

2014 Final Report: Low Frequency Predictive Skill Despite Structural Instability and Model Error

ONR Basic Research Challenge

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LONG-TERM GOALS

Identifying and quantifying the effects of uncertainty in long range prediction for complex systems such as long range weather forecasting or short term climate change,

OBJECTIVES

The development of new techniques to quantify the response of complex systems to changes in external conditions, to assess the behavior of imperfect models for long range forecasting for complex systems and their model errors, and to devise new strategies to mitigate these model errors through efficient algorithms. This includes strategies for using data assimilation to make judicious model errors.

APPROACH

The overall approach is to blend mathematical and physical reasoning to give new insight and new techniques for addressing these grand challenge and to develop prototype model problems, which despite their simplicity, capture key features of these complex systems where central issues can be addressed in an unambiguous fashion. The mathematical tools involve ideas from information theory, nonlinear dynamical systems, stochastic and statistical analysis, numerical analysis combined with ideas from statistical physics such as the fluctuation dissipation theorem applied in novel fashion.

PERSONNEL

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WORK COMPLETED

The work completed falls broadly into the following topics with many published results in each area.

- I) Mathematical Techniques for Quantifying Uncertainty in Complex Systems with Model Error with Prototype Applications (Majda, Branicki, Giannakis, Gershgorin, Yuan)
- II) Statistically Accurate Low Order Models for Uncertainty Quantification in Turbulent Dynamical Systems (Majda, Sapsis)
- III) New Algorithms and Techniques for Data Assimilation with Judicious Model Errors which can Capture Intermittent Extreme Events in Complex Systems (Majda, Branicki, Giannakis)
- IV) Algorithms for Response of Complex Dynamical Systems to External Forcing Based on the Fluctuation Dissipation Theorem (Abramov, Majda, Kjerland)

RESULTS

- I) Mathematical Techniques for Quantifying Uncertainty in Complex Systems with Model Error with Prototype Applications

The first three papers set-up and develop an information theoretic framework for identifying and mitigating model errors in long range forecasting.

1. Quantifying Uncertainty in Climate Change Science Through Empirical Information Theory

A.J. Majda (P.I., Courant Institute)
B.Gershgorin (Post doc, Courant Institute)

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 CO₂. Formulas for identifying the most sensitive climate change directions using statistics of the present climate or an AOS model approximation are developed here; they 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.

2. Improving Model Fidelity and Sensitivity for Complex Systems through Empirical Information Theory

A.J. Majda (P.I., Courant Institute)

B.Gershgorin (Post doc, Courant Institute)

In many situations in contemporary science and engineering, the analysis and prediction of crucial phenomena occur often through complex dynamical equations that have significant model errors compared with the true signal in nature. Here, a systematic information theoretic framework is developed to improve model fidelity and sensitivity for complex systems including perturbation formulas and multimodel ensembles that can be utilized to improve both aspects of model error simultaneously. A suite of unambiguous test models is utilized to demonstrate facets of the proposed framework. These results include simple examples of imperfect models with perfect equilibrium statistical fidelity where there are intrinsic natural barriers to improving imperfect model sensitivity. Linear stochastic models with multiple spatiotemporal scales are utilized to demonstrate this information theoretic approach to equilibrium sensitivity, the role of increasing spatial resolution in the information metric for model error, and the ability of imperfect models to capture the true sensitivity. Finally, an instructive statistically nonlinear model with many degrees of freedom, mimicking the observed non-Gaussian statistical behavior of tracers in the atmosphere, with corresponding imperfect eddy-diffusivity parameterization models are utilized here. They demonstrate the important role of additional stochastic forcing of imperfect models in order to systematically improve the information theoretic measures of fidelity and sensitivity developed here.

3. The Link Between Statistical Equilibrium Fidelity and Forecasting Skill for Complex Systems with Model Error

A.J. Majda (P.I., Courant Institute)

B.Gershgorin (Post doc, Courant Institute)

Understanding and improving the predictive skill of imperfect models for complex systems in their response to external forcing is a crucial issue in diverse applications such as for example climate change science. Equilibrium statistical fidelity of the imperfect model on suitable coarse-grained variables is a necessary but not sufficient condition for this predictive skill, and

elementary examples are given here demonstrating this. Here, with equilibrium statistical fidelity of the imperfect model, a direct link is developed between the predictive fidelity of specific test problems in the training phase where the perfect natural system is observed and the predictive skill for the forced response of the imperfect model by combining appropriate concepts from information theory with other concepts based on the fluctuation dissipation theorem. Here a suite of mathematically tractable models with nontrivial eddy diffusivity, variance, and intermittent non-Gaussian statistics mimicking crucial features of atmospheric tracers together with stochastically forced standard eddy diffusivity approximation with model error are utilized to illustrate this link.

These next three papers develop new strategies for coarse-grained long range forecasting with and without model error through information theory and clustering algorithms. The results are applied to ocean models for the double wind driven gyre.

4. Quantifying the Predictive Skill in Long-Range Forecasting. Part I: Coarse-grained Predictions in a Simple Ocean Model

A.J. Majda (P.I., Courant Institute)

D. Giannakis (Post doc, Courant Institute)

An information-theoretic framework is developed to assess the long-range coarse-grained predictive skill in a perfect-model environment. Central to the scheme is the notion that long-range forecasting involves regimes; specifically, that the appropriate initial data for ensemble prediction is the affiliation of the system to a coarse-grained partition of phase space representing regimes. The corresponding ensemble prediction probabilities, which are computable using ergodic signals from the model, are then used to quantify through relative entropy the information beyond climatology in the partition. As an application, the authors study the predictability of circulation regimes in an equivalent barotropic double-gyre ocean model using a partition algorithm based on K -means clustering and running-average coarse graining. Besides the established rolled up and extensional phases of the eastward jet, optimal partitions for triennial-scale forecasts feature a jet configuration dominated by the second empirical orthogonal function (EOF) of the streamfunction, as well as phases in which the jet interacts with eddies in higher EOFs. Due to mixing dynamics, the skill beyond three-state models is lost for forecast lead times longer than three years, but significant skill remains in the energy and the leading principal component of the streamfunction for septennial forecasts.

