ADVANCED MATHEMATICAL METHODS TO STUDY ATMOSPHERIC DYNAMICAL PROCESSES AND PREDICTABILITY

ISTVAN SZUNYOGH (Texas A&M University), OLIVIER TALAGRAND (Laboratorie de Meteorologie Dynamique) HEINI WERNLI (ETH Zurich), CRAIG BISHOP (Naval Research Laboratory Monterey

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1 Introduction

The summer school was organized by the Dynamical Processes and Predictability Working Group (PDP WG) of THORPEX¹. THORPEX is a 10-year international research and development program to accelerate improvements in the accuracy of one-day to two-week high impact weather forecasts for the benefit of society, the economy and the environment. The PDP WG provides the connection between the operational weather prediction and the academic communities in THORPEX. The summer school was organized for early career scientists working on mathematically challenging problems of weather prediction or mathematical problems which are highly relevant for weather forecasting.

The physical model of the atmosphere is a high-Reynolds-number, stratified fluid, which can be treated as an ideal fluid except for a narrow boundary layer at the surface of the Earth. Mathematical models of the atmosphere are typically based on the Eulerian equations of fluid dynamics. Since the independent variables in these differential equations are the spatial location and the time, the equations are partial differential equations. Analytical solutions to these equations exist only for very special initial and boundary conditions [35]; thus, the solution of the equations requires a numerical solution strategy for any realistic initial and boundary conditions.

The computer code implementation of a particular numerical solution strategy is called a (numerical) model. In addition to weather prediction, atmospheric models are also employed to simulate and predict changes in the climate, and to monitor and predict changes in the chemical composition of the atmosphere. As the skill of the models is continuously tested by operational forecast applications, *numerical weather prediction models provide the consistently most accurate solutions of the atmospheric governing equations for realistic initial conditions*. Hence, forecast models provide a unique opportunity to study the behavior of a truly complex physical system.

¹http://www.wmo.int/pages/prog/arep/wwrp/new/thorpex_new.html

2 Overview of the Field

The atmosphere is one of the most intensely studied complex physical system, which is, in large part, motivated by the never-ending quest for improved numerical weather prediction techniques. The development of such techniques has greatly benefitted from advances of applied mathematics. In return, the search for improved weather prediction techniques stimulated new research in dynamical system theory. Perhaps the best known example for atmospheric research that led to important developments in mathematics is the work by the late meteorologist Edward Lorenz², who was the first to use computer-aided simulations to explore the qualitative behavior of a dynamical system. His work played an important role in the emergence of the discipline of dynamical systems theory. A more recent example for a development in dynamical systems theory that was motivated by a practical problem of numerical weather prediction is the emergence of efficient computational algorithms for the estimation of Lyapunov vectors [19, 46]. While the development of these algorithms was motivated by practical challenges in operational ensemble weather forecasting, they are expected to play an important role in the investigation of such fundamental issues as the hyperbolicity of dynamical systems. Another recent example for atmospheric research leading to mathematical results of broader interest is the emergence of techniques to quantify the spatio-temporal propagation of information in complex physical systems. [28, 34].

Due to the time constraint imposed by the 5-day length of the summer school, the organizers had to be selective when choosing the particular topics covered by the summer school. Thus the present summary should be viewed as a collection of some of the most important and mathematically challenging research problems in weather forecasting rather than a comprehensive review of recent mathematical developments with some significance for the atmospheric sciences. In addition to lectures that were designed to provide an overview of the mathematical foundation of atmospheric modeling, covering such basic topics, as the derivation of the partial differential equations that govern atmospheric motions³ and the relevant basics of dynamical systems theory,⁴ the emphases were placed on such rapidly developing subjects, as the assimilation of observed information into the model initial conditions and the quantitative prediction of the spatio-temporal evolution of influences in the model forecasts.

3 Presentation Highlights

3.1 Heini Wernli: Potential Vorticity

Potential vorticity (PV) is a fundamental quantity of balanced flow dynamics. In essence, PV is defined as the scalar product between the absolute vorticity vector and the gradient of the potential temperature field. For adiabatic and frictionless motions (e.g., in cloud-free areas in the tropopause region) the PV is materially conserved. Moreover, according to the so-called invertibility principle, the distribution of PV anomalies in the interior of the atmosphere together with suitable boundary conditions (e.g., the surface potential temperature field) can be inverted in to obtain the balanced flow associated with the anomalies. The third essential aspect of PV is related to its diabatic production or destruction. PV thereby provides a unique framework to investigate the mutual relationship between diabatic processes (e.g., cloud condensation) and the large-scale atmospheric flow.

