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A Family of Second and Third Order Implicit-explicit Runge-Kutta Methods for Stiff Time-dependent Partial Differential Equations[1]

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Partitioned time-stepping

Want to solve initial value problems (IVPs) of

$$u_t = \underbrace{n(u,t)}_{\text{nonstiff terms}} + \underbrace{s(u,t)}_{\text{stiff terms}}, \quad \begin{bmatrix} v_t \\ w_t \end{bmatrix} = \begin{bmatrix} n(v,w,t) \\ s(v,w,t) \end{bmatrix}$$

- Implicit-explicit, partitioned, multi-rate, exponential Rosenbrock, etc (Sorry if your favorite isn't mentioned!).
- Efficiency balance: Large (and accurate) stable time-steps with cost/time-step.
- Analysis is trickier: partitioned $>$ implicit $>$ explicit ?

Additive and IMEX Runge-Kutta methods

$$\dot{u} = \underbrace{n(u,t)}_{\text{nonstiff terms}} + \underbrace{s(u,t)}_{\text{stiff terms}}, \quad u(t_0) = u_0.$$

An r-stage additive Runge-Kutta (RK) method with time step $\Delta t > 0$, $i = 1, \dots, r$:

$$u_{m+1} = u_m + \Delta t \sum_{j=1}^{r} \left(b_j n(g_{m,j}, t_m + \Delta t c_j) + \hat{b}_j s(g_{m,j}, t_m + \Delta t \hat{c}_j) \right)$$

$$g_{m,i} = u_m + \Delta t \sum_{j=1}^{r} \left(A_{i,j} n(g_{m,j}, t_m + \Delta t c_j) + \hat{A}_{i,j} s(g_{m,j}, t_m + \Delta t \hat{c}_j) \right)$$

Methods are represented using a double Butcher tableau:

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

The additive RK method is an IMEX RK method if one of the tables is implicit and the other is explicit.

IMKG methods

$$
\begin{array}{c|ccccc}
0 & & & & & \\
c_1 & a_1 & & & & \\
\vdots & b_1 & \ddots & & & \\
 & \vdots & & a_{s-2} & & \\
 & & & & a_{s-1} & \\
c_s & b_{s-1} & & & & a_s \\
\hline
 & b_{s-1} & & & & a_s
\end{array}
\qquad
\begin{array}{c|ccccc}
0 & & & & & \\
\hat{c}_1 & \hat{a}_1 & \hat{d}_1 & & & \\
\vdots & \hat{b}_2 & \ddots & \ddots & & \\
 & \vdots & & \hat{a}_{s-2} & \hat{d}_{s-2} & \\
 & & & & \hat{a}_{s-1} & \hat{d}_{s-1} \\
\hat{c}_s & \hat{b}_{s-1} & & & & \hat{a}_s \\
\hline
 & \hat{b}_{s-1} & & & & \hat{a}_s
\end{array}
$$

- IMKG2 methods (second order) have $b_j \equiv \hat{b}_j \equiv 0$, IMKG3 methods (third order) must have at least $b_{s-1}, \hat{b}_{s-1} \neq 0$ and $\hat{b}_j \equiv b_j$.[2]
- Explicit method has Kinnmark and Gray optimal[3]/near-optimal[4] stability on the imaginary axis, implicit method is I-stable.
- Explicit method is unique up to definition of $b_i \equiv \hat{b}_i$.

[2] A. Steyer, C. Vogl, M. Taylor, and O. Guba, *Efficient IMEX Runge-Kutta methods for nonhydrostatic dynamics.* In review. To appear on Arxiv.

[3] I. Kinnmark and W. Gray, *One step integration methods with maximum stability regions*, Math. Comput. Simulation, XXVI (1984), pp. 84-92.

[4] I. Kinnmark and W. Gray, *One step integration methods with third-fourth order accuracy with large hyperbolic stability limits*, Math. Comput. Simulation, XXVI (1984), pp. 101-108.

