Technical description of turbulent schemes in ICON-AES and ICON-LEM

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1 Introduction

This document explains in detail the formulations of two turbulent schemes in (ICOsahedral Nonhydro-static) ICON models: Total turbulent energy (TTE) scheme in ICON-AES and 3D Smagorinsky turbulent scheme in ICON-LEM. Their locations in the model codes are also provided.

2 ICON-AES: total turbulent energy (TTE) scheme

Total turbulent energy turbulent scheme was implemented into ICON-AES by Felix Pithan and Thorsten Mauritsen in 2016. This chapter will provide description of TTE scheme based on the codes and Louis (1979), Brinkop and Roeckner (1995), Mauritsen et al. (2007), Zilitinkevich et al. (2007), Angevine et al. (2010), Wan (2011), and Pithan (2014). These references will be referred as L79, BR95, M07, Z07, A10, W11, and P14 for the convenience.

2.1 Atmosphere process

Detail descriptions of exchange coefficient in atmosphere (from $k = 1$ to $k = $ nlev) are provided in this section, where nlev is the lowest model level.

All the equations in section 2.1 are in subroutine atm_exchange_coeff of mo_turbulence_diag.f90

2.1.1 Turbulent energies

The TTE scheme prognoses total turbulent energy ($E = E_k + E_p$) rather than turbulent kinetic energy unlike other turbulent prognostic schemes, where E_k is the turbulent kinetic energy and E_p is the turbulent potential energy. The prognostic equation is given by E is given by

$$\frac{DE}{Dt} = \tau \cdot S - \gamma - \frac{\partial F_E}{\partial z} + \begin{cases} 0 & \text{for } N^2 \geq 0 \\ 2\frac{g}{\theta}\overline{w'\theta'} & \text{for } N^2 < 0 \end{cases}, \tag{2.1}$$

from M07 Eq. (4), where τ is the turbulent stress, S is the wind shear and N is the Brunt-Väisälä frequency, $\gamma = \frac{C_\epsilon}{l}E^{3/2}$ is the dissipation rate, C_ϵ is empirical constant, $F_E = -|S|l^2\frac{\partial E}{\partial z}$ is the turbulent flux of total turbulent energy, and l is length scale (mixing length). E without vertical flux is computed using operator splitting method as

$$\frac{\partial E}{\partial t} = \left(\frac{\partial E}{\partial t}\right)_{local} + \left(\frac{\partial E}{\partial t}\right)_{diffusion}, \tag{2.2}$$

where the first term of r.h.s is local process and computed first, and the second term of r.h.s is vertical diffusion process and will be computed using VDIFF module like momentum and dry static. Local process term is given by

$$\left(\frac{\partial E}{\partial t}\right)_{local} = \mathcal{B}\sqrt{E} - \mathcal{C}(\sqrt{E})^3 \tag{2.3}$$

where $\mathcal{B}$ and $\mathcal{C}$ are

i) in stable case ($Ri \geq 0$):

$$\mathcal{B} = K_m\,S^2 \tag{2.4}$$

ii) in unstable case ($Ri < 0$):

$$\mathcal{B} = K_m\,S^2 - 2K_h\,N^2 \tag{2.5}$$

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and

$$\mathcal{C} = \frac{C_\epsilon}{l}. \tag{2.6}$$

Convert Eq. (2.3) into an equation of $\sqrt{E}$

$$\frac{D\sqrt{E}}{Dt} = \frac{\mathcal{B}}{2} - \frac{\mathcal{C}}{2}(\sqrt{E})^2, \tag{2.7}$$

and discretize using implicit time stepping

$$\frac{\sqrt{E^{(*)}} - \sqrt{E^{(t)}}}{\Delta t} = \frac{\mathcal{B}}{2} - \frac{\mathcal{C}}{2}(\sqrt{E^{(*)}})^2. \tag{2.8}$$

Finally, $E^{(*)}$ can be obtained by solving a quadrature equation

$$\sqrt{E^{(*)}} = \frac{-1 + \sqrt{1 + \mathcal{C}\ \Delta t\ \left[\mathcal{B}\Delta t + 2\sqrt{E^{(t)}}\right]}}{\mathcal{C}\ \Delta t} \tag{2.9}$$

from BR95 Eqs. (A3-A10) and W11 section 5.3, where $E^{(*)}$ is E at $t + \Delta t$, after local process, K_m and K_h exchange coefficients for momentum and heat. Then, E is updated once more to get $E^{(t+\Delta t)}$ by solving vertical diffusion process in VDIFF module like momentum and dry static energy in the TTE scheme.

Once total turbulent energy is updated, E_k and E_p are derived from $E^{(*)}$. The E_k and E_p can be obtained from that $E = E_k + E_p$ as follows

i) in stable case ($Ri \geq 0$):

$$E_k = E^{(t)}\left[1 + \frac{Ri}{3Ri + Pr_0}\right]^{-1}, \tag{2.10}$$

and

$$E_p = E_k\left[\frac{Ri}{3Ri + Pr_0}\right], \tag{2.11}$$

ii) in unstable case ($Ri < 0$):

$$E_k = E^{(t)}\left[1 + \frac{Ri}{2Ri - Pr_0}\right]^{-1}, \tag{2.12}$$

and

$$E_p = E_k\left[\frac{Ri}{2Ri - Pr_0}\right], \tag{2.13}$$

based on the relationship

$$\frac{E_p}{E_k} = \begin{cases} \dfrac{Ri}{3 \cdot Ri + Pr_0} & \text{for } Ri \geq 0 \\ \dfrac{Ri}{2 \cdot Ri - Pr_0} & \text{for } Ri < 0, \end{cases} \tag{2.14}$$

from P14 Eq. (5.9) and A10 Eq. (A10), where Ri is moist Richardson number, Pr_0 is turbulent Prandtl number.

