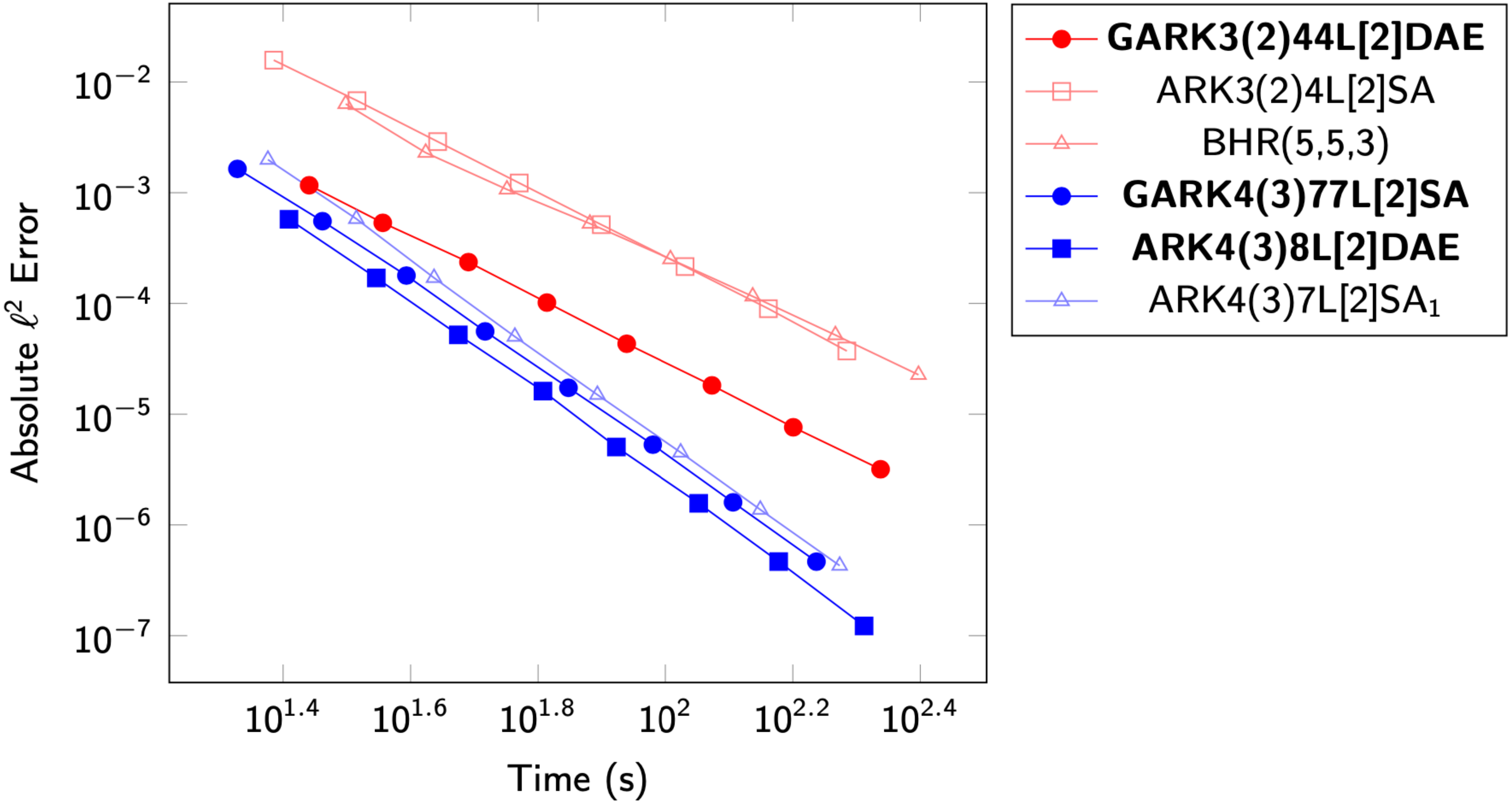
$$\frac{\partial u}{\partial t} = \nabla \cdot (D(x,y)\nabla \mathrm{u}) + 10(1 - \mathrm{u}^2)(\mathrm{u} + 0.6)$$

- Space-dependent diffusion term
- FEnicS used for finite element spatial discretization
- 100×100 quadrilateral mesh



1. Heineken, Wolfram, and Gerald Warnecke. "Partitioning methods for reaction–diffusion problems." *Applied numerical mathematics* 56.7 (2006): 981-1000.

Work-Precision Results for BSVD Problem



Conclusions

- The GARK framework is a more natural representation of IMEX methods.
- "Hidden" coupling coefficients are revealed.
- New IMEX GARK methods of order 3 and 4 have smaller error constants than highly-optimized ARK methods.
- Future work
  - Improving 4^{th} order methods
  - Deriving 5^{th} order methods?

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Questions?

Additional info at people.llnl.gov/roberts115