A dynamic subgrid-scale model for LES based on the Mori-Zwanzig formalism

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Subgrid scale models for Large Eddy Simulation (LES) are typically based on phenomenological assumptions which can be questionable in many complex problems. In this work, we explore the Mori-Zwanzig (M-Z) formalism – a concept from non-equilibrium statistical mechanics – for the development of coarse-grained models of turbulence. The appeal of these models is that their structural form is defined by the mathematics of the coarse-graining process. This work develops a new model that assumes memory effects decay in finite time, the length of which is approximated by a Germano-type identity. Successful predictions of rotating homogeneous turbulence and fully developed channel flow demonstrate the potential of this mathematically derived, parameter-free technique for LES closure.

1. Introduction

The LES technique has proved to be a computationally feasible alternative to DNS. In LES, the large-scale energy-containing features are resolved while the effect of the unresolved features are accounted for through a subgrid closure model. Subgrid models are traditionally based on phenomenological assumptions, such as scale-invariance, homogeneity, and rapid equilibration of small-scales. These models warrant improvement in many complex problems.

Developed by Mori (1965) and Zwanzig (1973) in the context of irreversible statistical mechanics, the Mori-Zwanzig (M-Z) formalism is a mathematically consistent coarse-graining scheme that is especially suitable for problems that lack scale-separation. The M-Z formalism provides a framework for recasting a high-dimensional Markovian dynamical system into a lower-dimensional non-Markovian (non-local) system. In this lower-dimensional system, which is commonly referred to as the generalized Langevin equation (GLE), the effects of the unresolved scales on the resolved scales appear as a convolution integral. Although the GLE is closed in the conventional sense, it is not tractable in general. However, the GLE provides a starting point for the development of closure models whose structural form is prescribed by the coarse-graining process.

The application of the M-Z formalism to model development is an emerging research topic. The optimal prediction framework developed by the Chorin group (Hald et al. 2000) uses the GLE to obtain a set of equations that describe the evolution of the resolved modes conditioned on the initial density of the unresolved modes. The framework additionally begins to consider models for the memory kernel, the most notable of which is the t-model. The t-model has since been applied to various problems of interest to fluid dynamics, including Burgers’ equation (Bernstein 2007), the Euler equations (Hald & Stinis 2007) and the triply periodic Navier-Stokes equations (Chandy & Frankel 2009). The t-model has been found to provide accurate predictions in decaying problems.

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(2006) proposed a class of models that are grounded in the assumption that the memory integrand has a finite support. The performance of these models was investigated for Burgers’ equation and the Euler equations.

Previous work by Parish & Duraisamy (2016) explored the validity of the finite memory approximation and investigated the performance of the t-model and Stinis’ finite memory models for Burgers’ equation, decaying homogeneous turbulence, and the Taylor Green Vortex. A heuristic that was related to the Jacobian of the resolved scales was presented to estimate the memory length. The finite memory models were found to produce accurate results, most notably for cases where the coarse-graining was moderate.

The objective of this work is to further develop the Mori-Zwanzig formalism as a closure model for coarse-grained simulations of the Navier-Stokes equations. A new dynamic model based on the Germano identity and a short memory assumption is presented. Rotating homogeneous isotropic turbulence and fully developed channel flow are considered. The channel flow is of particular interest as it is the first application of an M-Z-based model to a non-decaying fluid dynamics problem.

2. The Mori-Zwanzig Formulation

A brief description of the Mori-Zwanzig formalism is provided. See Hald et al. (2000) for a more complete description. Consider the semi-discrete system of ordinary differential equations

$$\frac{d\phi}{dt} = R(\phi),$$

(2.1)

where $\phi = \{\hat{\phi}, \tilde{\phi}\}$, with $\hat{\phi} \in \mathbb{R}^M$ being the resolved modes, and $\tilde{\phi} \in \mathbb{R}^{N-M}$ being the unresolved modes. The initial condition is $\phi(0) = \phi_0$ with $\phi_0 \in L^2$. The non-linear ODE can be posed as an N-dimensional linear partial differential equation by casting it into the Liouville form,

$$\frac{\partial}{\partial t} u(\phi_0, t) = \mathcal{L} u(\phi_0, t),$$

(2.2)

with $u(\phi_0, 0) = g(\phi(\phi_0, 0))$ and

$$\mathcal{L} = \sum_{k=1}^{N} R_k(\phi_0) \frac{\partial}{\partial \phi_0 k},$$

where $\phi_0 k = \phi_k(0)$. It can be shown that the solution to Eq. (2.2) is given by

$$u(\phi_0, t) = g(\phi(\phi_0, t)).$$

(2.3)

