Exponential Integrators with Fast and Slow Mode Splitting for Multilayer Ocean Models

Konstantin Pieper[1] K. Chad Sockwell[1,3] Max Gunzburger[1]

Part of a joint project with:

Thi-Thao-Phuong Hoang Lili Ju[2] Wei Leng Xucheng Meng[2] Zhu Wang[2]
Huanhuan Yang

[1]Department of Scientific Computing, Florida State University
[2]Department of Mathematics and Interdisciplinary Mathematics Institute, University of South Carolina
[3]LANL

January 17, 2018

State of time-stepping in MPAS-O

Time-stepping

- RK4: global time-step $\Delta t < \Delta t_{CFL}$
  - stable and easy to implement in parallel
  - does not exploit fast/slow dynamics
- Split-Explicit: coupling at global time-step Δt

  split into:
  - *barotropic mode (free surface)*:
    explicit time-step $\Delta t / M$ for $M > 1$
  - *dynamics minus barotropic mode*:
    explicit time-step Δt
  - *tracers* (explicit, split into vertical and horizontal)
  - *vertical mixing/diffusion* (implicit)

Multi-layer shallow water model

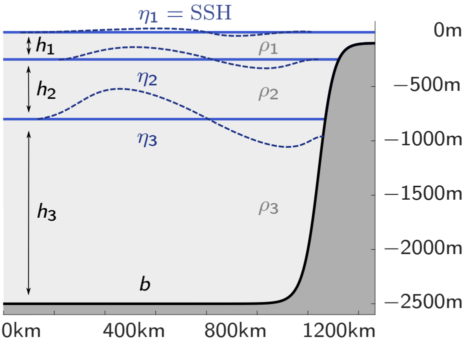
Model and solution variables

- L layers with uniform densities ρ_k, $k = 1, \ldots, L$
- bottom topography b
- layer thickness

$$h_k = \bar{h}_k + \Delta h_k$$

- layer velocity u_k (along isopycnal)
- layer interfaces

$$\eta_k = b + \sum_{i=k}^{L} h_i$$



Conserved quantities

Mass: $$m(h, u) = \sum_{k=1}^{L} \rho_k \int_{\Omega} h_k$$

Energy: $$H(h, u) = \frac{1}{2} \sum_{k=1}^{L} \int_{\Omega} \left[g\, \Delta\rho_k (\eta_k - \bar{\eta}_k)^2 + \rho_k h_k u_k^2 \right]$$

Hamiltonian view of the (multilayer) rotating shallow water equations

$$\partial_t V = F(V) = J(V)\delta H(V)$$

- prognostic variables $V = (h, u)^\top$ on C-grid at cell centers i and edges e (TRiSK-scheme[1])
- block diagonal differential operator $J(V) = \mathbf{diag}(J_k(V_k))$ and mass matrix M

$$J_k(V_k) = \frac{1}{\rho_k}\begin{pmatrix} 0 & -\boldsymbol{\nabla}\boldsymbol{\cdot}_{e\to i} \\ -\boldsymbol{\nabla}_{i\to e} & Q(h_k, u_k)_{e\to e} \end{pmatrix}, \quad M = \begin{pmatrix} M^i & 0 \\ 0 & M^e \end{pmatrix},$$

- discrete Hamiltonian/energy

$$H(V) = \frac{1}{2}\sum_{k=1}^{L}\left[g\,\Delta\rho_k\|\eta_k(h) - \bar{\eta}_k\|^2_{M^i} + \rho_k(\hat{h}_{k,e} * u_k, u_k)_{M^e}\right],$$

- symmetries[2]:

$$MJ(V) = -J(V)^\top M, \qquad M\,\delta^2 H(V) = \delta^2 H(V)^\top M$$

---

[1] Ringler et al. 2010.

[2] Eldred and Randall 2017; Thuburn and Cotter 2012.

