Progress in TOMS Stabilization

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Introduction

In TOUCANS, we have an option to include third order moments (TOMS) contributions to turbulent fluxes of heat (static energy) and moisture. These should provide important effects:

- Enhance (or reduce) 2nd order turbulent fluxes,
- maintain turbulent transport in a well-mixed PBL layer below capping cloud layer in no-gradient conditions,
- have a counter-gradient effect that can penetrate layers in an atmospherically stable situation.

Previous status

Routine for TOMS calculation (`ACDIFV3`) had known bugs. If corrected, TOMS solver becomes unstable. In previous stays:

- whole code checked and rederived,
- some more bugs found,
- instability traced to the infamous *ZZZ* bug - an auxiliary variable wrongly divided by timestep.

Suspects:

- wrong *ZZZ* definition,
- nonlinear instability protection algorithm,
- more undiscovered bugs.

After code and theory revision and testing, all disproven.

2nd order moments PBL system

This system is what we want to solve to get $\overline{w\theta}$ (no moisture included!):

$$\frac{\partial \overline{b_{ij}}}{\partial t} + D_{ij} = -P_{ij} + G_{ij} - \Pi_{ij} - \varepsilon_{ij},$$
$$\frac{\partial \overline{q^2}}{\partial t} + D^q = -P^q + G^q - 2\varepsilon,$$
$$\frac{\partial \overline{u_i\theta}}{\partial t} + D_i^\theta = -P_i^\theta + G_i^\theta - \Pi_i^\theta,$$
$$\frac{\partial \overline{\theta^2}}{\partial t} + D^\theta = -P^\theta - \varepsilon^\theta,$$

$b_{ij} = (\overline{u_i u_j} - \frac{1}{3}\delta_{ij}\overline{q^2})$ - Reynolds stress anisotropy, $\overline{q^2} = \overline{u_i u_i} = 2TKE$, D - turbulent transport (TOMS), P - mean production, G - buoyancy, Λ - pressure-velocity gradient, ε - dissipation.

System with prognostic *TKE*

Level 2.5 Mellor-Yamada:

$$
\begin{aligned}
\cancel{\frac{\partial \overline{b_{ij}}}{\partial t}} + \cancel{D_{ij}} &= -P_{ij} + G_{ij} - \Pi_{ij} - \varepsilon_{ij}, \\
\frac{\partial \overline{q^2}}{\partial t} + D^q &= -P^q + G^q - 2\varepsilon, \\
\cancel{\frac{\partial \overline{u_i \theta}}{\partial t}} + \cancel{D_i^\theta} &= -P_i^\theta + G_i^\theta - \Pi_i^\theta, \\
\cancel{\frac{\partial \overline{\theta^2}}{\partial t}} + \cancel{D^\theta} &= -P^\theta - \varepsilon^\theta,
\end{aligned}
$$

Downgradient (local) solution: $\overline{w\theta} = -K\frac{\partial \Theta}{\partial z}$, $K = L\sqrt{\overline{q^2}}S_\theta$
L - mixing length, S_θ - stability function

System with prognostic *TKE*, *TPE*

Level 3 MY:

$$
\begin{aligned}
\cancel{\frac{\partial \overline{b_{ij}}}{\partial t}} + \cancel{D_{ij}} &= -P_{ij} + G_{ij} - \Pi_{ij} - \varepsilon_{ij}, \\
\frac{\partial \overline{q^2}}{\partial t} + D^q &= -P^q + G^q - 2\varepsilon, \\
\cancel{\frac{\partial \overline{u_i \theta}}{\partial t}} + \cancel{D_i^\theta} &= -P_i^\theta + G_i^\theta - \Pi_i^\theta, \\
\frac{\partial \overline{\theta^2}}{\partial t} + D^\theta &= -P^\theta - \varepsilon^\theta,
\end{aligned}
$$

Still local solution, with additional TKE/TPE conversion term:

$$
\overline{w\theta} = -K' \frac{\partial \Theta}{\partial z} \left(1 - A \overline{w^2} \frac{TKE}{TPE} \right) = -K'' \frac{\partial \Theta}{\partial z}
$$

