Overview of evolution of computational kernel of ROMS: How different things add up to make an ocean model.

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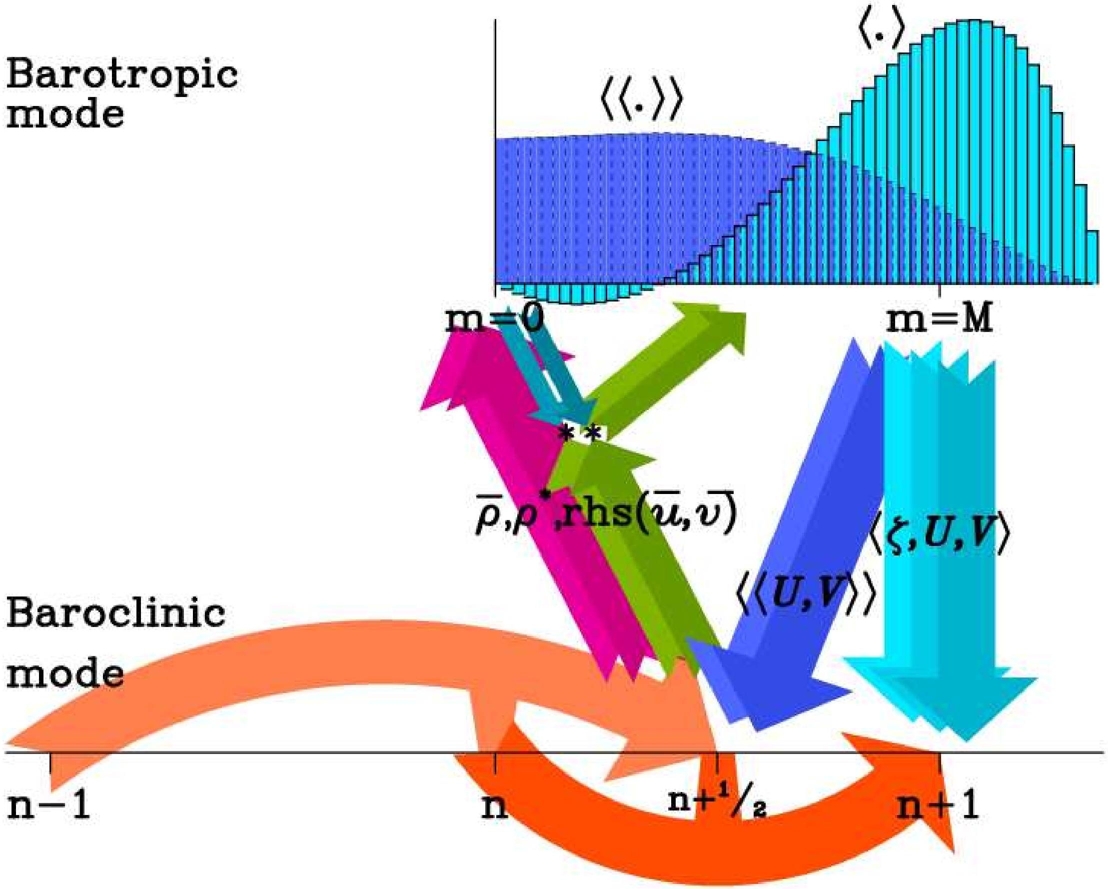
The purpose of this presentation is two-fold

- Overview of components of ROMS kernel as *a collection* of algorithms

- Focus on algorithm *interference*, *conflicts*, and *reconciliation* following ground-up design of ROMS



Why?

Computational kernel features

- kernel is part of the model which is present in any application and is not replaceable
- **vertical coordinate.** ROMS belongs to σ-class models, but code stores $z(x, y, \sigma)$ as an array $\Rightarrow$ can be used as a general vertical coordinate code.
- **time stepping engine** barotropic-baroclinic mode splitting and coupling
- built around new time-stepping algorithms for hyperbolic system equations
- **advection, pressure-gradient schemes, etc...**
- higher than second-order accuracy spatial discretization for critical terms
- ground-up design philosophy, focusing on multi-component interplay of normally remotely-related features and algorithms
- code architecture decisions involve optimization in multidimensional space, including model physics, numerical algorithms, computational performance and cost
- code infrastructure is distinct from *modular* design
- multiple computer architecture support: dual Open MP/MPI parallelization capability via 2D domain decomposition
- mounting points to interact with sub-models (biology, sediment transport, etc...)

Examples of algorithm interference

- Barotropic–baroclinic time splitting motivated by linear stability analysis interferes with finite-volume mass conservation in slow mode. This leads to the loss of *constancy preservation* property for tracer advection.

- Linear stability analysis favors Forward-Backward time step for momentum and tracers over predictor-corrector by the *stability* vs. *computational cost* criterion for internal waves alone. Yet, most suitable advection algorithms exist as two-stage procedures, which more naturally incorporate into predictor-corrector.

- In its turn, barotropic–baroclinic mode splitting makes it impossible to satisfy finite-volume continuity equation on slow baroclinic time during predictor sub-step, hence *loss of the constancy preservation property* of finite-volume conservative form of tracer advection.

- High-order polynomial interpolation requires monotonicity constraints to prevent spurious oscillations, if interpolated field is not smooth on grid scale. In context of pressure gradient it translates into the constraint of monotonicity of stratification, which eventually leads to complete redesign of Equation of State (EOS) of seawater to allow such constraint.

- In a time-split procedure barotropic mode requires knowledge of bottom stress *before* barotropic mode stepping begins within each main time step. This occurs naturally in time-explicit bottom stress formulation, but it also imposes unphysical limitation on bottom stress (remove no more that amount momentum within the bottom-most grid box per baroclinic time step).

Time stepping algorithms

Single hyperbolic equation [advection]:

$$\frac{\partial q}{\partial t} + c\frac{\partial q}{\partial x} = 0$$

wave system:

$$\frac{\partial \zeta}{\partial t} = -c\frac{\partial u}{\partial x}$$
$$\frac{\partial u}{\partial t} = -c\frac{\partial \zeta}{\partial x}$$

Time stepping in oceanic modeling, Griffies, et al, 2002:

- *Synchronous* (compute r.h.s. for all equations *at once* and apply it)

  LF + Asselin Filter (mostly; POM, MOM/POP, SPEM)

  LF-TR, LF-AM3, AB2-TR

  AB3 (Durran, 1991; *SPEM/SCRUM* family only)

same stability limit as for single advection equation, Canuto et al, 1988.

stability is limited by $\alpha_{\text{max}} = c\Delta t \cdot k_{\text{max}} \leq 1$, typically 0.7 per computation of r.h.s.

- *Forward-Backward* (systems only)

$$\zeta^{n+1} = \zeta^n - c\Delta t \cdot \frac{\partial u^n}{\partial x}\,; \qquad u^{n+1} = u^n - c\Delta t \cdot \frac{\partial \zeta^{n+1}}{\partial x}$$

twice as efficient, $\alpha_{\text{max}} \leq 2$ only in the simplest, classical version ever been used in oceanic modeling, and only for barotropic mode, Griffies, et al, 2002

Explicit time stepping for **single equation** $\dfrac{\partial q}{\partial t} = -i\omega \cdot q$ has general form

$$q^{n+1} = \mathcal{F}(q^n, q^{n-1}, \ldots) - i\alpha \cdot \mathcal{G}(q^n, q^{n-1}, \ldots)$$

where $\alpha = \omega \Delta t\,, \quad \mathcal{F}(q^n, q^{n-1}, \ldots) = \sum_{i=0}^{r} \beta_i q^{n-i}\,; \quad \mathcal{G}(q^n, q^{n-1}, \ldots) = \sum_{i=0}^{r} \gamma_i q^{n-i}$

and *characteristic equation* $\mathcal{P}(\lambda) = \lambda^{r+1} - \sum_{i=0}^{r} (\beta_i - i\alpha \cdot \gamma_i)\lambda^{r-i} = 0\,.$

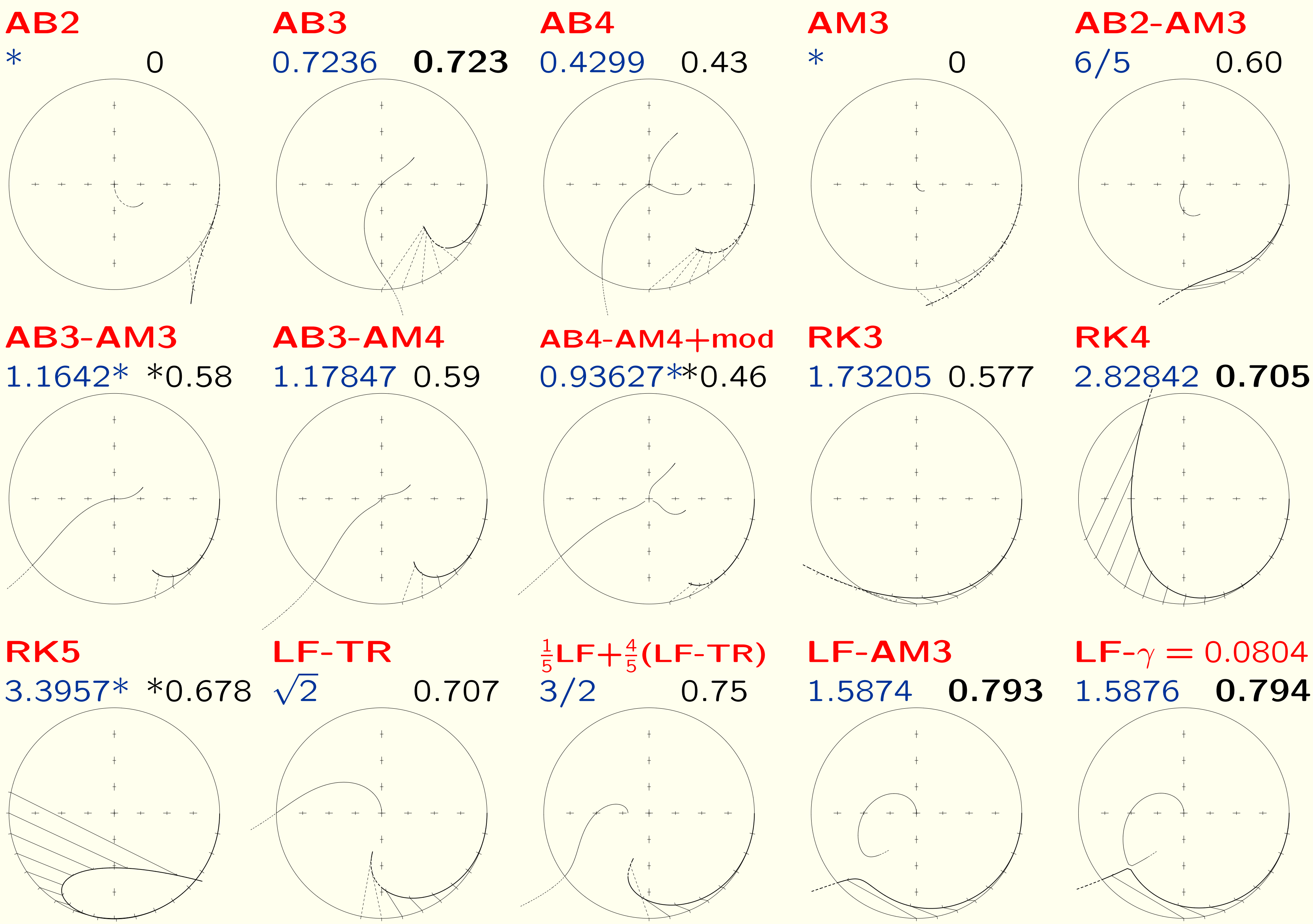
The same, but applied to **system** reads $\dfrac{\partial \zeta}{\partial t} = -i\omega \cdot u\,; \qquad \dfrac{\partial u}{\partial t} = -i\omega \cdot \zeta$

$$\begin{pmatrix}\zeta\\ u\end{pmatrix}^{n+1} = \mathcal{F}\left[\begin{pmatrix}\zeta\\ u\end{pmatrix}^{n}, \begin{pmatrix}\zeta\\ u\end{pmatrix}^{n-1}, \ldots\right] + \begin{pmatrix}0 & -i\alpha\\ -i\alpha & 0\end{pmatrix} \cdot \mathcal{G}\left[\begin{pmatrix}\zeta\\ u\end{pmatrix}^{n}, \begin{pmatrix}\zeta\\ u\end{pmatrix}^{n-1}, \ldots\right],$$

hence
$$\begin{vmatrix}\mathcal{F}(1, \lambda^{-1}, \ldots) - \lambda & -i\alpha \cdot \mathcal{G}(1, \lambda^{-1}, \ldots)\\ -i\alpha \cdot \mathcal{G}(1, \lambda^{-1}, \ldots) & \mathcal{F}(1, \lambda^{-1}, \ldots) - \lambda\end{vmatrix} = \left(\lambda - \sum_{i=0}^{r} (\beta_i - i\alpha \cdot \gamma_i)\lambda^{-i}\right) \times \left(\lambda - \sum_{i=0}^{r} (\beta_i + i\alpha \cdot \gamma_i)\lambda^{-i}\right) = 0$$

same set of roots λ and λ^* in complex-conjugate pairs $\Rightarrow$ **same stability limit**

Synchronous time stepping ...



Comparison of time stepping algorithms

Synchronous

- Well studied;
- Available to high orders of accuracy;
- *efficiency* $\leq 1 =$ *efficiency*(LF).
- less than optimal because the fastest processes occur as *interplay* between momenta and tracers

Forward-Backward

- **approximately twice as efficient;**
- purely dispersive;
- only first-order accurate for each equation, unless interpreted as u and ζ are staggered in time;
- What to do about advection? Coriolis terms?

Design Goals:

⇒We seek to generalize best known synchronous algorithms, such as RK2, LF-TR, LF-AM3, AB3, by introducing FB-like feedback, so that newly computed field *immediately* used for the update of the *partner* equation, rather at the next time step (or sub-step in predictor-corrector algorithm).

⇒ We also seek to generalize FB to higher orders of accuracy.

