Change of the baroclinic time stepping method

Second-order Adams-Bashforth method in MPAS-O

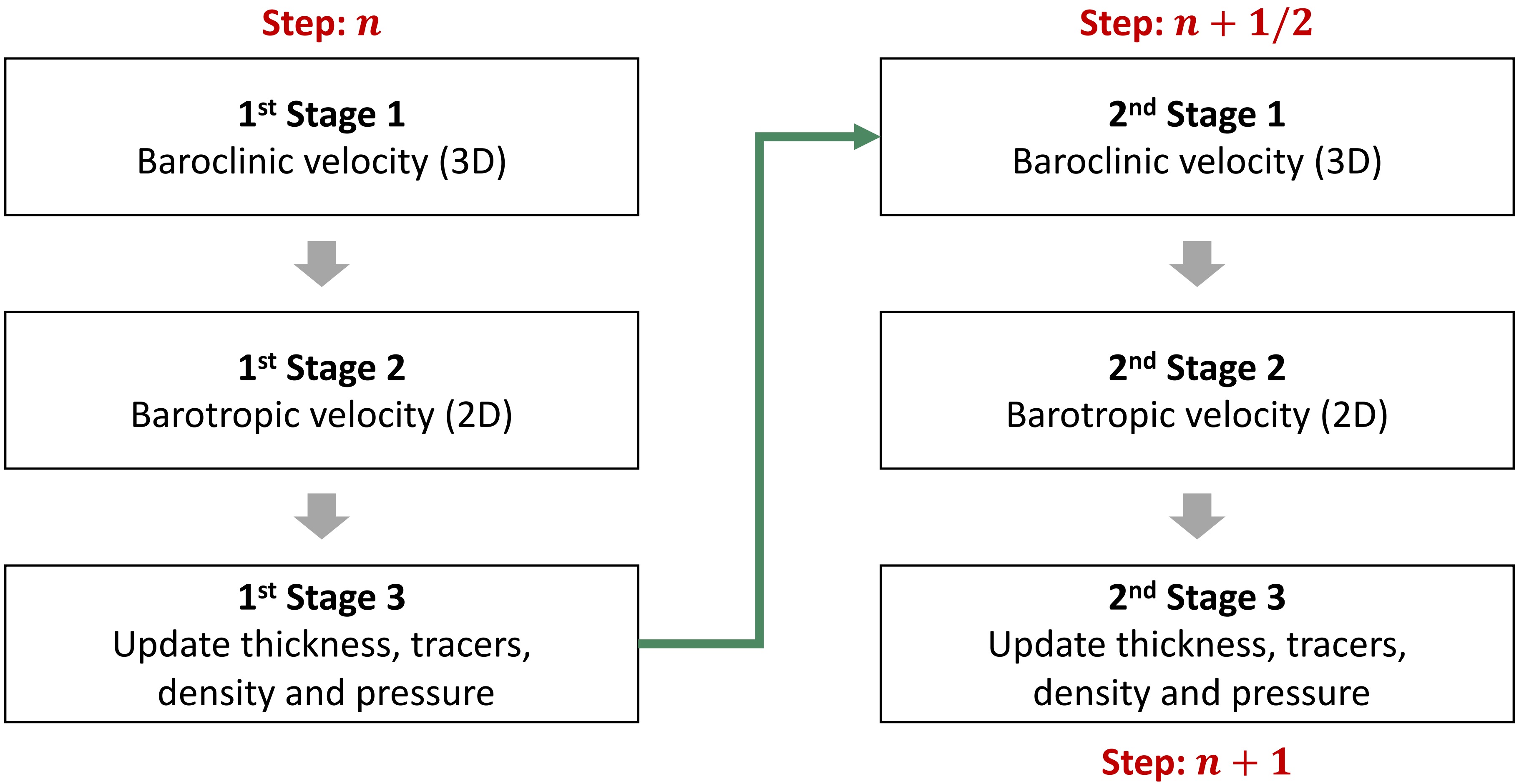
- Pros and Cons : Current vs AB2

	Forward-Backward (Current)	**Adams-Bashforth 2 (Plan)**
Order	2	2
Pros	- More stable scheme (broader stability region than AB2 method) - Use less memory - No initial value problem	- Compute S. 1~S. 3 once (approximately halved runtime compared to the current method)
Cons	- Repeat S. 1~S. 3 twice (computationally inefficient)	- Less stable scheme - Use more memory - Initial value problem due to $f(\mathbf{u}_{n-1})$

Change of the baroclinic time stepping method

Current: The forward-backward scheme (two-stage method)

- Achieve the second-order accuracy by repeating Stage1~3 **twice**



Change of the baroclinic time stepping method

Current: The forward-backward scheme (two-stage method)

- Achieve the second-order accuracy by repeating Stage1~3 **twice**

Example for baroclinic velocity in stage 1

1st Stage 1

Step n

u_n

↓

Compute tendency at n

$f(u_n)$

↓

Time advancing

$\hat{u}_{n+1} = u_n + \Delta t\, f(u_n)$

→

2nd Stage 1

Averaging for step $n + 1/2$

$u_{n+1/2} = 0.5(\hat{u}_{n+1} + u_n)$

↓

Compute tendency at $n + 1/2$

$f\left(u_{n+1/2}\right)$

↓

Time advancing

$u_{n+1} = u_n + \Delta t\, f(u_{n+1/2})$

Change of the baroclinic time stepping method

Plan: Second-order Adams-Bashforth method (two-step method)

- Computes Stage1~3 **once** to achieve the second-order accuracy

Example for baroclinic velocity in stage 1

Step n

u_n

↓

Compute tendency at n

$f(u_n)$

↓

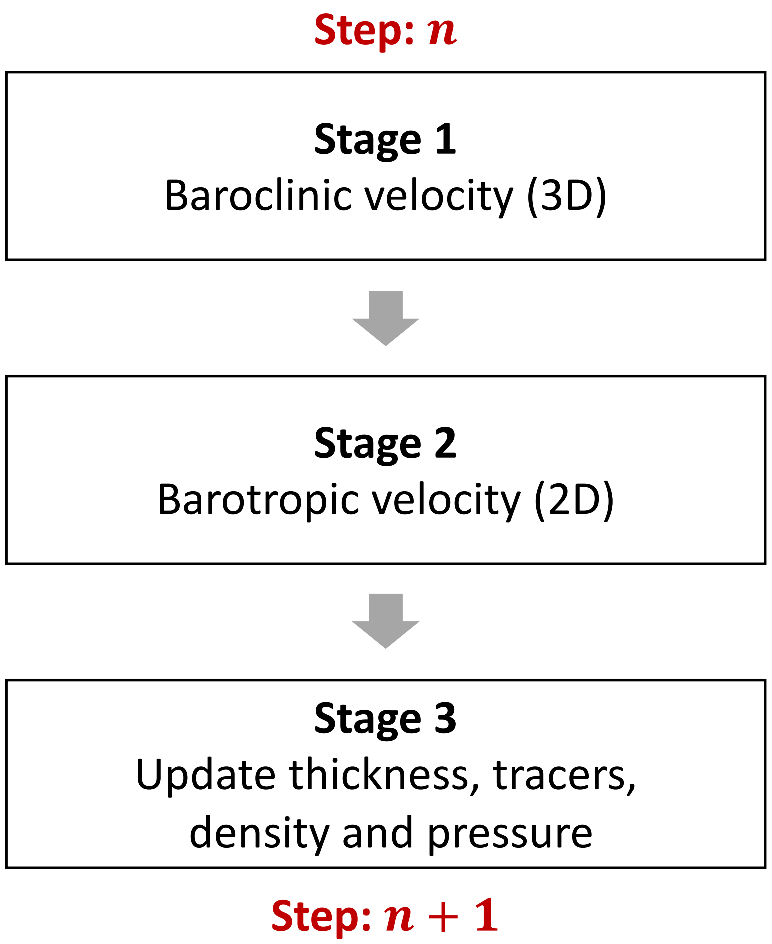
Time advancing

$$u_{n+1} = u_n + \frac{3}{2}\Delta t\, f(u_n) - \frac{1}{2}\Delta t\, f(u_{n-1})$$

Change of the baroclinic time stepping method

Plan: Second-order Adams-Bashforth method (two-step method)

- Computes Stage1~3 **once** to achieve the second-order accuracy



Change of the baroclinic time stepping method

Second-order Adams-Bashforth method in MPAS-O

- Computes Stage1~3 **once** to achieve the second-order accuracy

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \frac{3}{2}\Delta t\, \underline{f(\mathbf{u}_n)} - \frac{1}{2}\Delta t\, \underline{f(\mathbf{u}_{n-1})}$$

Compute at step n — Stored in a previous step $(n-1)$

Change of the baroclinic time stepping method

Second-order Adams-Bashforth method in MPAS-O

- AB2 for the baroclinic momentum equation

$$\mathbf{u}'_{k,n+1} = \mathbf{u}'_{k,n} + \frac{3}{2}\Delta t \mathcal{F}\left(\mathbf{u}_{k,n}\right) - \frac{1}{2}\Delta t \mathcal{F}\left(\mathbf{u}_{k,n-1}\right) - \underline{\bar{\mathbf{G}}}$$

$\bar{\mathbf{G}}$ includes all remaining terms in barotropic equations, so this term is not included in $\mathcal{F}(\mathbf{u})$

$$\mathcal{F}\left(\mathbf{u}_{k,n}\right) = -f\mathbf{u}'^{\perp}_{k,n} + T^{\mathbf{u}}\left(\mathbf{u}_{k,n}, w_{k,n}, p_{k,n}\right) + g\nabla\zeta_n$$

$$T^{\mathbf{u}}(\mathbf{u}_k, w_k, p_k) = -\frac{1}{2}\nabla|\mathbf{u}_k|^2 - (k\cdot\nabla\times\mathbf{u}_k)\mathbf{u}_k^{\perp} - w_k\frac{\partial \mathbf{u}_k}{\partial z} - \frac{1}{\rho_0}\nabla p_k + \underline{\nu_h\nabla^4\mathbf{u}_k}$$

A viscosity term does not need to be inside $\mathcal{F}(\mathbf{u})$. But for coding convenience, the terms is currently included.