2.1.2 Exchange coefficient

The K_m, exchange coefficients for momentum, and K_h, exchange coefficients for heat are derived from different formulas. Which formula will be used is determined by the height where K is computed and convective boundary layer height (h_d). The K_m and K_h are calculated as

i) $z > h_d$:

$$K_m = \frac{f_\tau^2 E_k^2}{C_\epsilon E_k \sqrt{E}/l - \beta f_\theta \sqrt{E_k \sigma_\theta^2}}, \tag{2.15}$$

and

$$K_h = \frac{2f_\theta^2 E_k l}{C_\phi \sqrt{E}}, \tag{2.16}$$

from M07 Eqs. (B1) and (B2),

ii) $z \leq h_d/2$:

$$K_m = \frac{f_{\tau 0}^2}{C_\epsilon} l_c \sqrt{E_k}, \tag{2.17}$$

and

$$K_h = Pr_0^{-1} K_m, \tag{2.18}$$

from A10 Eqs. (A21) and (A22),

iii) $h_d/2 < z \leq h_d$:

$$K_m = \text{Max}\left[\frac{f_\tau^2 E_k^2}{C_\epsilon E_k \sqrt{E}/l - \beta f_\theta \sqrt{E_k}\sigma_\theta^2}, \ \frac{f_{\tau 0}^2}{C_\epsilon} l_c \sqrt{E_k}\right], \tag{2.19}$$

and

$$K_h = \text{Max}\left[\frac{2f_\theta^2 E_k l}{C_\phi \sqrt{E}}, \ Pr_0^{-1} K_m\right], \tag{2.20}$$

if in unstable case ($Ri < 0$), there is one more procedure as

$$K_m = K_m\left[1 - \frac{2cRi}{1 + 3c^2 l^2 \left[\left(\frac{\Delta z}{z} + 1\right)^{1/3} - 1\right]^{3/2} \left[\frac{\sqrt{-Ri}}{(\Delta z)^{3/2}\sqrt{z}}\right]}\right], \tag{2.21}$$

and

$$K_h = K_h\left[1 - \frac{3cRi}{1 + 3c^2 l^2 \left[\left(\frac{\Delta z}{z} + 1\right)^{1/3} - 1\right]^{3/2} \left[\frac{\sqrt{-Ri}}{(\Delta z)^{3/2}\sqrt{z}}\right]}\right], \tag{2.22}$$

from ECHAM6 report Eqs. (2.165) and (2.166), where h_d is defined as the first model level whose dry static energy exceeds that of the lowest model level, f_τ (f_θ) is nondimensional stress (heat flux), C_ϕ ($= C_\epsilon$) is empirical constant related to the turbulence dissipation, l_c is convective length scale in convective condition, β is g/θ_v, $\sigma_\theta^2 = 2E_p\frac{|N^2|}{\beta^2}$ is potential temperature variation, $Pr_0 = K_m/K_h = f_\tau^2/2f_\theta^2$ is turbulent Prandtl number, and $c = 5.0$.

2.1.3 Moist Richardson number

Ri, moist Richardson number can be defined as

$$N^2 = \frac{g}{\theta_v}\frac{A\Delta\theta_L + \theta D\Delta q_t}{\Delta z} \tag{2.23}$$

$$S^2 = \frac{(\Delta U)^2 + (\Delta V)^2}{(\Delta z)^2} \tag{2.24}$$

$$Ri = \frac{N^2}{S^2} \tag{2.25}$$

from BR95 Eq. (11) and M07 Eq. (5), where θ_L is cloud water potential temperature, and q_t is total water content, last two variables are conserved under phase transitions and are defined as

$$\theta_L = \theta - \frac{L_v}{c_p}\frac{\theta}{T}m, \tag{2.26}$$

$$q_t = q + m, \tag{2.27}$$

from BR95 Eqs. (6) and (7), where T is temperature, θ is potential temperature, q is specific humidity and m is cloud water specific humidity (cloud liquid water + cloud ice specific humidity). The coefficients A and D are defined as

$$A = C_f A_s + (1 - C_f)A_u, \quad D = C_f D_s + (1 - C_f)D_u, \tag{2.28}$$

where C_f is cloud cover faction, A_s, A_u, D_s, and D_u are defined as

$$A_s = 1 + 0.61 q_t - \left[\frac{L}{c_p T}(1 + 0.61 q_t) - 1.622 \right] \frac{0.622 \dfrac{L}{R_d T} q_s}{1 + 0.622 \dfrac{L}{R_d c_p T^2} q_s}, \tag{2.29}$$

$$D_s = A_s \frac{L}{c_p T} - 1, \tag{2.30}$$

$$A_u = 1 + 0.61 q, \tag{2.31}$$

$$D_u = 0.61, \tag{2.32}$$

from BR95 Eqs. (8-10), where q_s is saturated specific himidity.

2.1.4 Nondimensional stress and heat flux

Nondimensional stress (f_τ) and heat flux (f_θ) are defined as

i) in stable case ($Ri \geq 0$):

$$f_\tau = \frac{|\tau|}{E_k} = f_{\tau 0} \left(0.25 + \frac{0.75}{1 + 4Ri} \right), \tag{2.33}$$

and

$$f_\theta = \frac{\overline{w\theta}}{\sqrt{E_k \sigma_\theta^2}} = -\frac{f_{\theta 0}}{1 + 4Ri}, \tag{2.34}$$

from M07 Eq. (6) and Mauritsen and Svensson (2007),

ii) in unstable case ($Ri < 0$):

$$f_\tau = f_{\tau 0}, \tag{2.35}$$

and

$$f_\theta = f_{\theta 0}, \tag{2.36}$$

where $f_{\tau 0} = 0.17$, $f_{\theta 0} = -\sqrt{\dfrac{f_{\tau 0}^2}{2 Pr_0}} = -0.1202081528$, and $Pr_0 = 1.0$. (In M07, $Pr_0 = 0.69$ and thus $f_{\theta 0} = -0.145$.)

2.1.5 Length scale

The l, length scale (mixing length) is derived as

$$\frac{1}{l} = \frac{1}{kz} + \frac{f}{C_f \sqrt{f_\tau E_k}} + \frac{N}{C_N \sqrt{f_\tau E_k}}, \tag{2.37}$$

from M07 Eq. (8) and A10 Eq. (A11), where $k = 0.4$ is von Kármán constant, f is the Coriolis parameter, $C_f = 0.185$ and $C_N = 2.0$.

