pTKE scheme as the extension of the K-diffusion scheme

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About this paper

This mini-documentation focuses to the extension of the Louis type vertical diffusion scheme by the pseudo-prognostic TKE scheme (hereafter pTKE). Hence to provide a complex view to the whole vertical diffusion scheme one should further complete this paper by the documentation of the (K-type) vertical diffusion scheme of ALADIN/ARPEGE physics (Gerard, 1999).

Basis about the pTKE concept

The prognostic TKE equation specifying the diffusion coefficients combined with the diagnostic length scale provides the simplest "higher order" closure with respect to the K-theory for vertical diffusion schemes. Having the prognostic TKE equation a diffusion scheme is provided by non-local turbulence aspects. This has been proven as advantageous for the realism of the turbulence simulation in atmospheric models.

On the other hand the higher sophistication for the turbulent scheme brings some negative drawbacks. Among the others it is namely reduced numerical stability, need for a consistent non-precipitating convection parameterization and sufficient model resolution to outperform first order schemes.

The pTKE tries to offer intermediate (at the moment) solution between the first order approach and the full TKE scheme. It aims to benefit from the both concepts: to keep the well proven NWP skills and stability of the first while extending it towards the non-local aspects by the prognostic TKE quantity. Moreover it still allows to use simple shallow convection parameterizations like the one modifying the Richardson number as proposed by Geleyn (1987). Additionally it offers an elegant and stable way to sequential convergence towards a fully sophisticated TKE scheme.

The current implementation of the pTKE extends the Louis scheme in the following:

- By diagnosing the TKE it keeps history for the diagnostic computation of the exchange coefficients.
- By application of TKE advection and auto-diffusion (along vertical and horizontal) it allows space-consistent variation around the static solution given by Louis scheme.

All this is additionally secured by the anti-fibrillation scheme for the vertical diffusion (Benard et al.,2000) and the extra treatment of the pTKE equation solver preventing TKE from negative values.

Setup level

The pTKE scheme is activated by the logical switch `LPTKE` in the NAMPHY namelist block. The only two tunable parameters are `GAMTKE` (default value is 0.5) and `NUPTKE` (default value is 0.52) belonging to the NAMPHY0 namelist.

As the pTKE scheme provides the TKE prognostic field, the adequate GFL structure has to be properly initialized. The related namelist values should be accessed as the attributes of the `YTKE_NL` field in the namelist block NAMGFL.

Data-flow

The full pTKE equation can be formally written as:

$$\frac{\partial e}{\partial t} + \mathrm{Adv}(e) = \frac{\partial}{\partial z}\left(K_e \frac{\partial e}{\partial z}\right) + \frac{1}{\tau_\epsilon}(\tilde{e} - e)$$

The advection of e is evaluated during the SL computation belonging to the model dynamics. The terms on the right hand side are evaluated in the (over)-implicit manner during the physical parameterization computation. The concerned routines of the model physics are APLPAR, ACCOEFK and ACDIFUS (the first one is calling the other two).

The consequent time-step organization is therefore as follows:

1. The e value of the previous time-step is bounded as $e = \max(e, e_{\min})$ with minimal allowed TKE $e_{\min}$=1.E-8 (hard-coded). This step take place in APLPAR before all the vertical diffusion related computation. (Note that this step is needed to correct resulting e values after advection. Usage of the quasi-monotone SL interpolation makes this procedure unnecessary.)
2. Physics gives the e^+_{phys} guess.
3. After completing the gridpoint dynamics, the final e^+ is obtained by evaluating the advection and horizontal diffusion (in case of active SLHD on e) contributions to e.

Note that at the moment the physics gives directly the tendency of the TKE (`PTENDPTKE`) instead of appropriate fluxes.

ACCOEFK computation related to e

The purpose of this routine is to diagnose the atmospheric static stability, the vertical exchange coefficients K_m and K_h for the Louis diffusion and their relevant diagnosed anti-fibrillation over-explicit weights.

The existence of the pTKE scheme requires computation of two more additional fields: The neutral exchange coefficient K_N and the anti-fibrillation coefficient β_e for the auto-diffusion of e. For computational efficiency reasons (to avoid multiple IF statements inside loop) and rather trivial computation of K_N and β_e both fields are automatically computed even in the case they are not needed (LPTKE=.F.).

