Quantifying uncertainty in climate change science through empirical information theory

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Quantifying the uncertainty for the present climate and the predictions of climate change in the suite of imperfect Atmosphere Ocean Science (AOS) computer models is a central issue in climate change science. Here, a systematic approach to these issues with firm mathematical underpinning is developed through empirical information theory. An information metric to quantify AOS model errors in the climate is proposed here which incorporates both coarse-grained mean model errors as well as covariance ratios in a transformation invariant fashion. The subtle behavior of model errors with this information metric is quantified in an instructive statistically exactly solvable test model with direct relevance to climate change science including the prototype behavior of tracer gases such as CO_2. Formulas for identifying the most sensitive climate change directions using statistics of the present climate or an AOS model approximation are developed here; these formulas just involve finding the eigenvector associated with the largest eigenvalue of a quadratic form computed through suitable unperturbed climate statistics. These climate change concepts are illustrated on a statistically exactly solvable one-dimensional stochastic model with relevance for low frequency variability of the atmosphere. Viable algorithms for implementation of these concepts are discussed throughout the paper.

model errors | practical algorithms | unbiased empirical estimates

The climate is an extremely complex coupled system involving significant physical processes for the atmosphere, ocean, and land over a wide range of spatial scales from millimeters to thousands of kilometers and time scales from minutes to decades or centuries (1, 2) Climate change science focuses on predicting the coarse-grained planetary scale long time changes in the climate system due to either changes in external forcing or internal variability such as the impact of increased carbon dioxide (3) For several decades the predictions of climate change science have been carried out with some skill through comprehensive computational atmospheric and oceanic simulation (AOS) models (1–4) which are designed to mimic the complex physical spatio-temporal patterns in nature. Such AOS models either through lack of resolution due to current computing power or through inadequate observation of nature necessarily parameterize the impact of many features of the climate system such as clouds, mesoscale and submesoscale ocean eddies, sea ice cover, etc. Thus, there are intrinsic model errors in the AOS models for the climate system and a central scientific issue is the effect of such model errors on predicting the coarse-grained large scale long time quantities of interest in climate change science.

The central difficulty in climate change science is that the dynamical equations for the actual climate are unknown. All that is available from the true climate in nature are some coarse-grained observations of functions such as mean or variance of temperature, tracer greenhouse gases such as carbon dioxide, or the large scale horizontal winds. Thus, climate change science must cope with predicting the coarse-grained dynamic changes of an extremely complex system only partially observed from a suite of imperfect models for the climate. Basic questions arise such as the following:

(**A**) How to measure the skill of a given model in reproducing the present climate and predicting the future climate in an unbiased fashion?

(**B**) How to make the best possible estimate of climate sensitivity to changes in external or internal parameters by utilizing the imperfect knowledge available of the present climate? What are the most sensitive parameters for climate change given uncertain knowledge of the present climate?

(**C**) How do coarse-grained measurements of different functionals of the present climate affect the assessments in (**A**, **B**)? What are the weights which should be assigned to different functionals of the present climate as targets to improve the performance of the imperfect AOS models? Which new functionals of the present climate should be observed in order to improve the assessments in (**A**), (**B**)?

With regards to the issues in (**A**), different metrics involving either suitable climate means or variances with the climate mean bias removed (5) or both in combination have been used (6, 7) as well as Bayesian statistics to utilize all the information in an imperfect multimodel ensemble of AOS models (8); these approaches are surveyed recently in ref. 7. These metrics are largely based on rms errors of either means or variances for a collection of variables and are not invariant under changes of variables; in other words, for example, if the geopotential height is used rather than the temperature, for the hydrostatically balanced large scale variables, then the metric of skill changes substantially even though the same physics is being described. Here, empirical information theory (9–11) is utilized systematically with the following goals regarding the issues in (**A**), (**B**), (**C**): (*i*) to provide a systematic framework to address the central issues in (**A**), (**B**), (**C**) which is unbiased and invariant under suitable changes of variables; (*ii*) to develop a simple calculus of empirical information theory, demonstrating how to build effectively computable algorithms in addressing (**A**), (**B**), (**C**) in practical climate models; (*iii*) to illustrate the use of these techniques explicitly on two instructive simplified test climate models with independent interest for climate change science.