2.1.6 Convective length scale

The l_c, convective length scale is used to define the length scale in convective boundary layer. The l_c is computed as

$$\frac{1}{l_c} = \frac{1}{kz} + \frac{f}{C_f \sqrt{f_\tau E_k}} + \frac{3}{k(h_d - z)} \quad \text{for} \ \ z < h_d, \tag{2.38}$$

from A10 Eq. (A20). The second term of r.h.s. is included in the code, but that is not included in A10 Eq. (A20). In personal conversation with Felix Pithan and Thorsten Mauritsen, they believe eddies in unstable condition should also feel the coriolis force (the second term of r.h.s) like in stable condition. Thus, I leave this as in the code.

2.2 Surface process

Detail descriptions of surface transfer coefficient is provided in this section.
All the equations in section 2.2 are in subroutine sfc_exchange_coeff of mo_turbulence_diag.f90

2.2.1 Turbulent energies

To obtain E, first E_k and E_p are computed as Eqs. (2.10-13) and then E is computed as

i) in stable case ($Ri \geq 0$):

$$E^{(*)} = \left(1 + \frac{E_p}{E_k}\right) \frac{u_*^2}{f_\tau} \tag{2.39}$$

ii) in unstable case ($Ri < 0$):

$$E^{(*)} = \left(1 + \frac{E_p}{E_k}\right) \frac{(u_*^3 + 2l\frac{g}{\theta_v}\overline{w'\theta'})^{2/3}}{f_\tau} \tag{2.40}$$

from P14 Eq. (5.17).

Again, E is updated once more to get $E^{(t+\Delta t)}$ by solving vertical diffusion process in VDIFF module like momentum and dry static energy in the TTE scheme.

2.2.2 Surface transfer coefficient

Surface transfer coefficient for momentum (C_d) and heat (C_h) are defined as

$$C_d = C_{N,d} \cdot f_d, \tag{2.41}$$

and

$$C_h = C_{N,h} \cdot f_h, \tag{2.42}$$

from ECHAM6 report Eq. (2.173) where $C_{N,d}$ and $C_{N,h}$ are surface transfer coefficients in neutral case for momentum and heat, and f_d and f_h are stability functions for momentum and heat.

Both of surface transfer coefficients are suggested as

$$C_{N,d} = \frac{l_s^2}{(f_{sl}\ z_1)^2 \left[\ln\left(\frac{z_1}{z_0}\right)\right]^2}, \tag{2.43}$$

and

$$C_{N,h} = \frac{l_s^2}{(f_{sl}\ z_1)^2 \left[\ln\left(\frac{z_1}{z_0}\right)\right]\left[\ln\left(\frac{z_1}{z_{0h}}\right)\right]} \frac{1}{Pr_0}, \tag{2.44}$$

from M07 Eqs. (9) and (10) and P14 Eqs. (5.15) and (5.16) where z_1 is height of the first model full level, l_s is length scale at the surface, $f_{sl} = 0.4$ is the fraction of the first level height at which the surface fluxes are nominally evaluated, z_0 is roughness length for momentum, and z_{0h} is roughness length for heat.

Both of stability functions can be obtained

i) in stable case ($Ri \geq 0$):

$$f_d = \frac{f_\tau}{f_{\tau 0}}, \tag{2.45}$$

and

$$f_h = \frac{f_\theta}{f_{\theta 0}}\sqrt{\frac{f_\tau}{f_{\tau 0}}}, \tag{2.46}$$

from M07 Eqs. (9) and (10) and P14 Eqs. (5.15) and (5.16)

ii) in unstable case ($Ri < 0$):

$$f_d = \left[1 - \frac{2cRi}{1 + 3c^2 C_{N,d}\sqrt{-Ri\left(\frac{z_1}{z_0} + 1\right)}}\right], \tag{2.47}$$

and

$$f_h = \left[1 - \frac{3cRi}{1 + 3c^2 C_{N,h}\sqrt{-Ri\left(\frac{z_1}{z_{0h}} + 1\right)}}\right], \tag{2.48}$$

from ECHAM6 report Eqs. (2.180) and (2.181) where $c = 5$.

2.2.3 Moist Richardson number

The Ri at surface is determined same as Eq. (2.25) except S. In case of surface S is suggested as

$$S^2 = \frac{(U_1)^2 + (V_1)^2 + (c_w w_*)^2}{z_1^2}, \tag{2.49}$$

from P14 Eq. (5.16) where U_1 and V_1 are wind speed at model full level and $c_w = 0.5$ is the ratio of the mean absolute wind at the first level to the convective velocity scale under free convection.

2.2.4 Surface length scale

The l_s, surface length scale is calculated as
i) in stable case ($Ri \geq 0$):

$$\frac{1}{l_s} = \frac{1}{k f_{sl} z_1} + \frac{f}{C_f \sqrt{f_\tau E_k}} + \frac{N}{C_N \sqrt{f_\tau E_k}} + \frac{3}{k(h_d - f_{sl} z_1)}, \tag{2.50}$$

ii) in unstable case ($Ri < 0$):

$$\frac{1}{l_s} = \frac{1}{k f_{sl} z_1} + \frac{f}{C_f \sqrt{f_\tau E_k}} + \frac{3}{k(h_d - f_{sl} z_1)}. \tag{2.51}$$

There is no reference for equation and it has a terms for unstable condition (the fourth term of r.h.s). In personal conversation with Felix Pithan and Thorsten Mauritsen, they think h_d in stable condition are small enough so including this term does not make big differences from the case that this term is not included.

2.3 Tendency (VDIFF module)

Detail description of momentum (and E) and temperature (and scalar) tendencies are provided in this section. The tendency in ICON-AES is calculated by VDIFF module which is implicit time stepping solver, since turbulent mixing is a very fast process compared to the typical time step used by global hydrostatic models (ECHAM6 report).

2.3.1 Discretization

The tendency of prognostic variable (ψ), which can be momentum (and E) or heat (and scalar), due to turbulent motion is obtained from

$$\begin{aligned}
\left(\frac{\partial \psi}{\partial t} \right)_{turb} &= \frac{\psi_k^{(t+\Delta t)} - \psi_k^{(t)}}{\Delta t} \\
&= -\frac{\partial \overline{w'\psi'}}{\partial p} = \frac{\partial}{\partial p} \left[\rho g K_\psi \left(-\frac{\partial \hat{\psi}}{\partial z} \right) \right].
\end{aligned} \tag{2.52}$$

in subroutine vdiff_tendencies of mo_vdiff_solver.f90

To integrate Eq. (2.52), the model from time instance t to $t + \Delta t$, the r.h.s of Eq. (2.52) has to be evaluated at intermediate time level $\hat{\psi}$ defined by

$$\hat{\psi}_k = \alpha \, \psi_k^{(t+\Delta t)} + (1 - \alpha) \, \psi_k^t, \tag{2.53}$$

where $\alpha = 1.5$ denotes the implicitness factor and follows its value the IFS model of the ECMWF.