System with prognostic *TKE*, *TPE* and TOMS

Level 3.25 (?) MY system:

$$
\begin{aligned}
\cancel{\frac{\partial \overline{b_{ij}}}{\partial t}} + D_{ij} &= -P_{ij} + G_{ij} - \Pi_{ij} - \varepsilon_{ij}, \\
\frac{\partial \overline{q^2}}{\partial t} + D^q &= -P^q + G^q - 2\varepsilon, \\
\cancel{\frac{\partial \overline{u_i \theta}}{\partial t}} + D_i^\theta &= -P_i^\theta + G_i^\theta - \Pi_i^\theta, \\
\frac{\partial \overline{\theta^2}}{\partial t} + D^\theta &= -P^\theta - \varepsilon^\theta,
\end{aligned}
$$

Solved by *Canuto et al. (2005)* for convective case ($\frac{\partial U}{\partial z} = \frac{\partial V}{\partial z} = 0$):

$$
\overline{w\theta} = -K'' \frac{\partial \Theta}{\partial z} + A_1^\theta \frac{\partial \overline{w^3}}{\partial z} + A_2^\theta \frac{\partial \overline{w\theta^2}}{\partial z} + A_3^\theta \frac{\partial \overline{w^2\theta}}{\partial z}
$$

TOMS expressions

$$\overline{w\theta} = -K'' \frac{\partial \Theta}{\partial z} + A_1^\theta \frac{\partial \overline{w^3}}{\partial z} + A_2^\theta \frac{\partial \overline{w\theta^2}}{\partial z} + A_3^\theta \frac{\partial \overline{w^2\theta}}{\partial z}$$

- A_i^θ coefficients are functions of closure constants, mean temperature gradient, TKE and stability functions.
- For TOMS, use approximation by *Canuto et al. (2007)*:

$$\begin{aligned} \overline{w^3} &= -0.06 \frac{g}{\Theta} \tau^2 \overline{w^2} \frac{\partial \overline{w\theta}}{\partial z}, \\ \overline{w\theta^2} &= -\tau \overline{w\theta} \frac{\partial \overline{w\theta}}{\partial z}, \\ \overline{w^2\theta} &= -0.3 \tau \overline{w^2} \frac{\partial \overline{w\theta}}{\partial z}. \end{aligned}$$

TOUCANS

More complex:

- Adds moisture q_T and uses dry static energy instead of temperature (s_{sL}) - more equations,
- has a specific closure which eliminates critical Richardson number,
- $A_i^{s_{sL}}$ and $A_i^{q_T}$ have more complex expressions, due to moisture addition,
- TOMS approximations are adapted to include moisture,
- Equations for $\overline{ws_{sL}}$ and $\overline{wq_T}$ are coupled.

Discretize prognostic equations in time, and where needed, average terms from full to half levels or vice versa. Finally use local solutions (without TOMS) in some terms (to simplify the solving).

Solver equations

TOMS contribution to dry static energy and moisture (δs_{sL}^{+}, δq_{T}^{+}):

$$\frac{\delta s_{sL}^{+[i+1]}}{\delta t} = \frac{1}{1+\frac{A^t}{\delta t}}\frac{\partial}{\partial p}\Bigg[\Big(-g\rho K''(1-\frac{T''T_{**}^{s_{sL}}}{\delta t})\Big)\frac{\partial \delta s_{sL}^{+[i+1]}}{\partial z} + \rho K''T''\Big(\widehat{T_*^{-1,s_{sL}}\frac{\delta s_{sL}^{+[i+1]}}{\delta t}}\Big)-$$

$$-g\rho K''\frac{T''T_{**}^{s_{sL}}}{\delta t}\frac{\partial(s_{sl}^{loc}-s_{sL}^{-})}{\partial z} + \rho K''T''\Big(\widehat{T_*^{-1,s_{sL}}\frac{(s_{sl}^{loc}-s_{sL}^{-})}{\delta t}}\Big)-$$

$$-g\rho K''\frac{T''T_{cr}^{sq}}{\delta t}\frac{\partial(\overbrace{K_{cr}^{sq}}e_k(q_T^{+[i]}-q_T^{-}))}{\partial z}\Bigg],$$