Empirical Information Theory and Climate Science

With a subset of variables $\vec{u} \in R^N$ and a family of measurement functionals $\vec{E}_L(\vec{u}) = (E_j(\vec{u}))$, $1 \le j \le L$, for the present climate, following Jaynes, empirical information theory (9, 10) builds the least biased probability measure $\pi_L(\vec{u})$ consistent with the L measurements of the present climate, $\vec{\bar{E}}_L$. There is a unique functional on probability densities (9, 10) to measure this given by the entropy

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$$\mathcal{S} = -\int \pi \ln \pi, \quad [1]$$

and $\pi_L(\vec{u})$ is the unique probability so that $\mathcal{S}(\pi_L(\vec{u}))$ has the largest value among those probability densities consistent with the measured information, $\bar{\vec{E}}_L$. All integrals as in [1] are over the phase space R^N unless otherwise noted. Standard calculations (see ref. 10 for many geophysical examples and applications) show that $\pi_L(\vec{u})$ is given by

$$\pi_L(\vec{u}) = e^{-\alpha_0 - \vec{\alpha}_L \cdot \vec{E}_L(\vec{u})}, \quad [2]$$

where the L Lagrange multipliers $\vec{\alpha}_L = (\alpha_1, \ldots, \alpha_L)$ are chosen so that

$$\bar{\vec{E}}_L = \int \vec{E}(\vec{u}) e^{-\alpha_0 - \vec{\alpha}_L \cdot \vec{E}_L(\vec{u})}, \quad [3]$$

while α_0 is determined by the normalization

$$e^{\alpha_0} = \int e^{-\vec{\alpha}_L \cdot \vec{E}_L(\vec{u})}, \quad [4]$$

needed to guarantee that $\pi_L(\vec{u})$ is a probability density. Here, the variables $\vec{u}$ reflect a choice of the coarse-grained climate statistics. The functionals $\vec{E}(\vec{u})$ measured in [3] can represent both quantities actually observed in the present climate as well as other functionals which measure the actual climate but are hidden from the current measurements. A natural choice for $\vec{E}(\vec{u})$ are all the moments up to some order p, i.e.,

$$E_j(\vec{u}) = \int (\vec{u})^j \pi(\vec{u}), \qquad |j| \le p. \quad [5]$$

For example, measurements of the mean and second moments of the present climate necessarily lead to a Gaussian approximation (10, 12) to the climate from measurements, $\pi_L(\vec{u}) = \pi_G(\vec{u})$. Any model of the climate produces a probability density, $\pi^M(\vec{u})$. The natural way (10, 13) to measure the lack of information in one probability density, $q(\vec{u})$, compared with the true probability density, $p(\vec{u})$, is through the relative entropy, $\mathcal{P}(p,q)$, given by

$$\mathcal{P}(p,q) = \int p \ln\left(\frac{p}{q}\right). \quad [6]$$

This asymmetric functional on probability densities, $\mathcal{P}(p,q)$, has two attractive features (10, 12, 13) as a metric for climate change science : (*i*) $\mathcal{P}(p,q) \ge 0$ with equality if and only if $p = q$; (*ii*) $\mathcal{P}(p,q)$ is invariant under general nonlinear changes of variables.

The first issue to contend with is the fact that $\pi_L(\vec{u})$ is not the actual climate density but only reflects the best unbiased estimate of the present climate given the L measurements, $\bar{\vec{E}}_L$. Let $\pi(\vec{u})$ denote the probability density of the present climate, which is not actually known. Nevertheless,

$\mathcal{P}(\pi,\pi_L)$ precisely quantifies the intrinsic error in using the L measurements of the present climate, $\bar{\vec{E}}_L$. [7]

Consider an AOS model for the present climate with its associated probability density, $\pi^M(\vec{u})$; then the intrinsic model error in the climate statistics is given by

$$\mathcal{P}(\pi,\pi^M). \quad [8]$$

In practice, $\pi^M(\vec{u})$ is determined by no more information than that available in the present climate. Thus, by repeating the reasoning above in [1–3] there is a subset of functionals $\vec{E}_{L'}(\vec{u}) = (E_1(\vec{u}), \ldots, E_{L'}(\vec{u}))$, $L' \le L$ so that

$$\pi^M(\vec{u}) \equiv \pi^M_{L'}(\vec{u}) = e^{-\alpha_0^M - \vec{\alpha}^M_{L'} \cdot \vec{E}_{L'}(\vec{u})}, \quad [9]$$

with α_0^M and $\vec{\alpha}^M_{L'}$ determined as in [3, 4] above with a crucial difference, the model climate $\pi^M_{L'}$ has averaged values $\bar{\vec{E}}^M_{L'}$ which do not necessarily agree with $(\bar{E}_1, \ldots, \bar{E}_{L'})$ for the actual climate due to model error. The most typical case for a climate model is that $\vec{E}^M_{L'}$ reflects the means and variances of the climate variables $\vec{u}$ as predicted by the model so that $L' = 2$ and $\pi^M_2(\vec{u})$ is necessarily a Gaussian distribution (see refs. 10 and 12), i.e., $\pi^M_2(\vec{u}) \equiv \pi_G(\vec{u})$ is uniquely characterized by the predicted climate mean, $\bar{\vec{u}}_M$, and covariance matrix, R_M. On the other hand, $\pi_L(\vec{u})$ represents the idealized least biased estimate for the climate distribution with at least as many actual and hypothetical measurements, $\bar{\vec{E}}_L(\vec{u})$ with $L \ge L'$. Consider a class of imperfect models, $\mathcal{M}$, for the climate, the best climate model for the coarse-grained variable $\vec{u}$ is the $M_* \in \mathcal{M}$ so that the true climate has the smallest additional information beyond the modeled climate distribution $\pi^{M_*}(\vec{u})$, i.e.,

$$\mathcal{P}(\pi,\pi^{M_*}) = \min_{M \in \mathcal{M}} \mathcal{P}(\pi,\pi^M). \quad [10]$$