After discretization of Eq. (2.52) and substitution of Eq. (2.53) in to Eq. (2.52), we can get

$$-A_{k+1/2} \frac{\hat{\psi}_{k+1}}{\alpha} + B_{k+1/2} \frac{\hat{\psi}_k}{\alpha} - C_{k+1/2} \frac{\hat{\psi}_{k-1}}{\alpha} = \frac{\psi_k^{(t)}}{\alpha}, \tag{2.54}$$

where $A_{k+1/2}$, $B_{k+1/2}$, and $C_{k+1/2}$ are obtained as

$$A_{k+1/2} = \frac{1}{\Delta p_k} \Delta t \alpha g \frac{\rho_{k+1/2} \, K_{\psi,k+1/2}}{z_k - z_{k+1}}, \tag{2.55}$$

$$C_{k+1/2} = \frac{1}{\Delta p_k} \Delta t \alpha g \frac{\rho_{k-1/2} \, K_{\psi,k-1/2}}{z_{k-1} - z_k}, \tag{2.56}$$

$$B_{k+1/2} = 1 + A_{k+1/2} + C_{k+1/2}, \tag{2.57}$$

i) for $k = 1$
$C_{k+1/2}$ should be rewritten as

$$C_{k+1/2} = 0, \tag{2.58}$$

ii) for $k = $ nlev

$A_{k+1/2}$ should be rewritten as

$$A_{k+1/2} = C_\psi \Delta t \alpha \frac{\rho_k}{M_k} \sqrt{(U_1)^2 + (V_1)^2 + (c_w w_*)^2}, \tag{2.59}$$

M_k is air mass $[kg\ m^{-2}]$

in subroutine matrix_setup_elim of mo_vdiff_solver.f90

2.3.2 Tridiagonal matrix

Firstly, $E_{k+1/2}$ and $F_{k+1/2}$ are computed from $k = 1$ to $k = $ nlev as

$$E_{k+1/2} = \frac{A_{k+1/2}}{B_{k+1/2} - C_{k+1/2}\ E_{k-1/2}} \tag{2.60}$$

and in subroutine matrix_setup_elim of mo_vdiff_solver.f90
for $k = $ nlev, in subroutine matrix_to_richtmyer_coeff of mo_vdiff_solver.f90

$$F_{k+1/2} = \frac{\psi_k^{(t)}/\alpha + C_{k+1/2}\ F_{k-1/2}}{B_{k+1/2} - C_{k+1/2}\ E_{k-1/2}}. \tag{2.61}$$

in subroutine rhs_elim of mo_vdiff_solver.f90
for $k = $ nlev, in subroutine matrix_to_richtmyer_coeff of mo_vdiff_solver.f90

Then, $\hat{\psi}_k$ is computed from $k = $ nlev to $k = 1$ as

$$\hat{\psi}_k = E_{k+1/2}\ \hat{\psi}_{k+1} + F_{k+1/2}. \tag{2.62}$$

in subroutine rhs_bksub of mo_vdiff_solver.f90

Finally, $\psi_k^{(t+\Delta t)}$ is calculated using Eq. (2.53) according to $\psi_k^{(t+\Delta t)} = \frac{1}{\alpha}\hat{\psi}_k - \frac{(1-\alpha)}{\alpha}\psi_k^{(t)}$ and the tendency is calculated as $\left(\frac{\partial \psi}{\partial t}\right)_{\text{turb}} = \frac{\psi_k^{(t+\Delta t)} - \psi_k^{(t)}}{\Delta t}$.

3 ICON-LEM: 3D Smagorinsky turbulent scheme

3D Smagrinsky turbulent scheme was implemented into ICON-LEM by Anurag Dipankar in 2013. This chapter will provide description of 3D Smagorinsky turbulent scheme based on the codes and Dipankar et al., 2015. I will refer Dipankar et al. (2015) as D15 for the convenience.

3.1 Atmospheric process

Detail descriptions of exchange coefficient in atmosphere are provided in this section. You can find further detail on grid system in Wan (2009) and Dipankar et al. (2015).

3.1.1 Exchange coefficient

The K_m at grid center and interface level is given by

$$K_m = \lambda^2 \rho |S| \left(1 - \frac{Ri}{Pr}\right)^{1/2} \quad \text{for} \left(1 - \frac{Ri}{Pr}\right) > 0, \tag{3.1}$$

and

$$K_h = \frac{K_m}{Pr}, \tag{3.2}$$

from D15 Eq. (10), where λ is subgrid length scale, $|S| = |D|/\sqrt{2}$, D is shear strain tensor, and $Pr = 0.33333$. There is a comment on K_m in the code: note that the factor $\sqrt{2}$ with λ^2 is considered into the Smagorinsky constant.

in subroutine smagorinsky_model of mo_sgs_turbulence.f90

3.1.2 Richardson number

Richardson number, Ri, is obtained as

$$Ri = \frac{N^2}{S^2}, \tag{3.3}$$

where N^2 and S^2 are

$$N^2 = \frac{g}{\theta_v} \frac{\Delta \theta_v}{\Delta z}, \tag{3.4}$$

in subroutine brunt_vaisala_freq of mo_les_utilities.f90
and

$$S^2 = \frac{D^2}{2}. \tag{3.5}$$

in subroutine smagorinsky_model of mo_sgs_turbulence.f90

3.1.3 Subgrid length scale

The λ subgrid length scale is given by

$$\frac{1}{\lambda^2} = \frac{1}{(C_s \Delta)^2} + \frac{1}{(kz)^2}, \tag{3.6}$$

where $C_s = 0.23$ is Smagorinsky constant and $\Delta = (\Delta x \Delta y \Delta z)^{1/3}$.
in subroutine smagorinsky_model of mo_sgs_turbulence.f90