Change of the baroclinic time stepping method

Second-order Adams-Bashforth method in MPAS-O

- AB2 for the baroclinic momentum equation

$$\mathbf{u}'_{k,n+1} = \mathbf{u}'_{k,n} + \frac{3}{2}\Delta t\mathcal{F}\left(\mathbf{u}_{k,n}\right) - \frac{1}{2}\underline{\Delta t\mathcal{F}\left(\mathbf{u}_{k,n-1}\right)} - \bar{\mathbf{G}}$$

This term raises an initial value problem at $n = 0$.

- Cold start:
  - 1st step : the current scheme (forward-backward)
    - The term $\mathcal{F}\left(\mathbf{u}_{k,0}\right)$ is stored during the 1st step.
  - 2nd step ~: AB2 method
- Restart:
  - 1st step: AB2 method by using tendencies at previous time step (saved in restart files)

Change of the baroclinic time stepping method

Second-order Adams-Bashforth method in MPAS-O

- Coriolis term linear iteration with AB2

Iter = 1

$$u'_n \rightarrow f u'^{\perp}_n$$

$$u'_* = u'_n + \Delta t \frac{3}{2}[T(u_n) + f u'^{\perp}_n + g\nabla\zeta_n] - \Delta t \frac{1}{2}[T(u_{n-1}) + f u'^{\perp}_{n-1} + g\nabla\zeta_{n-1}]$$

$$\bar{\mathbf{G}}_{n+1} = \frac{1}{D\Delta t}\sum_{k=ks}^{k=ke} L_{n,k} u'_*$$

$$u'_{n+0.5} = \frac{1}{2}(u'_n + u'_* - \Delta t G_{n+1})$$

Iter = 2

$$u'_n \rightarrow f u'^{\perp}_{n+0.5}$$

$$u'_{n+1} = u'_n + \Delta t \frac{3}{2}[T(u_n) + g\nabla\zeta_n] + f u'^{\perp}_{n+0.5} - \Delta t \frac{1}{2}[T(u_{n-1}) + g\nabla\zeta_{n-1}]$$

$$\bar{\mathbf{G}}_{n+1} = \frac{1}{D\Delta t}\sum_{k=ks}^{k=ke} L_{n,k} u'_{n+1}$$

$$u'_{n+0.5} = \frac{1}{2}(u'_n + u'_{n+1} - \Delta t G_{n+1})$$

Change of the baroclinic time stepping method

Second-order Adams-Bashforth method in MPAS-O

- Computes Stage1~3 **once** to achieve the second-order accuracy

  - AB2 for the baroclinic momentum equation

$$\mathbf{u}'_{k,n+1} = \mathbf{u}'_{k,n} + \frac{3}{2}\Delta t\mathcal{F}\left(\mathbf{u}_{k,n}\right) - \frac{1}{2}\Delta t\mathcal{F}\left(\mathbf{u}_{k,n-1}\right) - \bar{\mathbf{G}}$$

  - AB2 for the thickness equation

$$h_{k,n+1} = h_{k,n} + \frac{3}{2}\Delta t\mathcal{F}\left(h_{k,n}\right) - \frac{1}{2}\Delta t\mathcal{F}\left(h_{k,n-1}\right)$$

$$\mathcal{F}\left(h_{k,n}\right) = \left(-\nabla \cdot \left(h_k^{*edge}\mathbf{u}_k^{tr}\right) - \frac{\partial}{\partial z}\left(h_k^* w_k^*\right)\right)$$

Change of the baroclinic time stepping method

Second-order Adams-Bashforth method in MPAS-O

- After tons of tests, however, it is found that the AB2 method for the thickness equation is too sensitive to time step size.

$$h_{k,n+1} = h_{k,n} + \frac{3}{2}\Delta t \mathcal{F}\left(h_{k,n}\right) - \frac{1}{2}\Delta t \mathcal{F}\left(h_{k,n-1}\right)$$

$$\mathcal{F}\left(h_{k,n}\right) = \left(-\nabla \cdot \left(h_k^{*edge} \mathbf{u}_k^{tr}\right) - \frac{\partial}{\partial z}\left(h_k^* w_k^*\right)\right)$$

- So, use the forward-backward scheme for the thickness equation only.
  - AB2 for momentum, PC for thickness (kind of… a mixed scheme?)

$$\hat{h}_{k,n+1} = h_{k,n} + \Delta t \mathcal{F}\left(h_{k,n}\right)$$

$$\rightarrow h_k^* = \frac{1}{2}\left(\hat{h}_{k,n+1} + h_{k,n}\right)$$

$$\rightarrow h_{k,n+1} = h_{k,n} + \Delta t \mathcal{F}\left(h_k^*\right)$$

Change of the baroclinic time stepping method

Second-order Adams-Bashforth method in MPAS-O

- Use forward-backward scheme only for thickness equation

$$\hat{h}_{k,n+1} = h_{k,n} + \Delta t \mathcal{F}(h_{k,n})$$

$$h_k^* = \frac{1}{2}\left(\hat{h}_{k,n+1} + h_{k,n}\right)$$

$$h_{k,n+1} = h_{k,n} + \Delta t \mathcal{F}(h_k^*)$$

$$w_k^{*\,top} = w_{k+1}^{*\,top} - \nabla \cdot (\Delta z_k^* \mathbf{u}_k^{*\,tr})$$

$$\mathcal{F}(h_k^*) = \left(-\nabla \cdot \left(h_k^{*edge} \mathbf{u}_k^{*tr}\right) - \frac{\partial}{\partial z}(h_k^* w_k^*)\right)$$

AB2 advanced velocity

$$\mathbf{u}_k^{*tr} = \bar{\mathbf{u}}_{avg} + \mathbf{u}'_{k,n+0.5} + \mathbf{u}^{corr} + \mathbf{u}_k^{bolus}$$

$$\mathbf{u}^{corr} = \left(\bar{F} - \sum_{k=1}^{N^{edge}} h_k^{*\,edge}(\bar{\mathbf{u}}_{avg} + \mathbf{u}'_{k,n+0.5} + \mathbf{u}_k^{bolus})\right) \Big/ \sum_{k=1}^{N^{edge}} h_k^{*\,edge}$$

Change of the baroclinic time stepping method

Second-order Adams-Bashforth method in MPAS-O

- For now, different time stepping schemes are applied to each different equations:
  - Momentum equation: Adams-Bashforth 2nd order
  - Layer thickness equation: Forward-backward
  - Tracers: Forward Euler

- With 75% of the default del2 & del4 diffusion coefficient, current implementation is stable for a variety of simulations without the super cycle.

Change of the baroclinic time stepping method

Second-order Adams-Bashforth method in MPAS-O

- Computes Stage1~3 **once** to achieve the second-order accuracy

Example for velocity in stage 1

Stage 1

Step n

$\mathbf{u}_n$

↓

Compute tendency at n

$f(\mathbf{u}_n)$

↓

Time advancing

$$\mathbf{u}_{n+1} = \mathbf{u}_n + \frac{3}{2}\Delta t\, f(\mathbf{u}_n) - \frac{1}{2}\Delta t\, f(\mathbf{u}_{n-1})$$

← $f(\mathbf{u}_{n-1})$ is stored at the previous step. So, use more memory.

Change of the baroclinic time stepping method

Plan: Adams-Bashforth method

- Code example (a baroclinic velocity update part)

```
do iEdge = 1, nEdgesOwned
   cell1 = cellsOnEdge(1,iEdge)
   cell2 = cellsOnEdge(2,iEdge)
   uTemp(:,iEdge) = 0.0_RKIND
   sshGrad = splitFact * gravity * &
             (sshNew(cell2) - sshNew(cell1)) &
             /dcEdge(iEdge)
   do k = minLevelEdgeBot(iEdge), maxLevelEdgeTop(iEdge)
      uTemp(k,iEdge) = normalBaroclinicVelocityCur(k,iEdge) &
                + 1.50_RKIND * dt * (normalVelocityTend(k,iEdge) &
                + sshGrad) &
                -  0.5_RKIND * dt * normalVelocityTendOld(k,iEdge) &
                +                    dt * normalVelocityNew(k,iEdge)
   enddo ! vertical
enddo ! iEdge
```

$\frac{3}{2}\Delta t\, f(\mathbf{u}_n)$

Stored at the previous step

$\frac{1}{2}\Delta t\, f(\mathbf{u}_{n-1})$

Change of the baroclinic time stepping method

Performance check

- Test cases
  1) Surface gravity wave (1D)
  2) Internal tide test case (2D, x-z slice)
  3) Seamount test case (3D, idealized)
  4) High-resolution global ocean test case on RRS18to6 mesh (3D, Real world)