Also, actual improvements in a given climate model with distribution $\pi^M(\vec{u})$ either through higher resolution or improved parameterization resulting in a new $\pi^M_{\text{post}}(\vec{u})$ should result in improved information for the actual climate, so that

$$\mathcal{P}(\pi,\pi^M_{\text{post}}) \le \mathcal{P}(\pi,\pi^M), \quad [11]$$

otherwise, objectively, the model has not been improved compared with the original climate model. While the unbiased metrics proposed in equations **8–11** for quantifying uncertainty in the present climate have an extremely appealing mathematical basis, they suffer from a major defect, the climate statistical distribution, $\pi(\vec{u})$, is unknown and $\mathcal{P}(\pi,\pi^M)$ cannot be calculated directly. There is an important general mathematical fact established on pages 3 and 4 of ref. 14, which can be utilized to circumvent these major difficulties:

Fact1: A)

$$\mathcal{P}(\pi,\pi^M_{L'}) = \mathcal{P}(\pi,\pi_L) + \mathcal{P}(\pi_L,\pi^M_{L'}) = (\mathcal{S}(\pi_L) - \mathcal{S}(\pi)) + \mathcal{P}(\pi_L,\pi^M_{L'})$$

for $L' \le L$.

B)

With [2] and [9], $\mathcal{P}(\pi_L,\pi^M_{L'})$ is given explicitly by

$$\mathcal{P}(\pi_L,\pi^M_{L'}) = -\mathcal{S}(\pi_L) + \alpha_0^M + \vec{\alpha}^M_{L'} \cdot \bar{\vec{E}}_{L'}. \quad [12]$$

In particular, the unbiased intrinsic error in the finite number of climate measurements in Eq. **7** of the actual climate is exactly the entropy difference. With **Fact1** and a fixed family of L measurements of the actual climate, the optimization principles in equations **10** and **11** can be computed explicitly by replacing the unknown π by the hypothetically known π_L in these formulas so that for example, π^{M_*} in [10] is calculated by

$$\mathcal{P}(\pi_L,\pi^{M_*}_{L'}) = \min_{M \in \mathcal{M}} \mathcal{P}(\pi_L,\pi^M_{L'}). \quad [13]$$

In general in climate change science, there is calibration of the AOS models by comparison with statistics in the present climate (1–4) and $L = L'$ in these approximations for [**13**]; in other words, the AOS models attempt to use all the available observed climate information. Now, suppose new observations of the climate became available so that $L > L'$, then according to **Fact1**,

$$\mathcal{S}(\pi_L) + \mathcal{P}(\pi_L, \pi^M_{L'}) = \mathcal{S}(\pi_{L'}) + \mathcal{P}(\pi_{L'}, \pi^M_L). \quad [14]$$

Because π_L involves more climate measurements than $\pi_{L'}$, it follows immediately that the absolute uncertainty satisfies $\mathcal{S}(\pi_L)) < \mathcal{S}(\pi_{L'}))$ so from [**14**]

$$\mathcal{P}(\pi_L, \pi^M_{L'}) > \mathcal{P}(\pi_{L'}, \pi^M_{L'}), \quad [15]$$

and there is an increase of uncertainty of all the current AOS models, $\pi^M_{L'}$, due to the additional new measurements of the present climate; thus the current AOS models need to be recalibrated for their skill according to equations **10**, **11**. Clearly, the most appealing way to recalibrate the current climate models and improve them simultaneously is through active "on the fly" filtering or data assimilation (15), which is a systematic way to address the issues in (**B**), (**C**) using empirical information theory.