Accuracy

3rd order accuracy requires satisfaction of 22 equations:

$$\begin{cases} b^{\mathsf{T}}\mathbf{1}_{q+1} = 1 = \hat{b}^{\mathsf{T}}\mathbf{1}_{q+1}, \quad b^{\mathsf{T}}c = b^{\mathsf{T}}\hat{c} = \hat{b}^{\mathsf{T}}\hat{c} = \hat{b}^{\mathsf{T}}c = 1/2, \\ b^{\mathsf{T}}Ac = b^{\mathsf{T}}A\hat{c} = b^{\mathsf{T}}\hat{A}c = b^{\mathsf{T}}\hat{A}\hat{c} = \hat{b}^{\mathsf{T}}Ac = \hat{b}^{\mathsf{T}}A\hat{c} = \hat{b}^{\mathsf{T}}\hat{A}c = \hat{b}^{\mathsf{T}}\hat{A}\hat{c} = 1/6, \\ b^{\mathsf{T}}Cc = b^{\mathsf{T}}C\hat{c} = b^{\mathsf{T}}\hat{C}c = b^{\mathsf{T}}\hat{C}\hat{c} = \hat{b}^{\mathsf{T}}Cc = \hat{b}^{\mathsf{T}}C\hat{c} = \hat{b}^{\mathsf{T}}\hat{C}c = \hat{b}^{\mathsf{T}}\hat{C}\hat{c} = 1/3. \end{cases}$$

For IMKG3 methods this is equivalent to 8 or so equations:

$$a_q = 3/4 = \hat{a}_q, \quad b_{q-1} = 1/4 = \hat{b}_{q-1}$$

$$b_{q-1} + a_q = 1 = \hat{b}_{q-1} + \hat{a}_q$$

$$\hat{a}_{q-1} + \hat{d}_{q-1} + \hat{b}_{q-2} = 2/3 = a_{q-1} + b_{q-2},$$

$${}_{q-1}(\hat{a}_{q-2} + \hat{d}_{q-2} + \hat{b}_{q-3}) = 2/9 = a_{q-1}(a_{q-2} + b_{q-3}),$$

$$\hat{a}_{q-1}(\hat{a}_{q-2} + \hat{d}_{q-2} + \hat{b}_{q-3}) + \tfrac{2}{3}\hat{d}_{q-1} = 2/9 = \hat{a}_{q-1}(a_{q-2} + b_{q-3}) + \tfrac{2}{3}\hat{d}_{q-1}.$$

What's the point? Simplified conditions for accuracy free up coefficients to optimize coupled stability properties.

Deriving methods

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- We focus on deriving methods for atmosphere models.
- Not worried about conservation or find methods that are SSP or TVD.
- Stability $>$ Accuracy : require with a fast time-to-solution.
- Derive many methods to experiment with balances in number of explicit stages and implicit solves.
- Stability: Focus on coupled IMEX stability (good IM and EX stability necessary but not sufficient).

E3SM-HOMME aka HOMME-NH

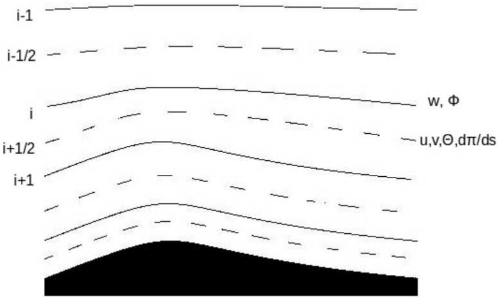
Laprise-like formulation[5] of primitive equations:

$$\begin{cases} \frac{Du}{Dt} + \text{coriolis terms} + \frac{1}{\rho}\nabla p = 0 \\ \frac{Dw}{Dt} + g + \frac{1}{\rho}\frac{\partial p}{\partial z} = 0 \\ \frac{D\phi}{Dt} - gw = 0, \quad \phi = gz \\ \frac{\partial \Theta}{\partial t} + \nabla \cdot (\Theta \mathbf{u}) = 0, \quad \Theta = c_p \frac{\partial \pi}{\partial \eta}\theta_v \\ \frac{\partial}{\partial t}\left(\frac{\partial \pi}{\partial \eta}\right) + \nabla \cdot \left(\frac{\partial \pi}{\partial \eta}\,\mathbf{u}\right) = 0 \end{cases}$$

