Epistemic uncertainty in statistical Markovian turbulence models

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1. Motivation and objectives

Diverse arrays of modern applications require accurate predictions of complex turbulent flows. These range from flows across aircraft and inside turbomachinery, over the planet for weather prediction and through the heart for cardiac auscultation, etc. Due to the disparate character of these complex flows, predictive methods must be robust so as to be applicable for most of these cases, yet possessing a high degree of fidelity in each. Furthermore, as the processes of analysis and engineering design involve repeated iterations, the predictive method must be computationally economical. In this light, Reynolds Averaged Navier Stokes (RANS)-based models represent the pragmatic approach for complex engineering flows.

However, the RANS-based modeling paradigm has significant shortcomings. In addition to the well recognized issues of fidelity and realizability for select flows, such models have an inherent degree of uncertainty associated with their predictions for all flows. This uncertainty arises due to specific assumptions utilized in the formulation of the closure. This can be expressed in a hierarchical manner as outlined in Figure 1, wherein each step of model formulation introduces additional variability in the predictions. These can be divided into the uncertainty due to:

The choice of a Markovian closure: Single-point turbulence closures assume that turbulence and its evolution can be described in terms of finite set of local tensors. For instance, in the two-equation model of Jones & Launder (1972), this set is composed of the turbulent kinetic energy and the dissipation rate. Similarly, in the Reynolds stress closure of Hanjalic & Launder (1972), this is composed of the Reynolds stress tensor and the mean gradients. This assumption does not adequately account for the history of the flow and leads to Markovian models attempting to replicate the Non-Markovian dynamics of turbulence. This introduces variability into the model's predictions. Successive steps build upon this uncertainty.

The form of the closure and the closure expression: This additional level of uncertainty arises due to the choice between different RANS closures (zero-/one-/two-equation models, or, a second moment closure). Thence, model formulation involves the choice of the exact closure expression with terms of different orders based on rational mechanics. This step may add further variability to the model prediction. The uncertainty resulting from these steps is typically designated as structural uncertainty.

The nature and the values of coefficients: The appropriation of the best-possible values of the coefficients and their functional form introduces additional uncertainty in the model framework. This would adhere to the classification of parameter uncertainty.

As is exhibited schematically in Figure 1, each level of assumptions may add to the inherent variability of the problem. Furthermore, a specific choice of the closure (or closure

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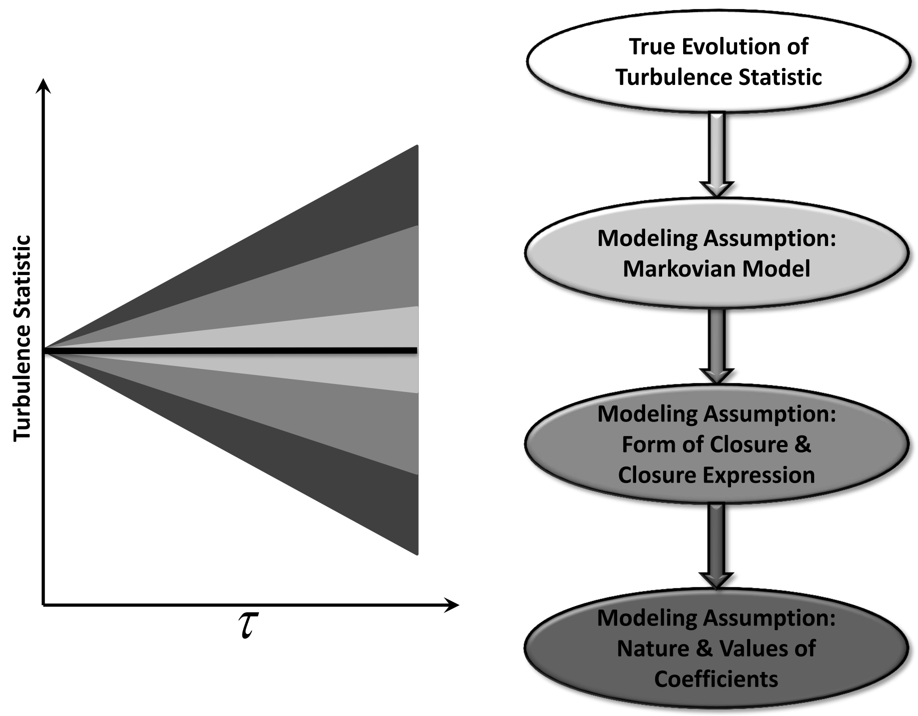


FIGURE 1. Schematic outlining the increment of the degree of uncertainty in predictions with every level of modeling assumptions.

expression, coefficients, etc) may restrict the model predictions to a subset of this space that may not even include the true solution. For instance, two-equation based models have a degree of uncertainty associated with the values of their coefficients. However, for flows with significant streamline curvature, the true evolution of turbulence is not replicable for any values of the coefficients.