Time stepping algorithm must be accurate and robust, even if run close to the limits of numerical stability. To do so in must have small numerical dumping of resolved time scales, but at the same time *dissipate* (not disperse) unresolved ones (hence prevent temporal aliasing in nonlinear terms), and also provide strong dumping of computational modes.

Although our primary focus is to find optimum algorithm for gravity waves, it should be also compatible with other terms, such as advection (both centered and upstream-biased) and Coriolis.

Inverse stability analysis method: use arbitrary coefficients and derive algorithms with desired eigen values for characteristic equations for discretized *coupled system*.

Generalized RK2

Predictor sub-step

$$\zeta^{n+1,*} = \zeta^n - i\alpha \cdot u^n$$
$$u^{n+1,*} = u^n - i\alpha \cdot \left[\beta\zeta^{n+1,*} + (1-\beta)\zeta^n\right]$$

corrector

$$\zeta^{n+1} = \zeta^n - \frac{i\alpha}{2} \cdot \left(u^{n+1,*} + u^n\right)$$
$$u^{n+1} = u^n - \frac{i\alpha}{2} \cdot \left[\epsilon\zeta^{n+1} + (1-\epsilon)\zeta^{n+1,*} + \zeta^n\right]$$

$\beta = \epsilon = 0 \Rightarrow$ standard RK2.

single-step matrix form:

$$\begin{pmatrix} \zeta \\ u \end{pmatrix}^{n+1} = \begin{pmatrix} 1 - \frac{\alpha^2}{2} & -i\alpha\left(1 - \frac{\alpha^2\beta}{2}\right) \\ -i\alpha\left(1 - \frac{\alpha^2\epsilon}{4}\right) & 1 - \frac{\alpha^2}{2} + \frac{\alpha^4\beta\epsilon}{4} \end{pmatrix} \begin{pmatrix} \zeta \\ u \end{pmatrix}^{n}$$

characteristic equation

$$\lambda^2 - \left(2 - \alpha^2 + \frac{\alpha^4\beta\epsilon}{4}\right)\lambda + 1 + \frac{\alpha^4}{4}(1 - 2\beta - \epsilon + \beta\epsilon) = 0$$

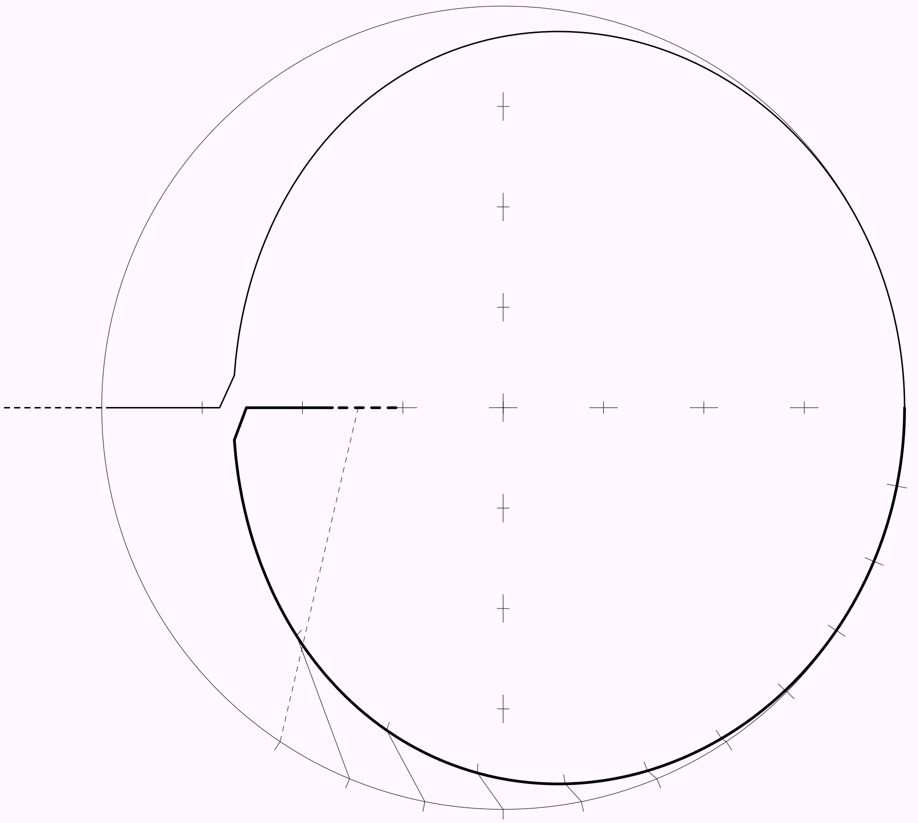
substitute $\lambda = e^{i\alpha}$ and expand in Taylor series:

$$\alpha^4\left(\frac{1}{3} - \frac{\beta}{2} - \frac{\epsilon}{4}\right) + i\alpha^5\left(\frac{1}{12} - \frac{\beta\epsilon}{4}\right) + \mathcal{O}\left(\alpha^6\right) = 0$$

setting $\epsilon = \frac{4}{3} - 2\beta$ eliminates $\mathcal{O}\left(\alpha^4\right)$-term, hence

$$+i\alpha^5\left[\frac{1}{36} + \frac{1}{2}\left(\beta - \frac{1}{3}\right)^2\right] + \mathcal{O}(\alpha^6) = 0 \qquad \Rightarrow \text{ optimum at } \begin{cases} \beta = 1/3 \\ \epsilon = 2/3 \end{cases}$$

Generalized RK2 continued ...



Characteristic roots for modified RK2 with $\beta = 1/3$, $\epsilon = 2/3$

third-order accurate **step multiplier**

stable $\alpha_{\max} = \sqrt{6\,(3-\sqrt{5})} = 2.14093$

all analysis carried out analytically

two-time-level scheme, comparable/exceeding that of Higdon 2002, attractive for *isopycnic* modeling, but less so for *sigma*/z.

dissipation-dominant leading-order truncation term

order of accuracy of representing *phase speed* exceeds that of individual terms in equations

stability is limited by one of the modes leaving unit circle through $\lambda = -1$, substituting *this* and $\epsilon = \frac{4}{3} - 2\beta$ into characteristic Eqn. yields

$$4 - \alpha^2 + \left[\frac{1}{36} - \left(\beta - \frac{1}{3}\right)^2\right]\alpha^4 = 0$$

$\Rightarrow$ settings for minimum truncation error *coincide* with maximum stability range

efficiency exceeds that of *any* synchronous scheme, yet is well below the classical FB

Generalized LF-TR/LF-AM3

Predictor sub-step

$$\begin{aligned} \zeta^{n+1,*} &= \zeta^{n-1} - 2i\alpha \cdot u^n \\ u^{n+1,*} &= u^{n-1} - 2i\alpha \cdot \left[(1-2\beta)\,\zeta^n + \beta\left(\zeta^{n+1,*} + \zeta^{n-1}\right)\right] \end{aligned}$$

corrector

$$\begin{aligned} \zeta^{n+1} &= \zeta^n - i\alpha\left\{\left(\frac{1}{2}-\gamma\right)u^{n+1,*} + \left(\frac{1}{2}+2\gamma\right)u^n - \gamma u^{n-1}\right\} \\ u^{n+1} &= u^n - i\alpha\left\{\left(\frac{1}{2}-\gamma\right)\left[\epsilon\zeta^{n+1} + (1-\epsilon)\zeta^{n+1,*}\right]\right. \\ &\qquad\qquad \left. + \left(\frac{1}{2}+2\gamma\right)\zeta^n - \gamma\zeta^{n-1}\right\} \end{aligned}$$

Standard (*no FB-feedback*) versions are identified as

$$\beta = \epsilon = 0 \quad \Rightarrow \begin{cases} \gamma = 0 & \Rightarrow \ \text{LF-TR} \qquad \alpha_{\text{max}} = \sqrt{2} \\ \gamma = 1/12 & \Rightarrow \ \text{LF-AM3} \qquad \alpha_{\text{max}} = 1.5874 \\ \gamma = 0.0804 & \Rightarrow \ \text{max stability} \qquad \alpha_{\text{max}} = 1.5876 \end{cases}$$

these are known as the most robust among synchronous algorithms.

Generalized LF-TR/LF-AM3 continued...

single-step matrix form

$$\begin{pmatrix}\zeta\\ u\end{pmatrix}^{n+1} = \begin{pmatrix} A & -iB\\ -iC & D\end{pmatrix}\begin{pmatrix}\zeta\\ u\end{pmatrix}^{n} + \begin{pmatrix} E & -iF\\ -iG & H\end{pmatrix}\begin{pmatrix}\zeta\\ u\end{pmatrix}^{n-1}$$

characteristic equation

$$\begin{aligned}\lambda^2 - (A+D)\lambda + AD + BC - H - E + (AH + ED + BG + FC)\lambda^{-1}\\ +(EH+FG)\lambda^{-2} = 0\end{aligned}$$

where

$$A = 1 - 2\alpha^2\left(\frac{1}{2}-\gamma\right)(1-2\beta) \qquad B = \alpha\left\{\frac{1}{2}+2\gamma-4\alpha^2\left(\frac{1}{2}-\gamma\right)\beta\right\}$$

$$C = \alpha\left\{\frac{1}{2}+2\gamma+\epsilon\left(\frac{1}{2}-\gamma\right)\left[1-2\alpha^2\left(\frac{1}{2}-\gamma\right)(1-2\beta)\right]\right\}$$

$$D = 1-2\alpha^2\left(\frac{1}{2}-\gamma\right)\left\{1-\epsilon\left[\frac{3}{4}-\gamma+2\alpha^2\left(\frac{1}{2}-\gamma\right)\beta\right]\right\}$$

$$G = \alpha\left\{\frac{1}{2}-2\gamma-\epsilon\left(\frac{1}{2}-\gamma\right)\left[1+4\alpha^2\left(\frac{1}{2}-\gamma\right)\beta\right]\right\}$$

$$E = -4\alpha^2\left(\frac{1}{2}-\gamma\right)\beta \qquad F = \alpha\left(\frac{1}{2}-2\gamma\right) \qquad H = -\alpha^2\left(\frac{1}{2}-\gamma\right)\left(\frac{1}{2}-2\gamma\right)\epsilon$$

Generalized LF-TR/LF-AM3 continued...

Substitute $\lambda = e^{i\alpha}$ and expand in Taylor series:

$$-\alpha^4\left(\frac{1}{6}-2\gamma\right)+i\alpha^5\left\{\frac{1}{12}+\left(\frac{1}{2}-2\gamma\right)^2-\left(\frac{1}{2}-\gamma\right)\left[2\beta+\epsilon\left(\frac{1}{2}-2\gamma\right)\right]\right\}$$
$$+\alpha^6\left\{\frac{133}{720}-\frac{\gamma}{2}+\frac{7}{3}\gamma^2-\left(\frac{1}{2}-\gamma\right)\left[\frac{4}{3}\beta+\epsilon\left(\frac{5}{12}-\frac{4}{3}\gamma\right)\right.\right.$$
$$\left.\left.-4\beta\epsilon\left(\frac{1}{2}-\gamma\right)\right]\right\}+\mathcal{O}\left(\alpha^7\right)=0$$

third-order accuracy condition

$$\gamma = \frac{1}{12} \qquad \forall\,\beta,\epsilon$$

fourth-order

$$\text{above and} \quad \beta = \frac{7}{30}-\frac{\epsilon}{6}$$

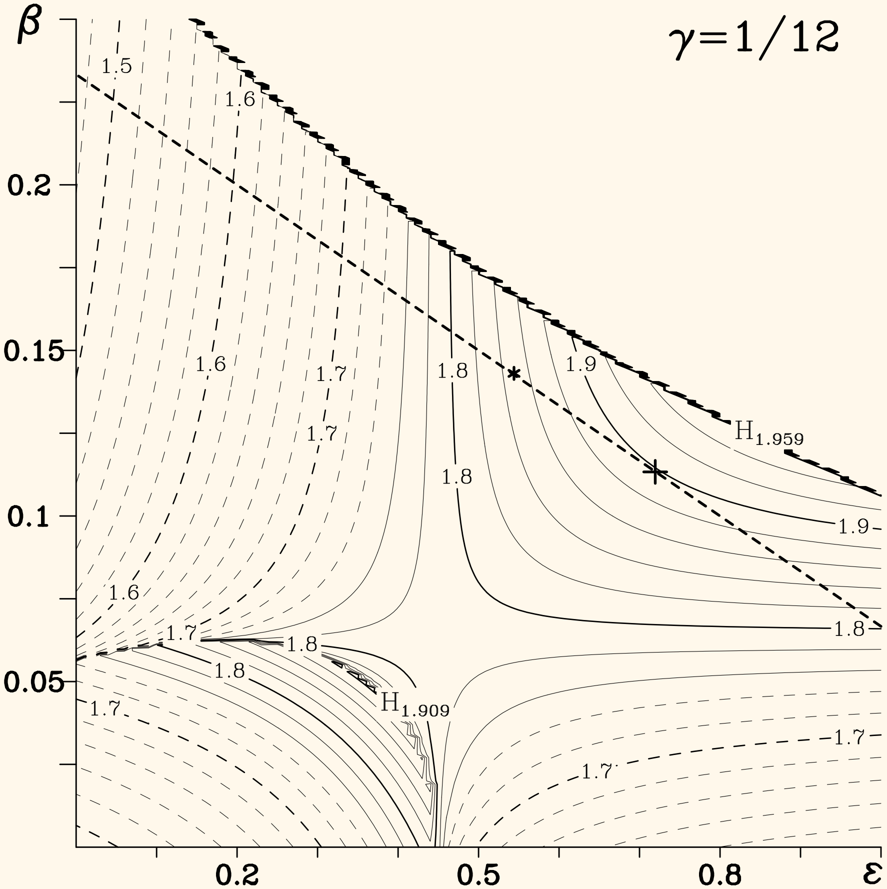
fifth-order (*no solution*)

$$\text{both above and} \quad -\frac{5}{6}\left(\epsilon-\frac{11}{20}\right)^2-\frac{1603}{2400}=0$$

minimal possible truncation error

$$\epsilon = \frac{11}{20} \qquad \beta = \frac{17}{120} \qquad \gamma = \frac{1}{12} \qquad\qquad \Rightarrow \quad \alpha_{\mathrm{max}} = 1.851640$$

Generalized LF-AM3 continued...



