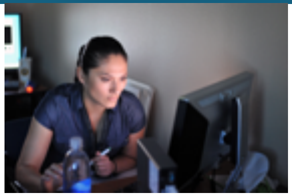
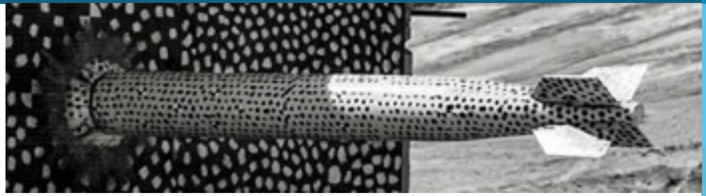
Exponential Integrators for the HOMME-NH Nonhydrostatic Dycore





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Time-stepping in HOMME-NH

The E3SM atmosphere model (EAM) targets high-resolution (3 km horizontal grid spacing) simulations. HOMME-NH uses a horizontally explicit vertically implicit (HEVI) partitioning of the nonhydrostatic (NH) equations:

$$\mathbf{u}_t + (\nabla_\eta \times \mathbf{u} + 2\Omega) \times \mathbf{u} + \tfrac{1}{2}\nabla_\eta(\mathbf{u}\cdot\mathbf{u}) + \dot\eta \frac{\partial \mathbf{u}}{\partial \eta} + \frac{1}{\rho}\nabla_\eta p + \mu \nabla_\eta \phi = 0, \quad \dot\eta := d\eta/dt$$

$$w_t + \mathbf{u}\cdot\nabla_\eta w + \dot\eta\frac{\partial w}{\partial \eta} + \boxed{\mathfrak{g}(1-\mu)} = 0, \quad \mu := \frac{\partial p}{\partial \eta}\Big/\frac{\partial \pi}{\partial \eta}$$

$$\phi_t + \mathbf{u}\cdot\nabla_\eta \phi + \dot\eta\frac{\partial \phi}{\partial \eta} + \boxed{-\mathfrak{g}w} = 0$$

$$\Theta_t + \nabla_\eta\cdot(\Theta\mathbf{u}) + \frac{\partial}{\partial\eta}(\Theta\dot\eta) = 0, \quad \Theta := \frac{\partial \pi}{\partial \eta}\theta_v$$

$$\frac{\partial}{\partial t}\left(\frac{\partial \pi}{\partial \eta}\right) + \nabla_\eta\cdot\left(\frac{\partial \pi}{\partial \eta}\mathbf{u}\right) + \frac{\partial}{\partial \eta}\left(\frac{\partial \pi}{\partial \eta}\dot\eta\right) = 0.$$

- Accurate and efficient time-stepping is critical for the atmosphere to be performant.
- Semi-implicit and implicit-explicit (IMEX) methods are the “industry standard” for time-stepping in HEVI NH models.
- Exponential-type (e.g. exponential time difference (ETD) and integrating factor methods) are an attractive alternative in the HEVI context.
- Big unknown: Are nonlinear solves (IMEX) cheaper than matrix exponentials (ETD) in NH models.

ETD Runge-Kutta (ETD-RK) methods

Consider a partitioned initial value ODE $q_t = n(q) + s(q)$ where $n(q)$ represent non-stiff terms and $s(q)$ represents stiff terms.

Given an approximate solution $q_m \approx q(t_m)$ at time-step m, we linearize the stiff part $s(q)$ along q_m. Let $L_m = \partial s/\partial q(q_m)$ and let $N_m(q) = f(q) - L_m q$. Now our additive partitioning becomes:

$$q_t = f(q) = L_m q + N_m(q).$$

An ETD-RK solution is given by

$$q_{m+1} = e^{L_m \Delta t} q_m + \Delta t \sum_{i=1}^{r} b_i(L_m \Delta t) N_m(t_m + c_i \Delta t, g_{mi}),$$

with stage values

$$g_{mj} = e^{c_j L_m \Delta t} q_m + \Delta t \sum_{i=1}^{r} a_{ij}(L_m \Delta t) N_m(t_m + c_i \Delta t, g_{mi}).$$

where the method coefficients a_{ij} and b_i depend on the so-called phi-functions:

$$\varphi_0(z) = \exp(z) \quad \varphi_{k+1}(z) = z^{-1}(\varphi_k(z) - \varphi_k(0))$$