The quantifications of margins and uncertainty (QMU) as a characterization of the reliability of the predictions of turbulence models has emerged as a salient subject. A multitude of recent investigations have attempted to quantify the bounds on the uncertainty in the model predictions of quantities of interest. Margheri *et al.* (2014) have focused on parameter uncertainty, using generalized Polynomial Chaos to investigate the sensitivity of the model predictions upon the values of the model coefficients. Cheung *et al.* (2011) and Oliver & Moser (2011) have utilized a Bayesian uncertainty quantification approach to RANS-based models. Herein, the authors attempt to address both structural and parameter uncertainty. In this investigation, we address the intrinsic component of the uncertainty that is independent of the choice of turbulence model or model coefficients. Figure 1 attempts to illustrate this schematically. The true evolution of turbulence is depicted as a dark line. Thereupon, the initial degree of uncertainty arises due to the use of Markovian closures to represent the evolution of turbulence. Due to this limited modeling basis, the evolution of the modeling problem is not unique and a range of evolution is permissible, leading to an incipient grade of uncertainty. Thereon, the choice of modeling paradigm and closure coefficients add on to this uncertainty. In Figure 1, the prediction ranges due to the uncertainty introduced in these subsequent steps is depicted in correspondingly darker shades. While the evolution of the stochastic velocity field governed by the Navier Stokes equations is Markovian, the evolution of the Reynolds stresses is unclosed and non-Markovian (Kraichnan 1959). However, engineering models assume that turbulence and its evolution can be described by local tensors such as the Reynolds stresses, the mean gradients, etc. This assumption enforces all such models to be Markovian. This attempt to model a non-Markovian process via a Markovian closure has its drawbacks. The most obvious are that of fidelity and realizability wherein the model may not be able to replicate the true dynamics of turbulence. A more subtle ramification is that of variability. Ignoring the history of the flow implies that specifying the macro state leads to a unique specification of the micro states: specifically, that all turbulent flows with the same Reynolds stresses will behave identically under similar conditions. As will be shown, this assumption is patently inaccurate. The uncertainty arising due to this Markovian assumption is universal and is independent of the choice of modeling paradigm, expression or coefficients. The best-possible turbulence closure, with an optimal closure expression and coefficients, would still have this degree of uncertainty. Furthermore, this type of uncertainty is not restricted to single-point models. As an illustration, the rapid pressure strain correlation can be expressed as

$$\left\langle p^{(r)} s_{ij} \right\rangle = -\frac{1}{2\pi}\frac{\partial U_k}{\partial x_l}\iiint\limits_D \frac{1}{|\vec{r}|}\left(\frac{\partial^2 R_{il}}{\partial r_j \partial r_k} + \frac{\partial^2 R_{jl}}{\partial r_i \partial r_k}\right) d\vec{r}. \tag{1.1}$$

Thus, the value of this statistic at any location is dependent on the flow conditions at all points in the domain. The true evolution of the Reynolds stress is non-Markovian at any level of countable multi-point statistics. While this investigation focuses on single-point closures, this epistemic uncertainty is extant in multi-point closure approaches as well.

An analogous problem occurs in the specification of the near-wall velocity boundary conditions for LES. Prior investigations in this problem have shown that detailing correct statistics up to the second order at the boundary is insufficient to obtain the correct core flow (Baggett 1997). Imposition of just the mean velocities and mean turbulent stresses at the artificial boundaries leads to unsatisfactory agreement, even in simple channel flow simulations (Nicoud et al. 1998). These investigations have concluded that while estimation of moments beyond the second-order is unnecessary, additional information about the structure of the turbulent flow is imperative to obtain a satisfactory core flow. In a similar vein, just the specification of a finite set of local tensors does not constitute a well-posed problem in the sense of Hadamard (1902) for RANS modeling. At this level of description, the evolution of the real flow is non-unique. We show that there is a broad envelope of possible evolution for the system, often with diametric behavior. The RANS models, being deterministic, may (at best) replicate a singleton member from this family. At this level of specification, the disparity between the broad range of possible evolution for the real flow and the unique evolution predicted by the RANS model introduces epistemic uncertainty in the model's predictions.

Herein, we study this degree of uncertainty in the context of non-local effects in turbulence evolution. Due to the incompressibility condition, pressure has to react instantaneously to changes in the velocity field at any location in the flow domain. Thus, the action of pressure is highly non-local, reflected in the fact that its evolution is governed by a Poisson equation. In any single-point closure, this non-local action is modeled via a basis of local tensors. However, the Reynolds stresses do not describe the complete internal structure of the turbulent flow field. For the same Reynolds stress tensor, the spectrum of the turbulent flow is not uniquely defined. Thus, this choice of a limited basis introduces an inherent degree of variability in the mapping between model predictions and flow evolution. This degree of variability is present in both explicit models for pressure, such as in the second moment closure approach, and also in modeling paradigms where the action of pressure is implicitly contained, such as those adhering to an eddy-viscosity assumption.

