On the discretization of vertical diffusion in the turbulent surface and planetary boundary layers

F. Lemarié – Inria (EPC AIRSEA), Laboratoire Jean Kuntzmann, Grenoble, France

In collaboration with: E. Blayo & S. Théry (UGA), C. Pelletier (UCLouvain), F. Nazari (Inria)

Context: representation of mixing in PBLs

▷ **Reynolds averaging ($\phi = \langle\phi\rangle + \phi'$)**

$$\partial_t \langle\phi\rangle = \ldots + \mathrm{div}(\langle \mathbf{u}'\phi' \rangle) + \ldots$$

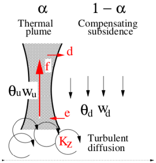
▷ **Diffusive approach for "local" mixing (K-theory)**

$\Rightarrow$ Boundary layer approximations: horiz. homogeneity and eddy diffusion

$$\langle w'\phi' \rangle = -K\partial_z \langle\phi\rangle \quad \rightarrow \quad \partial_t \langle\phi\rangle = \ldots + \partial_z(K\partial_z \langle\phi\rangle) + \ldots$$

$\rightarrow$ Down-gradient fluxes

$\rightarrow$ Turbulence acts as a "mixing"



▷ **Mass flux approach for "non-local" mixing**
(e.g. Chatfield & Brost, 1987; Siebesma, 2007)

$$\langle w'\phi' \rangle = -K\partial_z \langle\phi\rangle + \alpha w_u(\phi_u - \langle\phi\rangle) \quad \rightarrow \quad \partial_t \langle\phi\rangle = \partial_z(K\partial_z \langle\phi\rangle) - \partial_z(\alpha w_u \langle\phi\rangle) + \ldots$$

$\Rightarrow$ advection-diffusion operator to parametrize unresolved scales in PBLs and beyond (e.g. internal wave breaking or convective adjustment)

Context: representation of mixing in PBLs

Standard schemes to provide K:

- 0-equation: algebraic computation of the eddy parameters from bulk properties
- 1-equation: prog. eqn for turbulent kinetic energy (TKE) + diagnostic mixing length
- 2-equations: prog. eqn for TKE and for a ”generic” length scale (ϵ, ω, ...)

The resulting turbulent viscosity/diffusivity K

$\rightarrow$ strongly varies spatially (internal & boundary layers), i.e. large values of $\frac{h(\partial_z K)}{K}$

$\rightarrow$ depends nonlinearly on model variables

$\rightarrow$ induces stiffness i.e. large vertical parabolic Courant numbers $\sigma^{(2)} = \dfrac{K \Delta t}{h^2}$

Usual approach (e.g. WRF, LMDZ, all oceanic models):

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

Context: standard approach

- **What could be wrong with second-order scheme in space ?**
  - Nothing . . . if pure diffusion (i.e. with constant K) is considered

$$\partial_z \left(K \partial_z \phi\right)_k^{(\mathrm{C2})} = \partial_z (K \partial_z \phi)_k + \frac{h^2}{12} \left\{ K \partial_z^4 \phi \right\} + \mathcal{O}(\Delta z^4)$$

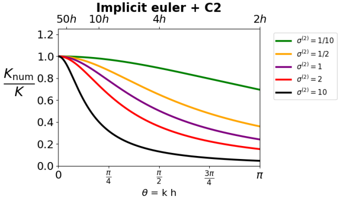
  - but with $\mathrm{Pe}^{(n)} = \dfrac{h^n \partial_z^n K}{K} \neq 0, \; n \geq 1$

$$\partial_z \left(K \partial_z \phi\right)_k^{(\mathrm{C2})} = \partial_z (K \partial_z \phi)_k + \frac{1}{24} \partial_z \left(K \left[\mathrm{Pe}^{(2)} \partial_z \phi + 2 \Delta z \mathrm{Pe}^{(1)} \partial_z^2 \phi + 2 \Delta z^2 \partial_z^3 \phi \right] \right) + \mathcal{O}(\Delta z^4)$$

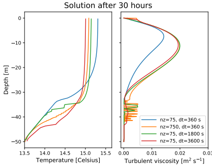
- **What could be wrong with (semi)-implicit scheme in time ?**
  - Lack of monotonic damping (e.g. **Manfredi & Ottaviani, 1999**; **Wood et al., 2007**) possibly leaving noise uncontrolled (+ trigger conv. adjust.)
  - Inexact damping for large $\sigma^{(2)}$
  - $\mathcal{O}(\Delta t)$ errors in coupling with physical parameterizations

