Three-Dimensional Planetary Boundary Layer Parameterization for High-Resolution Mesoscale Simulations

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Abstract. Wind energy applications including wind resource assessment, wind power forecasting, and wind plant optimization require high-resolution mesoscale simulations. High resolution mesoscale simulations are essential for accurate characterization of atmospheric flows over heterogeneous land use and complex terrain. Under such conditions, the assumption of grid-cell homogeneity, used in one-dimensional planetary boundary layer (1D PBL) parameterizations, breaks down. However, in most numerical weather prediction (NWP) models, boundary layer turbulence is parameterized using 1D PBL parameterizations. We have therefore developed a three-dimensional (3D) PBL parameterization to better account for horizontal flow heterogeneities. We have implemented and tested the 3D PBL parameterization in the Weather Research and Forecasting (WRF) numerical weather prediction model. The new parameterization is validated using observations from the Wind Forecast Improvement 2 (WFIP 2) project and compared to 1D PBL results.

1. Introduction

In numerical weather prediction (NWP) models, evolution of the flow field including: velocity, potential temperature, moisture and other constituents is represented using Reynolds Averaged Navier-Stokes (RANS) equations. The RANS equations are usually truncated at some higher moments of field variables and therefore do not represent a closed system of equations. In order to close the system of equations it is necessary to provide parameterizations of higher order moments. Until recently, these parameterizations applied to scales of tens of kilometers as NWP models utilized computational grids with grid-cell sizes of ten or more kilometers. Accurate characterization of wind resource and wind power prediction over heterogeneous surfaces and in complex terrain requires resolving land use and terrain effects on the flow. Surface heterogeneity effects need to be resolved with high-resolution numerical grids with grid-cell sizes of one kilometer or less. Such grid scales fall in the range labeled “gray zone” or “Terra Incognita” [1]. Recently, continuous development of high-performance computing (HPC) platforms enabled increased resolution of NWP models and grid-cell sizes below 1 km. In NWP models, turbulent stresses and fluxes are commonly parameterized using 1D PBL parameterizations based on the assumption of horizontal homogeneity and thus do not include horizontal gradients of turbulent stresses and fluxes. If horizontal grid-cell sizes are relatively large (e.g., greater than ten kilometers) this assumption is justified. As the grid-cell size of mesoscale simulations decreases, the assumption of horizontal homogeneity is violated and the effect of horizontal gradients should be accounted for [2]. Recently there were a number of attempts to develop scale aware PBL parameterizations, however they focused on modifying length scales in 1D PBL parameterizations [2,3]. For high-
resolution NWP including wind energy applications we have implemented 3D PBL parameterization in the WRF model.

Improving NWP models in complex terrain requires an improved understanding of flows and processes in complex terrain. High-resolution, high-quality flow observations are essential to achieve a better understanding of flows in complex terrain. However, various terrain-induced flow phenomena represent a challenge not only for wind forecasting, but also for observations and analysis. These phenomena include: mountain waves, topographic wakes, gap flows, cold pools, drainage flows, etc. Until recently, only a few field studies comprehensively addressed complex terrain flow phenomena.

The Wind Forecast Improvement Project 2 (WFIP2) project was designed to provide the observations needed to improve wind forecasting. A 18-month-long observational field study in the Columbia River Gorge area provided a wealth of data for better characterization of the phenomena that undermine wind forecasts [5]. We therefore use the data from the WFIP2 field study to assess the performance of the 3D PBL parameterization.

2. Model Development

We have developed and implemented a 3D PBL parameterization in the WRF model to account for 3D effects on turbulent kinetic energy (TKE) and turbulent stresses and scalar fluxes. The 3D PBL parameterization is an algebraic stress and flux parameterization based on the developments of Mellor and Yamada (1974, 1982) [6,7]. The parameterization involves solving a system of thirteen linear algebraic equations at each grid cell to solve for turbulent stresses and scalar fluxes. Once all six components of turbulent stress and three components of turbulent scalar fluxes are available, the full divergences of stresses and fluxes are computed and added to the right-hand side of prognostic equations for momentum, potential temperature, and water vapor mixing ratio.