5. Quantifying the Predictive Skill in Long-Range Forecasting. Part II: Model Error in Coarse-Grained Markov Models with Application to Ocean-Circulation Regimes

A.J. Majda (P.I., Courant Institute)

D. Giannakis (Post doc, Courant Institute)

An information-theoretic framework is developed to assess the predictive skill and model error in imperfect climate models for long-range forecasting. Here, of key importance is a climate equilibrium consistency test for detecting false predictive skill, as well as an analogous criterion describing model error during relaxation to equilibrium. Climate equilibrium consistency enforces the requirement that long-range forecasting models should reproduce the climatology of prediction observables with high fidelity. If a model meets both climate consistency and the analogous criterion describing model error during relaxation to

equilibrium, then relative entropy can be used as an unbiased superensemble measure of the model's skill in long-range coarse-grained forecasts. As an application, the authors investigate the error in modeling regime transitions in a 1.5-layer ocean model as a Markov process and identify models that are strongly persistent but their predictive skill is false. The general techniques developed here are also useful for estimating predictive skill with model error for Markov models of low-frequency atmospheric regimes.

6. **Information Theory, Model Error, and Predictive Skill of Stochastic Models for Complex Nonlinear Systems**

A.J. Majda (P.I., Courant Institute)

D. Giannakis (Post doc, Courant Institute)

Many problems in complex dynamical systems involve metastable regimes despite nearly Gaussian statistics with underlying dynamics that is very different from the more familiar flows of molecular dynamics. There is significant theoretical and applied interest in developing systematic coarse-grained descriptions of the dynamics, as well as assessing their skill for both short- and long-range prediction. Clustering algorithms, combined with finite-state processes for the regime transitions, are a natural way to build such models objectively from data generated by either the true model or an imperfect model. The main theme of this paper is the development of new practical criteria to assess the predictability of regimes and the predictive skill of such coarse-grained approximations through empirical information theory in stationary and periodically-forced environments. These criteria are tested on instructive idealized stochastic models utilizing K-means clustering in conjunction with running-average smoothing of the training and initial data for forecasts. A perspective on these clustering algorithms is explored here with independent interest, where improvement in the information content of finite-state partitions of phase space is a natural outcome of low-pass filtering through running averages. In applications with time-periodic equilibrium statistics, recently developed finite-element, bounded-variation algorithms for nonstationary autoregressive models are shown to substantially improve predictive skill beyond standard autoregressive models.

These next three papers illustrate new strategies for long range forecasting with model errors based on I) 1, 2, 3 for large dimensional systems and systems with extreme events including the development of judicious test problems.

7. **Quantifying uncertainty for climate change and long range forecasting scenarios with model errors. Part I: Gaussian models**

B.Gershgorin (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

Information theory provides a concise systematic framework for measuring climate consistency and sensitivity for imperfect models. A suite of increasingly complex physically relevant linear Gaussian models with time periodic features mimicking the seasonal cycle is utilized to elucidate central issues that arise in contemporary climate science. These include the role of model error, the memory of initial conditions, and effects of coarse graining in producing short-, medium-, and long-range forecasts. In particular, this study demonstrates how relative entropy can be used to improve climate consistency of an overdamped imperfect model by inflating stochastic forcing. Moreover, the authors show that, in the considered models, by improving climate consistency, this simultaneously increases the predictive skill of an imperfect model in

response to external perturbation, a property of crucial importance in the context of climate change. The models range in complexity from a scalar time periodic model mimicking seasonal fluctuations in a mean jet to a spatially extended system of turbulent Rossby waves to, finally, the behavior of a turbulent tracer with a mean gradient with the background turbulent field velocity generated by the first two models. This last model mimics the global and regional behavior of turbulent passive tracers under various climate change scenarios. This detailed study provides important guidelines for extending these strategies to more complicated and non-Gaussian physical systems.

8. Quantifying uncertainty for predictions with model error in non-Gaussian systems with intermittency

M. Branicki (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

Here, we discuss implications of such important effects as intermittency and coarse-graining on the prediction skill of non-Gaussian imperfect models. A suite of increasingly complex nonlinear models, some with intermittent hidden instabilities and with time-periodic features mimicking seasonal cycle, are utilized to illustrate a number of important issues in contemporary climate science. These include the role of model errors due to coarse-graining, moment closure approximations, and the memory of initial conditions in producing short, medium and long range forecasts. Importantly, we show that the predictive skill of the considered imperfect nonlinear models and their sensitivity to external perturbations is improved by assuring their climate consistency via appropriate inflation of the stochastic forcing. Furthermore, the discussed link between climate fidelity and sensitivity via the fluctuation-dissipation theorem opens up an enticing prospect of developing techniques for improving imperfect model sensitivity based on specific tests carried out in the training phase of the unperturbed climate.