Impact on model solutions

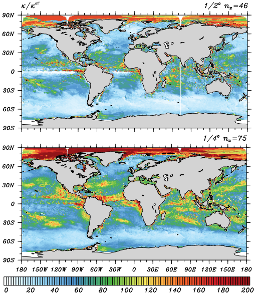
numerical vs exact damping rate



Sensitivity to Δt and Δz



Single-column exp. (Wind-induced deepening of BL)



Maps of K/K^{num} from oceanic realistic simulations

- K^{num} is the diffusivity in the continuous equation with same damping as the numerical damping
- $K/K^{\mathrm{num}} \gg 1 \;\Rightarrow$ the damping seen by the model is smaller than the theoretical damping.
- $\sigma^{(2)} = \overline{\sigma^{\mathrm{mld}}}$, $\theta = \dfrac{2\pi}{N_{\mathrm{mld}}}$.

Objectives

- Have a better control of numerical sources of error independently from the physical principles of the subgrid scheme
- Consistency between the parameterizations and the resolved fluid dynamics (for bottom boundary condition & $K(z)$ computation)

Outline

1. Spatial discretization

2. Treatment of the bottom boundary condition (MO consistency)

3. Combination with time discretization

4. Combination with subgrid closure schemes

1

Spatial discretization

Objectives & motivations

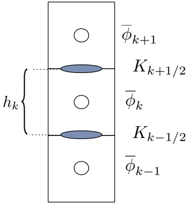
Constraints

- 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.**McKinnon & Johnson, 1991**; **Tian & Dai, 2007**)
$\rightarrow$ Specifically designed for accuracy with large Peclet numbers

▷ Padé compact finite volume discretization



General form of the discretization

$$\partial_z(K\partial_z\phi) = \frac{K_{k+1/2}d_{k+1/2} - K_{k-1/2}d_{k-1/2}}{h_k}, \qquad d_{k+1/2} = (\partial_z\phi)_{k+1/2}$$

for standard discretization: $d_{k+1/2} = (\phi_{k+1} - \phi_k)/h$ (h : vertical layers thickness)

Parabolic splines reconstruction

Suppose a given set of $\{\overline{\phi}_k, k = 1, \dots, N\}$ and assume a subgrid parabolic reconstruction

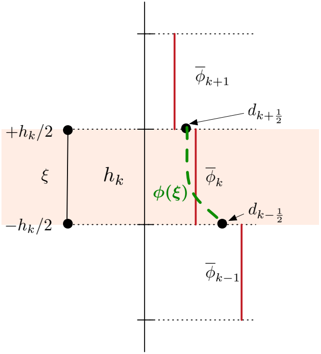
$$\phi(\xi) = a\xi^2 + b\xi + c, \qquad \xi \in \left] -\frac{h_k}{2}, \frac{h_k}{2} \right[$$

under the constraints

- $\displaystyle \frac{1}{h_k} \int_{-\frac{h_k}{2}}^{\frac{h_k}{2}} \phi(\xi) d\xi = \overline{\phi}_k$
- $\partial_z \phi(+h_k/2) = d_{k+1/2}$, $\partial_z \phi(-h_k/2) = d_{k-1/2}$

+ Impose the continuity of ϕ at cell interfaces :

$$\frac{1}{6} \mathbf{d_{k+3/2}} + \frac{2}{3} \mathbf{d_{k+1/2}} + \frac{1}{6} \mathbf{d_{k-1/2}} = \frac{\overline{\phi}_{k+1} - \overline{\phi}_k}{h}$$



$$\phi(\xi) = \overline{\phi}_k + \frac{d_{k+\frac{1}{2}} + d_{k-\frac{1}{2}}}{2} \xi + \left(\frac{d_{k+\frac{1}{2}} - d_{k-\frac{1}{2}}}{2h_k} \right) \left(\xi^2 - \frac{h_k}{12} \right)$$

- necessitates inversion of an implicit linear system of equations
- *compact* accuracy (4th-order for advection, 2nd for diffusion)
- Widely used for vertical advection in oceanic models