Methods are represented with the Butcher notation:
$$\begin{array}{c|ccc} c_1 & a_{1,1} & \cdots & a_{1,r} \\ \vdots & \vdots & \ddots & \vdots \end{array}$$

HEVI matrix exponentials in HOMME-NH

In HOMME-NHLinearizing the stiff terms results in:

$$L_m = \begin{bmatrix} 0 & & & & \\ & 0 & \mathfrak{g}\frac{\partial \mu}{\partial \phi} & & \\ & \mathfrak{g}I & 0 & & \\ & & & 0 & \\ & & & & 0 \end{bmatrix} \qquad e^{\alpha L_m} = \begin{bmatrix} I & & & \\ & \exp\left(\begin{bmatrix} 0 & \mathfrak{g}\alpha\frac{\partial \mu}{\partial \phi} \\ \mathfrak{g}\alpha I & 0 \end{bmatrix}\right) & & \\ & & I & \\ & & & I \end{bmatrix}, \quad \alpha \neq 0$$

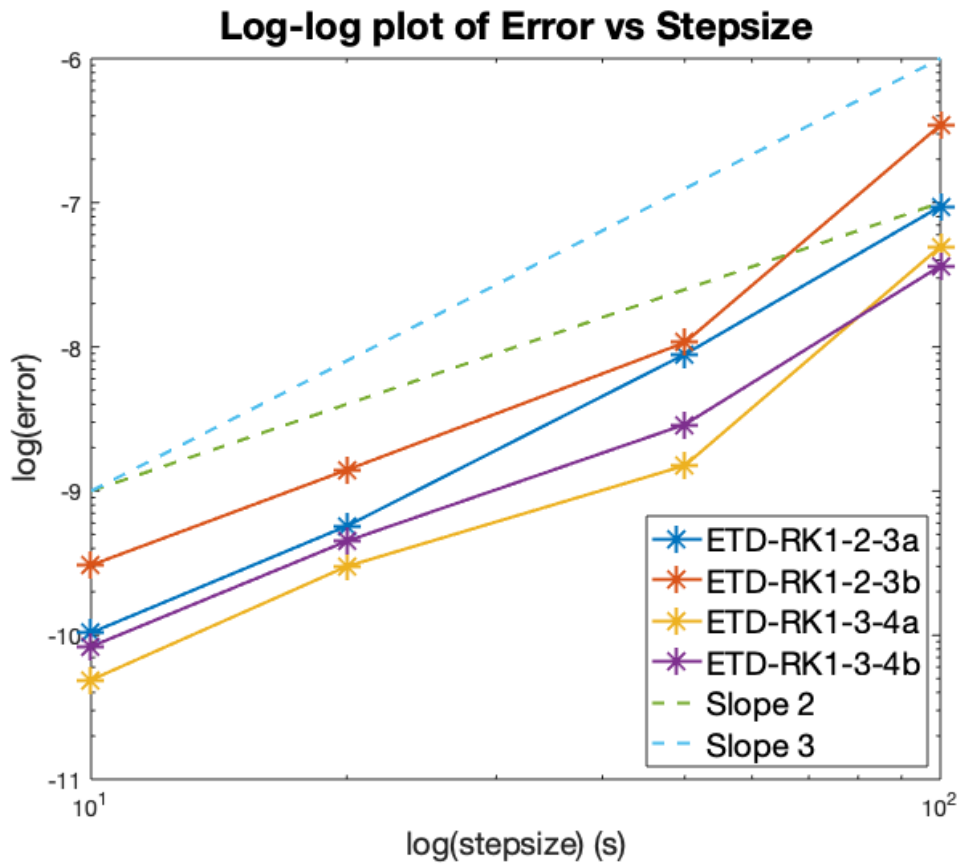
where $\frac{\partial \mu}{\partial \phi}$ is tridiagonal. We implement a (p,q)-Padé approximation to approximate the exponential of a matrix A as $e^A \approx \left[Q_{pq}(A)\right]^{-1} P_{pq}(A)$, where $P_{pq}(A)$ and $Q_{pq}(A)$ are defined as