The semigroup notation is now used, i.e., $u(\phi_0, t) = g(e^{t\mathcal{L}} \phi_0)$. By taking $g(\phi_0) = \phi_{0j}$, an equation for the trajectory of a resolved variable can be written as

$$\frac{\partial}{\partial t} e^{t\mathcal{L}} \phi_{0j} = e^{t\mathcal{L}} \mathcal{L} \phi_{0j}.$$  

(2.4)

The right-hand side can be partitioned into resolved and unresolved components through the use of projection operators. Let the space of the resolved variables be denoted by $\hat{L}^2$. Further, define $\mathcal{P} : L^2 \rightarrow \hat{L}^2$, as well as $\mathcal{Q} = I - \mathcal{P}$. In this work, a simple projection operator is used. For a function $f(\hat{\phi}_0, \tilde{\phi}_0)$, application of the projection operator yields $\mathcal{P} f(\hat{\phi}_0, \tilde{\phi}_0) = f(\hat{\phi}_0, 0)$. More complex projections are possible (see Hald et al. 2000). Using the identity $I = \mathcal{P} + \mathcal{Q}$, the right-hand side of Eq. (2.4) can be split into resolved
and unresolved components,
\[
\frac{\partial}{\partial t} e^{t\mathcal{L}} \phi_{0j} = e^{t\mathcal{L}} \mathcal{P} \mathcal{L} \phi_{0j} + e^{t\mathcal{L}} \mathcal{Q} \mathcal{L} \phi_{0j}.
\] (2.5)

At this point the Duhamel formula is utilized,
\[
e^{t\mathcal{L}} = e^{t\mathcal{Q} \mathcal{L}} + \int_0^t e^{(t-s)\mathcal{L}} \mathcal{P} \mathcal{L} e^{s\mathcal{Q} \mathcal{L}} ds.
\]

Inserting the Duhamel formula into Eq. (2.4), the generalized Langevin equation is obtained,
\[
\frac{\partial}{\partial t} e^{t\mathcal{L}} \phi_{0j} = e^{t\mathcal{L}} \mathcal{P} \mathcal{L} \phi_{0j} + e^{t\mathcal{L}} \mathcal{Q} \mathcal{L} \phi_{0j} + \int_0^t e^{(t-s)\mathcal{L}} \mathcal{P} \mathcal{L} e^{s\mathcal{Q} \mathcal{L}} \mathcal{Q} \mathcal{L} \phi_{0j} ds.
\] (2.6)

The system described in Eq. (2.6) is exactly equivalent to the original ODE system. Equation 2.6 demonstrates that coarse-graining leads to memory effects. For notational purposes, define
\[
F_j(\phi_0, t) = e^{t\mathcal{Q} \mathcal{L}} \mathcal{Q} \mathcal{L} \phi_{0j}, \quad K_j(\phi_0, t) = \mathcal{P} \mathcal{L} F_j(\phi_0, t).
\] (2.7)

By definition, \(F_j(\phi_0, t)\) satisfies the orthogonal dynamics equation
\[
\frac{\partial}{\partial t} F_j(\phi_0, t) = \mathcal{Q} \mathcal{L} F_j(\phi_0, t),
\] (2.8)

where \(F_j(\phi_0, 0) = \mathcal{Q} \mathcal{L} \phi_{0j}\). It can be shown that solutions to the orthogonal dynamics equation are in the null space of \(\mathcal{P}\), meaning \(\mathcal{P} F_j(\phi_0, t) = 0\). A simplification comes from projecting Eq. (2.6) to eliminate the dependence on the noise term,
\[
\frac{\partial}{\partial t} \mathcal{P} \phi_j(\phi_0, t) = \mathcal{P} R_j(\hat{\phi}(\phi_0, t)) + \mathcal{P} \int_0^t K_j(\hat{\phi}(\phi_0, t-s), s) ds.
\] (2.9)

Equations 2.8 and 2.9 provide a closed set of equations for the resolved modes \(\hat{\phi}\). Evaluation of the memory kernel is, however, not tractable as it involves solving a high-dimensional partial differential equation. Instead, Eq. (2.9) provides a starting point for the derivation of mathematically consistent closure models.

