F: Exponential Time Differencing And Parallel Implementation

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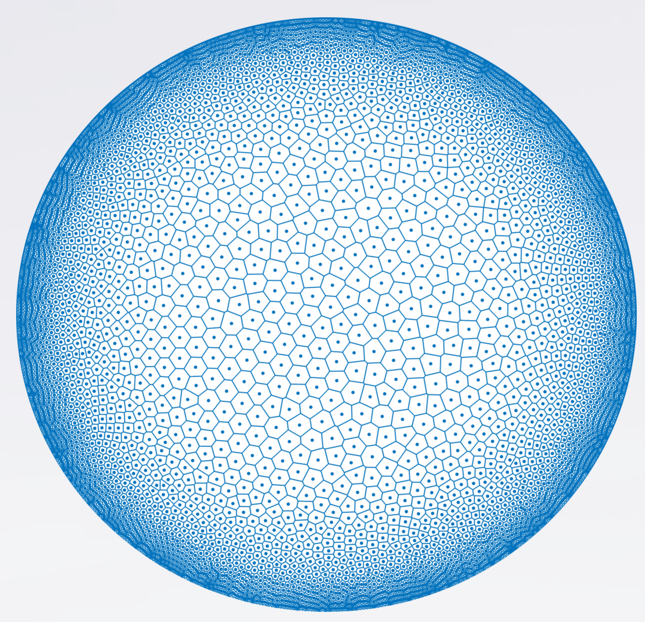
Hypothesis

Time Resolution In Ocean Models

- Multiresolution meshes allow to resolve areas of interest at finer scales. Future developments require increases in resolution difference.
- Explicit time stepping methods couple the global time step to the size of the smallest grid cell (restricted by the CFL condition).
- Long term stability and conservation (over decades) of the scheme is essential.



Research question:

Investigate different time discretization methods that allow for:

- Large time steps **independent of the CFL**.
- Accurate resolution of **conserved quantities** (mass, energy, etc.).
- **Decoupled time-discretization** in different regions.

Hypothesis: Exponential time differencing enables large time steps while retaining conservation properties and efficiency. Domain decomposition decouples different temporal scales in subdomains, enabling further efficiencies.

Developments Required

ETD For Rotating Shallow Water Equations

- The rotating shallow water equations: Hamiltonian $\mathcal{H}$, and skew-symmetric operator $\mathbf{J}$, where

$$\mathcal{H} = \int_\Omega \frac{1}{2} h|\mathbf{v}|^2 + \frac{1}{2} gh(h+b)\, d\Omega \,,\ \mathbf{J} = \begin{pmatrix} 0 & -\nabla\cdot \\ -\nabla & -\mathbf{q}(h\hat{\mathbf{k}}\times) \end{pmatrix}$$

$$\mathbf{u}_t = \mathbf{J}(\mathbf{u}) \frac{\delta \mathcal{H}(\mathbf{u})}{\delta \mathbf{u}} \,,\ \mathbf{u} = (h, \mathbf{v})$$

- Equations are split into linear and nonlinear parts:

$$\mathbf{u}_t = F(\mathbf{u}) \to \mathbf{u}_t = \mathbf{A}^n u + R(\mathbf{u})$$

- Approximate remainder, e.g. ETD-Euler (higher order possible):

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t \phi_1(\Delta t \mathbf{A}^n) F(\mathbf{u}^n)$$

- Reduce the size of matrix functions by Krylov Methods:

$$\phi_0(\mathbf{A}) = \exp(\mathbf{A}) \,,\ \phi_1(\mathbf{A}) = \int_0^1 \exp((1-s)\mathbf{A})\, ds$$

Structural Properties For Conservation:

- ETD methods conserve mass to machine precision.
- Operator $\mathbf{J}$ is skew-symmetric with respect to symmetric operator $\mathbf{M}$. Symmetry corresponds to energy conservation.
- ETD-wave (ETDW): Evaluate Jacobian at resting state

$$\mathbf{A} = \mathbf{J}(\mathbf{u}_0) \frac{\delta^2 \mathcal{H}(\mathbf{u}_0)}{\delta \mathbf{u}^2}$$

- Skew-symmetry of $\mathbf{A}$ with respect to special inner product.

Pros & Cons: Allows for the use of the $\mathcal{O}(N)$ Skew-Lanczos iteration compared to the $\mathcal{O}(N^2)$ Arnoldi iteration; lower convergence order.

Test Case Results

Energy Conservation Results

- Energy conservation to a time discretization error while maintaining time step sizes above the CFL limit (Table 1).
- ETD2W yields a computational speed-up over RK4, while maintaining a constant energy resolution error.

