

Localized Exponential Time Differencing Methods Based on Domain Decomposition

Zhu Wang
Department of Mathematics
University of South Carolina

Collaborators:

T.-T.-P. Hoang (USC/Auburn), L. Ju and X. Meng (USC)

E3SM Concall Meeting
January 17, 2019



Work overview

Idea

Applying **parallel Schwarz algorithms** with overlapping domain decomposition to **time evolution problems** discretized in time by the **exponential time differencing** methods.

Advantages

- Using exponential integrator allows **large time step sizes**.
- Solving **subdomain problems of smaller sizes in parallel**, possibly with **different time steps** in different subdomains.
- Reducing **computational cost** without affecting the **accuracy** of the approximate solution.

Global numerical solution

- PDE models: parabolic or hyperbolic types such as shallow water equations

Spatial discretization: $\mathbf{u}'(t) = \mathbf{L}\mathbf{u}(t) + \mathbf{R}(t, \mathbf{u}(t), \psi(t)), \quad 0 < t < T, \quad \mathbf{u}(0) = \mathbf{u}_0.$

Time integration: exponential time differencing

- Given solution \mathbf{u}_m at t_m and a time step $\Delta t = t_{m+1} - t_m.$

$$\mathbf{u}_{m+1} = e^{\Delta t \mathbf{L}} \mathbf{u}_m + \int_0^{\Delta t} e^{(\Delta t - s) \mathbf{L}} \left[\frac{\mathbf{R}(t_{m+1}) - \mathbf{R}(t_m)}{\Delta t} s + \mathbf{R}(t_m) \right] ds \quad (1)$$

$$= e^{\Delta t \mathbf{L}} \mathbf{u}_m + \Delta t \varphi_1(\Delta t \mathbf{L}) \mathbf{R}(t_m) + \Delta t \varphi_2(\Delta t \mathbf{L}) [\mathbf{R}(t_{m+1}) - \mathbf{R}(t_m)] \quad (2).$$

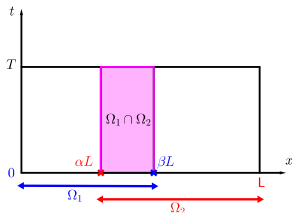
- Denote $\mathbf{R}(t) \equiv \mathbf{R}(t, \mathbf{u}(t), \psi(t))$; define $\varphi_1(z) = \frac{e^z - 1}{z}$ and $\varphi_2(z) = \frac{\varphi_1(z) - 1}{z}.$

- Second-order accuracy in time, named **ETD2**.

It can be formulated as a two stage approach (see Konstantin's slides).

- High performance computing \Rightarrow localized ETD based on domain decomposition

Multidomain formulation



- Partition Ω into overlapping subdomains Ω_1 and Ω_2 .

Partition \mathbf{u} into overlapping subsets \mathbf{u}_1 and \mathbf{u}_2 .

Solve subdomain problems separately.

Transmission conditions on the interfaces:

$$\mathbf{u}_1(N_\beta, t) = \mathbf{u}_2(N_{\beta,\alpha}, t) \text{ and } \mathbf{u}_2(1, t) = \mathbf{u}_1(N_\alpha, t),$$

where $N_\alpha h = \alpha L$, $N_\beta h = \beta L$, $N_{\beta,\alpha} = N_\beta - N_\alpha + 1$.

- Recall a two-stage ETD2:

$$\tilde{\mathbf{u}}_{m+1} = e^{\Delta t \mathbf{L}} \mathbf{u}_m + \Delta t \varphi_1(\Delta t \mathbf{L}) \mathbf{R}(t_m, \mathbf{u}_m, \psi_1, \psi_2);$$

$$\mathbf{u}_{m+1} = \tilde{\mathbf{u}}_{m+1} + \Delta t \varphi_2(\Delta t \mathbf{L}) [\mathbf{R}(t_{m+1}, \tilde{\mathbf{u}}_{m+1}, \psi_1, \psi_2) - \mathbf{R}(t_m, \mathbf{u}_m, \psi_1, \psi_2)].$$

- Assume that subdomain solutions at time t_m , $\mathbf{u}_{1,m}$ and $\mathbf{u}_{2,m}$, are obtained.

Second-order localized ETD (LETD) algorithm

- First compute subdomain solutions $\tilde{\mathbf{u}}_{1,m+1}$ and $\tilde{\mathbf{u}}_{2,m+1}$.

For instance, in Ω_1 ,

$$\tilde{\mathbf{u}}_{1,m+1} = e^{\Delta t \mathbf{L}_1} \mathbf{u}_{1,m} + \Delta t \varphi_1(\Delta t \mathbf{L}_1) \mathbf{R}_1(t_m, \mathbf{u}_{1,m}, \psi_1(t_m), \mathbf{u}_{2,m}(N_{\beta,\alpha})).$$

- Set $\mathbf{u}_{1,m+1}^{(0)}(N_\alpha) = \tilde{\mathbf{u}}_{1,m+1}(N_\alpha)$ and $\mathbf{u}_{2,m+1}^{(0)}(N_{\beta,\alpha}) = \tilde{\mathbf{u}}_{2,m+1}(N_{\beta,\alpha})$.
- Start the iteration: for $k = 0, 1, \dots$, compute $\mathbf{u}_{1,m+1}^{(k+1)}$ and $\mathbf{u}_{2,m+1}^{(k+1)}$.