The K'_N (`PKNROV`) [1] is evaluated as:

$$K'_N = -\frac{\rho g}{\Delta\phi} K_N = -\frac{\rho g}{\Delta\phi} l_m^2 \left|\frac{\Delta \bar{\mathbf{V}}}{\Delta z}\right| \texttt{ZRRCOR}$$

Here $\bar{\mathbf{V}}$ represents the large scale horizontal flow, Δz represents the layer thickness and `ZRRCOR` stands for the gustiness correction when `LRRGUST`=.T.. (Note that similarly to the other exchange coefficients K'_N is the half-level quantity.)

The anti-fibrillation coefficients for the TKE diffusion β_e (`PXPTKEROV`) are set equal to those of momentum β_m at this stage.

[1] The tilded values of exchange coefficients K' represent their form with dimension [kg m^{-2} s^{-1}] better suited for p-system.

ACDIFUS computation related to e

This routine computes turbulent fluxes according to the K-theory. Here the extra computation related to the pTKE is mostly under the LPTKE switch, thus quite well traceable.

The first step concerns the anti-fibrillation coefficients β_e for the auto-diffusion of e. Consistently with the computation of $\tilde{K}'_*$ (ZKESROV) β_e is computed as:

$$\beta_e = \beta_m{}^{\texttt{GAMTKE}}$$

To avoid the space oscillations caused by the anti-fibrillation scheme, the β_e are additionally secured to be of monotonic vertical profile increasing toward the bottom boundary.

Step two is the preparation and pre-computation of all the necessary half-level quantities needed for evaluation of the pTKE equation or for the subsequent modification of K'_m and K'_h exchange coefficients. Namely, those are:

$$\texttt{ZCONVERT} = -\frac{\rho g}{\Delta\phi} l'_m \nu$$

$$\texttt{ZKESROV} = \tilde{K}'_* = \frac{l'_m}{l_m} K'_N{}^{(1-\texttt{GAMTKE})} K'_m{}^{\texttt{GAMTKE}}$$

$$\texttt{ZTKETILD} = \tilde{e} = \left(\frac{\tilde{K}_*}{\nu l'_m}\right)^2$$

$$\texttt{ZKERV} = K'_e = \begin{cases} \frac{\tilde{K}'_*}{\nu^2} & \text{at first time-step when } e \text{ is not initialized,} \\ \frac{l'_m}{\nu}\sqrt{e} & \text{for all the other cases.} \end{cases}$$

$$\texttt{ZTAUITKE} = \frac{\Delta t}{\tau_\epsilon} = \begin{cases} \Delta t \frac{\nu^2 \tilde{K}_*}{l'^2_m} & \text{at first time-step when } e \text{ is not initialized,} \\ \Delta t \frac{\nu^3}{l'_m}\sqrt{e} & \text{for all the other cases.} \end{cases}$$

In the previous $\nu = \texttt{NUPTKE}$ and l'_m is the modified mixing length avoiding the positive off-diagonal terms in the solver evaluated for a (half) level $\tilde{i}$ as:

$$l'_{m\tilde{i}} = \max\left[l_{m\tilde{i}}, \sqrt{\frac{\nu^4 \beta_\tau}{2g} \frac{\Delta z_{\tilde{i}}}{\beta_{e\tilde{i}} \rho_{\tilde{i}}} \max\left(\frac{\Delta p_i \alpha_i}{\delta_i}, \frac{\Delta p_{i+1}(\delta_{i+1} - \alpha_{i+1})}{\delta_{i+1}}\right)}\right] \quad .$$

Step three is to solve the pTKE equation (Table 1) by elimination. Here subscripts represent the model levels being numbered downwards (1...L) and superscripts the time level (either "+" for $t + \Delta t$ or no superscript for a quantity at the actual model time t). The surface condition is derived from the following identity: $\tilde{e}_{\tilde{L}} = \alpha u*^2 = \frac{1}{\nu^2} u_*^2 = \frac{1}{\nu^2} C_V |\bar{\mathbf{V}}^2|$. Assuming then that mixing length is equal to the one of Ekman layer: $l_m = \kappa(z + z_0)$ and setting $e_L = e_{\tilde{L}}$ one can derive $\frac{1}{\tau_{\epsilon\tilde{L}}}$ similarly to the standard level procedure as: $\frac{1}{\tau_{\epsilon\tilde{L}}} = \frac{\nu^3\sqrt{\tilde{e}_{\tilde{L}}}}{\kappa(z_L + z_0)}$. Note that after the elimination process the PTENDPTKE array contains the e^+ values.

