

# Time-Stepping Methods for PDEs and Ocean Models

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1. On the Spatial and Temporal Order of Convergence of PDEs
  - 1.1 Analytical Derivation
  - 1.2 Derivation by Symbolic Algebra
  - 1.3 Numerical Experiments
  
2. Time-Stepping Methods for Ocean Models
  - 2.1 Barotropic-Baroclinic Splitting and Filtering of Barotropic Modes
  - 2.2 Verification Suite of Shallow Water Test Cases

## 1. On the Spatial and Temporal Order of Convergence of PDEs

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## 2. Time-Stepping Methods for Ocean Models

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# 1. On the Spatial and Temporal Order of Convergence of PDEs

Pop Quiz: Order of Convergence of Global Solution Error Norm with Respect to Exact Solution

You are modeling the PDE  $u_t = \mathcal{F}(u, u_x, u_{xx}, \dots, x, t)$

Numerical Method $\mathcal{O}(\Delta x^\alpha), \mathcal{O}(\Delta t^\beta)$	Refinement in Space: $\Delta x \rightarrow 0, \Delta t$ fixed	Refinement in Time: $\Delta t \rightarrow 0, \Delta x$ fixed	Refinement in Space and Time: $\Delta x \rightarrow 0, \Delta t \rightarrow 0, \Delta t/\Delta x$ fixed
$\alpha = 2, \beta = 1$			
$\alpha = 2, \beta = 2$			
$\alpha = 2, \beta = 3$			

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- With a stable numerical scheme, the order of accuracy of the global solution error is the same as that of the global truncation error,

$$\hat{\tau}_G = \mathcal{O}(\Delta x^\alpha) + \Delta t \mathcal{O}(\Delta x^\alpha) + \Delta t^2 \mathcal{O}(\Delta x^\alpha) + \dots + \Delta t^{\beta-1} \mathcal{O}(\Delta x^\alpha) + \mathcal{O}(\Delta t^\beta)$$

which can be approximated as

$$\hat{\tau}_G \approx \mathcal{O}(\Delta x^\alpha) + \mathcal{O}(\Delta t^\beta), \text{ for } \Delta t \ll 1$$

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$\alpha = 2, \beta = 1$	Convergence		
$\alpha = 2, \beta = 2$	Not Attained: Why?		
$\alpha = 2, \beta = 3$	$\mathcal{O}(\Delta t^\beta)$ dominates		

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$\alpha = 2, \beta = 2$	Not Attained: Why?	Not Attained: Why?	
$\alpha = 2, \beta = 3$	$\mathcal{O}(\Delta t^\beta)$ dominates	$\mathcal{O}(\Delta x^\alpha)$ dominates	

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- A simultaneous refinement of  $\Delta t$  and  $\Delta x$ , while maintaining their ratio  $\Delta t/\Delta x = \gamma$ , a constant, yields

$$\hat{\tau}_G \approx \mathcal{O}(\Delta x^\alpha) + \mathcal{O}(\Delta t^\beta) = \mathcal{O}(\Delta x^\alpha) + \mathcal{O}(\gamma^\beta \Delta x^\beta) = \mathcal{O}(\Delta x^\alpha) + \mathcal{O}(\Delta x^\beta) \approx \mathcal{O}(\Delta x^{\min(\alpha, \beta)})$$



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$\alpha = 2, \beta = 2$	Not Attained: Why?	Not Attained: Why?	$\min(\alpha, \beta) = \min(2, 2) = 2$
$\alpha = 2, \beta = 3$	$\mathcal{O}(\Delta t^\beta)$ dominates	$\mathcal{O}(\Delta x^\alpha)$ dominates	$\min(\alpha, \beta) = \min(3, 2) = 2$

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- A simultaneous refinement of  $\Delta t$  and  $\Delta x$ , while maintaining their ratio  $\Delta t/\Delta x = \gamma$ , a constant, yields

$$\hat{\tau}_G \approx \mathcal{O}(\Delta x^\alpha) + \mathcal{O}(\Delta t^\beta) = \mathcal{O}(\Delta x^\alpha) + \mathcal{O}(\gamma^\beta \Delta x^\beta) = \mathcal{O}(\Delta x^\alpha) + \mathcal{O}(\Delta x^\beta) \approx \mathcal{O}(\Delta x^{\min(\alpha, \beta)}).$$

- Strategy:** Given  $\alpha$ , we need  $\beta \geq \alpha$  to obtain maximum possible order of accuracy. But we gain no improvement in order of convergence for  $\beta > \alpha$  despite more work. So, optimum choice is  $\beta = \alpha$ .

# 1. On the Spatial and Temporal Order of Convergence of PDEs

Order of convergence of the error norm in the asymptotic regime at constant ratio of time-step to grid spacing for varying orders of spatial and temporal discretizations

Order of Spatial Discretization $\alpha$	Time-Stepping Method Employed	Order of Time-Stepping Method $\beta$	Order of Convergence of Error Norm in Asymptotic Regime at Constant Ratio of Time-Step to Grid Spacing $\min(\alpha, \beta)$
1	FE	1	$\min(1,1) = 1$
1	RK2 or AB2	2	$\min(1,2) = 1$
1	RK3 or AB3	3	$\min(1,3) = 1$
1	RK4 or AB4	4	$\min(1,4) = 1$
2	FE	1	$\min(2,1) = 1$
2	RK2 or AB2	2	$\min(2,2) = 2$
2	RK3 or AB3	3	$\min(2,3) = 2$
2	RK4 or AB4	4	$\min(2,4) = 2$
3	FE	1	$\min(3,1) = 1$
3	RK2 or AB2	2	$\min(3,2) = 2$
3	RK3 or AB3	3	$\min(3,3) = 3$
3	RK4 or AB4	4	$\min(3,4) = 3$
4	FE	1	$\min(4,1) = 1$
4	RK2 or AB2	2	$\min(4,2) = 2$
4	RK3 or AB3	3	$\min(4,3) = 3$
4	RK4 or AB4	4	$\min(4,4) = 4$

FE  $\equiv$  forward Euler, RK  $\equiv$  Runge-Kutta, and AB  $\equiv$  Adams-Bashforth

# 1. On the Spatial and Temporal Order of Convergence of PDEs: Motivation

- A graduate level textbook on numerical analysis typically contains standard predictor-corrector and multistep time-stepping methods applied to ODEs in one chapter, followed by spatial discretization operators of PDEs in another.
- In real-world applications, the discretization of the PDE consists of both spatial and temporal components.
- The order of convergence of a PDE with spatial and/or temporal refinement is a function of both the mesh spacing  $\Delta x$  and the time step  $\Delta t$ .
- I investigate this simultaneous dependence of the local truncation error of the numerical solution of a PDE on  $\Delta x$  and  $\Delta t$ , for varying orders of spatial and temporal discretizations.