$\mathbf{u} = (u, v)^T$ – horiz. vel. ϕ – geopotential π – hydrostatic press.
w – vert. vel. g – grav. constant c_p^* – thermo. constant
θ – potential temperature

[5] R. Laprise, *The Euler equations of motion with hydrostatic pressure as an independent variable*, Mon. Wea. Rev., 102 (1992), pp. 197-207.

Spatial discretization



- Horizontal: 4th order mimetic spectral elements on cubed sphere[6] .
- Vertical: 2nd order mimetic SB81 with Lorenz staggering[7].
- Terrain following hydrostatic pressure vertical coordinate coordinate.

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[6] M. Taylor and A. Fournier, *A compatible and conservative spectral element method on unstructured grids*, J. Comput. Phys., 229 (2010), pp. 5879-5895.

[7] A. Simmons and D. Burridge, *An Energy and Angular-Momentum Conserving Vertical Finite-Difference Scheme and Hybrid Vertical Coordinates*, Mon. Wea. Rev., 109 (1981), pp. 758-766.

HOMME-NH HEVI IMEX splitting

$$
\begin{cases}
\frac{D\mathbf{u}}{Dt} + \text{coriolis terms} + \frac{1}{\rho}\nabla p = 0 \\
\frac{Dw}{Dt} + \boxed{g(1-\mu)} = 0, \quad \mu = \frac{\partial p/\partial \eta}{\partial \pi/\partial \eta} \\
\frac{D\phi}{Dt} + \boxed{-gw} = 0, \quad \phi = gz \\
\frac{\partial \Theta}{\partial t} + \nabla \cdot (\Theta \mathbf{u}) = 0, \quad \Theta = c_p \frac{\partial \pi}{\partial \eta}\theta_v \\
\frac{\partial}{\partial t}\left(\frac{\partial \pi}{\partial \eta}\right) + \nabla \cdot \left(\frac{\partial \pi}{\partial \eta}\right) = 0
\end{cases}
$$

Boxed terms above are the implicitly treated terms: so-called HEVI splitting. Summer student (Cassidy Krause, U. of Kansas) will use this splitting as basis for exponential Rosenbrock methods.

HEVI and fast-slow wave Stability

Test equation for HEVI or fast-wave-slow-wave IMEX splitting[8] [9] :

$$\dot{u} = -ik_x N u - ik_z N u, \quad N = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \mathcal{S} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

k_x and k_z are horizontal and vertical wave numbers.

$$u_{m+1} = R_H(\Delta t k_x, \Delta t k_z) u_m, \qquad \text{IMEX RK solution}$$

HEVI or H-stability region:

$\mathcal{S}_H := \{(x, z)$: eigenvalues of $R_H(x, y)$ all have modulus at most 1$\}$.

Use to determine stability at various aspect ratios k_z/k_x.

[8] D. Durran and P. Blossey, *Implicit-explicit multistep methods for fast-wave-slow-wave problems.* Mon. Weather Rev., pp. 1307-1325.

[9] H. Weller, S.-J. Lock, and N. Wood, *Numerical analyses of Runge-Kutta implicit-explicit schemes for horizontally explicit, vertically implicit solutions of atmospheric models.* Q. J. Roy. Meteor. Soc., pp. 1654-1669.

