On the spatial and temporal discretization of vertical diffusion in the turbulent planetary boundary layer

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Context: advection-diffusion operator to parameterize unresolved scales in PBLs (and beyond)

The resulting turbulent viscosity/diffusivity $K$

- strongly varies spatially, i.e. large values of $K_{ij}$
  
- depends nonlinearly on model variables
- induces stiffness, i.e. large $\frac{1}{K_{ij}}$

Usual approach: use of (semi-)implicit temporal schemes with 2nd-order FD discretization

What could be wrong with 2nd-order in space?

- With $K^{(m)} = \frac{1}{\Delta x^2}$, $m \geq 2$
  
- $K^{(m)}(x) < K_{ij}$ for $x \approx j$

What could be wrong with (semi-)implicit scheme in time?

- Lack of monotonic damping / Inexact damping for large $\frac{1}{K_{ij}}$
- of errors with physical parameterizations
- Maps of $\frac{\partial K}{\partial t}$ from realistic simulations

Objective:

- Have a better control of numerical sources of error independently from the physical principles of the subgrid scheme
- Ensure the consistency between the parameterization and the resolved fluid dynamics (e.g. for air-sea B.C. & $K(z)$ computation)

1 - Spatial discretization

Constraints

- limit ourselves to tridiagonal linear problems
- possibility to have a joint treatment of vertical advection and diffusion
- allow a finite-volume interpretation

Possible alternatives

- Exponential Compact scheme, e.g. [Tian & Dai, 2007]
- Specifically designed for accuracy with large Peclet numbers
- Pade compact finite volume discretization

General form of the discretization

\[ \frac{dK_{ij}}{dt} + \frac{1}{\Delta x} \left( K_{ij} - K_{i+1,j} - K_{i-1,j} \right) \frac{\Delta x}{2} = \frac{\Delta x}{2} \left( \psi_{i+1} - \psi_i \right) \]

for standard discretization: $d_{i+1/2} = (\psi_{i+1} - \psi_{i})/\Delta x$ (the vertical layers thickness)

Compact Padé Finite Volume methods, e.g. [Kobayashi, 1999]

Unknowns: derivatives $d_{i+1/2}$ on cell interfaces, for $m, n \in N$

\[ \sum d_{i+1/2} + d_{i-1/2} = \left( \sum \psi \right) / \Delta x \]

For $(m,n) = (1,1), \frac{1}{\Delta x} \left( d_{i+1/2} + d_{i-1/2} \right) + \frac{\Delta x}{\Delta t} \left( \frac{\sum \psi}{\Delta x} \right) = \frac{\Delta x}{\Delta t} \left( \frac{\sum \psi}{\Delta x} \right) - \frac{\sum \psi}{\Delta t} \]

\[ \left( \frac{\Delta x}{\Delta t} \right) = \frac{1}{2} \left( \frac{\Delta x}{\Delta t} \right) \frac{1}{2} \rightarrow 48$-order discretization of $d_{i+1/2}$ for $K = \text{const}$

\[ \left( \frac{\Delta x}{\Delta t} \right) = \frac{1}{2} \left( \frac{\Delta x}{\Delta t} \right) \frac{1}{2} \rightarrow \text{equivalent to parabolic splines reconstruction.} \]

Can be reinterpreted in terms of subgrid reconstruction as parabolic splines

- Flexibility provided by $\alpha$ and $\gamma$ parameters

2 - Treatment of the boundary condition (Monin-Obukhov consistency)

no-slip boundary condition is never applied in practice

- replaced by a flux condition consistent with wall laws

For $\phi = \psi, \theta$

\[ \frac{\partial \phi}{\partial x} + \frac{\partial \phi}{\partial y} = 0 \]

\[ \phi = \phi_{\text{wall}} \]

IV approach with $h_1 = h_2$:

\[ \phi = \phi_{\text{wall}} \]

Asymptotics:

- Resolved case (combining the first 2 lines of the matrix)

\[ \frac{\partial \phi}{\partial z} + \frac{\partial \phi}{\partial z} = 0 \]