The key questions that are addressed involve the nature of this variability. First, we wish to circumscribe the magnitude of this uncertainty. This is a fundamentally important query from an engineering perspective. If this variability introduced due to the single-point modeling assumption is within engineering tolerance, then this investigation is of academic interest only. Additionally, the evolution of this uncertainty magnitude is important as it indicates the time windows wherein classical turbulence models may give predictions of engineering utility. Finally, we establish the dependence of this uncertainty on the initial state of the Reynolds stress tensor and the mean gradient. This provides invaluable guidance regarding the potential accuracy of turbulence closures for different flows.

2. Mathematical formulation

While focusing on the linear aspects of the evolution, the Navier-Stokes system is analyzed in the rapid distortion limit. At the rapid distortion limit, the turbulence-to-mean-shear time scale ratio, Sk/ϵ, is arbitrarily large. In the governing equations, the terms scaling with S dominate, while other terms become negligible in comparison. This causes the non-linear terms, representing the interactions amongst the fluctuating field, to drop out. The consequent rapid distortion equations in physical space are given by

$$\frac{\bar{D}{u'}_j}{\bar{D}t} = -{u'}_i \frac{\partial U_j}{\partial x_i} - \frac{1}{\rho}\frac{\partial p^{(r)}}{\partial x_j}, \tag{2.1}$$

$$\frac{1}{\rho}\nabla^2 p^{(r)} = -2\frac{\partial U_j}{\partial x_i}\frac{\partial {u'}_i}{\partial x_j}. \tag{2.2}$$

In the computations for this investigation, these equations are examined in Fourier space, via the projection

$${u'}_i(\mathbf{x},t) = \sum \hat{u}_i(\boldsymbol{\kappa},t)exp(i\boldsymbol{\kappa}\cdot\mathbf{x}), \quad p^{(r)}(\mathbf{x},t) = \sum \hat{p}(t)(\boldsymbol{\kappa},t)exp(i\boldsymbol{\kappa}\cdot\mathbf{x}). \tag{2.3}$$

In the Fourier analysis, the fluctuations are characterized in terms of the wavenumber vector, $\boldsymbol{\kappa}(t)$ and $\hat{\mathbf{u}}$, $\hat{p}$, the corresponding Fourier amplitudes and pressure coefficients. As Eqs. (2.1)-(2.2) are linear, each Fourier mode evolves independently and hence the equations can be decomposed and written for each mode separately. Starting from the incompressible Navier-Stokes equations at the rapid distortion limit, the modal evolution equations are

$$\frac{d\kappa_l}{dt} = -\kappa_j\frac{\partial U_j}{\partial x_l}, \tag{2.4}$$

$$\frac{d\hat{u}_j}{dt} = -\hat{u}_k\frac{\partial U_l}{\partial x_k}\left(\delta_{jl} - 2\frac{\kappa_j\kappa_l}{\kappa^2}\right), \tag{2.5}$$

and the incompressibility constraint is given by $\hat{\mathbf{u}}\cdot\boldsymbol{\kappa} = 0$. This indicates that the wavenumber vector, $\boldsymbol{\kappa}$, and Fourier amplitude vector, $\hat{\mathbf{u}}$, remain orthogonal to each other. For the solution of these equations, a fourth-order Runge-Kutta solver was utilized. In

Regime of Flow	**Width of Prediction Interval**	**Evolution of Prediction Interval**
Hyperbolic	Significantly Consequential	Exponential Growth
Planar Shear	Moderately Consequential	Linear Growth
Elliptic	Inconsequential	No Growth

TABLE 1. Characteristics of the prediction intervals with respect to the mean gradient

the discussion of the results, we utilize the unit wavenumber vector, $\vec{e} = \vec{\kappa}/|\vec{\kappa}|$. The unit wavenumber vector evolves on S^3 and thus, its phase space is compact and bounded. In the discussion of the results, the mean strain is applied in the $x - y$ plane, whilst the mean axis of rotation is along the $z - axis$. Additionally, for boundedness, the results are reported with respect to the Reynolds stress anisotropies, defined as $b_{ij} = R_{ij}/2k - \sigma_{ij}/3$.

For the results subscribing to the Monte-Carlo paradigm, the samples consist of over 5000 ensembles of Fourier modes, wherein each ensemble consists of over $20,000$ individual modes. In line with the axiom of least bias, the Fourier amplitudes were sampled from a Gaussian distribution with the requisite mean and covariance matrix. Given a Fourier amplitude vector, the corresponding wavenumber vector has to lie on an orthogonal plane to maintain continuity. However, the alignment of the wavenumber vector in this plane is not biased in any manner. Thus, the corresponding wavenumber vectors were selected from a uniform distribution over the orthogonal plane. To report the turbulence statistics, initial conditions of ensembles were generated corresponding to an isotropic initial state of the Reynolds stress tensor.

