Beyond second-order centered differencing: An alternative view on grid staggering

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Background

- Von Neumann Linearized Analysis - introduced in any CFD classes
  - Stability
  - Dissipation
  - Dispersion
- Arakawa Grid system - Projected to 1D
  - staggered vs unstaggered

“The unstaggered schemes have poor dispersion properties.”
A quick recap how to get this conclusion

1D Linearized Shallow Water Equations:

\[
\frac{\partial \phi}{\partial t} = -gH \frac{\partial u}{\partial x} \\
\frac{\partial u}{\partial t} = -\frac{\partial \phi}{\partial x}
\]

Analytical solutions (a=\sqrt{gH} grav-wave speed):

\[
\hat{\phi} = \hat{\phi}_k e^{i(kx \pm akt)} \\
\hat{u} = \mp \frac{1}{a} \hat{\phi}_k e^{i(kx \pm akt)}
\]

Exact amplification factor (pick \Rightarrow direction):

\[
\hat{G} = \exp(-iak\Delta t)
\]

When at same time level, for any \eta (with \theta=k\Delta x):

\[
\eta_{j+1} = \eta_j \exp(i\eta\theta)
\]

Unstaggered Forward-Backward Discretization:

\[
\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} = -\frac{a^2}{2\Delta x} (u_{j+1}^n - u_{j-1}^n) \\
\frac{u_j^{n+1} - u_j^n}{\Delta t} = -\frac{1}{2\Delta x} (\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1})
\]

Resulting numerical amp-factor (c is CFL):

\[
G = 1 - \frac{c^2}{2} \sin^2 \theta \pm i\frac{c}{2} \sin \theta \sqrt{4 - c^2 \sin^2 \theta}
\]

Staggered Forward-Backward Discretization:

\[
\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} = -\frac{a^2}{\Delta x} (u_{j+0.5}^n - u_{j-0.5}^n) \\
\frac{u_{j+0.5}^{n+1} - u_{j+0.5}^n}{\Delta t} = -\frac{1}{\Delta x} (\phi_{j+1}^{n+1} - \phi_j^{n+1})
\]

Resulting numerical amp-factor:

\[
G = 1 - c^2(1 - \cos \theta) \pm ic \sqrt{(1 - \cos \theta)(c^2 \cos \theta - c^2 + 2)}
\]
Dissipation and dispersion errors - Staggered rules!

Dissipation error - the ratio of the numerical and theoretical amplification amplitude (Both are 1):

$$\epsilon_{\nu} = \frac{|G|}{|G'|} = |G'| = \exp(\Phi_i)$$

$$G' = e^{\Phi_i} e^{-i\Phi_r} = e^{\omega_i \Delta t} e^{-i\omega_r \Delta t}$$

Dispersion error - the ratio between the numerical and the analytical phase speed (a):

$$\epsilon_{\phi} = \frac{\Phi_r}{ak\Delta t} = \frac{\Phi_r}{c\theta} = \frac{\omega_r/k}{a} = \frac{a_{num}}{a}$$

$$\tan \Phi_r = -\frac{\Im(G)}{\Re(G)}$$

(a) Dispersion Error - a-grid ng1

(d) Dispersion Error - c-grid ng1

Unstaggered: Stationary 2-delta waves

Staggered: Better resolved phase speeds

Unstaggered schemes do seem like to have incorrect (slower) phase speed.
However...

Apparently, many factor alters wave speed. Grid staggering choice does not look like the deterministic one.
Beyond the traditional perception...

Linearized analysis applies to:

- Linearized problems...
- 2nd order interpolation
- Central differencing
- No diffusion
- Smooth solutions

Linearized analysis cannot address:

- Solution with big perturbations
- Higher order interpolation
- Upwinding or more sophisticated directional splitting
- Discontinuities (fronts, small scales, etc.)

1st gen climate models for planetary scales (thousands of kms) - 2D mean flow

The modern weather/climate models (hundreds to a few kms), LES (meters!) - 3D full scales of motions

Kalnay Book, fcst geopotential height at 24 hr

Numeric technique and DA improves a lot over the years. Need to advance analysis (or perspectives)
How about high order linearized analysis?

