

Exponential Time Differencing for the Tracer Equations Appearing in Primitive Equation Ocean Models

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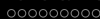
joint work with Konstantin Pieper and Max Gunzburger

LANL Meeting

January 17, 2019

Outline

- Tracer equation
- ETD solver for the tracer equation
- Numerical tests
- Future Work



Tracer Equation with vertical discretization

$$\frac{\partial(h_k T_k)}{\partial t} = -\nabla \cdot (h_k u_k T_k) - \bar{T}_k^t w_k^t + \bar{T}_{k+1}^t w_{k+1}^t + [D_h^T]_k + [D_\nu^T]_k ,$$

$$[D_h^T]_k = \nabla \cdot (h_k \kappa_h \nabla T_k) , \quad [D_\nu^T]_k = h_k \delta z_k^m (\kappa_\nu \delta z^t(T)) .$$

- m, t : location as the middle or top of the layer k in the vertical
- “:” in subscripts: multiple vertical layers were used for a vertical operator
- κ_h, κ_ν : diffusion
- $\bar{\phi}_k^t = \frac{\phi_{k-1} + \phi_k}{2}$
- $\delta z_k^m(\phi^t) = \frac{\phi_k^t - \phi_{k+1}^t}{h_k}$
- $\delta z_k^t(\phi^m) = \frac{\phi_{k-1}^m - \phi_k^m}{(\bar{h})_k^t}$

Full ETD Solver

Denote by T the tracer (temperature) and by $T_n \approx T(t_n)$ the current solution at time t_n . Let

$$\partial_t T = F(T) = A_n T + r_n(T) .$$

This equation is actually linear (u , h and w are constants), so the remainder is zero, namely

$$\partial_t T = F(T) = A_n T .$$

In this case, we can simply consider the exponential Euler method to find the solution, thus at the time step $n + 1$

$$T_{n+1} = T_n + \Delta t \varphi_1(\Delta t A_n) F(T_n) .$$

By taking $A_n = F'[T_n]$ (Exponential Rosenbrock Euler), this method gives the exact solution.

Splitting Scheme - One stage method

The transport and mixing in the vertical direction cause, in general, more restrictive requirements than the ones for the horizontal. Therefore, the linear operator A_n may be split into

$$A_n = A_n^z + A_n^x .$$

Thus,

$$\partial_t T = F(T) = A_n^z T + A_n^x T = A_n^z T + r_n(T) .$$

Using exponential Euler, $r_n(T)$ ($= A_n^x T$) is simply neglected, so the solution is given by

$$T_{n+1} = T_n + \Delta t \varphi_1(\Delta t A_n^z) F(T_n) .$$

Splitting Scheme - Two stages method

Using a second stage method following a predictor/corrector approach, we would get

$$T_{n+1}^{1st\ stage} = T_n + \Delta t \varphi_1(\Delta t A_n^Z) F(T_n),$$

$$T_{n+1} = T_{n+1}^{1st\ stage} + \frac{1}{2} \Delta t \varphi_1(\Delta t A_n^Z) (N_{n+1}^{1st\ stage} - N_n),$$

where $N_n = F(T_n) - A_n^Z T_n$, and

$N_{n+1}^{1st\ stage} = F(T_{n+1}^{1st\ stage}) - A_n^Z T_{n+1}^{1st\ stage}$, so N takes into account only the contribution from the horizontal terms.

Computationally, to build $N_{n+1}^{1st\ stage}$ I don't need to construct the full $F(T_{n+1}^{1st\ stage})$, but only the horizontal terms evaluated at $T_{n+1}^{1st\ stage}$.

Matrix A_n^z

Block diagonal structure of A_n^z :

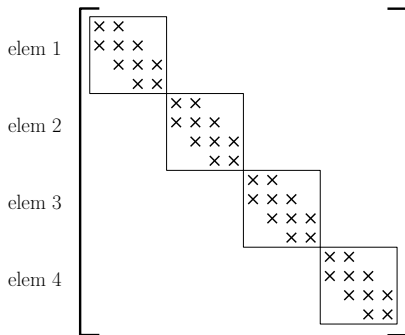


Figure: Simplified case with 4 horizontal elements and 4 vertical layers.

