Mixed nonlinear LES for DES suitable flows

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It is shown that a new mixed nonlinear/eddy viscosity LES model reproduces profiles better than a number of competing nonlinear and mixed models for plane channel flow. The objective is an LES method that produces a fully resolved turbulent boundary layer and could be applied to a variety of aerospace problems that are currently studied with RANS, RANS-LES, or DES methods that lack a true turbulent boundary layer. There are two components to the new model. One an eddy viscosity based upon the advected subgrid scale energy and a relatively small coefficient. Second, filtered nonlinear terms based upon the Leray regularization. Coefficients for the eddy viscosity and nonlinear terms come from LES tests in decaying, isotropic turbulence. Using these coefficients, the velocity profile matches measurements data at $Re_\tau \approx 1000$ exactly. Profiles of the components of kinetic energy have the same shape as in the experiment, but the magnitudes differ by about 25%. None of the competing LES gets the shape correct. This method does not require extra operations at the transition between the boundary layer and the interior flow.

Nomenclature

\[ A_{\mu}, A_{\epsilon} \] = turbulence model constants
\[ \alpha \] = filter scale of added nonlinear terms
\[ C_c, C_e, C_k, C_L, C_s, C_{\alpha}, C_e \] = turbulence model constants
\[ \Delta x, \Delta y, \Delta y', \Delta x^+, \Delta z^+ \] = mesh and dimensionless grid spacings
\[ \Delta v, \Delta' \] = averaged and maximum mesh sizes
\[ Ko \] = Kolmogorov constant
\[ k \] = wave number
\[ k_e \] = subgrid turbulent kinetic energy
\[ l \] = modeled turbulence length scale
\[ L, \overline{N} \] = linear and filtered nonlinear contributions to subgrid stress
\[ P_{ke} \] = subgrid turbulence energy production term
\[ Re_\tau \] = Reynolds number based on friction velocity

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\( S_{ij}, \tau_w, \tau_{ij} \) = mean strain rate tensor and wall and subgrid stresses  
\( \mathbf{u}, \mathbf{u}, u, v, w' \) = full vector, filtered, and fluctuating velocity components  
\( x, y, z \) = Cartesian coordinates  
\( y^+ = y\sqrt{\rho \tau_w/\mu} \) = dimensionless wall distance  
\( \mathbf{\omega}, \mathbf{\omega}' \) = full and fluctuating vorticity vectors

I. Introduction

For unsteady separated flows, URANS (Unsteady Reynolds Average Navier Stokes), has inherent difficulties\(^1\) that in principle LES (Large Eddy Simulations) should be able to address. The argument is that in LES the true large-scale equations are used, and thus the proper large-scale instabilities should exist. In practice, LES tends to smooth the small-scale instabilities, suppress the streak-like structures near solid surface and does not properly represent wall-bounded flows except for methods presently applicable to a few special cases. The problem is more than lack of resolution. Even allowing for generous increases in computing power that would not be available for many years,\(^2\) full LES as presently posed might have inherent problems.

If these inherent problems could be solved, many of the outstanding problems in aerodynamic turbulence could be addressed without major increases in computing power. One objective would be to accurately predict drag and lift for flows with significant separation using LES. From a combustion perspective, could a proper fluctuating turbulent velocity be generated that could mix reactants directly?

Our approach will be nonlinear LES with a modified eddy viscosity. We propose this as an alternative to the hybrid RANS-LES or DES (Detached Eddy Simulation) approach.\(^3\) In DES there are different terms for within and outside the boundary layer. The boundary layer is (U)RANS modeled to force the boundary layer to have correct profile. Outside the boundary layer, true LES is applied. In our approach, the same equations are used throughout the turbulent parts of the flow. The difference with standard LES is that additional nonlinearity is injected into the simulations. Done properly, this allows the turbulent fluctuations of the primitive velocities to directly provide the drag that leads to the correct profiles.

This paper will be organized as follows. The recent history of RANS-LES and nonlinear models proposed by the engineering community is discussed. Then a new perspective on nonlinear models as mathematical regularizations of the Euler equations is reviewed. Next our system of equations and the numerical method is described in detail. Finally, the single case we have used to compare the models is discussed.

