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Time-stepping in the E3SM nonhydrostatic atmosphere dynamic core

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E3SM Energy Exascale Ear

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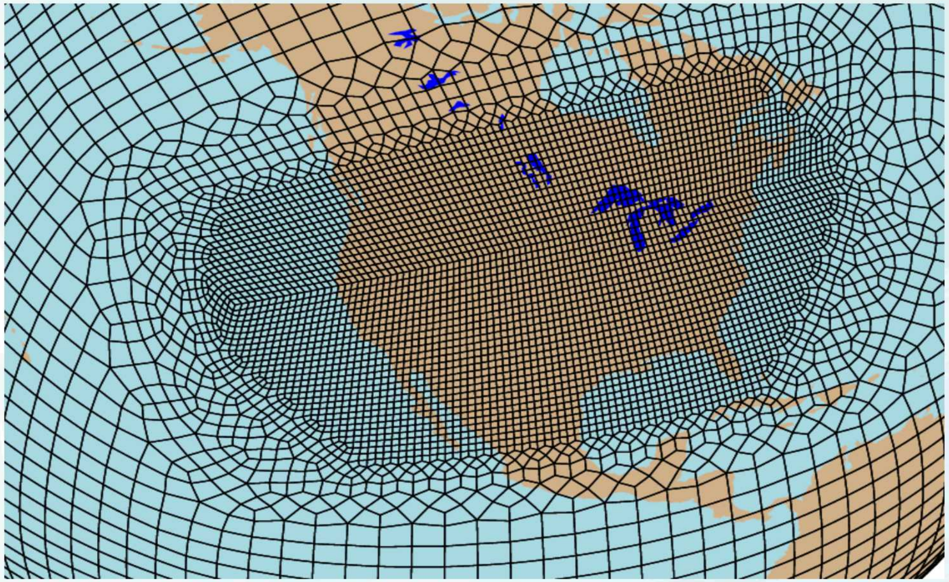
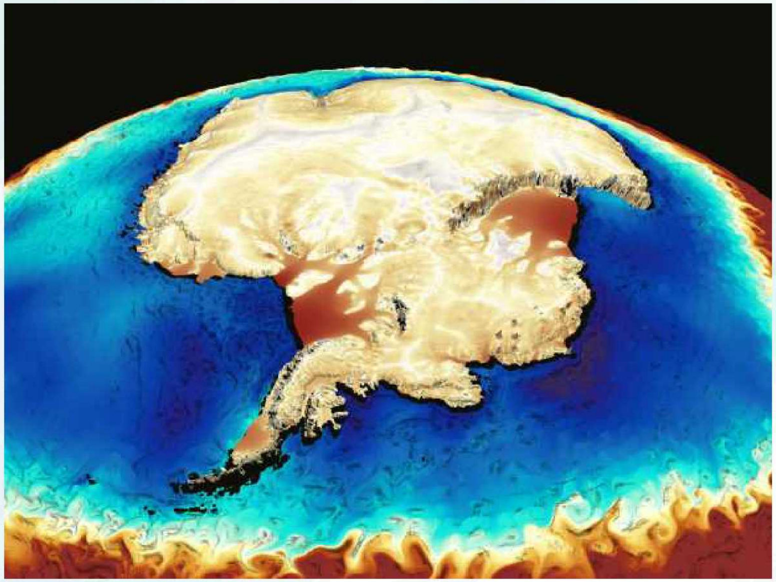
E3SM: Energy, Exascale, Earth system model

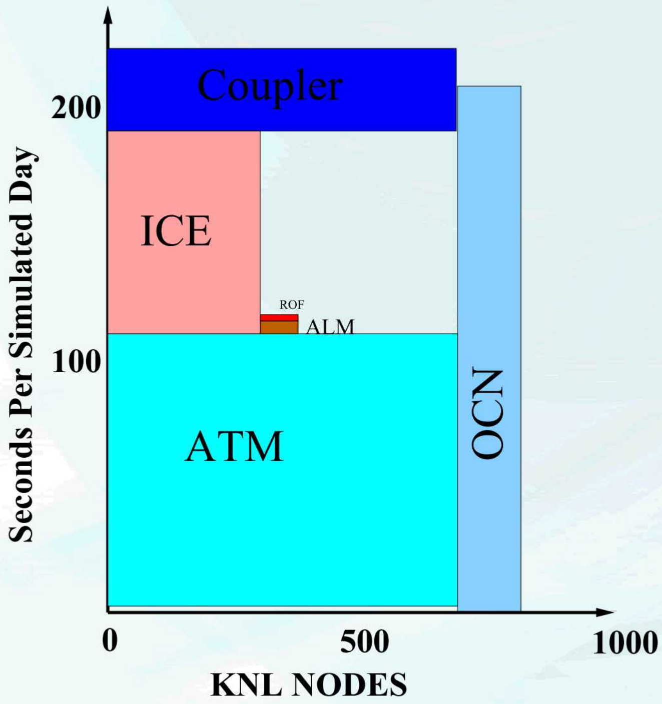
- Focused on Department of Energy (DOE) missions (energy, economic, water issues over next 40 years) and DOE leadership computing facilities.
- Science drivers: water cycle, cryosphere, biogeochemistry.
- Supports variable resolution in all components and targets next-gen machines and at-scale computing (e.g. 1 elem/core). V1 was released in April 2018, V2 coming soon!