$$
\begin{pmatrix}
1+\frac{g\Delta t}{\delta p_1}\beta_{e\tilde{1}}K'_{e\tilde{1}}+\frac{\beta_\tau}{2}\frac{\alpha_1}{\delta_1}\frac{\Delta t}{\tau_{\epsilon\tilde{1}}} & \frac{g\Delta t}{\delta p_1}\beta_{e\tilde{1}}K'_{e\tilde{1}}-\frac{\beta_\tau}{2}\frac{\alpha_1}{\delta_1}\frac{\Delta t}{\tau_{\epsilon\tilde{1}}} & \cdot & \cdot \\
\frac{g\Delta t}{\delta p_2}\beta_{e\tilde{1}}K'_{e\tilde{1}}-\frac{\beta_\tau}{2}\frac{\delta_2-\alpha_2}{\delta_2}\frac{\Delta t}{\tau_{\epsilon\tilde{1}}} & 1+\frac{g\Delta t}{\delta p_2}(\beta_{e\tilde{1}}K'_{e\tilde{1}}+\beta_{e\tilde{2}}K'_{e\tilde{2}})+\frac{\beta_\tau}{2}(\frac{\delta_2-\alpha_2}{\delta_2}\frac{\Delta t}{\tau_{\epsilon\tilde{1}}}+\frac{\alpha_2}{\delta_2}\frac{\Delta t}{\tau_{\epsilon\tilde{2}}}) & \frac{g\Delta t}{\delta p_2}\beta_{e\tilde{2}}K'_{e\tilde{2}}-\frac{\beta_\tau}{2}\frac{\alpha_2}{\delta_2}\frac{\Delta t}{\tau_{\epsilon\tilde{2}}} & \cdot \\
 & & \ddots & \\
\cdot & \cdot & \cdot & \frac{g\Delta t}{\delta p_{L-1}}\beta_{e\tilde{L}-1}K'_{e\tilde{L}-1}-\frac{\beta_\tau}{2}\frac{\alpha_{L-1}}{\delta_{L-1}}\frac{\Delta t}{\tau_{\epsilon\tilde{L}-1}} \\
\cdot & \cdot & \frac{g\Delta t}{\delta p_L}\beta_{e\tilde{L}-1}K'_{e\tilde{L}-1}-\frac{\beta_\tau}{2}\frac{\delta_L-\alpha_L}{\delta_L}\frac{\Delta t}{\tau_{\epsilon\tilde{L}-1}} & 1+\frac{g\Delta t}{\delta p_L}\beta_{e\tilde{L}-1}K'_{e\tilde{L}-1}+\frac{\beta_\tau}{2}(\frac{\delta_L-\alpha_L}{\delta_L}\frac{\Delta t}{\tau_{\epsilon\tilde{L}-1}}+2\frac{\alpha_L}{\delta_L}\frac{\Delta t}{\tau_{\epsilon\tilde{L}}})
\end{pmatrix}
\cdot
\begin{pmatrix} e_1^+ \\ e_2^+ \\ \vdots \\ e_{L-1}^+ \\ e_L^+ \end{pmatrix} =
$$