3. Results

To characterize the uncertainty, we utilize prediction intervals. While confidence intervals are associated with population parameters, prediction intervals correspond to future realizations. In essence, the prediction interval addresses the range of possible evolution of the statistic at a specified level of probability, given the mean gradient and an isotropic initial state of the Reynolds stress tensor. As can be seen in the series of Figures 2(a,b,c), the uncertainty in the predictions, characterized by the width of the prediction interval, is highly dependent on the mean gradient. For hyperbolic streamline flows (Figure 2(a)), there is a significant range of possible evolution for the turbulent kinetic energy. Additionally, this range grows exponentially with respect to time. However, for elliptic streamline flows (Figure 2(c)), the prediction intervals are of insignificant width. Furthermore, the extent of this interval stays constant in its temporal evolution. At the interface of these regimes of flow for a planar sheared mean flow (Figure 2(b)), the prediction interval is moderately substantial and grows with time. However, this growth is linear.

Moving from planar to three-dimensional flows, we consider the cases of a mean flow undergoing axisymmetric contraction and axisymmetric expansion. As can be seen in Figures 3(a,b), the dependence of the predictive variability on the mean gradient is emphasized again. For the case of axisymmetric contraction, the prediction interval is trivial and does not evolve in time. However, for the axisymmetric expansion mean flow, the prediction interval is significant and exhibits growth during the phase of instability in

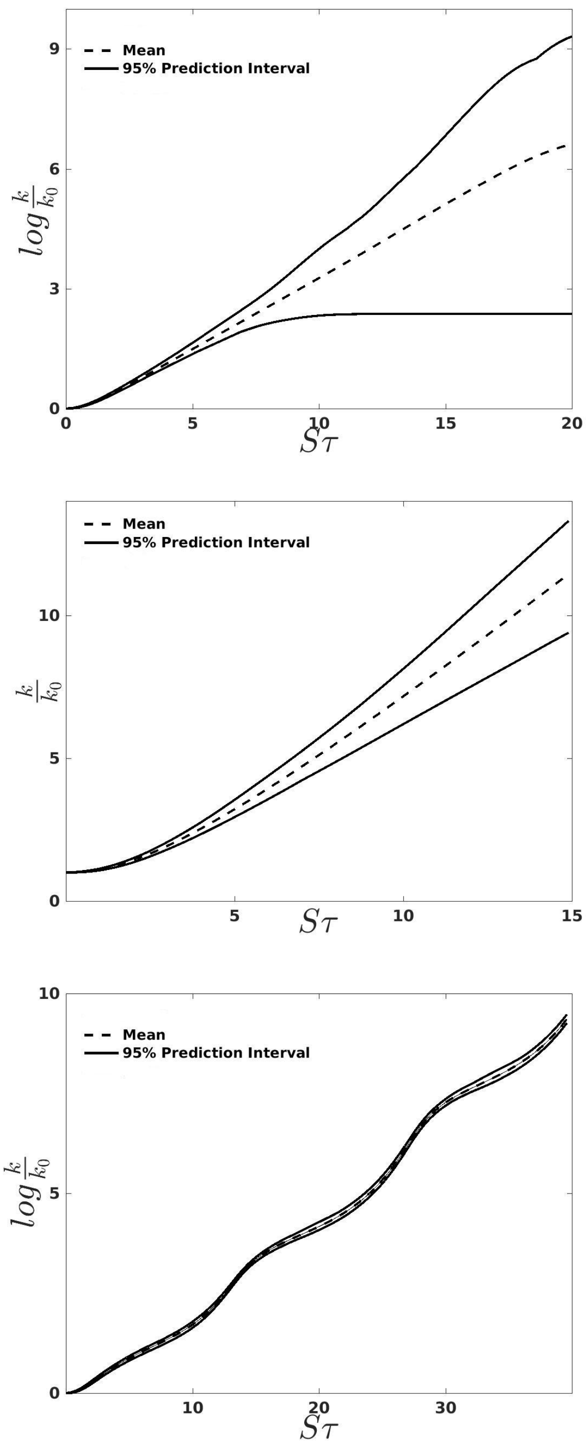
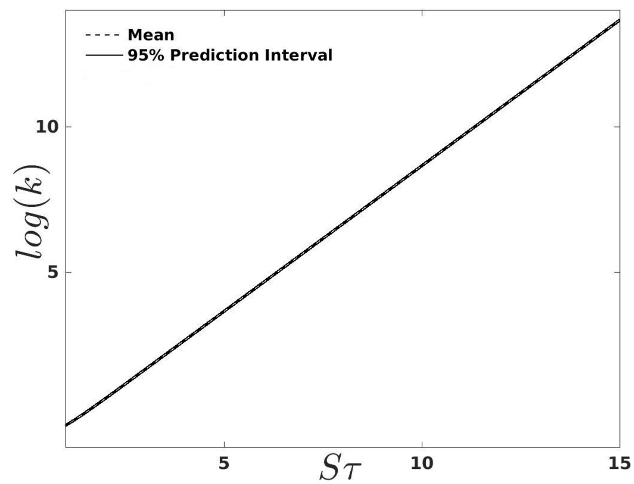