E3SM Atmosphere model (EAM)

- Atmosphere model composed of three parts: dynamics + tracer transport (dycore) and physics.
- Check out our movie on youtube (E3SM has a whole channel): E3SM Nonhydrostatic Dynamical Core Animation
- SCREAM Project developing simplified (but not too simple) physics for high-resolution (3km) nonhydrostatic atmosphere.



EAM Component	% time
Transport	0.35*(1/3)
Dynamics	0.13*(1.8)
Physics/Chem	0.52*(?)

Time-stepping nonhydrostatic dynamics in operational models

- Exascale: finer horizontal resolutions (<10km) motivates switch from hydrostatic (nonstiff) to nonhydrostatic (stiff) dynamic core
- E3SM: atmosphere dynamic core needs to efficiently chug through millions of time-steps for decadal-length simulations.
- CFL/stability/efficiency is still a major challenge in operational atmosphere models (fully-implicit too expensive, dt never goes to zero).
- HEVI (Horizontally explicit, vertically implicit) partitioning of nonhydrostatic (nh) atmospheric flow (e.g. nh-Euler equations).
- Stiff vertical acoustic waves are negligible for forecast and climate problems - treated implicitly.
- Can be used as partitioning for implicit-explicit (IMEX), exponential, or multirate methods.
- HEVI nh models should run at hydrostatic time-step.
- Multistep methods? Have issues when coupled to ``physics'' - instead, use one-step e.g. IMEX Runge-Kutta (RK).

Mimetic and compatible spatial discretizations

Taylor, M. and Fournier, A., *A compatible and conservative spectral element method on unstructured grids,* J. Comput. Phy. (2010).

Bovev, P. and Hyman, J (2006), *Principles of mimetic discretizations of differential operators,* n: Arnold D.N., Bochev P.B., Lehoucq R.B., Nicolaides R.A., Shashkov M. (eds) Compatible Spatial Discretizations. The IMA Volumes in Mathematics and its Applications, vol 142. Springer, New York, NY.

Conservation of important quantities (e.g. mass, energy, potential vorticity) is important In atmosphere modeling. To achieve this, use numerical methods that mimic various vector calculus identities such as integration by parts:

$$\Omega - \text{ periodic domain}$$

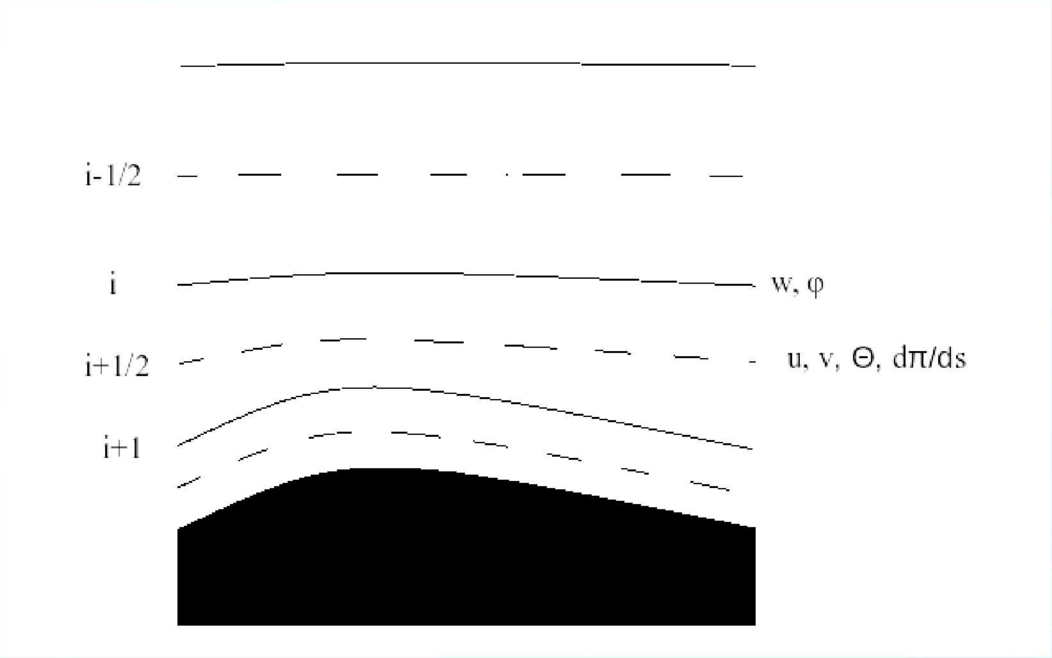
$$\int_\Omega \mathbf{v} \cdot \nabla f d\Omega + \int_\Omega f \nabla \cdot \mathbf{v} d\Omega = 0, \quad \forall f \in V, \mathbf{v} \in V^3$$