Compact Padé Finite Volume methods

Lele, 1992; Kobayashi, 1999

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

$$\sum_{i=1}^{m} \alpha_i \boldsymbol{d}_{\boldsymbol{k+\frac{1}{2}-i}} + \boldsymbol{d}_{\boldsymbol{k+\frac{1}{2}}} + \sum_{i=1}^{m} \alpha_i \boldsymbol{d}_{\boldsymbol{k+\frac{1}{2}+i}} = \frac{1}{h}\left(\sum_{j=1}^{n} \gamma_j \overline{\phi}_{k+j} - \sum_{j=1}^{n} \gamma_j \overline{\phi}_{k-j+1}\right)$$

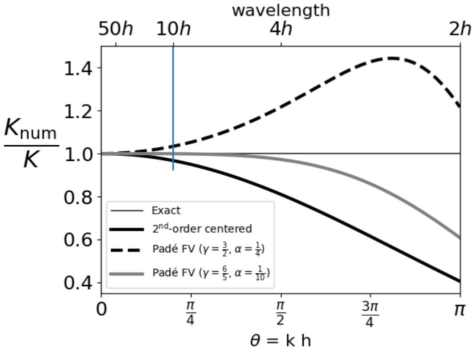
- For $(m, n) = (1, 1)$: $\alpha_1 d_{k-\frac{1}{2}} + d_{k+\frac{1}{2}} + \alpha_1 d_{k+\frac{3}{2}} = \gamma_1 \left(\frac{\overline{\phi}_{k+1} - \overline{\phi}_k}{h}\right)$

  $(\alpha_1, \gamma_1) = \left(\frac{1}{10}, \frac{6}{5}\right)$ $\quad\rightarrow$ 4th-order discretization of $d_{k+\frac{1}{2}}$ (for $K = \text{cste}$)

  $(\alpha_1, \gamma_1) = \left(\frac{1}{4}, \frac{3}{2}\right)$ $\quad\rightarrow$ equivalent to parabolic splines reconstruction.

- Can be reinterpreted in terms of subgrid reconstruction as parabolic splines
- Flexibility provided by α and γ parameters

Effective viscosity/diffusivity



- At this point relevant only for internal layers
  $\rightarrow$ not directly applicable to turbulent boundary layers

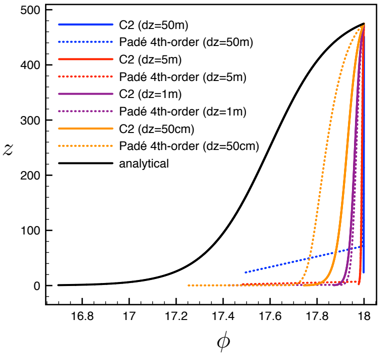
- Illustration : stationary problem

$$\begin{cases} \partial_z \left(K(z) \partial_z \phi \right) &= \dfrac{\partial_z \mathcal{R}}{\rho C_p} \\ \phi(0) &= \phi_{\text{bot}} \\ \phi\left(\dfrac{19 h_{\text{bl}}}{20} \right) &= \phi_{\text{top}} \end{cases}$$

with

$$K(z) = \kappa \phi_\star \frac{z}{h_{\text{bl}}} (h_{\text{bl}} - z) + K_{\text{mol}}$$

$$\mathcal{R}(z) = \mathcal{R}_0 \left(\alpha e^{-z/\zeta_0} + (1-\alpha) e^{-z/\zeta_1} \right)$$



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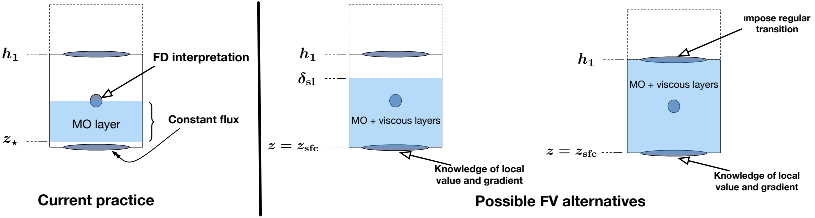
Treatment of the bottom boundary condition (MO consistency)

Treatment of boundary cells (neutral case)

Dirichlet boundary condition is never applied in practice
$\rightarrow$ replaced by a flux condition consistent with wall laws