The lecture first introduced the definition of PV, its typical atmospheric values and the climatological mean structure of atmospheric PV. The main characteristics (material conservation, invertibility and diabatic effects) have been discussed and illustrated with examples from the literature and a case study of a North Atlantic cyclone. In the final part of the lecture, a series of classical papers on the theory and application of PV has been briefly reviewed starting with the historical paper [29] and seminal paper [23] that led into the decades of "PV thinking" and provided a novel concept for understanding extratropical cyclogenesis. Also discussed was the paper [8], which pointed out the conceptual analogy between PV thinking and classical electrostatics, underlining the fundamental physical significance of the PV concept. Finally, the papers [21, 22, 41], which discuss the PV concept from a flux-form perspective, were mentioned.

²1917-2008

³John Methven: 'Atmospheric Dynamics: Equations and Wave Phenomena' 'Atmospheric Dynamics: Effects of Moisture'

⁴Eward Ott: 'Introduction to Chaotic Dynamics'.

3.2 Peter Lynch: The Emergence of Numerical Weather Prediction: from Richardson to the ENIAC

The development of computer models for numerical simulation of the atmosphere and oceans is one of the great scientific triumphs of the past fifty years. These models have added enormously to our understanding of the complex processes in the atmosphere and oceans. The consequences for humankind of ongoing climate change will be far-reaching. Earth system models are the best means we have of predicting the future of our climate.

The basic ideas of numerical forecasting and climate modeling were developed about a century ago, long before the first electronic computer was constructed. However, advances on several fronts were necessary before numerical prediction could be put into practice. A fuller understanding of atmospheric dynamics allowed the development of simplified systems of equations; regular observations of the free atmosphere provided the initial conditions; stable finite difference schemes were developed; and powerful electronic computers provided a practical means of carrying out the calculations required to predict the changes in the weather.

In his lecture, P. Lynch traced the history of computer forecasting from Richardsons prodigious manual computation [32], through the ENIAC (Electronic Numerical Integrator and Computer) integrations [33] to the early days of operational numerical weather prediction and climate modeling [20]. The useful range of deterministic prediction is increasing by about one day each decade. This talk had set the scene for the story of the remarkable progress in weather forecasting and in climate modeling over the past fifty years, which was treated in subsequent lectures.

3.3 Dale Durran: Strengths and Weaknesses of Common Numerical Methods for Simulating Atmospheric Flows

This presentation focused on key properties of broad categories of numerical schemes as they relate to modeling atmospheric flows. These categories included spatially discrete (finite difference and finite volume) methods, truncated series expansions (spectral, pseudo-spectral and finite elements), hybrid methods (spectral element and discontinuous Galerkin) and the fluid dynamical viewpoint used to formulate the governing equations (Eulerian, Lagrangian and semi-Lagrangian). Specific topics addressed in this general context included: (i) the utility of high order methods, (ii) when it is necessary to avoid overshoots and undershoots in scalar conservation laws (and strategies to achieve this), (iii) the sense in which discontinuous Galerkin methods are high-order finite volume schemes and the potential advantages of this approach on MPI computer architectures, and (iv) the relation between large time steps and the CFL condition in semi-Lagrangian methods. An up-to-date comprehensive treatment of the topic can be found in the recent edition of the standard textbook [17] by the lecturer.

3.4 Peter Lynch: Balance in the Atmosphere: Implications for NWP

Earth's atmosphere is in a constant state of near balance. There are many instances where large forces nearly cancel each other: the vertical attraction due to gravity is almost exactly balanced by the vertical gradient of pressure; the horizontal pressure force is approximately equal and opposite to the effective force due to the Earth's rotation; and so on. When the equilibrium is disturbed, extreme weather may result on a short time scale, or substantial changes in climate regime over longer periods. The lecture looked at some of the close balances in the atmosphere and considered what happens when they are disturbed.

The spectrum of atmospheric motions is vast, encompassing phenomena having periods ranging from seconds to millennia. The motions of interest to the forecaster typically have timescales of a day or longer, but the mathematical models used for numerical prediction describe a broader span of dynamical features than those of direct concern. For many purposes these higher frequency components can be regarded as noise contaminating the motions of meteorological interest. The elimination of this noise is achieved by adjustment of the initial fields, a process called initialization. The lecture reviewed the principal methods of initialization and considered their relative merits. An up-to-date description of these methods can be found in [32].