9. Lessons in Uncertainty Quantification for Turbulent Dynamical System

A.J. Majda (P.I., Courant Institute)

M. Branicki (Post doc, Courant Institute)

The modus operandi of modern applied mathematics in developing very recent mathematical strategies for uncertainty quantification in partially observed high-dimensional turbulent dynamical systems is emphasized here. The approach involves the synergy of rigorous mathematical guidelines with a suite of physically relevant and progressively more complex test models which are mathematically tractable while possessing such important features as the two-way coupling between the resolved dynamics and the turbulent fluxes, intermittency and positive Lyapunov exponents, eddy diffusivity parameterization and turbulent spectra. A large number of new theoretical and computational phenomena which arise in the emerging statistical-stochastic framework for quantifying and mitigating model error in imperfect predictions, such as the existence of information barriers to model improvement, are developed and reviewed here with the intention to introduce mathematicians, applied mathematicians, and scientists to these remarkable emerging topics with increasing practical importance.

These next papers illustrate fundamental limitations of popular methods for UQ such as polynomial chaos and adhoc nonlinear regression.

10. Fundamental Limitations of Polynomial Chaos for Uncertainty Quantification in Systems with Intermittent Instabilities

M. Branicki (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

Here, we examine the suitability of truncated Polynomial Chaos Expansions (PCE) and truncated Gram-Charlier Expansions (GrChE) as possible methods for uncertainty quantification (UQ) in nonlinear systems with intermittency and positive Lyapunov exponents. These two methods rely on truncated Galerkin projections of either the system variables in a fixed polynomial basis spanning the “uncertain” subspace (PCE) or a suitable eigenfunction expansion of the joint probability distribution associated with the uncertain evolution of the system (GrChE). Based on a simple, statistically exactly solvable non-linear and non-Gaussian test model, we show in detail that methods exploiting truncated spectral expansions, be it PCE or GrChE, have significant limitations for uncertainty quantification in systems with intermittent instabilities or parametric uncertainties in the damping. Intermittency and fat-tailed probability densities are hallmark features of the inertial and dissipation ranges of turbulence and we show that in such important dynamical regimes PCE performs, at best, similarly to the vastly simpler Gaussian moment closure technique utilized earlier by the authors in a different context for UQ within a framework of Empirical Information Theory. Moreover, we show that the non-realizability of the GrChE approximations is linked to the onset of intermittency in the dynamics and it is frequently accompanied by an erroneous blow-up of the second-order statistics at short times.

11. Fundamental Limitations of Ad Hoc Linear and Quadratic Multi-Level Regression Models for Physical Systems

A.J. Majda (P.I., Courant Institute)

Y. Yuan (Grad student, Courant)

A central issue in contemporary applied mathematics is the development of simpler dynamical models for a reduced subset of variables in complex high dimensional dynamical systems with many spatio-temporal scales. Recently, ad hoc quadratic multi-level regression models have been proposed to provide suitable reduced nonlinear models directly from data. The main results developed here are rigorous theorems demonstrating the non-physical finite time blow-up and large time instability in statistical solutions of general scalar multi-level quadratic regression models with corresponding unphysical features of the invariant measure. Surprising intrinsic model errors due to discrete sampling errors are also shown to occur rigorously even for linear multi-level regression dynamic models. All of these theoretical results are corroborated by numerical experiments with simple models. Single level nonlinear regression strategies with physical cubic damping are shown to have significant skill on the same test problems.

Important unambiguous test models for prediction, state estimation, and uncertainty quantification are developed in the next papers

12. Elementary models for turbulent diffusion with complex physical features: eddy diffusivity, spectrum and intermittency

A.J. Majda (P.I., Courant Institute)

B. Gershgorin (Post doc, Courant Institute)

This paper motivates, develops and reviews elementary models for turbulent tracers with a background mean gradient which, despite their simplicity, have complex statistical features mimicking crucial aspects of laboratory experiments and atmospheric observations. These statistical features include exact formulas for tracer eddy diffusivity which is non-local in space and time, exact formulas and simple numerics for the tracer variance spectrum in a statistical steady state, and the transition to intermittent scalar probability density functions with fat exponential tails as certain variances of the advecting mean velocity are increased while satisfying important physical constraints. The recent use of such simple models with complex statistics as unambiguous test models for central contemporary issues in both climate change science and the real-time filtering of turbulent tracers from sparse noisy observations is highlighted throughout the paper.

13. **Non-Gaussian Test Models for Prediction and State Estimation with Model Errors**

M. Branicki (Post doc, Courant Institute)

Nan Chen (Grad student Courant)

A.J. Majda (P.I., Courant Institute)

Turbulent dynamical systems involve dynamics with both a large dimensional phase space and a large number of positive Lyapunov exponents. Such systems are ubiquitous in applications in contemporary science and engineering where the statistical ensemble prediction and the real time filtering/state estimation are needed despite the underlying complexity of the system. Statistically exactly solvable test models have a crucial role to provide firm mathematical underpinning or new algorithms for vastly more complex scientific phenomena. Here, a class of statistically exactly solvable non-Gaussian test models is introduced, where a generalized Feynman-Kac formulation reduces the exact behavior of conditional statistical moments to the solution to inhomogeneous Fokker-Planck equations modified by linear lower order coupling and source terms. This procedure is applied to a test model with hidden instabilities and is combined with information theory to address two important issues in the contemporary statistical prediction of turbulent dynamical systems: the coarse-grained ensemble prediction in a perfect model and the improving long range forecasting in imperfect models. The models discussed here should be useful for many other applications and algorithms for the real time prediction and the state estimation.

II) **Statistically Accurate Low Order Models for Uncertainty Quantification in Turbulent Dynamical Systems**

Majda and Sapsis have achieved a potential major breakthrough with a new class of methods for UQ in the four papers listed below and summarized here.