Current practice :

$$\begin{cases} \partial_z \left(\kappa|\phi_\star|(z+z_\star)\partial_z\phi\right) = 0 \\ \phi(z_\star) = \chi_{\mathrm{sfc}} \\ \phi(h_1/2) = \phi_1 \end{cases}$$

$$\phi(z) = (\phi_1 - \chi_{\mathrm{sfc}}) \left(\frac{\ln\left(\frac{1}{2} + \frac{z}{2z_\star}\right)}{\ln\left(\frac{1}{2} + \frac{h_1}{4z_\star}\right)} \right) + \chi_{\mathrm{sfc}}$$

FV approach with $h_1 = \delta_{\mathrm{sl}}$:

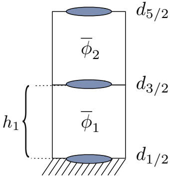
$$\begin{cases} \partial_z \left(\kappa|\phi_\star|(z+z_\star)\partial_z\phi\right) = 0 \\ \phi(z_{\mathrm{sfc}}) = \chi_{\mathrm{sfc}} \\ \phi(h_1) = \phi_{3/2} \end{cases}$$

$$\phi(z) = (\phi_{3/2} - \chi_{\mathrm{sfc}}) \left(\frac{\ln\left(1 + \frac{z}{z_\star}\right)}{\ln\left(1 + \frac{h_1}{z_\star}\right)} \right) + \chi_{\mathrm{sfc}}$$

Treatment of boundary cells with Parabolic splines

2nd-order polynomial subgrid reconstruction for $z \in]-\frac{h_k}{2},\frac{h_k}{2}[$:

$$\phi(z) = \overline{\phi}_k + \left(\frac{d_{k+1/2}+d_{k-1/2}}{2}\right) z + \frac{d_{k+1/2}-d_{k-1/2}}{2h_k}\left(z^2-\frac{h_k}{12}\right)$$



Usual treatment of boundary cell (with Dirichlet B.C.)

$$\phi\left(-\frac{h_1}{2}\right) = \overline{\phi}_1 - \frac{h_1}{3} d_{1/2} - \frac{h_1}{6} d_{3/2} = \chi_{\rm sfc} \quad \rightarrow \frac{1}{3} d_{1/2} + \frac{1}{6} d_{3/2} = \frac{\overline{\phi}_1 - \chi_{\rm sfc}}{h_1}$$

Alternative treatment

$$\phi(z) = (\phi_{3/2} - \chi_{\rm sfc}) \left(\frac{\ln\left(1+\frac{z}{z_\star}\right)}{\ln\left(1+\frac{h_1}{z_\star}\right)}\right) + \chi_{\rm sfc} = d_{3/2}(h_1 + z^\star) \ln\left(1+\frac{z}{z_\star}\right) + \chi_{\rm sfc}$$

$$\rightarrow \; d_{1/2} = d_{3/2}\left(1+\frac{h}{z_\star}\right)$$ (consistant with constant flux layer)

$$\rightarrow \; \frac{1}{6} d_{5/2} + \left[\frac{1}{3} + \left(1+\frac{z_\star}{h}\right)\ln\left(1+\frac{h}{z_\star}\right)\right] d_{3/2} = \frac{\overline{\phi}_2 - \chi_{\rm sfc}}{h}$$ (impose regularity)

Treatment of boundary cells with Parabolic splines

- **Asymptotics :**

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

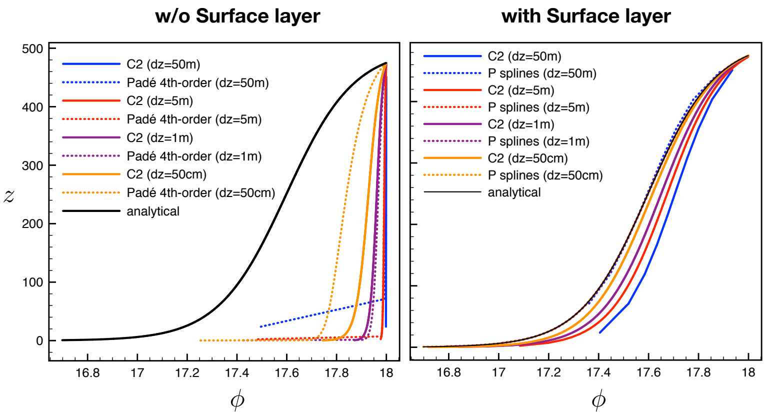
$$\frac{1}{6}d_{5/2} + \frac{5}{6}d_{3/2} + \frac{1}{2}d_{1/2} = \frac{\overline{\phi}_2 - \chi_{\rm sfc}}{h}$$

Unresolved case (for $h \to 0$)

$$\frac{1}{6}d_{5/2} + \underbrace{\left(\frac{1}{3} + \left[1 + \frac{h}{2z_\star}\right]\right) d_{3/2}}_{\frac{5}{6}d_{3/2}+\frac{1}{2}d_{1/2}} = \frac{\overline{\phi}_2 - \chi_{\rm sfc}}{h}$$

Smooth transition between the unresolved and the resolved limit.