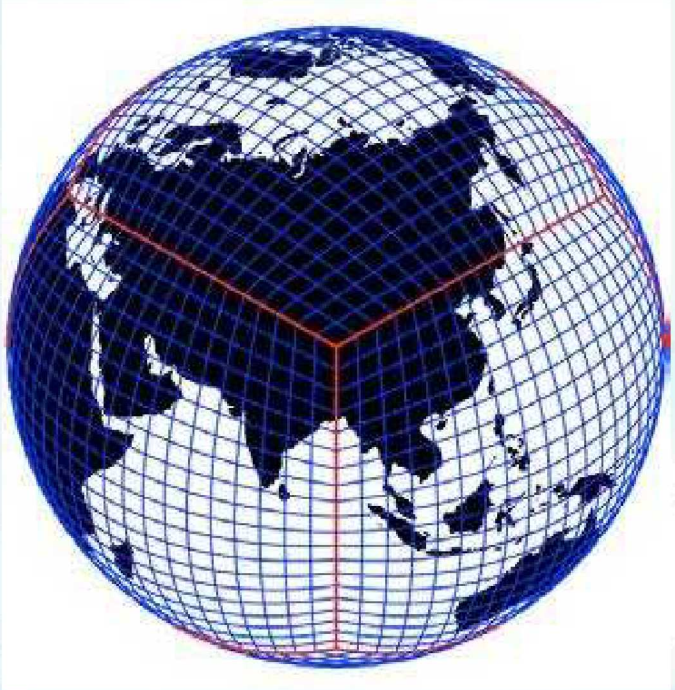
$$\langle \mathbf{v}_h, \nabla f_h \rangle + \langle f_h, \nabla \cdot \mathbf{v}_h \rangle = 0, \quad \forall f_h \in V_h, \mathbf{v}_h \in V_h^3$$

Other properties: $\text{Stokes' Theorem}, \quad \nabla \times \nabla f = 0, \quad \nabla \cdot \nabla \psi = 0$

PDEs on spheres (spatial discretization)

- Cubed sphere with terrain following vertical coordinate.
- Horizontal: 4th order mimetic spectral elements on cubed sphere (M. Taylor and A. Fournier, *A compatible and conservative spectral element method on unstructured grids,* J. Comput. Phys., 229 (2010), pp. 5879-5895) .
- Vertical: 2nd order mimetic SB81 with Lorenz staggering (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).





Laprise-like formulation of nh-Euler equations

Laprise-like (R. Laprise, *The Euler equations of motion with hydrostatic pressure as an independent variable,* Mon. Wea. Rev., 102 (1992), pp. 197-207), (Taylor et al, *An energy consistent discretization of the nonhydrostatic equations in primitive variables, arxiv:1908.04430)*

formulation of nh-Euler equations posed on spherical domain:

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

$\mathbf{u}-$ hor. veloc.

$w-$ vert. veloc.

$\phi-$ nh geopotential

$\Theta-$ virtual pot. temp. dens.

$\tilde{\rho}-$ pseudo-density

$\eta-$ terrain following vertical coordinate.

HEVI splitting isolates terms (boxed) responsible for fast vertical acoustic wave propagation. (Steyer et al, *Efficient IMEX Runge-Kutta methods for nonhydrostatic dynamics, arxiv:1906.07219).*

Hypervisocity and vertical remap (not discussed) are applied separate from the time-stepping.

E3SM Energy Exascale Earth System Model

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Time-stepping operator-split initial value problems

Philosophy: Balance cost of taking large time-steps with cost-per-time-step – treat stiff terms with a stiff integrator and non-stiff terms with a cheap nonstiff integrator.

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

Example (~Math 783):

$$u_t + u_x - u_{xx} = 0 \Longrightarrow \dot{u}_j + \frac{u_{j+1} - u_{j-1}}{2\Delta x} + \frac{u_{j+1} - u_{j-1} - 2u_j}{\Delta x^2} = 0$$

IMEX Euler: $u_{m+1} = u_m + \Delta t \cdot n(u_m) + \Delta t \cdot s(u_m).$

Types of methods: Low-order operator splitting, Implicit-explicit RK and multistep methods, multirate methods, exponential methods.

Error analysis is more challenging (but doable) and stability analysis is essentially case-by-case (opinion).