Turbulent dynamical systems are characterized by both a large dimensional phase space and a large dimension of instabilities i.e. a large number of positive Lyapunov exponents on the attractor.

Turbulent dynamical systems are ubiquitous in many complex systems with fluid flow such as for example, the atmosphere, ocean, and coupled climate system, confined plasmas, and engineering turbulence at high Reynolds numbers. In turbulent dynamical systems, these linear instabilities are mitigated by energy conserving nonlinear interactions which transfer energy to the linearly stable modes where it is dissipated resulting in a statistical steady state. Uncertainty quantification (UQ) in turbulent dynamical systems is a grand challenge where the goal is to obtain statistical estimates such as the change in mean and variance for key physical quantities in the nonlinear response to changes in

external forcing parameters or uncertain initial data. These key physical quantities are often characterized by the degrees of freedom which carry the largest energy or variance and an even more ambitious grand challenge is to develop truncated low order models for UQ for a reduced set of important variables with the largest variance. This is the topic of the research by Sapsis and Majda. In the work of Sapsis and Majda a systematic strategy is developed for building statistically accurate low order models for UQ in turbulent dynamical systems. First, exact dynamical equations for the mean and the covariance are developed; the possibly intermittent effects of the third order statistics on these low-order statistics are present in the exact equations. Secondly, an approximate nonlinear dynamical system for the evolution of the mean and covariance constrained by covariance forcing from minimal damping and random forcing on the unperturbed attractor is formulated; it is required that this dynamical system has the unperturbed mean and covariance as a stable fixed point. In the third calibration step, the effect of the third moments on the mean and the covariance in the approximate dynamical system for the statistics are calibrated efficiently at the unperturbed steady state using only the measured first and second moments. The result at this stage is a very recent algorithm for UQ called Modified Quasilinear Gaussian (MQG) closure which applies on the entire phase space of variables. In the fourth step, the MQG algorithm is projected on suitable leading EOF patterns with further efficient calibration of the effect of the unresolved modes at the unperturbed statistical steady state. This final step defines the reduced order MQG (ROMQG) method for UQ in turbulent dynamical systems. The research of Sapsis and Majda includes two highly nontrivial applications of the ROMQG method to UQ. The first application involves the Lorenz 96 (L-96) model which is a non-trivial forty dimensional turbulent dynamical system which mimics mid-latitude atmospheric turbulence and is a popular model for testing methods for statistical prediction, data assimilation or filtering, FDT, and UQ. The advantage of the forty mode L-96 with many features of turbulent dynamical systems is that very large ensemble Monte-Carlo simulations can be utilized for validation in transient regimes. Here the ROMQG algorithm has remarkably robust skill for UQ in the transient response to general random external forcing for truncations as low as one, two or three leading Fourier (EOF) modes. The second application involves a prototype example of two-layer ocean baroclinic turbulence. Here the turbulent system has over 125,000 degrees of freedom so validation through transient Monte-Carlo simulations is impossible and only the nonlinear statistical steady state response to the change in shear can be tested for various perturbed shear strengths. Here the ROMQG algorithms for UQ utilizing 252 EOF modes (less than 0.2% of the total modes) are able to capture the nonlinear response of both the one-dimensional energy spectrum and heat flux spectrum at each wavenumber with remarkable skill for a wide range of shear variations.

1. Statistically Accurate Low Order Models for Uncertainty Quantification in Turbulent Dynamical Systems

T. Sapsis (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

2. A statistically accurate modified quasilinear Gaussian closure for uncertainty quantification in turbulent dynamical systems

T. Sapsis (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

3. Blending Modified Gaussian Closure and Non-Gaussian Reduced Subspace Methods for Turbulent Dynamical Systems

T. Sapsis (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

4. Blended reduced subspace algorithms for uncertainty quantification of quadratic systems with a stable mean state

T. Sapsis (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

III) **New Algorithms and Techniques for Data Assimilation with Judicious Model Errors which can Capture Intermittent Extreme Events in Complex Systems**

The first two papers describe a new technique to capture unresolved intermittent features of turbulent signals in data assimilation by a new technique proposed by the PI, Majda, based on earlier theoretical work.

1. Dynamic Stochastic Superresolution of sparseley observed turbulent systems

M. Branicki (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

Real-time capture of the relevant features of the unresolved turbulent dynamics of complex natural systems from sparse noisy observations and imperfect models is a notoriously difficult problem. The resulting lack of observational resolution and statistical accuracy in estimating the important turbulent processes, which intermittently send significant energy to the large-scale fluctuations, hinders efficient parameterization and real-time prediction using discretized PDE models. This issue is particularly subtle and important when dealing with turbulent geophysical systems with an vast range of interacting spatio-temporal scales and rough energy spectra near the mesh scale of numerical models. Here, we introduce and study a suite of general Dynamic Stochastic Superresolution (DSS) algorithms and show that, by appropriately filtering sparse regular observations with the help of cheap stochastic exactly solvable models, one can derive stochastically ‘superresolved’ velocity fields and gain insight into the important characteristics of the unresolved dynamics, including the detection of the so-called black swans. The DSS algorithms operate in Fourier domain and exploit the fact that the coarse observation network aliases high-wavenumber information into the resolved waveband. It is shown that these cheap algorithms are robust and have significant skill on a test bed of turbulent solutions from realistic nonlinear turbulent spatially extended systems in the presence of a significant model error. In particular, the DSS algorithms are capable of successfully capturing time-localized extreme events in the unresolved modes, and they provide good and robust skill for recovery of the unresolved processes in terms of pattern correlation. Moreover, we show that DSS improves the skill for recovering the primary modes associated with the sparse observation mesh which is equally important in applications. The skill of the various DSS algorithms depends on the energy spectrum of the turbulent signal and the observation time relative to the decorrelation time of the turbulence at a given spatial scale in a fashion elucidated here.