$\alpha_{\max}$ as function of ϵ, β with $\gamma = 1/12$.

Contours below $\alpha = 1.75$ are shown in dashed lines.

Stability properties of *third*- and *fourth*-order subsets among Generalized LF-TR/LF-AM3 family schemes

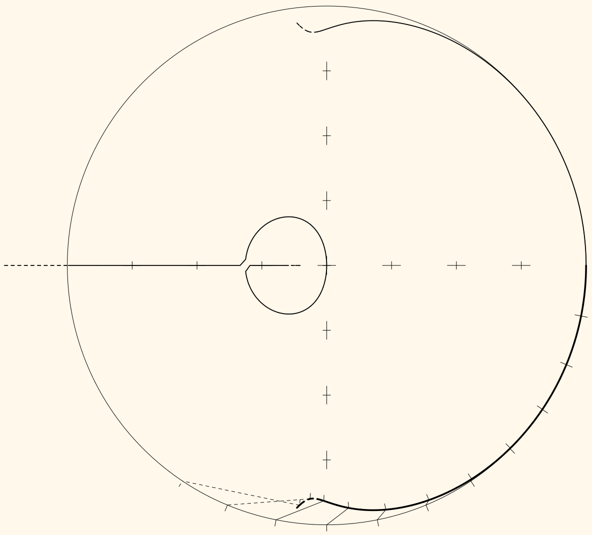
The empty area in the upper-right corner corresponds to schemes with an asymptotic instability of the physical modes.

Note the appearance of two maxima of stability, at (ϵ, β)=(0.83,0.126) just on the edge of asymptotic instability, and (0.39,0.044).

The straight dashed line $\beta = 7/30 - \epsilon/6$ approximately parallel to the edge corresponds to a zero $\mathcal{O}\left(\alpha^5\right)$ truncation term.

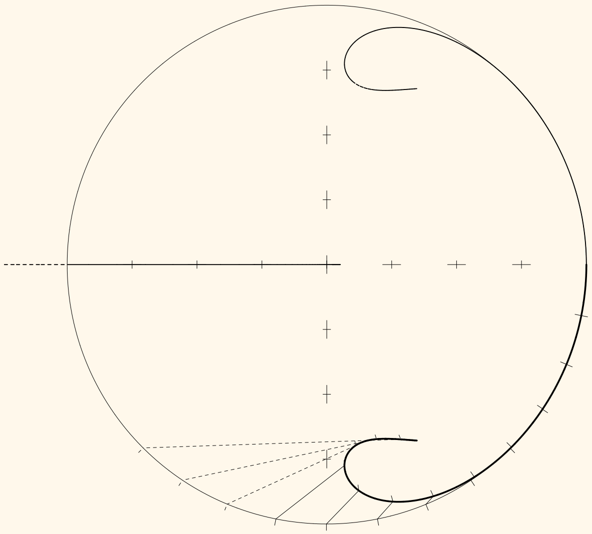
The asterisk * and cross + on this line denote locations of the minimal truncation error and maximum stability limit among the forth-order algorithms, which are not far away from each other.

Generalized LF-AM3 continued... γ=1/12



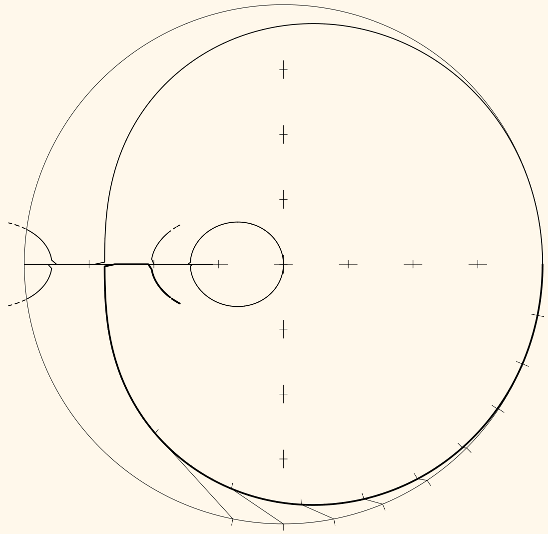
$\beta = 17/120$, $\epsilon = 11/20$,
α_{max}**=1.851640**

minimal truncation error among all *fourth*-order accuracy schemes



β=0.126, ϵ=0.83,
α_{max}**=1.958537**

maximum stability range among $\gamma = 1/12$



β=0.044, ϵ=0.39,
α_{max}**=1.908525**

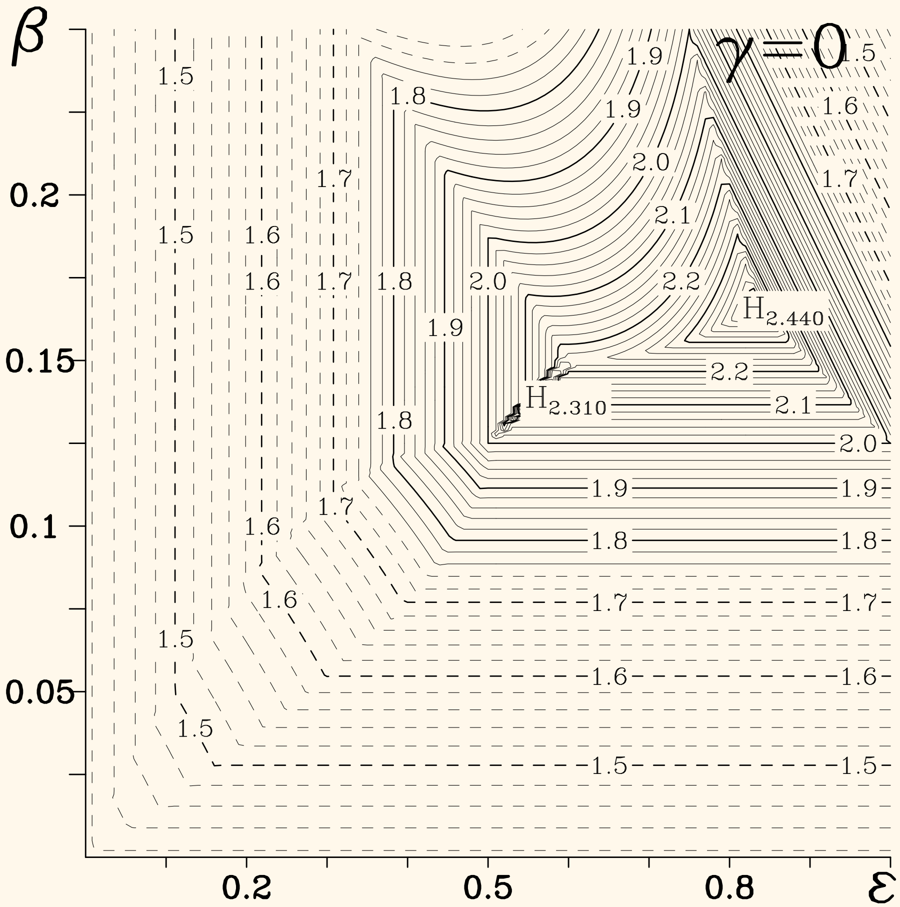
secondary stability maximum

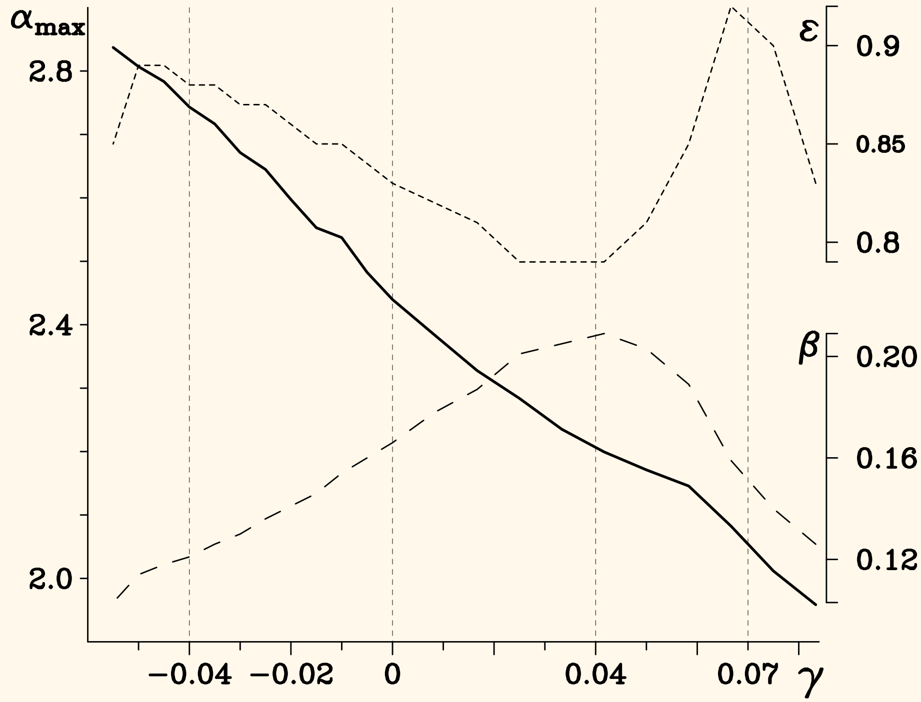
At best 24% gain in stability range relatively to LF-AM3 with $\beta = \epsilon = 0$.

Unprecedentally small numerical dissipation and dispersion, if desired.

Generalized LF-TR/LF-AM3 continued...

Search for maximum stability range among all γ, β, ϵ, while maintaining *second*-order accuracy. Treat γ, β, ϵ as free parameters. Sweep (β, ϵ)-plane for each γ.

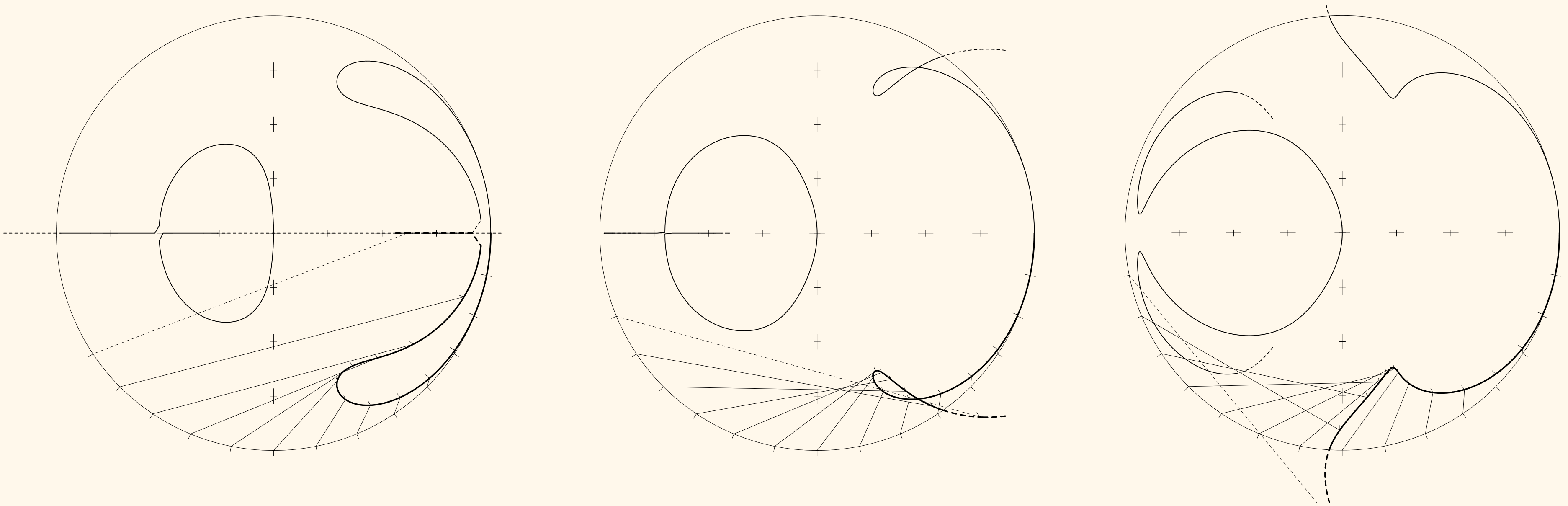




Left: Map of $\alpha_{\max} = \alpha_{\max}(\epsilon, \beta)$ for γ=0.

Right: $\alpha_{\max}$ and the corresponding ϵ, β as functions of γ

Generalized LF-TR/LF-AM3 continued...



$\gamma = 0$, $\beta = 0.166$, $\epsilon = 0.84$ α_{max}**=2.4114**

$\gamma = -0.025$, $\beta = 0.130$, $\epsilon = 0.84$ α_{max}**=2.6078**

$\gamma = -0.05$, $\beta = 0.105$, ϵ=0.84, α_{max}**=2.8010**

Dissipative algorithms optimized for stability range. Stability increases with decrease of γ, but accuracy degrades. Suitable for barotropic mode.

LF-TR($\gamma = 0$): **70% gain in stability range relatively to** $\beta = \epsilon = 0$

Going beyond $\gamma < 0$ is not desirable because of accuracy loss. Still much less efficient than FB.