3. A Short-time Dynamic Approach to Model the Memory Kernel

Previous work by the current authors has suggested that, for coarse-grained simulations of turbulent flow, the memory kernel has a finite support. This insight has been used to construct tractable approximations to the memory kernel. Most notably, a class of finite memory models that evolve an additional set of differential equations for the memory integrand has been investigated. In this work, an alternative zeroth-order model is used. The most straightforward derivation is to use a right-hand side quadrature to the memory integrand and assume a temporal support of \(\tau_p\). In this case, the memory kernel can be simplified as
\[
\mathcal{P} \int_{t - \tau_p}^t e^{s\mathcal{L}} \mathcal{P} \mathcal{L} e^{(t-s)\mathcal{Q} \mathcal{L}} \mathcal{Q} \mathcal{L} \phi_{0j} ds \approx \tau_p e^{t\mathcal{L}} \mathcal{P} \mathcal{L} \mathcal{Q} \mathcal{L} \phi_{0j}.
\] (3.1)

Equation 3.1 will be referred to as the \(\tau\)-model (in contrast to the \(t\)-model (Hald et al. 2000) which assumes long or infinite memory).
An outstanding question for the previously explored finite memory models and the \( \tau \)-model described above is the selection of the memory length \( \tau_P \). Here, a dynamic procedure using the Germano identity is derived for the \( \tau \)-model. To proceed, decompose the resolved variable \( \hat{\phi} \) into two sets such that

\[
\hat{\phi} = \{ \bar{\phi}, \phi' \}, \quad \phi = \{ \bar{\phi}, \phi', \tilde{\phi} \}.
\]

Further, define the sharp cutoff filters \( \mathcal{G} \) and \( G' \) that satisfy

\[
\mathcal{G}\phi = \hat{\phi}, \quad G' \phi = \bar{\phi}.
\]

Note that these filters are not Zwanzig projection operators (i.e., \( \mathcal{G} f(\phi) \neq f(\hat{\phi}) \)) and they do not commute with non-linear functions; instead they act as a traditional sharp spectral cutoff filter. To derive an expression for \( \tau_P \), note that for the zero-variance projection (with fully resolved initial conditions) the memory kernel can be written as

\[
P \int_0^t K_j(\hat{\phi}(s), t-s) ds = \mathcal{G} R_j(\phi) - R_j(\mathcal{G}\phi).
\]

Equation 3.2

\[
\mathcal{G}'\mathcal{P} \int_0^t K_j(\hat{\phi}(s), t-s) ds = [\mathcal{G}' R_j(\phi) - R_j(\mathcal{G}\phi)] + [R_j(\bar{\phi}) - \mathcal{G}' R_j(\hat{\phi})],
\]

where we have used the identities \( \mathcal{G}' \mathcal{G} f(\phi) = \mathcal{G}' f(\phi) \) and \( \mathcal{G}' \phi = \bar{\phi} \). The first term in the RHS is simply the unclosed term that arises from coarse-graining at a level \( \mathcal{G}' \). Equation 3.3 is a statement of the Germano identity. The second bracketed term on the RHS can be computed from the under-resolved simulation. The memory length \( \tau_P \) can be approximated by using the \( \tau \)-model to model the LHS and the first term on the RHS,

\[
\mathcal{G}' e^{t \mathcal{P}_P} \mathcal{L} \mathcal{Q} \mathcal{L} \phi_{0j} = e^{t \mathcal{P}_P} \mathcal{L} \mathcal{Q}' \mathcal{L} \phi_{0j} + [R_j(\bar{\phi}) - \mathcal{G}' R_j(\hat{\phi})],
\]