IMEX RK methods

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

$$\begin{cases} u_{m+1} = u_m + \Delta t \sum_{k=1}^{r} \Big(b_k n(g_{m,k}, t_{m,k}) + \hat{b}_k s(g_{m,k}, \hat{t}_{m,k}) \Big) \\ g_{m,j} = u_m + \Delta t \sum_{j=1}^{j-1} \Big(A_{j,k} n(g_{m,k}, t_{m,k}) + \hat{A}_{j,k} s(g_{m,k}, \hat{t}_{m,k}) \Big) + \Delta t \hat{A}_{j,j} s(g_{m,j}, \hat{t}_{m,j}) \\ t_{m,j} := t_m + c_j \Delta t, \quad \hat{t}_{m,j} := t_m + \hat{c}_j \Delta t \quad j = 1, \ldots, r \quad m = 0, 1, 2, \ldots. \end{cases}$$

Methods are represented with a double Butcher tableau:

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

Accuracy: both methods must be accurate and satisfy additional coupled order conditions.

IMEX RK methods accuracy

$$
\begin{aligned}
u(t+\Delta t) = u(t) + \Delta t(n'(t) + s'(t)) \\
&+ \frac{\Delta t^2}{2}(n'n + n's + s'n + s's) \\
&+ \frac{\Delta t^3}{6}\Big(s''(n+s)^2 + n'(n'+s')(n+s) \\
&+s''(n+s)^2 + s'(n'+s')(n+s)\Big) \\
&+ \ldots
\end{aligned}
$$

- Requires analysis of coupling conditions. (Hairer, E., *Order conditions for numerical methods for partitioned ordinary differential equations,* Numer. Math., 36 (1981), pp. 431–445).
- B-series type analysis.
- Coupling conditions increase much faster than standard order conditions means higher order methods (> 4) not commonly used.

IMEX RK: Limitations of scalar test equations In pure imaginary setting

$$\dot{u} = Au \equiv Nu + Su, \quad N = \begin{bmatrix} 1 & -1 \\ 2 & -1 \end{bmatrix}, \quad S = \begin{bmatrix} 1 & \frac{5}{4} \\ -100 & -1 \end{bmatrix}.$$

A, N, S have pure imaginary eigenvalues: $\{\pm i\sqrt{\frac{41}{2}}\}, \{\pm i\}, \{\pm i\sqrt{124}\}$

$$\dot{z} = inz + isz, \quad n \in \{\pm i\}, s \in \{\pm i\sqrt{124}\}$$

Solve $\dot{u} = Au, u(0) = u_0$ with the following 1st order IMEX RK method:

$$\begin{array}{c|cc} 0 & 0 & \\ 1 & 1 & \\ 1 & & 1 \\ \hline & & 1 \end{array} \qquad \begin{array}{c|cc} 0 & 0 & \\ \frac{3}{4} & 0 & \frac{3}{4} \\ 1 & & 1 \\ \hline & & 1 \end{array},$$

exp. method has stability on imaginary axis
imp. method is A-stable

As $\Delta t \to 0$: one eigenvalue of $R(\Delta tN, \Delta tS)$ is always greater than 1 in modulus, $|R(i\Delta t n_j, i\Delta t s_k)| \leq 1$ for $j, k = 1, 2$ where R represents stability matrix/function for method applied to $\dot{u} = Nu + Su$ or $\dot{z} = in_j z + is_k z$.

HEVI and fast-wave slow-wave stability

Proposed test equation for stability of HEVI IMEX RK Lock et al, *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.)

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

$k_x, k_z > 0$ - horizontal and vertical wave numbers

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

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 $\Delta t (K_x \times K_z) \subseteq \mathcal{S}_H$

Derivation of HEVI test equation

HEVI test equation arises from solving a 2D linear acoustic wave problem with an IMEX RK method and assuming solutions are exact in space:

$$\begin{bmatrix} u_t \\ v_t \\ p_t \end{bmatrix} = - \begin{bmatrix} 0 & 0 & \partial_x \\ 0 & 0 & 0 \\ \partial_x & 0 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \\ p \end{bmatrix} - \begin{bmatrix} 0 & 0 & 0 \\ 0 & \partial_z & 0 \\ 0 & 0 & \partial_z \end{bmatrix} \begin{bmatrix} u \\ v \\ p \end{bmatrix}$$