For instance, in Ω_1 ,

$$\mathbf{u}_{1,m+1}^{(k+1)} = \tilde{\mathbf{u}}_{1,m+1} + \Delta t \varphi_2(\Delta t \mathbf{L}_1) \cdot \left[\mathbf{R}_1(t_{m+1}, \tilde{\mathbf{u}}_{1,m+1}, \psi_1(t_{m+1}), \mathbf{u}_{2,m+1}^{(k)}(N_{\beta,\alpha})) - \mathbf{R}_1(t_m, \mathbf{u}_{1,m}, \psi_1(t_m), \mathbf{u}_{2,m}(N_{\beta,\alpha})) \right].$$

- Stop if interface values from subdomain solutions are close enough.

Model problem

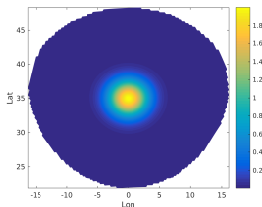
Rotating Shallow water equation (SWE)

$$\begin{cases} \partial_t h + \nabla \cdot (h\mathbf{u}) = 0, & \text{in } \Omega \times (0, T), \\ \partial_t \mathbf{u} + (f + \omega)\mathbf{k} \times \mathbf{u} + \nabla \left(\frac{|\mathbf{u}|^2}{2} + g(h + b) \right) = \mathbf{0}, & \text{in } \Omega \times (0, T), \end{cases}$$

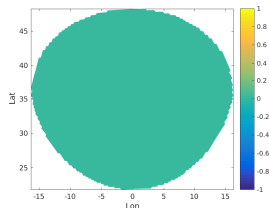
- h the fluid thickness, \mathbf{u} the velocity field, $\omega = \mathbf{k} \cdot (\nabla \times \mathbf{u})$ the relative vorticity, \mathbf{k} is the surface normal vector, g the acceleration of gravity, b the bottom topography and f the Coriolis parameter.
- Application of TRiSK scheme leads: $\mathbf{U}' = \mathbf{F}(\mathbf{U}, \psi)$ (see Lili's slides).
 - Approach I: $\mathbf{F} = \mathbf{J}_m \mathbf{U} + \mathbf{R}_m$,
where \mathbf{J}_m the Jacobian of \mathbf{F} at $\mathbf{U}(t_m)$ and $\mathbf{R}_m = \mathbf{F}(\mathbf{U}) - \mathbf{J}_m \mathbf{U}$ the remainder.
 - Approach II: $\mathbf{F} = \mathbf{A}_{ref} \mathbf{U} + \mathbf{R}_{ref}$, using Hamiltonian view (see Konstantin's slides).
- Application of LETD2 (Approach I \rightarrow LETD2; Approach II \rightarrow LETD2-wave).

Gaussian pulse test case

- SOMA test case inspired geometry (Ocean basin) with no forcing or smoothing.
- Primal SCVT mesh consists of 8521 cells, 25898 edges, and 17378 vertices.
- Gaussian initial condition:



Sea surface height



Velocity field

- No normal flow boundary condition $\mathbf{u} \cdot \mathbf{n} = 0$

Performance of LETD2

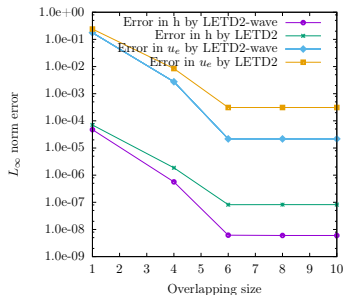
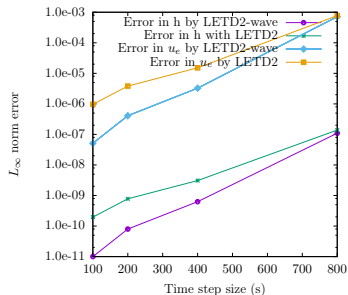
- 10 subdomains with nearly equal parts generated by METIS.
Overlapping 6 cells, and $\Delta t = 200$ s.
- Relative L_∞ error in h , using RK4 with $\Delta t = 1$ s as benchmark.
Average CPU time per step (CPU time per processor is shown for localized algorithms).

Methods	# Krylov vectors=20		# Krylov vectors=30	
	error	time	error	time
ETD2	8.2e-8	2.39e-01 s	8.2e-8 [h]	3.15e-01 s
LETD2	8.2e-8	5.12e-02 s	8.2e-8 [h]	7.01e-02 s
ETD2-wave	6.0e-9	5.84e-02 s	6.0e-9 [h]	8.00e-02 s
LETD2-wave	6.0e-9	1.73e-02 s	6.0e-9 [h]	2.10e-02 s

- No iteration needed** for LETD2 or LETD2-wave.

Localized schemes achieve the **same accuracy** as the associated global schemes, while **accelerating the simulations**; **ETD-wave** models are computationally more efficient than ETD models.

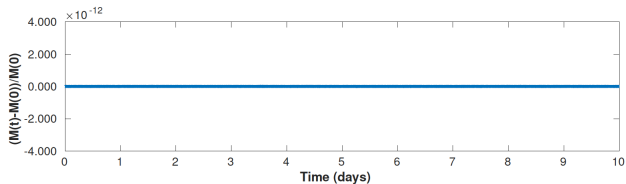
- 10 subdomains, 30 Krylov vectors.
- Relative L_∞ error in h and \mathbf{u} , using RK4 with $\Delta t = 1$ s as benchmark.

Error vs overlapping size when $\Delta t = 200$ s.

Error vs time step when overlapping 8 cells.

- 10-day simulation using LETD2-wave

10 subdomains, 30 Krylov vectors, and $\Delta t = 200$ s when overlapping 8 cells.



- Mass conservation** up to machine precision.

Conclusion

Summary

- Localized ETD algorithms with overlapping subdomains.

Reach the **same accuracy** as global schemes.

Speed up simulations through parallel performance.

Next steps

- **Convergence analysis** for Localized ETD applied to SWEs.

Extensions to **multi-layer SWEs**, and more complicated systems.