where \( \mathcal{P}' \) and \( \mathcal{Q}' \) are the corresponding projection/remainder operators for coarse-graining at the level \( \mathcal{G}' \) (i.e., \( \mathcal{P}' f(\phi) = f(\bar{\phi}) \)), \( \tau_P \) is the time-scale for coarse-graining at the level \( \mathcal{P} \), and \( \tau_{P'} \) is the time-scale for coarse-graining at the level \( \mathcal{P}' \). Previous work by the present authors has shown that the memory length is approximately linearly related to the spectral radius of the Jacobian of the resolved variables. In the present work, \( \tau_{P'} \) is scaled by the ratio of largest resolved wavenumber squared (the viscous contribution to the spectral radius is \( \nu k^2 \)) at level \( \mathcal{P} \) to level \( \mathcal{P}' \). The memory length is then determined by equating the subgrid energy transfer between the two scales. For example, in the triply periodic Navier-Stokes equations where the test filter is twice as coarse as the true filter, we use

\[
\tau_P = \frac{\sum_j [R_j(\bar{\phi}) - \mathcal{G}' R_j(\hat{\phi})]}{\sum_j e^{t \mathcal{P}_P} \mathcal{L} \mathcal{Q} \mathcal{L} \phi_{0j} - 4 \sum_j e^{t \mathcal{P}_P} \mathcal{P}' \mathcal{L} \mathcal{Q}' \mathcal{L} \phi_{0j}}.
\]

4. Mori-Zwanzig Model Forms

Mori-Zwanzig-based models for Fourier-Galerkin approximations to the Navier-Stokes equations are considered. The incompressible Navier-Stokes equations subject to rotation are given by

\[
\frac{\partial u_i}{\partial x_i} = 0
\]

(4.1)
Dynamic MZ-SGS model

\[
\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \nu \frac{\partial u_i}{\partial x_j} \right) - 2 \epsilon_{ijk} \Omega_j u_k. \quad (4.2)
\]

In this work we consider triply periodic problems (rotating homogeneous turbulence) and doubly periodic problems (fully developed channel flow). The model derivation will be provided for both formulations in the following sections.

4.1. Triply Periodic Formulation

For triply periodic problems, Eqs. 4.1 and 4.2 can be Fourier-transformed in all directions. The pressure Poisson equation can be directly solved in Fourier space, allowing the governing equations to be written compactly as

\[
\left( \frac{\partial}{\partial t} + \nu k^2 \right) \hat{u}_i(k, t) + \left( \delta_{im} - \frac{k_i k_m}{k^2} \right) \sum_{p+q=k, \ p,q \in F,G} \hat{u}_j(p, t) \hat{u}_m(q, t) + 2 \epsilon_{ijm} (1 + i \frac{k_i k_j}{k^2}) \Omega_j \hat{u}_m(k, t) = 0 \quad k \in F \cup G, \quad (4.3)
\]

where the Fourier modes have been written to belong to the union of two sets (with \(F\) being the resolved set and \(G\) being the unresolved set). Separating the modes into the resolved and unresolved sets yields the reduced system

\[
\left( \frac{\partial}{\partial t} + \nu k^2 \right) \hat{u}_i(k, t) + \left( \delta_{im} - \frac{k_i k_m}{k^2} \right) \sum_{p+q=k, \ p,q \in F} \hat{u}_j(p, t) \hat{u}_m(q, t)
+ 2 \epsilon_{ijm} (1 + i \frac{k_i k_j}{k^2}) \Omega_j \hat{u}_m(k, t) = - \left( \delta_{im} - \frac{k_i k_m}{k^2} \right) \sum_{p+q=k, \ p \in F, q \in G} \hat{u}_j(p, t) \hat{u}_m(q, t) + \sum_{p \neq k} \hat{u}_j(p, t) \hat{u}_m(q, t), \quad k \in F, \quad (4.4)
\]

where

\[
\hat{\tau}_{jm}(k, t) = \sum_{p \neq k} \hat{u}_j(p, t) \hat{u}_m(q, t) + \sum_{p \neq k} \hat{u}_j(p, t) \hat{u}_m(q, t) + \sum_{p \neq k} \hat{u}_j(p, t) \hat{u}_m(q, t).
\]