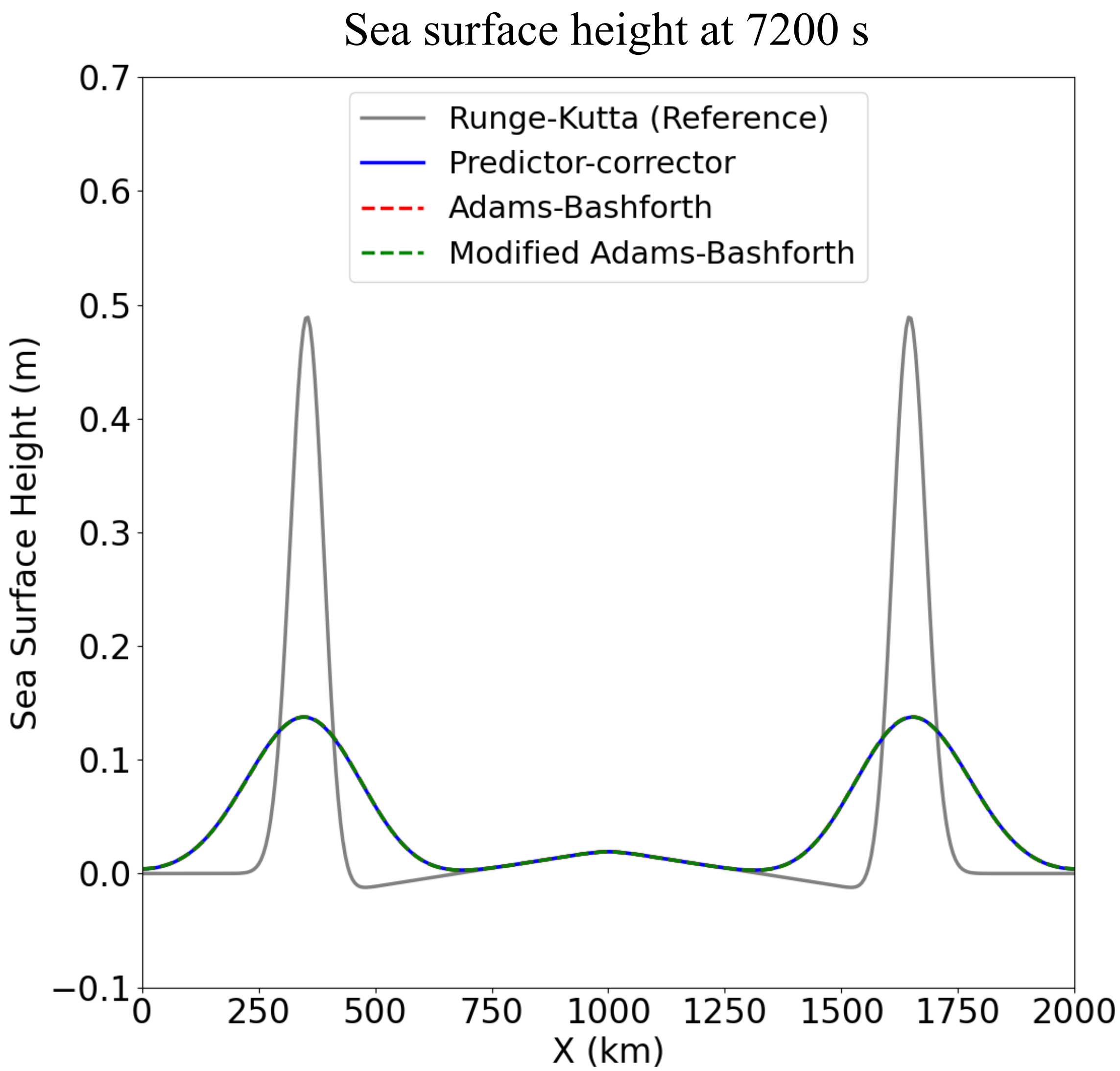
Change of the baroclinic time stepping method

Surface gravity wave test (1D)

- Initial SSH travels opposite direction.
- Tested on my Mac using 1 core
- $\Delta t = 300$ s

Method	Runtime (main loop)
Forward-backward	3.23260 s
Adams-Bashforth	1.78725 s

1.81x speedup



Change of the baroclinic time stepping method

Surface gravity wave test (1D)

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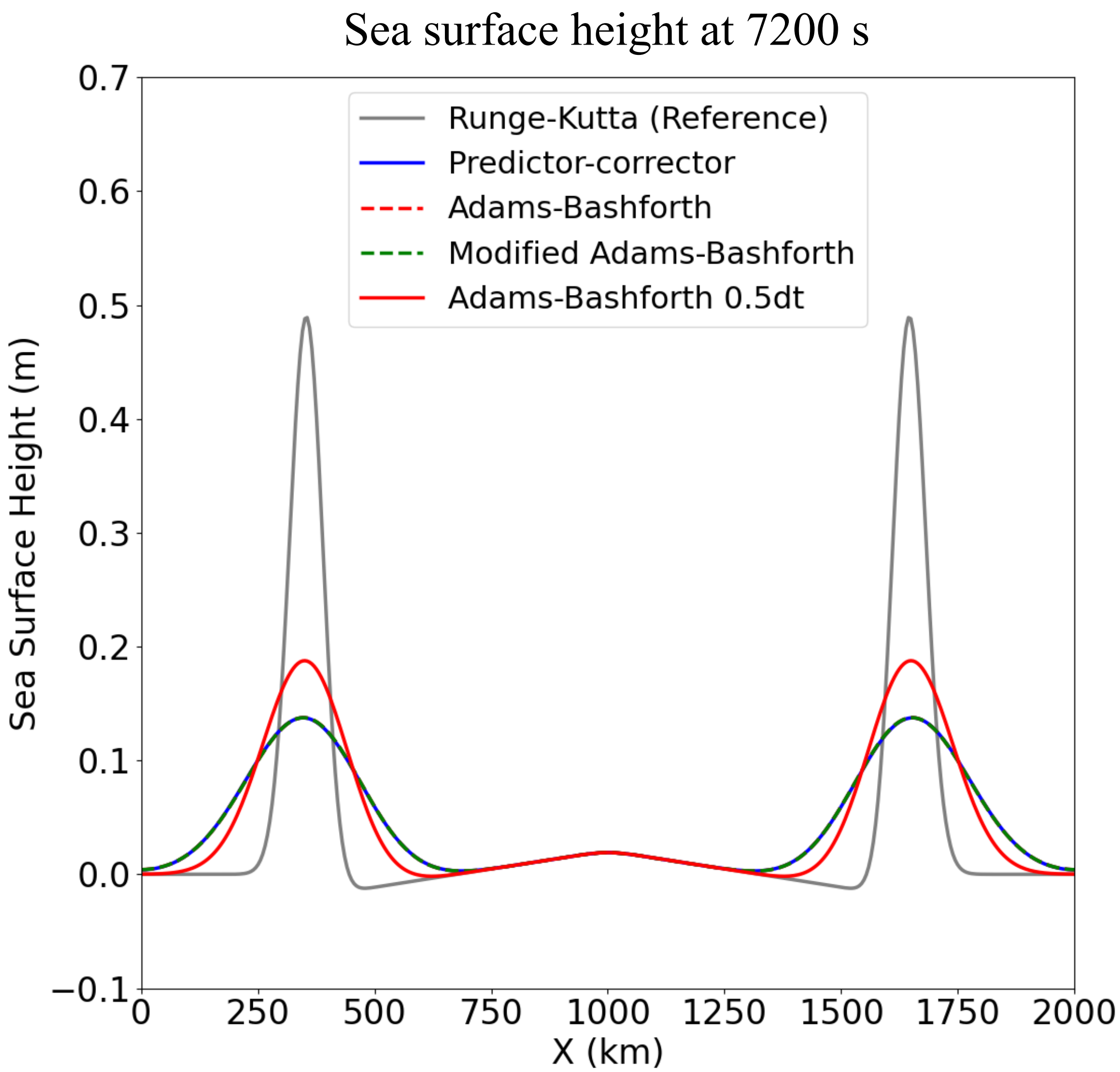
- $\Delta t = 300$ s

Method	Runtime (main loop)
Forward-backward	3.23260 s
Adams-Bashforth	1.78725 s
Adams-Bashforth (0.5dt)	2.57797 s



Change of the baroclinic time stepping method

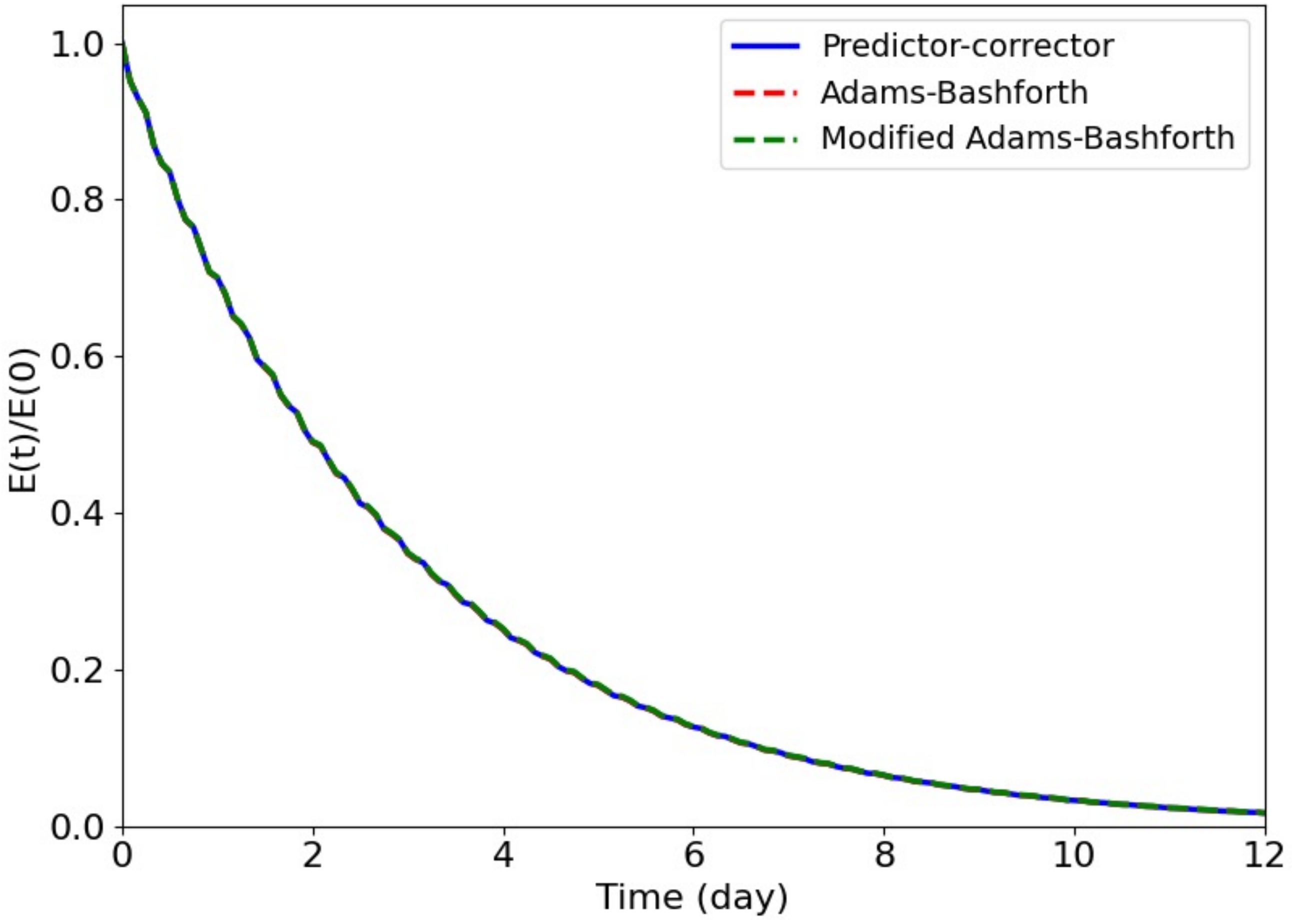
Internal tide test case (2D, x-z slice)