Generalized Forward–Backward algorithm for system

Starting with logically AB2-like step for ζ followed by logically AM3-like for u

$$
\begin{aligned}
\zeta^{n+1} &= \zeta^n - i\alpha\left[(1+\beta)u^n - \beta u^{n-1}\right] \\
u^{n+1} &= u^n - i\alpha\left[(1-\gamma-\epsilon)\zeta^{n+1} + \gamma\zeta^n + \epsilon\zeta^{n-1}\right]
\end{aligned}
$$

reverts to Classical FB if $\beta = \gamma = \epsilon = 0$
characteristic equation

$$
\lambda^2 - \left[2 - \alpha^2(1-\gamma-\epsilon)(1+\beta)\right]\lambda + 1 - \alpha^2(\beta - \gamma - 2\beta\gamma - \beta\epsilon) \\
+\alpha^2(\epsilon + \beta\epsilon - \beta\gamma)\lambda^{-1} - \alpha^2\beta\epsilon\lambda^{-2} = 0
$$

substitute $\lambda = e^{i\alpha}$ and expand in Taylor series

$$
(\beta - \gamma - 2\epsilon)\, i\alpha^3 + \left(\frac{1}{12} - \frac{\beta}{2} + \frac{\gamma}{2} + \beta\gamma + 2\beta\epsilon\right)\alpha^4 + \left(\frac{1}{12} - \frac{\beta}{6} + \frac{\gamma}{6} + \frac{\epsilon}{3} - \beta\epsilon\right) i\alpha^5 \\
+\mathcal{O}\left(\alpha^6\right) = 0
$$

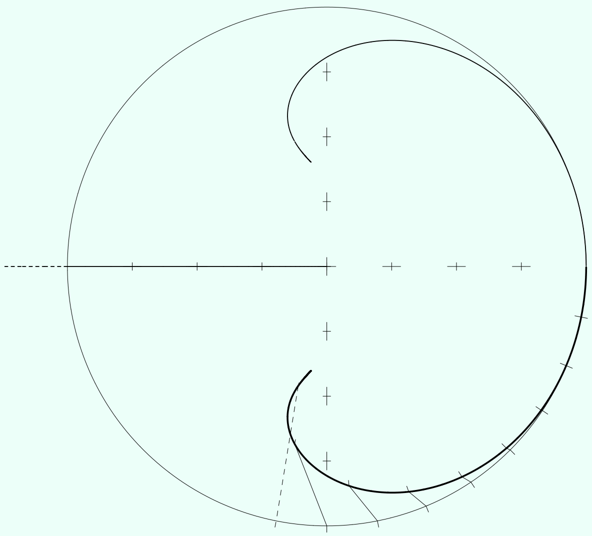
Always respect $\beta - \gamma - 2\epsilon = 0$ to ensure *second*-order accuracy. *Time-centering* balance: once r.h.s. for ζ is placed at $t_n + \left(\frac{1}{2} - \delta\right)\Delta t$, then r.h.s. for u is centered at $t_n + \left(\frac{1}{2} + \delta\right)\Delta t$ with the same offset $\delta \equiv \frac{1}{2} - \beta$. Classical FB respects this rule.

Setting $\gamma = \beta - 2\beta^2 - \dfrac{1}{6}$ and $\epsilon = \beta^2 + \dfrac{1}{12}$ eliminates both $\mathcal{O}\left(\alpha^3\right)$ and $\mathcal{O}\left(\alpha^4\right)$ terms, resulting in *third*-order accuracy for any β.

Above and $\dfrac{1}{12} - \dfrac{\beta}{12} - \beta^3 = 0 \quad \Rightarrow \quad \beta = 0.3737076$ eliminates $\mathcal{O}\left(\alpha^5\right)$

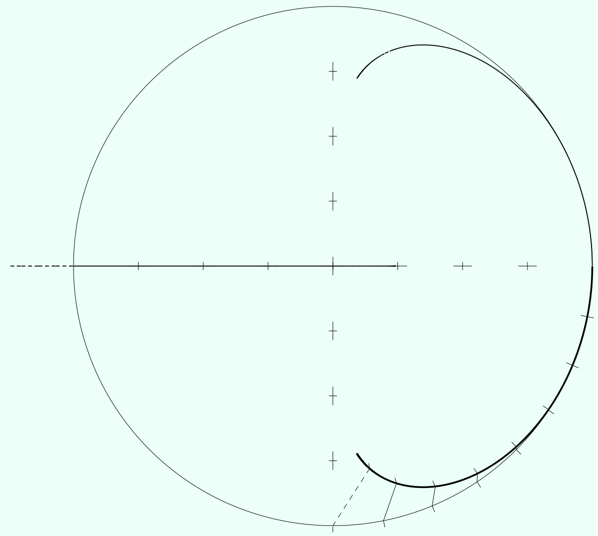
Generalized FB continued...

AB2-AM3



$\beta = 0, \ \gamma = -\frac{1}{6}, \ \epsilon = \frac{1}{12}$

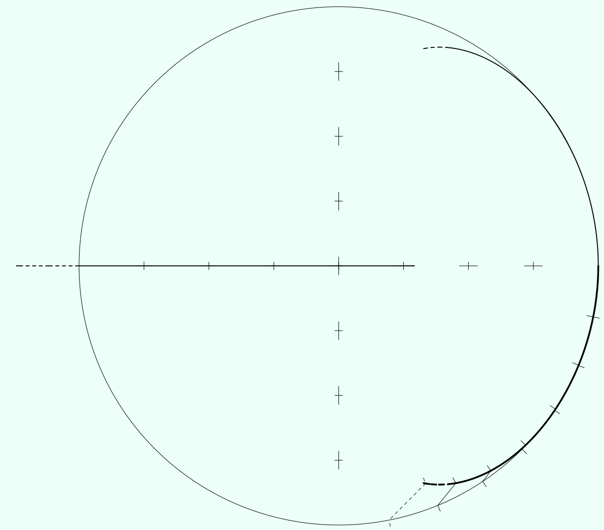
$\alpha_{\text{max}} = \sqrt{3}$



$\beta = 0.3737076,$

fourth-order accurate

$\alpha_{\text{max}} = \sqrt{2}$



$\beta = \frac{1}{2}, \ \gamma = -\frac{1}{6}, \ \epsilon = \frac{1}{3}$

$\alpha^*_{\text{max}} = \sqrt{3/2} \approx$ **1.2247**

Strong instability occurs when one of the computational modes leaves unit circle at $\lambda = -1$, hence $\alpha_{\text{max}} = \sqrt{3} \Big/ \sqrt{1 + \dfrac{\beta}{2} + 6\beta^3}$ decreases with β. In addition to that, physical modes become asymptotically unstable if $\beta > 0.3737076$.

Logically-AB2 time step is asymptotically unstable for single hyperbolic equation when $\beta \leq 1/2$. Although attractive, this algorithm does not combine well with the other hyperbolic *SWE* terms (advection, Coriolis) because of no overlap in β.

Generalized FB

AB3—AM4

Logically-AB3 — logically-AM4 like step:

$$\zeta^{n+1} = \zeta^n - i\alpha\left[\left(\frac{3}{2}+\beta\right)u^n - \left(\frac{1}{2}+2\beta\right)u^{n-1} + \beta u^{n-2}\right]$$
$$u^{n+1} = u^n - i\alpha\left[\left(\frac{1}{2}+\gamma+2\epsilon\right)\zeta^{n+1} + \left(\frac{1}{2}-2\gamma-3\epsilon\right)\zeta^n + \gamma\zeta^{n-1} + \epsilon\zeta^{n-2}\right]$$

where r.h.s. for both equations are *already* centered around $t_n + \Delta t/2$, regardless of settings of $\beta, \gamma, \epsilon \Rightarrow$ Second-order accuracy is always guaranteed.

Logically-AB3 step for **single advection equation** becomes stable if $\beta > 1/6$ (asymptotic instability of AB2, if below), and gets *third*-order accuracy if $\beta = 5/12$; $\beta = 0.281105$ yields the largest stability range. $\Rightarrow$ Naturally combines with computation of Coriolis and advection terms.

characteristic equation

$$\lambda^2 - \left[2 - \alpha^2\left(\frac{3}{2}+\beta\right)\left(\frac{1}{2}+\gamma+2\epsilon\right)\right]\lambda + 1 - \alpha^2\left[\frac{7}{2}\gamma + \frac{11}{2}\epsilon - \frac{1}{2} + \beta\left(\frac{1}{2}+4\gamma+7\epsilon\right)\right]$$
$$-\alpha^2\left[\frac{1}{4} - \frac{5}{2}\gamma - \frac{3}{2}\epsilon + \beta\left(\frac{1}{2}-6\gamma-4\epsilon\right)\right]\lambda^{-1} + \alpha^2\left[\beta\left(\frac{1}{2}-4\gamma-2\epsilon\right) - \frac{\gamma}{2} + \frac{3}{2}\epsilon\right]\lambda^{-2}$$
$$+\alpha^2\left[\beta\left(\gamma-2\epsilon\right) - \frac{\epsilon}{2}\right]\lambda^{-3} + \alpha^2\beta\epsilon\lambda^{-4} = 0$$

Requires finding roots of *sixth-order* polynomials: $\Rightarrow$ trace physical modes by continuation (using Newton's iterations), then reduce power to *fourth*.

Generalized FB continued... AB3—AM4

set $\lambda = e^{i\alpha}$ and expand in Taylor series

$$\alpha^4\left[\frac{1}{3}-\beta-\gamma-3\epsilon\right]+\frac{1}{2}i\alpha^5\left[\frac{1}{6}+\beta-\gamma-\epsilon\right]+\alpha^6\left[-\frac{47}{720}-\frac{1}{6}\gamma-\frac{1}{2}\epsilon+\beta\left(\frac{1}{3}+\gamma+3\epsilon\right)\right]$$
$$+\mathcal{O}(\alpha^7)=0$$

third-order accuracy condition $\quad \gamma = \frac{1}{3} - \beta - 3\epsilon \quad \forall\beta,\epsilon$

fourth-order $\quad \beta = \frac{1}{12} - \epsilon$ and $\gamma = \frac{1}{4} - 2\epsilon \quad \forall\epsilon$

fifth-order $\quad \frac{7}{120} + \frac{2}{3}\epsilon + \epsilon^2 = 0 \quad \Rightarrow \quad \epsilon = -\frac{1}{3} \pm \frac{\sqrt{190}}{60}$

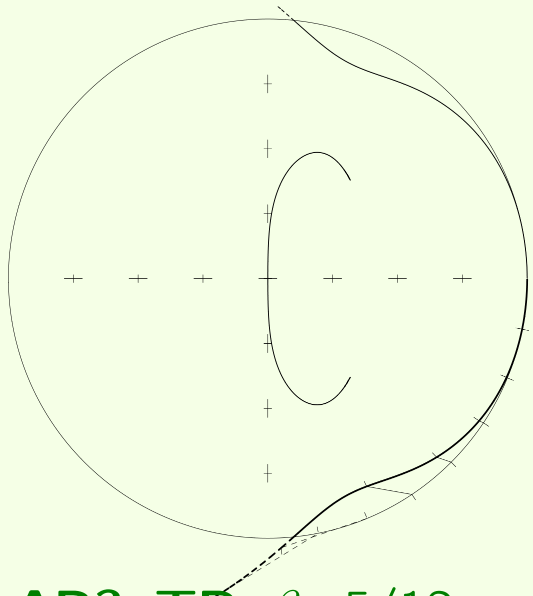
- *Fifth*-order algorithm is asymptotically unstable and has $\alpha_{\mathrm{max}} = 1.01$ limited by computational mode.

- *Fourth*-order algorithms are asymptotically stable for $\epsilon > -0.03655$ and has widest stability range $\alpha_{\mathrm{max}} = 1.727$ if $\epsilon = 0.083$.

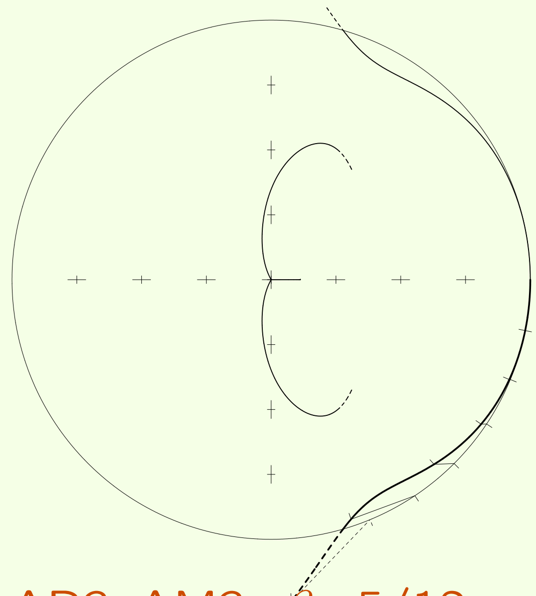
- *Third*-order 2-parametric (β,ϵ) family can reach up to $\alpha_{\mathrm{max}} = 1.96$ and can be made with desirable dissipation.

- Compromise *second*-order choice $\beta = 0.281105$, $\gamma = 0.088$ and $\epsilon = 0.013$ for barotropic mode.

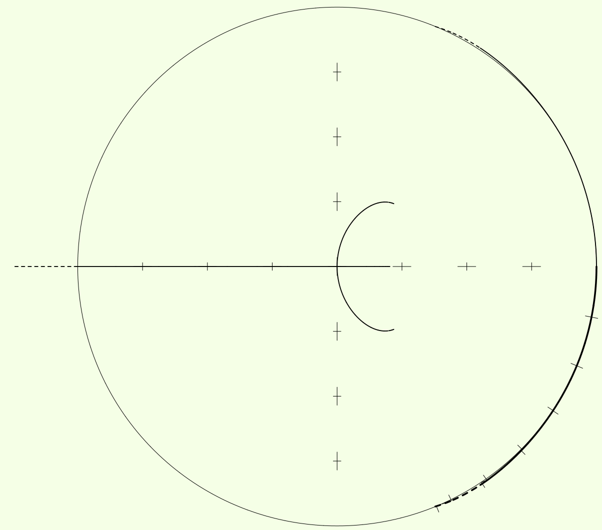
Generalized FB continued... AB3—AM4



AB3–TR: β=5/12,
γ=ϵ=0
α_{max}=1.1441551



AB3–AM3: β=5/12,
$\gamma = -1/12$, ϵ=0
α_{max}=1.003859



β, γ, ϵ set to achieve
fifth-order accuracy
α_{max}=1.0145*
not a viable choice

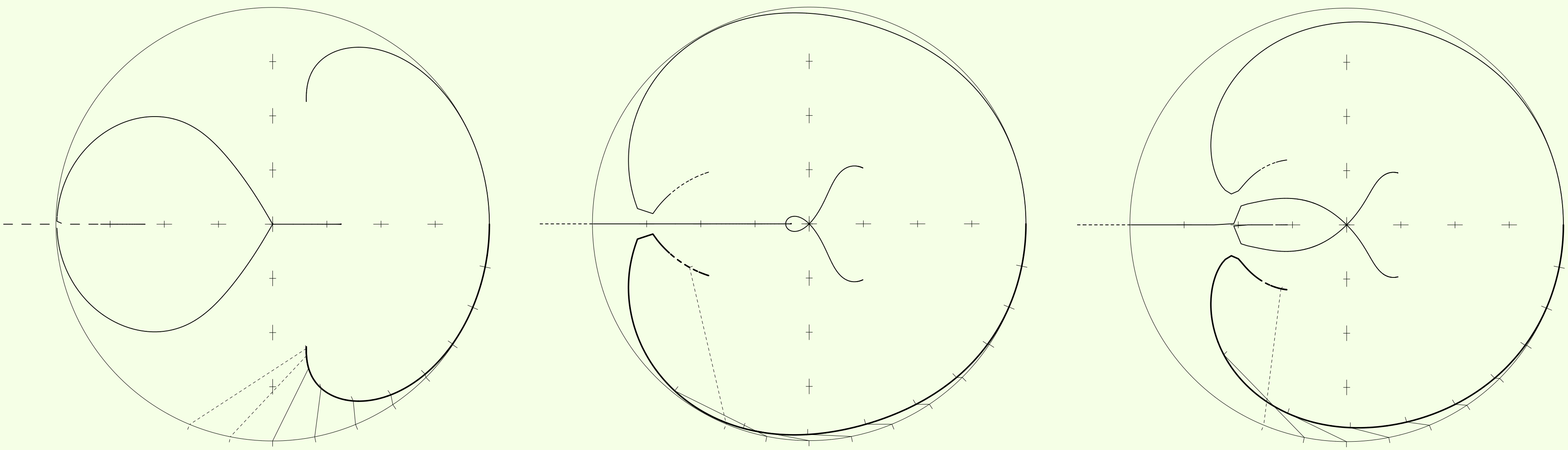
AB3–TR is historically the first Generalized FB step in ROMS family codes (1998): Rutgers versions 1.8, 1.9, 2.0/TOMS, 2.1 still use it for main 3D step. Approx 50% more efficient than AB3 of SCRUM model, but is below of what is coming.

Setting β, γ, ϵ to achieve the largest possible order of accuracy (*fifth*) results in asymptotic instability, $|\lambda| = 1.014$ at $\alpha \approx \pm 1$; (above value of α_{max}=1.0145* is limited by computational mode at $\lambda = -1$).

The most crucial step to expand stability limit beyond shown above is to reduce AB3-curvature by setting β <5/12. Note that β <1/6 leads to asymptotic instability for AB3 for centered advection and Coriolis terms.

Generalized FB continued... AB3—AM4

Search for maximum stability limit, while maintaining *at least third*-order accuracy, hence $\gamma = 1/3 - \beta - 3\epsilon$ in all cases shown here. Parameter(s) ϵ or β, ϵ are treated as adjustable.



$\epsilon = 0.083, \quad \beta = 1/12 - \epsilon$
fourth-order accuracy
$\alpha_{\max} = 1.727$ maximum $\forall\epsilon$

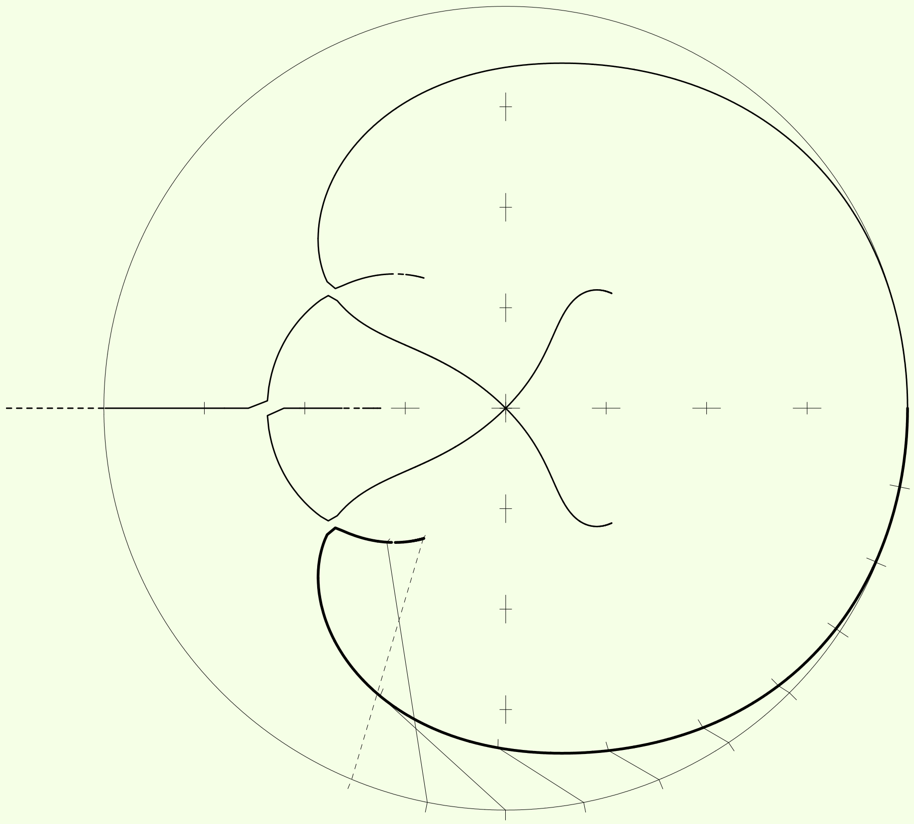
β=0.232, ϵ=0.00525
$\alpha_{\max}$=1.939
maximum $\forall\beta,\epsilon$

β=0.21, ϵ=0.0115
$\alpha_{\max} = 1.874$
monotonic dissipation

Maintaining fourth-order accuracy leads to $\beta \approx 0 \Rightarrow$ Coriolis and advection terms needs to be dealt with separately.

β=0.232 of maximum stability range falls into the favorable range of $1/6 < \beta < 5/12$, and is close to the maximum stability for AB3 alone, β=0.281105. It naturally combines with computation of Coriolis and advection terms. However it weekly dissipates under-resolved time scales (similarly to classical FB). β=0.21, ϵ=0.0115 deviates from maximum stability to achieve proper dissipation.

Conclusions (time stepping)



β=0.281105, ϵ=0.013, γ=0.0880

α_{max}=1.7802

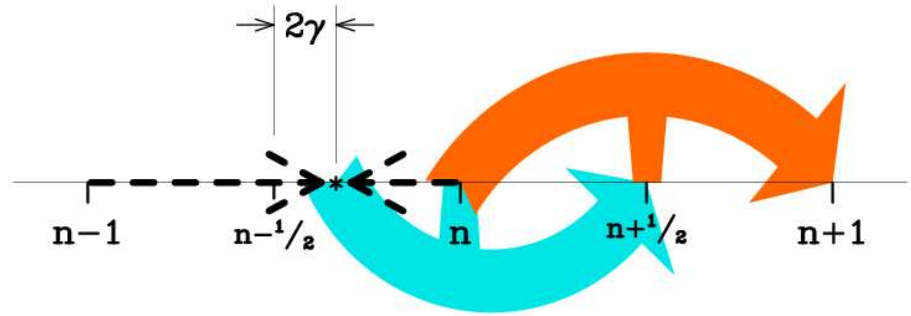
Predictor–Corrector

- LF-TR stability range $\approx 2.4 \Rightarrow$ 70% gain relatively to its prototype

Forward-Backward AB3-AM4

- stability range up to $\approx$ 1.8 while maintaining *third*-order accuracy
- nearly *twice* as efficient relatively to LF, AB3, LF-TR, LF-AM3
- both r.h.s-des are time-centered at $n+1/2$ Coriolis and advection terms are computed naturally using *the same* AB3-extrapolation
- *third*-order accurate, if $\gamma = \frac{1}{3} - \beta - 3\epsilon$
- *fourth*-order $\gamma = \frac{1}{4} - 2\epsilon\,, \quad \beta = \frac{1}{12} - \epsilon$
- *small* numerical dispersion
- *dissipative* leading-order truncation term

Time stepping of nonlinear equations LF-TR/LF-AM3



Predictor

$$\zeta^{n+1,*} = \zeta^{n-1} - 2i\alpha \cdot u^n$$
$$u^{n+1,*} = u^{n-1} - 2i\alpha \cdot [(1-2\beta)\,\zeta^n + \beta\left(\zeta^{n+1,*} + \zeta^{n-1}\right)]$$

corrector

$$\zeta^{n+1} = \zeta^n - i\alpha\left\{\left(\frac{1}{2}-\gamma\right)u^{n+1,*} + \left(\frac{1}{2}+2\gamma\right)u^n - \gamma u^{n-1}\right\}$$
$$u^{n+1} = u^n - i\alpha\left\{\left(\frac{1}{2}-\gamma\right)\left[\epsilon\zeta^{n+1} + (1-\epsilon)\zeta^{n+1,*}\right] + \left(\frac{1}{2}+2\gamma\right)\zeta^n - \gamma\zeta^{n-1}\right\}$$

Original form: $i\alpha\{...\}$ translate into computationally expensive nonlinear terms stored from one step to another.

Predictor

$$\zeta^{n+\frac{1}{2}} = \left(\frac{1}{2}-2\gamma\right)\zeta^{n-1} + \left(\frac{1}{2}+2\gamma\right)\zeta^n - i\alpha\,(1-2\gamma)\,u^n$$
$$u^{n+\frac{1}{2}} = \left(\frac{1}{2}-2\gamma\right)u^{n-1} + \left(\frac{1}{2}+2\gamma\right)u^n - i\alpha\left[(1-2\gamma)\,\zeta^n + \beta\left(2\zeta^{n+\frac{1}{2}} - 3\zeta^n + \zeta^{n-1}\right)\right]$$

corrector

$$\zeta^{n+1} = \zeta^n - i\alpha\cdot u^{n+\frac{1}{2}}$$
$$u^{n+1} = u^n - i\alpha\left\{(1-\epsilon)\,\zeta^{n+\frac{1}{2}} + \epsilon\left[\left(\frac{1}{2}-\gamma\right)\times\zeta^{n+1} + \left(\frac{1}{2}+2\gamma\right)\zeta^n - \gamma\zeta^{n-1}\right]\right\}$$

Alternative form: Eliminates the need to store r.h.s. between time steps

Time stepping of nonlinear equations — AB3–AM4

forward AB3-extrapolation

$$\begin{pmatrix}\zeta\\ \overline{\mathbf{u}}\end{pmatrix}^{m+\frac{1}{2}} = \left(\frac{3}{2}+\beta\right)\begin{pmatrix}\zeta\\ \overline{\mathbf{u}}\end{pmatrix}^{m} - \left(\frac{1}{2}+2\beta\right)\begin{pmatrix}\zeta\\ \overline{\mathbf{u}}\end{pmatrix}^{m-1} + \beta\begin{pmatrix}\zeta\\ \overline{\mathbf{u}}\end{pmatrix}^{m-2}$$

finite-volume fluxes

$$D^{m+\frac{1}{2}} = h + \zeta^{m+\frac{1}{2}} \qquad \overline{U}^{m+\frac{1}{2}} = D^{m+\frac{1}{2}}\overline{u}^{m+\frac{1}{2}}\Delta\eta \qquad \overline{V}^{m+\frac{1}{2}} = D^{m+\frac{1}{2}}\overline{v}^{m+\frac{1}{2}}\Delta\xi$$

free-surface step

$$\zeta^{m+1} = \zeta^{m} - \Delta t_{*}\,\mathrm{div}\,\overline{\mathbf{U}}^{m+\frac{1}{2}}$$

half-step-back interpolation

$$\zeta' = \left(\frac{1}{2}+\gamma+2\epsilon\right)\zeta^{m+1} + \left(\frac{1}{2}-2\gamma-3\epsilon\right)\zeta^{m} + \gamma\zeta^{m-1} + \epsilon\zeta^{m-2}$$

momentum step

$$\overline{\mathbf{u}}^{m+1} = \frac{1}{D^{m+1}}\left\{D^{m}\overline{\mathbf{u}}^{m} + \Delta t_{*}\left[\mathcal{F}\left(\zeta'\right) - D^{m+\frac{1}{2}}f\mathbf{k}\times\overline{\mathbf{u}}^{m+\frac{1}{2}} + \ldots\right]\right\}$$

- pressure gradient term $\mathcal{F}(\zeta')$ is *nonlinear* function of its argument; (...) denotes other terms: advection, viscous, etc.
- Stable without need for viscosity or upstream-bias of ζ in $\overline{\mathbf{U}}$-terms; Naturally combines with advection (centered and/or upstream-biased), and Coriolis terms
- **There is no need to store r.h.s. terms between time steps**

Time splitting: Constancy preservation for tracers

Tracer equation

advective form	$\dfrac{\partial q}{\partial t} + (\mathbf{u} \cdot \nabla) q = 0$	$\Rightarrow$	Lagrangian conservation
conservation form	$\dfrac{\partial q}{\partial t} + \nabla (\mathbf{u} q) = 0$	$\Rightarrow$	integral content conservation
nondivergence	$(\nabla \cdot \mathbf{u}) = 0$	$\Rightarrow$	**coexistence of the above**

- If tracer field q is initially uniform in space, it remains so at all times later: *constancy preservation property*

- For numerical reasons oceanic models always use conservation form as prototype for discrete tracer equations
- in a time-split free-surface model nondivergence is linked with free-surface equations in *fast* time, hence, strictly speaking

$$\langle \zeta \rangle^{n+1} \neq \langle \zeta \rangle^{n} - \Delta t \cdot \mathrm{div} < D\overline{\mathbf{u}} >$$

  where n and $n+1$ correspond to baroclinic *slow* time step, $\langle ... \rangle$ means fast-time averaging; $\overline{\mathbf{u}}$ means vertical averaging.

- In a hydrostatic *free-surface* model vertical velocity is computed from 3D continuity equation and it must be consistent with *changes* in control volumes to ensure integral volume conservation.

How constancy preservation is lost

discrete tracer advection

$$\Delta\mathcal{V}^{n+1}_{i,j,k} q^{n+1}_{i,j,k} = \Delta\mathcal{V}^{n}_{i,j,k} q^{n}_{i,j,k} - \Delta t \Big[\widetilde{q}_{i+\frac{1}{2},j,k} U_{i+\frac{1}{2},j,k} - \widetilde{q}_{i-\frac{1}{2},j,k} U_{i-\frac{1}{2},j,k} + \widetilde{q}_{i,j+\frac{1}{2},k} V_{i,j+\frac{1}{2},k}$$
$$- \widetilde{q}_{i,j-\frac{1}{2},k} V_{i,j-\frac{1}{2},k} + \widetilde{q}_{i,j,k+\frac{1}{2}} W_{i,j,k+\frac{1}{2}} - \widetilde{q}_{i,j,k-\frac{1}{2}} W_{i,j,k-\frac{1}{2}} \Big]$$

where $\Delta\mathcal{V}_{i,j,k} = H_{i,j,k}\Delta\mathcal{A}_{i,j,k}$ is control volume, and

$$q_{i,j,k} = \frac{1}{\Delta\mathcal{V}^{n}_{i,j,k}} \int\limits_{\Delta\mathcal{V}^{n}_{i,j,k}} q(x,y,z)\; \mathrm{d}^3\mathcal{V}$$

discrete continuity: formally set $q_{i,j,k} \equiv 1$ in the above

$$\Delta\mathcal{V}^{n+1}_{i,j,k} = \Delta\mathcal{V}^{n}_{i,j,k} - \Delta t \cdot \Big[U_{i+\frac{1}{2},j,k} - U_{i-\frac{1}{2},j,k} + V_{i,j+\frac{1}{2},k} - V_{i,j-\frac{1}{2},k} + W_{i,j,k+\frac{1}{2}} - W_{i,j,k-\frac{1}{2}} \Big]$$

...however, because of time splitting, $\Delta\mathcal{V}^{n+1}_{i,j,k}$ does not come from here, but is controlled by free-surface ζ via

$$H^{n+1}_{i,j,k} = H^{(0)}_{i,j,k} \cdot \left(1 + \frac{\langle\zeta\rangle^{n+1}_{i,j}}{h_{i,j}} \right) \qquad \Rightarrow \qquad \Delta\mathcal{V}^{n+1}_{i,j,k} = H^{n+1}_{i,j,k}\Delta\mathcal{A}_{i,j,k}$$

which uses different time stepping algorithm, different time step, and furthermore, is subject to fast-time averaging $\zeta \rightarrow \langle\zeta\rangle$ to prevent aliasing of barotropic frequencies unresolved in *slow* time. Above $H^{(0)}_{i,j,k}$ is *unperturbed* ($\zeta \equiv 0$) vertical grid spacing.

$\Rightarrow$ unless the finite-volume fluxes $U_{i+\frac{1}{2},j,k}$ and $V_{i,j+\frac{1}{2},k}$ are computed in a very special way, it is *not automatically guaranteed* that $\Delta\mathcal{V}^{n+1}_{i,j,k}$ and $\Delta\mathcal{V}^{n}_{i,j,k}$ are related via discrete continuity equation above.

How constancy preservation is lost, continued...

Equivalently

$$W_{i,j,\frac{1}{2}} \equiv 0 \qquad \text{at the sea floor, and}$$

$$W_{i,j,k+\frac{1}{2}} = -\sum_{k'=1}^{k} \left\{ \frac{\Delta\mathcal{V}^{n+1}_{i,j,k'} - \Delta\mathcal{V}^{n}_{i,j,k'}}{\Delta t} + U_{i+\frac{1}{2},j,k'} - U_{i-\frac{1}{2},j,k'} + V_{i,j+\frac{1}{2},k'} - V_{i,j-\frac{1}{2},k'} \right\}$$

$$\text{for all} \qquad k = 1, 2, ..., N$$

defines $W_{i,j,k+\frac{1}{2}}$ as *finite-time-interval finite-volume* flux across *moving* interface between vertically adjacent grid boxes $\Delta\mathcal{V}_{i,j,k}$ and $\Delta\mathcal{V}_{i,j,k+1}$.

What guarantees that surface kinematic boundary condition

$$W_{i,j,N+\frac{1}{2}} \equiv 0$$

is respected, if $\Delta\mathcal{V}^{n+1}_{i,j,k}$ come from the barotropic mode with different time stepping?

Solution: enforce $\displaystyle\sum_{k=1}^{N} U_{i+\frac{1}{2},j,k} = \langle\!\langle \overline{U} \rangle\!\rangle^{n+\frac{1}{2}}_{i+\frac{1}{2},j}$ and $\displaystyle\sum_{k=1}^{N} V_{i,j+\frac{1}{2},k} = \langle\!\langle \overline{V} \rangle\!\rangle^{n+\frac{1}{2}}_{i,j+\frac{1}{2}}$ where

$$\Delta\mathcal{A}_{i,j}\langle\zeta\rangle^{n+1}_{i,j} = \Delta\mathcal{A}_{i,j}\langle\zeta\rangle^{n}_{i,j} - \Delta t\left[\langle\!\langle \overline{U} \rangle\!\rangle^{n+\frac{1}{2}}_{i+\frac{1}{2},j} - \langle\!\langle \overline{U} \rangle\!\rangle^{n+\frac{1}{2}}_{i-\frac{1}{2},j} + \langle\!\langle \overline{V} \rangle\!\rangle^{n+\frac{1}{2}}_{i,j+\frac{1}{2}} - \langle\!\langle \overline{V} \rangle\!\rangle^{n+\frac{1}{2}}_{i,j-\frac{1}{2}}\right]$$

consistently with change in *fast-time-averaged* free surface $\langle\zeta\rangle$ between two consecutive baroclinic time steps. **How to define $\langle\!\langle ... \rangle\!\rangle$?**

Time splitting continued...

barotropic time stepping

$$\zeta^{m+1} = \zeta^m - \frac{\Delta t}{M} \cdot \text{div}\overline{\mathbf{U}}^{m+\frac{1}{2}} \qquad \forall\, m = 1, ..., M^*$$

yields $$\zeta^m = \zeta^0 - \frac{\Delta t}{M} \sum_{m'=0}^{m-1} \text{div}\overline{\mathbf{U}}^{m'+\frac{1}{2}}$$

where ζ^0 (meaning $m = 0$) corresponds to baroclinic step n. Apply operation $\langle ... \rangle$ to both sides:

$$\sum_{m=1}^{M^*} a_m \zeta^m = \zeta^0 - \frac{\Delta t}{M} \cdot \text{div} \sum_{m=1}^{M^*} \left[a_m \sum_{m'=1}^{m} \overline{\mathbf{U}}^{m'-\frac{1}{2}} \right]$$

which translates into

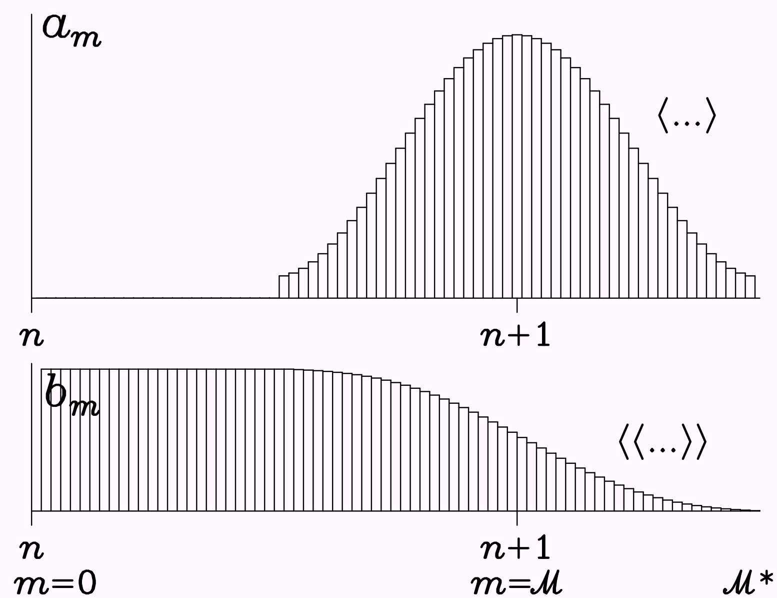
$$\langle \zeta \rangle^{n+1} = \langle \zeta \rangle^n - \Delta t \cdot \text{div} \sum_{m'=1}^{M^*} b_{m'} \overline{\mathbf{U}}^{m'-\frac{1}{2}}$$

where $$b_{m'} = \frac{1}{M} \sum_{m=m'}^{M^*} a_m\,, \qquad \forall m = 1, ..., M^*$$

NOTE: barotropic mode *restarts* at every baroclinic time step, $\langle \zeta, \overline{U}, \overline{V} \rangle^{n+1} \rightarrow \zeta^0, \overline{U}^0, \overline{V}^0$

$$\langle \zeta \rangle^{n+1} \equiv \sum_{m=1}^{M^*} a_m \zeta^m$$

$$\sum_{m=1}^{M^*} a_m \equiv 1 \qquad \sum_{m=1}^{M^*} \frac{m}{M} a_m \equiv 1$$



$$\Rightarrow \quad \langle\langle \overline{\mathbf{U}} \rangle\rangle^{n+\frac{1}{2}} \equiv \sum_{m=1}^{M^*} b_m \overline{\mathbf{U}}^{m-\frac{1}{2}} \quad \textbf{exact}$$

slow-time volume conservation

Time splitting continued...

Fluxes $U_{i+\frac{1}{2},j,k}$, $V_{i,j+\frac{1}{2},k}$, $W_{i,j,k+\frac{1}{2}}$ are consistent with barotropic mode only at $n+1/2$, after barotropic stepping is finished for current 3D step. What to do during predictor step for 3D?

Nonconservative (pseudo-compressible) step via artificial continuity equation
"continuity" step(s)

$$\Delta\mathcal{V}^{n\pm\frac{1}{2}}_{i,j,k} = \Delta\mathcal{V}^{n}_{i,j,k} \mp \frac{1}{2}\Delta t \cdot \left[U^n_{i+\frac{1}{2},j,k} - U^n_{i-\frac{1}{2},j,k} + V^n_{i,j+\frac{1}{2},k} - V^n_{i,j-\frac{1}{2},k} + W^n_{i,j,k+\frac{1}{2}} - W^n_{i,j,k-\frac{1}{2}}\right]$$

pseudo-compressible tracer step

$$\Delta\mathcal{V}^{n+\frac{1}{2}}_{i,j,k} q^{n+\frac{1}{2}}_{i,j,k} = \Delta\mathcal{V}^{n-\frac{1}{2}}_{i,j,k} \frac{q^n_{i,j,k} + q^{n-1}_{i,j,k}}{2} - \Delta t \left[\widetilde{q}^n_{i+\frac{1}{2},j,k} U^n_{i+\frac{1}{2},j,k} - \widetilde{q}^n_{i-\frac{1}{2},j,k} U^n_{i-\frac{1}{2},j,k} + \widetilde{q}^n_{i,j+\frac{1}{2},k} V^n_{i,j+\frac{1}{2},k} \right.$$
$$\left. - \widetilde{q}^n_{i,j-\frac{1}{2},k} V^n_{i,j-\frac{1}{2},k} + \widetilde{q}^n_{i,j,k+\frac{1}{2}} W^n_{i,j,k+\frac{1}{2}} - \widetilde{q}^n_{i,j,k-\frac{1}{2}} W^n_{i,j,k-\frac{1}{2}}\right]$$

discard $\Delta\mathcal{V}^{n\pm\frac{1}{2}}_{i,j,k}$ after computing $q^{n+\frac{1}{2}}_{i,j,k}$.
[*alternative* LF-TR version is shown for simplicity. The actual code uses LF-AM3.]

- **this is constancy preserving for** $q^{n+\frac{1}{2}}_{i,j,k}$
- **content conservation property for** $q^{n+\frac{1}{2}}_{i,j,k}$ **is lost** because $\Delta\mathcal{V}^{n+\frac{1}{2}}_{i,j,k}$ has nothing to do with the actual $\Delta\mathcal{V}^{n+1}_{i,j,k}$ set by the barotropic mode
- this is OK because $q^{n+\frac{1}{2}}_{i,j,k}$ is used **exclusively** to compute fluxes at $n+1/2$. Subsequent corrector step from n to $n+1$ is both conservative and constancy preserving

Time splitting continued... Fast-time averaging shape

Purpose: to prevent temporal aliasing of barotropic signals unresolved by baroclinic time step.