A. Background

In RANS-LES, the physical processes modeled by URANS and LES are very different. The LES equations invoke spatial filtering in the interior and the URANS temporal averaging in a portion of the boundary layer. Despite this, the governing equations arising from these two procedures appear virtually identical and easy to interface, which could be a key reason for their limited success.\(^2,3\) However, major problems can arise. For example, buffeting from the LES zone introduces fluctuations into the domain modeled by URANS. This can make the near wall sum of the resolved and modeled turbulence energy levels is too high, hence a mean velocity profile kink results. This has been demonstrated using \( k - \omega \) for the inner part of the logarithmic boundary layer region i.e. \( y^+ \leq 60 \), with the LES in the interior using an eddy viscosity based upon the \( k - l \) equations with the small coefficient of \( C_e = 0.07 \) in front of the eddy viscosity.\(^4\) This is a model that is more LES than
most. Attempts have been made to smooth the velocity profile kink, either by damping modeled stresses in the URANS region,\textsuperscript{5} damping resolved stresses,\textsuperscript{6} and increasing resolved kinetic energy levels in the LES zone.\textsuperscript{7,8} All of these \textit{ad hoc} procedures make both the U(RANS) and VLES (Very Large Eddy) modeling assumptions questionable.\textsuperscript{4,9}

Physically, it has been proposed that the limitation upon LES in the boundary layer is that the subgrid scales not only extract energy from the resolved scales, but feed fluctuations back into the resolved scales, a phenomena known as ‘backscatter’.\textsuperscript{10} Backscatter was first introduced into eddy-viscosity parametrization for second-order closures.\textsuperscript{11} The LES backscatter problem is that a cheap, flexible method that generates the correct small-scale instabilities does not exist. Only for simple flows, such as a plane channel, has backscatter based upon extra inversion operations been able to reproduce the results of DNS.\textsuperscript{12,13} Attempts to remedy the hybrid RANS-LES model deficiences by injecting turbulent energy into the mean flow\textsuperscript{7,8} are more akin to stochastically forced LES\textsuperscript{14} than true dynamic calculations.

To understand the origin of backscatter, systematic analyses of the energy transfer between the large and small scales in direct numerical simulations and experiments\textsuperscript{15–17} have been done. The study most relevant to the present work\textsuperscript{17} showed that the full subgrid transfer terms could be divided into two primary components. A component that looks like a traditional eddy viscosity and another term that represents the convection of the subgrid vorticity by the resolved scales and contains all the backscatter. In rotation form, this implies that a nonlinear part of the divergence of the subgrid scale stress should go as $\partial_j t^\text{NL}_{ij} = -\mathbf{u} \times \mathbf{\omega}'$, where $\mathbf{\omega}'$ is some estimate of the subgrid vorticity. This has spawned some successful ‘estimation’ models\textsuperscript{13} designed to represent this subgrid convection, but these still suffer from the need for extra inversions.

What we propose is the use of added nonlinear terms taken from the mathematics of regularizations of the Euler equations as a cheap, deterministic means of introducing the backscatter due to subgrid convection. The objective of including the added terms is to sensitize the mean flow to the instabilities responsible for anisotropic turbulence structures.

### II. Modeling Approach

#### A. Nonlinear LES models

Although not phrased in this context, Clark et al.\textsuperscript{18} introduced the first nonlinear model for subgrid stress terms in an LES in 1979. These nonlinear terms complemented the linear Smagorinsky model for dissipation.\textsuperscript{19} If these nonlinear terms could be related to the subgrid terms responsible for backscatter in the DNS analysis, then they could provide a means of introducing backscatter dynamically without extra inversions or new parameterizations of a stochastic component. To date no such nonlinear method has generated the proper mean profiles and therefore the idea has lain dormant since 1979.

There have been a few attempts to revive the concept for boundary layers since then. In nonlinear RANS modeling, a standard Boussinesq (linearized) approximation similar to those for non-Newtonian fluids has been added\textsuperscript{20} and a cubic eddy-viscosity model has been used.\textsuperscript{21} The explicit algebraic stress model can also be viewed as a non-linear RANS model.\textsuperscript{22} Nonlinear LES of meteorological boundary layers has also been used,\textsuperscript{23} which are another high Reynolds number system.