2. New methods for estimating poleward eddy heat transport using satellite altimetry

S. Keating (U. New South Wales)

A.J. Majda (P.I., Courant Institute)

K.S. Smith (Courant Institute)

The role of ocean eddies in redistributing heat from the tropics to the poles remains

a poorly constrained feature of the global energy balance. Attempts to monitor poleward eddy heat transport using satellite altimetry are severely limited by the sparseness of the observations in the vertical and the horizontal as well as in time, and consequently underrepresent heat transport by mesoscale eddies, particularly at high latitudes. In this article, we examine a suite of cheap, skillful, and robust filtering strategies for estimating poleward heat transport in idealized, eddy-resolving simulations of oceanic turbulence at high and low latitudes. A range of observation scenarios are considered, allowing us to explore the interplay of eddy length and time scales with the spatiotemporal resolution capability of satellite observations.

We show that, by extracting high-wavenumber information aliased into the low wavenumber band, one can derive "superresolved" velocity fields from sparse satellite observations, increasing the effective resolution of altimetric maps by a factor of four or more. As a result, the measured magnitude and temporal variability of the poleward eddy heat transport is much closer to the true value. The speed and stability of the filters are also dramatically increased by employing stochastic turbulence models for the unresolved scales, effectively parameterizing them with a model that can be learned "on-the-fly" from the satellite observations themselves. Implications for estimating poleward eddy heat transport using current and next-generation altimeters are discussed.

An important new way to assess and improve filters with model error through information theory is developed in the next paper.

3. Quantifying Bayesian Filter Performance for Turbulent Dynamical Systems through Information Theory

M. Branicki (U. Edinburgh, unsupported)

A.J. Majda (Courant)

This work develops families of information measures involving the entropy of the forecast error (a generalization of RMS error), the mutual information (a generalization of anomaly pattern correlation), and the relative entropy (a nonlinear statistical measure of forecast fidelity) to cope with imperfect model errors in filtering and prediction. All three measures are optimized by the Kalman filter for perfect models but emphasize different properties of the filter or forecast distribution for imperfect models. This paper introduces a new optimization principle over parameters for imperfect models which combines all three probabilistic measures and incorporates both means and covariances of the imperfect model in assessing skill. This tool should have wide use for the training phase of low order imperfect models for data assimilation and prediction as well as for targeted statistics in more complex models.

Filtering turbulent tracers and also moisture-coupled waves in the tropics have large practical importance. The next papers develop unambiguous test problems for these issues as well as study the phenomenon of catastrophic filter divergence.

4. Test Models for Filtering and Prediction of Moisture-Coupled Tropical Waves

J. Harlim (Penn State)

A.J. Majda (Courant)

The filtering/data assimilation and prediction of moisture-coupled tropical waves is a contemporary topic with significant implications for extended-range forecasting. The development of efficient algorithms to capture such waves is limited by the unstable multiscale features of tropical convection which can organize large-scale circulations and the sparse observations of the moisture-coupled wave in both the horizontal and vertical. The approach proposed here is to address these difficult issues of data assimilation and prediction through a suite of analogue models which, despite their simplicity, capture key features of the observational record and physical processes in moisture-coupled tropical waves. The analogue models emphasized here involve the multicloud convective parametrization based on three cloud types (congestus, deep, and stratiform) above the boundary layer. Two test examples involving an MJO-like turbulent travelling wave and the initiation of a convectively coupled wave train are introduced to illustrate the approach. A suite of reduced filters with judicious model errors for data assimilation of sparse observations of tropical waves, based on linear stochastic models in a moisture-coupled eigenmode basis is developed here and applied to the two test problems. Both the reduced filter and 3D-Var with a full moist background covariance matrix can recover the unobserved troposphere humidity and precipitation rate; on the other hand, 3D-Var with a dry background covariance matrix fails to recover these unobserved variables. The skill of the reduced filtering methods in recovering the unobserved precipitation, congestus, and stratiform heating rates as well as the front-to-rear tilt of the convectively coupled waves exhibits a subtle dependence on the sparse observation network and the observation time.

5. Filtering a Statistically Exactly Solvable Test Model for Turbulent Tracers from Partial Observations

B.Gershgorin (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

A statistically exactly solvable model for passive tracers is introduced as a test model for the authors' Nonlinear Extended Kalman Filter (NEKF) as well as other filtering algorithms. The model involves a Gaussian velocity field and a passive tracer governed by the advection-diffusion equation with an imposed mean gradient. The model has direct relevance to engineering problems such as the spread of pollutants in the air or contaminants in the water as well as climate change problems concerning the transport of greenhouse gases such as carbon dioxide with strongly intermittent probability distributions consistent with the actual observations of the atmosphere. One of the attractive properties of the model is the existence of the exact statistical solution. In particular, this unique feature of the model provides an opportunity to design and test fast and efficient algorithms for real-time data assimilation based on rigorous mathematical theory for a turbulence model problem with many active spatiotemporal scales. Here, we extensively study the performance of the NEKF which uses the exact first and second order nonlinear statistics without any approximations due to linearization. The role of partial and sparse observations, the frequency of observations and the observation noise strength in recovering the true signal, its spectrum, and fat tail probability distribution are the central issues discussed here. The results of our study provide useful guidelines for filtering realistic turbulent systems with passive tracers through partial observations.

