Regional Cooperation for Limited Area Modelling in Central Europe

RC LACE Stay Report

Topic: Solving instabilities of solver in ACDIFV3 routine

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1 Introduction

TOUCANS (Third Order moments Unified Condesation Accounting and N-dependent Solver for turbulence and diffusion) is a compact turbulence parameterization, used in the ALARO-1 physical package [1], [2].

One of its features is the parameterization of third order moments, used to calculate their contribution to turbulent fluxes of total moisture ($\overline{w'q'_T}$) and static energy ($\overline{w'{s'}_{sL}}$) In the code, this calculation is done in the `ACDIFV3` routine. There are known bugs in this routine, which have already been investigated in previous stays [4], [5]. In these stays, some new bugs were also discovered. It was found out that all of these bugs, when corrected, have little impact on results and stability of the solver, except one. The problematic bug is in an auxiliary variable `ZZZ` of the ACDIFV3 routine, which should not be divided by the time step (`TSPHY` in code). When this bug is corrected, the solver becomes unstable and crashes the model after two steps of forecast for all tried cases.

2 State of solver before stay

In the stay in the year 2024 [6], after theory revision, we determined that the solver equations contain a time term A_t, coming from the parameterization of the time derivatives. This term is present in the equations in the documentation [3], but was not included in the code.

After adding the time term to the code and correcting the `ZZZ` bug, the solver was less unstable, but still crashed. After some investigation, the value of TKE was limited from below to 10^{-4} only in ACDIFV3 routine in order to limit magnitude of terms that contain TKE in the denominator. After both corrections, the solver was stable for 24 hours of forecast for a predominantly dry case from 7 Sep 2023 with strong dry convection (dry case).

After the stay, I ran a 72h forecast for the the dry case and also for a moist convective case from 24 June 2022 (moist case) and a case with stable conditions from 11 Nov 2021 (stable case). While the dry case was stable for the whole 72h, unfortunately the moist and stable cases crashed because of numerical instabilities after 11 and 15 hours of forecast, respectively.

After some more code investigation, I found that for the bottom level `KLEV`, equations for the solver were missing a term, which would imply that a variable in the code (`ZXSTAP`, see [5]) is 0 on `KLEV`, although there is no theoretical reason for this to be true. When I included the term in the code, the stability somewhat improved, but forecasts still crashed. This could be linked not just to general numerical instability but also to the fact that nonzero `ZXSTAP` value at level `KLEV` was not included in the algorithm for nonlinear instability protection, because it is not clear how to theoretically include it. It should be investigated further.

3 Investigations during stay

3.1 `ACDIFV3` code and theory revision. First, the whole code of `ACDIFV3` routine was revised and checked against the documentation. The following issues were found:

- In `ACMRIP` routine, there is a local variable `Z2AZ0` corresponding to Q^I (eq. (24) in the documentation), which is coded as $1 - 3\lambda_3 - \lambda_2$, but should be $1 - 3\lambda_3 + \lambda_2$,
- In `ACMRIP` and `ACPTKE` routines, the variable `PTH_FUN` should correspond to T''_h in the documentation, but is actually coded as $\frac{1}{2}T''_h$,
- Additionally, in `ACTPKE`, the variable `PTH_FUN` is multiplied erroneously by a factor `ZTKE_OLAMC3`, corresponding to $\frac{3O_\lambda}{4C_3}$,
- There is a bug in the documentation in eq. (7), where the second term should be divided by e.

When fixed, these bugs had insignificant impact on the results.

In the theory revision, only the derivation of eq. (232)-(238) is not yet done, but will be done after the stay.

3.2 Time term. During the code revision, it was found out that the time term A_t was already coded in `ACDIFV3` routine, by modifying the `ZKTROV` (K''_H variable in documentation), which features in every term on the RHS of the solver equation. However, this A_t was multiplied in the code by an additional factor F_ϵ^{-2} (`PF_EPS` in the code), which we believe is a bug, because in the documentation A_t has no such multiplication. Also, because K''_H in the solver equation is differentiated by $\frac{\partial}{\partial p}$, the vertical dependence of A_t was not taken into account.

In addition, in the A_t that was added in the previous stay, I made a mistake that resulted in A_t time term being effectively multiplied by $\frac{4}{C_\epsilon^2} \sim 6$.

The code was corrected by deleting the newly added A_t, removing the multiplication with F_ϵ^{-2} from the already coded A_t and adding a term corresponding to $\frac{\partial A_t}{\partial p}$ to the RHS of the solver equation. However, this correction did not improve the stability.