A numerical example (with $z_\star = K_{\rm mol}/(\kappa|\phi_\star|)$)



3

Combination with time discretization

Combination with implicit time discretization

Combine Padé-type schemes with implicit Euler :

$$\begin{cases} \alpha d_{k+3/2}^{n+1} + d_{k+1/2}^{n+1} + \alpha d_{k-1/2}^{n+1} = \gamma \dfrac{\overline{\phi}_{k+1}^{n+1} - \overline{\phi}_k^{n+1}}{h} \\ \overline{\phi}_k^{n+1} = \overline{\phi}_k^{n} + \dfrac{\Delta t}{h}\left[K_{k+1/2} d_{k+1/2}^{n+1} - K_{k-1/2} d_{k-1/2}^{n+1}\right] + \Delta t \, \mathrm{rhs}_k \\ \overline{\phi}_{k+1}^{n+1} = \overline{\phi}_{k+1}^{n} + \dfrac{\Delta t}{h}\left[K_{k+3/2} d_{k+3/2}^{n+1} - K_{k+1/2} d_{k+1/2}^{n+1}\right] + \Delta t \, \mathrm{rhs}_{k+1} \end{cases}$$

to end up with the following single tridiagonal problem

$$\begin{aligned} \left(\frac{\alpha}{\gamma} - \frac{K_{k+3/2}\Delta t}{h^2}\right) d_{k+3/2}^{n+1} &+ \left(\frac{1}{\gamma} + 2\frac{K_{k+1/2}\Delta t}{h^2}\right) d_{k+1/2}^{n+1} + \left(\frac{\alpha}{\gamma} - \frac{K_{k-1/2}\Delta t}{h^2}\right) d_{k-1/2}^{n+1} \\ &= \frac{\overline{\phi}_{k+1}^{n} - \overline{\phi}_k^{n}}{h} + \frac{\Delta t}{h}(\mathrm{rhs}_{k+1} - \mathrm{rhs}_k) \end{aligned}$$

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

Temporal discretization for diffusion

Relevant properties for a well-behaved numerical solution

(e.g. **Manfredi & Ottaviani (1999)**; **Wood et al. (2007)**)

- Unconditional stability
- Monotonic damping (damping increases with increasing wavenumber, i.e. $\partial_\theta \mathcal{A} < 0$)
- Non-oscillatory (i.e. $\mathcal{A} \geq 0$)
- Proper control of grid-scale noise $\forall \sigma^{(2)}$

→ Convergence & stability are often not sufficient

Temporal discretization for diffusion

Existing alternatives :

1. Crank-Nicolson : ill-behaved for large time-steps
   $\rightarrow$ short wave-lengths not damped efficiently

2. 2nd-order "Padé" 2-step scheme (e.g **Manfredi & Ottaviani 1999; Wood et al. 2007**) :

$$\begin{cases} (1 + a(K\Delta t)\widetilde{k}^2)\phi^\star = (1 + b(K\Delta t)\widetilde{k}^2)\phi^n \\ (1 + b(K\Delta t)\widetilde{k}^2)\phi^{n+1} = \phi^\star \end{cases} \qquad \begin{aligned} a &= 1 + \sqrt{2}, \\ b &= 1 + 1/\sqrt{2} \end{aligned}$$

