Uncertainty estimation is becoming an important new research discipline, cross-cutting through many scientific areas. Mathematical concept of uncertainty estimation is based on probability theory and statistics, estimation theory, information theory, and control theory. Theoretical aspects of uncertainty estimation are generally well understood for linear models (operators) and Gaussian probability distribution functions. In geosciences applications, however, nonlinear models are typically used, thus the Gaussian probability assumption may not be the best option. In addition, geosciences systems are typically high-dimensional, with state variable dimensions of the order of $10^6$-$10^7$. At the same time, the mathematical concept of uncertainty estimation, algorithmically defined by smoothing and/or filtering, is relatively simple, and common mathematical framework can be applied across disciplines. These facts create challenging problem for uncertainty estimation, requiring new scientific development and cross-disciplinary research efforts.

A progress in uncertainty estimation research related to high-dimensional geosciences applications in particular can be significantly accelerated only by bringing practitioners and theoreticians together, and exposing them to the common mathematical formalism of uncertainty estimation. By creating new ties and collaborations between seemingly unrelated scientific disciplines, the research on uncertainty estimation can be greatly advanced and facilitated. This workshop was a step in that direction, especially aimed at young scientists from all facets of applications and mathematics. The idea of the workshop was to bring together applied and theoretical researchers from different disciplines, to learn about and to discuss common mathematical concepts behind the uncertainty estimation. Predictability, data assimilation, ensemble forecasting, ensemble Kalman filters, information theory, were all seen as components of a general uncertainty estimation theory, working together toward achieving the same goal, the reduction of uncertainty in high-dimensional nonlinear systems. The workshop was supported by the School of Computational Science (SCS) at Florida State University (FSU) and by the National Science Foundation (NSF).

Background of the workshop participants encompassed broad scientific areas, ranging from weather and climate, hydrology, to geology, nuclear sciences and mathematics. The workshop had more than 50 attendees, many of them students from Florida State University (FSU) and neighboring universities. The workshop lasted for three days, and 22 papers were presented, related to uncertainty estimation in Climate, Weather, Hydrology, Nuclear Science, and Geology. Due to close relationship between the Predictability and Uncertainty, many of the presented works included results in the context of Chaos theory. Workshop was generally divided in two parts: presentations, and
discussions. The discussions were very helpful by allowing better understanding of the issues and terminology used in different disciplines and applications.

It is interesting to note that model error and parameter estimation were quickly established as most relevant issues for ensemble-based uncertainty estimation. Few presenters even had this as a topic of presentation, but many others mentioned the importance of estimating the model-related uncertainty, including empirical parameter estimation as well as the multi-model ensembles.

The workshop was opened by Dr. John Travis, Dean of the College of Arts and Sciences at FSU, followed by welcoming remarks from Max Gunzburger, Professor of Mathematics and Director of the School of Computational Science at FSU, and by Michael Navon, [SCS and Department of Mathematics at FSU], a co-organizer of the workshop.

**CHAOS THEORY AND UNCERTAINTY ESTIMATION**

Importance of chaos theory in uncertainty estimation is underlined by presentation of Ed Lorenz [Massachusetts Institute of Technology, Boston, Massachusetts]. In an inspiring manner, he explained the fundamentals of chaos. He defined the chaos as “when the present determines the future, but approximate present does not approximately predict the future”, as opposed to randomness “when the present does not determine the future uniquely”. He considered three differential equation systems, a second order, a third order (Fibonacci map) and an M-order ordinary differential equation, and showed that chaos is abundant, but also a regime dependent phenomenon. Zoltan Toth [National Oceanic and Atmospheric Administration (NOAA) National Centers for Environmental Prediction (NCEP), Camp Springs, Maryland] stressed that initial conditions obtained from data assimilation are not on the model attractor, causing a “drift” of the forecast. He related this to an estimation of “drift-induced” model errors. He suggested one could perform a “remapping” of observations in order to produce the initial conditions consistent with the model attractor. He presented encouraging results using Lorenz 3-variable chaotic model. Stephane Vannitsem [Royal Meteorological Institute, Belgium] also examined model error in chaotic systems. He pointed out two types of model error, a parametric error, and a phase space truncation error. Theoretical considerations, supported by a simple model results, suggest that the role of Lyapunov vectors is important, and that larger scales of model error have more profound and longer impact than the small scales. This was indirectly supported by Eugenia Kalnay [Department of Meteorology, University of Maryland, College Park, Maryland], who showed that low-dimensional estimation of model error may be advantageous in ensemble data assimilation system.