Without any diffusion, the amp-factor for the simplest 5-point polynomial scheme:

\[
G = \frac{23c^2}{100} \cos(\phi) + \frac{19c^2}{200} \cos^2(2\phi) + \frac{43c^2}{80} \cos(2\phi) - \frac{9c^2}{40} \cos(3\phi) \\
- \frac{c^2}{200} \cos(5\phi) + \frac{c^2}{3600} \cos(6\phi) - \frac{1139c^2}{1800} + 1 \\
\pm \frac{\sqrt{2}c}{3600} i \sqrt{(-684c^2 \sin^4(\phi) + 2619c^2 \sin^2(\phi) + c^2 \sin^2(3\phi) - \\
414c^2 \cos(\phi) + 405c^2 \cos(3\phi) + 9c^2 \cos(5\phi) - 3600)} \\
\sqrt{(828 \cos(\phi) + 342 \cos^2(2\phi) + 1935 \cos(2\phi) - \\
810 \cos(3\phi) - 18 \cos(5\phi) + \cos(6\phi) - 2278)}
\]

Calculated from a Python script, and I do not know if it is correct or not...need better solutions
Single step discretization in the matrix form

Every single-step spatial discretization can be written in the matrix form:

$$\sum_l L^{(l)} \begin{bmatrix} \phi \\ u \end{bmatrix}_{j+l}^{n+1} = \sum_l R^{(l)} \begin{bmatrix} \phi \\ u \end{bmatrix}_{j+l}^n$$

When at same time level, for any \( \eta \) (with \( \theta = k \Delta x \)):

$$\eta_{j+l} = \eta_j \exp(il\theta)$$

With single step amp-factor \( G \):

$$G \sum_l \left\{ L^{(l)} \exp(i l \theta) \right\} \begin{bmatrix} \phi \\ u \end{bmatrix}_0 = \sum_l \left\{ R^{(l)} \exp(i l \theta) \right\} \begin{bmatrix} \phi \\ u \end{bmatrix}_0$$

Take a inverse:

$$P = \left( \sum_l \left\{ L^{(l)} \exp(i l \theta) \right\} \right)^{-1} \left( \sum_l \left\{ R^{(l)} \exp(i l \theta) \right\} \right)$$

The amp-factor \( G \) is the eigenvalue of \( P \) (2x2):

$$G \begin{bmatrix} \hat{\phi} \\ \hat{u} \end{bmatrix}_0 = P \begin{bmatrix} \hat{\phi} \\ \hat{u} \end{bmatrix}_0$$

Properties of \( P \):

- Deterministic 2 by 2 matrix of variables: \( c \) and \( \theta \); Grav-speed \( a \) is cancelled
- Multi-step extension can be analogous: \( P = P_1 \times P_2 \times ... \)
- For any \( (c, \theta) \), if the solution \( |G| > 1 \), indicating the numerical scheme is not stable
- \( c > 0 \); \( 0 < \theta \leq \pi \)

Let's solve this system in the \( (c, \theta) \) space
Examples: Forward-Backward Central differencing

Unstaggered:

\[
\begin{align*}
\phi_j^{n+1} &= \phi_j^n - ac \sum_{l=-N_g}^{N_g} A^{(l)} u_{j+i}^n \\
u_j^{n+1} &= u_j^n - \frac{c}{a} \sum_{l=-N_g}^{N_g} A^{(l)} \phi_{j+l}^{n+1}
\end{align*}
\]

In matrix form (expanded, explicit P):

\[
\begin{bmatrix}
\phi_j^{n+1} \\
u_j^{n+1}
\end{bmatrix} = \begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix} + \sum_{l=-2N_g}^{2N_g} \begin{bmatrix}
0 & -acA^{(l)} \\
-\frac{c}{a}A^{(l)} & c^2C^{(l)}_{FB}
\end{bmatrix} \begin{bmatrix}
\phi_j^n \\
u_j^n
\end{bmatrix} \exp(i\theta)
\]

where

\[
C^{(p)}_{FB} = \sum_{l=-N_g}^{N_g} A^{(l)} A^{(p-l)}
\]

Staggered:

\[
\begin{align*}
\phi_j^{n+1} &= \phi_j^n - ac \sum_{l=-N_g}^{N_g} A^{(l)} u_{j+i}^n \\
u_j^{n+1} &= u_j^n - \frac{c}{a} \sum_{l=-N_g}^{N_g} A^{(l)} \phi_{j+l}^{n+1}
\end{align*}
\]

In matrix form:

\[
\begin{bmatrix}
\phi_j^{n+1} \\
u_j^{n+1}
\end{bmatrix} = \begin{bmatrix}
1 & 0 \\
0 & 1
\end{bmatrix} + \sum_{l=-2N_g}^{2N_g} \begin{bmatrix}
0 & -acA^{(l)} \\
-\frac{c}{a}B^{(l)} & c^2C^{(l)}_{FB}
\end{bmatrix} \begin{bmatrix}
\phi_j^n \\
u_j^n
\end{bmatrix} \exp(i\theta)
\]

where

\[
B^{(l)}_c = A^{(l+1)}_c \\
C^{(p)}_{FB} = \sum_{l=-N_g}^{N_g} B^{(l)}_c A^{(p-l)}_c
\]

Bonus: one can achieve equivalent effect to FB scheme by adding a second order diffusion term

Otherwise, explicit central-differencing scheme is not stable.
High order dispersion errors

Here we have the plot of the similar dispersion errors for high order schemes.