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# 1.1. Analytical Derivation of Local Truncation Error

## Local Truncation Error of a Generic Hyperbolic PDE

**Theorem 1.** Given the exact solution  $u_j^n$  of a hyperbolic PDE  $u_t = \mathcal{F}(u, u_x, x, t)$  on a uniform mesh with spacing  $\Delta x$ , at spatial locations  $x_j$  for  $j = 1, 2, \dots$ , and at time level  $t^n$ , the exact solution at time level  $t^{n+1} = t^n + \Delta t$  may be obtained by Taylor expanding  $u_j^n$  about time level  $t^n$  as

$$u_j^{n+1} = u_j^n + \sum_{k=1}^{\infty} \frac{\Delta t^k}{k!} \left( \frac{\partial^k u}{\partial t^k} \right)_j^n \equiv u_j^n + \sum_{k=1}^{\infty} \frac{\Delta t^k}{k!} (\mathcal{F}^{(k)})_j^n,$$

where  $(\mathcal{F}^{(k)})_j^n = \left( \frac{\partial^k u}{\partial t^k} \right)_j^n$  is the  $k^{\text{th}}$ -order spatial derivative at  $x_j$  and  $t^n$ . The numerical solution at time level  $t^{n+1}$ , obtained with a time-stepping method belonging to the Method of Lines, may be written in the general form

$$\hat{u}_j^{n+1} = u_j^n + \sum_{k=1}^{\infty} \frac{\Delta t^k}{k!} \left( \hat{\mathcal{F}}^{(k)} + \mathcal{O}(\Delta x^\alpha) \right)_j^n,$$

where  $\alpha$  is the order of the spatial discretization and  $\hat{\mathcal{F}}^{(k)}$  is specified by the time-stepping method. If  $\beta$  represents the order of the time-stepping method,

$$\left( \hat{\mathcal{F}}^{(k)} \right)_j^n = \left( \mathcal{F}^{(k)} \right)_j^n \equiv \left( \frac{\partial^k u}{\partial t^k} \right)_j^n, \text{ for } k = 1, 2, \dots, \beta.$$

The local truncation error is then

$$\begin{aligned} \hat{\tau}_j^{n+1} &= u_j^{n+1} - \hat{u}_j^{n+1} \\ &= \frac{\Delta t}{1!} \mathcal{O}(\Delta x^\alpha) + \frac{\Delta t^2}{2!} \mathcal{O}(\Delta x^\alpha) + \frac{\Delta t^3}{3!} \mathcal{O}(\Delta x^\alpha) + \dots + \frac{\Delta t^\beta}{\beta!} \mathcal{O}(\Delta x^\alpha) + \frac{\Delta t^{\beta+1}}{(\beta+1)!} (c_{\beta+1} + \mathcal{O}(\Delta x^\alpha))_j^n + \mathcal{O}(\Delta t^{\beta+2}) \\ &= \Delta t \mathcal{O}(\Delta x^\alpha) + \Delta t^2 \mathcal{O}(\Delta x^\alpha) + \Delta t^3 \mathcal{O}(\Delta x^\alpha) + \dots + \Delta t^\beta \mathcal{O}(\Delta x^\alpha) + \mathcal{O}(\Delta t^{\beta+1}), \end{aligned}$$

where  $(c_{\beta+1})_j^n = (\mathcal{F}^{(\beta+1)})_j^n - \left( \hat{\mathcal{F}}^{(\beta+1)} \right)_j^n \neq 0$ .

**Bishnu, S., Petersen, M., Quaife, B., "On the Spatial and Temporal Order of Convergence of Hyperbolic PDEs", *Journal of Computational Physics* (submitted)**



# 1.1. Analytical Derivation of Local Truncation Error

But wait! I can still verify the order of accuracy by refining only  $\Delta x$  or  $\Delta t$ !

- Assume a stable numerical scheme,  $\Delta t \ll 1$ , and the the global solution error is of the same order of accuracy as the global truncation error  $\hat{\tau}_G \approx \mathcal{O}(\Delta x^\alpha) + \mathcal{O}(\Delta t^\beta) \approx \zeta \Delta x^\alpha + \zeta_{\beta+1} \Delta t^\beta$ .
- Convergent behavior as  $\Delta t \rightarrow 0$ , keeping  $\Delta x$  fixed (refinement only in time)
  - Given  $\Delta x$  and  $\Delta t$ , measure the global solution error at a time horizon.
  - Reduce  $\Delta t$  by a constant ratio, say  $p$ , but keep  $\Delta x$  fixed.
  - Measure the global solution error at the same time horizon.
  - Plot the norm of the difference between the errors against  $\Delta t$ .
- **Proof:** For two time steps  $\Delta t_i$  and  $\Delta t_{i+1}$ , with  $\Delta t_{i+1}/\Delta t_i = p < 1$ , we can write

$$(\hat{\tau}_{G_i})_j \approx \zeta \Delta x^\alpha + \zeta_{\beta+1} \Delta t_i^\beta, \quad (\hat{\tau}_{G_{i+1}})_j \approx \zeta \Delta x^\alpha + \zeta_{\beta+1} \Delta t_{i+1}^\beta,$$

$$\Delta \left\{ (\hat{\tau}_{G_{i,i+1}})_j \right\} = (\hat{\tau}_{G_i})_j - (\hat{\tau}_{G_{i+1}})_j = \zeta_{\beta+1} \left( \Delta t_i^\beta - \Delta t_{i+1}^\beta \right) = \zeta_{\beta+1} \Delta t_{i+1}^\beta \left( p^{-\beta} - 1 \right).$$

Taking logarithm of both sides,

$$\log \left[ \Delta \left\{ (\hat{\tau}_{G_{i,i+1}})_j \right\} \right] = \theta + \beta \log(\Delta t_{i+1}), \quad \text{where } \theta = \log \left\{ \zeta_{\beta+1} \left( p^{-\beta} - 1 \right) \right\} \text{ is constant.}$$

- Note that the exact solution is independent of  $\Delta x$  or  $\Delta t$ . So,

$$\Delta \hat{\tau}_G \equiv \hat{\tau}_{G^1} - \hat{\tau}_{G^2} = (u_{\text{exact}} - u_{\text{numerical}}^1) - (u_{\text{exact}} - u_{\text{numerical}}^2) = u_{\text{numerical}}^2 - u_{\text{numerical}}^1.$$

- By plotting norm of error (or numerical solution) difference between successive spatial resolutions, we can attain convergence with spatial order of accuracy.

# 1.1. Analytical Derivation of Local Truncation Error

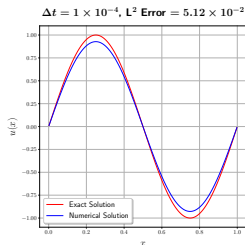
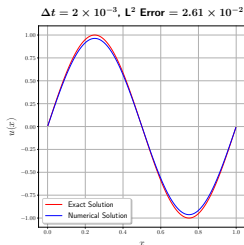
## Increase in Global Solution Error with only Temporal Refinement

For certain PDEs and discretization methods, the global solution error can increase with only temporal refinement. A simple example is the one-dimensional linear homogeneous constant-coefficient advection equation  $u_t + au_x = 0$ , discretized in space with the first-order upwind finite difference scheme and advanced in time with the first-order Forward Euler method. The global truncation error, approximating the global solution error, is

$$\left[ (\hat{\tau}_G)_j \right]_{\text{leading order}} = -\frac{1}{2}|a|\Delta x \left( 1 - \frac{|a|\Delta t}{\Delta x} \right) (u_{xx})_j^n = -\frac{1}{2}|a|\Delta x (1 - C) (u_{xx})_j^n.$$

where  $C = |a|\Delta t/\Delta x$  is the Courant number, which is positive and must be less than one to ensure numerical stability. Maintaining  $C < 1$ , if  $\Delta x$  is held constant and  $\Delta t$  is refined, then  $(1 - C)$  increases towards 1, and the magnitude of the global truncation error increases. Moreover, the error will be diffusive in nature.