FIGURE 2. Sample mean and 95% prediction intervals for a) representative hyperbolic (plane strain), b) planar sheared and c) representative elliptic mean flow at the rapid distortion limit.



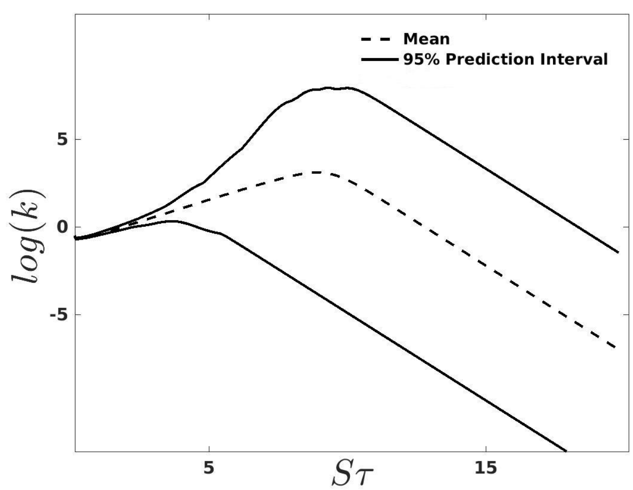


FIGURE 3. Sample mean and 95% prediction intervals for a mean flow undergoing a) axisymmetric contraction, b) axisymmetric expansion at the rapid distortion limit.

the flow. In physical terms, for a flow undergoing axisymmetric contraction, the evolution of the flow for an isotropic state is almost independent of the internal structuring of the turbulent flow field. On the other hand, for a mean flow undergoing axisymmetric expansion, the flow evolution is highly dependent on the internal structure of the flow field. This mean flow case exhibits transient growth. Thus, in a collection of ensembles of modes, each corresponding to an isotropic initial state of the Reynolds stresses, there are ensembles that exhibit kinetic energy growth up to many orders of magnitude. There are also ensembles in this collection that circumvent any growth, and the turbulence decays straightaway.

4. Discussion

The degree of uncertainty for a particular mean flow depends on two features:

a. The stability characteristics of the flow: The flow evolution defines a reflexive map onto the phase space of the fluctuating velocity. Clearly, a volume-expanding map will be able to exhibit a higher degree of variability than a volume-preserving (or contracting) map. For instance, if we consider the case of decaying turbulence, the dissipation process leads to a contraction in phase space with time. Due to this contraction, any variability in flow evolution will decrease in magnitude. In the asymptotic limit, all initial states of the turbulent flow field will end up at the origin where $u = v = w = 0$. In unstable flows, there is no such contraction of the permissible phase space, and such variability in flow evolution can increase. For instance, if the map is uniformly volume expanding, then the variability should increase as well.

b. The topology of the unstable set: For the system being considered, the nature of flow evolution is dependent on the alignment of the wavenumber vectors. A key consideration is the subset of unit wavenumber vectors that exhibit unstable behavior. Herein, the topological property is the measure (more specifically, the zero-dimensionality vis-à-vis the inductive dimension) of these subsets.

For a general hyperbolic streamline flow, such as the case of plane strain, the evolution of the unit wavevectors is exhibited in Figure 4. As can be seen, almost all modes evolve quickly to stationary states along the attractors in the phase space, representing a state of alignment with the extensional principal axis. However, a very small set of modes are initially attracted to the saddle point (at the north pole in the figure). These modes are characterized by their initial alignment along the seperatrix (trajectory joining the repeller to the saddle point). If we observe Figure 4(b), we find that it is this set of modes that exhibit any degree of instability. Thus, the instability of the flow is contingent on this set of modes of zero measure. Accordingly, the evolution of the instability (and the flow) depends on the dynamics of this very small set of modes. A mode having a perfect initial alignment with the seperatrix would stay so and would exhibit sustained unstable behavior. However, in any real flow such perfect alignment is not possible (and there will be minor perturbations due to, say, the nonlinear effects). Thus, these modes are forced off the set of instability and start to decay. Furthermore, as this set is of very small measure, there are very few unstable modes in such a flow and the evolution of each one has significant effect on the flow evolution. The highly sensitive nature of this forcing off phenomenon (Mishra & Girimaji 2010, 2013) determines the time till which the instability persists and the extent of growth of turbulent kinetic energy. This sensitivity is observed in the prediction intervals, where we see that ensembles with very few modes in this unstable set (or very few modes having close to such a perfect alignment) exhibit a much lower degree of instability than ensembles having significant modes with such a perfect alignment and thus, exhibiting exponential growth throughout the span of the simulation. In terms of the Reynolds stress anisotropies, the forcing off of the unstable modes is exhibited as a transfer of turbulent kinetic energy from the R_{22} to the R_{33} component (physically, energy transfer due to pressure out of the plane of applied shear). This can be observed in Figure 5, exhibiting the prediction intervals for the Reynolds stress anisotropies, where this shift is evident in the mean.