3.5 Olivier Talagrand: Introduction to Data Assimilation

Data Assimilation, which originated from the need of defining initial conditions for Numerical Weather Prediction, is the process by which observations of the atmosphere or the ocean are combined together with a numerical model of the dynamics of the flow in order to determine as accurately as possible the state of that flow.

All the information that is used in assimilation (observations and model) will always be affected with some uncertainty, which will propagate to the final estimate. From a theoretical point of view, it is convenient to consider assimilation as a problem in Bayesian estimation, viz., determine the conditional probability distribution for the state of the flow, conditioned by the available information [27, e.g.]. Because of the very large numerical size of the problem, and of the poor knowledge of the uncertainty affecting a large part of the available information, Bayesian estimation is impossible in practice. The notion of Bayesian estimation is nevertheless very useful in that it provides guidelines for continuous research and development.

In most algorithms used at present for assimilation, a background estimate coming from the past is updated with new observations. Most algorithms are heuristic extensions to mildly nonlinear situations of statistical linear estimation, which achieves Bayesian estimation in the circumstances when the link between the data and the unknowns is linear, and the errors affecting the data are additive and gaussian. Two large classes of algorithms exist at present. In sequential assimilation, the optimal form of which is Kalman Filter, the background produced by the assimilating model is constantly updated with new observations. In variational assimilation, the model is globally adjusted to the background and to the observations available over a period time. Both those classes of algorithms were described in later lectures.

A third class of algorithms, the particle filters, are independent of any linear or gaussian hypothesis. Particle filters evolve an ensemble of points in state space that are meant to sample the current conditional probability distribution for the state of the flow. The ensemble is updated with new observations according to Bayes rule on conditional probabilities. Particle filters for atmospheric and oceanic applications are actively studied [45]. One major difficulty is at present their high numerical cost [42]. Data assimilation, from its origin in Numerical Weather Prediction, has progressively extended to many diverse applications in geophysical sciences, and is related to many aspects of, among others, probability theory, dynamical systems and stability theory, and algorithmics.

3.6 Pierre Gauthier: 3D and 4D variational data assimilation

All major operational weather prediction centers use variational schemes for data assimilation. Most of the operational systems are based on the 4D formulation: the first 4D system was introduced by the European Centre for Medium Range Weather Forecasts (1997) and was followed by Meteo-France (2000), UK Met Office (2004), Japan Meteorological Agency (2005), Meteorological Service of Canada (2005) and the Fleet Numerical Meteorological and Oceanography Center (2009). The 4D-Var approach allows for an inclusion of a digital filter initialization procedure in the data assimilation process [18], an online observation quality control procedure [25, 1, 26] and an online observation bias correction procedure for satellite radiances [16, 14, 2]. Current implementations of 4D-Var do not include an explicit representation of the effects of model errors on the background.

The most intense ongoing research and development efforts focus on introducing an online estimation of the model errors into the data assimilation algorithms. Since these algorithms do not use the model as a strong constraints, that is, they do not assume that the model provides a perfect representation of the dynamics, they are called weak-constraint 4D-Var schemes. While the general idea of weak-constraint 4D-Var is not new [40], the search for specific schemes that could be applied in practice started only very recently[44, 43]. Another interesting development is the growing interest in ensemble-based variational schemes [9, 10].

3.7 Istvan Szunyogh: Ensemble-based Kalman Filters

The first correct formulations of Ensemble-based Kalman Filter (EnKF) schemes were published in 1998 [24, 11]. EnKF schemes rapidly became the most popular class of data assimilation schemes in academic research, as the development of a high-quality EnKF-based data assimilation system is a more feasible than the development of a 4D-Var scheme for a small academic research group. The relative simplicity of an

EnKF-based system is due to the general features of EnKF scheme that (i) they provide a straightforward, computationally efficient approach to obtain spatio-temporally varying estimates of the background error covariance and (ii) do not require the availability of a code of the tangent-linear dynamics and its adjoint and a code of the linearized observation operator and its adjoint.

EnKF schemes restrict all calculations to the linear space spanned by the ensemble perturbations, which are defined by the difference between the members of a background ensemble and the ensemble mean of the background. The key assumption made by all practical implementations of EnKF schemes is that a sufficiently accurate correction to the background state estimate can be made in the low-dimensional linear space spanned by a small ensemble of forecasts. (Without making this assumption, the computation cost of an EnKF scheme would be unaffordable in practice.) The results of a large number of independent numerical experiments suggest that the background error covariance, or at least its flow-dependent part, can be efficiently estimated by a small, operationally affordable, ensemble. These results has generated a growing interest in ensemble-based schemes at the operational centers. At the time of the summer school, all major operational schemes. These schemes employ an ensemble to estimate the flow-dependent part of the background error and use a variational approach to find the minimizer of the cost function.