Finally it was decided that the time term should not be present in the solver equation at all. There are two main reasons for this decision. The first one is that in the Mellor-Yamada second order system that is solved to get the approximations for the third order moments, the time derivatives are neglected. The second reason is that even though stability improved when the time term was added, the time term was ~ 10x bigger than it should be because of bugs, but the model still crashed after some time. This means that if the RHS of the solver equation is dampened enough, the stability improves, but at the same time, we also dampen the physical contributions to the flux by TOMS.

3.3 Final version of `ACDIFV3` routine. A final version of the `ACDIFV3` routine was then prepared. This version has:

- Refactorized code to remove the C_ϵ and F_ϵ occurrences from the terms where they effectively cancel out - both variables now appear only in the calculation of secure TKE time scale.
- Code was also optimized, local variables were renamed to better reflect what they represent and local variables not used were removed.

- Minor bugs that were already known to exist (as they are mentioned in the documentation [3]) were corrected:
  - The terms `ZTSTAR_TERM3A` and `ZTSTARQ_TERM3A` were divided by F_ϵ instead of F_ϵ^{-2} - corrected by code refactorization,
  - The terms `ZTSTAR2_TERM2` and `ZTSTAR2Q_TERM2`, were multiplied by $\frac{C_\epsilon^2}{4}$ two times instead of one time - corrected by code refactorization,
  - In terms `ZRHSS` and `ZRHSQ`, the second term was multiplied by g^3 instead of g^2.
- New minor bugs that were discovered during code investigation, were also corrected:
  - Term `ZKTROV2Q` was not initialized at the top level.
  - Terms `ZDSLOC` and `ZDQLOC`, representing starting values of δs_{sL} and δq_T for the solver, were initialized inside the solver loop, so they were moved before the solver loop,
  - Lines with the `cheat?` comment that set terms `ZDS` and `ZDQ`, representing current values of δs_{sL} and δq_T in the solver loop to starting values, were removed.
- Corrected **`ZZZ` bug**: The auxilliary variable `ZZZ` used throughout the `ACDIFV3` routine was wrongly divided by time step `TSPHY`.
- Time term was completely removed (both previous implementation inside the `ZKTROV` variable and our new implementation with `ZAT` variable).
- Value of TKE was limited below to 10^{-4} only for the `ACDIFV3` routine.

The final version was then checked against the spectral norms and determined that it was equivalent to the nonrefactorized version.

3.4 MUSC analysis. With the final version of `ACDIFV3`, the 3D model integration blows up after one time step, which happens beacuse of numerical instability of the solver in just a few suspicious points. For this reason, the configuration was tested with MUSC, on idealized cases ARMCU (a shallow convection case [7]) and GABLS1 (a stable boundary case [8]). For these cases, the configuration in MUSC works, so the stability of the model could be analyzed.

First thing we noticed were oscillations in flux Richardson number (Rif) and subsequently F_ϵ everywhere outside the PBL (Fig. 1) even when TOMS were not included. In this region turbulence energies are small but bigger than threshold 10^{-8} (here the threshold is not 10^{-4} because Rif is calculated in `ACMRIP`). These were mitigated by increasing the `ETKE_CRIT` (e_{crit}, see [9]) parameter from 10^{-7} to 10^{-4}, forcing Rif to $\text{Rif}_{max} = 0.3338$ whenever TKE and TTE are smaller than e_{crit}.

After this correction, the values of F_ϵ were sometimes still very high, which was caused by the fact that the lower bound for Rif, Rif_{min} was set to -1000. These values were suppressed by setting Rif_{min} to -3 as in [9]. Correction of both thresholds suppressed the oscillations, but had no significant effect on the results in the PBL.

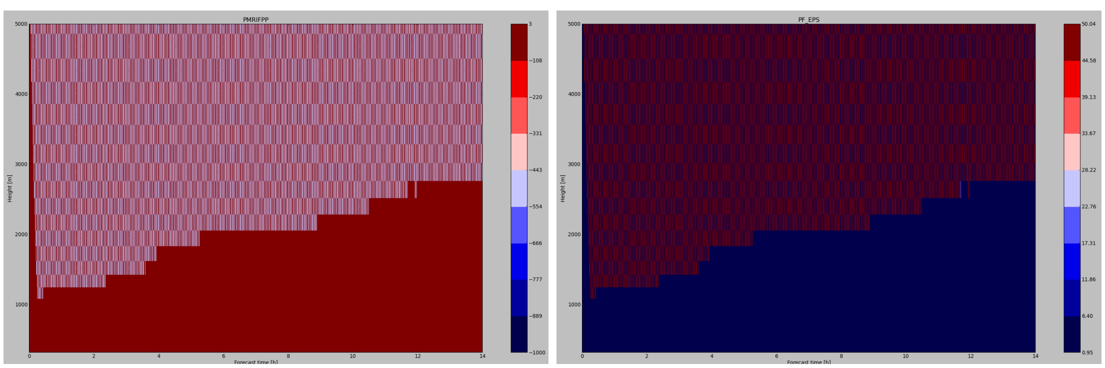

FIGURE 1. Flux Richardson number (left) and F_ϵ (right) for heights up to 5000 m and a 14 hour forecast of ARMCU case with MUSC with 50 s time step and 87 height levels and no TOMS included, showing oscillations above PBL.