- Unresolved case (for $K = 0$)

\[ \frac{\partial \phi}{\partial z} - \frac{1}{\gamma} \frac{\partial \phi}{\partial z} = 0 \]

Smooth transition between the unresolved and the resolved limit

\[ \phi = \phi_{\text{wall}} \]

Numerical experiment:

\[ \frac{\partial \phi}{\partial t} + \frac{\partial \phi}{\partial z} = 0 \]

3 - Combination with time discretization

Combining Padé type schemes with implicit Euler leads to

\[ \frac{dK_{ij}}{dt} + \frac{1}{\Delta x} \left( K_{ij} - K_{i+1,j} - K_{i-1,j} \right) \frac{\Delta x}{2} + \frac{1}{\Delta t} \left( K_{ij} - K_{i+1,j} - K_{i-1,j} \right) \frac{\Delta x}{2} = \frac{1}{\Delta t} \left( \psi_{i+1} - \psi_i \right) \]

\[ \frac{dK_{ij}}{dt} + \frac{1}{\Delta x} \left( K_{ij} - K_{i+1,j} - K_{i-1,j} \right) \frac{\Delta x}{2} = \frac{1}{\Delta t} \left( \psi_{i+1} - \psi_i \right) \]

- easy to generalize for non-constant grid-size
- The tridiagonal solve provides the flux and not $\phi$

Properties for well-behaved numerical solutions

- Unconditional stability
- Monotonic damping (damping increases with increasing wavenumber, i.e. $\alpha_k > 0$)
- Non-oscillatory (i.e. $A \geq 0$)
- Proper control of grid-scale noise $\nu_{\text{grid}}$

- Convergence & stability are often not sufficient

With implicit Euler scheme:

\[ A(\gamma, \theta) = \frac{1}{1 + 2 \alpha_k \cos \theta + 1 + 2 \alpha_k \cos \theta \cos \gamma} \]

\[ 2 \text{-nd order accurate in space} \quad \gamma = \frac{1}{2} \]

\[ 2 \text{-nd order accurate in time} \quad \gamma = \frac{1}{2} \]

\[ 4 \text{-th order in space} \quad \gamma = \frac{1}{2} \]

\[ 4 \text{-th order in time} \quad \gamma = \frac{1}{2} \]

\[ 6 \text{-th order in space and time} \quad \gamma = \frac{1}{2} \]

4 - Combination with subgrid closure schemes and energy consistent

For $X$-equation closures with $X > 0$ a global energy budget can be derived

\[ \frac{\partial X}{\partial t} + \frac{\partial \phi}{\partial x} = 0 \]

- Energy budget in a water column (ignoring the contribution of B.C.) with the TKE dissipation

\[ E = \int_{z_{\text{sfc}}}^{z_{\text{bottom}}} (\phi E + \phi \frac{\partial \phi}{\partial z}) dz \]

\[ \text{Discrete counterpart of it tells you exactly how to discretize forcing terms in the TKE equation} \]

- Numerical experiment: single column with 0-equation closure (KPP, [Large et al., 1994])
- Use subgrid reconstruction to detect critical F number
- 'Energy consistent' discretization of the Richardson number

5 - Summary & Perspectives

Summary

- Pade FV approach provides a good combination of simplicity and flexibility to handle diffusive terms with minimal changes in existing codes
- Allows a good combination with surface layer param. and existing time-stepping
- Provides degrees of freedom to mitigate numerical errors in time or to impose desired properties
- Simple single column test (Kato & Philips) indicates a reduced sensitivity to numerical parameters

Perspectives

- Nonlinear stability
- Extension to mass-flux scheme
- Air-sea interface boundary condition
- Neutral case → stratified case
- Single column tests & global ocean simulation
- Add representation of oceanic molecular sublayer + MO layer in the top most oceanic grid box for OA coupling purposes, e.g. [Zeng & Beljaars, 2005]

References