The origin of our model stems from mathematical analysis of the Euler and Navier-Stokes equations where you want to prove regularity, that is smoothness, of some terms in the equations so as to isolate the truly intractable terms that might not be smooth and might have singularities.\textsuperscript{24} In the regularized models, similar to LES, the full velocity $\mathbf{u}$ is the sum of the filtered velocity $\mathbf{\bar{u}}$ and the sub-filter velocity fluctuations $\mathbf{u}'$. In our model, we will estimate the fluctuations using...
\( u' = -\alpha^2 \nabla^2 \bar{u} \), where \( \alpha \) is a filter length scale and the full velocity is \( u = \bar{u} + u' = (1 - \alpha^2 \nabla^2) \bar{u} \). Alternatively, one can think of the resolved velocity \( \bar{u} \) as a Helmholtz filtered velocity, which in physical and Fourier spaces is

\[
\bar{u}(x) = \int d^3x' \frac{1}{1 - \alpha^2 \nabla^2} u(x') \quad \bar{u}(k) = \frac{1}{1 + \alpha^2 k^2} u(k)
\]

Three models have been tested that can be derived from different nonlinear components in the expansion of the convection term into \( u, u' \) and \( \bar{u}' \). These terms will be added to the large-scale convection, which can be written either as \((u \cdot \nabla)u\) or \(-u \times \bar{\omega}'\). Unlike earlier nonlinear models, all the added nonlinearities are filtered. One model adds \(-u \times \bar{\omega}'\), as suggested by the DNS analysis.\(^{17}\) This formulation conserves circulation and is equivalent to the recently introduced Lagrangian averaged Navier-Stokes equations or \( \alpha \)-model.\(^{25}\) Another model will be based upon \((u \cdot \nabla)u'\), which was originally introduced in the classic mathematical study of regularization by Leray.\(^{26}\) The third filtered model is \((u \cdot \nabla)u' + (u' \cdot \nabla)u\), which is the nonlinearity suggested by Clark et al.\(^{18}\)

The reason for filtering stems from the energy-like conservation laws of the first two regularized models, the \( \alpha \) and Leray models. With the filter and after some manipulation of the Laplacian terms that takes advantage of incompressibility, the \( \alpha \) model,\(^{27}\) the Leray model,\(^{26, 28}\) and Clark model,\(^{18}\) can all be converted into simple quadratic products of the velocity derivative tensor, as given in Table 1. Therefore, after the application of a physical space approximation of the Helmholtz filter, all three models could be used in complicated domains using non-uniform meshes.

In the analysis of DNS,\(^{17}\) it was found that in addition to backscatter generated by subgrid terms, there was a second term that was dissipative and was similar to the prediction of an eddy viscosity model. It has been claimed that the regularization models, without eddy viscosities, are an alternative method of LES.\(^{28, 29}\) Our tests of decaying, isotropic turbulence show that by adjusting the filter scale \( \alpha \) of the added nonlinearities that a constant viscosity can maintain the correct decay rates and spectra for short periods, but at the cost of generating unphysical small-scale structures. The problem appears to be that the regularization models tend to suppress the true energy cascade and energy is dissipated only after it cannot be held back any longer, and then at too great a rate. A following paper addressing LES of decaying, isotropic turbulence will discuss how this problem can be resolved using eddy viscosities.

<table>
<thead>
<tr>
<th>Model</th>
<th>( \tau_{ij} ) (nonlinear part)</th>
<th>centerline error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yoshizawa (1993)(^\text{30})</td>
<td>( C_c \rho \alpha^2 u_{i,k} u_{j,k} )</td>
<td>7.2%</td>
</tr>
<tr>
<td>Clark et al (1979)(^{18})</td>
<td>( C_k \rho \alpha^2 [u_{i,k}u_{k,j} + 3u_{i,k}u_{j,k} - u_{k,i}u_{i,j}] )</td>
<td>-4.6%</td>
</tr>
<tr>
<td>Kosovic (1997)(^{23})</td>
<td>( C_\alpha \rho \alpha^2 [u_{i,k}u_{k,j} + u_{i,k}u_{j,k}u_{k,i}u_{i,j}] )</td>
<td>10.6%</td>
</tr>
<tr>
<td>( \alpha )(^{27})</td>
<td>( C_L \rho \alpha^2 [u_{i,k}u_{k,j} + u_{i,k}u_{j,k}] )</td>
<td>-0.1%</td>
</tr>
</tbody>
</table>