After these corrections, we analysed the ARMCU case, where we focused on the total heat flux ($\overline{ws_{sl}}$). With no TOMS, the results are as expected, when the cumulus appears, we get an unstable layer below the cloud layer and a stable layer above. After 8 hours, positive heat flux regions (downward in model convention) appear above the cloud layer at a height of around 2 km (Fig. 2 top).

If we include TOMS, temporal oscillations appear at the top of the positive heat flux regions above the cloud layer (Fig. 2 bottom). These oscillations can be traced to TOMS contributions

(Fig. 3) and again occur in regions where turbulent energies are small. The oscillations do not dissappear even when the time step is decreased to 5 s or increased to 200 s.

As for the general behaviour of the TOMS contributions, we can see by comparing Figs. 2 and 3 that they have a mostly counter gradient effect (TOMS contribution in Fig. 3 has typically an opposite sign that the down gradient flux in top panel of Fig. 2) and are active around the height of 1 km at the cloud layer, which is an expected behaviour. At some points, they can attain values of around $40W/m^2$ and even dominate the total flux.

3.5 Conclusions and future work. Unfortunately there was no time left to thoroughly analyse the reason for the oscillations in the heat flux caused by the TOMS contributions, which are likely also linked to the crash of the 3D model, but I will continue the analysis from Slovenia.

Ideas for further investigation are:

- Analyse the solver matrix, that can be positive definite (invertible), but still ill-conditioned,
- continue the MUSC analysis of several `ACDIFV3` variables (moisture flux, cloud layer, flux Richardson number, TKE, ...), which is not yet done,
- compare the MUSC results with LES results (from Ivan Baštak Duran).
- In the 3D model, analyse interaction with dynamics,
- in the 3D model, suppress the TOMS contributions at higher levels, as difficulties could arise from strong gradients in the tropopause region,
- check the code for bugs also in other routines, as bugs were already found there,
- finish the checking of theoretical derivation in the documentation,
- determine how to include the missing term on `KLEV` in the algorithm for protection against nonlinear instability.

The main conclusion of the stay is that the code of `ACDIFV3` is no longer the reason for numerical instabilities anymore as it is completely debugged. The reason is most probably an inherent numerical instability in the solver, most likely occuring in the regions above PBL where turbulent energies are small, which is not yet understood and taken care of. The

