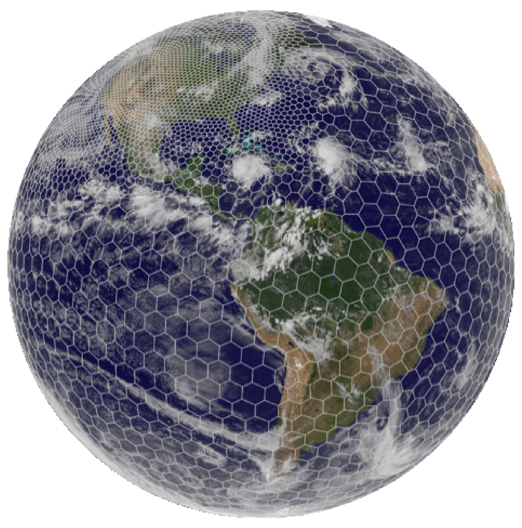
Conservation Properties and Performance of Exponential Integrators for Nonlinear Conservation Laws

Chad Sockwell[1], Konstantin Pieper[1], Zhu Wang[2], Lili Ju[2], Max Gunzburger[1]

[1] *University of Florida State: Department of Scientific Computing* [2] *University of South Carolina: Department of Mathematics*

1) Introduction

- Climate modeling is a computationally intense effort that benefits greatly from the use of multi-resolution, non-uniform, spatial grids. The DOE OS's *Model for Prediction Across Scales* (MPAS) models the Earth's climate using this idea (right) and the Primitive Equations.
- Currently MPAS does not have a matching multi-resolution temporal scheme. Such a scheme would need to be conservative and negate the restrictive CFL condition generated by the smallest grid cells.
- Exponential Integrators solve linear problems exactly (CFL independent), and solve stiff problems well, but are they conservative?



2) Exponential Integrators(EI)

Consider the following system of nonlinear conservation laws with periodic boundary conditions

$$u_t = F(u) = f_x(u)\ , \tag{1}$$

$$\Omega := \{a < x < b\}\ ,\ 0 < t < \Delta t\ ,\ u(t_n, x) = u_n$$

and expanding $F(u)$ at u_0

$$u_t = F(u_n) + J_n(u - u_n) + R(u) = Ju + \tilde{R}(u)$$

where $J_n = F'(u_n)$.

The 2nd order Exponential Rosenbrock-Euler method, using the variation of constants formula and freezing F at u_n, has the form

$$u(\Delta t) = u_n + \left(\int_0^{\Delta t} e^{J_n(\Delta t - s)} ds \right) F(u_n)$$

$$\Rightarrow \vec{\mathbf{U}}^{n+1} = \vec{\mathbf{U}}^{n} + \Delta t \phi_1(\Delta t \mathbf{J}_n)\vec{\mathbf{F}}^{n}\ , \tag{2}$$

where

$$\phi_s(\mathbf{A}) = \sum_{k=0}^{\infty} \frac{\mathbf{A}^k}{(k+s)!}\ . \tag{3}$$

This can be calculated efficiently in several ways:

1. Krylov Methods: Assume $\phi_1(\Delta t J_n)F^n$ lies in the space $K_m(\mathbf{J}_n, \mathbf{F}^n)$, for $m < n$, then

   $$\vec{\mathbf{U}}^{n+1} = \vec{\mathbf{U}}^{n} + \Delta t ||\vec{\mathbf{F}}^n|| \mathbf{V}_m \phi_1(\Delta t \mathbf{H}_m)\vec{\mathbf{e}}_1.$$

   Typically the number of Krylov vectors required for an accurate, non-oscillatory solution is one to three times the $\Delta t/\Delta x$ ratio. Thus more Krylov vectors are needed for larger time steps.
2. Sub-stepping methods: The quantity $\vec{\mathbf{R}}(1) = \phi_1(\Delta t \mathbf{J}_n)\vec{\mathbf{F}}^n$ is solution of the following ODE:

   $$\vec{\mathbf{R}}'(t) = \mathbf{J}_n\vec{\mathbf{R}}(t) + \vec{\mathbf{F}}^n\ , 0 < t < 1\ , \vec{\mathbf{R}}(0) = \vec{0}\ .$$

   Thus $\vec{\mathbf{R}}(1) = \phi_1(\Delta t \mathbf{J}_n)\vec{\mathbf{F}}^n$ can be found by sub-stepping (perhaps RK4) instead of explicitly evaluating matrix exponentials.
3. Open software packages such as Expokit combine these methods in some way and provide error control.
4. Chebyshev interpolation for the ϕ_s functions over the domain containing the spectrum (not yet implemented).