The prognostic equations for the mean momentum and potential temperature are:

\[
\frac{\partial V_i}{\partial t} + V_j \frac{\partial V_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} - \frac{\partial (u_i u_j)}{\partial x_j} \tag{1}
\]

\[
\frac{\partial \theta}{\partial t} + V_j \frac{\partial \theta}{\partial x_j} = -\frac{\partial (u_i \theta)}{\partial x_j} \tag{2}
\]

Here, angle brackets denote grid-cell-volume averaging and capital letters denote grid-cell-volume-averaged quantities, \( V_j \) denotes velocity components and, \( \theta \) potential temperature. Lower case letters denote fluctuating quantities, \( u_j \) are fluctuating velocity components, and \( \theta \) is a fluctuating potential temperature. Repeated indices indicate summation. All six components of the symmetric turbulent stress tensor need to be parameterized and a full divergence of the stress tensor computed. Similarly, all three components of the turbulent scalar flux must be parameterized and a full divergence of the flux vector computed. The homogeneity assumption significantly simplifies RANS equations, resulting in equations for horizontal components of velocity of the following form

\[
\frac{\partial V_1}{\partial t} + V_j \frac{\partial V_1}{\partial x_j} = -\frac{\partial P}{\partial x_1} - \frac{\partial (u_1 u_3)}{\partial x_3} \tag{3}
\]

\[
\frac{\partial V_2}{\partial t} + V_j \frac{\partial V_2}{\partial x_j} = -\frac{\partial P}{\partial x_2} - \frac{\partial (u_2 u_3)}{\partial x_3} \tag{4}
\]

\[
\frac{\partial \theta}{\partial t} + V_j \frac{\partial \theta}{\partial x_j} = -\frac{\partial (u_3 \theta)}{\partial x_3} \tag{5}
\]
Under the homogeneity assumption, horizontal gradients of turbulent stresses and fluxes are identically zero. This means that only two components of turbulent stress, \( \langle u_1 u_3 \rangle \) and \( \langle u_2 u_3 \rangle \), and one component of turbulent flux, \( \langle u_3 \theta \rangle \), and their vertical gradients affect the evolution of mean fields. Therefore, 1D PBL parameterizations include only these three terms.

Three-dimensional parameterizations of turbulent stresses and fluxes are commonly used in engineering RANS equations-based model. However, due to large grid-cell aspect ratios previously used in NWP models, horizontal gradients in a boundary layer were many orders of magnitude smaller than vertical gradients. Therefore, the effect of horizontal gradients on boundary layer turbulence development and evolution was neglected. Nevertheless, following development of limited area models in early 1970s Mellor and Yamada [6] outlined a hierarchy of turbulence parameterizations for atmospheric flow simulations that included a fully 3D PBL parameterization. They classified turbulence parameterizations in four levels based on the assumptions made deriving them, with Level 4 representing the full three-dimensional parameterization including prognostic equations for all the second order turbulence moments. In this work we follow the developments of Mellor and Yamada (1982) [7], variants of which were also implemented in the Mellor-Yamada-Nakanishi-Niino (MYNN) PBL parameterization [8–11]. While the MYNN parameterization includes a prognostic equation for TKE, we implemented the Mellor-Yamada [6] Level 2 parameterization that neglects material derivatives of second order moments including the TKE and instead diagnostic equations are provided. In contrast to 1D PBL version of Level 2 parameterization, the horizontal velocity gradients are retained. First, the TKE is computed using a diagnostic equation

\[
\frac{q^3}{\Lambda_1} = -\langle u^2 \rangle \frac{\partial U}{\partial x} - \langle v^2 \rangle \frac{\partial V}{\partial y} - \langle w^2 \rangle \frac{\partial W}{\partial z} - \langle uv \rangle \left( \frac{\partial U}{\partial y} + \frac{\partial V}{\partial x} \right) - \langle uw \rangle \left( \frac{\partial U}{\partial z} + \frac{\partial W}{\partial x} \right) - \langle vw \rangle \left( \frac{\partial V}{\partial z} + \frac{\partial W}{\partial y} \right) - \beta g \langle w \theta \rangle
\]