## Numerical Example: $\Delta x = 1/2^8$ (fixed)



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## 1.2. Derivation by Symbolic Algebra

Developed a Symbolic Python (SymPy) library (consisting of  $\sim 12,600$  lines of code) that contains

- Taylor Series expansion in  $x, y, z$ ,
- routines for determining the local truncation error of
  - the generic ODE  $u_t = \mathcal{F}(u, t)$ , and the generic hyperbolic PDE  $u_t = \mathcal{F}(u, u_x, x, t)$
  - a specific ODE  $u_t + (p_0 + q_1)u = f(t)$ , and specific PDEs, such as the inhomogeneous, linear variable-coefficient and non-linear advection equations

$$u_t + p(x)u + (q(x)u)_x = f(x, t),$$
$$u_t + uu_x = f(x, t).$$

If  $p(x) = p_0$ ,  $q(x) = q_0 + q_1x$ ,  $u$  and  $f$  are only functions of  $t$ , the linear PDE reduces to the ODE, and so does its truncation errors. I have used

- first-, second-, and third-order spatial discretizations for the PDEs
- five explicit time-stepping methods
  - first-order Forward Euler method
  - second-order explicit midpoint method
  - Williamson's low-storage third-order Runge-Kutta method
  - second-order Adams-Bashforth method
  - third-order Adams-Bashforth method
- three implicit time-stepping methods
  - first-order Backward Euler method
  - second-order implicit midpoint method
  - second-order Crank-Nicholson method (Trapezoidal Rule)

# 1.2. Derivation by Symbolic Algebra

## Relevant Terms in the Local Truncation Error of the Generic One-Dimensional Advection Equation

	$\frac{1}{3!}\widehat{\mathcal{F}}^{(3)}$	$\frac{1}{4}\mathcal{F}\mathcal{F}_u\mathcal{F}_{uv}v + \frac{1}{4}\mathcal{F}\mathcal{F}_{uv}\mathcal{F}_v w_1 + \frac{1}{4}\mathcal{F}\mathcal{F}_{uv}\mathcal{F}_x + \frac{1}{8}\mathcal{F}_{tt}$
Explicit Midpoint Method	$\frac{1}{3!}c_3$	$\frac{1}{6}\mathcal{F}\mathcal{F}_u^2 + \frac{1}{12}\mathcal{F}\mathcal{F}_u\mathcal{F}_{uv}v + \frac{1}{4}\mathcal{F}\mathcal{F}_{uv}\mathcal{F}_v w_1 + \frac{1}{12}\mathcal{F}\mathcal{F}_{uv}\mathcal{F}_x + \frac{1}{6}\mathcal{F}\mathcal{F}_{ux}\mathcal{F}_v + \frac{1}{6}\mathcal{F}_t\mathcal{F}_u + \frac{1}{24}\mathcal{F}_{tt}$ $+ \frac{1}{3}\mathcal{F}_u^2\mathcal{F}_v v + \frac{1}{6}\mathcal{F}_u\mathcal{F}_{uv}\mathcal{F}_v v^2 + \frac{1}{2}\mathcal{F}_u\mathcal{F}_v^2 w_1 + \frac{1}{6}\mathcal{F}_u\mathcal{F}_v\mathcal{F}_{vx}v + \frac{1}{3}\mathcal{F}_u\mathcal{F}_v\mathcal{F}_x + \frac{1}{2}\mathcal{F}_{uv}\mathcal{F}_v^2 v w_1$ $+ \frac{1}{6}\mathcal{F}_{uv}\mathcal{F}_v\mathcal{F}_x v + \frac{1}{3}\mathcal{F}_{ux}\mathcal{F}_v^2 v + \frac{1}{6}\mathcal{F}_v^3 w_2 + \frac{1}{2}\mathcal{F}_v^2\mathcal{F}_{vx}w_1 + \frac{1}{6}\mathcal{F}_v^2\mathcal{F}_{xx} + \frac{1}{6}\mathcal{F}_v\mathcal{F}_{vx}\mathcal{F}_x + \frac{1}{6}\mathcal{F}_v\mathcal{F}_{xt}$
Implicit Midpoint Method	$\frac{1}{3!}\widehat{\mathcal{F}}^{(3)}$	$\frac{1}{4}\mathcal{F}\mathcal{F}_u^2 + \frac{1}{4}\mathcal{F}\mathcal{F}_u\mathcal{F}_{uv}v + \frac{1}{2}\mathcal{F}\mathcal{F}_{uv}\mathcal{F}_v w_1 + \frac{1}{4}\mathcal{F}\mathcal{F}_{uv}\mathcal{F}_x + \frac{1}{4}\mathcal{F}\mathcal{F}_{ux}\mathcal{F}_v + \frac{1}{4}\mathcal{F}_t\mathcal{F}_u + \frac{1}{8}\mathcal{F}_{tt}$ $+ \frac{1}{2}\mathcal{F}_u^2\mathcal{F}_v v + \frac{1}{4}\mathcal{F}_u\mathcal{F}_{uv}\mathcal{F}_v v^2 + \frac{3}{4}\mathcal{F}_u\mathcal{F}_v^2 w_1 + \frac{1}{4}\mathcal{F}_u\mathcal{F}_v\mathcal{F}_{vx}v + \frac{1}{2}\mathcal{F}_u\mathcal{F}_v\mathcal{F}_x + \frac{3}{4}\mathcal{F}_{uv}\mathcal{F}_v^2 v w_1$ $+ \frac{1}{4}\mathcal{F}_{uv}\mathcal{F}_v\mathcal{F}_x v + \frac{1}{2}\mathcal{F}_{ux}\mathcal{F}_v^2 v + \frac{1}{4}\mathcal{F}_v^3 w_2 + \frac{3}{4}\mathcal{F}_v^2\mathcal{F}_{vx}w_1 + \frac{1}{4}\mathcal{F}_v^2\mathcal{F}_{xx} + \frac{1}{4}\mathcal{F}_v\mathcal{F}_{vx}\mathcal{F}_x + \frac{1}{4}\mathcal{F}_v\mathcal{F}_{xt}$
	$\frac{1}{3!}c_3$	$-\frac{1}{12}\mathcal{F}\mathcal{F}_u^2 + \frac{1}{12}\mathcal{F}\mathcal{F}_u\mathcal{F}_{uv}v + \frac{1}{12}\mathcal{F}\mathcal{F}_{uv}\mathcal{F}_x - \frac{1}{12}\mathcal{F}\mathcal{F}_{ux}\mathcal{F}_v - \frac{1}{12}\mathcal{F}_t\mathcal{F}_u + \frac{1}{24}\mathcal{F}_{tt} - \frac{1}{6}\mathcal{F}_u^2\mathcal{F}_v v$ $- \frac{1}{12}\mathcal{F}_u\mathcal{F}_{uv}\mathcal{F}_v v^2 - \frac{1}{4}\mathcal{F}_u\mathcal{F}_v^2 w_1 - \frac{1}{12}\mathcal{F}_u\mathcal{F}_v\mathcal{F}_{vx}v - \frac{1}{6}\mathcal{F}_u\mathcal{F}_v\mathcal{F}_x - \frac{1}{4}\mathcal{F}_{uv}\mathcal{F}_v^2 v w_1 - \frac{1}{12}\mathcal{F}_{uv}\mathcal{F}_v\mathcal{F}_x v$ $- \frac{1}{6}\mathcal{F}_{ux}\mathcal{F}_v^2 v - \frac{1}{12}\mathcal{F}_v^3 w_2 - \frac{1}{4}\mathcal{F}_v^2\mathcal{F}_{vx}w_1 - \frac{1}{12}\mathcal{F}_v^2\mathcal{F}_{xx} - \frac{1}{12}\mathcal{F}_v\mathcal{F}_{vx}\mathcal{F}_x - \frac{1}{12}\mathcal{F}_v\mathcal{F}_{xt}$