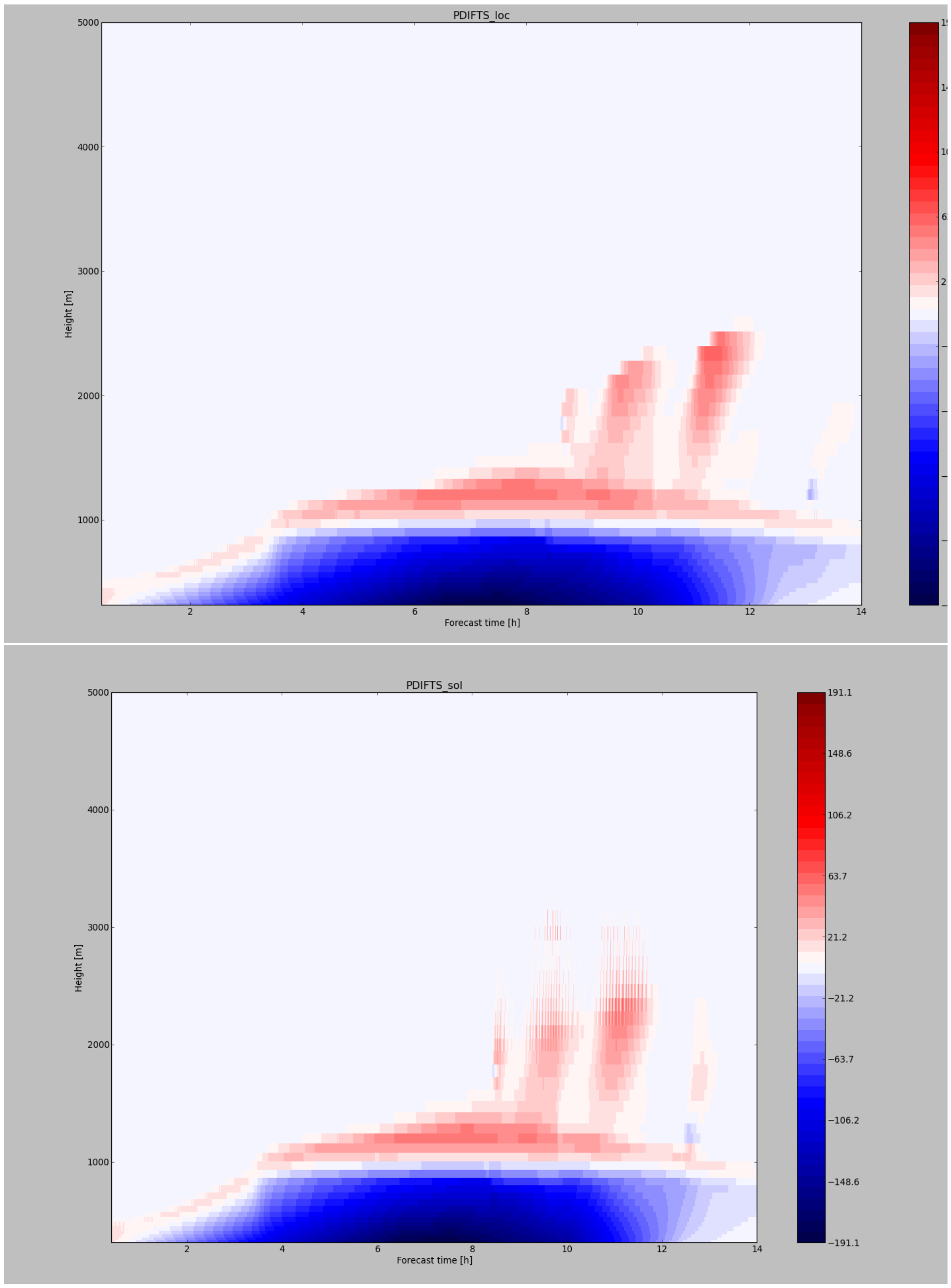

FIGURE 2. Total heat flux $\overline{ws_{sl}}$ (positive downwards) with no TOMS (top) and with TOMS (bottom) for heights up to 5000 m and a 14 hour forecast of ARMCU case with MUSC with 50 s time step and 87 height levels.

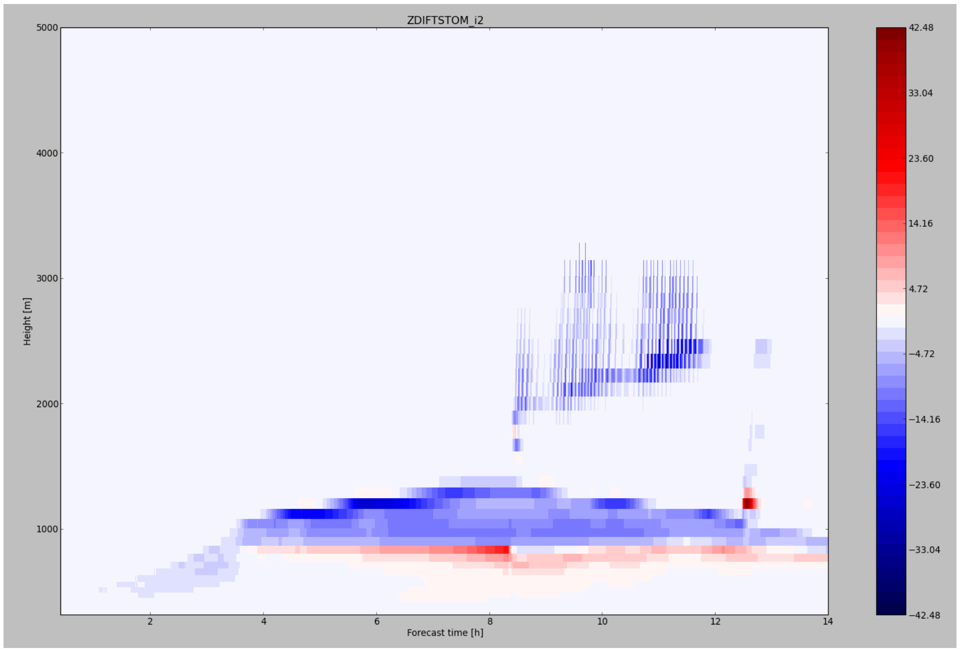

FIGURE 3. TOMS contributions to heat flux $\overline{ws_{sl}}$ (positive downwards) for heights up to 5000 m and a 14 hour forecast of ARMCU case with MUSC with 50 s time step and 87 height levels.

second thing is that with MUSC, we were able to show that the general behaviour of TOMS contributions is as expected, although more analysis is needed.

I want to thank Ján Mašek for many interesting and useful conversations, and Ján and I. Bašták-Ďurán for many ideas on how to proceed further. Thanks also goes to David Němec, who's work on MUSC enabled us to proceed further.

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