Similar to the situation with variational schemes, finding efficient mathematical algorithms for the estimation and representation of errors in the model dynamics in ensemble-based schemes is a major theoretical and practical challenge [6, 5, 15]. In addition, while efficient algorithms for the estimation of observation bias, whose availability is essential for the gainful assimilation of satellite radiances, exist for the variational schemes [16, 14], observation bias correction schemes for the EnKF schemes are in their infancy[37, 4].

3.8 Edward Ott: Using a limited area model to enhance global analyses

E. Ott proposed a data assimilation scheme that produces the analyses for a global and a nested limited area model simultaneously, considering forecast information from both model. The proposed scheme minimizes a cost function in which the control variable is the joint state of the global and the limited area model. The initial results obtained with idealized models are very encouraging: the scheme led to an improvement of both the global and the limited area analyses compared to the case where the state of the two models were analyzed independently [47].

3.9 Craig Bishop: Observational network design and the forecast error variance reduction due to observations

In this talk, Craig Bishop began by describing how, in principle, the Kalman filter could be used to quantitatively predict the reduction in analysis and forecast error variance due to supplemental targeted observations. Noting that the computational costs of the Kalman filter are prohibitive in atmospheric and oceanic applications, he went on to describe how an approach known as the Ensemble Transform Kalman Filter (ETKF) [7, 36] provides predictions of the reduction in analysis and forecast error variance due to supplemental targeted observations in the same way as the Kalman filter but at a much lower computational cost. The cost saving is obtained via the assumption that the forecast error covariance can be perfectly described by the perturbations of a K-member ensemble forecast - where K is much smaller than both the number of observations and the number of state variables. Another assumption of the ETKF theory is that the square root of forecast error covariances conditioned on the assimilation of targeted observations can be represented in terms of an ensemble that is a linear transformation of the original or raw ensemble. The cost saving enabled by these assumptions and associated mathematical analysis enables the ETKF to compute the forecast error variance associated with a very large number of specific deployments of observational resources in a short amount of time. The technique has been used over the last decade at the National Centers Environmental Prediction Center Winter Storms Reconnaissance program to direct aircraft to locations where observations are likely to reduce the error in 2 to 4 day forecasts of high impact winter weather over the contiguous United States and Alaska. It has also been used to direct Underwater Autonomous observation Vehicles (UAVs) in oceanographic experiments. Methods to quantify the accuracy of ETKF predictions of the reduction in forecast error variance were discussed and shown to have been qualitatively correct in the Winter Storms Reconnaissance program. Craig concluded by noting that much work was still needed in order to achieve the ultimate aim of making such predictions of forecast error variance reduction due to supplemental observations quantitatively accurate.

3.10 Craig Bishop: Uncertainty quantification in geophysical systems

In this talk, Craig Bishop began by noting that although some aspects of the uncertainty in forecasts for geophysical systems, such as observation error variance, could be empirically quantified, chaos rendered flow-dependent forecast error variance formally unobservable. To better understand the distribution of true error covariances given a single imperfect ensemble covariance, he considered an idealized univariate model in which Bayes' theorem could be used to derive the distribution of true error variances given an imperfect ensemble variance. He went on to note that advanced regression techniques could be used to derived all of the parameters defining this model from a large number of realizations of (innovation, ensemble-variance) pairs. Consequently, the analysis provides a new (1st) method for estimating (a) the climatological pdf of true error variances, (b) the pdf of ensemble variances given a true error variance, and (c) The Posterior pdf of true error Variances Mean (PVM). The equation for this PVM of this distribution showed that a Hybrid error variance formulation that linearly combines a climatological estimate of the error variance with a flow-dependent ensemble based estimate was more accurate than estimates based solely on ensemble variances or estimates based solely on static climatological variances. The approach assumed that the climatological distribution of true error variances was an inverse-gamma distribution and that the distribution of ensemble variances given a single true error variance was a gamma distribution. To help explain and justify this approach a "replicate Earth" paradigm was realized with the help of an application of the Ensemble Transform Kalman filter applied to Lorenz's (2005) simple model 1. The theoretically derived weights were then applied to the newly built Navy-Hybrid-4DVAR scheme. The forecast performance using the theoretical weights was found to be as good as that from weights obtained from a much more computationally expensive brute force tuning method. Thus, the new theory provided a justification for the Hybrid plus tools to facilitate its implementation.