3.1.4 Shear strain tensor

Shear strain tensor, D, will be suggested this subsection. It is better to define the coordinate system of the ICON before moving on the detail. x_1 is the horizontal axis normal to the triangle edge, x_2 is the horizontal axis to the triangle edge, x_3 is vertical axis (Figs. 1 and 2). Velocity components (v_1, v_2, v_3) increase along with these axises. v_1 is velocity component normal to the triangle edges at triangle edge and full level (can be referred as v_n), v_2 is tangential velocity component at triangle edge and full level (can be referred as v_t), and v_3 is vertical velocity component at triangle center and interface level. Furthermore, I would like to define notations used here. Position letters denote e: triangle edge, v: triangle vertex, c: triangle center, f: full level, and i: interface level (Fig. 1). The arrow on the superscript indicates interpolation from left letter to right letter. Δ operator with subscript indicate difference between the variables at right letter and left letter. Δ_{x_3} operator means difference between the variables at two interface levels. For example, $\Delta_{ab} v_1^{(e \to v)}$ indicates v_1 at b minus v_1 at a and two v_1 are interpolated into triangle vertex from triangle edge before subtraction.

Shear strain tensor is given by

$$\begin{aligned} D_{11} &= 2 \left(\frac{\partial v_1}{\partial x_1} \right) \\ &= 2 \left(\frac{\Delta_{ab} v_1^{(e \to v)}}{\Delta_{ab} x_1} \right), \end{aligned} \tag{3.7}$$

$$\begin{aligned} D_{12} &= \left(\frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1} \right) \\ &= \left(\frac{\Delta_{dc} v_1^{(e \to v)}}{\Delta_{dc} x_2} + \frac{\Delta_{ab} v_2^{(e \to v)}}{\Delta_{ab} x_1} \right), \end{aligned} \tag{3.8}$$

$$\begin{aligned} D_{13} &= \left(\frac{\partial v_1}{\partial x_3} + \frac{\partial v_3}{\partial x_1} \right) \\ &= \left(\frac{\Delta_{x_3} v_1^{(f \to i)}}{\Delta x_3} + \frac{\Delta_{qp} v_3^{(i \to f)}}{\Delta_{qp} x_1} \right), \end{aligned} \tag{3.9}$$

$$D_{21} = D_{12}, \tag{3.10}$$

$$D_{22} = 2\left(\frac{\partial v_2}{\partial x_2}\right)$$
$$= 2\left(\frac{\Delta_{dc}\, v_2^{(e\to v)}}{\Delta_{dc}\, x_2}\right), \tag{3.11}$$

$$D_{23} = \left(\frac{\partial v_2}{\partial x_3} + \frac{\partial v_3}{\partial x_2}\right)$$
$$= \left(\frac{\Delta_{x_3}\, v_2^{(f\to i)}}{\Delta\, x_3} + \frac{\Delta_{dc}\, v_3^{(c\to v)(i\to f)}}{\Delta_{dc}\, x_2}\right), \tag{3.12}$$

$$D_{31} = D_{13}, \tag{3.13}$$

$$D_{32} = D_{23}, \tag{3.14}$$

$$D_{33} = 2\left(\frac{\partial v_3}{\partial x_3}\right)$$
$$= 2\left(\frac{\Delta_{x_3}\, v_3^{(c\to e)}}{\Delta\, x_3}\right), \tag{3.15}$$

$$D^2 = D_{11}^2 + D_{22}^2 + D_{33}^2 + 2\left(D_{12}^2 + D_{13}^2 + D_{23}^2\right), \tag{3.16}$$

from D15 Eqs. (20-28).

in subroutine smagorinsky_model of mo_sgs_turbulence.f90

The subgrid-scale stress tensor is parameterized

$$\tau_{ij} = K_m \left(D_{ij} - \frac{1}{3}\delta_{ij}\sum_{m=1}^{3} D_{mm}\right) \tag{3.17}$$
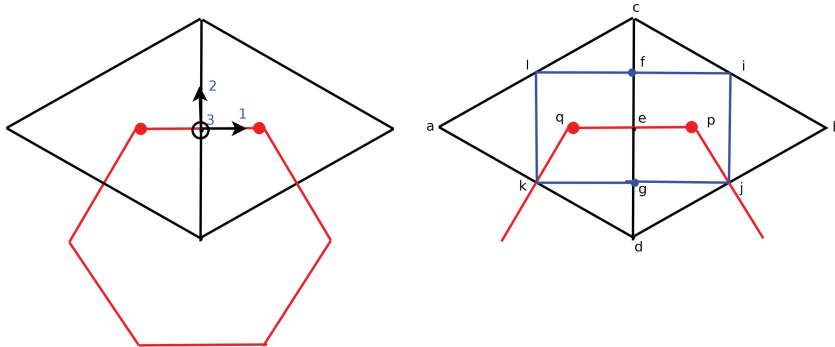

Figure 1: (left) Schematic showing the primal (black triangles) and dual (red hexagons) cells, and the associated local coordinate system. Unit vectors 1, 2, and 3 point in the direction of edge normal, tangent, and vertically upward, respectively. (right) Schematic of two adjacent triangles in ICON grid identifying the various locations used to discretize the turbulent diffusion term. The figure is taken from D15.

3.2 Surface process

There is nothing to describe. Surface sensible heat flux (H), latent heat flux, and friction velocity (u_*) are calculated in simple surface layer scheme.
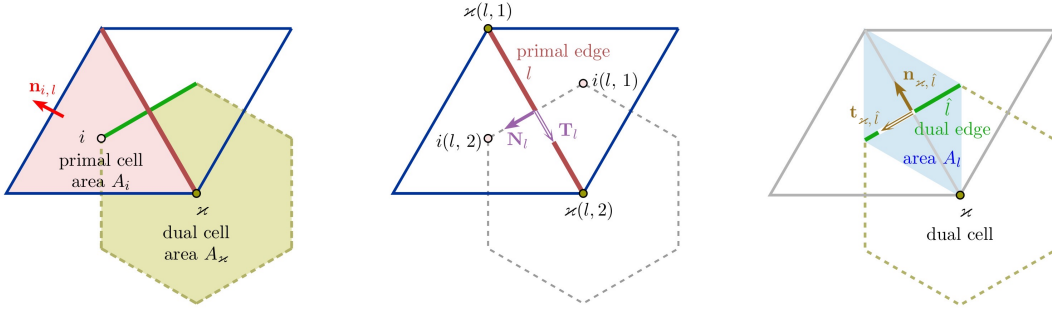
in subroutine surface_condition of mo_surface_les.f90

Figure 2: The primal and dual cells and edges, and the associated unit vectors and areas. The figure is taken from Wan, 2009.