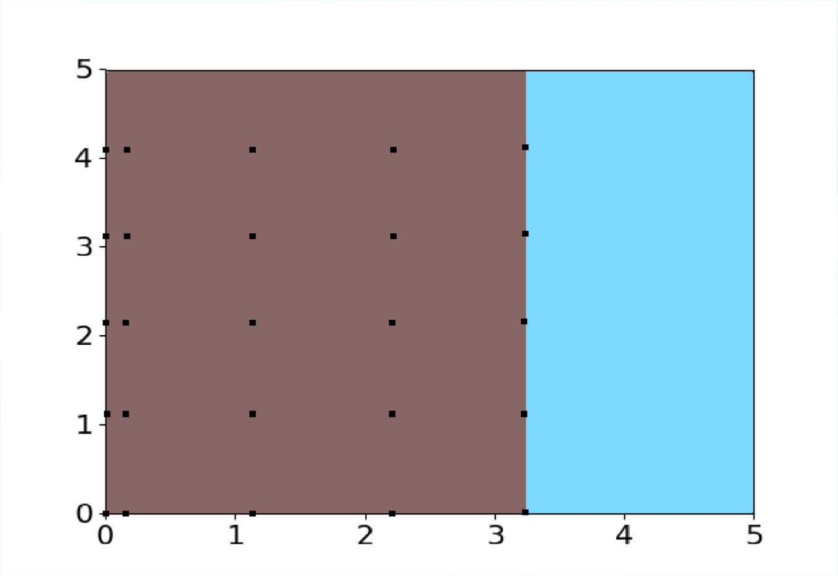
Derived by linearizing either Eulerian fluid about some simplified reference thermodynamics state (e.g constant density or buoyancy) and various approximations on e.g. scale height of the atmosphere.

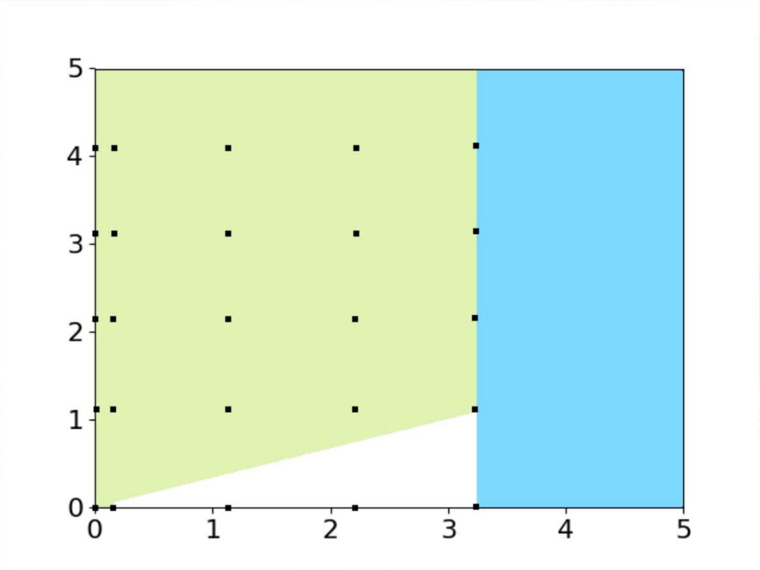
O. Guba (SNL): Obtain shifted system taking into account other effects differences in linearizations.

Getting to the hydrostatic time-step

- Goal: Run NH-model with a hydrostatic time-step.
- Optimal case: H-stability region 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: H-stability region is a ``shrub'' with slope given by:

$$\gamma = \min(K_z \cap (0, \infty))/\max(K_x)$$





IMKG2-3 methods

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

- Explicit method has Kinnmark and Gray optimal stability on the imaginary axis, implicit method is I-stable, H-stability regions is a trunk or a shrub.
- 2nd or 3rd order accurate. 2nd order accuracy can be obtained with:

$$b_j = \hat{b}_j = 0, \quad j = 1, \ldots, r-1$$

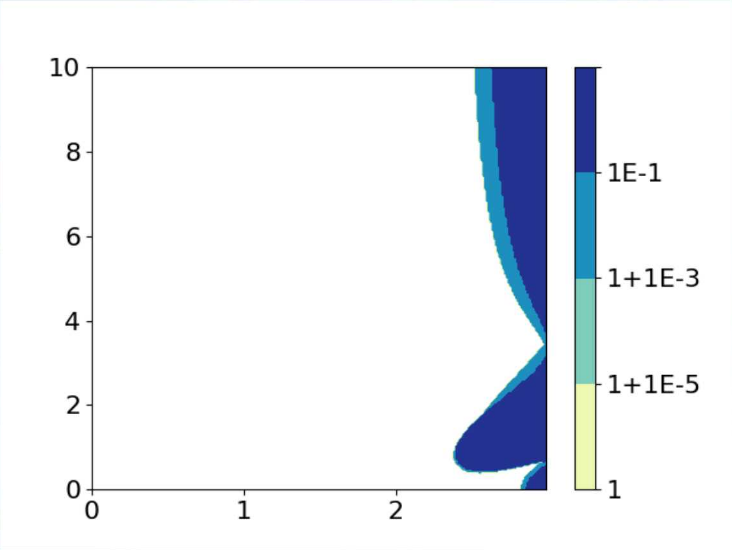
- Low-storage to minimize memory foot-print.