Recall that for second-order time-stepping methods,  $\widehat{\mathcal{F}}^{(1)} = \mathcal{F}^{(1)}$ ,  $\widehat{\mathcal{F}}^{(2)} = \mathcal{F}^{(2)}$ , but  $\widehat{\mathcal{F}}^{(3)} \neq \mathcal{F}^{(3)}$  leading to  $c_3 = \mathcal{F}^{(3)} - \widehat{\mathcal{F}}^{(3)} \neq 0$ .

# 1.2. Derivation by Symbolic Algebra

Terms containing  $\Delta t^l \Delta x^k$   $l \times k \in \{\{1, 2\} \times \{0, 1, 2\}\} \cup \{\{3\} \times \{0\}\}$  within local truncation error of the numerical solution of the linear inhomogeneous variable-coefficient advection equation  $u_t + p(x)u + (q(x)u)_x = f(x, t)$ , discretized in space with first order upwind finite difference and advanced in time with explicit midpoint method

$l$	$k$	Term containing $\Delta t^l \Delta x^k$ within the Local Truncation Error
	0	0
1	1	$\Delta t \left[ \Delta x \left\{ -\frac{1}{2}qu_{xx} - q_x u_x - \frac{1}{2}q_{xx}u + \dots \right\} \right]$
	2	$\Delta t \left[ \Delta x^2 \left\{ \frac{1}{6}qu_{xxx} + \frac{1}{2}q_x u_{xx} + \frac{1}{2}q_{xx}u_x + \frac{1}{6}q_{xxx}u + \dots \right\} \right]$
	0	0
2	1	$\Delta t^2 \left[ \Delta x \left\{ -\frac{1}{4}f_{xx} - \frac{1}{2}f_x q_x - \frac{1}{4}f_{xx}q + \frac{1}{2}pqu_{xx} + pq_x u_x + \frac{1}{2}pq_{xx}u \right. \right.$ $\left. + \frac{1}{2}p_x q u_x + \frac{1}{2}p_x q_x u + \frac{1}{4}p_{xx}qu + \frac{1}{2}q^2 u_{xxx} + \frac{3}{2}q q_x u_{xx} \right. \left. + \frac{1}{4}qq_{xx}u_x + \frac{1}{2}qq_{xxx}u + \frac{3}{2}q_x^2 u_x + q_x q_{xx}u + \dots \right]$
	2	$\Delta t^2 \left[ \Delta x^2 \left\{ \frac{1}{12}f_{xxx} + \frac{1}{4}f_x q_{xx} + \frac{1}{4}f_{xx}q_x + \frac{1}{12}f_{xxx}q - \frac{1}{6}pqu_{xxx} - \frac{1}{2}pq_x u_{xx} - \frac{1}{2}pq_{xx}u_x \right. \right.$ $\left. - \frac{1}{8}pq_{xxx}u - \frac{1}{4}p_x q u_{xx} - \frac{1}{2}p_x q_x u_x - \frac{1}{4}p_x q_{xx}u - \frac{1}{4}p_{xx}q u_x - \frac{1}{4}p_{xx}q_x u - \frac{1}{12}p_{xxx}qu \right. \left. - \frac{1}{4}qq_x u_{xxx} - \frac{1}{8}qq_{xx}u_{xx} - \frac{3}{4}qq_{xx}u_x - \frac{1}{4}q_x^2 u_{xx} - \frac{3}{2}q_x q_{xx}u_x - \frac{3}{8}q_x q_{xxx}u - \frac{3}{8}q_x^2 u + \dots \right]$
	0	$\Delta t^3 \left[ \frac{1}{6}fp^2 + \frac{1}{3}fpq_x + \frac{1}{6}fp_x q + \frac{1}{6}fq q_{xx} + \frac{1}{6}fq_x^2 - \frac{1}{6}fp - \frac{1}{6}f_x q_x + \frac{1}{24}f_{tt} + \frac{1}{3}fpq \right.$ $\left. + \frac{1}{2}f_x q q_x - \frac{1}{6}f_{xx}q + \frac{1}{6}f_{xx}q^2 - \frac{1}{6}p^3 u - \frac{1}{2}p^2 q u_x - \frac{1}{2}p^2 q_x u - \frac{1}{2}p p_x q u - \frac{1}{2}p q_x^2 u_{xx} \right.$ $\left. - \frac{3}{2}p q q_x u_x - \frac{1}{2}p q q_{xx}u - \frac{1}{2}p q_x^2 u - \frac{1}{2}p_x q^2 u_x - \frac{2}{3}p_x q q_x u - \frac{1}{6}p_{xx}q^2 u - \frac{1}{6}q^3 u_{xxx} \right.$ $\left. - q^2 q_x u_{xx} - \frac{2}{3}q^2 q_{xx}u_x - \frac{1}{6}q^2 q_{xxx}u - \frac{7}{6}qq_x^2 u_x - \frac{2}{3}qq_x q_{xx}u - \frac{1}{6}q_x^3 u + \dots \right]$

By specifying all spatial gradients to zero, the local truncation error reduces to that of the ODE  $u_t + (p_0 + q_1)u = f(t)$ , advanced with the explicit midpoint method,  $\Delta t^3 \left[ \frac{1}{6}fp_0^2 + \frac{1}{3}fp_0q_1 + \frac{1}{6}fq_1^2 - \frac{1}{6}ft_0 - \frac{1}{6}ft_0q_1 + \frac{1}{24}ft_{tt} - \frac{1}{6}p_0^3u - \frac{1}{2}p_0q_1^2u - \frac{1}{2}p_0q_1^2u - \frac{1}{6}q_1^3u \right] + \mathcal{O}(\Delta t^4)$