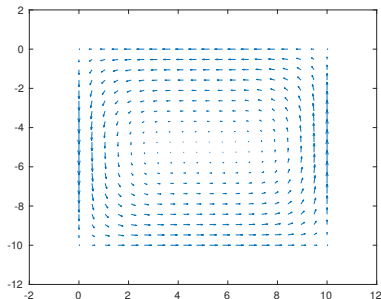
Pros of a block diagonal structure:

- ① Solving many small problems instead of a large one.
- ② Easy for parallelization purposes.

Box with a circular velocity field

Numerical Tests - Box shape geometry

Velocity Field $(u, w) = (-\psi_1(x)\psi_2'(z), \psi_1'(x)\psi_2(z))$



$$\psi_1(x) = 1 - \frac{(x - \frac{x_{max}}{2})^4}{(\frac{x_{max}}{2})^4}, \quad \psi_2(z) = 1 - \frac{(z - \frac{z_{min}}{2})^2}{(\frac{-z_{min}}{2})^2}$$

with $x_{max} = 10$ and $z_{min} = -10$.

Numerical Tests - Box shape geometry

40 layers of height $\Delta z = 0.25$ m

$\Delta x = 1$ m so 10 horizontal elements

$$\text{CFL}_x = \frac{\max u \cdot dt}{\Delta x} \quad \text{and} \quad \text{CFL}_z = \frac{\max w \cdot dt}{\Delta z}$$

3 solvers:

- Exponential Rosenbrock Euler (ERE)
- Splitting ETD 2 stages
- RK4 + implicit Euler

Numerical Tests - Box shape geometry

ERE ($dt = 6$): $CFL_z = 19.2$, $CFL_x = 2.4$

Splitting ETD 2 stages ($dt = 3$): $CFL_z = 9.6$, $CFL_x = 1.2$

RK4 + implicit Euler ($dt = 0.5$): $CFL_z = 1.6$, $CFL_x = 0.2$

Constant CFL ratio: $\frac{CFL_z}{CFL_x} = 8$

	$k_\nu = 2.5 \cdot 10^{-5}$		
	dt	time steps	computational time
ERE	6	750	16.5680
Splitting ETD 2 stages	3	1500	31.8529
RK4 + implicit Euler	0.5	9000	89.3249

Table: Results for the three solvers, all times are in seconds (s).

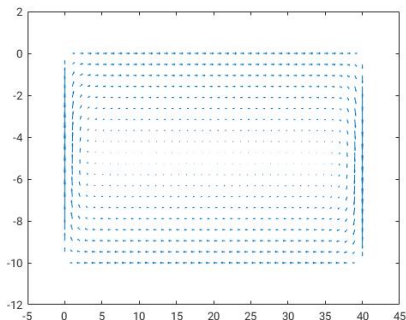
Note: n. of vectors in the Krylov basis:

4 vectors for the four central elements and 8 for the six external ones.

Rectangle with a circular velocity field

Numerical Tests - Rectangle shape geometry

Velocity Field $(u, w) = (-\psi_1(x)\psi_2'(z), \psi_1'(x)\psi_2(z))$



$$\psi_1(x) = 1 - \frac{(x - \frac{x_{max}}{2})^{16}}{(\frac{x_{max}}{2})^{16}}, \quad \psi_2(z) = 1 - \frac{(z - \frac{z_{min}}{2})^2}{(\frac{-z_{min}}{2})^2}$$

with $x_{max} = 40$ and $z_{min} = -10$.

Numerical Tests - Rectangle shape geometry

40 layers of height $\Delta z = 0.25$ m

$\Delta x = 1$ m so 40 horizontal elements

CFL ratio: $\frac{CFL_z}{CFL_x} = 8$

	$k_\nu = 2.5 \cdot 10^{-5}$		
	dt	time steps	computational time
Splitting ETD 2 stages	2.8	5,000	244.0533
RK4 + implicit Euler	0.5	28,000	669.9195

Table: Results for the three solvers, all times are in seconds (s).