Additional dissipation and source terms (in momentum equation)

$$\partial_t V = F(V) = \underbrace{J(V)\delta H(V)}_{\substack{\text{contains fast modes} \\ CFL_{\mathrm{wave}} \sim \sqrt{g|b|}/\Delta x}} + \underbrace{S(V) + F_{\mathsf{drag}}(V) + F_{\mathsf{wind}}(V)}_{\substack{\text{slow processes} \\ CFL \ll CFL_{\mathrm{wave}}}}$$

- wind forcing in top layer $F_{\mathsf{wind}}(V)$
- drag terms in bottom layer:

$$F_{\mathsf{drag}}(V) = -c_{\mathsf{drag}} \begin{pmatrix} 0 \\ |u_L| u_L / h_L \end{pmatrix}$$

- dissipation term:

$$S_k(V_k) = -\nu_{\Delta x} \begin{pmatrix} 0 \\ (1/h_k) D_{\substack{-\Delta \\ e \to e}} h_k D_{\substack{-\Delta \\ e \to e}} u_k \end{pmatrix}$$

  - biharmonic smoothing operator
  - turbulence closure

Double gyre test case (based on SOMA[3])

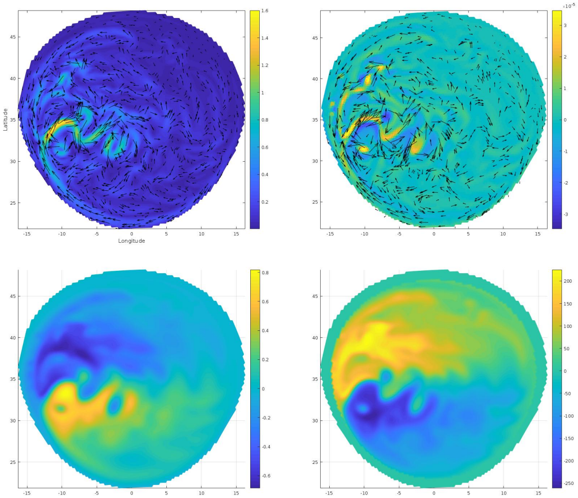


Figure: velocity and vorticity $\nabla \times u$ in top layer (first row) sea surface height η_1 and layer η_2 (second row)

Parameters

- three layer
- wind forcing in zonal direction in top layer
- 32km or 16km resolution
- five year spin-up

CFL-requirements (RK4 on 32km)

- *full model:* $\Delta t < 3.7$[min] (wave speed: 156[m/s])
- *minus waves:* $\Delta t < 414$[min] (advection: 1.6[m/s])

[3] Wolfram et al. 2015.

Exponential Runge Kutta methods[4]

- split the forcing term in linear part and remainder

$$
\begin{aligned}
\partial_t V &= F(V) \\
&= AV + \left[F(V) - AV\right] \\
&= \underbrace{F(V_n) + A(V - V_n)}_{\text{Linear approximation}} + \underbrace{\left[F(V) - F(V_n) - A(V - V_n)\right]}_{\text{Residual } R(V)}
\end{aligned}
$$

  - Taylor-expansion: $A_n = F'(V_n)$ (Rosenbrock-ETD)

- Exponential Euler method

$$V_{n+1} = V_n + \Delta t \varphi_1(\Delta t A_n) F(V_n)$$

- Exponential RK2 method (for $A_n \neq F'(V_n)$)

$$
\begin{aligned}
V_n^1 &= V_n + \Delta t \varphi_1(\Delta t A_n) F(V_n) && \text{“Exponential Euler”} \\
V_{n+1} &= V_n^1 + \Delta t \varphi_2(\Delta t A_n) R(V_n^1) && \text{“Second order correction”}
\end{aligned}
$$

- φ-functions:

$$\varphi_0(z) = \exp(z), \quad \varphi_1(z) = (\exp(z) - 1)/z, \quad \varphi_2(z) = (\exp(z) - 1 - z)/z^2, \quad \ldots$$

[4] Hochbruck and Ostermann 2010.