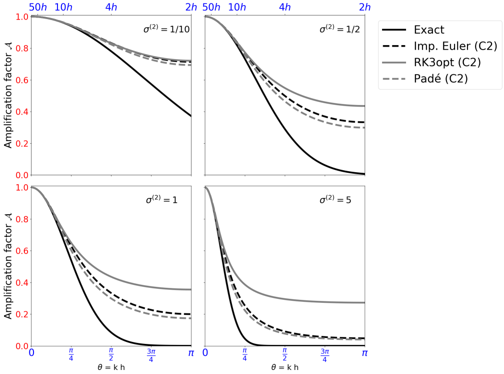
3. Diagonally-implicit RK (e.g **Nazari et al., (2013,2014)**)

$$\begin{cases} \phi^{(1)} = \phi^n + (K\Delta t)\widetilde{k}^2\, a_{11}\phi^{(1)} \\ \phi^{(2)} = \phi^n + (K\Delta t)\widetilde{k}^2(a_{21}\phi^{(1)} + a_{22}\phi^{(2)}) \\ \phi^{(3)} = \phi^n + (K\Delta t)\widetilde{k}^2(a_{31}\phi^{(1)} + a_{32}\phi^{(2)} + a_{33}\phi^{(3)}) \\ \phi^{n+1} = \phi^n + (K\Delta t)\widetilde{k}^2(b_1\phi^{(1)} + b_2\phi^{(2)} + b_3\phi^{(3)}) \end{cases}$$

Temporal discretization for diffusion

Existing alternatives :

2. 2nd-order two-step scheme
3. Diagonally-implicit RK



- Preserves qualitatively the features of the original equation

Temporal discretization with FV Padé scheme

Illustration with implicit Euler scheme :

$$\mathcal{A}(\sigma^{(2)},\theta) = \frac{1+2\alpha\cos\theta}{1+2\alpha\cos\theta+4\gamma\sigma^{(2)}(\sin\frac{\theta}{2})^2}$$

- 2nd-order accurate in space : $\alpha = \dfrac{\gamma-1}{2}$
- $\forall\gamma \neq 0,\ \partial_\theta\mathcal{A} < 0 \ \rightarrow$ non-oscillatory if $\mathcal{A}(\sigma^{(2)},\pi) \geq 0$
- Two possibilities :
  - $\mathcal{A}(\sigma^{(2)},\pi) = 0 \ \rightarrow \ \gamma = 2$
  - 2nd-order in time, 4th-order in space $\rightarrow \ \gamma = \dfrac{6}{5-6\sigma^{(2)}}$

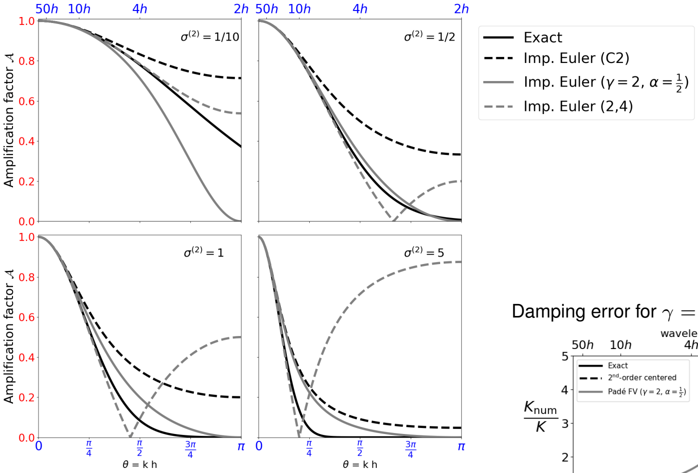
Implicit Euler + C2

$$\mathcal{A} = \frac{1}{1+4\sigma^{(2)}\sin(\theta/2)^2}$$

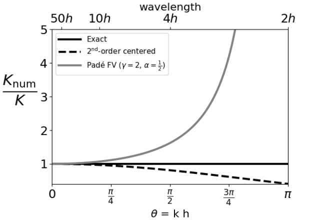
Implicit Euler + Padé FV ($\gamma = 2, \alpha = 1/2$)

$$\mathcal{A} = \frac{1}{1+4\sigma^{(2)}\tan(\theta/2)^2}$$

Temporal discretization for diffusion



Damping error for $\gamma = 2$ and $\alpha = 1/2$



→ Padé FV scheme provides flexibility in the spatial discretization to counteract time discretization errors.