## 1. On the Spatial and Temporal Order of Convergence of PDEs

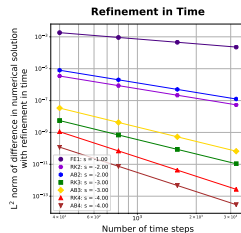
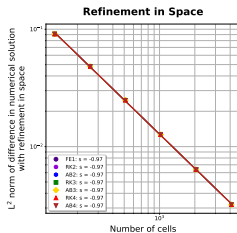
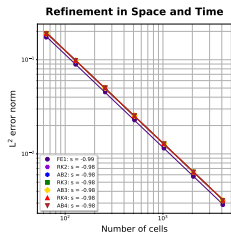
- 1.1 Analytical Derivation
- 1.2 Derivation by Symbolic Algebra
- 1.3 Numerical Experiments

## 2. Time-Stepping Methods for Ocean Models

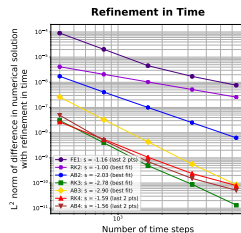
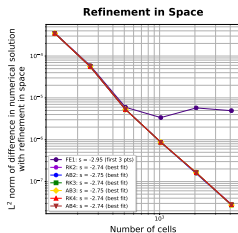
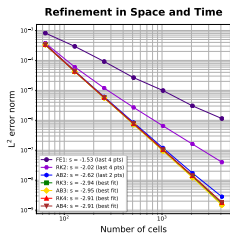
- 2.1 Barotropic-Baroclinic Splitting and Filtering of Barotropic Modes
- 2.2 Verification Suite of Shallow Water Test Cases

# 1.3. Numerical Experiments: Linear Advection

Convergence of Linear Advection using First-Order Upwind (Finite Difference) in Space ( $\alpha = 1$ )



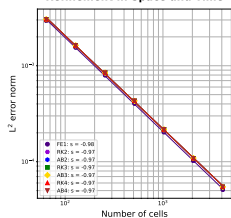
Convergence of Linear Advection using Piecewise Parabolic Reconstruction (Finite Volume) in Space ( $\alpha \approx 3$ )



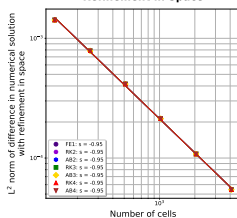
# 1.3. Numerical Experiments: Non-Linear Burgers' Advection

Convergence of Non-Linear Advection using First-Order Upwind (Finite Difference) in Space ( $\alpha = 1$ )

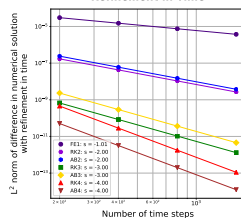
Refinement in Space and Time



Refinement in Space

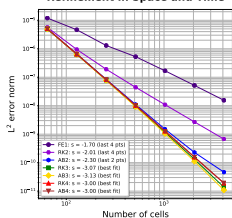


Refinement in Time

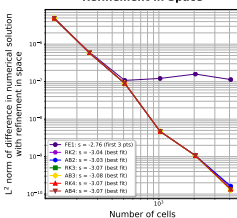


Convergence of Non-Linear Advection using Piecewise Parabolic Reconstruction (Finite Volume) in Space ( $\alpha \approx 3$ )

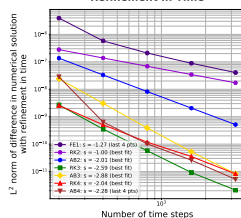
Refinement in Space and Time



Refinement in Space



Refinement in Time

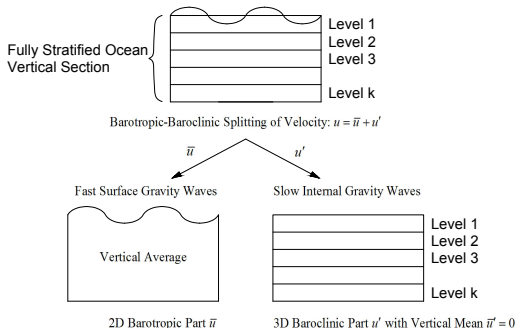


1. On the Spatial and Temporal Order of Convergence of PDEs
  - 1.1 Analytical Derivation
  - 1.2 Derivation by Symbolic Algebra
  - 1.3 Numerical Experiments
2. Time-Stepping Methods for Ocean Models
  - 2.1 Barotropic-Baroclinic Splitting and Filtering of Barotropic Modes
  - 2.2 Verification Suite of Shallow Water Test Cases

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# 2.1. Barotropic-Baroclinic Splitting

- Ocean circulation models deal with disparate time scales by splitting the momentum equations into two parts:
  - a **barotropic** part for solving the depth independent **fast** 2D barotropic waves (advanced in time either explicitly using a small time-step or implicitly using a long time-step) and
  - a **baroclinic** part for solving the much **slower** 3D baroclinic waves
- Before reconciling the barotropic variables with their baroclinic counterparts to arrive at the total 3D states, a time-averaging filter is applied over the barotropic solutions, to minimize aliasing and mode-splitting errors.

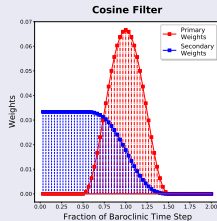
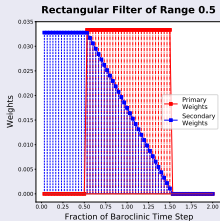
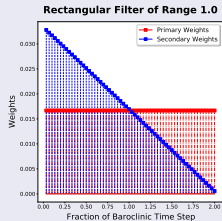


Kang, H., Evans, K., Petersen, M., Jones, P., and **Bishnu, S.**, (2021), "A scalable semi-implicit barotropic mode solver for the MPAS-Ocean", *Journal of Advances in Modeling Earth Systems*

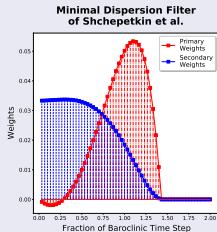
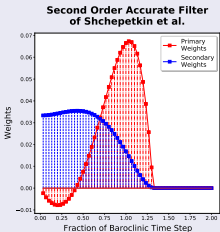
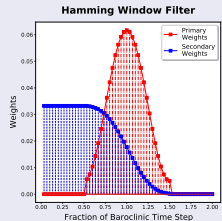


# 2.1. Time-Averaging Filters Incorporated in MPAS-Ocean

## Rectangular and Cosine Filters with Primary (Red) & Secondary (Blue) Weights



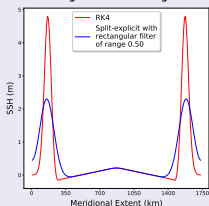
## Hamming Window and Shchepetkin's Filters with Primary (Red) & Secondary (Blue) Weights



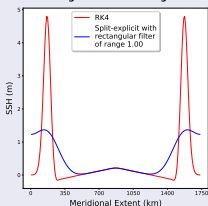
# 2.1. Surface Gravity Wave Simulation in MPAS-Ocean with Various Filters