Example (IMKG 343a)

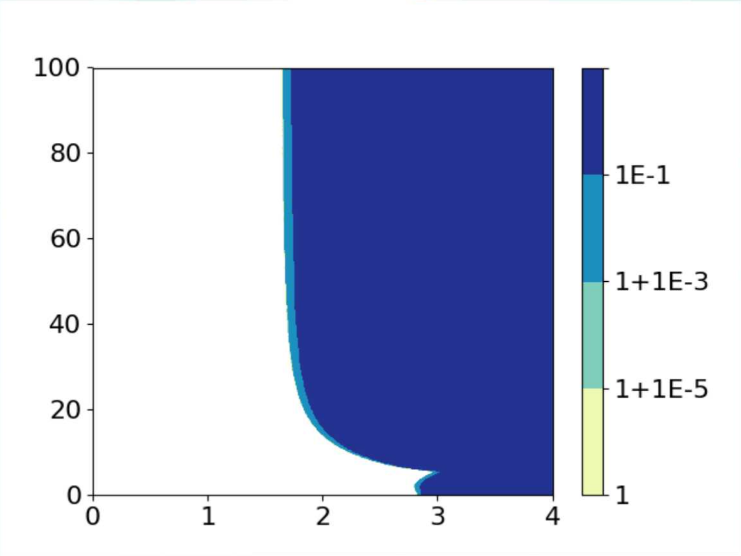
0	0			
1/4	1/4			
2/3	0	2/3		
2/3	1/3		1/3	
1	1/4			3/4
	1/4			3/4

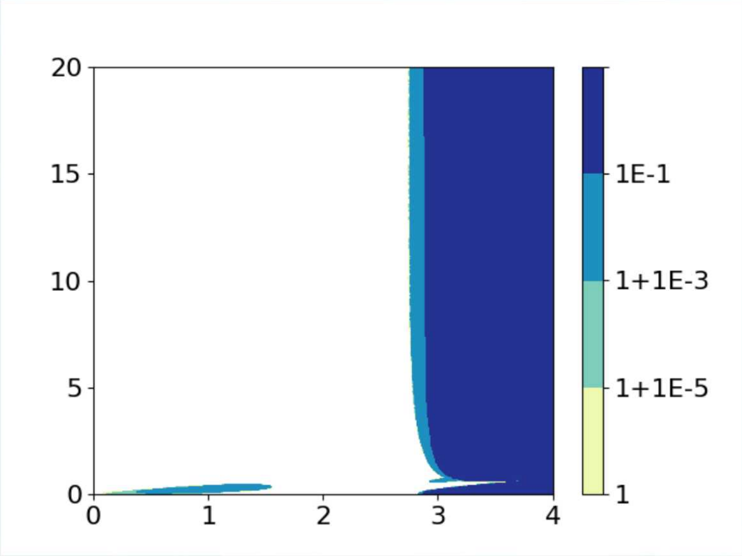
0	0			
−1/3	0	−1/3		
2/3	0	−1/3	1	
2/3	1/3		−2/3	1
1	1/4			3/4
	1/4			3/4

Third order accurate, explicit method has CFL ~2.85, implicit method is I-stable, coupled IMEX stability has CFL ~2.5 (H-stability region to the right).



H-stability of IMKG242a-b





H-stability regions of the IMKG242a (left) and IMKG242b (right) methods. Max. stable time-steps at v-to-h aspect ratios 1/100, 1/10, and 1: IMKG242a 175, 17.5, 2.25; IMKG242b 225, 27.5, 2.75. Hydrostatic time-steps 275, 27.5, 2.75.

$$\begin{array}{c|cccc} 0 & 0 & & & \\ \frac{1}{4} & \frac{1}{4} & & & \\ \frac{1}{3} & & \frac{1}{3} & & \\ \frac{1}{2} & & & \frac{1}{2} & \\ 1 & & & & 1 \\ \hline & & & & 1 \end{array}$$

with

$$\begin{array}{c|cccc} 0 & 0 & & & \\ 0 & & 0 & & \\ \frac{2-\sqrt{2}}{2} & & & \frac{2-\sqrt{2}}{2} & \\ \frac{1}{2} & & & \frac{\sqrt{2}-1}{2} & \frac{2-\sqrt{2}}{2} \\ 1 & & & & 1 \\ \hline & & & & 1 \end{array}$$

IMKG242a

or

$$\begin{array}{c|cccc} 0 & 0 & & & \\ 0 & & 0 & & \\ \frac{2+\sqrt{2}}{2} & & & \frac{2+\sqrt{2}}{2} & \\ \frac{1}{2} & & & -\frac{1+\sqrt{2}}{2} & \frac{2+\sqrt{2}}{2} \\ 1 & & & & 1 \\ \hline & & & & 1 \end{array}$$