Choice of the linear operator

Splitting of the forcing term at step n

$$F(V) = J(V)\delta H(V) \approx F(V_n) + A_n(V - V_n)$$

- Taylor expansion[5]

$$A_n = F'(V_n) = \underbrace{J(V_n)}_{\substack{\text{frozen}\\ J\text{-operator}}} \underbrace{\delta^2 H(V_n)}_{\substack{\text{quadratic}\\ \text{approximation}\\ \text{of energy}}} + \underbrace{J'(V_n)(\cdot)}_{\substack{\text{derivatives}\\ \text{of potential vorticity } q}} \delta H(V_n)$$

- wave operator approximation[6]:
  linearize at $\bar{V} = (\bar{h}, 0)$ for a reference heights $\bar{h}$, zero velocities

$$A_n = \bar{A} = F'(\bar{V}) = J(\bar{V})\delta^2 H(\bar{V})$$

Multilayer rotating wave equation

$$\partial_t V = J(\bar{V})\delta^2 H(\bar{V})\ V \quad \rightsquigarrow \quad \begin{cases} \partial_t h = -\nabla \cdot (\bar{h}\, u) \\ \partial_t u = -g\nabla \hat{\mathrm{R}}\, h + f\, k \times u \end{cases}$$

[5] Gaudreault and Pudykiewicz 2016.
[6] Haut and Wingate 2014.

Barotropic vs. baroclinic components of the wave operator

Eigenvalue problem (reference state $\bar{V} = (\bar{h}, 0)$)

$$\lambda V_\lambda = \bar{A} V_\lambda = J(\bar{V})\delta^2 H(\bar{V})\, V_\lambda \quad \rightsquigarrow \quad \begin{cases} \lambda h_\lambda = -\nabla \cdot (\bar{h}\, u_\lambda) \\ \lambda u_\lambda = -g \nabla \hat{\mathrm{R}}\, h_\lambda + f\, k \times u_\lambda \end{cases}$$

- vertical structure of the velocity-modes $u_\lambda = \mathbf{diag}(1/\bar{h}_k)\mathrm{D}\eta_\lambda$:

$$\lambda^2\, \mathbf{diag}(\Delta \rho_k)\, \eta_\lambda = \mathrm{D}^*\, \mathbf{diag}(\rho_k/\bar{h}_k)\mathrm{D}\, \eta_\lambda$$

$$\lambda^2 \rho'(z)\eta_\lambda(z) = \nabla \cdot (\rho \nabla \eta_\lambda(z))$$

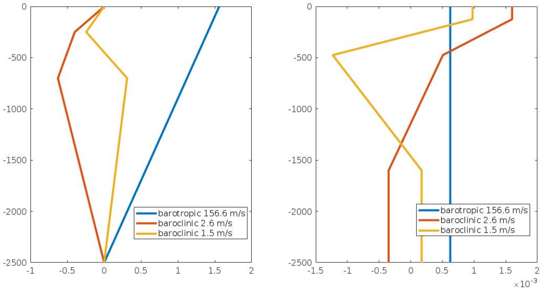


Figure: Vertical η- and velocity-modes and corresponding wave speeds.

Reduction to barotropic mode (similar to split-explicit scheme[7])

- most energy contained in the barotropic mode (variables $(\boldsymbol{h}, \boldsymbol{u})$)

$$u_{\text{baro},k} \approx \mathbf{u}, \quad h_{\text{baro},k} \approx \mathbf{h}\,\frac{\bar{h}_k}{\sum_k \bar{h}_k}, \quad k = 1, \ldots, L.$$

- corresponding Ansatz

$$\begin{pmatrix} h_{\text{baro}} \\ u_{\text{baro}} \end{pmatrix} = G \begin{pmatrix} \boldsymbol{h} \\ \boldsymbol{u} \end{pmatrix}$$

- corresponding left inverse with $G^\dagger G = \text{Id}$

$$\begin{pmatrix} \boldsymbol{h} \\ \boldsymbol{u} \end{pmatrix} = G^\dagger \begin{pmatrix} h \\ u \end{pmatrix}$$

- replace multilayer operator A by projected version

$$PAP = G \underbrace{G^\dagger A G}_{=\boldsymbol{A}} G^\dagger; \qquad\qquad P = GG^\dagger$$

[7] Higdon 2005.