(6)

Here, \( q \), is twice the TKE, \( \Lambda_1 \) is the length scale (sometimes labeled the “dissipation length scale”), \( \beta \), is the coefficient of thermal expansion, and \( g \) is gravitational acceleration. Once the TKE is diagnosed, second order moments are computed by inverting the following system of linear algebraic equations at each grid cell. The full system includes 13 simultaneous algebraic equations, here we present a system of 10 equations for six turbulent stresses, three turbulent sensible heat fluxes and potential temperature variance. The three additional equations, not shown here, are solved for turbulent scalar fluxes of specific humidity, liquid water content, and ice water content.

\[
\begin{bmatrix}
\begin{array}{cccccccccc}
\frac{\partial^2}{\partial x^2} & \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{\partial}{\partial x} & \frac{\partial^2}{\partial y^2} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial^2}{\partial z^2} & \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{\partial}{\partial y} & \frac{\partial^2}{\partial z^2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} & \frac{\partial^2}{\partial y^2} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0 & 0 & 0 \\
0 & 0 & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial^2}{\partial y^2} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{\partial^2}{\partial y^2} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{\partial}{\partial z} & \frac{\partial^2}{\partial z^2} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial z} & \frac{\partial^2}{\partial z^2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\partial^2}{\partial y^2} \\
\end{array}
\end{bmatrix}
\begin{bmatrix}
\frac{q^3}{\Lambda_1} \\
\frac{q^3}{\Lambda_1} \\
\frac{q^3}{\Lambda_1} \\
\frac{q^3}{\Lambda_1} \\
\frac{\partial q^3}{\partial x} \\
\frac{\partial q^3}{\partial y} \\
\frac{\partial q^3}{\partial z} \\
\frac{\partial \theta}{\partial y} \\
\frac{\partial \theta}{\partial z} \\
\frac{\partial \theta}{\partial y} \\
\end{bmatrix}
= \begin{bmatrix}
\frac{q^3}{\Lambda_1} \\
\frac{q^3}{\Lambda_1} \\
\frac{q^3}{\Lambda_1} \\
\frac{q^3}{\Lambda_1} \\
\frac{\partial q^3}{\partial x} \\
\frac{\partial q^3}{\partial y} \\
\frac{\partial q^3}{\partial z} \\
\frac{\partial \theta}{\partial y} \\
\frac{\partial \theta}{\partial z} \\
\frac{\partial \theta}{\partial y} \\
\end{bmatrix}
\begin{bmatrix}
\alpha_1 \\
\alpha_2 \\
\alpha_3 \\
\alpha_4 \\
\beta_1 \\
\beta_2 \\
\beta_3 \\
\beta_4 \\
\beta_5 \\
\beta_6 \\
\end{bmatrix}
\]

(7)
Here, $\ell_1$, $A_1$, $\ell_2$, and $A_2$ are length scales that are proportional to each other, so they can be expressed in terms of a master length scale $\ell$:

$$[\ell_1 \ A_1 \ \ell_2 \ A_2] = \ell [A_1 \ B_1 \ A_2 \ B_2] \quad (8)$$

The master length scale is defined as:

$$\ell = \frac{\int_0^h q z \, dz}{\int_0^h q \, dz} \quad (9)$$

The constants, $A_1$, $B_1$, $A_2$, $B_2$, and $C_1$ are determined from experimental data. The original values used by Mellor and Yamada (1982) [7] are

$$[A_1 \ B_1 \ A_2 \ B_2 \ C_1] = [0.92 \ 16.6 \ 0.74 \ 10.1 \ 0.08] \quad (10)$$