- All have no dissipative errors ($e_{\text{diff}} = 1$)
- Unstaggered schemes still produce stationary 2-delta waves.
- Staggered scheme still has smaller dispersion errors, but the gap is closing
- Note there are $e_{\text{disp}} > 1$ cases, what does this mean to realistic simulations? Will explore it in the following slides.

Now we have a numerical way to perform the linearized analysis!
“Numerical” linearized analysis to a practical scheme

Let’s change gear: in GFDL, we are exploring a Riemann solver based unstaggered dynamical core to extend FV3 (https://www.gfdl.noaa.gov/fv3/).

- The Low Mach-number Approximate Riemann Solver (LMARS, Chen et al. 2013)
- The vertical lagrangian coordinate (same as FV3)
- Cubed-sphere geometry with the curvilinear coordinates (same as FV3)
- Two-substep update with forward-backward in each substep (same as FV3)
- Implicit diffusion packed in the LMARS

We will project the Riemann solver based scheme to 1D and perform the linearized analysis to it.
LMARS in a nutshell

Assumptions to create LMARS:
- Low Mach number flow
- Weak discontinuities
- Locally constant group speed (sound, grav-waves)

Simpler Riemann problem structure:

\[ U_l = [\phi_l, u_l]^T \quad U_r = [\phi_r, u_r]^T \]

Different stencil creates mismatch at the cell interfaces

Stencil: \( N_c = 2N_g - 1 \)
Ng is the number of ghost cells required

\[ \phi_{1/2} = \frac{1}{2} (\phi_l + \phi_r) + \frac{a}{2} (u_l - u_r) \]
\[ u_{1/2} = \frac{1}{2} (u_l + u_r) + \frac{1}{2a} (\phi_l - \phi_r) \]

- Resulting math expression is extremely clean compared to traditional solvers (Roe, HLL, AUSM+-up, etc.)
- Accurate, low diffusive (need to see supplement slides for proof)
Dissipation-dispersion error evaluation

Numerical discretization (LMARS expanded):

\[ \phi_{j}^{n+1} = \phi_{j}^{n} - ac \sum_{l} A^{(l)} u_{j+l}^{n} + c \sum_{l} C_{vm,RS}^{(l)} \phi_{j+l}^{n} \]

\[ u_{j}^{n+1} = u_{j}^{n} - \frac{c}{a} \sum_{l} A^{(l)} \phi_{j+l}^{n+1} + c \sum_{l} C_{vm,RS}^{(l)} u_{j+l}^{n} \]

In matrix form:

\[
L \begin{bmatrix} \phi \\ u \end{bmatrix}_{j+l}^{n+1} = R \begin{bmatrix} \phi \\ u \end{bmatrix}_{j+l}^{n}
\]

\[
L = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \sum_{l} \begin{bmatrix} 0 & 0 \\ A^{(l)} & 0 \end{bmatrix} \exp(\imath l \theta)
\]

\[
R = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \sum_{l} \begin{bmatrix} cC_{vm,RS}^{(l)} & -acA^{(l)} \\ 0 & cC_{vm,RS}^{(l)} \end{bmatrix} \exp(\imath l \theta)
\]

\[ P = L^{-1} R \]

Bonus: Riemann solver (sounds like a black box) merely adds a high order diffusion term into the scheme
Final thoughts to the “numerical” linearized analysis

Pros:

- It finds the max stable CFL number
- The results applies to full spectrum of CFL (stable ones) numbers and wavenumbers. It is a continuous mapping between \((c, \theta)\) to \((e_{\text{dissipation}}, e_{\text{dispersion}})\)
- No need to solve the amplification factor analytically, which is almost impossible for high-order schemes or scheme with complex diffusion terms

Cons:

- We found diffusion can alter the dispersion relationship significantly. Testing the response for different diffusion settings populates your plots too quickly.
- Although doable, formulating the matrix form and perform linearized analysis is still a burden.
- It takes a pretty hard “numerical imagination” to form a picture of the combined effect for both dispersive and dissipative properties. (Try to tell everyone that you have developed a numerical scheme that has super-optimal dispersive relation, and the diffusive property damps the false waves effectively...)

Visualize the dispersion and dissipation properties by a set of numerical tests.
Before moving on...

Disclaimer of responsibilities: Please do not generalize the results of the staggered and unstaggered schemes to all staggered and unstaggered schemes. Because:

- No one runs a realistic simulation with zero damping effect. This work choose the numerical schemes to isolate the dispersive properties.
- As shown before, diffusion alters the dispersion relations. Other works also show time-marching schemes alters linearized analysis results too (Ullrich 2014, Kent 2014)

So, it only takes one counter-example to challenge "the non-staggered scheme has stationary grid-scale waves."

- You have two examples now.
- Diffusion alters the dispersion relations (repeated intentionally).
Introducing a new test case for dispersion-dissipation analysis

The numerical domain size: [-10000, 10000] M, with grid size Δ x=100 M.

Combine two waves within [-1000,1000] M range (20 grid cells):

\[ h_1 = h_0 \sin(kx - akt) \]
\[ u_1 = \sqrt{g/H} h_0 \sin(kx - akt) \]
\[ h_2 = h_0 \sin(kx + akt) \]
\[ u_2 = -\sqrt{g/H} h_0 \sin(kx + akt) \]

with \( g=10 \) M/s/s; \( H=10 \) M; \( h_0 =1 \) M. Denote \( m \) is the number of waves within the init region. The longest resolvable wave contains 20 grid points (\( m=1 \)). The shortest resolvable wavelength is \( 2 \Delta x=200 \) M.

\[ \theta_{deg} = k_m \Delta x = \frac{180m}{N} = 18m, \quad m = 1, \ldots, 10 \]

The reference solution with wave number \( m=1 \)
Choose CFL=0.8 for all schemes

- Replotted w.r.t. Wavelengths (much less dramatic than the phase plot, right?)
- Focus on lowest and highest orders of accuracy (Ng=1 and Ng=3) to save time
- Focus on wavelengths in 4-delta to 20-delta (m=5 and m=1)
- Simple to DIY if you want to expand the tests
Low wavenumber, low order schemes (theoretical)

- Unstaggered - slower
- Staggered - perfect
- RS - damped out
Unstaggered - slower
Staggered - perfect (almost - due to discontinuity)
RS - damped out (considered useless for practical usage)
Low wavenumber, high order schemes (theoretical)

- All should be perfect
All are perfect (almost - due to discontinuity)

High order schemes should handle 20-delta waves properly
High wavenumber, low order schemes (theoretical)

- Unstaggered - terrible, stationary
- Staggered - less “stationary”, but should look better
- RS - damped out
High wavenumber, low order schemes

- Unstaggered - terrible, stationary
- Staggered - less “stationary”, but still out of phase
- RS - damped out (low-order RS already considered useless regardless)
High wavenumber, high order schemes (theoretical)

- Unstaggered - nice phase
- Staggered - phase speed too fast
- RS - damped out
High wavenumber, high order schemes

- Unstaggered - better speed, but noise is so big! The downwind noise is stationary
- Staggered - waves travel too fast! The trailing waves might be exited by discontinuity
- RS - damped out
- All do a horrible job at ultra-short waves, maybe simply damp it out is a good choice
In fact...

ECMWF production runs simply DROP ultra-short waves completely.

FV3 damps ultra-short wave effectively with high-order diffusion terms.
We see discontinuities create plenty of surprises...

Finally, let’s construct a more “stressful” test - wavenumber m=0:

\[
\begin{align*}
    h_1 &= h_0 \\
    u_1 &= \sqrt{g/H}h_0 \\
    h_2 &= h_0 \\
    u_2 &= -\sqrt{g/H}h_0
\end{align*}
\]
Wavenumber zero, low order schemes (theoretical)

- Unstaggered - stationary noises
- Staggered - less “stationary”
- RS - smearing
- Unstaggered - stationary noise
- Staggered - stationary noise, nothing in the upwind region
- RS - little noise, but shape is too smeared (low-order RS already considered useless regardless)
Wavenumber zero, high order schemes (theoretical)

- Unstaggered - “very” stationary noise at 2-delta
- Staggered - phase speed too fast at low wavelengths
- RS - damp high-freq noise effectively
Wavenumber zero, low order schemes

- Unstaggered - stationary noise, evenly distributed
- Staggered - noise travels at a faster speed, causing aliasing!
- Staggered - Even the short ones are damped out, the remaining longer waves are false information, but look realistic
- RS - little noise, and the shape is conserved well!
Conclusions

- We introduce a numerical approach to perform Von Neumann linearized analysis on high-order methods with complex time-marching schemes.

- A new set of test cases are designed to demonstrate the dispersion and dissipation properties of numerical schemes, and validated against the linearized analysis.

- The advantages based on grid staggering choice, such as correct phase speed and allowing larger maximum Courant number, are diminished with high-order schemes.

- Our unstaggered Riemann Solver scheme effectively filters grid-scale (2-delta) and ultra-small (4-delta) waves, which could contain false information due to noise caused by discontinuities.
Thank you!

What gets us into trouble is not what we don't know. It's what we know for sure that just ain't so.

-- Mark Twain
Supplementary plots
(In case you wonder if unstaggered dynamical core really works in a full model)
W92 case 5
W92 case 6, resolution = C192, last frame = Day 80
BW (Jablonowski) test, NH
BW (Jablonski) test, NH-zoomed
BW (Jablonski) test, SH

ac C384 SP vort850-mean

fv3 C384 SP vort850-mean
Held-Suarez test