Barotropic method

- consider ETD-methods based on $A = J(\bar{V})\delta^2 H(\bar{V})$ with

$$\partial_t V = F(V) = PAP\,V + r(V); \qquad P = GG^\dagger$$

- symplectic structure preserved: $\boldsymbol{A} = G^\dagger A G = \boldsymbol{J}\ \boldsymbol{\delta^2 H}$

$$\boldsymbol{\delta^2 H} = G^\top \delta^2 H(\bar{V}) G$$
$$\boldsymbol{J} = G^\dagger J(\bar{V})(G^\dagger)^\top$$

- computation of the φ-functions

$$\varphi_s(\Delta t PAP) = \frac{1}{s!}(\mathrm{Id} - P) + G\varphi_s(\Delta t \boldsymbol{A})G^\dagger$$

- corresponding exponential Euler

$$V_{n+1} = V_n + \Delta t(\mathrm{Id} - P)F(V_n) + \Delta t\, G\varphi_1(\Delta t \boldsymbol{A})G^\dagger F(V_n)$$

Computation of φ-functions

- any S-stage ETD-RK requires $\geq S$ computations of

$$w(\Delta t) = \Delta t \varphi_s(\Delta t A) b, \quad s \in \{ 1, \ldots, S \}$$

- equivalent to solution of

$$w'(t) = A w(t) + c_s t^{s-1}\, b, \quad t \in (0, \Delta t), \quad w(0) = 0 \,,$$

Polynomial approximation

$$\varphi_s(\Delta t A) b \approx p_K(A) b$$

- explicit time-stepping (substepping)
- Krylov methods (skew-Lanzcos for skew-symmetric A)
- Chebychev-polynomials

Rational approximation

$$\varphi_s(\Delta t A) b \approx \begin{cases} p_K((I + \gamma A)^{-1}) b \\ p_{K-1}(A) / p_k(A) b \end{cases}$$

- implicit time-stepping (substepping)
- rational Krylov methods (shift-inverse Arnoldi; SIA)
- optimal rational polynomials

K *much smaller* than for polynomial approximation

Spectral filters with Arnoldi

- high frequency error can accumulate over long times ($\sim$ months)
- including a biharmonic smoothing in the linear operator A
  - loss of skew-symmetry
  - can be detrimental for performance
- alternative approach: substitute

$$\varphi_s(\Delta t H_K) \rightsquigarrow \varphi_s^{\gamma}(\Delta t H_K) = \varphi_s(\Delta t H_K - \Delta t^{2p}/\gamma^{2p}(H_K^* H_K)^p)$$

  - can be interpreted as additional p-order harmonic viscosity $\Delta t^{\mathbf{2}p-\mathbf{1}}/\gamma^{\mathbf{2}p}(A^*A)^p$
  - vanishes for $\Delta t \to 0$ (of order $2p-1$)
  - no additional cost

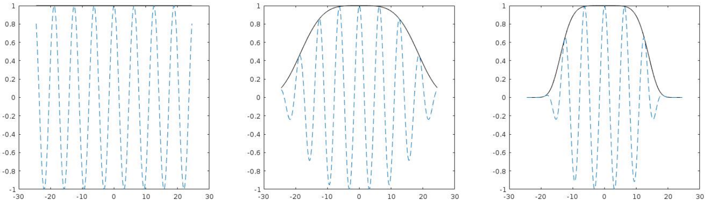


Figure: Visualization for $\Delta t = 10\Delta t_{\mathbf{RK4}}$. From left to right: $\exp(z)$, $\exp^{\gamma}(z) = \exp\big(z - |z/\gamma|^{\mathbf{4}}\big)$ for $\gamma = 20$, and matrix exponential obtained from ten RK4 steps.