As an intermediate step to implementing a full 3D PBL parameterization, we have developed a hybrid approach where all the six components of turbulent stress tensor and three components of the sensible heat gradient vector are diagnosed and the full divergence of both stress tensor and flux vector computed, but a 1D PBL approximation (i.e. neglecting horizontal derivatives) is used to develop diagnostic equations. The 1D PBL approximation assumes that horizontal gradients appearing in the matrix in Equation 7 can be neglected leading to the following simplified set of linear algebraic equations

$$\begin{bmatrix}
\frac{\partial}{\partial z} & 0 & 0 & 0 & 2\frac{\partial U}{\partial z} & \frac{\partial V}{\partial z} & 0 & 0 & \rho g \\
0 & \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & \rho g & 0 & 0 \\
0 & 0 & \frac{\partial}{\partial z} & 0 & -\frac{\partial U}{\partial z} & \frac{\partial V}{\partial z} & -2\rho g & 0 & 0 \\
0 & 0 & 0 & \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{\partial}{\partial z} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{\partial}{\partial z} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{\partial}{\partial z} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{\partial}{\partial z} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{\partial}{\partial z} & 0 \\
\end{bmatrix}
= \begin{bmatrix}
C_{1g} \frac{\partial U}{\partial z} \\
\frac{\partial V}{\partial z} \\
\frac{\partial U}{\partial z} \\
-2\rho g \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
\end{bmatrix} \quad (11)$$

3. Model Testing and Validation

3.1. Mesoscale Simulations over Idealized Heterogeneous Terrain

The new PBL scheme is able to account for horizontal heterogeneity of boundary-layer flows not only due to complex topography and heterogeneous land use, but also due to large convective eddies, convective cells and rolls. Convective rolls and cells generally scale with the boundary layer height. Therefore, as the grid-cell size approaches boundary-layer height, these structures are captured by NWP models but are under-resolved (12). Since the structures are under-resolved, their characteristic length scales are not realistic. It is therefore important to account for the effects of velocity and potential temperature gradients induced by convective structures that result in enhanced turbulence.
diffusion. Other convectively induced secondary circulations caused by, for example, heterogeneous surface characteristics, are often not resolved properly using NWP models with 1D PBL parameterizations and grid-cell size in “terra incognita” (i.e. gray zone) range.

Before proceeding with simulations over heterogeneous terrain, model parameters were tuned using simulations of a convective boundary layer over homogeneous terrain. We found that when using parameters determined by Bougeault and Lacarrere (1989) \cite{13}, the 3D PBL parameterization produces the correct mixed layer ABL structure while the original set of parameters presented by Mellor and Yamada (1982) \cite{7} result in a diabatic profile of potential temperature (Martilli, personal communication). Therefore, the parameters that we used in all the simulations presented here are:

\[
[A_1, B_1, A_2, B_2, C_1] = [0.3, 8.4, 0.33, 6.4, 0.08] \tag{12}
\]

Not accounting for the effects of horizontal gradients on turbulence production, transport, and dissipation results in inaccurate levels of turbulence and therefore inaccurate turbulent diffusion. We demonstrated this by carrying out idealized mesoscale simulations of an ABL over heterogeneous surface. The results of these simulations are verified by comparing them to the results of an ensemble of LES. The idealized mesoscale simulation setup includes periodic lateral boundary conditions with a weak, 2 m s\(^{-1}\), southerly wind and surface heat flux of 160 W m\(^{-2}\) on the west half of the domain and 320 W m\(^{-2}\) on the east half of the domain. The horizontal grid-cell size in both directions was 200 m. Two mesoscale simulations were carried out, one using the MYNN 1D PBL parameterization and the other using the new 3D PBL parameterization. Additionally, an ensemble of 20 LES was carried out over the lateral boundary conditions and the same domain but with grid-cell size of 50 m. The ensemble was created by adding a uniformly distributed random perturbation to the surface heat flux. All the simulations were run for two hours of physical time. The results of these simulations are shown in Figure 1 and 2. In these Figures shown are contour plots of meridional and vertical velocity components at 250 m above the surface, respectively. In the left panel of Figure 1 presented are mesoscale simulation results obtained using the 1D PBL parameterization while on the right are results from the simulation with the 3D PBL parameterization. In Figure 2 the left and middle panel show mesoscale simulation results with the 1D and 3D PBL parameterizations, respectively, while the right panel shows the ensemble average vertical velocity from the LES.