Note that, in Fourier space, the pressure term appears as a projection. This projection leads to additional non-linear interactions between the resolved and unresolved scales. Through the use of the Mori-Zwanzig formalism, the RHS of Eq. (4.4) can be alternatively written as a convolution integral

\[
\hat{u}_i(k, t) = \sum_{p \neq k} \hat{u}_j(p, t) \hat{u}_m(q, t) + \int_0^t K(\hat{u}(t), t-s) ds, \quad k \in F \quad (4.5)
\]
The integral is approximated by the model described in Section 2, which requires the evaluation of

\[ e^{tL}PQLQ\hat{u}_i(k, 0) = \left( \frac{-\delta_{im} + \frac{k_i k_m}{k^2}}{L} \right) 
\sum_{p+q = k} \hat{u}_j(p, t) e^{tL}PQL\hat{u}_m(q, 0) - \left( \frac{\delta_{im} + \frac{k_i k_m}{k^2}}{L} \right) 
\sum_{p+q = k} u_m(p, t) e^{tL}PQL\hat{u}_j(q, 0), \] (4.6)

where \( e^{tL}PQLu_j \) is the coarse-grained right-hand side. Note that, while the linear viscous and rotational terms do not appear in the first-order M-Z models, they are present in higher-order terms (i.e., \( PQLQQLu_i \)).

### 4.2. Doubly Periodic Formulation

The construction of Mori-Zwanzig models for fully developed turbulent channel flow is now outlined. The flow is taken to be streamwise \((x)\) and spanwise \((z)\) periodic. The models are constructed by coarse-graining in the periodic directions. No rotational forces are considered. Fourier transforming Eqs. 4.1 and 4.2 in the \(x\) and \(z\) directions yields

\[ \frac{\partial}{\partial x_j} \hat{u}_j(k, t) = 0 \] (4.7)

\[ \frac{\partial}{\partial t} \hat{u}_i(k, t) + \frac{\partial}{\partial x_j} \sum_{p+q = k} \hat{u}_i(p, t) \hat{u}_j(q, t) = -\frac{1}{\rho} \frac{\partial}{\partial x_i} \hat{p}(k, t) + \nu \frac{\partial^2}{\partial x_j^2} \hat{u}_i(k, t), \] (4.8)

where

\[ \frac{\partial}{\partial x_j} = \{ik_1, \partial_y, ik_3\}. \]

Unlike in the triply periodic case, the continuity equation cannot be implicitly satisfied by a simple solution to the pressure Poisson equation in Fourier space. Solutions of the pressure Poisson equation are complicated by inhomogeneity in the \(y\) direction and boundary conditions. However, the effect of the pressure projection on the subgrid scale models for triply periodic problems was confirmed to be minimal. The M-Z models are thus formulated by neglecting the effects induced by coarse-graining the pressure. In this case one can derive

\[ PQLQ\hat{u}_i(k) = -\frac{\partial}{\partial x_j} \sum_{p+q = k} \hat{u}_j(p) PQL\hat{u}_i(q) - \frac{\partial}{\partial x_j} \sum_{p+q = k} \hat{u}_i(p) PQL\hat{u}_j(q), \quad k \in F. \] (4.9)

### 5. Numerical Results

#### 5.1. Computational Details

In the case of rotating homogeneous turbulence, the triply periodic Navier-Stokes equations are solved using a Fourier-Galerkin pseudo-spectral method with an explicit low-storage RK4 time integration scheme. For the channel flow, the Navier-Stokes equations are solved in skew-symmetric form via a Fourier-Chebyshev pseudo-spectral method.
coupled semi-implicit Adams-Bashforth scheme is used for time integration, as in Moin & Kim (1980). The continuity equation is directly enforced at each time-step, bypassing the need for pressure boundary conditions. The main solvers are written in Python and utilize mpi4py for parallelization. All FFT calculations (including the Chebyshev transforms) are de-aliased by the 3/2 rule.

5.2. Rotating Homogeneous Turbulence

Rotating homogeneous turbulence is first discussed. The DNS velocity field is initialized using the Rogallo (1981) procedure. The initial spectrum is taken to be

$$E(k, 0) = \frac{q^2}{2A k_p^{\sigma+1}} k^\sigma \exp\left[-\frac{\sigma}{2} \left(\frac{k}{k_p}\right)^2\right],$$

where $k_p$ is the wavenumber at which the energy spectrum is maximum, $\sigma$ is a parameter set to 4, and $A = \int_0^{\infty} k^\sigma \exp(-\sigma k^2/2)dk$. The parameters used are $\sigma = 4$, $k_p = 5$, and $q^2 = 3$. The DNS simulation is evolved on a 512$^3$ mesh until realistic homogeneous turbulence is present. The resulting filtered field is used for initial conditions in the LES simulations. A summary of computational details is given in Table 1.

