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Efficient IMEX Runge-Kutta integrators for the HOMME-NH dycore

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Context

- E3SM atm. hydrostatic (nonstiff, HE) → nonhydrostatic (stiff, HEVI).
- Horizontally explicit, vertically implicit (HEVI).
- Climate: atmosphere model runs close to CFL stability limit to chug through rather lengthy simulations.
- Need flexible methods for range resolutions and vert.-to-hor. aspect ratios.
- Purely imaginary eigenvalues. Want IMEX version of the KGU35 3rd order explicit Runge-Kutta (RK) method [1,2] :

$$
\begin{array}{c|ccccc}
0 & 0 & & & & \\
1/5 & 1/5 & & & & \\
1/5 & & 1/5 & & & \\
1/3 & & & 1/3 & & \\
2/3 & & & & 2/3 & \\
1 & 1/4 & & & & 3/4 \\
\hline
 & 1/4 & & & & 3/4
\end{array}
$$

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

[2] 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.

HOMME-NH dycore

Laprise-like formulation of nonhydrostatic Euler equations [3,4]:

$$\begin{cases} \frac{D\mathbf{u}}{Dt} + \text{coriolis terms} + \left\{\frac{1}{\rho}\nabla p\right\}_h = 0, \quad \frac{Dw}{Dt} + g + \frac{1}{\rho}\frac{\partial p}{\partial z} = 0 \\ \frac{D\phi}{Dt} - g w = 0, \quad \frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{u}\cdot\nabla_\eta + \dot{\eta}\frac{\partial}{\partial\eta} \\ \frac{\partial\Theta}{\partial t} + \nabla_\eta\cdot(\Theta\mathbf{u}) + \frac{\partial}{\partial\eta}(\dot{\eta}\Theta) = 0, \quad \Theta = \tilde{\rho}\theta_v \\ \frac{\partial}{\partial t}(\tilde{\rho}) + \nabla_\eta\cdot(\tilde{\rho}\mathbf{u}) + \frac{\partial}{\partial\eta}(\dot{\eta}\tilde{\rho}) = 0 \end{cases}$$

$\mathbf{u} = (u, v)^T$ – horiz. vel., ϕ – geopotential, π – hydrostatic press.

w – vert. vel., g – grav. constant, c_p – thermo. constant

θ_v – virtual pot. temp., η – vertical coordinate, $\tilde{\rho}$ – pseudo density.

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

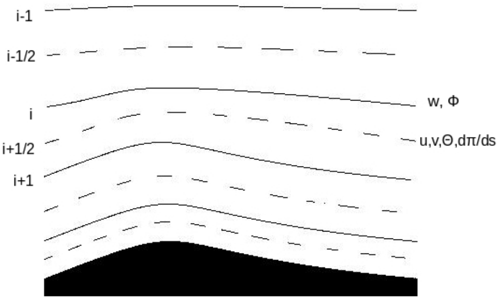
[4] M. Taylor et al, *The E3SM non-hydrostatic atmosphere dynamical core*, Preprint.

HOMME-NH HEVI IMEX splitting

$$
\begin{cases}
\frac{D\mathbf{u}}{Dt} + \text{coriolis terms} + \left\{\frac{1}{\rho}\nabla p\right\}_h = 0 \\
\frac{Dw}{Dt} + \boxed{g + \frac{1}{\rho}\frac{\partial p}{\partial z}} = 0 \\
\frac{D\phi}{Dt} + \boxed{-gw} = 0 \\
\frac{\partial \Theta}{\partial t} + \nabla_\eta \cdot (\Theta \mathbf{u}) + \frac{\partial}{\partial \eta}(\dot{\eta}\Theta) = 0, \qquad \Theta = \tilde{\rho}\theta_v \\
\frac{\partial}{\partial t}(\tilde{\rho}) + \nabla_\eta \cdot (\tilde{\rho}\mathbf{u}) + \frac{\partial}{\partial \eta}(\dot{\eta}\tilde{\rho}) = 0
\end{cases}
$$

HEVI splitting: boxed terms generate fast and vertically propagating acoustic waves that are implicitly treated, all other terms (including vertical advection) are expcplicitly treated. Summer student (Cassidy Krause, U. of Kansas) will use this splitting as basis for split-exp-RK methods.

Spatial discretization



- Horizontal: 4th order mimetic spectral elements on cubed sphere[5] .
- Vertical: 2nd order mimetic SB81 with Lorenz staggering[6].
- Terrain following hydrostatic pressure vertical coordinate η.

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

[6] 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.