Long Term Stability: Double Gyre Test Case

- Stability of ETD2W maintained over one year in double-gyre test case (Figures 1 & 2).
- Meshes with increasing resolution resolved at a coarsest time scale (Table 2).

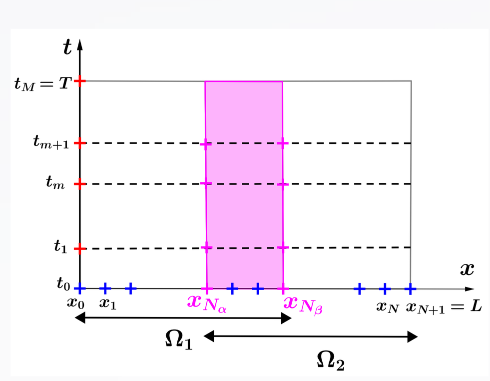
Ongoing Investigation

- Multiresolution, faster, and parallel matrix functions.
- Explore different choices of the linear operator (stability, conservation, and computational efficiency).

Parallel Implementation of ETD

- The spatial domain is decomposed into overlapping sub-domains.
- Phi-functions and residual localized to each subdomain.

Coupling of The Subdomain Problems



- Coupling by Dirichlet BCs at local interfaces.
- Parallel Schwarz iteration applied at each time level (Method 1) or over whole time interval (Method 2).

Method 1: Space L-ETD2 First discretize globally in time, then apply domain decomposition at each time step:

$$\begin{aligned} \boldsymbol{u}_{1,m+1}^{(k+1)} &= \phi_0(\Delta t \boldsymbol{A}_1)\boldsymbol{u}_m + \Delta t\, \phi_1(\Delta t \boldsymbol{A}_1)\boldsymbol{R}_1\left(\boldsymbol{u}_{2,m}(N_{\beta,\alpha})\right) \\ &+ \Delta t \phi_2(\Delta t \boldsymbol{A}_1)\Big[\boldsymbol{R}_1\left(\boldsymbol{u}_{2,m+1}^{(k)}(N_{\beta,\alpha})\right) - \boldsymbol{R}_1\left(\boldsymbol{u}_{2,m}(N_{\beta,\alpha})\right)\Big]. \end{aligned}$$

Pros & Cons: Cheap cost per iteration, fast convergence but only works for conforming time grids.

Method 2: Space-Time L-ETD2 Discretize in time separately in each subdomain and perform global-in-time domain decomposition:

$$\begin{aligned} \boldsymbol{u}_{1,m+1}^{(k+1)} &= \phi_0(\Delta t \boldsymbol{A}_1)\boldsymbol{u}_{1,m}^{(k+1)} + \Delta t\, \phi_1(\Delta t \boldsymbol{A}_1)\boldsymbol{R}_1\left(\boldsymbol{u}_{2,m}^{(k)}(N_{\beta,\alpha})\right) \\ &+ \Delta t \phi_2(\Delta t \boldsymbol{A}_1)\Big[\boldsymbol{R}_1\left(\boldsymbol{u}_{2,m+1}^{(k)}(N_{\beta,\alpha})\right) - \boldsymbol{R}_1\left(\boldsymbol{u}_{2,m}^{(k)}(N_{\beta,\alpha})\right)\Big]. \end{aligned}$$

Pros & Cons: Different time steps in different subdomains, super-linear convergence on short time intervals; larger cost per iteration.

- The larger the overlap size, the faster the convergence.

Numerical Performance of Localized ETD

1. Two Dimensional Diffusion Equation (Table 3)

- L-ETD2 solutions reach the same accuracy as the global ETD2 after a few iterations.
- Method 1 seems more efficient than Method 2 on conforming time grids.

2. One Dimensional Shallow Water Equation (Table 4)

- Significant speed-ups by L-ETD2 compared to Global ETD2, especially with nonuniform meshes (Figure 3).
- L-ETD2 solution conserves mass.

Future Work

- Implementation of L-ETD with nonconforming time grids & non-uniform meshes for the 2D SOMA test case.
- Nonoverlapping domain decomposition with more general transmission conditions and optimized parameters.