6. Filtering Skill for Turbulent Signals for a Suite of Nonlinear and Linear Extended Kalman Filters

M. Branicki (Post doc, Courant Institute)

B.Gershgorin (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

The filtering skill for turbulent signals from nature is often limited by errors due to utilizing an imperfect forecast model. In particular, real-time filtering and prediction when very limited or no a posteriori analysis is possible (e.g. spread of pollutants, storm surges, tsunami detection, etc.) introduces a number of additional challenges to the problem. Here, a suite of filters implementing stochastic parameter estimation for mitigating model error through additive and multiplicative bias correction is examined on a nonlinear, exactly solvable, stochastic test model mimicking turbulent signals in regimes ranging from configurations with strongly intermittent, transient instabilities associated with positive finite-time Lyapunov exponents to laminar behavior. Stochastic Parameterization Extended Kalman Filter (SPEKF), used as a benchmark here, involves exact formulas for propagating the mean and covariance of the augmented forecast model including the unresolved parameters. The remaining filters use the same nonlinear forecast model but they introduce model error through different moment closure approximations and/or linear tangent approximation used for computing the second-order statistics of the augmented stochastic forecast model. A comprehensive study of filter performance is carried out in the presence of various moment closure errors which are enhanced by additional model errors due to incorrect parameters inducing additive and multiplicative stochastic biases. The estimation skill of the unresolved stochastic parameters is also discussed and it is shown that the linear tangent filter, despite its popularity, is completely unreliable in many turbulent regimes for both parameter estimation and filtering; moreover, regimes of filter divergence for the linear tangent filter are identified. The results presented here provide useful guidelines for filtering turbulent, high-dimensional, spatially extended systems with more general model errors, as well as for designing more skillful methods for superparameterization of unresolved intermittent processes in complex multi-scale models. They also provide unambiguous benchmarks for the capabilities of linear and nonlinear extended Kalman filters using incorrect statistics on an exactly solvable test bed with rich and realistic dynamics.

7. A mechanism for catastrophic filter divergence in data assimilation for sparse observation networks

G. Gottwald (U. Sydney)

A.J. Majda (P.I., Courant Institute)

We study catastrophic filter divergence in data assimilation procedures whereby the forecast model develops severe numerical instabilities leading to a blow-up of the solution. Catastrophic filter divergence can occur in sparse observational grids with small observational noise for intermediate observation intervals and finite ensemble sizes. Using a minimal five-dimensional model, we establish that catastrophic filter divergence is a numerical instability of the underlying forecast model caused by the filtering procedure producing analyses which are not consistent with the true dynamics, and stiffness caused by the fast attraction of the inconsistent analyses towards the attractor during the forecast step.

New advanced nonlinear time series techniques which are suitable for capturing intermittency and low frequency variability in large dimensional time series for massive data sets are introduced and developed in the next three papers.

8. **Nonlinear Laplacian spectral analysis for time series with intermittency and low-frequency variability**

D. Giannakis (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

Many processes in science and engineering develop multiscale temporal and spatial patterns, with complex underlying dynamics and time-dependent external forcings. Because of the importance in understanding and predicting these phenomena, extracting the salient modes of variability empirically from incomplete observations is a problem of wide contemporary interest. Here, we present a technique for analyzing high-dimensional, complex time series that exploits the geometrical relationships between the observed data points to recover features characteristic of strongly nonlinear dynamics (such as intermittency and rare events), which are not accessible to classical singular spectrum analysis. The method employs Laplacian eigenmaps, evaluated after suitable time-lagged embedding, to produce a reduced representation of the observed samples, where standard tools of matrix algebra can be used to perform truncated singular-value decomposition despite the nonlinear geometrical structure of the dataset. We illustrate the utility of the technique in capturing intermittent modes associated with the Kuroshio current in the North Pacific sector of a general circulation model and dimensional reduction of a low-order atmospheric model featuring chaotic intermittent regime transitions, where classical singular spectrum analysis is already known to fail dramatically.

9. **Comparing low-frequency and intermittent variability in comprehensive climate models through nonlinear Laplacian spectral analysis**

D. Giannakis (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

Nonlinear Laplacian spectral analysis (NLSA) is a recently developed technique for spatiotemporal analysis of high-dimensional data, which represents temporal patterns via natural orthonormal basis functions on the nonlinear data manifold. Through such basis functions, determined efficiently via graph-theoretic algorithms, NLSA captures intermittency, rare events, and other nonlinear dynamical features which are not accessible through linear approaches (e.g., singular spectrum analysis (SSA)). Here, we apply NLSA to study North Pacific SST monthly data from the CCSM3 and ECHAM5/MPI-OM models. Without performing spatial coarse graining (i.e., operating in ambient-space dimensions up to 1.6×10^5 after lagged embedding), or seasonal-cycle subtraction, the method reveals families of periodic, low-frequency, and intermittent spatiotemporal modes. The intermittent modes, which describe variability in the Western and Eastern boundary currents, as well as variability in the subtropical gyre with year-to-year reemergence, are not captured by SSA, yet are likely to have high significance in a predictive context and utility in cross-model comparisons.