Note: n. of vectors in the Krylov basis:

4 vectors for the thirty-four central elements and 8 for the six external ones.

Primitive equations tests - Qualitative Results

Lock Exchange:

Test Description:

- 20 layers, each of which has a thickness of 1 m
- Initial condition for velocity: $u = 0$ in every layer
- Initial condition for temperature:

$$T(x, z) = \begin{cases} 5, & x < 32 \text{ km}, \\ 30, & x \geq 32 \text{ km}. \end{cases}$$

All diffusion are turned off, so the correct solution is where no mixing occurs, and the front propagates with no intermediate temperatures between 5° C and 30° C.

With z-level coordinates, the intermediate layers have temperature in between 5° C and 30° C.

Primitive equations tests - Qualitative Results

Lock Exchange test case with $\nu_h = 100$:

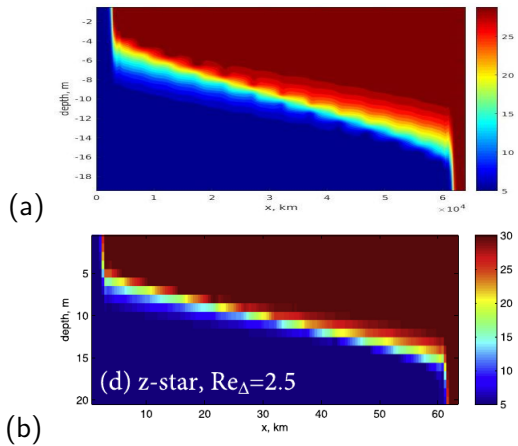


Figure: (a) our ETD solver, (b) MPAS Ocean.

Primitive equations tests - Qualitative Results

Internal Waves:

The initial temperature distribution is $T_0(z) + T'(x, z)$, where

$$T_0(z) = T_{bot} + (T_{top} - T_{bot}) \frac{z_{bot} - z}{z_{bot}}, \text{ and}$$

$$T'(x, z) = -A \cos\left(\frac{\pi}{2L}(x - x_0)\right) \sin\left(\pi \frac{z + 0.5\Delta z}{z_{bot} + 0.5\Delta z}\right),$$

where $T_{bot} = 10.1^\circ \text{ C}$, $T_{top} = 20.1^\circ \text{ C}$, $z_{bot} = -487.5 \text{ m}$, $L = 50 \text{ km}$, $x_0 = 125 \text{ km}$, $x_0 - L < x < x_0 + L$, $\Delta z = 25 \text{ m}$, and $A = 2^\circ \text{ C}$.

The perturbation is a single hump of displaced isotherms that initiate symmetric waves propagating out from the center.

Primitive equations tests - Qualitative Results

Internal Waves:

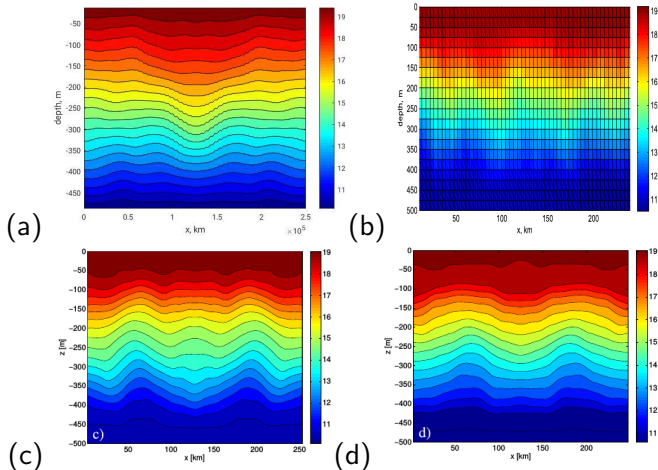


Figure: (a) our ETD solver, (b) MPAS Ocean, (c) MITgem, (d) MOM

Future Work

- Further testing of the splitting ETD scheme with two stages.
- Testing the performances of the proposed solver on more realistic applications.
- Simulating the behavior of multiple tracers in addition to the temperature, such as contaminants and salinity.
- Investigating spatial grid refinements so that passive tracer transport (of, e.g., contaminants) can be handled.

References

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