## Numerical SSH with RK4 vs split-explicit method using rectangular and cosine filters

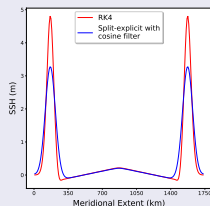
**RK4 vs Split-Explicit Method with Rectangular Filter of Range 0.50**



**RK4 vs Split-Explicit Method with Rectangular Filter of Range 1.00**

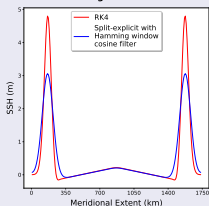


**RK4 vs Split-Explicit Method with Cosine Filter**

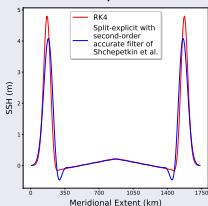


## Numerical SSH with RK4 vs split-explicit method using Hamming Window and Shchepetkin's filters

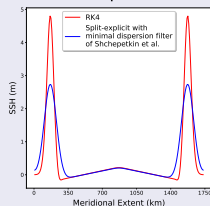
**RK4 vs Split-Explicit Method with Hamming Window Cosine Filter**



**RK4 vs Split-Explicit Method with Second-Order Accurate Filter of Shchepetkin et al.**



**RK4 vs Split-Explicit Method with Minimal Dispersion Filter of Shchepetkin et al.**



# 2.1. Shallow Water Solver Simulating Surface Gravity Wave

- To understand the combined stabilizing effect of various barotropic time-averaging filters and the forward-backward (FB) parameters, I developed a non-linear shallow water solver in object-oriented Python and tested it against the simulation of a surface gravity wave.

- I obtain a near-exact solution using a truncated Fourier series approximation, which is spectrally accurate in space, and the classic fourth-order Runge-Kutta (RK4) method in time. I treat it as the reference benchmark to compare to my numerical solution, employing piecewise parabolic reconstruction in space and the forward-backward (FB) time-stepping method with parameter  $\gamma$ ,  $u^{n+1} = u^n + \mathcal{F}(u^n, \eta^n) \Delta t$ ;  $\eta^{n+1} = \eta^n + \{(1 - \gamma)\mathcal{G}(u^n, \eta^n) + \gamma\mathcal{G}(u^{n+1}, \eta^n)\} \Delta t$ , where  $u_t = \mathcal{F}(u, \eta)$ ;  $\eta_t = \mathcal{G}(\eta, t)$  represent the non-linear shallow water equations in functional form.

- The following table lists maximum error norms of the surface elevation of the gravity wave after 1 hour (30 baroclinic time steps, each consisting of 2 minutes and 20 barotropic subcycles) for a variety of filters and FB parameter  $\gamma$ .

Surface Elevation Maximum Error Norm  $\times 10^{-3}$

FB Parameter $\gamma$	No Filter	Rectangular Filter with Range $R$					Cosine Filters		Shchepetkin Filters	
		$R = 0.25$	$R = 0.375$	$R = 0.50$	$R = 0.75$	$R = 1.00$	ROMS	HW	2 <sup>nd</sup> Order	Min. Disp.
-0.50	2.322	2.611	1.780	2.277	<b>2.408</b>	<b>3.039</b>	1.945	1.573	<b>1.951</b>	<b>1.629</b>
-0.25	2.192	2.514	1.703	2.191	2.441	3.073	1.834	1.452	1.976	1.685
+0.00	2.065	2.417	1.607	2.107	2.474	3.121	1.737	1.333	2.003	1.741
+0.25	1.946	2.327	1.521	<b>2.075</b>	2.506	3.238	1.641	1.230	2.035	1.822
+0.50	1.847	2.240	1.453	2.101	2.537	3.354	1.554	1.138	2.088	1.902
+0.75	1.750	2.154	<b>1.386</b>	2.126	2.567	3.470	1.486	1.048	2.141	1.983
+1.00	1.653	2.070	1.461	2.151	2.601	3.592	<b>1.418</b>	<b>1.016</b>	2.197	2.080
+1.25	1.583	1.986	1.542	2.184	2.640	3.718	1.477	1.106	2.274	2.182
+1.50	<b>1.515</b>	<b>1.964</b>	1.628	2.220	2.678	3.843	1.558	1.214	2.352	2.284

HW  $\equiv$  Hamming Window Cosine Filter and Min. Disp  $\equiv$  Shchepetkin Filter Optimized for Minimal Numerical Dispersion

1. On the Spatial and Temporal Order of Convergence of PDEs
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## 2.2. Verification Suite of Barotropic Test Cases

**Motivation:** The development of any numerical ocean model warrants a suite of verification exercises for testing its spatial and temporal discretizations. I have designed a set of shallow water test cases for verifying the barotropic solver of ocean models.

### Geophysical Waves and Barotropic Tide

- 1 Non-Dispersive Coastal Kelvin Wave
- 2 Low Frequency Dispersive Planetary Rossby Wave
- 3 Low Frequency Dispersive Topographic Rossby Wave
- 4 High Frequency Dispersive Inertia Gravity Wave
- 5 Non-Dispersive Equatorial Kelvin Wave
- 6 Dispersive Equatorial Yanai Wave
- 7 Low Frequency Dispersive Equatorial Rossby Wave
- 8 High Frequency Dispersive Equatorial Inertia Gravity Wave
- 9 Barotropic Tide

### Standard Mathematical Test Cases

- 1 Diffusion Equation
- 2 Viscous Burgers Equation
- 3 Non-linear Manufactured Solution

## 2.2. Verification Suite of Barotropic Test Cases

I developed a new unstructured-mesh ocean model (consisting of  $\sim 12,600$  lines of code) in object-oriented Python, employing TRISK-based spatial discretization, and the following set of time-stepping algorithms:

### Standard Mathematical Time-Stepping Algorithms

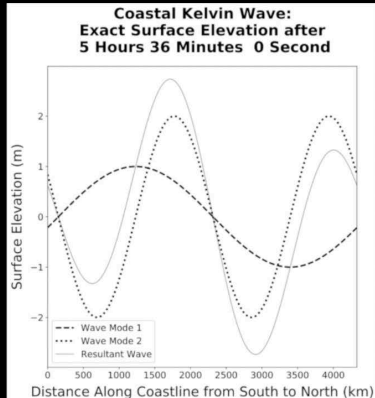
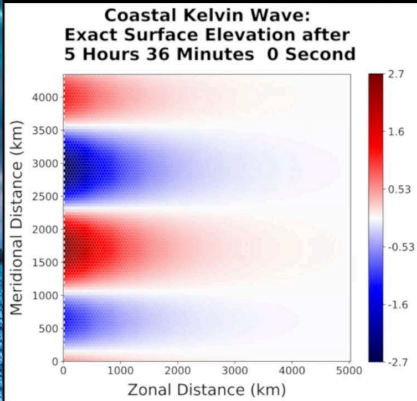
- 1 Forward Backward Method or Implicit Euler Method
- 2 Explicit Midpoint Method, a Form of Second-Order Runge-Kutta Method
- 3 Low-Storage Third-Order Runge-Kutta Method of Williamson
- 4 Low-Storage Fourth-Order Runge-Kutta Method of Carpenter and Kennedy
- 5 Second-Order Adams-Bashforth Method
- 6 Third-Order Adams-Bashforth Method
- 7 Fourth-Order Adams-Bashforth Method