10. **Nonlinear Laplacian spectral analysis: Capturing intermittent and low-frequency spatiotemporal patterns in high-dimensional data**

D. Giannakis (Post doc, Courant Institute)

A.J. Majda (P.I., Courant Institute)

We present a technique for spatiotemporal data analysis called nonlinear Laplacian spectral analysis (NLSA), which generalizes singular spectrum analysis (SSA) to take into account the nonlinear manifold structure of complex data sets. The key principle underlying NLSA is that the functions used to represent temporal patterns should exhibit a degree of smoothness on the nonlinear data manifold M ; a constraint absent from classical SSA. NLSA enforces such a notion of smoothness by requiring

that temporal patterns belong in low-dimensional Hilbert spaces V_l spanned by the leading l Laplace-Beltrami eigenfunctions on M . These eigenfunctions can be evaluated efficiently in high ambient-space dimensions using sparse graph-theoretic algorithms. Moreover, they provide orthonormal bases to expand a family of linear maps, whose singular value decomposition leads to sets of spatiotemporal patterns at progressively finer resolution on the data manifold. The Riemannian measure of M and an adaptive graph kernel width enhances the capability of NLSA to detect important nonlinear processes, including intermittency and rare events. The minimum dimension of V_l required to capture these features while avoiding overfitting is estimated here using spectral entropy criteria.

IV) Algorithms for the response of Complex Dynamical Systems to External Forcing Based on the Fluctuation Dissipation Theorem

1. **“High skill in low frequency climate response through fluctuation dissipation theorems despite structural instability”**, Proc. Natl. Acad. Sci., 2010, vol. 107, no. 2, 581-586.
 A.J. Majda (P.I., Courant Institute)
 R.V. Abramov (Co-PI, U. Illinois, Chicago)
 B.Gershgorin (Post doc, Courant Institute)

In this work, we developed a systematic approach to mitigate the irreducible imprecision emerging in comprehensive Atmospheric Ocean Simulation models due to nonlinear chaos and multiple scales. This approach was advocated through algorithms based on the Fluctuation Dissipation Theorem (FDT). The high skill of FDT in predicting climate change, despite structural instability, was developed in an unambiguous fashion using mathematical theory as guidelines in three different test models: a generic class of analytical models mimicking the dynamical core of the computer climate models, reduced stochastic models for low frequency variability, and models with a significant new type of irreducible imprecision involving many fast, unstable modes.

2. **“Approximate linear response for slow variables of dynamics with explicit time scale separation”**, J. Comp. Phys., 2010, vol. 229, no. 20, 7739-7746.
 R.V. Abramov (Co-PI, U. Illinois, Chicago)

In this article I developed a new linear response algorithm based on the approximate averaged dynamics of two-scale dynamical systems with optional stochastic forcing at fast variables. The new method allows to compute the response operators directly at slow variables using existing FDT formulas, improving numerical stability and reducing computational expense as compared to the existing methods.

3. **“Improved linear response for stochastically driven systems”**, Front. Math. China, 2012, vol. 7, no. 2, 199-216.
 R.V. Abramov (Co-PI, U. Illinois, Chicago)

In this article I developed the new stochastic short-time fluctuation-dissipation formula (SST-FDT) for stochastically driven systems which does not require the probability measure of the statistical state of the system to be known explicitly. This formula is the analog of the general linear response formula for chaotic (but not stochastically driven) nonlinear systems.

4. **“Low Frequency Climate Response of Quasigeostrophic Wind-Driven Ocean Circulation”**, J. Phys. Oceanogr., 2012, vol. 42, no. 2, 243-260.
R.V. Abramov (Co-PI, U. Illinois, Chicago)
A.J. Majda (P.I., Courant Institute)

In this article we computed the linear response of the climatological statistics of the four leading empirical orthogonal functions for the wind-driven ocean circulation model, finding interesting cross-response patterns.

5. **“Suppression of chaos at slow variables by rapidly mixing fast dynamics through linear energy-preserving coupling”**, Comm. Math. Sci., 2012, vol. 10, no. 2, 595-624.
R.V. Abramov (Co-PI, U. Illinois, Chicago)

In this article I discovered a mathematical mechanism which suppresses chaos of slow climate dynamics through turbulent mixing of fast scales and energy preserving coupling, thus questioning a common understanding that turbulence at fast scales should make climate more chaotic. It turned out that, if the linear coupling between the slow and fast variables has the property of preserving the energy (in a general sense, a positive definite quadratic form) which is transferred between the slow and fast variables, then coupled slow variables in a full-scale system tend to be less chaotic and mixing than if they were uncoupled from the fast variables. Since climate models generally involve uncoupling large-scale slow dynamics from the fast unresolved processes, it may be the case that the climate models currently in use are more chaotic and unpredictable than the actual climate.

6. **“A simple linear response closure approximation for slow dynamics of a multiscale system with linear coupling”**, Multiscale Model. Simul., 2012, vol. 10, no. 1, 28-47.
R.V. Abramov (Co-PI, U. Illinois, Chicago)

In this article I designed a new closure method for slow variables of multiscale systems based on his previous work. This method allows to build computationally inexpensive reduced models for multiscale systems which capture key features of statistics of those multiscale systems. The findings of the previous work were vividly demonstrated as a contrast between the generic constant-forcing parameterization of coupling and the new method which involves computing the linear coupling term through the Fluctuation-Dissipation Theorem: the former demonstrated much more chaotic and mixing behavior than was in the fully coupled model, while the new method provided much better approximation for chaos and mixing.

7. chapter **“Climate Change: Is It More Predictable Than We Think?”** of the book **“Modern Climatology”** (ISBN 978-953-51-0095-9)
R.V. Abramov (Co-PI, U. Illinois, Chicago)

In this book chapter I projected my new findings in the area of multiscale dynamical system onto predictability of atmospheric low frequency variability and global climate.