3.3 Tendency

Detail description of momentum and temperature (and scalar) tendencies are described in this section. The tendency in ICON-LEM is derived from horizontal diffusion terms and a vertical diffusion term. The horizontal diffusion is calculated explicitly whereas the vertical diffusion is calculated implicitly. Calculation processes for v_1, v_3, and temperature are different since v_1 is stored at triangle edge and full level, v_3 is stored at triangle center and interface level, and temperature is stored at triangle center and full level. Thus, I separate this section into three subsections.

3.3.1 Normal velocity tendency

Total tendency:

$$\left(\frac{\partial v_1}{\partial t}\right) = \left(\frac{\partial v_1}{\partial t}\right)_{\text{hori,turb}} + \left(\frac{\partial v_1}{\partial t}\right)_{\text{vert,turb}}, \tag{3.18}$$

Horizontal tendency:

$$\left(\frac{\partial v_1}{\partial t}\right)_{\text{hori,turb}} = \frac{1}{\rho}\left(\frac{\partial \tau_{11}}{\partial x_1} + \frac{\partial \tau_{12}}{\partial x_2}\right)$$

$$= \frac{1}{\rho_k^{(c\to e)}}\left(\frac{\Delta_{qp}\ \tau_{11}}{\Delta_{qp}\ x_1} + \frac{\Delta_{gf}\ \tau_{12}}{\Delta_{gf}\ x_2}\right), \tag{3.19}$$

$$\Delta_{qp}\ \tau_{11} = K_m^{(i\to f)}\left[2\left(\frac{\Delta_{eb}\ v_1}{\Delta_{eb}\ x_1}\right) - \frac{2}{3}\text{Div.}\right] - K_m^{(i\to f)}\left[2\left(\frac{\Delta_{ae}\ v_1}{\Delta_{ae}\ x_1}\right) - \frac{2}{3}\text{Div.}\right], \tag{3.20}$$

from D15 Eq. (B1) where Div. $= \frac{1}{2}(D_{11} + D_{22} + D_{33})$ and

$$\Delta_{gf}\ \tau_{12} = K_m^{(c\to v)(i\to f)}\left[\frac{\Delta_{ec}\ v_1}{\Delta_{ec}\ x_2} + \frac{\Delta_{ab}\ v_2}{\Delta_{ab}\ x_1}\right] - K_m^{(c\to v)(i\to f)}\left[\frac{\Delta_{de}\ v_1}{\Delta_{de}\ x_2} + \frac{\Delta_{ab}\ v_2}{\Delta_{ab}\ x_1}\right], \tag{3.21}$$

from D15 Eq. (B2).
in subroutine diffuse_hori_velocity of mo_sgs_turbulence.f90

Vertical tendency (implicit method):

$$\left(\frac{\partial v_1}{\partial t}\right)_{\text{vert,turb}} = \frac{v_1^{(t+\Delta t)} - v_1^{(t)}}{\Delta t}$$

$$= \frac{1}{\rho}\left(\frac{\partial \tau_{13}}{\partial x_3}\right) \tag{3.22}$$

$$= \frac{1}{\rho_k^{(c\to e)}}\left(\frac{\Delta_{x_3}\ \tau_{13}}{\Delta\ x_3}\right),$$

$$\Delta_{x_3}\tau_{13} = K_{m,k-1/2}^{(c\to e)}\left[\frac{\Delta_{x_3}v_1}{\Delta x_3} + \frac{\Delta_{qp}\ v_3}{\Delta_{qp}\ x_1}\right] - K_{m,k+1/2}^{(c\to e)}\left[\frac{\Delta_{x_3}v_1}{\Delta x_3} + \frac{\Delta_{qp}\ v_3}{\Delta_{qp}\ x_1}\right], \tag{3.23}$$

where $v_1^{(t+\Delta t)}$ is v_1 at time $t + \Delta t$. For vertical tendency, implicit method is used. It is noticeable that the implicitness factor, α, is different from that of ICON-AES as $\alpha = 1$ is used here.

After discretization, Eq. (3.22) can be rewritten as

$$A_{k+1/2}\ v_{1,k-1}^{(t+\Delta t)} + B_{k+1/2}\ v_{1,k}^{(t+\Delta t)} + C_{k+1/2}\ v_{1,k+1}^{(t+\Delta t)} = \frac{v_{1,k}^{(t)}}{\Delta t} + \Omega_k, \tag{3.24}$$

where $A_{k+1/2}$, $B_{k+1/2}$, $A_{k+1/2}$, and Ω_k are given by

$$A_{k+1/2} = -\frac{1}{\rho_k^{(c\to e)}\Delta x_3}\frac{K_{m,k-1/2}^{(c\to e)}}{z_{k-1}-z_k}, \tag{3.25}$$

$$C_{k+1/2} = -\frac{1}{\rho_k^{(c\to e)}\Delta x_3}\frac{K_{m,k+1/2}^{(c\to e)}}{z_k-z_{k+1}}, \tag{3.26}$$

$$B_{k+1/2} = \frac{1}{\Delta t} - A_{k+1/2} - C_{k+1/2}, \tag{3.27}$$

$$\Omega_k = \frac{1}{\rho_k^{(c\to e)}\Delta x_3}\left[K_{m,k-1/2}^{(c\to e)}\frac{\Delta_{qp}\,v_{3,k-1/2}}{\Delta_{qp}\,x_1} - K_{m,k+1/2}^{(c\to e)}\frac{\Delta_{qp}\,v_{3,k+1/2}}{\Delta_{qp}\,x_1}\right], \tag{3.28}$$

i) for $k=1$
$K_{m,k-1/2}$ should be rewritten as

$$K_{m,k-1/2}^{(c\to e)} = 0, \tag{3.29}$$

ii) for $k=\text{nlev}$
$K_{m,k+1/2}$ and Ω should be rewritten as

$$K_{m,k+1/2}^{(c\to e)} = 0, \tag{3.30}$$

and

$$\Omega_k = \frac{1}{\rho_k^{(c\to e)}\Delta x_3}\left[K_{m,k-1/2}^{(c\to e)}\frac{\Delta_{qp}\,v_{3,k-1/2}}{\Delta_{qp}\,x_1}\right] - \frac{u_*^2}{\Delta z_{k-1/2}}, \tag{3.31}$$

where u_* is friction velocity.
in subroutine diffuse_hori_velocity of mo_sgs_turbulence.f90