**Figure 1.** Meridional velocity from mesoscale simulations with the 1D PBL parameterization (left) and 3D PBL parameterization (right).
In comparison to the simulation with the 1D PBL parameterization, which results in unphysical flow patterns in homogeneous flow direction, the simulation with the 3D PBL parameterization reproduces correctly homogeneous flow in the homogeneous direction. The flow field produced using the 3D PBL parameterization is similar to that produced by the ensemble LES simulation.

3.2. Mesoscale Simulations over Complex Terrain

We validated WRF-ARW with a new 3D PBL parameterization using field experiment data from the Columbia River Gorge. For this purpose, we focused on validation of the parameterization for all the components of turbulent stress and sensible heat flux and their full divergence, but with the use of a boundary-layer approximation. This approach was assessed first rather than the full 3D parameterization due to numerical stability issues related to the use of diagnostic equation for the TKE that can result in ill conditioning of the system of linear algebraic equations.

The validation of 3D PBL parameterization is based on one of the selected “ten-day” WFIP2 retrospective study periods [5], the period between August 13 and 24, 2016. We carried out three mesoscale simulations. We used the MYNN 1D PBL parameterization for the baseline mesoscale simulation. In the other two mesoscale simulations, we used the new 3D PBL with and without an additional two-dimensional (2D) Smagorinsky type diffusion parameterization commonly used in operational NWP models. Here, it should be pointed out that the role of the 2D Smagorinsky diffusion parameterization is not to represent unresolved physical processes and resulting diffusion [15,16], but instead to provide numerical stability through diffusion of numerical oscillations controlled by a strain-rate-dependent diffusivity. The initial and boundary conditions were derived from HRRR simulations with horizontal grid-cell size of 3 km. The HRRR output was obtained from the University of Utah data archive (http://home.chpc.utah.edu/~u0553130/Brian_Blaylock/hrrr.html) maintained by Brian Blaylock. Simulations were carried out for 30 hours. The first 6 hours represented simulation spin up time and the last six hours overlapped with the next day’s simulation. All the simulations started at 00 UTC and ended the next day at 06 UTC. The simulations were carried out using two domains. The parent domain was resolved using 750 m horizontal grid-cell sizes, while the inner, nested domain was resolved with 250 m horizontal grid-cell sizes (Figure 3). The inner domain was centered on the so-called Physics Site near just east of the Biglow Canyon wind plant. The outer domain resolution corresponded to the resolution of a special instance of HRRR that was run by the NOAA team over the WFIP2 study area during the duration of the field study.

The observations used to assess the model performance are from observational platforms located within the inner domain including: 2-meter tower at Wasco – wind only, 3-meter tower at the Physics site: wind data, relative humidity, temperature, and irradiance, and a 17-meter Physics site...
tower with sonic measurements at three levels: 3 m, 10 m, and 17 m. Sonic anemometers provide high-frequency measurements needed to compute turbulent fluxes.

In Figures 4 and 5 shown are comparisons of output from the three mesoscale simulations with observations at the two-meter tower at Wasco. In these figures shown are example comparisons based on observations from two simulated days. From Figure 4 we can see that all the mesoscale simulations capture quite well the diurnal temperature evolution. During nighttime between hours 12 and 19 UTC temperature is first only slightly underpredicted and then during the second day slightly overpredicted.