### Time-Stepping Algorithms Popular in Ocean Modeling

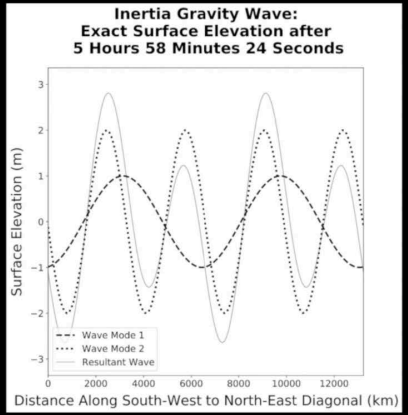
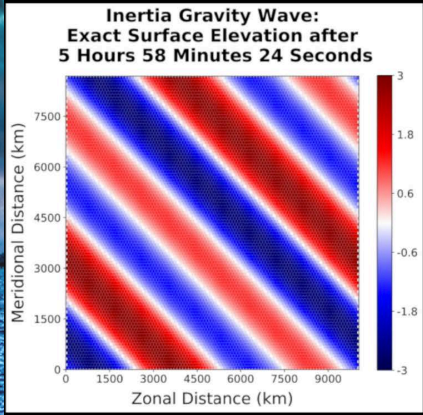
- 1 Leapfrog Trapezoidal Method
- 2 Leapfrog Adams Moulton Method
- 3 Forward Backward Method with RK2 Feedback
- 4 Generalized Forward Backward Method with AB2 - AM3 Step
- 5 Generalized Forward Backward Method with AB3 - AM4 Step



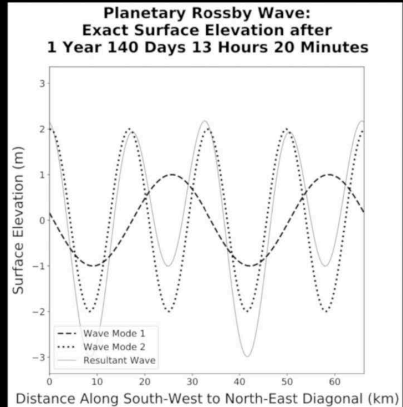
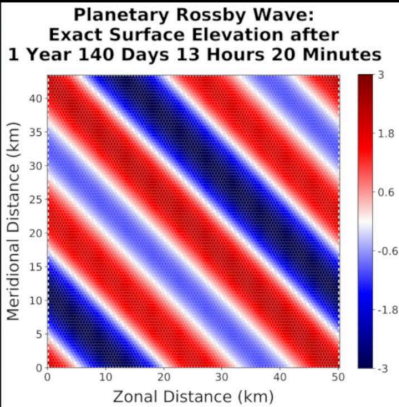
## 2.2. Verification Suite: Coastal Kelvin Wave



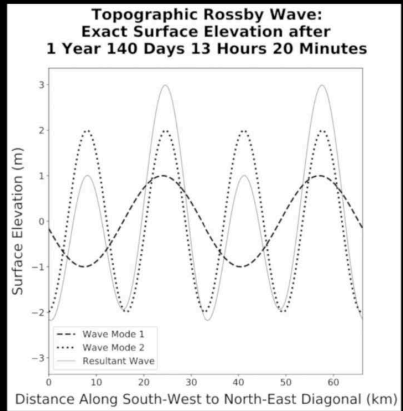
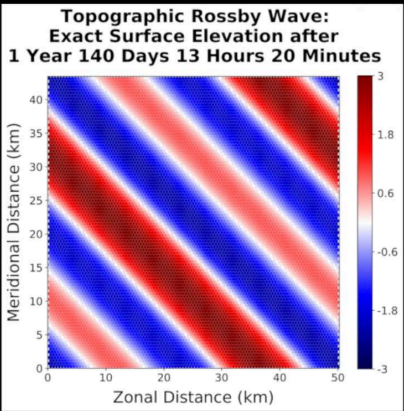
## 2.2. Verification Suite: High-Frequency Inertia-Gravity Wave



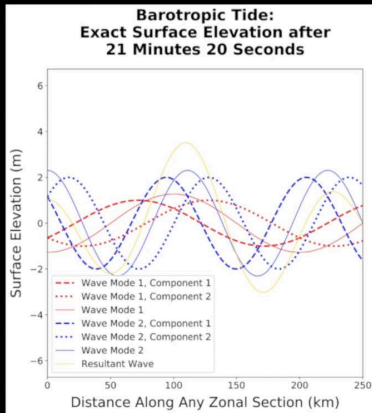
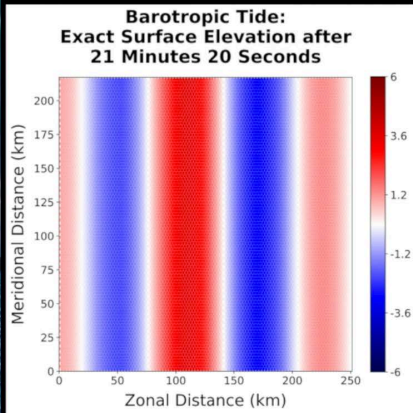
## 2.2. Verification Suite: Low-Frequency Planetary Rossby Wave



## 2.2. Verification Suite: Low-Frequency Topographic Rossby Wave

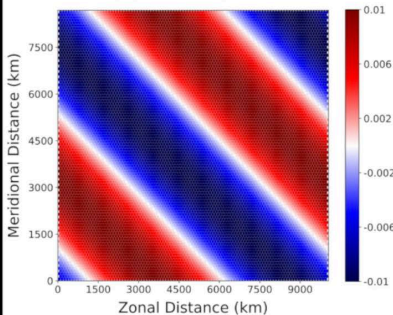


## 2.2. Verification Suite: Barotropic Tide

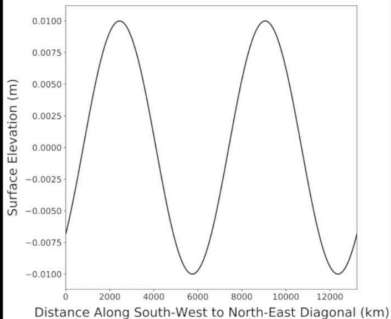


## 2.2. Verification Suite: Non-Linear Manufactured Solution

**Non-Linear Manufactured Solution:  
Exact Surface Elevation after  
2 Hours 10 Minutes 40 Seconds**



**Non-Linear Manufactured Solution:  
Exact Surface Elevation after  
2 Hours 10 Minutes 40 Seconds**



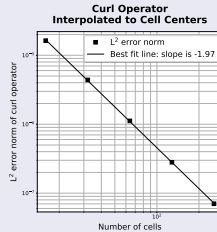
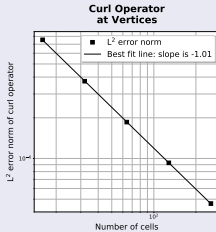
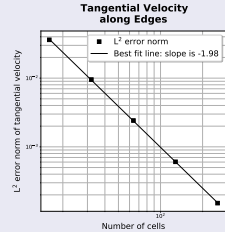
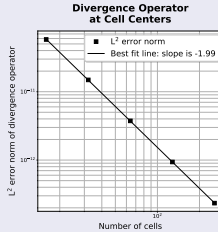
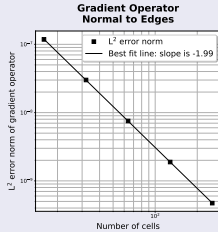
## 2.2. Verification Suite: Summary of Shallow Water Test Cases