Assuming $A(\tau)$ being continuous analog of $\{a_m | m = 1, ..., M^*\}$ with $\tau \sim m/M$, and $\tau_* \sim M^*/M$, *response function* $\mathcal{R}(\alpha)$, $\alpha \equiv \omega\Delta t$ is defined as

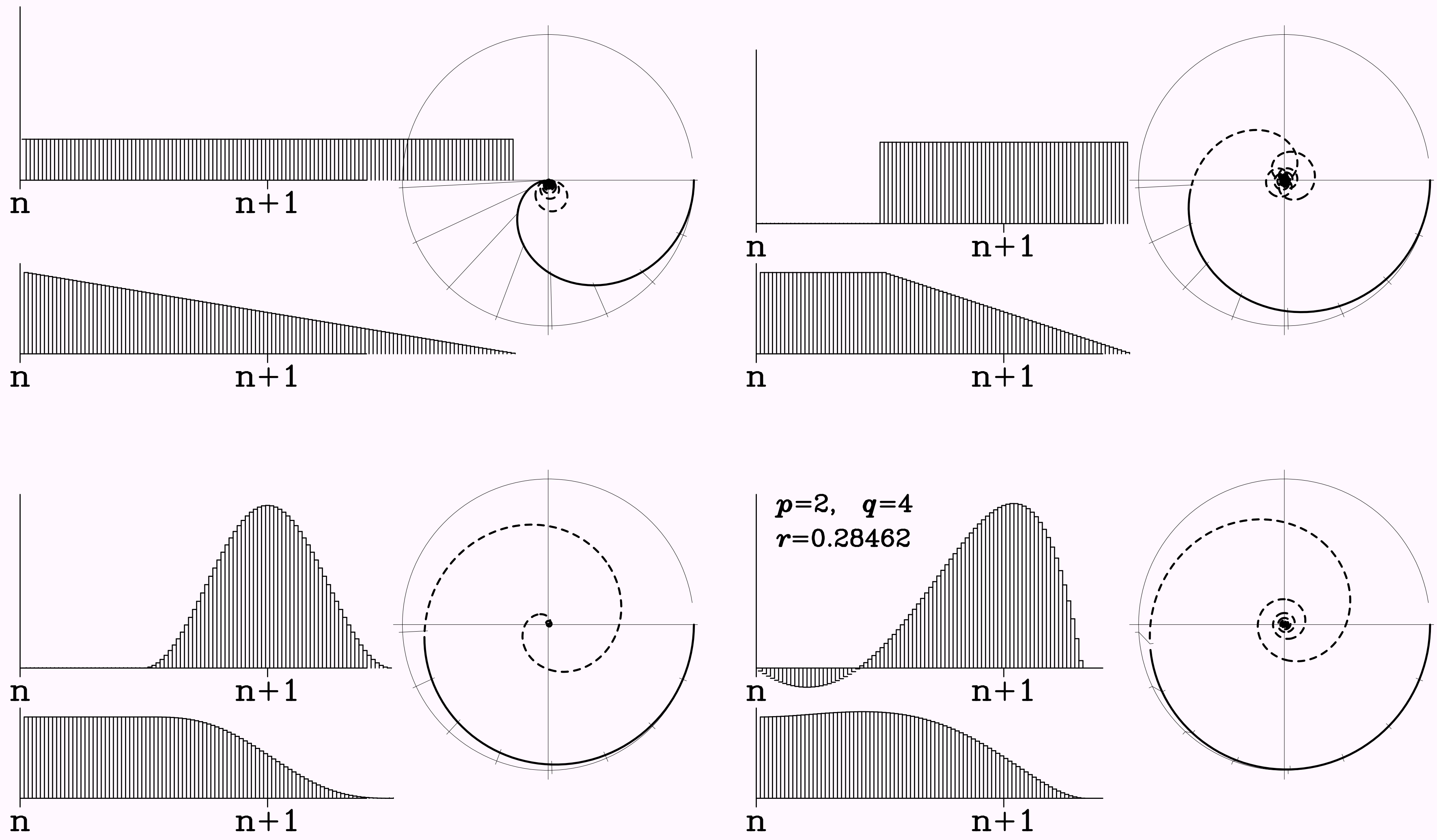
$$\lambda(\alpha) = \int_0^{\tau_*} \mathrm{e}^{-i\alpha\cdot\tau} A(\tau)\, d\tau = \mathcal{R}(\alpha)\mathrm{e}^{-i\alpha}$$

where $A(\tau)$ is assumed to satisfy appropriate normalization and centroid conditions.

Ideally $\mathcal{R}(\alpha) \approx 1$ for $\alpha \leq \alpha_0 \sim 1$, and $\mathcal{R}(\alpha) \to 0$ as fast as possible once $\alpha > \alpha_0$, $\alpha \to \infty$. In the vicinity of $\alpha \to 0$, $1 - \mathcal{R}(\alpha) = \mathcal{O}(\alpha^r)$ with r identified as *order of accuracy.*

- It is desirable that $\lambda(\alpha)$ be similar to step multiplier of time stepping algorithm for pressure-gradient terms in baroclinic mode
- Any *positive-definite* shape function $A(\tau)$ yields **at most first order of accuracy**
- S-shaped $A(\tau)$ (with some negative weights) can achieve *second*-order accuracy
- Split-explicit model in inherently more accurate in representing barotropic motions resolved by baroclinic time step (cf., tides, topographic Rossby waves) than implicit free-surface model (usually constraint to BE or weighted CN step for free-surface pressure-divergence terms). Even if $A(\tau)$ is positive definite.

Time splitting continued...   Fast-time averaging shape



$\lambda(\alpha)$ for four different shapes

Barotropic mode splitting for a stratified ocean

Baroclinic–barotropic mode splitting by Blumberg & Mellor, 1987, Bleck & Smith, 1990, Killworth, et. al., 1991, and Nadiga et. al., 1997

$$\frac{\partial}{\partial t}(D\overline{u}) + ... = -gD\nabla_x\zeta + \left\{gD\nabla_x\zeta + \mathcal{F}\right\}$$

where $-gD\nabla_x\zeta$ is "fast" and $\left\{....\right\}$ are "slow" terms, and

$$\mathcal{F} = \mathcal{F}\left[\nabla_x\zeta,\ \zeta,\ \nabla_x\rho(z),\ \rho(z)\right] = -\frac{1}{\rho_0}\int_{-h}^{\zeta}\frac{\partial P}{\partial x}dz \quad \text{with} \quad \frac{\partial^2\mathcal{F}}{\partial\zeta\,\partial\rho} \neq 0 \quad \text{due to nonlinearity}$$

Mode splitting error: after $\zeta \rightarrow \zeta'$ is updated by barotropic mode stepping,

$$-gD\nabla_x\zeta' + \left\{gD\nabla_x\zeta + \mathcal{F}\left[\nabla_x\zeta,\ \zeta,\ \nabla_x\rho(z),\ \rho(z)\right]\right\} \neq \mathcal{F}\left[\nabla_x\zeta',\ \zeta',\ \nabla_x\rho(z),\ \rho(z)\right]$$

i.e., *split-add* term no longer matches vertical integral of full (barotropic+baroclinic) PGF computed from new free surface and the same density. Usual arguments $\zeta \ll D$ and $\rho(x,y,z) = \rho_0 + \rho'(x,y,z)$ where $\rho'(x,y,z) \ll \rho_0$, so that the error is small,

$$\mathcal{O}\left(\max\left\{\frac{\rho'\nabla_x\zeta}{\rho_0}, \frac{\zeta\nabla_x\rho'}{\rho_0}\right\}\right) \qquad \text{vs.} \quad \mathcal{O}\left(\nabla_x\zeta\right)$$

...but what about stability?
POM, MICOM, SCRUM, ROMS are working for so many years, what is your problem?

Stratified barotropic mode continued...

Higdon & Bennett, 1996; Higdon & de Szoeke, 1997; Hallberg, 1997: (all in isopycnic coordinate framework) found instability of linearized split-coupled system in the case of nondissipative time stepping (FB, LF) and proposed remedies.

Their findings:

- the instability is of resonant nature due to aliasing of barotropic mode sub-sampled in at baroclinic steps, when barotropic step multipliers aliased in baroclinic Δt

- ideally barotropic-baroclinic modes are coupled via. nonlinear terms only (linearize $\Rightarrow$ uncouple); mode splitting error brings additional artificial coupling even in linearized version;

- perturbation analysis of weakly couples system;

- $\Rightarrow$ redefine barotropic mode pressure gradient term (make it to be **exactly** the vertical integral of 3D term and showed that it can be achieved in isopycnic coordinates);

- $\Rightarrow$ dissipative algorithms (via time filters to suppress barotropic mode aliasing, or dissipative predictor–corrector, Hallberg, 1997) for time stepping as an alternative.

Do we have similar problems in ROMS?

Can we do better than we usually do?

Stratified barotropic mode continued...

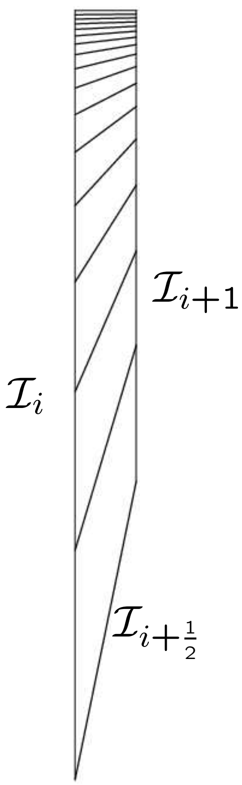
General guideline to replace SWE-like pressure gradient term $-gD\nabla_x\zeta$

$$\frac{\partial\mathcal{F}}{\partial\left(\nabla_x\zeta\right)}\nabla_x\zeta+\frac{\partial\mathcal{F}}{\partial\zeta}\zeta$$

hence

$$\mathcal{F}\left[\nabla_x\zeta,\ \zeta,\ ...\right]+\frac{\partial\mathcal{F}}{\partial\left(\nabla_x\zeta\right)}\nabla_x\left(\zeta'-\zeta\right)+\frac{\partial\mathcal{F}}{\partial\zeta}\left(\zeta'-\zeta\right)\approx\mathcal{F}\left[\nabla_x\zeta',\ \zeta',\ ...\right]$$

$\Rightarrow$ cancellation of the dominant part of mode splitting error.



$$\mathcal{F}_{i+\frac{1}{2}}=\int\limits_{-h_i}^{\zeta_i}P(x_i,z)\,dz-\int\limits_{-h_{i+1}}^{\zeta_{i+1}}P(x_{i+1},z)\,dz+\int\limits_{x_i}^{x_{i+1}}P(x,-h(x))\,\frac{\partial h(x)}{\partial x}dx$$

$$=\mathcal{I}_i-\mathcal{I}_{i+1}+\mathcal{I}_{i+\frac{1}{2}}$$

$$P_i(z)=g\int\limits_{z'_i}^{\zeta_i}\rho_i(z')\,dz'$$

$$\rho_i^*=\frac{1}{\frac{1}{2}D_i^2}\int\limits_{-h_i}^{\zeta_i}\left\{\int\limits_{z_i}^{\zeta_i}\rho_i(z')dz'\right\}dz$$

$$\overline{\rho}(x)=\frac{1}{D_i}\int\limits_{-h_i}^{\zeta_i}\rho_i(z')dz'$$

$$\rho_i^*\le\overline{\rho}_i$$

$$\Rightarrow\qquad\mathcal{F}_{i+\frac{1}{2}}=g\left\{\frac{\rho_i^*D_i^2}{2}-\frac{\rho_{i+1}^*D_{i+1}^2}{2}+\int\limits_{x_i}^{x_{i+1}}\overline{\rho}D\,\frac{\partial h}{\partial x}dx\right\}$$

Stratified barotropic mode continued... discrete version

Continuous pressure gradient term

$$\frac{\partial}{\partial t}(D\overline{u}) + \ldots = -\frac{1}{\rho_0} g \left\{ \frac{\partial}{\partial x}\left(\frac{\rho^* D^2}{2}\right) - \overline{\rho} D \frac{\partial h}{\partial x} \right\} = -\frac{1}{\rho_0} g D \left\{ \rho^* \frac{\partial \zeta}{\partial x} + \frac{D}{2}\frac{\partial \rho^*}{\partial x} + (\rho^* - \overline{\rho}) \frac{\partial h}{\partial x} \right\}$$

Separate $\mathcal{F}$ into zero-free-surface $\zeta = 0$ and perturbation

$$\mathcal{F}_{i+\frac{1}{2}} = \mathcal{F}^{(0)}_{i+\frac{1}{2}} + \mathcal{F}'_{i+\frac{1}{2}} ,$$

where

$$\mathcal{F}^{(0)}_{i+\frac{1}{2}} = g\left(\rho^*_i - \overline{\rho}_i\right)\frac{h_i^2}{2} - g\left(\rho^*_{i+1} - \overline{\rho}_{i+1}\right)\frac{h_{i+1}^2}{2} + g\left(\overline{\rho}_i - \overline{\rho}_{i+1}\right)\frac{h_i^2 + h_i h_{i+1} + h_{i+1}^2}{6}$$

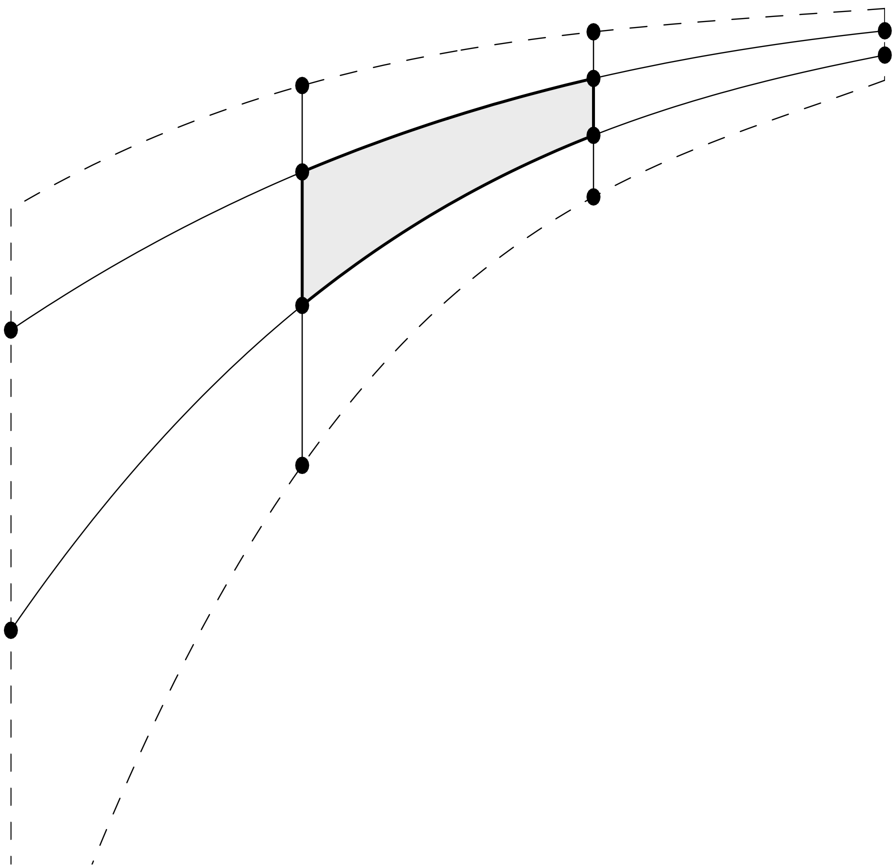
is purely baroclinic, and

$$\begin{aligned}\mathcal{F}'_{i+\frac{1}{2}} = -g \Bigg\{ & \frac{h_{i+1} + h_i}{2}\left(\rho^*_{i+1}\zeta_{i+1} - \rho^*_i \zeta_i\right) + \frac{\rho^*_{i+1}\zeta^2_{i+1}}{2} - \frac{\rho^*_i \zeta^2_i}{2} \\ & + (h_{i+1} - h_i)\Bigg[\frac{\left(\rho^*_{i+1} - \overline{\rho}_{i+1}\right)\zeta_{i+1} + \left(\rho^*_i - \overline{\rho}_i\right)\zeta_i}{2} \\ & \qquad + \frac{1}{6}\left(\overline{\rho}_{i+1} - \overline{\rho}_i\right)\left(\zeta_{i+1} - \zeta_i\right)\Bigg]\Bigg\}\end{aligned}$$

consists of *modified SWE term* and *baroclinic topographic response term.*

splitting: ρ^* and $\overline{\rho}$ *do not depend* on free surface, hence are kept constant during time stepping of barotropic mode.