Table 1. Nonlinear stress expressions for different models using \( \alpha = \Delta' \), defined below. The error in the channel centerline velocity is given. The derivative \( u_{i,j} = \partial u_i / \partial x_j \) convention is used. For the finite-difference channel calculations, all the velocities derivatives are determined using a discrete 2nd order approximation to a Gaussian filter.\(^{31}\)

B. \( \nu_e \) and \( k - l \) equation

For the channel flow, a \( k_e - l \) formulation is used to ascertain the eddy viscosity \( \nu_e \)\(^{23, 30, 32}\) which the analysis of the DNS says should be part of the mixed model.\(^{17}\) Based upon dimensional consistency, the eddy viscosity is

\[
\nu_e = C_e \ell e (k_e)^{1/2}
\]

\[4\text{ of 10}\]

American Institute of Aeronautics and Astronautics
The equation for the sub-grid turbulent kinetic energy is

$$\partial_t k_e + \nabla \cdot (\bar{u}k_e) = \frac{1}{\rho} \partial_j \left[ \left( \nu + \frac{\nu}{\sigma_e} \right) (\partial_j k_e) \right] + P_{ke} - \epsilon_e \quad \text{with} \quad \epsilon_e = \frac{C_\epsilon k_e^{3/2}}{\ell_e}$$

where $P_{ke}$ is the standard turbulence production term and the damping functions are

$$\ell_{e,\mu} = \min \{ \Delta_v, C_{c} y \left[ 1 - \exp(-A_{c,y} y^+ \right) \} \} .$$

Two LES mesh scales are considered

$$\Delta_v = (\Delta x \Delta y \Delta z)^{1/3} \quad \text{and} \quad \Delta' = \max(\Delta x, \Delta y, \Delta z) .$$

The volume based length scale $\Delta_v$ is used for linear terms because this definition tends to zero at the wall, where we want the eddy viscosity to become inactive. As in RANS, this is aided by use of the damping functions in Eq. (4). For the nonlinear terms (see Table 1, $\alpha = \Delta'$, the maximum grid scale. This choice was based upon the decaying, isotropic LES tests, which worked best when $\alpha$ was the grid scale.

The following constants are used in Eqs. (2-4): $\sigma_e = 1$, $C_e = 1.05$, $C_c = 2.4$, $A_{\mu} = 0.016$, and $A_c = 0.263$. The constants in Eqs. (2-4) are taken from Wolfshtein$^{33}$ and the others are from Yoshizawa.$^{30}$ Calibration of $C_e$ and $\alpha$ is discussed below.

There are superficial similarities to perhaps the most sophisticated of dynamic backscatter models, one that modifies the coefficients of the $k-l$ equation used to determine $\nu_e$. However in that model backscatter comes from negative values of $\nu_e$. In our model, the eddy viscosity term will be strictly dissipative and our backscatter effects come entirely from the added nonlinear terms.

C. Numerical methods and parameterization of $C_e$ and $\Delta'$.

The subgrid scale stress can be decomposed as

$$\tau_{ij} = L + N \quad \text{where} \quad L = \partial_j \nu_e S_{ij}$$

is the linear eddy viscosity part, $N$ is the filtered nonlinear term and the nonlinearities $N$ are given in Table 1.

For the decaying, isotropic LES that determined the LES constants $C_e$ and $\alpha$, a Smagorinsky model for the eddy viscosity $\nu_e^{19}$ was used,

$$\nu_e = \Delta_v^2 |\bar{s}|, \quad \text{where} \quad |\bar{s}| = \sqrt{2 S_{ij} S_{ij}} \quad \text{and} \quad S_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) \quad \text{is the strain.}$$

The numerical method is a standard periodic, pseudospectral code with 2/3rd’s rule dealiasing and Helmholtz filtering in Fourier space of the added nonlinearities as in Eq. (1). The decaying, isotropic LES calculations were performed on a $64^3$ mesh and compared to a DNS on a $256^3$ mesh.$^{35}$

The details of our parameterization study of mixed models for decaying, isotropic turbulence will be discussed in a following paper. The objective is to obtain parameters where the decay rate and spectra behave at least as well as an LES using just the original Smagorinsky eddy viscosity model. This is in many ways still the best LES for decaying, isotropic turbulence. Therefore, it is not surprising that the value for the Smagorinsky constant $C_s$ we chose is within the traditional range ($0.2 < C_s < 0.1$) for decaying, isotropic turbulence.