Algorithms for Effective Calculation of the Empirical Metrics for Climate Uncertainty

The most practical setup for applying the framework of empirical information theory developed above to the calibration of contemporary AOS models arises when both the climate measurements and the model measurements involve only the mean and covariance of the variables $\vec{u}$ so that π_L is Gaussian with climate mean $\bar{\vec{u}}$ and covariance R while π^M is Gaussian with model mean $\bar{\vec{u}}_M$ and covariance R_M. In this case, $\mathcal{P}(\pi_L, \pi^M)$ has the explicit formula (10, 16, 17)

$$\mathcal{P}(\pi_L, \pi^M) = \left[\frac{1}{2}(\bar{\vec{u}} - \bar{\vec{u}}_M)^*(R_M)^{-1}(\bar{\vec{u}} - \bar{\vec{u}}_M)\right] + \left[-\frac{1}{2}\log\det(RR_M^{-1}) + \frac{1}{2}(\mathrm{tr}(RR_M^{-1}) - N)\right]. \quad [16]$$

Note that the first term in brackets in [**16**] is the signal, reflecting the model error in the mean but weighted by the inverse of the model covariance, R_M^{-1} while the second term in brackets, the dispersion, involves only the model error covariance ratio, RR_M^{-1}. There is extensive use of this signal-dispersion decomposition and its generalizations in quantifying uncertainty in ensemble predictions with perfect models (16–19). The role of these different contributions to the model error in the climate calibration metric is illustrated below in prototype climate test models. The intrinsic metric in [**16**] is invariant under any (linear) change of variables which maps Gaussian distributions to Gaussians and the signal and dispersion terms are individually invariant under these transformations; this property is very important for unbiased AOS model calibration. The formula in [**16**] with firm mathematical underpinning is our proposed answer to the interesting discussion at the end of ref. 7 regarding the search for a climate calibration metric for AOS models including both means and variances systematically with unbiased invariant properties. Improved future measurements of the climate and the AOS models might involve higher moments of coarse-grained variables, $\vec{u}$, such as the skewness and kurtosis as in [**5**]. There is a practical theory for bounds and algorithms (12, 16) with major recent advances in the algorithms to implement (20–23) **Fact 1** A), B) in the AOS model calibration principles in [**10**, **11**] in this non-Gaussian setting. Also, here for simplicity in exposition, the important issues of observation errors in measuring $\bar{\vec{E}}_L$ in the present climate are ignored; these issues have been studied systematically for the information metrics for calibration using equations **10**–**13** in ref. 24 and applied to finite member ensemble prediction. The work in ref. 24 provides an explicit link between the AOS model calibration metric proposed here and further practical developments on the issues in [**1**] utilizing Bayesian statistical theory (25, 26). Having discussed the important issue of AOS model calibration in the present climate, the next topic is systematic ways to assess climate change using empirical information.

Empirical Theory for Finding the Most Sensitive Climate Change Directions from the Present Climate

An important question in climate change science is how to assess the most sensitive directions for climate change given the imperfect AOS models for the present climate. To quantify these most sensitive directions for climate change, consider a family of parameters $\vec{\lambda} \in R^p$ with $\pi_{\vec{\lambda}}$ the true climate that occurs and $\vec{\lambda}$ normalized so that $\vec{\lambda} = 0$ corresponds to the present day climate distribution, $\pi(\vec{u})$. In practice $\vec{\lambda}$ can consist of external parameters such as changes in forcing or parameters of internal variability such as a change in dissipation. The uncertainty of the present climate in measuring the perturbed climate, $\pi_{\vec{\lambda}}(\vec{u})$, is given by $\mathcal{P}(\pi_{\vec{\lambda}}, \pi)$ and the most sensitive perturbed climate is the one with largest uncertainty of the present climate

$$\mathcal{P}(\pi_{\vec{\lambda}_*}, \pi) = \max_{\vec{\lambda} \in R^p} \mathcal{P}(\pi_{\vec{\lambda}}, \pi). \quad [17]$$

Here, the issue of calculating the most sensitive perturbations for the present climate through statistics of the present climate including the role of imperfect model errors is addressed through the framework of empirical information theory under the tacit assumption that $\pi_{\vec{\lambda}}$ is differentiable in the parameter $\vec{\lambda}$ (see refs. 27–29 for a discussion). Since $\pi_{\vec{\lambda}}|_{\vec{\lambda}=0} = \pi$, for small values of $\vec{\lambda}$,

$$\mathcal{P}(\pi_{\vec{\lambda}}, \pi) = \vec{\lambda} \cdot I(\pi)\vec{\lambda} + O(|\vec{\lambda}|^3), \quad [18]$$

where $\vec{\lambda} \cdot I(\pi)\vec{\lambda}$ is the quadratic form in $\vec{\lambda}$ given by the Fisher information (11, 14, 28, 30)

$$\vec{\lambda} \cdot I(\pi)\vec{\lambda} = \int \frac{(\vec{\lambda} \cdot \nabla_{\vec{\lambda}}\pi)^2}{\pi}. \quad [19]$$

It is understood in [**19**] and below that all gradients are evaluated at the present climate, $\vec{\lambda} = 0$. Thus, if the present climate distribution, $\pi(\vec{u})$, is known exactly, as well as $\vec{\lambda} \cdot \nabla_{\vec{\lambda}}\pi$, then we have

Fact2: With [**17**], the most sensitive climate change direction occurs along the unit direction $\vec{e}^*_\pi \in R^p$ which is associated with the largest eigenvalue, λ^*_π, of the quadratic form in [**19**]. **[20]**