$$\frac{\delta q_{T}^{+[i+1]}}{\delta t} = \frac{1}{1+\frac{A^t}{\delta t}}\frac{\partial}{\partial p}\Bigg[\Big(-g\rho K''(1-\frac{T''T_{**}^{q_T}}{\delta t})\Big)\frac{\partial \delta q_{T}^{+[i+1]}}{\partial z} + \rho K''T''\Big(\widehat{T_*^{-1,q_T}\frac{\delta q_{T}^{+[i+1]}}{\delta t}}\Big)-$$

$$-g\rho K''\frac{T''T_{**}^{q_T}}{\delta t}\frac{\partial(q_{T}^{loc}-q_{T}^{-})}{\partial z} + \rho K''T''\Big(\widehat{T_*^{-1,q_T}\frac{(q_{T}^{loc}-q_{T}^{-})}{\delta t}}\Big)-$$

$$-g\rho K''\frac{T''T_{cr}^{qs}}{\delta t}\frac{\partial(\overbrace{K_{cr}^{qs}}e_k(s_{sL}^{+[i]}-s_{sL}^{-}))}{\partial z}\Bigg],$$

Newly discovered bug

A new bug discovered in 2024: A^t term is missing in the solver code:

$$\frac{\delta s_{sL}^{+[i+1]}}{\delta t} = \frac{1}{1 + \frac{A^t}{\delta t}} \frac{\partial}{\partial p}\Bigg[\Big(- g\rho K''(1 - \frac{T'' T_{**}^{s_{sL}}}{\delta t})\Big)\frac{\partial \delta s_{sL}^{+[i+1]}}{\partial z} + +\rho K'' T''\Big(\widehat{T_*^{-1,s_{sL}} \frac{\delta s_{sL}^{+[i+1]}}{\delta t}}\Big) -$$

$$- g\rho K'' \frac{T'' T_{**}^{s_{sL}}}{\delta t}\frac{\partial (s_{sl}^{loc} - s_{sL}^{-})}{\partial z} + \rho K'' T''\Big(\widehat{T_*^{-1,s_{sL}} \frac{(s_{sl}^{loc}} - s_{sL}^{-})}{\delta t}\Big) -$$

$$- g\rho K'' \frac{T'' T_{cr}^{sq}}{\delta t}\frac{\partial (\overbrace{K_{cr}^{sq}} e_k(q_T^{+[i]} - q_T^{-}))}{\partial z}\Bigg],$$

$$A^t = -\overbrace{K'' T'' \hat{e}_k^{-1}} > 0.$$

Very important, as it multiplies the whole equation and is always positive and thus reduces the RHS, contributing to stability.

New discovered bug - code

Rewrite solver equation with variables from the code:

$$\mathtt{ZN1} = \frac{1}{1+\mathtt{ZAT}}\Big[\mathtt{ZIPOI}\Delta\big(\mathtt{ZKTROV2}\frac{\Delta\mathtt{ZN1}}{\Delta z}\big) + \mathtt{PRDELP}\Delta\big(2\mathtt{ZZZ}(\widehat{\mathtt{ZTSTAR}\cdot\mathtt{ZN1}})\big) + \mathtt{ZSCG0}\Big]$$

After discretization in height levels, for j-th level (using short notation):

$$X_j\Big[1 + A_j^t/\delta t + Z_j(K_{j-1}+K_j) + P_j(T_j^+ - T_j^-)\Big] +$$
$$X_{j-1}\Big[-Z_jK_{j-1} + P_jT_{j-1}^-\Big] + X_{j+1}\Big[-Z_jK_j - P_jT_{j+1}\Big] = S_j$$

$X = \mathtt{ZN1}$, $Z = \mathtt{ZIPOI}$, $K = \mathtt{ZKTROV2}$, $P = \mathtt{PRDELP}$, $T^+ = \mathtt{ZZZ}|\mathtt{ZTSTAR}|$,
$T^- = -\mathtt{ZZZ}|-\mathtt{ZTSTAR}|$, $S = \mathtt{ZSCG0}$.