Summary of Shallow Water Test Cases for the Barotropic Solver of Ocean Models

	<b>Coriolis Parameter</b>	<b>Bottom Topography</b>	<b>Numerical PDE</b>	<b>Boundary Conditions</b>
<b>Coastal Kelvin Wave</b>	Constant ( <i>f-plane</i> )	Flat Bottom	Linear, Homogeneous, Constant-Coefficient	Non-Periodic in $x$ , Periodic in $y$
<b>Inertia-Gravity Wave</b>	Constant ( <i>f-plane</i> )	Flat Bottom	Linear, Homogeneous, Constant-Coefficient	Periodic in $x$ , Periodic in $y$
<b>Planetary Rossby Wave</b>	Linear in $y$ ( <i>beta plane</i> )	Flat Bottom	Linear, Inhomogeneous, Variable-Coefficient	Periodic in $x$ , Non-Periodic in $y$
<b>Topographic Rossby Wave</b>	Constant ( <i>f-plane</i> )	Linear in $y$ , Sloping Bottom	Linear, Inhomogeneous, Variable-Coefficient	Periodic in $x$ , Non-Periodic in $y$
<b>Barotropic Tide</b>	Constant ( <i>f-plane</i> )	Flat Bottom	Linear, Homogeneous, Constant-Coefficient	Non-Periodic in $x$ , Non-Periodic in $y$
<b>Manufactured Solution</b>	Constant ( <i>f-plane</i> )	Flat Bottom	Non-Linear, Inhomogeneous, Constant-Coefficient	Periodic in $x$ , Periodic in $y$

## 2.2. Verification Suite: Convergence of Spatial Operators

### Convergence of TRiSK-based gradient, divergence, curl, and flux interpolation operators





# Recap Slide 1. On the Order of Convergence of PDEs

Order of convergence of the error norm in the asymptotic regime at constant ratio of time-step to grid spacing for varying orders of spatial and temporal discretizations

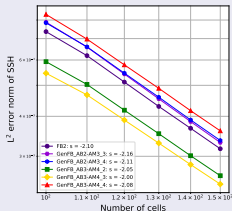
Order of Spatial Discretization $\alpha$	Time-Stepping Method Employed	Order of Time-Stepping Method $\beta$	Order of Convergence of Error Norm in Asymptotic Regime at Constant Ratio of Time-Step to Grid Spacing $\min(\alpha, \beta)$
1	FE	1	$\min(1,1) = 1$
1	RK2 or AB2	2	$\min(1,2) = 1$
1	RK3 or AB3	3	$\min(1,3) = 1$
1	RK4 or AB4	4	$\min(1,4) = 1$
2	FE	1	$\min(2,1) = 1$
2	RK2 or AB2	2	$\min(2,2) = 2$
2	RK3 or AB3	3	$\min(2,3) = 2$
2	RK4 or AB4	4	$\min(2,4) = 2$
3	FE	1	$\min(3,1) = 1$
3	RK2 or AB2	2	$\min(3,2) = 2$
3	RK3 or AB3	3	$\min(3,3) = 3$
3	RK4 or AB4	4	$\min(3,4) = 3$
4	FE	1	$\min(4,1) = 1$
4	RK2 or AB2	2	$\min(4,2) = 2$
4	RK3 or AB3	3	$\min(4,3) = 3$
4	RK4 or AB4	4	$\min(4,4) = 4$

FE  $\equiv$  forward Euler, RK  $\equiv$  Runge-Kutta, and AB  $\equiv$  Adams-Bashforth

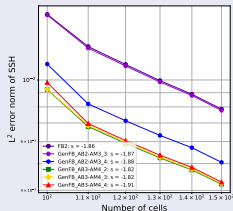
## 2.2. Verification Suite: Convergence of Shallow Water Test Cases

Convergence of the coastal Kelvin wave, the high-frequency inertia-gravity wave, the barotropic tide, and the non-linear manufactured solution with simultaneous refinement in space and time

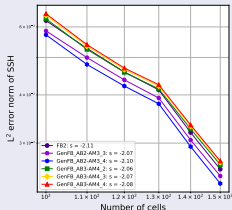
**Coastal Kelvin Wave:  
Refinement in Space and Time**



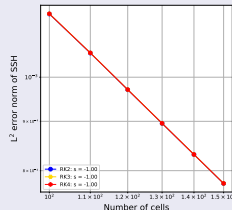
**Inertia Gravity Wave:  
Refinement in Space and Time**



**Barotropic Tide:  
Refinement in Space and Time**



**NonLinear Manufactured Solution:  
Refinement in Space and Time**



# Conclusions, Future Work and Current Status

## Conclusions

### On the Spatial and Temporal Order of Convergence of Hyperbolic PDEs

- The order of convergence at constant ratio of time step to cell width is determined by the minimum of the orders of the spatial and temporal discretizations.
- Convergence of the error norm cannot be guaranteed under only spatial or temporal refinement.

### Time-Stepping Methods for Ocean Models

- The amount of dissipation applied to stabilize the barotropic modes can be controlled by (a) the time-averaging filter, or (b) the forward-backward time-stepping parameters. Too much dissipation can damp the entire solution, not just the spurious oscillations.
- The order of convergence of an ocean model under simultaneous refinement in space and time is limited by minimum of the orders of accuracy of the time-stepping method, and all spatial operators like gradient, divergence, curl etc.

## Ongoing and Future Work

- Extend truncation error analysis and the convergence studies to parabolic equations, higher order and spectral discretizations in space and time, and time integrators beyond Method of Lines.
- Design verification exercises with complexity in between the barotropic and the full primitive equations, involving stratification, a complex bathymetry, and the ability to test both the barotropic and baroclinic components separately.

## Relevant Publications

- **Bishnu, S.**, Petersen, M., Quaife, B., "On the Spatial and Temporal Order of Convergence of Hyperbolic PDEs", *Journal of Computational Physics* (submitted)
- **Bishnu, S.**, Petersen, M., Quaife, B., "A Suite of Verification Exercises for the Barotropic Solver of Ocean Models" (in preparation)

## Current Status

- Successfully defended PhD Dissertation on June 10, 2021.
- Hoping to continue working at the Los Alamos National Laboratory (LANL) as a postdoctoral researcher and collaborate with scientists working on E3SM at LANL and other national laboratories.