While this is the theoretical solution to the climate sensitivity of the present climate, it is hampered by both our lack of information in both the present climate and for the gradients, $\vec{\lambda} \cdot \nabla_{\vec{\lambda}}\pi$. The abstract formula in [**19**] is useful as a platonic ideal for climate change science and simplifies considerably when the observed climate distribution $\pi_L(\vec{u})$ defined by $\bar{\vec{E}}_L(\vec{u})$ in [**3**, **4**] is utilized for the present and perturbed climates. We have the following

$$\textbf{Fact3}: \mathcal{P}(\pi_{\vec{\lambda},L}, \pi_L) = \vec{\lambda} \cdot I(\pi_L)\vec{\lambda} + O(|\vec{\lambda}|^3), \quad [21]$$

with

$$\vec{\lambda} \cdot I(\pi_L)\vec{\lambda} = (\vec{\lambda} \cdot \nabla_{\vec{\lambda}}\bar{\vec{E}}_L)^T \mathcal{C}_L^{-1} \vec{\lambda} \cdot \nabla_{\vec{\lambda}}\bar{\vec{E}}_L, \quad [22]$$

and $\mathcal{C}_L$ is the $L \times L$ climate correlation matrix

$$\mathscr{C}_L = \overline{(\vec{E}_L(\vec{u}) - \bar{\vec{E}}_L)(\vec{E}_L(\vec{u}) - \bar{\vec{E}}_L)^T}, \quad [23]$$

with $\bar{F}(\vec{u}) = \int F(\vec{u})\pi_L$. If fewer measurements $L' \le L$ are available, then **Fact 3** applies to produce the quadratic form $\vec{\lambda} \cdot I(\pi_{L'})\vec{\lambda}$. In practice, it is also interesting to compute the compressed quadratic form involving fewer measurements, $L' \le L$ with the approximate climate π_L, $\vec{\lambda} \cdot I(\pi_L)\vec{\lambda}$ with

$$\vec{\lambda} \cdot I(\pi_L)\vec{\lambda} = (\vec{\lambda} \cdot \nabla_{\vec{\lambda}}\bar{\vec{E}}_{L'})^T \mathscr{C}_L^{-1} \vec{\lambda} \cdot \nabla_{\vec{\lambda}}\bar{\vec{E}}_{L'}, \quad [24]$$

where $\vec{E}_{L'} = (E_1,\ldots,E_{L'},0,\ldots,0)^T$. The compressed quadratic form in [**24**] is relevant in determining the important practical information regarding whether, for example, changes in the mean climate statistics alone determine the most sensitive directions of climate change. Obviously, the same formulas in [**22**, **23**] can be applied also to any AOS model by utilizing π_L^M in [**22**, **24**]. For such a climate model, one can calculate the unknown information $\nabla_{\vec{\lambda}}\bar{\vec{E}}_L(\vec{u})$ through statistics of the present modeled climate from a suitable version of algorithms based on the fluctuation-dissipation theorem (FDT) (see refs. 14, 27, 28, and 31–38). There is even a systematic use of Fisher information for the most sensitive perturbation direction for linear response based on FDT (14, 28) which also applies to time varying ensemble predictions in a climate change scenario. Of course, the most crucial issue for the AOS models is whether the eigenvector associated with the largest eigenvalue with model error of the quadratic forms in [**22**, **24**] is suitably close to the actual sensitive direction, $\vec{e}_\pi^*$, associated with [**19**]; in other words, are the eigenvectors associated with the largest eigenvalue of the quadratic forms $I(\pi_L)$, $I(\pi_{L'})$, $I_{L'}(\pi_L)$, and $I_{L'}(\pi_{L'}^M)$ close to $\vec{e}_\pi^*$? Lack of space prevents a detailed development here and instead these issues are demonstrated explicitly next in an instructive model. The use of Fisher information here for the sensitive climate change directions is physics based through [**17**, **18**] rather applied as conventionally used in statistics. From a purely statistical viewpoint, the leading empirical orthogonal functions carry the most variance and are most sensitive statistically; however, the example of the L-96 model in refs. 34 and 38 shows the most sensitive climate directions do not necessarily carry the largest variance but the sensitive directions carry the dynamical response to a change in external forcing.

In a general mathematical sense, the sensitive directions depend on the coordinate system chosen for the parameters λ and the metric utilized to measure the gradient in refs. 22 and 23; however, in physical applications to climate change, the coordinate parameters such as dissipation and external forcing are clearly defined by very specific physical processes and the metric for these parameters, guided for example by energy principles, is known in advance through the physical setting.