For the case of a planar shear mean flow, the topology and measure of the unstable sets is homeomorphic to the hyperbolic flow case. However, the flow instability exhibits polynomial growth (explicitly, linear under the rapid distortion assumption), in contrast to the exponential growth for the hyperbolic flow cases. Thus, we observe that the variabil-

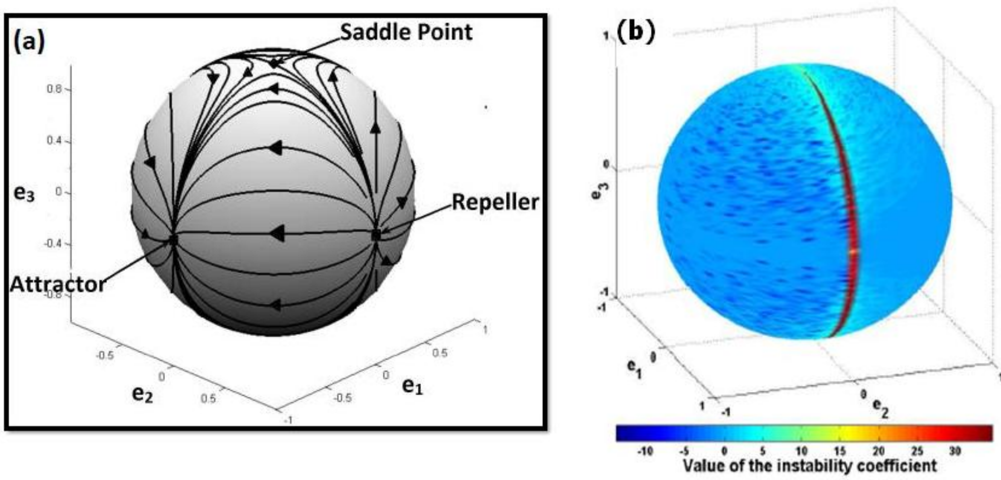


FIGURE 4. a) Phase space and sample evolution trajectories for the unit wavenumber vector under plane strain, b) heat map exhibiting the relationship between modal alignment and modal stability.

Regime of Flow	Measure of set of unstable modes	Nature of the instability
Hyperbolic	Zero Measure	Exponential
Planar Shear	Zero Measure	Linear
Elliptic	Finite Measure	Exponential

TABLE 2. Characteristics of the flow instability with respect to the mean gradient

ity is significant but grows linearly in time. For the elliptic flows, the instability exhibits exponential growth just like the hyperbolic flows. However, the set of unstable modes form bands in unit wavevector space, as exhibited in Figure 6(a). These bands of unstable modes have finite measure and cover a significant ratio of the phase space (unlike the zero measure set for hyperbolic flows) Due to this, there are always unstable wavevector alignments in almost all such elliptic flows. Secondly, wavevector evolution trajectories are not repelled from these unstable zones as they are neutrally stable, exhibited in Figure 6(b). Thus, any modes that are unstable, remain unstable. Clearly, such a system is less sensitive to small random perturbations. This is reflected in the insignificant prediction intervals for elliptic flows.

The qualitative nature of the flow variability characteristics with respect to the mean gradient is outlined in Table 2. A contrast of Tables 1 and 2 provides an unequivocal guide to the variation of the uncertainty in different flow regimes and the underlying rationale. The dependence of the uncertainty on the mean gradient is schematically outlined in Figure 7(a). In addition to the mean gradient, the magnitude of the uncertainty is contingent upon the initial state of the Reynolds stress tensor. This is exhibited in Figure 7(b). As can be observed, the two component states have lesser variance associated