What our tests have shown is that for the nonlinear terms to have an appreciable effect one needs $\alpha \sim \Delta$ (some mesh size) and that given this, a Smagorinsky coefficient on the low side is possible. This is because the extra nonlinearity creates more fluctuations at the small scales and the
same amount of dissipation can then be obtained with a smaller eddy viscosity coefficient. Using $C_s = 0.126$ and $C_e = \pi C_s^2$, which comes from a spectral re-derivation Lilly's relations,$^{32}$ we chose $C_e = 0.05$. The differences with earlier constant coefficient eddy viscosity models is that in our case $\nu_e$ is based upon $k_e$, not the strain, we have damping functions, and we have added nonlinearities. Note that $C_e = 0.05$ will not give the correct law of the wall in RANS, only in LES.

Details of the numerical method for the plane channel flow simulations have been given earlier.$^1$ In brief, it is finite difference/volume code using a staggered grid, a geometric grid expansion factor of 1.15 in the vertical ($y$), derivatives are based upon second order central differences and an iterative Crank-Nicolson implicit method is used for the time advancement of both the convective and the diffusion terms. A discrete approximation to a Gaussian$^{31}$ is applied to the added nonlinear terms $N$, replacing the Helmholtz filter, and for channel flow stability the added nonlinearities are clipped relative to the linear such that $|N| \leq |L|$.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{velocity_profile.png}
\caption{Profile of the mean horizontal velocity for plane channel flow as a function of $y^+ = y\sqrt{\tau_w/\mu}$ produced by several mixed nonlinear models. Circles are the benchmark experiment at $Re_e \approx 1000$, the solid line is the mixed Leray model described, dashed is the linear (only an eddy viscosity) model of Yoshizawa,$^{30}$ and dotted is the modified mixed nonlinear model of Kosovic$^{23}$ as described. The mixed Leray model has a particularly good law of the wall.}
\end{figure}

The channel flow ($x, y, z$) domain of $2\pi \times 2 \times \pi$ is discretized using a $33 \times 65 \times 33$ grid. The non-uniform vertical mesh ensures that $y^+$ values at first off-wall nodes are around unity. The grid is such that $\Delta x^+ \sim 200$ and $\Delta z^+ \sim 100$. The chosen grid was originally developed for a hybrid RANS-LES,$^9$ which gave poor turbulent statistics when compared with the benchmark LES data at
$Re_\tau \approx 1000$. The effective $Re_\tau$ of our LES is determined by the true viscous terms in the viscous sublayer, where the wall damping functions shut off any eddy viscosity.

### III. Case details

Figure 1 compares the mixed Leray, modified Kosovic and linear Yoshizawa LES results with the benchmark experimental law of the wall at $Re_\tau \approx 1000$. There were three phases leading to this figure. In the first phase, the plain linear (that is only eddy viscosity) model of Yoshizawa and original Kosovic model were tested, then combined to create a modified Kosovic model, where the original linear eddy viscosity terms were replaced with Eqs. (2-4). The original Kosovic model gave results in the direction of, and far worse than, the Yoshizawa model. In the second phase, the best parameters and nonlinearity determined from decaying, isotropic turbulence were implemented. The amazing result was that the first try gave the Leray curve in the Fig. 1. In the final stage, the other nonlinearities were checked and the filter scale $\alpha$ was varied for the channel flow. The results of all these subsequent tests were negative. That is, the original mixed Leray model suggested by the decaying, isotropic tests was the best. Not shown are the Clark and $\alpha$ model tests that used the same coefficients as the Leray model shown.