- Nonlinear internal tide generation by small but sharp bathymetry
- Comparison of total barotropic mechanical energy
- Tested on my Mac using 8 cores
- $\Delta t = 600$ s

Method	Runtime (main loop)
Forward-backward	398.91979 s
Adams-Bashforth	205.64063 s

1.94x speedup

Time evolution of Total barotropic M.E.



Change of the baroclinic time stepping method

Seamount test case (3D, idealized)

- A Gaussian bell-shape bathymetry located at the center of domain
- The ocean is initially at rest
- Designed to evaluate pressure gradient error arising from numerical discretization in terrain-following coordinates
- Non-zero values for the velocity can be interpreted as numerical errors.

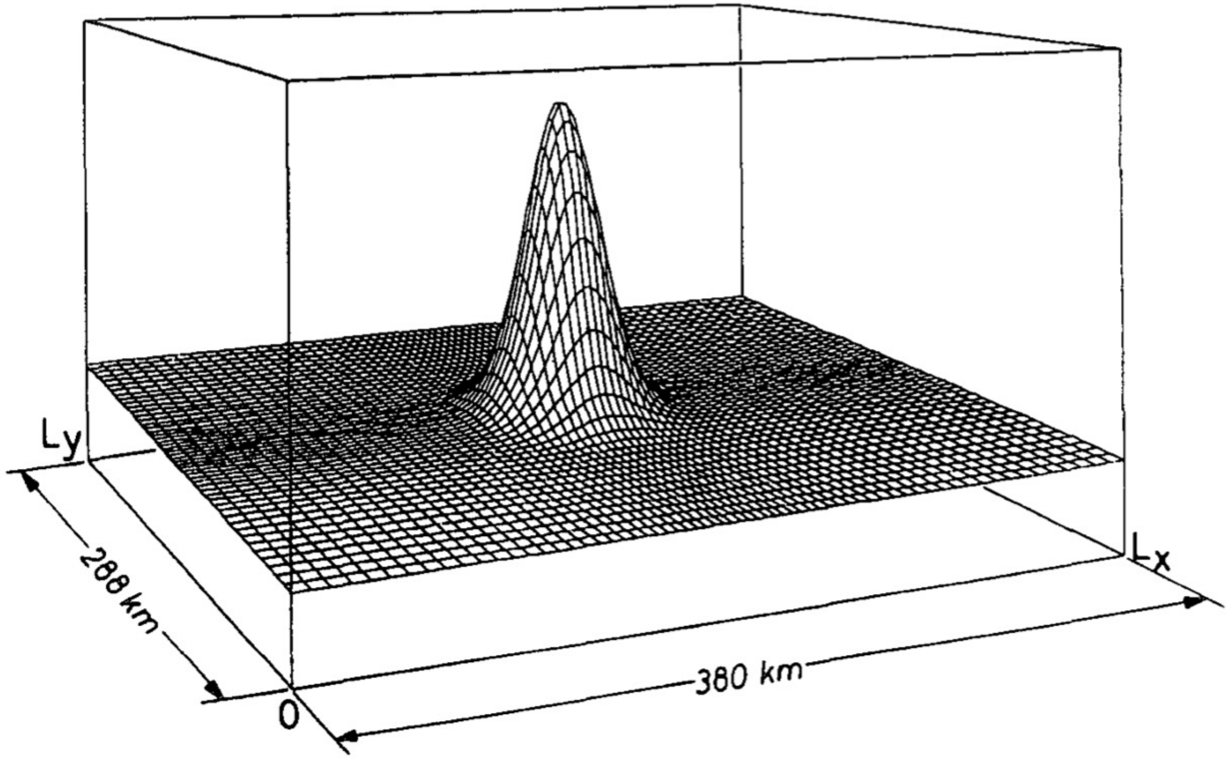


FIG. 2. Perspective view of the seamount geometry. The stretching of the grid that leads to higher horizontal resolution in the center (across the seamount) can be seen best at the boundaries.

Figure 2 of
Beckmann and Haidvogel (1993)

Change of the baroclinic time stepping method

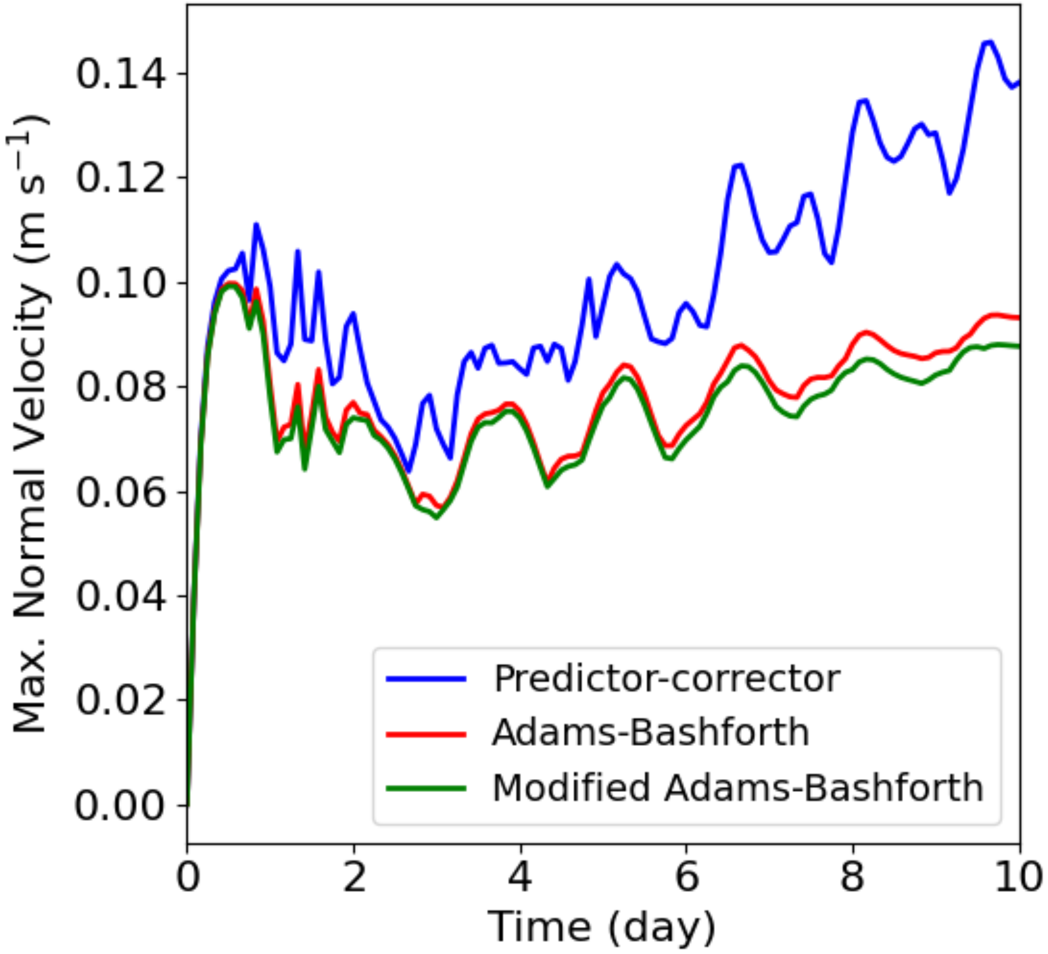
Seamount test case (3D, idealized)

- Tested on my MacBook using 8 cores
- Non-zero values for the velocity can be interpreted as numerical errors.
- Smaller error in AB2 and M-AB2 methods
  - Smaller error in M-AB2, since numerical modes are dominant in this test case.