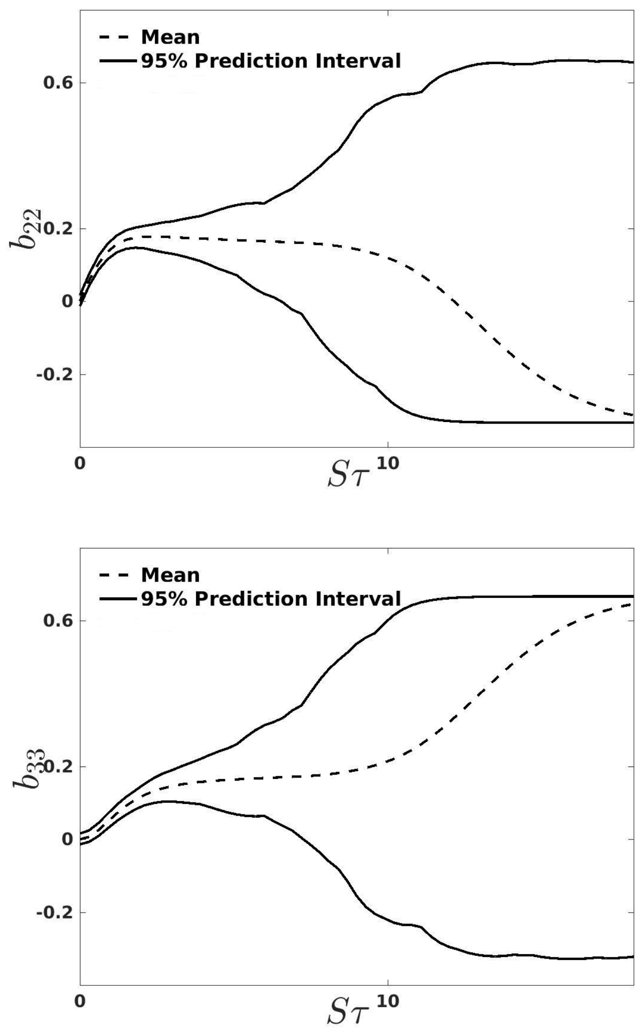


FIGURE 5. Sample mean and 95% prediction intervals for the Reynolds stress anisotropies for a plane strain mean flow.

with them. This favors modeling approaches as a lower degree of uncertainty ameliorates predictions and additionally, the 2C limit arises often in inhomogeneous problems like wall-bounded turbulence. However, as prior investigations have shown, in the vicinity of 2C state, RANS based closures have very unsatisfactory realizability adherence (Mishra & Girimaji 2014). Lack of fidelity, realizability and uncertainty are engendered due to the use of a Markovian closure for a non-Markovian process. In this vein, moving from an isotropic state to one of the limiting states of anisotropy only changes the relative influence of these problems.