Additive and IMEX RK 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 $\Delta t > 0$:

$$\begin{aligned}
u_{m+1} &= u_m + \Delta t \textstyle\sum_{j=1}^{r} \left(b_j n(g_{m,j}, t_{m,j}) + \hat{b}_j s(g_{m,j}, \hat{t}_{m,j}) \right) \\
g_{m,i} &= u_m + \Delta t \textstyle\sum_{j=1}^{r} \left(A_{i,j} n(g_{m,j}, t_{m,j}) + \hat{A}_{i,j} s(g_{m,j}, \hat{t}_{m,j}) \right) \\
t_{m,j} &:= t_m + c_j \Delta t, \quad \hat{t}_{m,j} := t_m + \hat{c}_j \Delta t \quad i = 1, \ldots, r \quad m = 0, 1, 2, \ldots
\end{aligned}$$

Methods are represented using a double Butcher tableau:

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

IMEX RK method: one tableau is implicit, the other is explicit.

HOMME-NH stage equations

HEVI simplifies solution of HOMME-NH RK stage equations:

$$s(q) = (0, 0, -\mathfrak{g}(1-\mu), \mathfrak{g}w, 0, 0)^T, \quad \mu = \frac{\partial p}{\partial \eta} / \frac{\partial \pi}{\partial \eta}, \quad n(q) := \text{everything else.}$$

$$\begin{cases} g^w_{m,j} = E^w_{m,j} + \Delta t \mathfrak{g} \hat{A}_{j,j}(1 - \mu_{m,j}) \\ g^\phi_{m,j} = E^\phi_{m,j} + \Delta t \mathfrak{g} \hat{A}_{j,j} g^w_{m,j} \end{cases}, \quad m \in \mathbb{N}, \quad j = 1, \ldots, r$$

Newton solve for $g^\phi_{m,j}$ then set $g^w_{m,j} = (g^\phi_{m,j} - E^\phi_{m,j})/(\mathfrak{g}\Delta t \hat{A}_{j,j})$.

- Embarrassingly parallel full Newton to machine precision (typically takes 2-4 iterations).
- Direct tridiagonal solves with Lapack.
- Implicit stage costs roughly 50 % of an explicit function evaluation.

IMKG methods

$$
\begin{array}{c|ccccc}
0 & & & & & \\
c_1 & a_1 & & & & \\
\vdots & b_1 & \ddots & & & \\
 & \vdots & & a_{r-2} & & \\
 & & & & a_{r-1} & \\
c_r & b_{r-1} & & & & a_r \\
\hline
 & b_{r-1} & & & & a_r
\end{array}
\qquad
\begin{array}{c|ccccc}
0 & & & & & \\
\hat{c}_1 & \hat{a}_1 & \hat{d}_1 & & & \\
\vdots & \hat{b}_2 & \ddots & \ddots & & \\
 & \vdots & & \hat{a}_{r-2} & \hat{d}_{r-2} & \\
 & & & & \hat{a}_{r-1} & \hat{d}_{r-1} \\
\hat{c}_r & \hat{b}_{r-1} & & & & \hat{a}_r \\
\hline
 & \hat{b}_{r-1} & & & & \hat{a}_r
\end{array}
$$

- Assume $c_j = a_j + b_{j-1}$ and $\hat{c}_j = \hat{a}_j + \hat{b}_{j-1} + \hat{d}_i$ for $j \geq 1$.
- IMKG2 methods (second order) have $b_j \equiv \hat{b}_j \equiv 0$, IMKG3 methods (third order) must have at least $b_{r-1}, \hat{b}_{r-1} \neq 0$ and $\hat{b}_j \equiv b_j$.[7]
- Explicit method has Kinnmark and Gray optimal stability on the imaginary axis, implicit method is I-stable.
- Methods are low storage (2- or 3-registers).

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

Example

The IMKG343a method:

$$
\begin{array}{c|cccc}
0 & 0 & & & \\
1/4 & 1/4 & & & \\
2/3 & 0 & 2/3 & & \\
2/3 & 1/3 & & 1/3 & \\
1 & 1/4 & & & 3/4 \\
\hline
 & 1/4 & & & 3/4
\end{array}
\qquad
\begin{array}{c|ccccc}
0 & 0 & & & & \\
-1/3 & 0 & -1/3 & & & \\
2/3 & 0 & -1/3 & 1 & & \\
2/3 & 1/3 & & -2/3 & 1 & \\
1 & 1/4 & & & 3/4 & \\
\hline
 & 1/4 & & & 3/4 &
\end{array}
$$

Third order accurate, explicit method has CFL ≈ 2.85, implicit method is I-stable, coupled IMEX stability has CFL ≈ 2.5.

HEVI and fast-slow wave stability

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

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

k_x and k_z are horizontal and vertical wave numbers, $K_x := \{k_x\}$, $K_z \in \{k_z\}$.