Method	Runtime (main loop)
Forward-backward	362.45233 s
Adams-Bashforth	197.34885 s

1.83x speedup

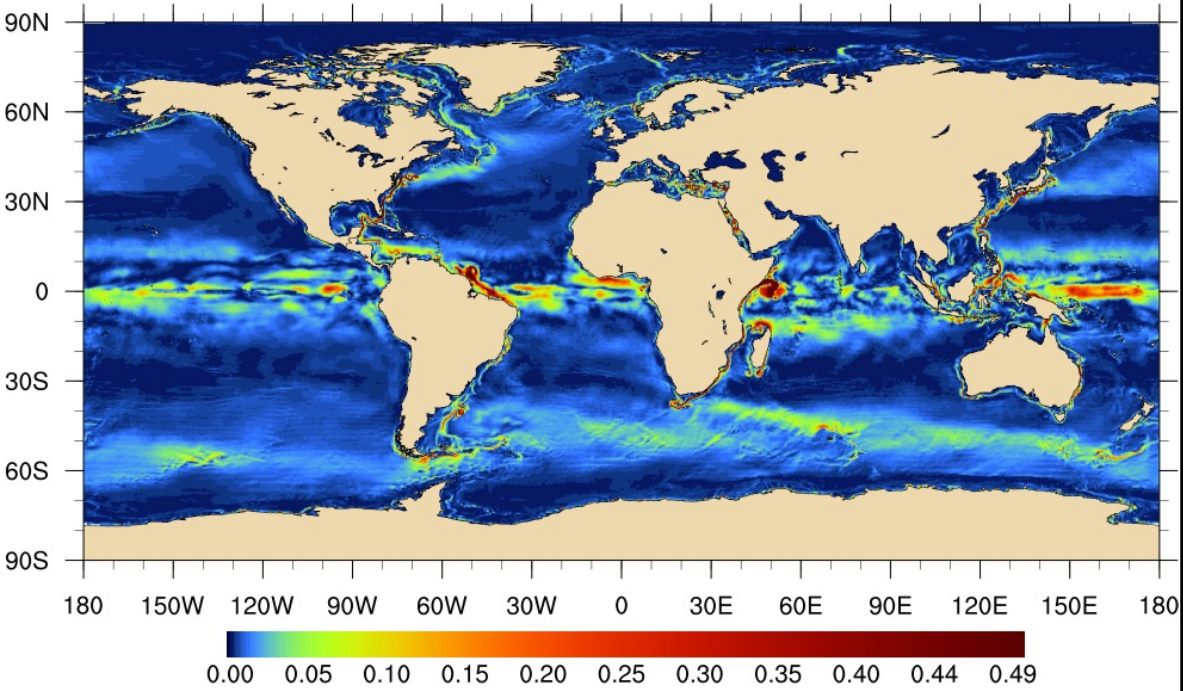
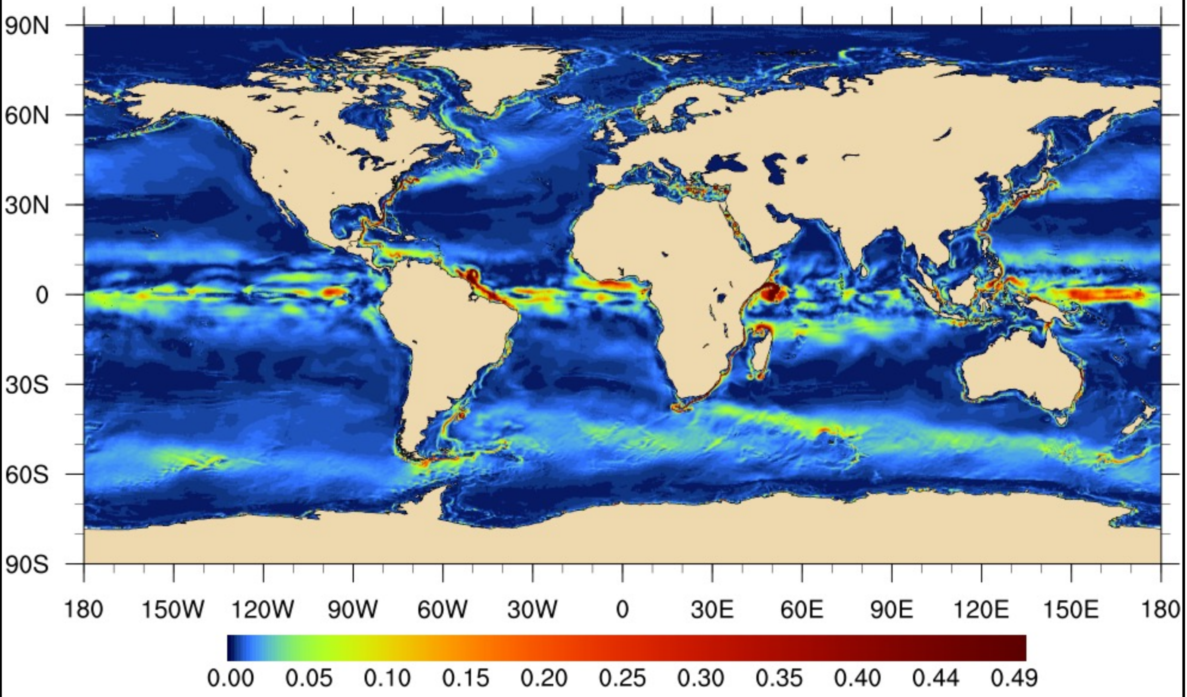
Time evolution of Max. normal velocity



Change of the baroclinic time stepping method

High-resolution global ocean test case on RRS18to6 mesh

- Tested on NERSC-Cori KNL using 8160 cores
- Time integrated for 30 model days with $\Delta t = 300\ s$

	Forward-backward (Current)	**Adams-Bashforth (Plan)**
Runtime (Main loop)	**7354.18854 s**	**4023.81048 s**
Surface kinetic energy field at day 30		

Change of the baroclinic time stepping method

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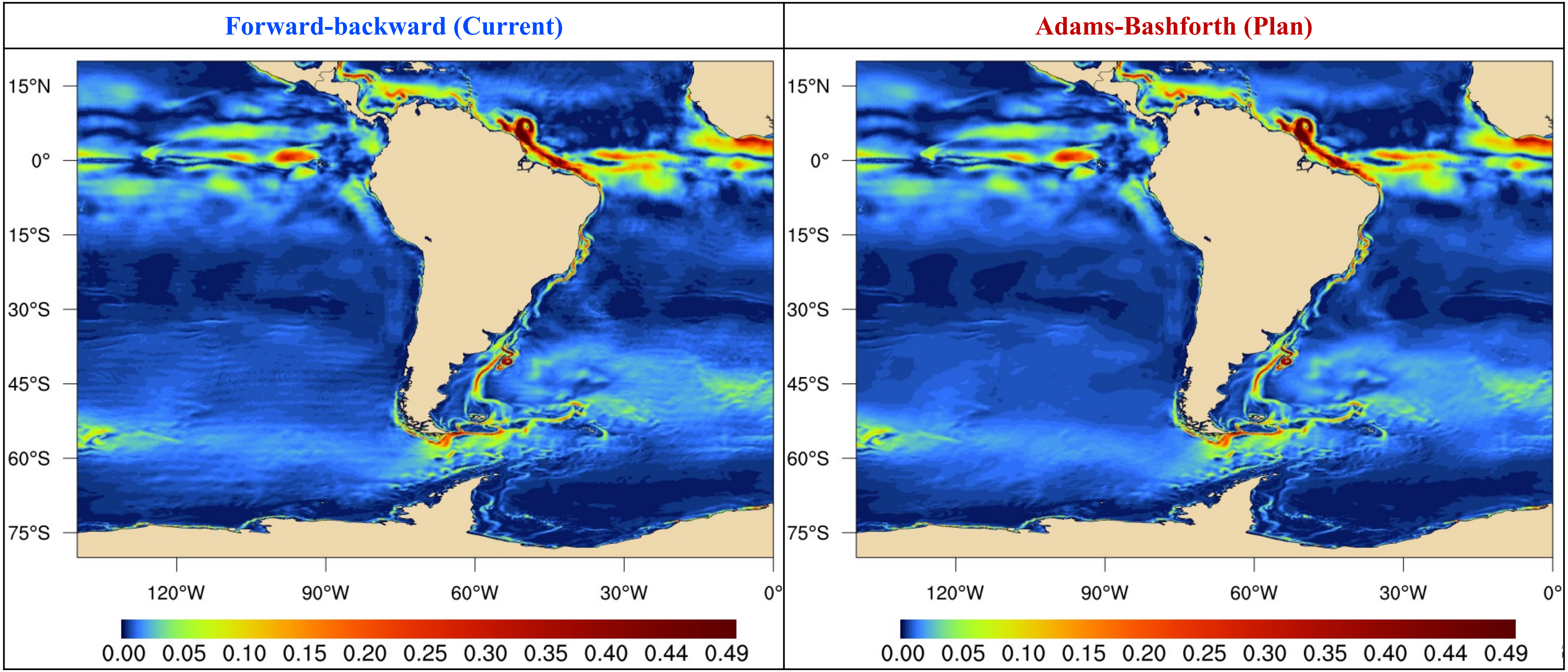