Figure 1 shows the evolution of the total resolved kinetic energy in the simulation. The energy decay rate is suppressed by the rotational forces, which introduce significant anisotropy to the turbulence field. The dynamic Smagorinsky model slightly overpredicts the dissipation of energy, but still compares well to the DNS data. The Mori-Zwanzig models slightly underpredict the decay of kinetic energy, but also compare well to the DNS data. The energy spectra at $t = 2.0$ and $t = 3.0$ are shown in Figure 2. The dynamic Smagorinsky and Mori-Zwanzig models again compare well to the DNS data. The dynamic Smagorinsky model slightly underpredicts the energy content at mid to high wavenumbers while the M-Z model slightly overpredicts the energy content.

Although the Smagorinsky and M-Z models produce similar results, the dynamics of the models are significantly different. This is seen by observing the energy transfer induced by the subgrid model, as shown in Figure 3. The dynamic Smagorinsky model is seen to actively remove energy from all wavenumbers. It overpredicts the energy removed for low wavenumbers ($k \leq 20$), but underpredicts the energy removed for highwave numbers. The M-Z-based models act in the opposite fashion, removing too little energy at low wavenumbers (a small amount of energy is seen to be added at low wavenumbers) and removing too much energy at high wavenumbers.

5.3. Channel Flow

M-Z-based LES of channel flow at $Re_\tau = 180$ is now discussed. The solutions are compared to the Smagorinsky model. In the Smagorinsky model, the filter width $\Delta$ is taken to include the Van Driest damping function

$$\Delta = (1 - e^{y^+}/A) \left(\Delta_1 \Delta_2 \Delta_3\right)^3,$$
where $\Delta_i$ is the filter width in the $i$-th direction and $A^+ = 25$. The Smagorinsky constant was set to $C_s = 0.065$. No such explicit damping is used in the dynamic M-Z model.

The LES simulations are evolved using $32 \times 64 \times 32$ resolved modes in the $x, y,$ and $z$ directions, respectively. Simulation parameters are given in Table 2. Statistical properties of the LES solutions are compared to unfiltered DNS data from Moser et al. (1999) in Figure 4. The filtering process will not affect the mean velocity profiles, but the filtered Reynolds stress profiles are expected to be slightly different. The M-Z-based models are seen to offer improved solutions similar to that produced from the wall-damped
Smagorinsky model. In particular, the mean velocity profiles are much improved, and the model correctly reduces the Reynolds stresses.

6. Conclusions

The Mori-Zwanzig formalism provides a mathematical framework to derive closure models in problems that lack scale separation. The appeal of the M-Z-based models is that they are derived directly from the governing equations and require minimal heuristics. Under the assumption that the memory kernel has a short time support, an approximation was derived to represent the impact of the unresolved modes on the resolved modes. A Germano-type dynamical procedure was used to determine the memory length for the $\tau$-model. The model was applied to rotating turbulence and turbulent channel flow. For rotating turbulence, the model was seen to provide accurate predictions for the decay of energy as well as spectral content. The mechanisms through which the subgrid model removes energy from the flow field have qualitative similarities to the DNS data. In the context of channel flow, the M-Z-based model was seen to provide predictions that were similar to that seen from the Smagorinsky model with Van-Driest damping. The
results from the channel are particularly encouraging as they are the first application of M-Z-based models to a non-decaying fluid dynamic system.

The results presented in this work highlight the promise of Mori-Zwanzig-based techniques as the structural form of the closure is imposed by the mathematics of the coarse-graining and not by the specific physics at play. The applicability of M-Z-based methods to more complex problems requires further development and will require a formulation that makes use of specialized scale separation operators. The variational multiscale approach and spectral element method are two such candidates. In addition to pursuing a general framework, we are currently exploring the performance of M-Z-based models for higher Reynolds numbers and are developing tools to further dissect the memory kernel.

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