Firstly, $E_{k+1/2}$ and $F_{k+1/2}$ are computed from $k=1$ to $k=\text{nlev}$ as

$$E_{k+1/2} = \frac{C_{k+1/2}}{B_{k+1/2} - A_{k+1/2}\,E_{k-1/2}}, \tag{3.32}$$

and

$$F_{k+1/2} = \frac{v_{1,k}^{(t)}/\Delta t + \Omega_k - A_{k+1/2}F_{k-1/2}}{B_{k+1/2} - A_{k+1/2}\,E_{k-1/2}}. \tag{3.33}$$

Then, $v_{1,k}^{(t+\Delta t)}$ is computed from $k=\text{nlev}$ to $k=1$ as

$$v_{1,k}^{(t+\Delta t)} = -E_{k+1/2}\,v_{1,k+1}^{(t+\Delta t)} + F_{k+1/2}. \tag{3.34}$$

in subroutine tdma_solver of mo_math_utilities.f90

Finally, the tendency is calculated as $\left(\frac{\partial v_1}{\partial t}\right)_{\text{vert,turb}} = \frac{v_1^{(t+\Delta t)} - v_1^{(t)}}{\Delta t}$.

3.3.2 Vertical velocity tendency

Total tendency:

$$\left(\frac{\partial v_3}{\partial t}\right) = \left(\frac{\partial v_3}{\partial t}\right)_{\text{hori,turb}} + \left(\frac{\partial v_3}{\partial t}\right)_{\text{vert,turb}}, \tag{3.35}$$

Horizontal tendency:

$$\left(\frac{\partial v_3}{\partial t}\right)_{\text{hori,turb}} = \frac{1}{\rho}\left(\frac{\partial\tau_{31}}{\partial x_1} + \frac{\partial\tau_{32}}{\partial x_2}\right)$$
$$= \frac{1}{\rho_k^{(f\to i)}}\left(\frac{\Delta_{qp}\,\tau_{31}}{\Delta_{qp}\,x_1} + \frac{\Delta_{gf}\,\tau_{32}}{\Delta_{gf}\,x_2}\right), \tag{3.36}$$

$$\Delta_{qp}\tau_{31} = K_m\left[\frac{v_{1,k-1}^{(e\to c(p))} - v_{1,k}^{(e\to c(p))}}{z_{k-1}-z_k} + \frac{\Delta_{eb}\,v_3}{\Delta_{eb}\,x_1}\right] - K_m\left[\frac{v_{1,k-1}^{(e\to c(q))} - v_{1,k}^{(e\to c(q))}}{z_{k-1}-z_k} + \frac{\Delta_{ae}\,v_3}{\Delta_{ae}\,x_1}\right], \tag{3.37}$$

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$$\Delta_{gf}\tau_{32} = K_m^{(c\to v)} \left[\frac{v_{2,k-1}^{(e\to v(c))} - v_{2,k}^{(e\to v(c))}}{z_{k-1} - z_k} + \frac{\Delta_{ec}\, v_3}{\Delta_{ec}\, x_2} \right] - K_m^{(c\to v)} \left[\frac{v_{2,k-1}^{(e\to v(d))} - v_{2,k}^{(e\to v(d))}}{z_{k-1} - z_k} + \frac{\Delta_{de}\, v_3}{\Delta_{de}\, x_2} \right], \quad (3.38)$$

where $c(p)$ is interpolation to triangle center at p, $c(q)$ is interpolation to triangle center at q, $v(c)$ is interpolation to triangle vertex at c, and $v(d)$ is interpolation to triangle vertex at d.

Vertical tendency (implicit method):

$$
\begin{aligned}
\left(\frac{\partial v_3}{\partial t} \right)_{\text{vert,turb}} &= \frac{v_{3,k-1/2}^{(t+\Delta t)} - v_{3,k-1/2}^{(t)}}{\Delta t} \\
&= \frac{1}{\rho} \left(\frac{\partial \tau_{33}}{\partial x_3} \right) \\
&= \frac{1}{\rho_k} \left(\frac{\tau_{33,k-1} - \tau_{33,k}}{z_{k-1} - z_k} \right),
\end{aligned}
\qquad (3.39)
$$

$$\tau_{33,k-1} - \tau_{33,k} = K_{m,k-1}^{(i\to f)} \left[2 \left(\frac{v_{3,k-3/2} - v_{3,k-1/2}}{z_{k-3/2} - z_{k-1/2}} \right) - \frac{2}{3}\text{Div}_{k-1} \right] - K_{m,k}^{(i\to f)} \left[2 \left(\frac{v_{3,k-1/2} - v_{3,k+1/2}}{z_{k-1/2} - z_{k+1/2}} \right) - \frac{2}{3}\text{Div}_k \right]. \qquad (3.40)$$

After discretization, Eq. (3.39) can be rewritten as

$$A_k\, v_{3,k-3/2}^{(t+\Delta t)} + B_k\, v_{3,k-1/2}^{(t+\Delta t)} + C_k\, v_{3,k+1/2}^{(t+\Delta t)} = \frac{v_{3,k-1/2}^{(t)}}{\Delta t} + \Omega_{k-1/2}, \qquad (3.41)$$

where A_k, B_k, C_k, and $\Omega_{k-1/2}$ are computed as

$$A_k = -2\frac{1}{\rho_k(z_{k-1} - z_k)}\frac{K_{m,k-1}^{(i\to f)}}{\Delta x_3}, \qquad (3.42)$$

$$C_k = -2\frac{1}{\rho_k(z_{k-1} - z_k)}\frac{K_{m,k}^{(i\to f)}}{\Delta x_3}, \qquad (3.43)$$

$$B_k = \frac{1}{\Delta t} - A_k - C_k, \qquad (3.44)$$

$$\Omega_{k-1/2} = -\frac{2}{3}K_{m,k-1}^{(i\to f)}\text{Div}_{k-1} + \frac{2}{3}K_{m,k}^{(i\to f)}\text{Div}_k, \qquad (3.45)$$