Change of the baroclinic time stepping method

Time step size sensitivity

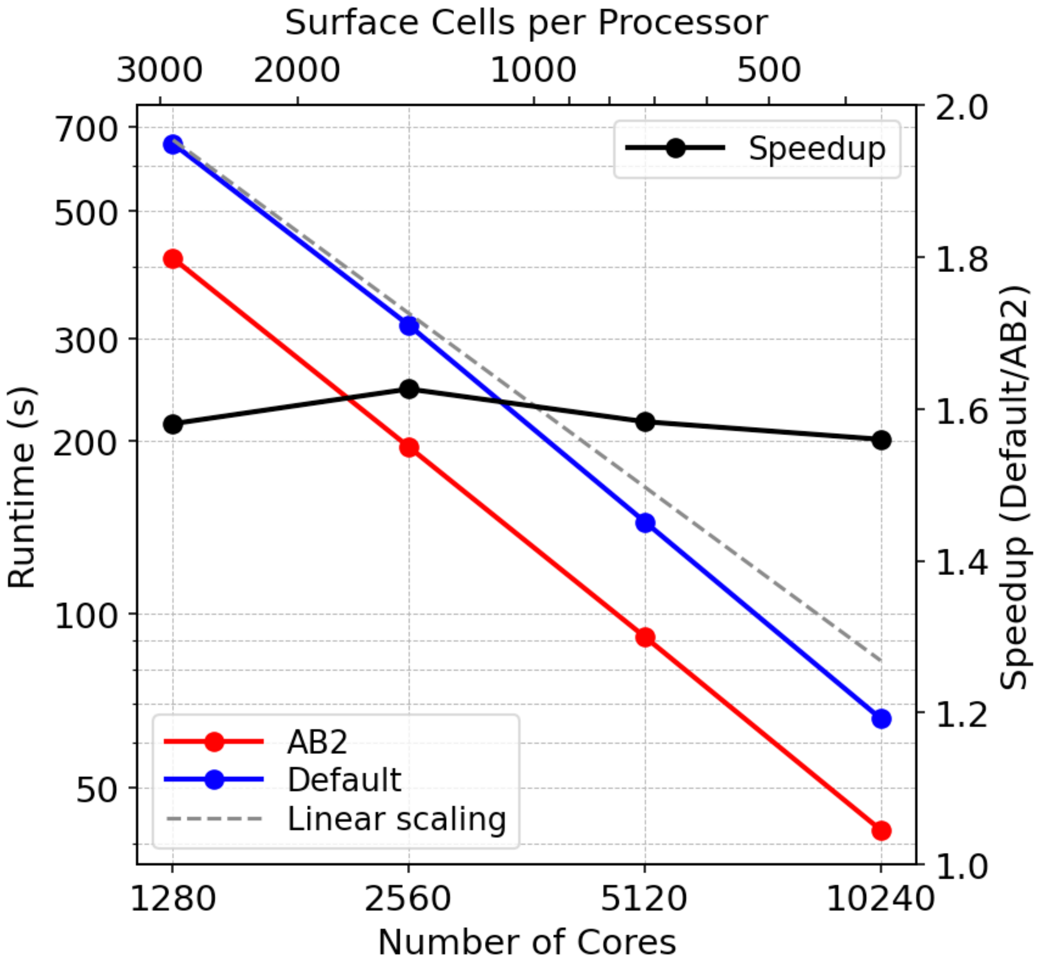
- After some modifications, the AB2 method with less hyperviscosity (~25%) can use the same time step size with the PC method.
  - Time step size test using the 18 km to 6 km resolution mesh

Time step size	PC	AB2
180 s	O	O
300 s	O	O
360 s	O	O
480 s	O	O
600 s	X	X

Change of the baroclinic time stepping method

Computational performance

- A whole model runtime comparison
  - one day integration on 18to6km mesh (real-world configuration)
    - Tested on HPC11 (miller), which is the AF machine at OLCF (identical architecture to Perlmutter)
  - ~1.6x speedup for AB2

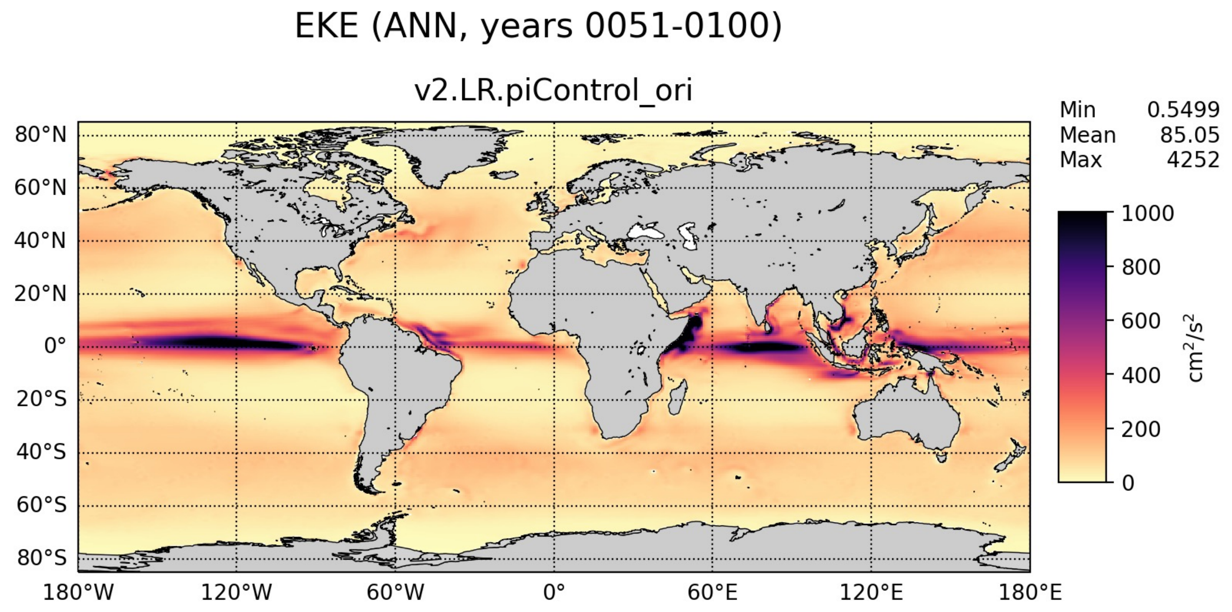


Change of the baroclinic time stepping method

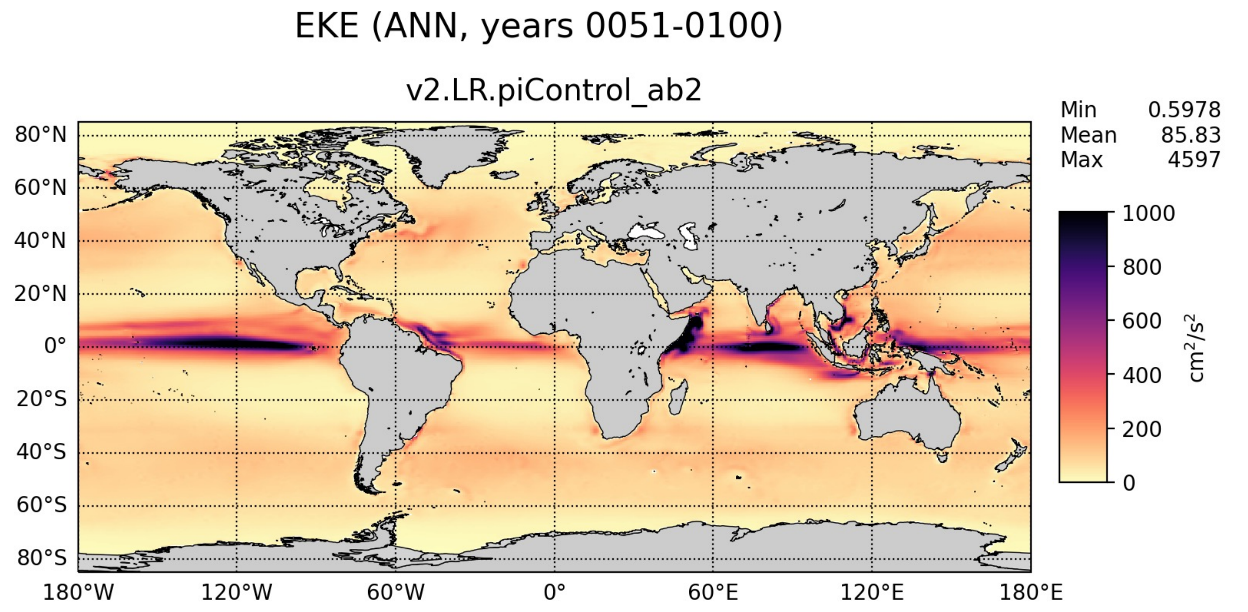
WCYCL simulation : A fully-coupled simulation using E3SM

Surface Eddy Kinetic Energy
(years 051-100)

Default (PC)



AB2



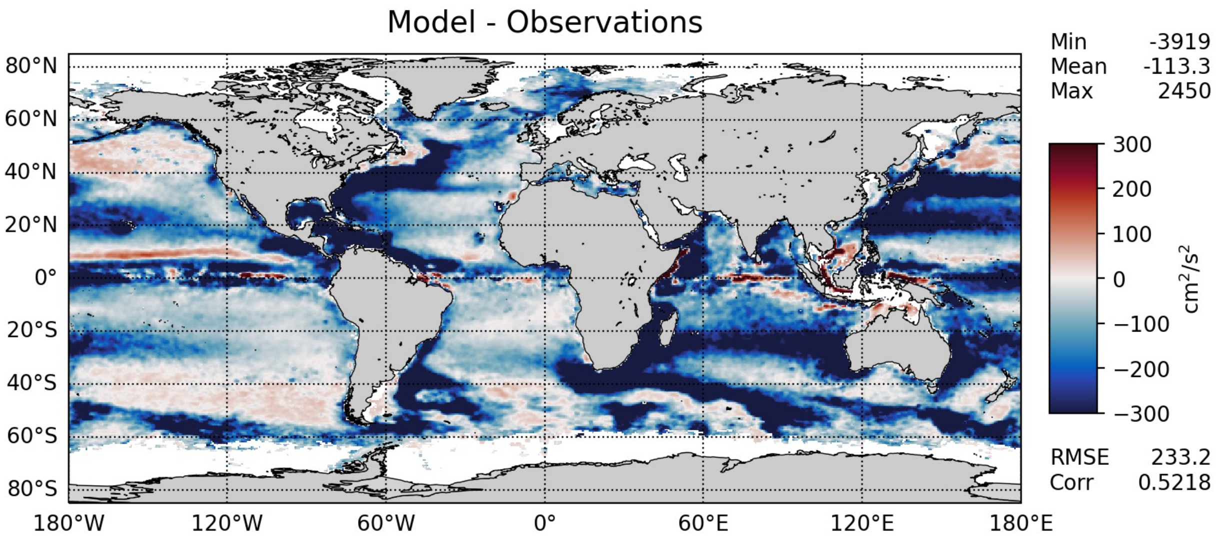
AB2 uses 25% less diffusion from default setup
(Laplacian, hyper-Laplacian)