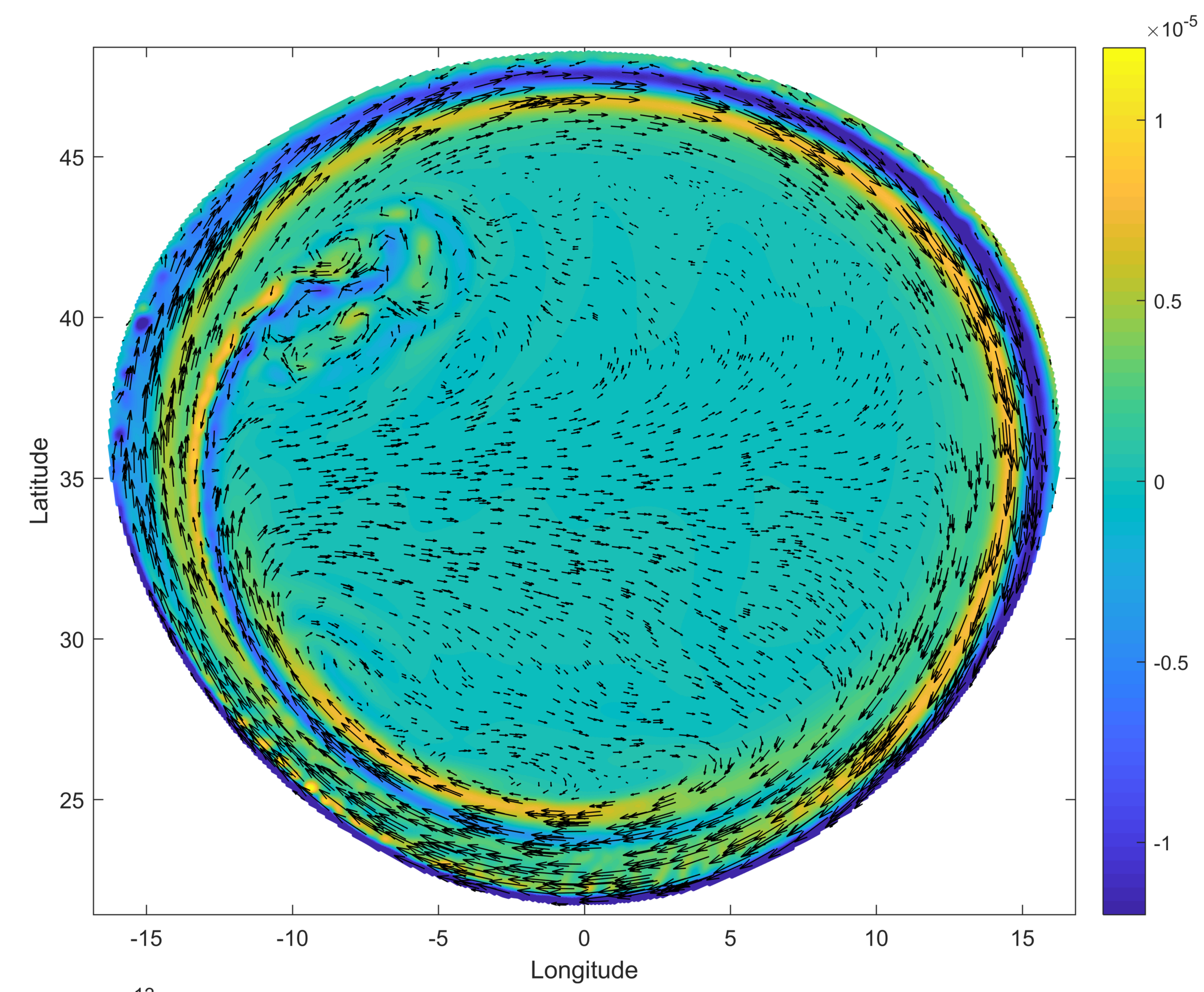


Figure 1. Velocity (vectors), relative vorticity (density), and energy for double gyre test case for one year on 8 km grid using ETDW2. Bottom drag constant c=-1E-6. This test case consists of a circular ocean with a variable bathymetry, wind forcing in the zonal direction, and a single layer.

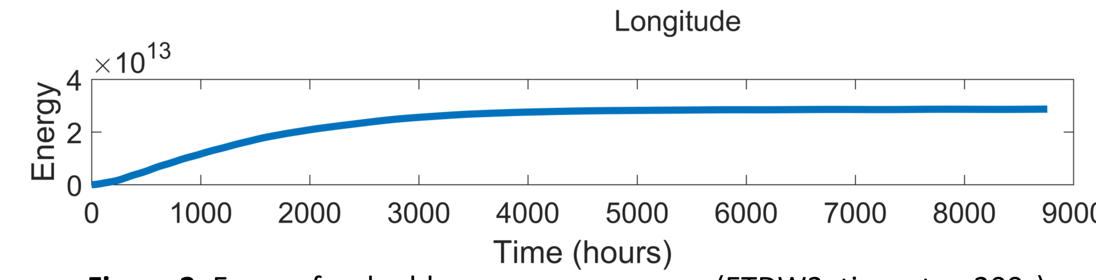


Figure 2. Energy for double gyre over one year (ETDW2, time step 200s).