IMKG242b

Solution of implicit stage equations

Recall implicitly treated equations:

$$Dw/Dt = \mathfrak{g}(\mu - 1), \quad D\phi/Dt = \mathfrak{g}w, \quad \mu = \frac{\partial p/\partial \eta}{\partial \pi/\partial \eta}.$$

Implicit stage equations for IMEX DIRK methods:

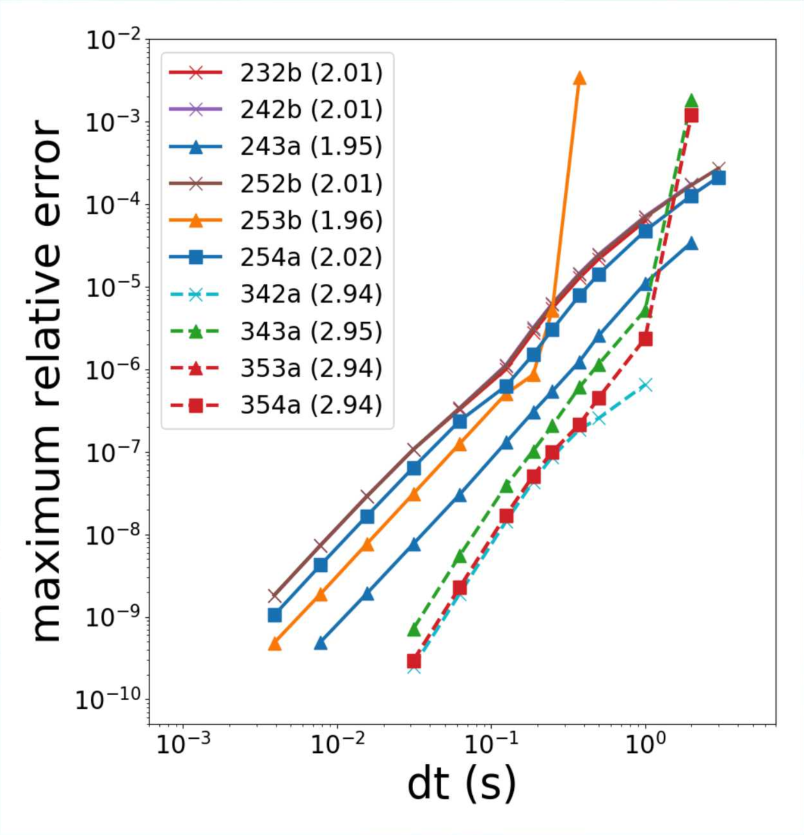
$$\text{Solve for } g_{m,j} : g_{m,j} = \begin{bmatrix} g^w_{m,j} \\ g^\phi_{m,j} \end{bmatrix} = \begin{bmatrix} E^w_{m,j} \\ E^\phi_{m,j} \end{bmatrix} + \Delta t \mathfrak{g} \hat{A}_{j,j} \begin{bmatrix} (\mu(g^\phi_m) - 1) \\ g^w_m \end{bmatrix}$$

- Static condensation (the math version!): iterate only one equation.
- \item Explicit update is used as the initial guess in Newton iteration.
- Tridiagonal direct linear solves (2nd order differences $\partial/\partial\eta$ terms above) in the Newton iteration - sparse in general case.
- No (horizontal) parallel communication.

Consequence: on large computers, implicit solves can cost as little at 20-30% of the explicit function evaluations.

Convergence study

Methods implemented with HOMME-ARKode interface (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) Thanks to the SUNDIALS-ARKODE team: Chris Vogl, Carol Woodward, David Gardner (LLNL), Dan Reynolds (SMU)!



(Left) Error in solution of 5 hour run of DCMIP 2012 non-hydrostatic gravity wave test case, 1.25km horizontal resolution, 20 vertical levels. Hyperviscosity and vertical remap were disabled.

Time-stepping in presence of topography

- The goal is to run nonhydrostatic dycore with same dt as hydrostatic dycore.
- Preliminary runs on nonhydrostatic core without topography did well.
- With topography, time steps were too small. ← It is not a bug, it is a feature.