Runtimes and statistics for three layer SOMA-testcase

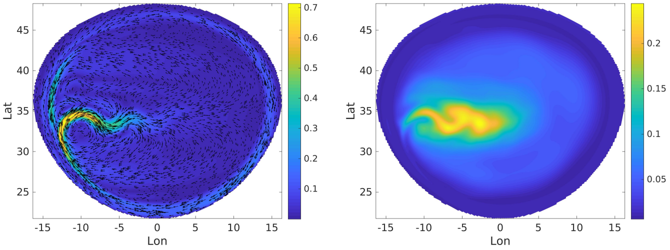


Figure: SOMA simulation statistics: The mean flow of the velocity, vectors and magnitude (left) and the RMS-SSH (right) over ten years.

Method	K	$\Delta t/\Delta t_{\mathrm{RK4}}$	SYPD	mean-flow (rel.)	SSH-RMS
RK4	–	3/4	0.9	0.054	0.054
ETD2wave	63	15	2.8	0.044	0.060
B-ETD2wave	35	7	4.6	0.037	0.071
B-ETD3wave	98	25	5.3	0.064	0.085
ETD2wave (SIA)	7	50	5.3	0.064	0.082

Table: Comparison of the ETD methods against the base-line RK4 method: the number of Krylov vectors K, the average simulated years per real day (SYPD), the relative mean velocity error in the $L^2_{\bar{h}}$ norm, and the RMS-SSH error in the L^∞ norm.

Conclusions and Outlook

Conclusions

- mode splitting with exponential integrators
- several ways to approximate the φ-functions

Outlook

- investigate multiple vertical modes in practice (e.g., barotropic & first baroclinic)
- most costly operation: computation of the φ-functions
  - inverse Arnoldi
  - specialized methods based on domain decomposition
  - reduced order modeling (talk by Chad Sockwell)
- combination of ETD and domain decomposition (talk by Zhu Wang)

Pieper, K., K. C. Sockwell, and M. Gunzburger (2018). "Exponential time differencing for mimetic multilayer ocean models".

References

Eldred, C. and D. Randall (2017). "Total energy and potential enstrophy conserving schemes for the shallow water equations using Hamiltonian methods-Part 1: Derivation and properties". In: *Geoscientific Model Development* 10.2.

Gaudreault, S. and J. A. Pudykiewicz (2016). "An efficient exponential time integration method for the numerical solution of the shallow water equations on the sphere". In: *Journal of Computational Physics* 322.

Haut, T. and B. Wingate (2014). "An asymptotic parallel-in-time method for highly oscillatory PDEs". In: *SIAM Journal on Scientific Computing* 36.2.

Higdon, R. L. (2005). "A two-level time-stepping method for layered ocean circulation models: further development and testing". In: *Journal of Computational Physics* 206.2.

Hochbruck, M. and A. Ostermann (2010). "Exponential integrators". In: *Acta Numerica* 19.

Ringler, T. D. et al. (2010). "A unified approach to energy conservation and potential vorticity dynamics for arbitrarily-structured C-grids". In: *Journal of Computational Physics* 229.9.

Thuburn, J. and C. J. Cotter (2012). "A framework for mimetic discretization of the rotating shallow-water equations on arbitrary polygonal grids". In: *SIAM Journal on Scientific Computing* 34.3.

Wolfram, P. J. et al. (2015). "Diagnosing isopycnal diffusivity in an eddying, idealized midlatitude ocean basin via Lagrangian, in Situ, Global, High-Performance Particle Tracking (LIGHT)". In: