

‘ACDIFUS_prog’ (or ‘pseudo-TKE’) and its ingredients

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A) What is the aim of the method?

- Starting from the usual ‘static’ exchange coefficients obtained by the ‘Louis’ technique within the ACCOEFK routine, we are searching a method of evolution of a prognostic TKE E which gives in return an equilibrium position corresponding to the said coefficients but which also allows for space-consistent time variations around it. The whole procedure symbolically reads:

$$\tilde{K}_m(ACCOEFK), \tilde{K}_n(ACCOEFK) \Rightarrow \tilde{K}_* \Rightarrow \tilde{E}, K_E, \tau_\varepsilon$$

$$dE/dt = f(E, \tilde{E}, K_E, \tau_\varepsilon)$$

$$E \Rightarrow K_*$$

$$K_*, \tilde{K}_*, \tilde{K}_m \text{ \& } \tilde{K}_h(ACCOEFK) \Rightarrow K_m \text{ \& } K_h$$

In the above, the tilded values correspond to the static part of the computation and the non-tilded ones correspond to the prognostic aspects. The final K_m (for momentum) and K_h (for energy) vertical exchange coefficients will be those used for the ‘classical’ part of the vertical diffusion computations; for that they simply replace their tilded equivalents, all other things unchanged. K_n represents the vertical exchange coefficients at neutrality, while K_* is an equivalent vertical exchange coefficient chosen in such a way that the relationship between itself and E is as independent as possible of the K_m/K_n (stability dependent) ratio. K_E is the auto-diffusion vertical coefficient for the TKE and τ_ε its dissipation time scale (ratio E/ε of the TKE to its own dissipation rate).

- This rather simple algorithm (where the third line of course uses the inverse operator of that of the first line) will allow to keep results close to that of the current well tuned scheme, while introducing a prognostic component for the TKE (advective + diffusive in the horizontal [SLHD] + auto-diffusive in the vertical). This in fact allows to treat three basic problems in a simplified but still hopefully realistic environment:
 - i. The time stability of the TKE prognostic algorithm at long time steps;
 - ii. The vertical staggering problem between E and the various K values;
 - iii. The anti-fibrillation properties of this pseudo-TKE scheme.

B) Two ‘arbitrary’ choices for keeping simplicity

- For treating all aspects of static stability, we shall simply write:

$$K_m = K_* \cdot (\tilde{K}_m / \tilde{K}_*)$$

$$K_h = K_* \cdot (\tilde{K}_h / \tilde{K}_*)$$

with

$$\tilde{K}_* = R_l \cdot \tilde{K}_n^{1-\gamma} \cdot \tilde{K}_m^\gamma$$

R_l will be defined later (in Section ‘E’). Let us assume for the time being that it is equal to one (which indeed happens in the PBL where most of the TKE exists).

If γ is zero, one computes E as if the atmosphere was neutral and the influence of the stability just comes afterwards from the ‘static’ (tilded) ratios. This solution is stable for E but decouples its computation from the (implicit) buoyancy term. If γ is one, one captures the full spirit of the proposal but the assumption that the stability dependency is everywhere the same is erroneous and leads to some chaotic behaviour for E . The use of some intermediate value for γ allows a good compromise (see below). Once this is done, the problem is reduced to the one for momentum and TKE at an intermediated state between neutrality and the full stability-dependent computation of the ‘static’ K values.

- In this special case, for going from the full TKE formalism to the one corresponding to the ‘static’ computations, we use the method proposed by Redelsperger, Mahé and Carlotti (2001) [thereafter RMC01] for the link between TKE and surface similarity laws. We shall simply arbitrarily extend it to other cases than $l = \kappa z$ for $z \rightarrow 0$ (with κ the von-Karman constant). In such a case, the choice of γ is in fact related to approximations we must do for the so-called ϕ_L & ψ_L functions of RMC01. If we consider them as equal to one-another γ is one, while if we say that their ratio is equal to K_m/K_n γ is zero. Following some additional assumptions (detailed in Annex 1), we elected to have a single $\gamma = 0.5$ value for all the range of stabilities, looking mostly at the problem from the point of view of the near neutral transition regimes.

C) The basic equations for momentum and TKE (using the additional notations of RMC01)

$$\frac{dE}{dt} = A_{dv}(E) + \frac{1}{\rho} \frac{\partial}{\partial z} \rho K_E \frac{\partial E}{\partial z} + \frac{1}{\tau_\varepsilon} (\tilde{E} - E)$$

$$K_* = C_K L_K \sqrt{E} = C_K A_K \frac{l_m}{\kappa} \sqrt{E} \Leftrightarrow \tilde{E} = \left(\frac{\kappa \tilde{K}_*}{C_K A_K l_m} \right)^2$$

$$K_E = \alpha K_*$$

$$\frac{1}{\tau_\varepsilon} = \frac{C_\varepsilon \sqrt{E}}{L_\varepsilon} = \frac{C_\varepsilon \kappa \sqrt{E}}{A_\varepsilon l_m}$$

Here, α , C_K and C_ε are ‘universal’ constants, L_K and L_ε are the related mixing lengths in the sense of a full TKE scheme, not to be confused with the Prandtl-type mixing length for momentum l_m (which corresponds to the one previously used in the computation of the tilded K values). Indeed, RMC01 show that the two types of mixing lengths are proportional to each other near the surface, where one may also assume that $L_K = L_\varepsilon$. Beware that $L_{K/\varepsilon}$ should not be confused with the Monin-Obukhov length scale (a completely different concept this time) which will be noted L_{MO} . Given the first of our two simplifying assumptions of Section ‘B’, the l_h equivalent of l_m (for energy) never appears in the pseudo-TKE algorithm (but it is of course used for the computation of the tilded K values).

In the first of the above equations, the last term represents a simple version of the balance between shear plus buoyancy production/destruction on the one hand and dissipative effects on the other hand. As already mentioned, the Newtonian time scale is chosen to be the one of the dissipation in a full TKE formalism.

It should be mentioned at this point that the method described here is in principle able to mimic any full TKE scheme, but with the advantage of a well defined and stability oriented discretisation. For that we need only two things: an independent definition of L_K and/or L_ε as well as a computation of the last term of the first of the above equations so that its tilded part corresponds to the shear plus buoyancy production/destruction. We shall not come back in this note on this property, but there is here an obvious area of further research as well as a basis for clean comparisons of competing methods.

D) The application of the second ‘arbitrary’ choice

We have (RMC01):

$$A_K = \frac{1}{\sqrt{\alpha}} \frac{\kappa}{C_K} \quad \& \quad A_\varepsilon = \alpha \sqrt{\alpha} \kappa C_\varepsilon$$

and (RMC01 again) we want $A_K = A_\varepsilon$. Then, introducing ν with

$$C_K C_\varepsilon = \frac{1}{\alpha^2} = \nu^4$$

we finally get the very simple set of equations:

$$K_* = \nu l_m \sqrt{E} \quad \Leftrightarrow \quad \tilde{E} = \left(\frac{\tilde{K}_*}{\nu l_m} \right)^2$$

$$K_E = \frac{l_m \sqrt{E}}{\nu} \quad \text{or} \quad K_E = \frac{\tilde{K}_*}{\nu^2}$$

$$\frac{1}{\tau_\varepsilon} = \frac{\nu^3 \sqrt{E}}{l_m} \quad \text{or} \quad \frac{1}{\tau_\varepsilon} = \nu^2 \frac{\tilde{K}_*}{l_m^2}$$

E) Time and space discretisation algorithm

The last two equations are written here in two shapes. This is done in order to symbolically indicate that there were indeed two possible ways of solving the time-loop of the algorithm. It was sure that we should need the new value of E to compute K_* , but whether we should (before that) use the ‘ E ’ information of the past time-step or the ‘ K -tilded’ one of the present time-step for computing the diffusion and Newtonian-relaxation coefficients of the evolution equation for E remained an open question. In fact one could even consider having an iterative (predictor-corrector) step for this aspect with a provisional (predictor) new value of E also used for getting K_E and $1/\tau_\varepsilon$ in the corrector part. The three issues were studied both separately and together and the outcome was unambiguous: an iterative procedure is unnecessary (and even slightly detrimental) and the use of the past E values leads to better stability for both auto-diffusion and Newtonian-relaxation aspects. Hence, only at the first time step is the second version of the above-mentioned equations needed (since one then does not have the guarantee of getting a non-zero historical value of E). Otherwise, one systematically uses the first version of the said equations.

The anti-fibrillation treatment (Bénard, Marki, Neytchev and Prtenjak, 2000) may (our first implementation choice) or may not be associated to the ACCOEFK/ACDIFUS computations for the ‘usual’ prognostic variables, a fact that allows a transparent evaluation of its impact for the diffusive part of a prognostic turbulent scheme, something otherwise quasi-impossible to obtain, to our knowledge. Of course this application involves an approximation since the coefficients are computed for the tilded values and applied together with the non-tilded coefficients, but it is expected that this slight discrepancy will be of little impact compared to the yes/no choice about the anti-fibrillation procedure itself.

Additionally, there is the question whether the (slightly approximated, see above) anti-fibrillation treatment should also be applied to the auto-diffusion process for E , when indeed activated for other variables. The answer is difficult to assess a priori since the Richardson number is not directly dependent on K_E but remains related to it (provided γ is non zero, see above), and this question thus deserves some empirical testing. As first trial we elected to have an amplifying factor (space and time-dependent) β' for K_E equal to the γ power of the one for the momentum diffusion process.

Even if it is not strictly speaking a fibrillation problem, there is also the risk of a stiff behaviour for the Newtonian-relaxation part of the prognostic equation for E . But we are here in a textbook example of the analysis by Kalnay and Kanamitsu (1988) with the P exponent equal to 0.5 (since the inverse Newtonian time scale is proportional to the square root of the TKE). Hence using an over-implicitness factor $\beta=1.5$ everywhere at each time step gives the closest possible solution to the fully implicit scheme, without the complexity of the change of variables of Brinkop and Roeckner (1995).

A staggering problem apparently comes from the $K_{E/*}$ and I_m presence on half levels while E is needed on full levels (for instance in order to be advected like all other prognostic variables). However the problem is symmetric: a (non-advecting) shifted E on half levels would see its relaxation towards its target values becoming straightforward, but the vertical diffusion of this quantity would loose its direct character (one would probably need to vertically interpolate diffusion coefficients and to invent a special treatment at the surface). On the contrary, keeping E on full-levels means: (a) a simple diffusion process alike that for other prognostic variables but (b) the need to get the relaxation for a given layer as the weighted average of two relaxations happening on the bounding half-levels (which is fortunately compatible with the use of a uniform over-implicitness β factor, see above). This obviously means a three-level stencil in the vertical (the E values on the half-levels must also be interpolated -and this gives the I/τ_ε value where needed-) for the matrix of the implicit operator. But the latter is fortunately alike the one of the diffusion operator (except that the signs for the off-diagonal elements are opposite). Furthermore, using (like we elected to do) the same choice (past time step E or tilded K -only for the first time step in the latter case-) for both processes, the said coefficients are proportional to each other (by a factor related to $(\alpha_m/\Delta z)^2$) and one can thus readily verify that the combined matrix is diagonal-dominant and that its solution is linearly stable.

However the staggered Newtonian-relaxation process then possesses a potentially oscillating mode while the diffusion process does not. It was thus found interesting to make sure that the latter is always dominant in term of coefficients (keeping in mind for instance that E may go to zero while K^* cannot). This makes it necessary to impose something proportional to $(\Delta z/\alpha)$ as a minimum value for I_m , this ensuring that the off-diagonal element of the implicit matrix are negative or zero (the computations are detailed in Annex 2). Indeed such a choice was shown to definitely further stabilise the numerical behaviour of the scheme. However the change from I'_m (the value used in ACCOEFK) to the above-defined bounded I_m value does create an inconsistency within the whole scheme. Noting (i) that the inconsistency primarily concerns the 'tilded' relation between the exchange coefficients and the equilibrium position of the TKE and (ii) that K^* (except at the first time step) is only used for computing this equilibrium position, it is easy to solve the problem through the use of the R_l factor which becomes I_m/I'_m whenever this quantity is bigger than one. Indeed this solution keeps the 'targets' for K_m and K_h unchanged and leads to reasonable values of E when the I_m stabilising enhancement is applied (otherwise they become too small).

For all the above reasons it was found that a direct staggering operator with E on full-levels is totally compatible with the spirit of the 'pseudo-TKE' scheme and does not show any sign of worrying numerical behaviour, even at long time-steps. In principle

this should remain true when extending the scope of the method like hinted at in the last paragraph of Section ‘C’ above.

F) Numerical values

Measurements seem to indicate a value of $\nu \approx 0.52$ for the first tuning constant of the scheme, if indeed the hypotheses and simplifications of Annex 1 hold (this meaning a still unique value for ν). Furthermore, following the computations of Annex 2, this 0.52 value leads to $L_{K/\varepsilon} \approx \Delta z$ when the limitation on l_m is applied for a regular vertical discretisation and with $\beta^2=1$. The hypothesis of a minimum value Δz for $L_{K/\varepsilon}$ is something rather common in full TKE schemes, something that creates another bridge between both types of formulation.

As shown in Annex 1, the study of the ϕ_m , ϕ_L and ψ_L expressions of RMC01 suggest that $\gamma = 0.5$ is a justified choice for the second tuning constant of the scheme.

Annex 1

Stability dependency of the tuning of pseudo-TKE

Warnings: (i) the ensuing development does not aim at fitting the graphical expressions shown by RMC01, since the latter are based on MO functions quite differing from those used in the derivation of the Louis-type functions of ACCOEFK; (ii) the two central hypotheses below are however a kind of bridge between both formalisms, even if only around neutrality.

We study now the problem of the stability dependency of the basic equations of pseudo-TKE. If one refers to RMC01, two of them can be written in all generality:

$$K_m = \nu l_m \Phi_L \left(\frac{K_m}{K_n} \right) \sqrt{E}$$

$$\frac{1}{\tau_\varepsilon} = \nu^3 \frac{1}{l_m \Psi_L \left(\frac{K_m}{K_n} \right)} \sqrt{E}$$

If we decide that l_m is not to be dealt with here (for reasons linked to the topic of Annex 2), still in all generality, the idea of a change of variables can be applied to $[K_*, \nu_*]$ with:

$$\nu_* = \frac{\nu}{(\Psi_L)^{1/3}} \quad K_* = \frac{K_m}{\Phi_L (\Psi_L)^{1/3}}$$

Arrived there, and reintroducing the third basic equation, we get (in the time-stepping mode used for all time steps except the first one), and indeed without any need to touch l_m :

$$K_* = \nu_* l_m \sqrt{E} \quad \Leftrightarrow \quad \tilde{E} = \left(\frac{\tilde{K}_*}{\nu_* l_m} \right)^2$$

$$K_E = \frac{l_m \sqrt{E}}{\nu_*}$$

$$\frac{1}{\tau_\varepsilon} = \frac{\nu_*^3 \sqrt{E}}{l_m}$$

Now we shall write (still in the notations of RMC01) $\phi_E \phi_m^2 = g$ and make the two hypotheses (strictly valid only around neutrality but acceptable elsewhere) $f \phi_m = 1$ & $\phi_m^2 = K_n / K_m$.

With this and the RMC01 developed expressions for Φ_L and Ψ_L , one gets:

$$\Phi_L = \frac{1}{\phi_m g^{1/2}} \quad \& \quad \Psi_L = g^{3/2}$$

$$\Rightarrow$$

$$K_* = \sqrt{K_m K_n} \quad (\gamma = 1/2)$$

$$\nu_* = \nu / \sqrt{g}$$

If we follow RMC01: (a) in the stable case $g=1$ so we do not need to make ν a locally dependent parameter; (b) in the unstable case, pushing the above method to its last consequences gives:

$$\nu_* = \frac{\nu}{\left[1 + \delta \left(\sqrt{\frac{K_m}{K_n}} - 1 \right)^{2/3} \right]^{1/2}} \quad \text{with} \quad \delta \approx 0.10$$

For $-z/L_{MO}=1$ (quite unstable) we get $\nu_* \approx 0.89 \nu$ and hence we may continue for the time being with a constant ν and address this additional refinement only at a later stage (see below). But γ really ought to be 0.5 .

All the above development was made with one idea in mind: to get a better justification for the introduction of K_* and to do it without touching l_m . It is interesting that it works so fine (a stability independent value for γ and $\nu_* = \nu$ as an excellent approximation), but it is even more interesting to notice that things would not be so easy to justify with a $[K_*, l_m^*]$ pairing. This is good because we shall indeed need to keep a ‘clean hand’ on l_m for two reasons:

- We want to further experiment with its formulation in a completely independent manner, as hinted at in the last paragraph of Section ‘C’ of the main text.
- As already mentioned, an in depth modification of the role of l_m would interfere in a quite cumbersome way with the development explained in Annex 2.

Finally, coming back to the above analytical development of $\nu_*(\nu)$ (for the unstable case), a direct application together with $\nu_* = \nu$ in the stable case would be contradicting the Louis type computation of tilded K values which has continuity of derivatives across the neutral state. The challenge is thus rather to find a formulation that extends the above equation (or any good approximation of it) to the whole range of K_m/K_n values (our only available measure of stability in the pseudo-TKE formalism), without any divergent behaviour either for high stability cases.

Annex 2

Avoidance of a Lorentz-type spurious vertical mode in the solution of the implicit common algorithm for auto-diffusion and adjustment processes

We want local dominance of the diffusion process with respect to the Newtonian relaxation one, with the consequence that the +/- mode of the latter is sufficiently damped by the former. In numerical terms this corresponds to avoid positive off-diagonal terms in the matrix. This can be fixed by using a MAX(ZLMU,PLMU) rather than PLMU in our computations. The limiting value ZLMU can be prepared from purely geometrical considerations since K_E and l/τ_ε are always proportional to each other.

Given the chosen vertical discretisation, the minimum value for l_m must be the maximum of those obtained for each of the two off-diagonal elements (one for above, one for below, in geometrical terms) and this gives, with the usual IFS/ARPEGE/ALADIN notations for the vertical discretisation, the following:

$$l_{m\tilde{i}}^2(\text{lim}) = \frac{\nu^4 \beta}{2g} \frac{\Delta z_{\tilde{i}}}{\beta'_{\tilde{i}} \rho_{\tilde{i}}} \max\left(\frac{\Delta p_i \alpha_i}{\delta_i}, \frac{\Delta p_{i+1} (\delta_{i+1} - \alpha_{i+1})}{\delta_{i+1}}\right)$$

A rough estimate gives $l_m(\text{lim}) \approx \Delta z/6$ which means that the 'max' between PLMU and ZLMU will not be used in all the part of the vertical where $l \approx \kappa(z+z_0)$, an important fact because this is where we do not want to get away from the RMC01 method. Elsewhere we are rather free to apply this numerical security provided the inconsistency it might have as consequence is avoided through a modified definition of K_* (see main text).