Solver stability

Gaussian elimination of tridiagonal matrix:

$$\begin{bmatrix} \ddots & & & & \\ & a_j & b_j & c_j & \\ & & & \ddots & \end{bmatrix} \begin{bmatrix} \vdots \\ X_j \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ S_j \\ \vdots \end{bmatrix},$$

$$a_j = -Z_j K_{j-1} + P_j T^-_{j-1}, \quad c_j = -Z_j K_j - P_j T^+_{j+1},$$

$$b_j = 1 + A^t_j/\delta t + Z_j(K_{j-1} + K_j) + P_j(T^+_j - T^-_j).$$

$$A^t_j, Z_j, K_j, P_j, T^+_j > 0, \quad T^-_j < 0$$

Algorithm is stable if the matrix is positive definite:

$$d_j = |b_j| - |a_j| - |c_j| > 0.$$

As $A^t_j > 0$ and only present in b_j it increases positive definitness and solver stability.

Another correction - TKE limiting

Code tried on a predominantly dry case with strong dry convection (7.9.2023).

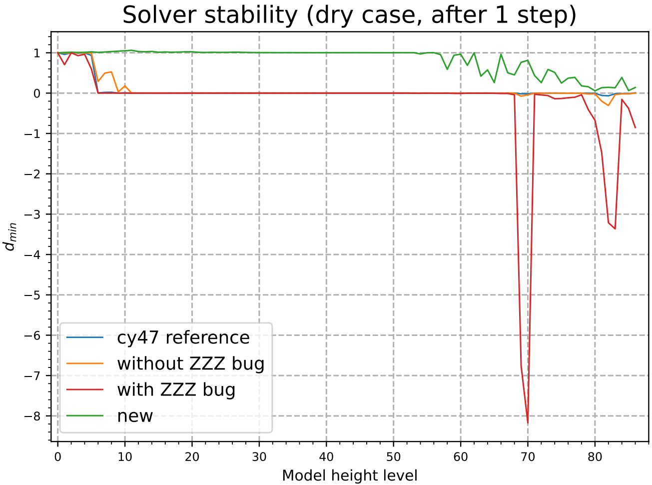
- After A^t addition, algorithm still not stable, but at least runs for more timesteps - debugging possible.
- Instability traced to terms that contain $\frac{1}{TKE}$.
- TKE is generally limited from below to $10^{-8} J$, above terms can attain very large values that cause big jumps in d_j which can drop below 0.

Solution: only in `ACDIVF3` routine, limit TKE from below to $10^{-4} J$.

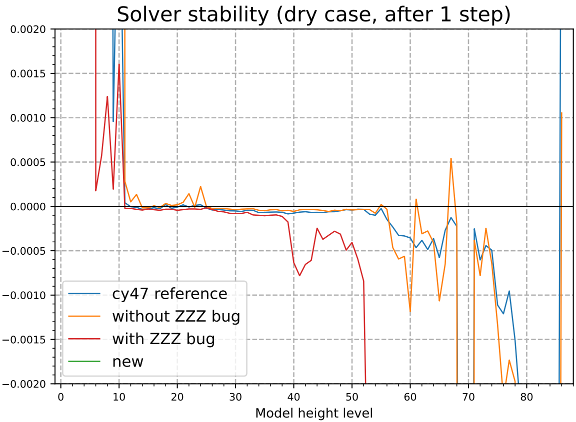
After both corrections, code is numerically stable for 24 hours of forecast. (IMPORTANT: Both corrections have to made for stable code)

Solver positive definitness - comparison at first step

Comparison of minimum value of d for each height level:

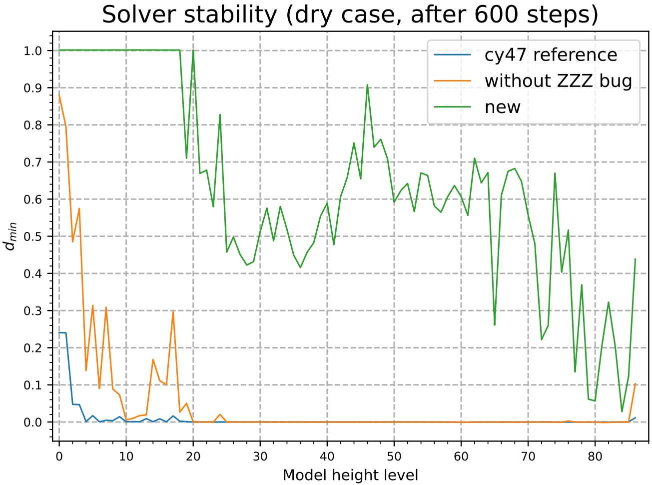


Solver positive definitness - comparison at first step

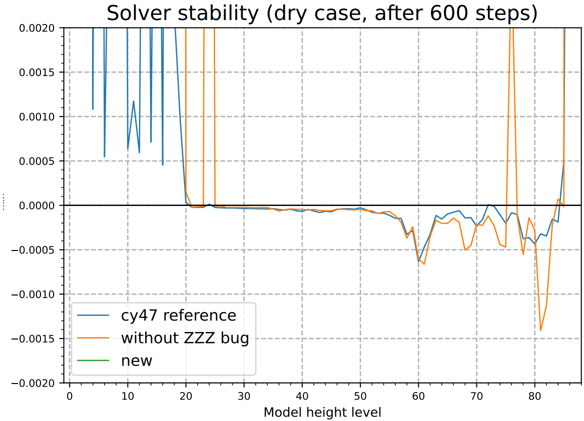


Without the two new corrections, the solver is on the edge of instability even for the reference code from cy47!

Solver positive definitness - comparison at 15:00

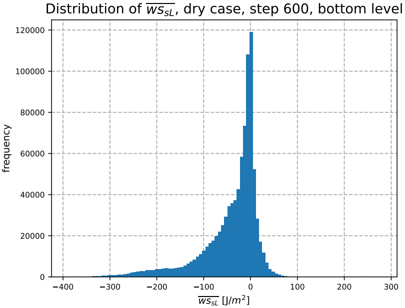


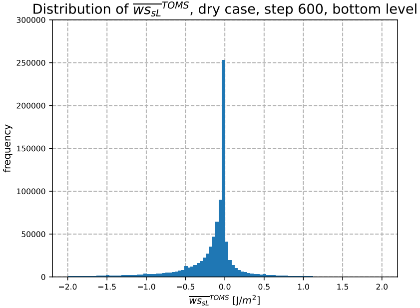
Solver positive definitness - comparison at 15:00



TOMS contribution to s_{sL} flux - distribution

TOMS contribution is about 0.5% of the whole s_{s_L} flux.





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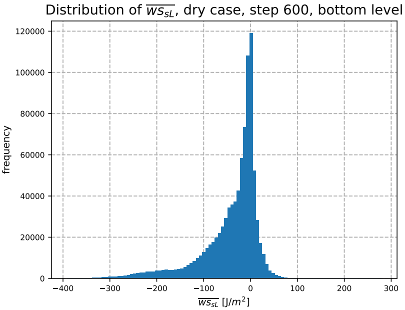

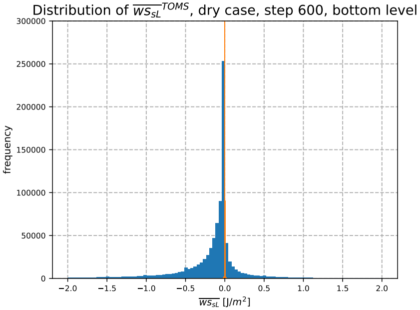

This is however, a big improvement compared to the cy47 reference version.

TOMS contributions s_{sL} flux - field

A local systematic effect of around 50 J$/m^2$:

Remaining instability

- Ran a 72 hour forecast with new code for three cases - a dry case with strong convection, a moist convective case and an atmosphericaly stable case.
- Dry case is stable, moist case crashes after 11 hours and stable case crashes after 15 hours.
- This remaining instability not yet properly investigated.
- One possibility is that the solver code is not correctly written for the lowest level - cases run longer if it is corrected - however, the nonlinear stabilization algorithm has to be changed - not yet known how.

To Do

- Try running cases with single precision code,
- more thorough investigation of various variables in `ACDIFV3`,
- figure out how to correct the nonlinear stabilization algorithm for lowest level,
- look for bugs at other routines that `ACDIVF3` depends on,
- revision of theory - ongoing (about 50 % done),
- run LES simulations (a student at ARSO will work on this for his masters degree).

At least some things will be done at a stay in Prague in April.