The kinematic sensible heat flux is shown in the top right panel of Figure 4. In this case the sensible heat flux from simulation with the MYNN parameterization was not included in the output and therefore it is zero. For the other two simulations the agreement between observations and model results is relatively good, however, during both days, daytime sensible heat flux is underpredicted. Finally, the wind speed and surface friction velocity (Figure 4, top and bottom panels, respectively) are predicted quite well. Wind speed is overpredicted during the first few hours on the first day.

Figure 3. Left panel - WFIP2 field study area with symbols indicating instrument locations; Right panel – WRF domains, D01 – 750 m grid-cell size, D02 – 250 m grid cell size. In D02 plus sign denotes Wasco tower and x denotes Physics site.

One of the reasons to replace a 1D PBL parameterization with a 3D PBL parameterization is the ability of the latter to represent normal turbulent stresses as well as their effects on the momentum evolution. The normal turbulent stress components from mesoscale simulations is compared to the observed normal stress components (Figure 5). The horizontal normal stress components are underpredicted by the 3D PBL parameterization while the vertical component is overpredicted. The observations indicate that at the scale of interest, normal stresses are significant. Their temporal variability, and therefore likely spatial variability is also significant. This points to the importance of including normal turbulent stresses and their gradients as grid-cell size of mesoscale simulations is reduced.

4. Summary
The new 3D PBL parameterization based on developments by Mellor and Yamada (1982) [7] was first assessed by carrying out idealized mesoscale simulations over heterogeneous terrain characterized by sharp differences in surface heat fluxes. These simulations demonstrated the deficiency of a 1D PBL parameterization when grid-cell size is in the so-called “terra incognita” range, between 100 m and 1 km. We used the MYNN 1D PBL parameterization in this study and it
resulted in unphysical secondary circulations. In contrast, the simulation with the 3D PBL parameterization correctly maintained homogeneity in one horizontally-homogeneous direction while capturing the dynamical effects of the heterogeneity in the other horizontal direction. We have demonstrated that the results obtained using the 3D PBL parameterization are consistent with the averages from an ensemble LES.

We have assessed the performance of an intermediate form of the 3D PBL parameterization which utilizes the boundary-layer approximation in order to directly solve a system of linear algebraic equations for all the turbulent stresses and fluxes. For that purpose, we have used observations during the “ten-day” retrospective period from August 13 to August 24, 2016. Horizontal normal turbulent stress components are underpredicted by the 3D PBL as well as one of the shear stress components, $\langle u'v' \rangle$, while the two turbulent shear stress components, $\langle u'w' \rangle$ and $\langle v'w' \rangle$ are accurately predicted. Based on the results of the assessment additional parameter tuning may be necessary to obtain optimal performance.

Figure 4. Comparison of the output from domain 2 of three mesoscale simulations with observations at two-meter tower at Wasco: 2 m temperature – top left panel, wind speed at 10 m – top right panel, surface kinematic sensible heat flux – bottom left panel, surface friction velocity –
bottom right panel. In all the panels different lines represent: simulation with the 3D PBL parameterization – blue line, simulation with the 3D PBL but with the 2D Smagorinsky parameterization turned off – orange line, simulation with MYNN PBL parameterization – yellow line, and observations – purple line.

Figure 5. Comparison of simulated and observed normal turbulent stresses: normal turbulent stress component in zonal direction – top left panel; normal turbulent stress component in meridional direction – top right panel; normal turbulent stress component in vertical direction – bottom right panel. In all the panels different lines represent: simulation with the 3D PBL parameterization – blue line, simulation with the 3D PBL but with the 2D Smagorinsky parameterization turned off – orange line, simulation with MYNN PBL parameterization – yellow line, and observations – purple line.

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