Res(Δx)		Δt(s)	Wtime(s)
32 km		100	4.46E+3
16 km		50	5.23E+4
8 km		25	4.95E+5
Res(Δx)	**#KV**	**Δt(s)**	**Wtime(s)**
32 km	(10,10)	200	6.75E+3
16 km	(14,10)	200	2.75E+4
8 km	(20,19)	200	1.36E+5

Table 2. Wall times for double gyre test case for one year. RK4 (top) and ETDW2 (bottom). KV is the number of Krylov vectors per internal stage.

Methods	min Δx	Δt=22.84s	CPU time/time step
Global ETD2	1431.3m	10 Δt_{CFL}	0.096s
Non-iterative L-ETD2	1431.3m	10 Δt_{CFL}	0.028s/proc
Global ETD2	238.56m	30 Δt_{CFL}	0.135s
Non-iterative L-ETD2	238.56m	30 Δt_{CFL}	0.034s/proc

Table 4. Computational cost per time step of global ETD2 and non-iterative L-ETD2 (with 10 procs) for the 1D SOMA test case, max Δx = 1431.35m.

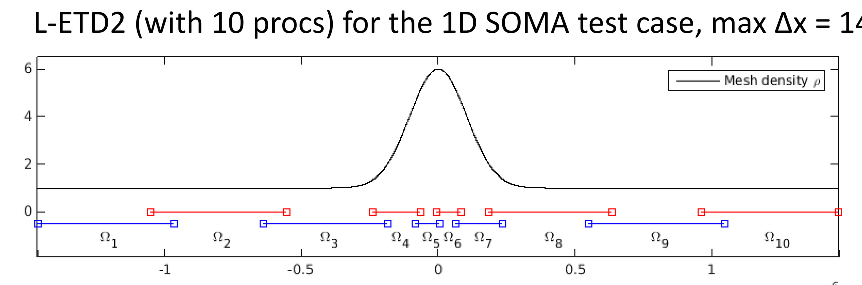


Figure 3. Density function used for mesh generation and overlapping subdomains for the 1D shallow water test case.

#Subdomains	1×1	2×2	4×4
Method 1	2.79E-3	2.79E-3 [2]	2.79E-3 [4]
Method 2		2.41E-1 [2] 2.79E-3 [14]	3.27E-1 [4] 2.79E-3 [23]

Table 3. Errors between global/localized ETD2 solutions and the exact solution for 2D diffusion problems. Numbers of Schwarz iterations shown in brackets.

Res(Δx)		Δt(s)	ΔE	Wtime(s)
32 km		200	2.40E-4	3.18
32 km		100	7.62E-6	5.78
16 km		50	2.40E-7	83.1
8 km		25	7.58E-9	756
4 km		12.5	2.38E-10	6135
Res(Δx)	**#KV**	**Δt(s)**	**ΔE**	**Wtime(s)**
32 km	(10,7)	200	2.01E-5	17.9
16 km	(12,10)	200	2.29E-5	55.3
8 km	(18,14)	200	2.34E-5	206
4 km	(30,24)	200	2.35E-5	1108

Table 1. Energy conservation for Gaussian pulse on SOMA geometry for 12 hours and for various grid resolutions. RK4 (top) and ETDW2 (bottom). KV is the number of Krylov vectors per internal stage. The first row for RK4 is the CFL compliant step, the rest are one half of CFL compliant.

Expected Impact

Time Step Selection Based On Accuracy Requirements

- **CFL Mitigation:** Time step size chosen based on accuracy not stability.

Nonuniform Time Step Size Selection by Domain Decomposition

- **Treatment of Domain Specific CFL Conditions:** Time step selection corresponding to local mesh size through domain decomposition.
- **Increased Work Distribution**: Local time stepping allows processors to be distributed based on mesh coarseness and time step size in each subdomain.

Impacts

- **Coastal Refinement:** Resolving coastal areas becomes feasible from a performance standpoint.
- **Time Scale Splitting:** Improved treatment of baroclinic and barotropic modes combining ETD and split-explicit method.
- **Coupling to local high-resolution models:** coastal (tidal / estuary) models for accurate modeling of inflows and tides.

ACME Accelerated Climate Modeling for Energy

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