Change of the baroclinic time stepping method

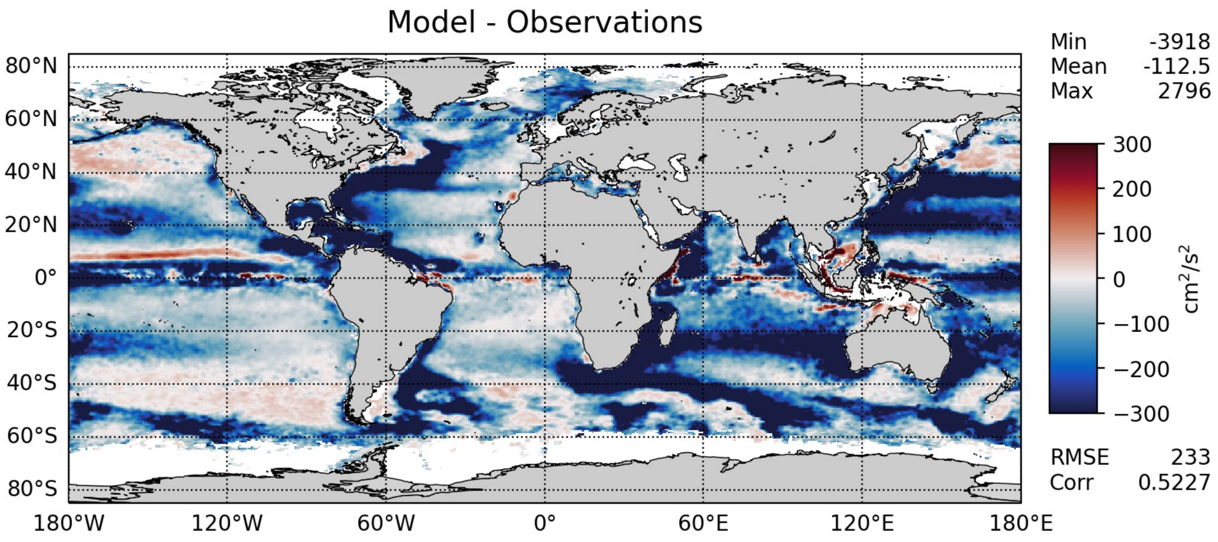
WCYCL simulation : A fully-coupled simulation using E3SM

Surface Eddy Kinetic Energy
(years 051-100)

Default (PC)



AB2



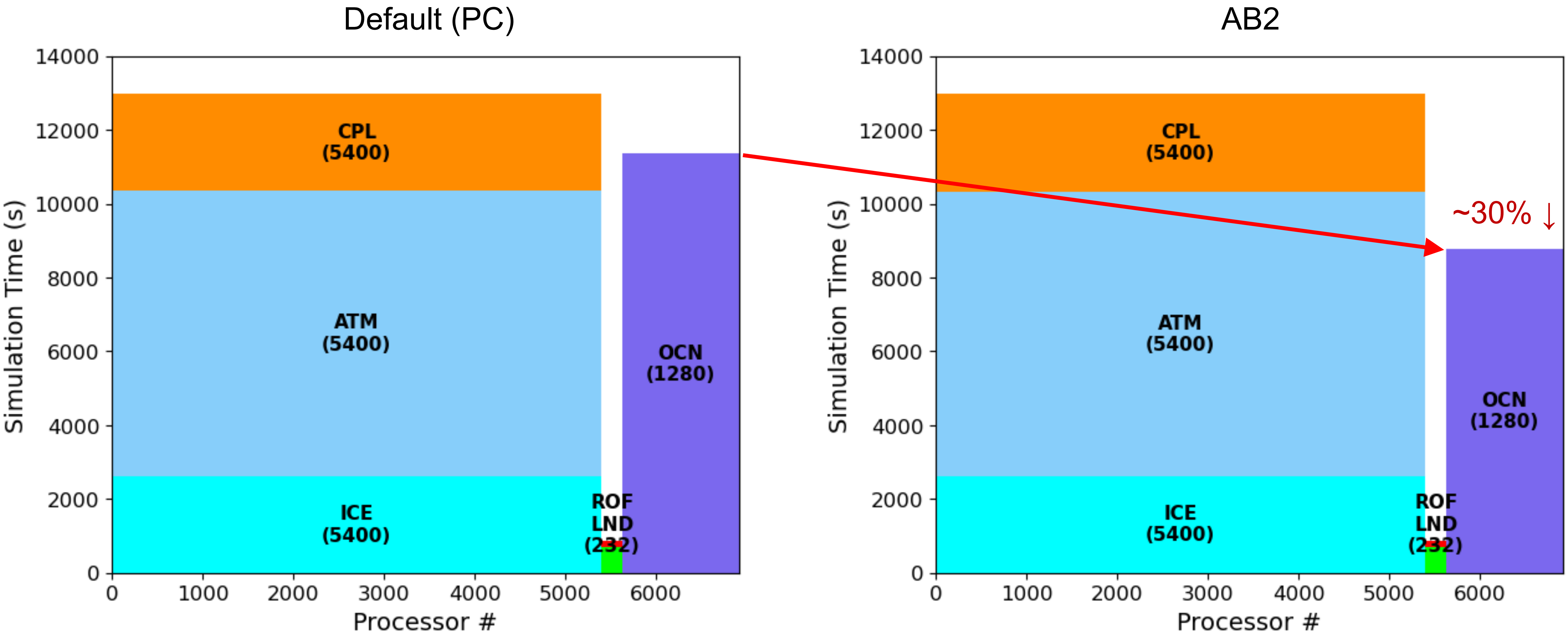
AB2 uses 25% less diffusion from default setup
(Laplacian, hyper-Laplacian)

Change of the baroclinic time stepping method

WCYCL simulation : A fully-coupled simulation using E3SM

- AB2 30% faster, but OCEAN Waiting time increased a lot ➔ Need to optimize PE layout

Performance on HPC11 machine (Air Force machine in OLCF)



Change of the baroclinic time stepping method

Stability region of time-stepping methods

- A model problem with an analytical solution

$$\frac{dy(t)}{dt} = \lambda y(t), \qquad y(0) = y_0 = 1, \qquad y(t) = e^{\lambda t}$$

- Amplification factors for each time-stepping method

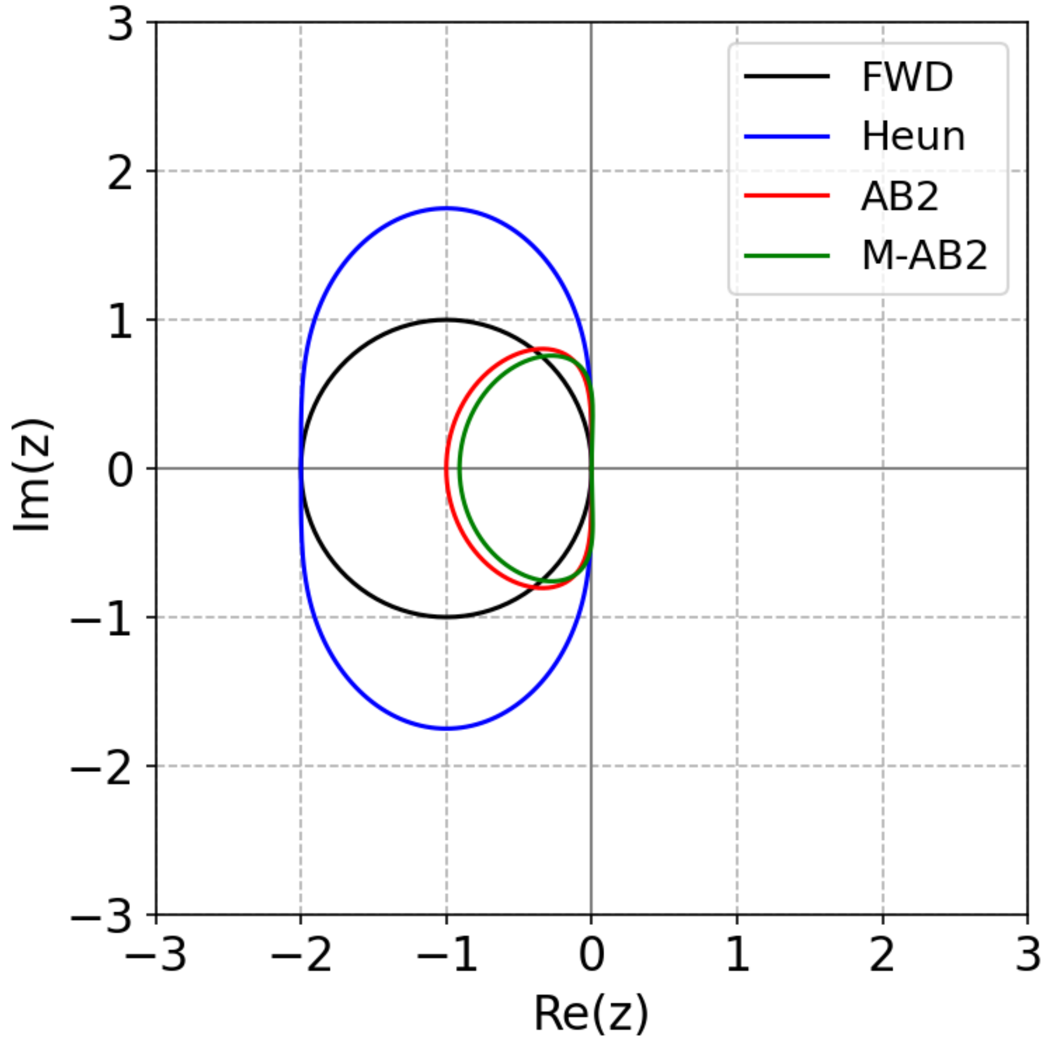
$$z = e^{i\theta}, 0 \le \theta \le 2\pi$$