The Most Sensitive Climate Change Directions in a Stochastic Model for Low Frequency Variability

The one-dimensional stochastic models (in Ito form)

$$\frac{du}{dt} = F + au + bu^2 - cu^3 + (A - Bu)\dot{W} + \sigma_A \dot{W}_A, \quad [25]$$

with $\dot{W}$, $\dot{W}_A$ independent white noises and $c > 0$ have been shown to be canonical normal forms for reduced stochastic models for low frequency variability with their general properties developed and applied in ref. 39 to low frequency atmospheric teleconnections; they have exactly solvable probability density functions with changing parameters (39) and have been used recently to demonstrate the high skill of FDT algorithms despite structural instability (27). Here, these models are utilized to illustrate the role of model error and the skill in identifying the most sensitive climate directions through various simpler climate statistical approximations using $I(\pi_L)$, $I(\pi_{L'})$, $I_{L'}(\pi_L)$, and $I_{L'}(\pi_L^M)$ to identify the most sensitive climate change directions. The advantage here is that in these models, we know the perturbed true climate, $\pi_{\vec{\lambda}}$, explicitly from ref. 39 so we also know the true climate change behavior explicitly. Here, the two dimensional parameters $\vec{\lambda} = (F,a)^T \in R^2$ for external forcing and dissipation are the natural parameters which are varied. Parameters for the normal form in [**25**] for the low frequency variability were estimated empirically from actual data projected on a comprehensive atmospheric model in ref. 39 for the North Atlantic Oscillation (NAO), a simplified low frequency teleconnection pattern for climate change science as well as the leading order principal component (PC-1) of the model, which carries the largest energy variance. Various approximations for the climate change response of these patterns utilizing FDT for [**25**] are developed recently in ref. 27. The mean and variance for the climate equilibrium were utilized as the measured climate functionals for identifying the most sensitive perturbation direction, $\vec{e}$, for climate change according to the theory in **Fact 3**. For PC-1, the exact most sensitive direction using [**19**] is given by $\vec{e}_\pi^* = (0.969,0.249)^T$ so that the projection on changes in external forcing is roughly 80% and this is reproduced exactly by the full two moment estimator through the formula in **Fact 3**; this is not surprising because $A = B = 0$ in [**25**], see *SI Text*. The functional with model error which utilizes the mean and covariance but a Gaussian approximate climate has the predicted most sensitive direction, $\vec{e}_G^* = (0.937,0.349)^T$ which has an error of 6.0° in the angle with $\vec{e}_\pi^*$; the model error functional using only the mean alone for climate sensitivity but the non-Gaussian climate as in [**23**] yields $\vec{e}_1^* = (0.989,0.150)^T$ with an error of −5.8° in the angle with $\vec{e}_\pi^*$. While the stochastic model for PC-1 is most sensitive to changes in external forcing, in contrast the most sensitive perturbation direction for the NAO is $\vec{e}_\pi^* = (-0.076,0.997)$ and is overwhelmingly dominated by changes in dissipation. Remarkably, all three approximations reproduce $\vec{e}_\pi^*$ here exactly within three significant figures. The *SI Text* both presents the details of these calculations and tables illustrating 16 different cases of [**25**] with both academic and practical interest as described here.

Finally, we complete this section by sketching the detailed calculations which lead us to **Fact 3** in [**22**, **23**] because [**24**] is an immediate consequence of **Fact 3**. With the approximate climate statistics defined by $\bar{\vec{E}}_L(\vec{\lambda})$ in [**3**, **4**], which determines $\pi_{L,\vec{\lambda}}$ in [**2**], the Lagrange multipliers $\alpha_0(\vec{\lambda})$, $\vec{\alpha}_L(\vec{\lambda})$ are regarded as functions of $\vec{\lambda}$ so that

$$\frac{((\vec{\lambda} \cdot \nabla_{\vec{\lambda}})\pi_{L,\vec{\lambda}})^2}{\pi_{L,\vec{\lambda}}} = \left((\vec{\lambda} \cdot \nabla_{\vec{\lambda}})(\alpha_0(\vec{\lambda}) + \vec{\alpha}_L(\vec{\lambda}) \cdot \vec{E}_L(\vec{u}))\right)^2 \pi_{L,\vec{\lambda}}. \quad [26]$$

Differentiating [**3**] and [**4**] with respect to $\vec{\lambda}$ yields

$$\nabla_{\vec{\lambda}}\bar{\vec{E}}_L = -\mathscr{C}_L \nabla_{\vec{\lambda}}\vec{\alpha}_L(\vec{\lambda}), \quad [27]$$

with the correlation matrix $\mathscr{C}_L$ in [**23**]. Inserting [**27**] into [**26**] and performing the required integration over $\vec{u}$ in the definition of $I(\pi_L)$ in [**19**] directly yields [**22**, **23**] from **Fact 3**.