8. **``A simple closure approximation for slow dynamics of a multiscale system: Nonlinear and multiplicative coupling``**, Multiscale Model. Simul., 2013, vol. 11, no. 1, 134-151.
R.V. Abramov (Co-PI, U. Illinois, Chicago)

In this article I extended the previously developed framework for reduced models onto those where the slow and fast variables are coupled nonlinearly and multiplicatively. I tested the new approach on the appropriately modified two-scale Lorenz 96 model which included nonlinear and multiplicative coupling terms. The reduced model successfully reproduced a wide range of statistics, including cross-correlation functions and energy autocorrelation functions of model variables.

9. **``A simple stochastic parameterization for reduced models of multiscale dynamics``**, submitted to Journal of Computational Dynamics, 2013.
R.V. Abramov (Co-PI, U. Illinois, Chicago)

In this article I developed a new practical framework of creating a stochastically parameterized reduced model for slow variables of complex nonlinear multiscale dynamics. I demonstrated that this framework is simple enough to be successfully applied even to complex models of multiscale phenomena with many degrees of freedom. Due to inclusion of stochastic parameterization, the new framework improves the dynamical properties of the reduced model in comparison with the previously developed deterministic approaches.

10. **``The response of reduced models of multiscale dynamics to small external perturbations``**, submitted to Communications in Mathematical Sciences, 2013.
R.V. Abramov (Co-PI, U. Illinois, Chicago)
M. Kjerland (Grad student, Courant)

In this article, Marc Kjerland (my student) and I studied the effectiveness of linear response prediction in reduced models for predicting the response to external perturbations in multiscale models. We found that the reduced models, built using the methods I described above, respond to small forcing in a very similar manner to that of the fully coupled models. In effect, we demonstrated that reduced models can be successfully used to predict the response of multiscale dynamics to external perturbations.

11. **``Linear response of the Lyapunov exponent to Linear response of the Lyapunov exponent to a small constant perturbation``**, submitted to Communications in Mathematical Sciences, 2014.
R.V. Abramov (Co-PI, U. Illinois, Chicago)

In this article I developed a fluctuation-dissipation prediction framework for the response of the largest Lyapunov exponent to small constant external perturbations. The approach was tested on the Lorenz 96 model in three different dynamical regimes with weak, moderate, and strong chaos. It was found that for the regimes with stronger chaotic properties the response of the Lyapunov exponent can be predicted reasonably well via a linear approximation via the FDT framework. For the regimes with weaker chaos, however, the Lyapunov exponent tends to respond to external forcing in a more nonlinear fashion.

IMPACT/APPLICATIONS

The new strategies to assess and mitigate model error in long range forecasting through information theory and linear response theory in the training phase and developed in I) are ready to be tested on intermediate complexity models for turbulent dynamical systems. These methods are also potentially very useful for overcoming model errors in classes of low order prediction models. The notion of information barriers in classes of imperfect models is an important new concept which can explain potentially the lack of improvement in some parameterizations of complex models and also point to strategies to overcome these barriers.

The new strategies from II) for low order models for UQ in turbulent dynamical systems are a potential breakthrough. They only involve the computational overhead of roughly two ensemble members of a complex system and leave already been demonstrated to have skill for models with intermediate complexity.

The novel strategy for resolving subgridscale turbulence through Dynamic Stochastic Superresolution utilizing aliased grids is a potential breakthrough for practical online estimation of complex turbulent signals in oceanography and meteorology. The unambiguous test models for filtering turbulent tracers and moisture coupled tropical waves can serve as an important test bed for practical filtering of extreme events.

Finally, the novel new machine time series techniques for capturing intermittency and low frequency variability in high dimensional massive datasets are ready for application to practical problems such as tropical intraseasonal variability and arctic sea ice reemergence mechanisms.

PUBLICATIONS

I)

(A.J. Majda, B. Gershgorin) "**Quantifying Uncertainty in Climate Change Science Through Empirical Information Theory**," *PNAS*, Vol. 107, No 34, August 2010, pp. 14958-1496 [published, refereed]

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(D. Giannakis, A.J. Majda) "**Nonlinear Laplacian spectral analysis: Capturing intermittent and low-frequency spatiotemporal patterns in high-dimensional data**", *American Statistical Association*, December 19, 2012, doi:10.1002/sam.11171 [published, refereed]

IV)

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High skill in low frequency climate response through fluctuation dissipation theorems despite structural instability. Proc. Natl. Acad. Sci., 107(2):581-586, 2010. [published, refereed]

HONORS/AWARDS/PRIZES

1. A. Majda was elected to American Academy of Arts and Sciences in 2010
2. A. Majda received the 2012 Norbert Wiener Prize of the American Math. Soc. and the Soc. For Industrial and Applied Math. His interdisciplinary work in applied math and geoscience is a prominent part of the citation.
3. A. Majda will receive the 2015 Lagrange Prize, awarded every four years by the International Congress of Industrial and Applied Mathematics, for outstanding research achievements throughout his career. His interdisciplinary work in applied math and geoscience is part of the citation including some of the work developed in the BRC challenge.

STATISTICS

Undergraduate students – 0

Grad students – 0

Women or minority - 0

Post docs – 3

Best/accomplishment

- I) Development of new strategies to assess and mitigate model errors in long range forecasting through information theory and linear response theory
- II) Development of ROMQ6 algorithms for accurate low order UQ in turbulent dynamics
- III) The development of novel Dynamic Stochastic Superresolution Algorithms, exploiting aliasing for online data assimilation of sub-grid scale feature of turbulent signals
- IV) Development of novel nonlinear time series methods to capture intermittency and low frequency variability in massive data sets