$$
\begin{pmatrix}
e_1-\left[\frac{g\Delta t}{\delta p_1}(1-\beta_{e\tilde{1}})K'_{e\tilde{1}}\right](e_1-e_2)-\frac{1-\beta_\tau}{2}\frac{\alpha_1}{\delta_1}\frac{\Delta t}{\tau_{\epsilon\tilde{1}}}(e_1+e_2)+\frac{\alpha_1}{\delta_1}\frac{\Delta t}{\tau_{\epsilon\tilde{1}}}\tilde{e}_1 \\
e_2-\left[\frac{g\Delta t}{\delta p_2}(1-\beta_{e\tilde{1}})K'_{e\tilde{1}}\right](e_2-e_1)-\left[\frac{g\Delta t}{\delta p_2}(1-\beta_{e\tilde{2}})K'_{e\tilde{2}}\right](e_2-e_3)-\frac{1-\beta_\tau}{2}\frac{\delta_2-\alpha_2}{\delta_2}\frac{\Delta t}{\tau_{\epsilon\tilde{1}}}(e_1+e_2)-\frac{1-\beta_\tau}{2}\frac{\alpha_2}{\delta_2}\frac{\Delta t}{\tau_{\epsilon\tilde{2}}}(e_2+e_3)+\frac{\delta_2-\alpha_2}{\delta_2}\frac{\Delta t}{\tau_{\epsilon\tilde{1}}}\tilde{e}_1+\frac{\alpha_2}{\delta_2}\frac{\Delta t}{\tau_{\epsilon\tilde{2}}}\tilde{e}_2 \\
\vdots \\
e_{L-1}-\left[\frac{g\Delta t}{\delta p_{L-1}}(1-\beta_{e\tilde{L}-2})K'_{e\tilde{L}-2}\right](e_{L-1}-e_{L-2})-\left[\frac{g\Delta t}{\delta p_{L-1}}(1-\beta_{e\tilde{L}-1})K'_{e\tilde{L}-1}\right](e_{L-1}-e_L)-\frac{1-\beta_\tau}{2}\frac{\delta_{L-1}-\alpha_{L-1}}{\delta_{L-1}}\frac{\Delta t}{\tau_{\epsilon\tilde{L}-2}}(e_{L-2}+e_{L-1}) \\
\qquad -\frac{1-\beta_\tau}{2}\frac{\alpha_{L-1}}{\delta_{L-1}}\frac{\Delta t}{\tau_{\epsilon\tilde{L}-1}}(e_{L-1}+e_L)+\frac{\delta_{L-1}-\alpha_{L-1}}{\delta_{L-1}}\frac{\Delta t}{\tau_{\epsilon\tilde{L}-2}}\tilde{e}_{L-2}+\frac{\alpha_{L-1}}{\delta_{L-1}}\frac{\Delta t}{\tau_{\epsilon\tilde{L}-1}}\tilde{e}_{L-1} \\
e_L-\left[\frac{g\Delta t}{\delta p_L}(1-\beta_{e\tilde{L}-1})K'_{e\tilde{L}-1}\right](e_L-e_{L-1})-\frac{1-\beta_\tau}{2}\frac{\delta_L-\alpha_L}{\delta_L}\frac{\Delta t}{\tau_{\epsilon\tilde{L}-1}}(e_{L-1}+e_L)-(1-\beta_\tau)\frac{\alpha_L}{\delta_L}\frac{\Delta t}{\tau_{\epsilon\tilde{L}}}e_L+\frac{\delta_L-\alpha_L}{\delta_L}\frac{\Delta t}{\tau_{\epsilon\tilde{L}-1}}\tilde{e}_{L-1}+\frac{\alpha_L}{\delta_L}\frac{\Delta t}{\tau_{\epsilon\tilde{L}}}\tilde{e}_L
\end{pmatrix}
$$

Table 1: Matrix form of the discretized pTKE equation

Next step (step four) is to update the exchange coefficients K'_m and K'_h of the Louis scheme according the e^+ values. Knowing that $K'_m = \nu^2 K'_e$ the updated value of K'_m (ZKURV) is computed as:

$$K'_m = -\frac{\rho g}{\Delta\phi} l'_m \nu \sqrt{\left.\frac{e_i^+ + e_{i+1}^+}{2}\right|_{\tilde{i}}}$$

The updated value of the thermal exchange coefficient K'_h (used for diffusion of dry static energy ZKSRV and moisture ZKQRV) is accordingly derived from K'_m by keeping the proportion of the original coefficients $\tilde{K}'_m$ and $\tilde{K}'_h$ as diagnosed by the ACCOEFK routine computation:

$$K'_h = K'_m \frac{\tilde{K}'_m}{\tilde{K}'_h} \quad .$$

Last step before leaving the ACDIFUS routine is to save the updated exchange coefficient K'_m and K'_h and to replace the e^+ values of the PTENDPTKE array by the e tendencies:

$$\texttt{PTENDPTKE} = \frac{e^+ - e}{\Delta t}$$

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