Test Models for Climate Change Science Illustrating Features of the Information Metric for Model Error and Climate Uncertainty

Here we introduce a family of test models for climate change science which have direct qualitative relevance for actual observed features for tracers in the atmosphere (40, 41) with the additional attractive feature of exactly solvable statistics for the mean and covariance (37, 42, 43) with many degrees of freedom despite the inherent statistical nonlinearity. Thus, they are physically relevant unambiguous test models for uncertainty in climate change science (37). The role of model error and the use of the information metric described earlier in **[16]** are demonstrated in an unambiguous fashion below for these test problems with direct analogues of the actual climate and an AOS model with model error. The models have a zonal (east-west) mean jet, $U(t)$, a family of planetary and synoptic scale waves with north-south velocity $v(x,t)$ with x, a spatially periodic variable representing a fixed midlatitude circle in the east-west direction, and tracer gas $T(x,t)$ with a north-south environmental mean gradient α and molecular diffusivity κ (40, 41). The dynamical equations for these variables are

$$\begin{aligned} &\text{A)}\quad \frac{dU}{dt} = -\gamma U + f(t) + \sigma \dot{W}, \\ &\text{B)}\quad \frac{\partial v}{\partial t} = P\left(\frac{\partial}{\partial x}\right)v + \sigma_v(x)\dot{W}_v + f_v(x,t), \\ &\text{C)}\quad \frac{\partial T}{\partial t} + U(t)\frac{\partial T}{\partial x} = -\alpha v(x,t) + \kappa \frac{\partial^2 T}{\partial x^2}, \end{aligned} \qquad \textbf{[28]}$$

The functions $f(t), f_v(x,t)$ are known time periodic functions with period of 1 yr reflecting the changing external forcing of the seasonal cycle, while $\dot{W}, \dot{W}_v$ represent random white noise fluctuations in forcing arising from hidden nonlinear interactions and other processes (15, 44). The equation in **[28]** for the turbulent planetary waves is solved by Fourier series with independent scalar complex variable versions of the equation in **[28]** A) for each different wave number k (15, 44); in Fourier space the operator $\hat{P}_k$ has the form $\hat{P}_k = -\gamma_k + i\omega_k$ with frequency $\omega_k = \frac{\beta k}{k^2+F_s}$ corresponding to the dispersion relation of baroclinic Rossby waves and dissipation $\gamma_k = \nu(k^2 + F_s)$ where β is the north-south gradient of rotation, F_s is the stratification, and ν is a damping coefficient; the white noise forcing for **[28]** B) is chosen to vary with each spatial wave number k to generate an equipartition energy spectrum for planetary scale wave numbers $1 \le |k| \le 10$ and a $|k|^{-5/3}$ turbulent cascade spectrum for $11 \le |k| \le 52$ (see refs. 15 and 44). The zonal jet $U(t) = \bar{U}(t) + U'(t)$, where $\bar{U}(t)$ is the climatological periodic mean with γ, and σ chosen so that this jet is strongly eastward while the random fluctuations, $U'(t)$, have a standard deviation consistent with such eastward dynamical behavior. See Fig. 1 for the mean zonal jet as a function of time of year and the energy spectrum of the Rossby waves. While $U(t)$, $v(x,t)$ have exactly solvable Gaussian statistics mimicking features of the atmosphere, the tracer $T(x,t)$ has non-Gaussian behavior due to the nonlinear tracer flux term $U'(t)\frac{\partial T}{\partial x}$ in **[28]** C); nevertheless, $T(x,t)$ has exactly solvable mean and covariance climate statistics following (37, 42, 43) with explicit formulas listed in the *SI Text*. These procedures define the exactly solvable statistics for the perfect climate. Actual AOS models utilized in climate change science typically have too much additional damping and we mimic this here in the representative AOS models by increasing the two parameters γ, ν for **[28]** A), B) by 10% to γ_M, ν_M to define the AOS model velocity fields $U^M(t) = \bar{U}^M(t) + U^{M,\prime}(t)$, $v^M(x,t)$, with model error. The turbulent tracer in an AOS model is usually calculated roughly by an eddy diffusivity (1–4) $\overline{U^{M,\prime}(t)\frac{\partial T}{\partial x}} = -\kappa_M^* T_{xx}$ and in the present models there is an exact explicit formula for κ_M^* as shown in the *SI Text*. Thus, the AOS model tracer satisfies

$$\frac{\partial T^M}{\partial t} + \bar{U}(t)\frac{\partial T^M}{\partial x} = -\alpha v^M(x,t) + (\kappa + \kappa_M^*)\frac{\partial^2 T^M}{\partial x^2}. \qquad \textbf{[29]}$$