**METHODOLOGIES FOR UNCERTAINTY ESTIMATION**

In general, deterministic and probabilistic uncertainty estimation methods were presented. Francois LeDimet [Department of Mathematics, Joseph Fourier University, Grenoble, France] and Allessandro Petrucci [University of Pisa, Italy] discussed
deterministic uncertainty estimation. LeDimet pointed out that the optimality system, which combines the model and data, should be used to predict uncertainties, rather than model prediction without considering data. He indicated that the second-order adjoint methodology, related to general sensitivity analysis, is a valuable tool in error covariance estimation in variational methods. Petruzzi described a method named the Code with the capability of Internal Assessment of Uncertainty (CIAU). The uncertainties in the NPP originate in system’s thermo-hydraulics calculations. He pointed the importance of estimating the uncertainty of the transient stage of a NPP, and the need for addressing the model errors. He also stressed the importance of estimating the timing and the quantity of uncertainties. Results with simulated NPP failure indicated satisfactory uncertainty estimate using the CIAU method, but also revealed the need for more advanced methods such as the EnKF and other ensemble methods.

Most often discussed ensemble-based uncertainty estimation algorithms presented at the workshop were the Maximum Likelihood Ensemble Filter (MLEF), described by Milija Zupanski [Cooperative Institute for Research in the Atmosphere (CIRA) at Colorado State University (CSU), Fort Collins, Colorado], the Ensemble Adjustment Kalman Filter (EAKF) presented by Jeffrey Anderson [National Centers for Atmospheric Research (NCAR), Boulder, Colorado], and the Localized Ensemble Transform Kalman Filter (LETKF) presented by Eugenia Kalnay.

The similarities and differences between the variational and ensemble-based methodologies were discussed in particular. Kalnay pointed out that 4d-Var with perfect model and very long time-windows may be better than an ensemble Kalman filter (EnKF), but very expensive. In practical applications, however, she suggested that there is an overall advantage of the EnKF. Also, she addressed the conceptual and methodological implications of using four-dimensional variational data assimilation (4d-Var) or ensemble filter in uncertainty estimation. Zupanski discussed the relation between variational and ensemble methods by considering Hessian preconditioning. He suggested that the advantage of using improved Hessian preconditioning in the MLEF can overcome the disadvantage related to the reduced-rank uncertainty estimation. He also stressed the importance of model error estimation and information content analysis in the development and applications of an ensemble filter. Anderson suggested the need for the EnKF capability to adjust parameters and other specification of the system in an adaptive manner. He suggested that the use of a Hierarchical Bayesian methodology for adaptive error correction in ensemble filters can be advantageous. The new methodology relies on the use of two interdependent filters with the same data, referred to as the “ensemble of an ensemble”, and it is feasible for use on the present-day computers.

Bill Hu [Department of Geology, FSU] underlined the problem of parameter uncertainty estimation in geology. He pointed out the need for using the control theory in uncertainty estimation, and presented the Sequential Self-Calibration (SSC) method. Results from applications to heterogeneous media and tracer test indicated the capability of the SSC method to also estimate the correlation structure of the state variable.
Improvements to the above mentioned methodologies are also discussed. Steven Fletcher [CIRA/CSU] suggested that current methodologies, typically based on the Gaussian error assumption, need to be further developed to allow for non-Gaussian errors as well. He pointed out potential problems for multivariate lognormal probability density function (PDF), the unbounded conditional mean and the non-uniqueness of the median estimate, eventually concluding that conditional mode is most advantageous. He suggested that a hybrid Gaussian-Lognormal data assimilation framework, developed within MLEF, can successfully deal with both the Gaussian and lognormal errors. Bahri Uzunoglu [SCS/FSU] presented a method for improving the efficiency of ensemble data assimilation, based on the Proper Orthogonal Decomposition method. Using this methodology, he was able to create an ensemble algorithm with adaptive change of the ensemble size, i.e. with inflation and reduction of the number of ensemble members. He suggested possible applications of the method for reduced order modeling and targeted observations.