Pressure Gradient Scheme



x-z plane view onto ROMS PG stencil: $\mathcal{J}(\rho, z)$ is approximated as a contour integral $\oint \rho dz$ around the shaded area

Shchepetkin & McWilliams, 2003

Pressure-Jacobian formulation: generalization of POM Jacobian to higher order of accuracy using *pseudo-flux form* based on 4-point polynomial fits for density and geopotential field

$$-\Delta x\, \Delta z \cdot \mathcal{J}(\rho, z) = FX_{i,k} - FX_{i+1,k} + FC_{i,k+1} - FC_{i,k}$$

where $\quad FX, FC = \int \rho dz = \int \rho \frac{\partial z}{\partial s} ds$

along the four segments

fourth-order accurate cancellation of hydrostatic σ-errors in PG

exact symmetry $\mathcal{J}(\rho, z) = -\mathcal{J}(z, \rho)$

formalism of *adiabatic differences* for compressible EOS $\Rightarrow$ guarantees positive stratification of cubic interpolant as long as discrete data is positively stratified

improved tolerance to "*hydrostatically inconsistent*" (Haney, 1991) grids

harmonic averaging $\Rightarrow$ does not lose accuracy on vertically non-uniform grids

Pressure Gradient continued...

High-order accurate pressure gradient schemes were constructed in the past (Beckmann & Haidvogel, 1993; Chu & Fan, 1997; 1998; 2003), they were shown to be very successful in idealized test cases, and ... earned reputation of being non-robust and practically useless in real-world oceanic modeling (e.g., Kliem & Pietrzak, 1999). In fact, even today most σ-modelers stick with POM Jacobian. **Why?**

- oscillation of high-order polynomial interpolants, when density is *not smooth* on grid scale

- mathematical criterion for field smoothness on *grid scale* is always based on ratio of consecutive differences

$$\frac{\rho_{i+1,k} - \rho_{i,k}}{\rho_{i,k} - \rho_{i-1,k}} < 3\,, \qquad \frac{\rho_{i,k+1} - \rho_{i,k}}{\rho_{i,k} - \rho_{i,k-1}} < 3\,, \qquad \text{etc...}$$

- the fact that field is "physically smooth" does not guarantee *smoothness on grid scale*: it is just a matter of grid spacing. One can easily get non-smooth data from Levitus. In fact, most trouble occurs in abyss, where stratification is weak and vertical grid spacing [either Δz or via projected $\Delta x \cdot \partial z / \partial x|_\sigma$] is too large.

- model "feels" polynomial oscillations within the discretization of stiff hydrostatic balance as *spurious negative stratification*, which leads to computational blowup

- In the case of Compressible EOS most of vertical gradient ($\Rightarrow$ also projected along-sigma horizontal gradient) occurs due to *passive* compressibility, effect i.e., $\partial\rho_{\text{in situ}}/\partial z \neq 0$ even if Θ, S=cost spatially uniform. Furthermore, maintaining non-oscillatory behavior of $\rho_{\text{in situ}}$ **does not guarantee** monotonic positive stratification, even if discrete density is positively stratified.

Pressure Gradient continued... What to do about oscillations?

Cubic polynomial fit

$$\rho(\xi) = \rho_{k+1}\left(\xi+\frac{1}{2}\right) + \rho_k\left(\xi-\frac{1}{2}\right) + \left(\xi^2+\frac{1}{4}\right)\left\{\left[d_{k+1}+d_k-2\left(\rho_{k+1}-\rho_k\right)\right]\xi + \frac{d_{k+1}-d_k}{2}\right\}$$

defined for $-1/2 \leq \xi \leq +1/2$ and

$$\rho\left(\xi\right)\Big|_{\xi=-\frac{1}{2}} \equiv \rho_k \qquad \rho\left(\xi\right)\Big|_{\xi=+\frac{1}{2}} \equiv \rho_{k+1} \qquad \frac{\partial\rho}{\partial\xi}\Big|_{\xi=-\frac{1}{2}} \equiv d_k \qquad \frac{\partial\rho}{\partial\xi}\Big|_{\xi=+\frac{1}{2}} \equiv d_{k+1}$$

How to estimate d_k and d_{k+1} from discrete data ρ_k?

algebraically averaged slope:

$$d_k = \frac{\delta\rho_{k+\frac{1}{2}} + \delta\rho_{k-\frac{1}{2}}}{2} \qquad \text{where} \qquad \delta\rho_{k+\frac{1}{2}} = \rho_{k+1} - \rho_k \quad \forall k$$

harmonic average

$$d_k = 1 \Bigg/ \left[\frac{1}{2}\left(\frac{1}{\delta\rho_{k+\frac{1}{2}}} + \frac{1}{\delta\rho_{k-\frac{1}{2}}}\right)\right] = \frac{2\delta\rho_{k+\frac{1}{2}}\cdot\delta\rho_{k-\frac{1}{2}}}{\delta\rho_{k+\frac{1}{2}} + \delta\rho_{k-\frac{1}{2}}} \quad \text{as long as} \quad \delta\rho_{k+\frac{1}{2}}\cdot\delta\rho_{k-\frac{1}{2}} > 0$$

and $d_k = 0$ if $\delta\rho_{k+\frac{1}{2}}\cdot\delta\rho_{k-\frac{1}{2}} \leq 0$.

As long as $\delta\rho_{k+\frac{1}{2}}$ and $\delta\rho_{k-\frac{1}{2}}$ have the same sign, d_k is **no greater than twice the smaller** of the two by magnitude,

$$|d_k| < 2\left|\mathrm{minmod}\left(\delta\rho_{k+\frac{1}{2}}, \delta\rho_{k-\frac{1}{2}}\right)\right|$$

which guarantees that $\rho(\xi)$ is **monotonic** as a **continuous function** of its argument within the whole area of its definition.

Pressure Gradient continued... Compressible EOS case

- **It is dangerous to compare and apply harmonic averaging to consecutive differences of in situ density. ROMS PGF scheme is not compatible with subtraction of horizontally uniform $\rho(z)$-profile.**

- **adiabatic differencing instead**

- EOS

$$\rho\left(\Theta,S,z\right)=\rho_1'\left(\Theta,S\right)+q_1\left(\Theta,S\right)\cdot z+q_1\left(\Theta,S\right)\cdot z^2+...$$

- adiabatic derivative

$$\left.\frac{\partial\rho\left(\theta,S,z\right)}{\partial s}\right|_{ad}=\frac{\partial\rho_1'\left(\theta,S\right)}{\partial s}+\sum_{n=1}^{n_{\text{max}}}z^n\frac{\partial q_n\left(\theta,S\right)}{\partial s}$$

- elementary adiabatic difference

$$\delta\rho_{i,k+\frac{1}{2}}^{(\text{ad})}={\rho_1'}_{i,k+1}-{\rho_1'}_{i,k}+\frac{z_{i,k+1}+z_{i,k}}{2}\left({q_1}_{i,k+1}-{q_1}_{i,k}\right)$$

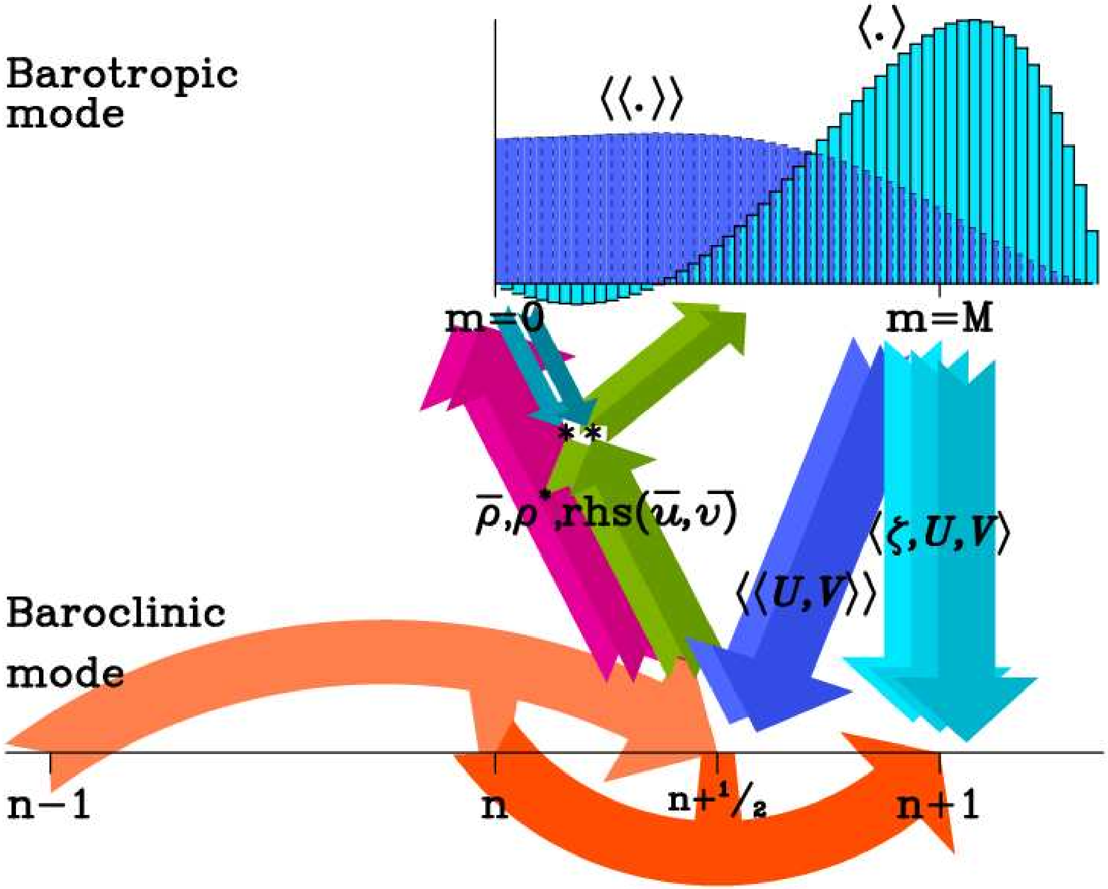
- averaged slope

$$d_{i,k}\equiv\left.\frac{\partial\rho}{\partial s}\right|_{i,k}=\frac{2\delta\rho_{i,k+\frac{1}{2}}^{(\text{ad})}\cdot\delta\rho_{i,k-\frac{1}{2}}^{(\text{ad})}}{\delta\rho_{i,k+\frac{1}{2}}^{(\text{ad})}+\delta\rho_{i,k-\frac{1}{2}}^{(\text{ad})}}+{q_1}_{i,k}\left.\frac{\partial z}{\partial s}\right|_{i,k}$$

Pressure Gradient continued...

- Jackett & McDougall, 1995 introduced *in situ* adiabatic derivatives of *in situ* density.
- They noticed that *potential density* — i.e., a scalar 3D field, spatial derivatives of which are equivalent *in situ* adiabatic differences of *in situ* density — can not be defined for realistic EOS. Isopycnic-coordinate modelers already faced this problem. In z-coordinate world Griffies, *et al*, 1998 had to reformulate isopycnic $\rightarrow$ *isoneutral* diffusion.
- Baroclinic pressure gradient can be expressed entirely in terms of *in situ* adiabatic differences of *in situ* density. This is independent of type of vertical coordinate.
- Besides pressure gradient, density and EOS participates in computation of vertical mixing parameterization (via BVF stability frequency and buoyancy fluxes) and in definition of isosurfaces of diffusion. It all cases density participates only via adiabatic derivatives. **Unified treatment of EOS throuhout the whole code?**
- Traditionally EOS is formulated as computation of *in situ* density via T, S, but in fact *in situ* density is irrelevant for anything in ocean modeling, except, perhaps recovering $\mathcal{O}\left(10^{-3}\right)$ differences between Boussinesque and non-Boussinesque models.
- Examination of EOS + Levitus data reveals that Taylor expansion in powers of z is sufficiently accurate, even if truncated after $(q_1 \cdot z)$-term. This is due to the fact that nonlinearity is extremely small in upper 1000 m, while below that World-wide variations in T, S are small.
- McDougall, *et al*, 2003 came up with new EOS using thermodynamic approach.

Conclusion



Barotropic-baroclinic mode exchange in ROMS time step

Generalized FB step for barotropic mode

Predictor–corrector LF-AM3 (with FB-feedback → 70% gain on stability range vs. standard LF-AM3) for baroclinic mode

Split-explicit barotropic mode, with 2-way temporal averaging via S-shaped filter → at least second-order temporal accuracy for resolved barotropic motions

Nonconservative (pseudo-compressible) predictor sub-step (via artificial continuity equation); Conservative and constancy preserving corrector sub-step.

Accounting for nonuniform density in barotropic mode via ρ^*, $\overline{\rho}$: accurate convergent split of pressure-gradient terms

Permissible time steps for ROMS applications

Configuration	Grid Size	Resolution *deg* or *km*	Time Step *sec*	Mode Splitting Ratio	Primary Time Step Limitation
Atlantic DAMEE	$128 \times 128 \times 20$	0.75^0	8640	60 (Gen. FB)	Coriolis force
Atlantic DAMEE	$256 \times 256 \times 20$	0.375^0	5760	92 (Gen. FB)	Coriolis/internal
Pacific	$384 \times 224 \times 30$	0.5^0	7200	78 (Gen. FB)	Coriolis force
US West Coast	$83 \times 168 \times 20$	15 *km*	2880	50 (LF-TR)	internal waves
US West Coast	$126 \times 254 \times 20$	10 *km*	2160	60 (LF-TR)	internal waves
Monterey Bay	$93 \times 189 \times 20$	5 *km*	960	60 (LF-TR)	internal waves

"(Gen. FB)" and "(LF-TR)" in the Mode Splitting Ratio column indicates time stepping algorithm for barotropic mode.