i) for $k = 2$
A_k and B_k should be rewritten as

$$A_k = 0, \qquad (3.46)$$

and

$$B_k = \frac{1}{\Delta t} + 2\frac{1}{\rho_k(z_{k-1} - z_k)}\frac{K_{m,k-1}^{(i\to f)}}{\Delta x_3} - C_k, \qquad (3.47)$$

ii) for $k = \text{nlev}$
B_k and C_k should be rewritten as

$$C_k = 0, \qquad (3.48)$$

and

$$B_k = \frac{1}{\Delta t} - A_k + 2\frac{1}{\rho_k(z_{k-1} - z_k)}\frac{K_{m,k}^{(i\to f)}}{\Delta x_3}. \qquad (3.49)$$

in subroutine diffuse_vert_velocity of mo_sgs_turbulence.f90

Firstly, E_k and F_k are computed from $k = 1$ to $k = \text{nlev}$ as

$$E_k = \frac{C_k}{B_k - A_k\, E_{k-1}}, \qquad (3.50)$$

and

$$F_k = \frac{v_{3,k-1/2}^{(t)}/\Delta t + \Omega_{k-1/2} - A_k F_{k-1}}{B_{k+1} - A_{k+1} \, E_{k-1}}. \tag{3.51}$$

Then, $v_{1,k-1/2}^{(t+\Delta t)}$ is computed from $k = \text{nlev}$ to $k = 1$ as

$$v_{3,k-1/2}^{(t+\Delta t)} = -E_k \, v_{3,k+1/2}^{(t+\Delta t)} + F_k. \tag{3.52}$$

in subroutine tdma_solver of mo_math_utilities.f90

Finally, the tendency is calculated by $\left(\frac{\partial v_3}{\partial t}\right)_{\text{vert,turb}} = \frac{v_{3,k-1/2}^{(t+\Delta t)} - v_{3,k-1/2}^{(t)}}{\Delta t}$.

3.3.3 Temperature tendency

Total tendency:

$$\left(\frac{\partial T}{\partial t}\right) = \left(\frac{\partial T}{\partial t}\right)_{\text{hori,turb}} + \left(\frac{\partial T}{\partial t}\right)_{\text{vert,turb}}, \tag{3.53}$$

Horizontal tendency:

$$\left(\frac{\partial T}{\partial t}\right)_{\text{hori,turb}} = -\left(\frac{\partial \overline{v_1'T'}}{\partial x_1} + \frac{\partial \overline{v_2'T'}}{\partial x_2}\right)$$
$$= \left[\nabla_{\text{tri}} \cdot \left(k_h^{(c\to e)} \frac{\Delta_{qp} T_k}{\Delta_{qp} x_1}\right)\right] \phi, \tag{3.54}$$

where ∇_{tri} is divergence at center of the triangular grid, and $\phi = \frac{c_p}{c_v}$ is coupler that converts the temperature tendency for the dynamics.

Vertical tendency (implicit method):

$$\left(\frac{\partial T}{\partial t}\right)_{\text{vert,turb}} = \frac{T_k^{(t+\Delta t)} - T_k^{(t)}}{\Delta t}$$
$$= -\frac{\partial \overline{v_3'T'}}{\partial x_3}$$
$$= \left[K_{h,k-1/2}\frac{T_{k-1} - T_k}{z_{k-1} - z_k} - K_{h,k+1/2}\frac{T_k - T_{k+1}}{z_k - z_{k+1}}\right]\phi. \tag{3.55}$$

After discretization, Eq. (3.55) can be rewritten as

$$A_{k+1/2} \, T_{k-1}^{(t+\Delta t)} + B_{k+1/2} \, T_k^{(t+\Delta t)} + C_{k+1/2} \, T_{k+1}^{(t+\Delta t)} = \frac{T_k^{(t)}}{\Delta t} + \Omega_k \tag{3.56}$$

where $A_{k+1/2}$, $B_{k+1/2}$, $C_{k+1/2}$, and Ω_k are obtained as

$$A_{k+1/2} = -\frac{1}{\Delta x_3}\frac{K_{h,k-1/2}}{z_{k-1} - z_k} \, \phi, \tag{3.57}$$

$$C_{k+1/2} = -\frac{1}{\Delta x_3}\frac{K_{h,k+1/2}}{z_k - z_{k+1}} \, \phi, \tag{3.58}$$

$$B_{k+1/2} = \frac{1}{\Delta t} - A_{k+1/2} - C_{k+1/2}, \tag{3.59}$$

$$\Omega_k = 0, \tag{3.60}$$

i) for $k = 1$
$A_{k+1/2}$ should be rewritten as

$$A_{k+1/2} = 0, \tag{3.61}$$

ii) for $k = \text{nlev}$
$C_{k+1/2}$ and Ω_k should be rewritten as

$$C_{k+1/2} = 0, \tag{3.62}$$

and

$$\Omega_k = \frac{1}{\Delta x_3} H\phi, \tag{3.63}$$

where H is surface sensible heat flux $[Kms^{-1}]$.
in subroutine diffuse_scalar of mo_sgs_turbulence.f90

Firstly, $E_{k+1/2}$ and $F_{k+1/2}$ are computed from $k = 1$ to $k = \text{nlev}$ as

$$E_{k+1/2} = \frac{C_{k+1/2}}{B_{k+1/2} - A_{k+1/2} \; E_{k-1/2}}, \tag{3.64}$$

and

$$F_{k+1/2} = \frac{T_k^{(t)}/\Delta t + \Omega_k - A_{k+1/2} F_{k-1/2}}{B_{k+1/2} - A_{k+1/2} \; E_{k-1/2}}. \tag{3.65}$$

Then, $v_{1,k}^{(t+\Delta t)}$ is computed from $k = \text{nlev}$ to $k = 1$ as

$$T_k^{(t+\Delta t)} = -E_{k+1/2} \; T_{k+1}^{(t+\Delta t)} + F_{k+1/2}. \tag{3.66}$$

in subroutine tdma_solver of mo_math_utilities.f90

Finally, the tendency is calculated by $\left(\frac{\partial T}{\partial t}\right)_{\text{vert,turb}} = \frac{T_k^{(t+\Delta t)} - T_k^{(t)}}{\Delta t}$.

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