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

HEVI or H-stability region:

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

Δt is a stable time-step if $\Delta t(K_x \times K_z) \subseteq \mathcal{S}_H$

[8] S.-J. Lock, N. Wood, and H. Weller *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.

Getting to the hydrostatic time-step

- Goal: Run NH-model with a hydrostatic time-step.
- Optimal case: $\mathcal{S}_H$ is a "trunk" with width equal to explicit stability limit; stability is enforced by ensuring $\Delta t K_x$ is contained in the stability region of the explicit method.
- Sub-optimal case: $\mathcal{S}_H$ is a "shrub" with slope small less than $\gamma = \min(K_z \cap (0,\infty))/\max(K_x)$.

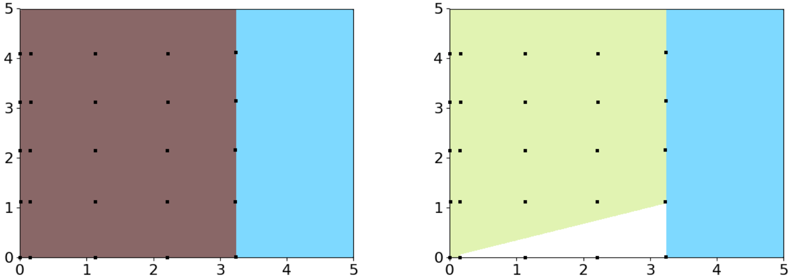


Figure: Dots represent $\Delta t(K_x \times K_z)$, brownish region is a trunk, green region is a shrub with slope less than γ.

H-stability of IMKG232a-b

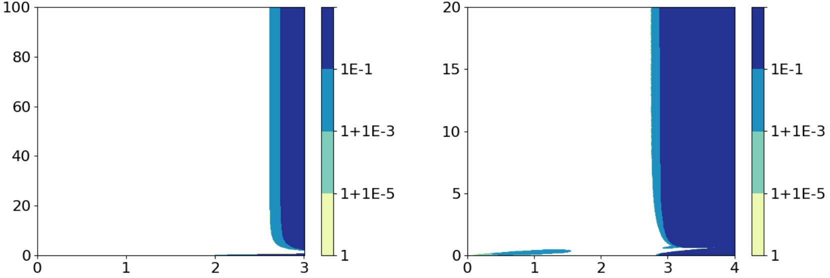


Figure: H-stability regions of the IMKG232b (left) and IMKG242b (right) methods. Max. stable time-steps at v-to-h aspect ratios $\approx 1/100$, $\approx 1/10$, and ≈ 1: IMKG232b 200, 17.5, 1.75; IMKG242b 225, 27.5, 2.5.

Convergence study

Methods implemented with HOMME-ARKode interface[9]: Thanks Chris Vogl, Carol Woodward, David Gardner (LLNL), Dan Reynolds (SMU)!

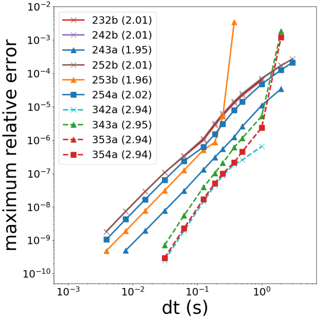
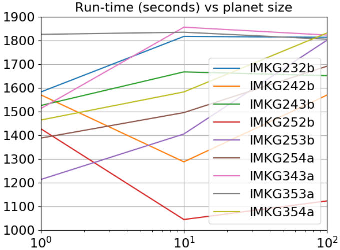
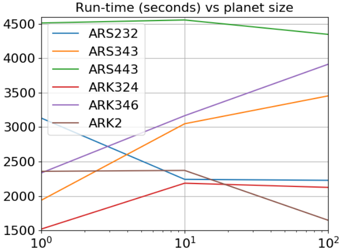


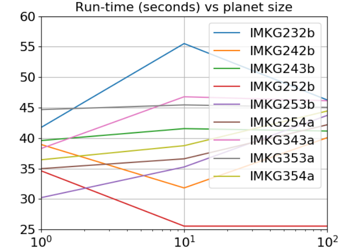
Figure: Error in solution of 5 hour run of DCMIP 2012 non-hydrostatic gravity wave test case, 1.25km horizontal resolution, 20 vertical levels.

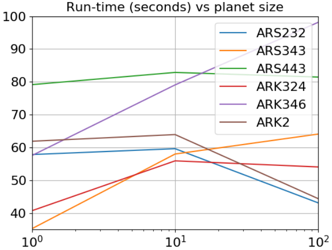
[9] C. Vogl, A. Steyer, D. Reynolds, P. Ullrich, and C. Woodward, *Evaluation of Implicit-Explicit Additive Runge-Kutta Integrators for the HOMME-NH Dynamical Core.* arxiv:1904.10115

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????