3.11 Olivier Talagrand: Verification of Probabilistic Forecasts

Accepting that the purpose of probabilistic prediction is to describe our uncertainty on the future state of the atmosphere, an obvious question is the following. How is it possible to objectively (and, if possible, quantitatively) evaluate the degree to which that purpose has been achieved ? In particular, how is it possible to objectively compare the performance of two different methods for probabilistic prediction? Except in rather extreme situations, it is not possible to say anything as to the quality of a particular probabilistic forecast, and objective validation of probabilistic forecasts can only be statistical. The point of view taken here is that is the quality of a probabilistic prediction system lies in the conjonction of two different properties. The first property is reliability, i. e., statistical consistency between the a priori predicted probabilities and the a posteriori observed frequencies of occurrence (it rains with frequency 40% in the circumstances when rain has been predicted to occur with probability 40%). In general terms, reliability is the property that, for any predicted probability distribution F, F(F) = F. where F(F) is the observed frequency distribution in the circumstances when F has been predicted. The second quality, which can be called resolution (it is also called sharpness) is that the reliably predicted probability distributions are mutually distinctly different (in the case of a binary event, the reliably predicted probabilities of occurrence are close to either 0 or 1). Both reliability and resolution can be objectively evaluated, provided a large enough number of realizations of the prediction system is available. A number of (non mutually equivalent) diagnostic tools and scores are commonly used for that purpose : as concerns reliability, reliability diagrams (for events), rank histograms and Reduced Centred Random Variable (for variables); as concerns resolution, Relative Operating Characteristics curve (for events). The Brier score (defined for events), and its generalization the Ranked Probability Score (defined for variables), decompose into a reliability and a resolution components. These various scores and diagnostic tools show over the years a slow but steady improvement of the quality of operational Ensemble Prediction Systems. The various scores saturate for ensemble sizes on the order of a few tens of units. The speed of saturation does not depend on the values of the scores, but on the dispersion of the predicted probabilities. The larger the dispersion, the faster the saturation (this can be shown analytically on the Brier score). The reason for the rapid saturation is that, because of the unavoidably limited size of the validation sample, only probabilistic forecasts for the occurrence of events or for values of one- or two-dimensional variables can be reliably validated. This suggests that using larger-size ensembles would be useless.

3.12 Dale Durran: Mesoscale Predictability

The classic Lorenz [31, 39] and the Anthes [3] viewpoints about mesoscale predictability were discussed and contrasted. More recent results involving the influence of the conditions imposed at the lateral boundaries of a mesoscale domain and the upscale influence of convection were reviewed. The focus then shifted to the question of whether the flow is more predictable over complex terrain.

Despite earlier research suggesting complex terrain might improve predictability, and that downslope windstorms in particular might be predictable well in advance, the recent evidence presented by the author and collaborators suggests otherwise [38]. In particular, ensemble simulations for two cases from the TREX experiment show that the development of strong downslope winds in the lee of the Sierra Nevada can be very sensitive to small perturbations in the initial conditions at forecast lead times of less than 6 to 12 hours.

Ensemble simulations of lowland snow in the Puget Sound region of the Pacific Northwest also showed high sensitivity to initial conditions at lead times as short as 36 hours. Uncertainties associated with micro-physical and boundary-layer parameterizations were side-stepped in this analysis by linking the snow forecast to the 850-hPa temperature during times of precipitation.

3.13 Peter Lynch: Laplace Transform Integration of the Shallow Water Equations

P. Lynch described a filtering integration scheme, which used a modification of the contour used to invert the Laplace transform (LT). It was shown to eliminate components with frequencies higher than a specified cut-off value. Thus it is valuable for integrations of the equations governing atmospheric flow. The scheme was implemented in a shallow water model with an Eulerian treatment of advection [12]. It was compared to a reference model using the semi-implicit (SI) scheme. The LT scheme was shown to treat dynamically important Kelvin waves more accurately than the SI scheme.

A model that combined the Laplace transform (LT) scheme with a semi- Lagrangian advection scheme in a shallow water model was also considered [13]. It was compared to a reference model using the semiimplicit (SI) scheme, with both Eulerian and Lagrangian advection. It was shown that the LT scheme was accurate and computationally competitive with these reference schemes. It was also shown, both analytically and numerically, that the LT scheme was free from the problem of orographic resonance that is found with semi-implicit schemes.

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