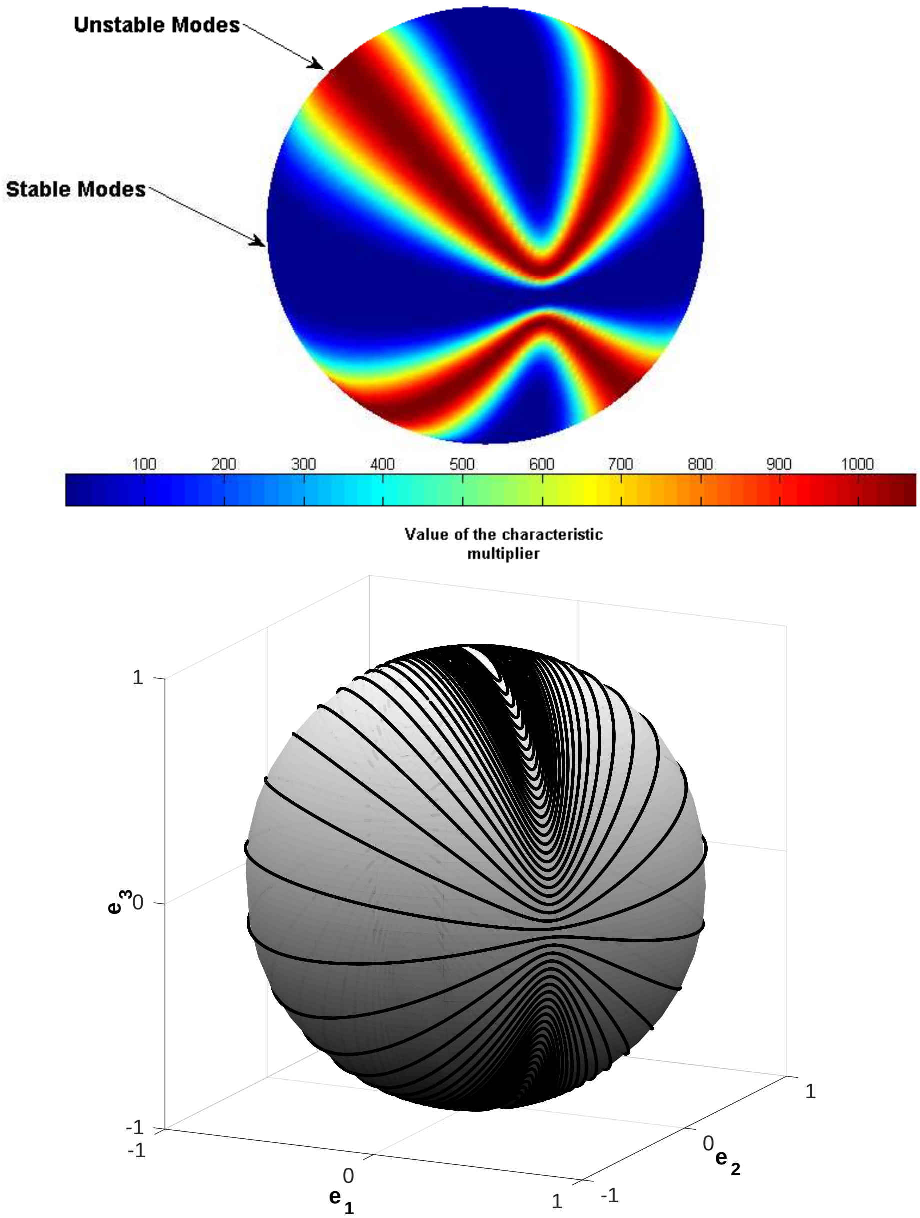


FIGURE 6. a) heat map exhibiting the relationship between modal alignment and modal stability, b)phase space and sample evolution trajectories for the unit wavenumber vector under an elliptic flow.

5. Conclusions

This investigation studies the degree of epistemic uncertainty in the RANS-based modeling paradigm, with an emphasis on the non-local processes in turbulence. In essence, the internal structure of turbulence, outlining the distribution of energy over different length scales and directions, contains information about the history of the flow. The true dynamics of turbulence are decidedly non-Markovian. However, single-point closures as-

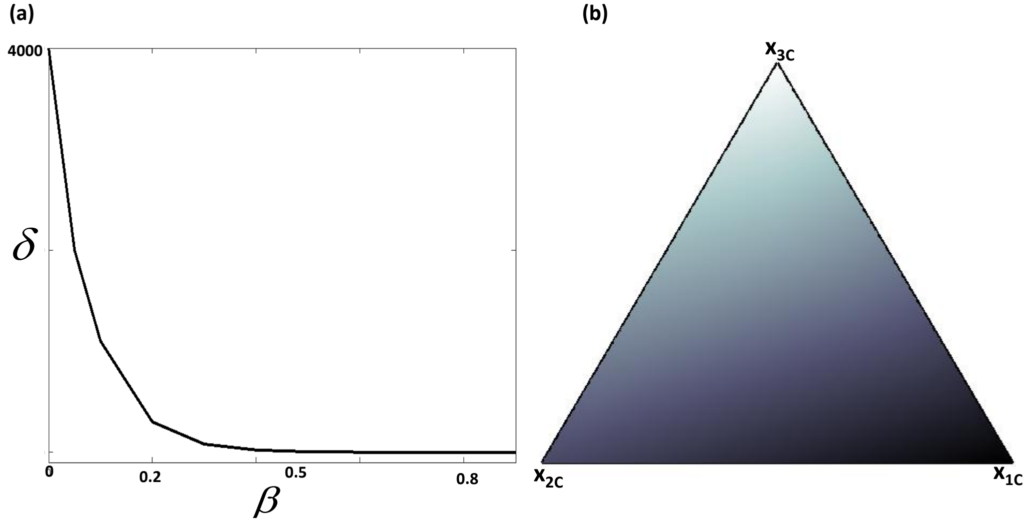


FIGURE 7. a) Variation of width of prediction interval at $\tau = 12$, δ, contra the ellipticity parameter, $\beta = W_{ij}W_{ij}/(S_{ij}S_{ij}+W_{ij}W_{ij})$; b)Barycentric map contours depicting the sensitivity on the initial Reynolds stress.

sume that turbulence and its evolution can be described by a finite set of local tensors. This assumption enforces all such models to be Markovian. This attempt to model a non-Markovian process via a Markovian closure has its drawbacks. The most obvious shortcoming is that of fidelity whereby the model may not be able to replicate the true dynamics of turbulence. A more subtle ramification is that of variability. Ignoring the history of the flow implies that all turbulent flows with the same Reynolds stresses will behave identically under matching gradients. As is shown, this is patently not true, as flows with the same Reynolds stresses can have diametrically different evolutions under the same mean gradient. This range of possible evolution forms an envelope that determines the lowest bound on the uncertainty in the predictions of such models. It is shown that the magnitude and evolution of this uncertainty are highly dependent on the type of mean flow. Traditionally, rotation-dominated flows such as the elliptic streamline flows have been a primary hurdle for single-point modeling vis-à-vis the fidelity of predictions. It is shown that in regard to uncertainty, it is the strain-dominated mean flows such as the hyperbolic streamline flows that are more challenging. All observations are explicitly explained in terms of the nature of the information in spectral space ignored by single-point closures.

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