We also increase κ_M^* by 10% over its predicted value. With **[29]**, the AOS model with (U^M, v^M, T^M) has Gaussian statistics so the model error information metric in **[16]** applies directly. Next, we briefly assess the signal and dispersion contributions to the model error for the zonal velocity field U and tracer T with various coarse-grained climate measurements in space to illustrate simple features of the information metric. In Fig. 2, the ratio of the signal to the total lack of information for U together with three spatial coarse-grainings T_1, $T_{1\text{–}3}$, and $T_{1\text{–}5}$ involving the first, first three, and first five Fourier modes of T is shown as a function of the time of year. To help with the physical interpretation, the reader should regard $t = 0$ as the late fall so that there is a peak of the mean jet in winter and a secondary peak in summer through the year. With U and T_1, the signal dominates the information metric but less significantly in the fall and spring; the attempt to calculate a more regional distribution of T through the AOS model through only the first five Fourier modes, $T_{1\text{–}5}$ is dominated by the dispersion by a factor of two while the case of $T_{1\text{–}3}$ is intermediate between these extremes. The total relative entropy in the model error from **[16]** increases from order 2.5 for U and T_1 to order 25 for U and $T_{1\text{–}3}$, to order 250 for U and $T_{1\text{–}5}$ which with Fig. 1 illustrates the increasing importance of the dispersion

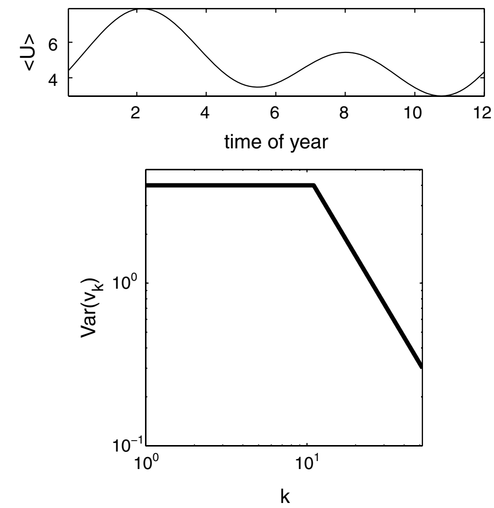

Fig. 1. (*Top*) Equilibrium mean of the zonal jet U as a function of time of year. (*Bottom*) Equilibrium energy spectrum of the shear flow v_k, the first part of the spectrum is white noise and the second part is a cascade $\sim|k|^{-5/3}$.

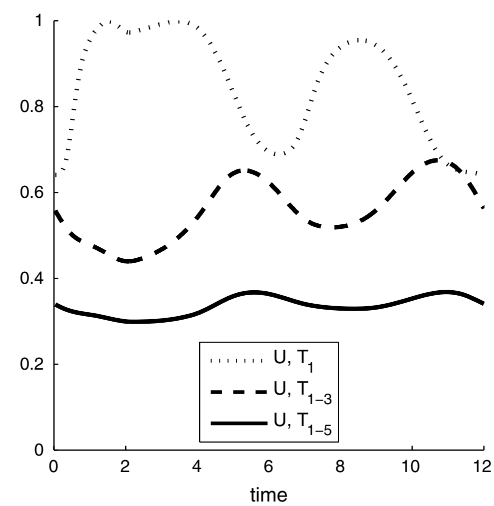

Fig. 2. Fraction of the signal part to the total lack of information $\mathcal{P}$ for the model with the jet U and either only one mode of scalar T_1 (dotted line) or three modes of scalar $T_{1\text{–}3}$ (dashed line) or five modes of scalar $T_{1\text{–}5}$ (solid line).

model errors when more fine scale information for T is required. See the *SI Text* for the details and more examples.

Future Directions and Concluding Discussion

A perspective on quantifying uncertainty in climate change science has been developed here systematically through empirical information theory (9–11, 14). A practical information metric with firm mathematical underpinning to quantify model error in the climate has been proposed here in [**16**] which incorporates both coarse-grained mean model errors as well as covariance ratios in an invariant fashion (7). The subtle behavior of model errors with this information metric has been quantified in an instructive statistically exactly solvable test model with direct relevance to climate change science (40, 41) which includes the prototype behavior of a tracer gas such as CO_2. Formulas to locate the most sensitive climate perturbation directions using only the present climate have been developed and tested on a statistically exactly solvable one-dimensional stochastic model with relevance for the low frequency variability of the atmosphere (27, 39). These formulas for most sensitive perturbation directions just involve finding the eigenvector associated with the largest eigenvalue of a quadratic form computed through the unperturbed climate statistics. For AOS models, a direct link with parallel developments for climate change science based on FDT (14, 27, 28, 31–38) has been developed. In this fashion, several aspects of the central issues in the list of basic questions from the beginning of this article regarding quantifying uncertainty for climate change science have been addressed here. The present approach blends naturally with Bayesian statistical methods (25, 26, 30) to address important future directions such as active data assimilation (15) to improve AOS climate model error "on the fly" and estimate statistical uncertainties in observational climate measurements as well as quantifying the additional uncertainty in multimodel ensembles (8). The present framework also applies to ensemble prediction with model error.

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