4

Combination with subgrid closure schemes

Mathematical stability of closure models (e.g. Deleersnijder et al., 2009)

- **An example :** analogy with a local Ri-dependent model

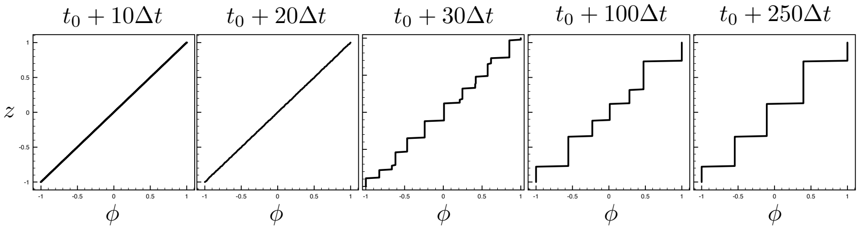
$$\partial_t \phi = \partial_z \left(K(z) \partial_z \phi \right), \qquad K(z) = (\partial_z \phi)^{-2}$$

  - ▷ $K(z) > 0 \;\rightarrow\; \phi$ remains bounded
  - ▷ Original equation can be reexpressed as

$$\partial_t \left(\partial_z \phi \right) = \partial_z \left(\widetilde{K}(z) \partial_z \left(\partial_z \phi \right) \right), \qquad \widetilde{K}(z) = -(\partial_z \phi)^{-2}$$

  $\rightarrow$ the gradient can grow unbounded

- **Numerical test :** $\phi(z, t = 0) = z$, $\phi(z = -1, t) = -1$, $\phi(z = 1, t) = 1$



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  $\rightarrow$ the gradient can grow unbounded

- Ill-behaved solution due to the continuous formulation of the closure model and not to the details of its numerical discretisation

  $\rightarrow$ 0-equation closures are hard to study since it can change the diffusive nature of the equation

- More generally, spurious oscillations generally noticed are of a mathematical or a numerical nature ?

Energetic consistency – mixing terms vs turbulent closure

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

$$\begin{array}{rclcrclcl} \partial_t u - \partial_z (K_m \partial_z u) & = & 0 & \rightarrow & \partial_t \mathrm{KE} - \partial_z (K_m \partial_z \mathrm{KE}) & = & -K_m (\partial_z u)^2 & = & -P \\ \partial_t b - \partial_z (K_s \partial_z b) & = & 0 & & \partial_t \mathrm{PE} - \partial_z ((-z) K_s \partial_z b) & = & K_s \quad \partial_z b & = & -B \end{array}$$

$$\partial_t \mathrm{TKE} - \partial_z (K_e \partial_z \mathrm{TKE}) = P + B - \varepsilon$$

Energy budget in a water column (ignoring the contribution of B.C.) :

$$E = \int_{z_{\mathrm{bot}}}^{z_{\mathrm{top}}} (\mathrm{KE} + \mathrm{PE} + \mathrm{TKE}) dz \qquad \rightarrow \qquad \partial_t E = - \int_{z_{\mathrm{bot}}}^{z_{\mathrm{top}}} \varepsilon dz$$

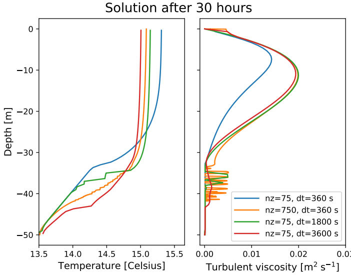
- The discrete counterpart of it tells you exactly how to discretize forcing terms in the TKE equation

Wind-induced deepening of boundary layer

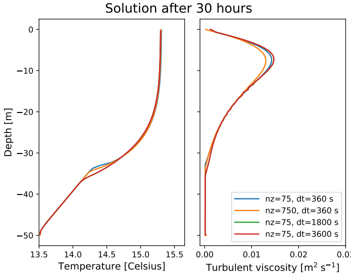
Kato & Phillips : *On the penetration of a turbulent layer into stratified fluid*, J. Fluid Mech., 1969
Price : *On the scaling of stress-driven entrainment experiments*, J. Fluid Mech., 1979

- Single column experiments with 0-equation closure (KPP, Large et al., 1994)
  - Use subgrid reconstruction to detect critical Ri-number
  - ”Energy consistent” discretization of the Richardson number

Standard approach



Implicit Euler + FV Padé ($\alpha = 1/2$, $\gamma = 2$)



Summary

- Padé 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 & Phillips) indicates a reduced sensitivity to numerical parameters

Perspectives

- Nonlinear stability (inputs on known pathological behaviors are welcome)
- Bottom boundary condition
  - Neutral case $\rightarrow$ stratified case
- Single column tests & global ocean simulation within NEMO
- Add representation of oceanic molecular sublayer + MO layer in the top most oceanic grid box for OA coupling purposes (e.g. Zeng & Beljaars, 2005)