Time-stepping method	Amplification factor (S)
Forward-Euler	$z - 1$
Heun's method (i.e., forward-backward)	$-1 \pm \sqrt{2(z-1)+1}$
Standard ($\epsilon_{AB} = 0$) or Modified ($\epsilon_{AB} = 0.1$) Second-order Adams-Bashforth	$\dfrac{z^2 - z}{\left(\frac{3}{2} + \epsilon_{AB}\right) z - \left(\frac{1}{2} + \epsilon_{AB}\right)}$

Change of the baroclinic time stepping method

Stability region of time-stepping methods

- Area of stability region: Heun > FWD > AB2 > M-AB2



Change of the baroclinic time stepping method

Oscillatory and damping feature of time-stepping methods

- A simple oscillation equation (without forcing and damping)

$$\frac{\partial u}{\partial t} + ifu = 0$$

  - Analytical solution: $u(t) = u_0 e^{ift},\ u_0 = 1$

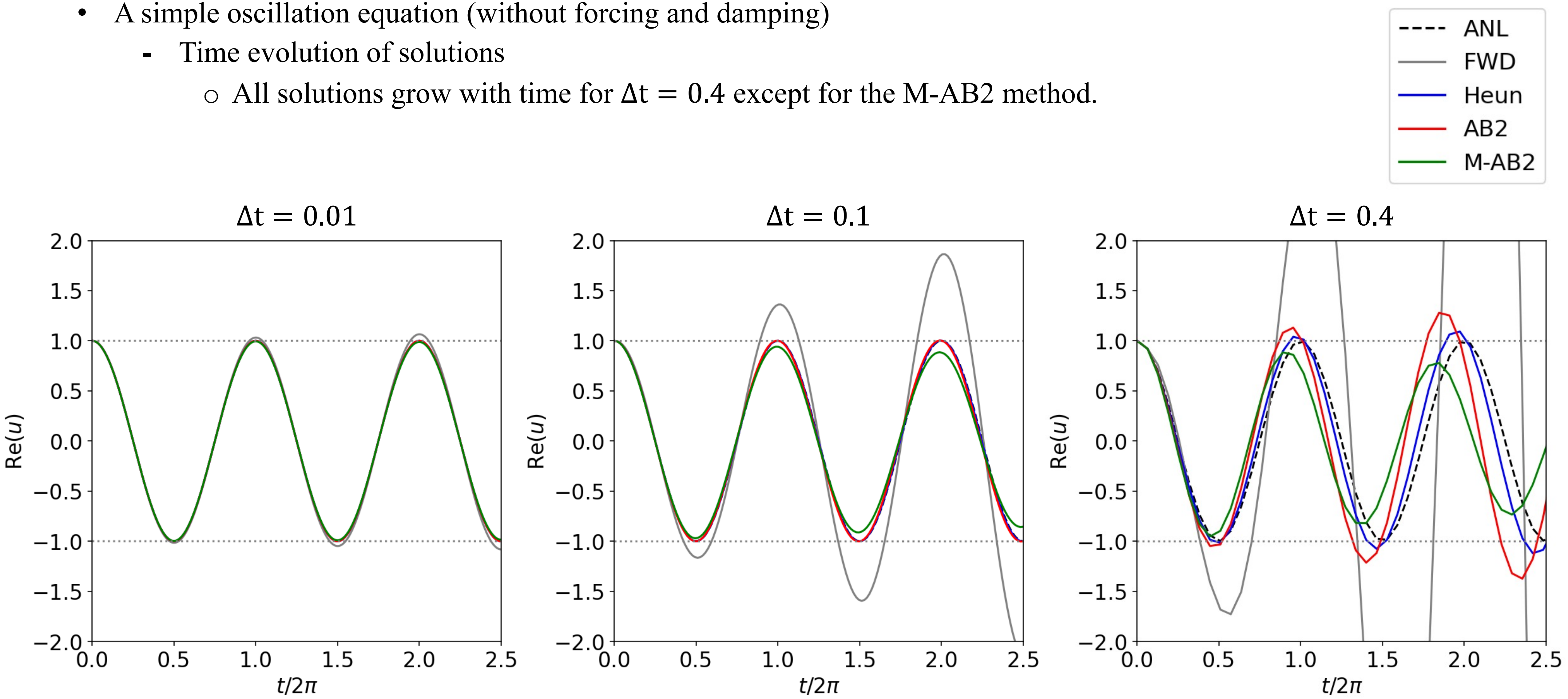
$P = i\Delta t f$

Time-stepping method	Time-discretized equation
Forward-Euler	$u^{n+1} = (1 - P)u^n$
Heun's method (i.e., forward-backward)	$\hat{u}^{n+\alpha} = u^n + \alpha P u^n$ $u^{n+1} = u^n + \Delta t(\beta P \hat{u}^{n+\alpha} + (1-\beta)Pu^n)$ $\alpha = 1, \beta = 1/2$
Standard ($\epsilon_{AB} = 0$) or Modified ($\epsilon_{AB} > 0$) Second-order Adams-Bashforth	$u^{n+1} = \left(1 - \left(\frac{3}{2} + \epsilon_{AB}\right)P\right)u^n + \left(\frac{1}{2} + \epsilon_{AB}\right)Pu^{n-1}$

Change of the baroclinic time stepping method

Oscillatory and damping feature of time-stepping methods

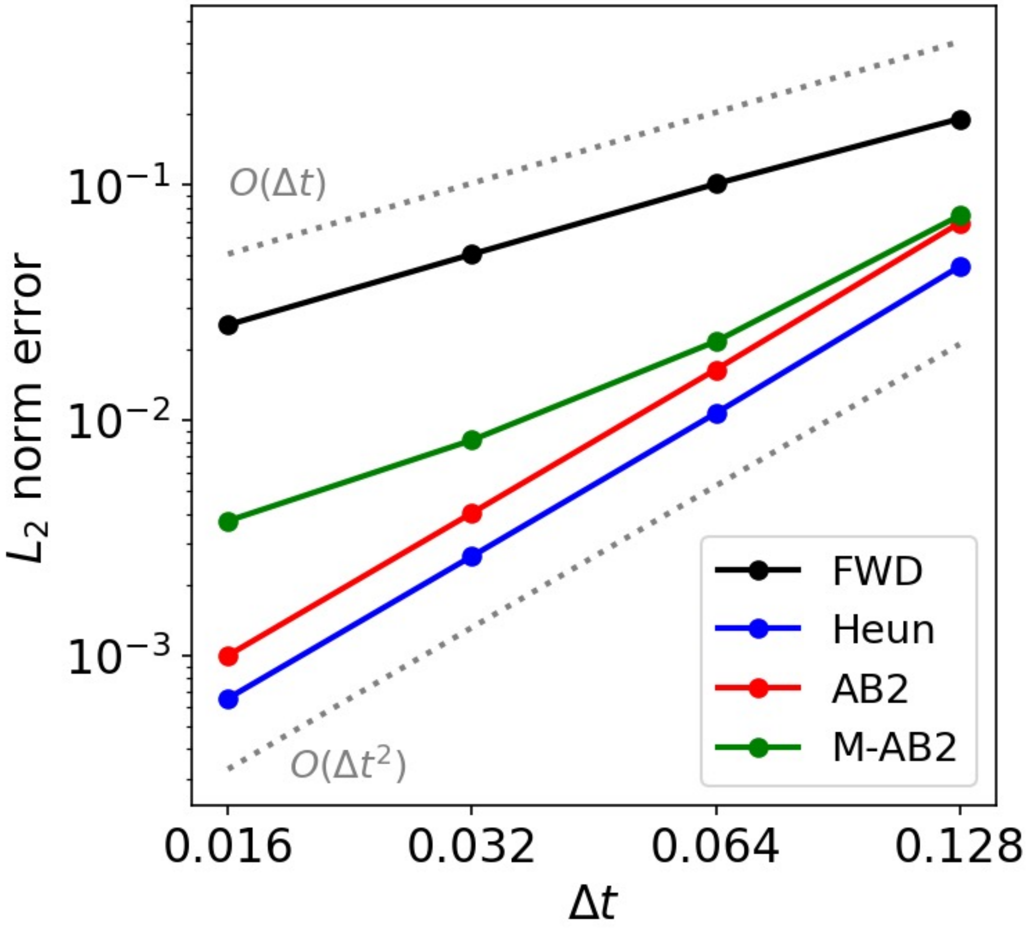
- A simple oscillation equation (without forcing and damping)
  - Time evolution of solutions
    - All solutions grow with time for $\Delta t = 0.4$ except for the M-AB2 method.



Change of the baroclinic time stepping method

Oscillatory and damping feature of time-stepping methods

- A simple oscillation equation (without forcing and damping)
  - Accuracy
    - Heun's (2nd) > AB2 (2nd) > M-AB2 (quasi 2nd) > FWD (1st)



Change of the baroclinic time stepping method

Second-order Adams-Bashforth method in MPAS-O

- Computes Stage1~3 **once** to achieve the second-order accuracy