All the models shown, as well as the mixed Clark and $\alpha$ model calculations, gave an excellent viscous sublayer, as might be expected because all of the calculations use the same damping functions for the eddy viscosity. Outside the viscous sublayer the mean horizontal velocity profile $\overline{U}(y)$ for all of the models, except the mixed Leray model, diverge from the benchmark data. The mixed Leray model gives an exceptionally good law of the wall all the way to the center of the channel. The mixed Clark model results overlay the Yoshizawa curve and the mixed $\alpha$-model performs particularly poorly, giving a centerline velocity much greater than Yoshizawa. The mixed Clark results would be consistent with the nonlinear terms in the Clark model creating what is in reality an LES for the full velocity $u$ with no added nonlinearities. The mixed $\alpha$-model results would be consistent with the extra conservation properties suppressing the energy cascade.

Figure 2 presents modeled and benchmark profiles of the fluctuating velocity squared profiles, which are twice the fluctuating kinetic energies. For the vertical kinetic energy profile, which was not reported experimentally, the comparison is to a dynamic subgrid LES. Only the Yoshizawa and mixed Leray results are shown. The different profiles are not labeled, but for each case their order in decreasing magnitude is $u'^2$, $w'^2$, and $v'^2$, or streamwise, spanwise, and vertical. For the mixed Leray model, $u'^2$ is consistently about 25% too large, $w'^2$ is in good agreement with the benchmark, and $v'^2$ is below the benchmark near the wall. For all three profiles, the shape is similar to the benchmark, in particular the position of the peak in $u'^2$ is predicted correctly.

The Yoshizawa model gives consistently smaller turbulent fluctuations than Leray and the profiles near the wall are smoother than the mixed Leray results and the benchmark. All of the other models tested gave still fewer fluctuations and their energy profiles were all smoother than Yoshizawa. Therefore, while not perfect, the mixed Leray model is again the best of this set of LES simulations. Only for special cases where an inexpensive Fourier filter can be used can comparable results on a comparable mesh be obtained.

### IV. Summary

These are the first tests of a new approach to large-eddy simulation that combines two approaches favored separately by the mathematics and engineering communities. What came from the mathematics community are nonlinearities related to regularizations of the Euler equation used
in mathematical analysis. From the engineering community we take a formulation for the eddy viscosity that uses a well-known $k-l$ equation for which parameterizations have been established experimentally. There are no additional inversions and filtering is applied only to the added nonlinear terms. The form of the nonlinearity and filtering could easily be applied to any physical space calculation with a non-uniform mesh and a complicated geometry. Any URANS (Unsteady Reynolds averaged Navier-Stokes) code using higher-order numerics could be converted into a true LES code using these steps, which means that testing could begin immediately to determine if this could be a viable alternative to hybrid DES/LES schemes.

![Figure 2. Mean square velocity profiles (2×kinetic energy components) for plane channel flow from the wall to the centerline compared to benchmark data. $u'^2$ and $w'^2$ are from measurements, and $v'^2$ is from a dynamic LES. Dot-dashed are the remaining profiles from the dynamic LES. In order of decreasing magnitude are $u'^2$, $w'^2$ and $v'^2$, the streamwise, spanwise and vertical components. The same symbols for the benchmark, mixed Leray and Yoshizawa models as before. The Leray model reproduces the shape better than the linear Yoshizawa model and has larger turbulent fluctuations.](image-url)

The approach and parameterizations are justified by DNS analysis and LES of decaying, isotropic turbulence. There are many differences between the DNS analysis, the parameterization tests using decaying, isotropic turbulence, and the channel flow LES. These are that a wavenumber cut-off filter was used in the DNS analysis instead of a Helmholtz filter as we now believe is correct, the Leray terms have never been tested in DNS analysis, and a Smagorinsky eddy viscosity was used for the decaying, isotropic LES tests instead of the $k-l$ eddy viscosity. New DNS analysis
is planned to determine the effect of these differences and the decaying, isotropic LES tests will be repeated with a $k$ -- $l$ eddy viscosity. We also want to do this type of analysis on more complicated flows, including a plane channel and a rotating channel and test our model against DNS of more complicated geometries such as a backward facing step.

Our hope is that with this method a wide range of new flows can now be studied with LES that previously had been amenable only to RANS. We believe that this approach has the potential for predicting flows with significant separation while still giving a satisfactory boundary layer treatment. Realistic turbulent fluctuations would also allow there to be realistic mixing of scalars such as is required in combustion.

Acknowledgments

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