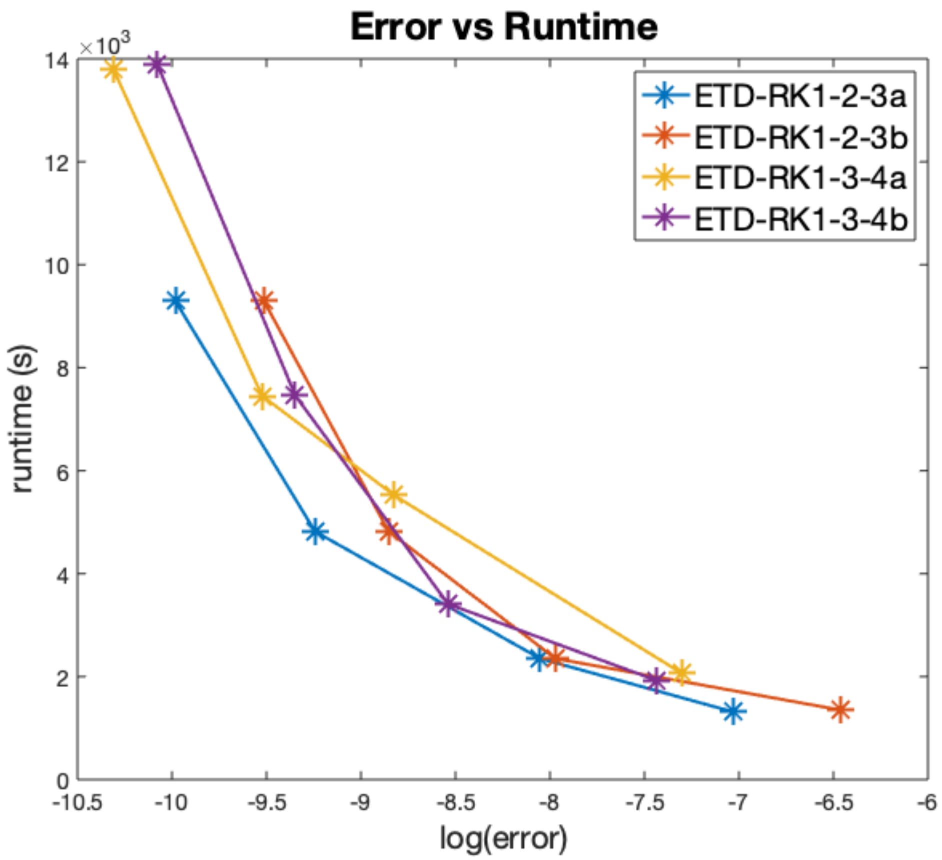
$$P_{pq}(A) = \sum_{j=0}^{p} \frac{(p+q-j)!\,p!}{(p+q)!\,j!\,(p-j)!} A^j \qquad Q_{pq}(A) = \sum_{j=0}^{q} \frac{(p+q-j)!\,q!}{(p+q)!\,j!\,(q-j)!} (-A)^j$$

Factoring the polynomial $Q_{pq}(A)$ and applying static condensation to L_m means $e^{\alpha L_m}$ can be. approximated with q tridiagonal solves and p tridiagonal multiplications. phi-functions φ_k with $k \geq 0$ are computed iteratively.

Taking L_m from a spin-up run of the DCMIP Test Case 3.1, the (3,3)-Padé approximation for e^{L_m} has an absolute error of $5.25e-13$.

Convergence and Efficiency





Convergence and efficiency study for several custom ETD-RK methods integrating the DCMIP2012 Test Case 3.1 (nonhydrostatic gravity wave). The error is the full L2-error of the solution found by comparison with a high-precision reference trajectory.

Future Work:

- Investigate parallel implementation of exponential calculations and function evaluations. Optimize performance relative to the best IMEX-RK methods.

References

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4. An energy consistent discretization of the nonhydrostatic equations in primitive variables. Taylor, M., Guba, O., Steyer, A., Ullrich P., Hall, D., Eldred, C. **arXiv:1908.04430.**