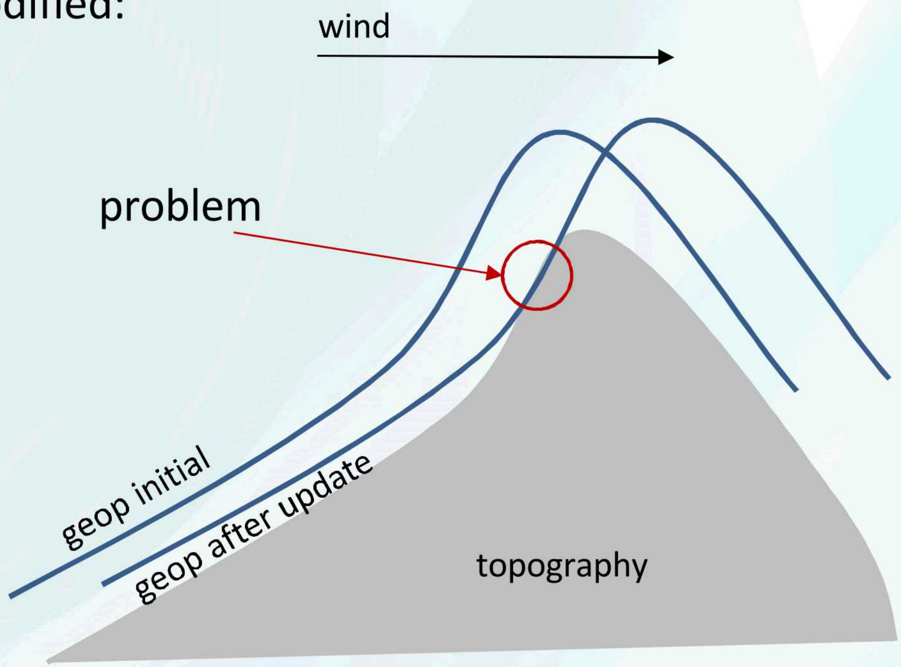
Hydrostatic dt	Held-Suarez, 1 degree, before	F case 1 degree, before	Held-Suarez, 1 degree, after	F case, 1 degree after
300 for 5 stage scheme	15	30	150 for 3 stage scheme	150 for 3 stage scheme
			5-stage scheme in works	5-stage scheme in works

Credit: Oksana Guba

Explicit stage with topography

IMEX in HOMME, RK Kinmark and Gray modified:

Explicit stage
  Implicit stage
Explicit stage
  Implicit stage
Explicit stage
  Implicit stage
Explicit stage
  Implicit stage
Explicit stage
  ? Implicit stage ?



This is not how current IMEX RK in HOMME works, but primitively, **explicit** stage solves transport

$$\underbrace{\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla_\eta \phi + \dot{\eta} \frac{\partial \phi}{\partial \eta}}_{\text{explicit terms}} - \underbrace{gw}_{\text{implicit term}} = 0$$

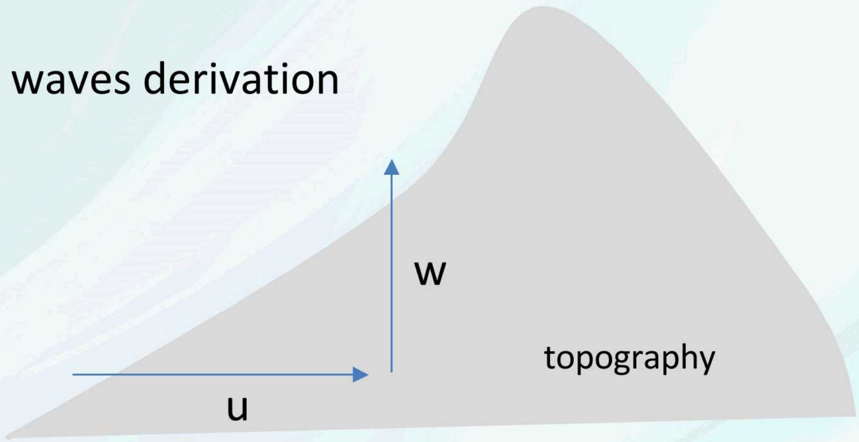
This equation is not solved in hydrostatic model.

Credit: Oksana Guba

New IMEX splitting in geopotential equation and moving last implicit stage

$$\frac{\partial \phi}{\partial t} + \underbrace{\mathbf{u} \cdot \nabla_s \phi - \mathbf{u} \cdot \nabla_s \phi_{surf} + \dot{s}\frac{\partial \phi}{\partial s}}_{\text{explicit terms}} = \underbrace{gw - \mathbf{u} \cdot \nabla_s \phi_{surf}}_{\text{implicit terms}}$$

New term is a ‘constant’ in IMEX and so, acoustic waves derivation from implicit terms stays the same.



Modify IMEX RK so that last stage is implicit and off-centered (slightly more dissipative) and all method coefficients are small and positive (ensures internal stage accuracy):

$$g_r = u_m + \text{ exp. terms } + \Delta t(\hat{b}_{r-1} s(g_1) + \hat{a}_r s(g_{r-1}) + \hat{d}_r s(g_r))$$

Credit: Oksana Guba

$$0 < \hat{b}_{r-1} < \hat{d}_r$$

Thanks! Questions?