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4) Shallow Water Setup

The Shallow water equations (which serve as a prototype for the Primitive Equations) for a given bathymetry are ($g \approx 9.8$ kg m s^{-2})

$$\partial_t h + \partial_x(uh) = 0$$

$$\partial_t u + \partial_x(u^2/2 + g(h - b(x))) = 0$$

$$b(x) = H_{shelf} + H_0/2(1 + \tanh(d(x)/\psi))\ .$$

The shallow water equations are discretized using a staggered central finite volume scheme.

$$h_i' = \frac{-1}{\Delta x}(u_{i+1/2}\hat{h}_{i+1/2} - u_{i-1/2}\hat{h}_{i-1/2})$$

$$u_{i+1/2}' = \frac{-1}{\Delta x}\{(\hat{u}_{i+1}^2/2 - \hat{u}_i^2/2)$$

$$+ g([h_{i+1} - b(x_{i+1})] - [h_i - b(x_i)])\}$$

$$\hat{u}_i = \frac{1}{2}(u_{i+1/2} + u_{i-1/2})\ ,\ \hat{h}_{i+1/2} = \frac{1}{2}(h_{i+1} + h_i)$$

$$\nu = \max_i(|\hat{u}_i \pm \sqrt{gh_i}|)\ ,\ \Delta t = \Delta x/\nu \approx 9.38 \text{ s}\ .$$

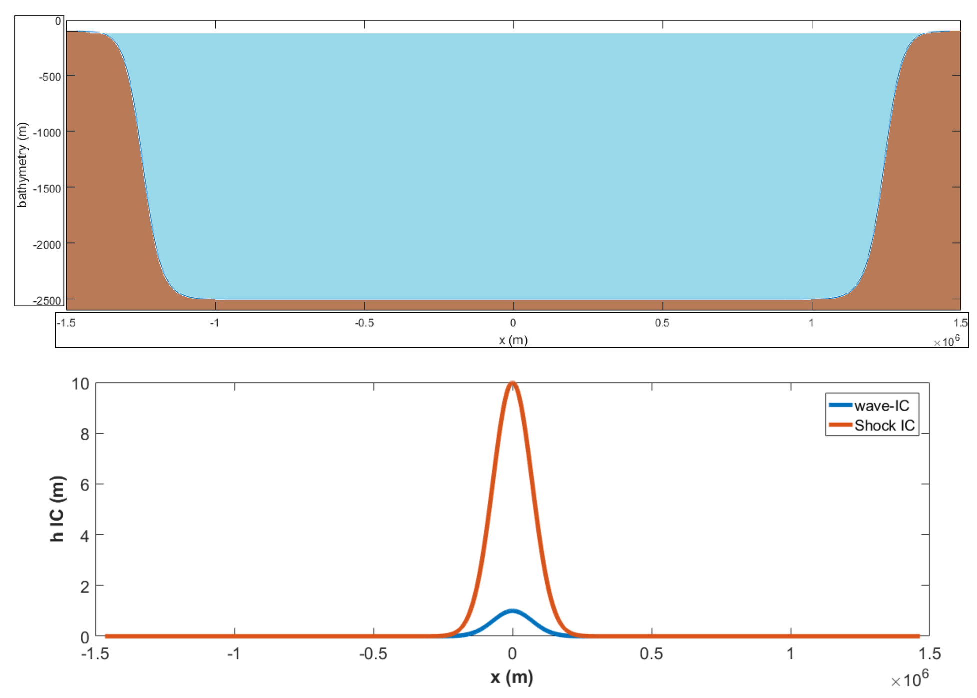

Figure 1: (Top) The bathymetry of the ocean given by the function $b(x)$. (Bottom) Initial conditions on h ($h_0(x) = ae^{-(x/10^5)^2}$ - $b(x)$) for wave-like behavior (a=1) and shock-like behavior (a=10).

3) Conservation of Mass of EI

Consider the system of nonlinear conservation law in (1) for the variable u. The linearization for $\tilde{u} = u + \tau v$ as $\tau \to 0$

$$\partial_t v(x,t) + \partial_x f'(x,u)v = 0\ , \tag{4}$$

and the weak form is given by

$$\partial_t \int_\Omega \phi v\ dx - \int_\Omega \partial_x(\phi) f'(x,u)v\ dx = 0\ ,\quad \forall \phi \in V\ . \tag{5}$$

Note the boundary terms cancel due to periodicity of v. Let $\Omega := \cup_{i=0}^{N-1} S_i$, $S_i := \{x_{i-1/2} < x < x_{1+1/2}\}$, $h = x_{i+1} - x_i$, and let $\phi^h = \vec{\mathbf{1}}$. Discretizating the weak form (5) on each S_i and summing all S_i gives

$$\sum_{S_i} \frac{d}{dt} \int_{S_i} v^h\ dx + \left(\hat{g}'_{i+1/2} - \hat{g}'_{i-1/2}\right) = \sum_{S_i} \frac{d}{dt} \int_{S_i} v^h\ dx = 0 \quad \forall t \in (0,T) \tag{6}$$

where $\hat{g}'_{i+1/2} = \frac{1}{2}(f'(x_{i+1/2}, u_i^{h,-})v^{h,-} + f'(x_{i+1/2}, u_i^{h,+})v^{h,+} - \alpha_i(v^{h,-} - v^{h,+}))$ is the Lax Friedrichs flux at the interface, where α_i is a penalty parameter. This is equivalent to matrix problem

$$\frac{d}{dt}\mathbf{M}_h\vec{\mathbf{V}}^h + F_h'(\vec{\mathbf{U}}^h)\vec{\mathbf{V}}^h = 0\ ;$$

$$\sum_{S_i}\left(\hat{g}'_{i+1/2} - \hat{g}'_{i-1/2}\right) = 0$$

$$\Rightarrow \vec{\mathbf{1}}^T F_h'(\vec{\mathbf{U}}^h)\vec{\mathbf{V}}^h = 0\ .$$