H-stability regions of IMKG232a-b

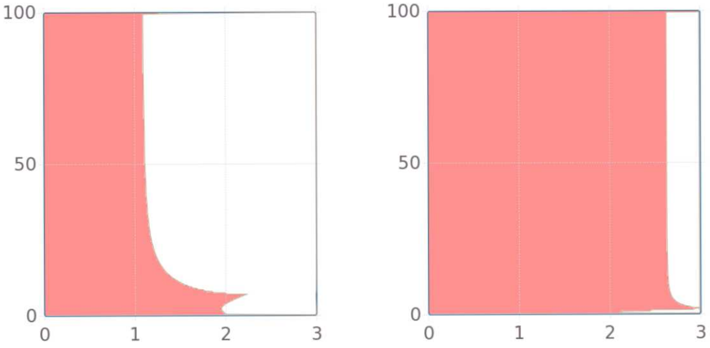


Figure: H-stability regions (z vs x where shaded area denotes stability) of the IMKG232a (left) and IMKG232b (right) methods.

Maximum usable time-step

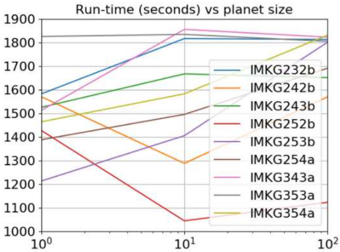
All IMEX methods implemented with HOMME-ARKode interface: Thanks Chris Vogl, Carol Woodward, David Gardner (LLNL) and also Dan Reynolds (SMU)!

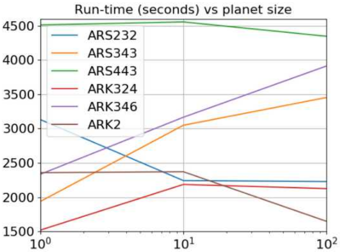
IMKG	232a	232b	242a	242b	243a	252a	253a	254a	254b	342a	343a	353a	354a
100	100	200	175	225	275	275	375	375	150	75	275	250	350
10	10	17.5	17.5	27.5	27.5	37.5	32.5	35	15	22.5	22.5	25	32.5
1	1.75	1.75	2.25	2.5	2.5	3.5	2.5	3.0	2.25	2.25	2.25	2.5	2.75

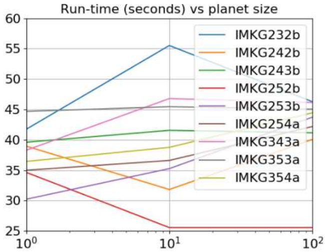
Method	KGU35	KGU35(H)	ARS232	ARS343	ARS443	ARK2	ARK324	ARK346
100	0.75	375	125	275	175	125	250	275
10	0.75	37.5	12.5	17.5	15	12.5	17.5	20
1	0.75	3.75	1.75	1.5	1.75	1.75	1.75	1.5

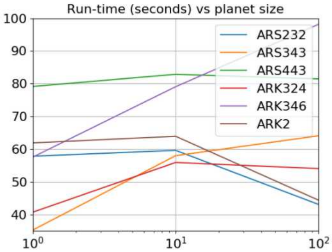
Table: Maximum usable step-sizes for various IMKG2-3, non-IMKG methods, the KGU35 explicit method, and the KGU35 method running in hydrostatic mode (KGU35(H)) with $ne = 30$, 30 vertical levels, and aspect ratios (vertical/horizontal) 100, 10, and 1. Solver tolerances 10^{-12}

Time trials


Run-time (seconds) vs planet size
1900
1800
1700
1600
1500
1400
1300
1200
1100
1000
10^0
10^1
10^2
IMKG232b
IMKG242b
IMKG243b
IMKG252b
IMKG253b
IMKG254a
IMKG343a
IMKG353a
IMKG354a


Run-time (seconds) vs planet size
4500
4000
3500
3000
2500
2000
1500
10^0
10^1
10^2
ARS232
ARS343
ARS443
ARK324
ARK346
ARK2


Run-time (seconds) vs planet size
60
55
50
45
40
35
30
25
10^0
10^1
10^2
IMKG232b
IMKG242b
IMKG243b
IMKG252b
IMKG253b
IMKG254a
IMKG343a
IMKG353a
IMKG354a


Run-time (seconds) vs planet size
100
90
80
70
60
50
40
10^0
10^1
10^2
ARS232
ARS343
ARS443
ARK324
ARK346
ARK2

Thanks!

Questions????