The EI method is of the form

$$\vec{\mathbf{U}}^{n+1} = \vec{\mathbf{U}}^{n} + \Delta t \phi_1(\mathbf{M}_h^{-1}F_h'(\vec{\mathbf{U}}^n))F_h(\vec{\mathbf{U}}^n)\ .$$

Testing $\phi_1(\cdot)$ by $\vec{\mathbf{1}}^T\mathbf{M}_h$ and using (3) yields

$$\vec{\mathbf{1}}^T\mathbf{M}_h\phi_1(\mathbf{M}_h^{-1}F_h'(\vec{\mathbf{U}}^n)) = \vec{\mathbf{1}}^T\mathbf{M}_h\ ,$$

yielding conservation of mass

$$\vec{\mathbf{1}}^T\mathbf{M}_h\vec{\mathbf{U}}^{n+1} = \vec{\mathbf{1}}^T\mathbf{M}_h\vec{\mathbf{U}}^{n} \quad \forall n\ .$$

5) 1-D Shallow Water (S.W.)

The S.W. system is discretized in time, using the 3 EI methods and RK4. KV is the # of Krylov vectors, Sub is the # of RK4 sub-steps, and in space using the FV discretization with $N = 2049$ points. The solutions are compared to an over-refined solution using RK4 and 10 times as many spatial points and time steps.

The wave-like IC in Fig. 1 is used and $u_0(x) = 0$, and homogeneous Dirichlet BC's on u. For small perturbations in h and u, S.W. → Wave Equation. This is where EI performs well since the problem is nearly linear. Large perturbations give rise to shocks, and the EI cannot propagate faster than the shock.

The time horizon for the simulation is one day, and $\alpha = 6.38\text{E}{-3}$. The EI-Sub method provides a performance advantage over RK4 by minimizing the number of nonlinear flux calculations and replaces them with sparse mat-vecs using the $\mathbf{J}_n$.

Method	$\Delta t/\Delta x$	Time (s)	Error$_h$	Error$_u$
RK4	α	6.59	6.4E-3	4.34E-4
EI-KV24	10α	15.3	6.4E-3	4.41E-4
Expokit-KV10	100α	7.69	2.8E-2	1.81E-3
Expokit-KV10	10α	15.7	6.5E-3	4.41E-4
EI-Sub-10	10α	5.43	6.5E-3	4.41E-4
EI-Sub-100	100α	2.67	2.8E-2	1.81E-3

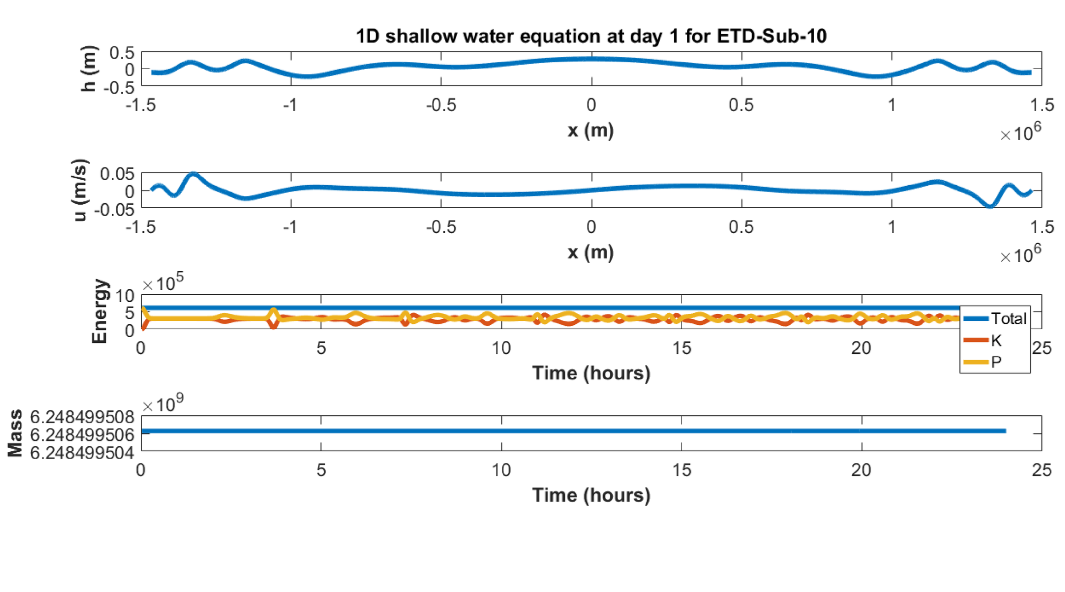

Figure 2: The S.W. equations at Day 1 using EI-Sub-10. Both energy and mass are conserved.