Some of the presented methodology improvements were related to the ensemble forecasting. Jun Du [NOAA/NCEP] indicated how the NCEP short-range ensemble forecasting (SREF) system is capable of bringing important new information, as opposed to deterministic forecasting. He pointed out the importance of not only estimating and reducing uncertainty, but also the way this information is conveyed to users and public. He suggested the need for multi-model ensembles, possibly using more physics diversity in the ensemble members. He mentioned NCEP plans to run SREF 4-times per day, replace the ETA model and Regional Spectral Model (RSM) by the Weather Research and Forecasting (WRF) model in 2007-2008, and to provide forecast uncertainty product for the upcoming 2008 Beijing Olympics. Jidong Gao [Center for Analysis and Prediction of Storms (CAPS) at University of Oklahoma, Norman, Oklahoma] suggested the use of a hybrid dual-resolution EnKF method, also mentioned by Du, capable of using low-resolution ensemble members to estimate error covariance and a high-resolution data assimilation system used to correct the mean estimate. He stressed that a computational savings of more than one order of magnitude can be achieved using this methodology, as opposed to using high-resolution EnKF.

CLIMATE UNCERTAINTY ESTIMATION

James Annan [Frontier Research Center for Global Change, Japan] described the parameter estimation in climate models with time scales of hundreds of years. He pointed out difficulties related to probabilistic multivariate parameter estimation, and suggested that an EnKF method can successfully perform the task, also being few orders of magnitude more efficient than other existing parameter estimation methods. He suggested the need for introducing particle filters, for addressing the nonlinear aspect of the problem, and for a cross-validation of climate forecasts. T. N. Krishnamurti [Department of Meteorology, FSU] addressed the problem of uncertainty estimation seasonal climate, hurricanes and numerical weather prediction (NWP), indicating the benefit of multi-model ensemble. Among other things, he pointed out the challenge of modeling a diurnal cycle, and the capability of the multi-model ensemble to predict it. He suggested there is a great promise for hurricane intensity and heavy precipitation multi-model ensemble
methodology. The need for model error and parameter uncertainty estimation was also stressed by Rolf Reichle [National Aeronautical Space Agency (NASA) Global Modeling and Assimilation Office (GMAO)], in applications to hydrology. In relation to the seasonal climate predictability associated with land surface, he pointed the need to use remote sensing observations of soil moisture and temperature. He suggested that a scaling approach may help in reducing large biases between satellite and model estimates. He also mentioned the need for more work in snow assimilation, and coupled land-atmosphere systems. The short-range climate problem of El Nino Southern Oscillation (ENSO) was addressed by Alicia Karspeck [NCAR]. In particular, she examined in detail the problem of error covariance inflation and localization, and found that localization was not beneficial, probably because of a low dimensionality of the system and the need to maintain the balance in the system. She concluded by indicating the benefits of EAKF analysis in recreating the thermocline depth and wind stress for certain areas of Pacific.

OTHER APPLICATIONS

In addition to the above mentioned presentations and discussions, there were few other novel applications of the ensemble and related methodologies for uncertainty estimation. Jiang Xiaowei [China Institute of Geology in Beijing, China and the Department of Geology, FSU] applied various kriging techniques, such as Ordinary, Universal and Indicator Kriging, to uncertainty of image restoration in geostatistical techniques using remote sensing. Since all these techniques produce similar results, he suggested that Ordinary Kriging, being the most efficient, is probably best suited for use in remote sensing image restoration. Martin William [CAPS] discussed a method for sensitivity analysis using an ensemble. He mentioned difficulties using the adjoint based sensitivity technique due to the assumed infinitesimal perturbations, and suggested using ensembles for both the forward and backward sensitivity analysis, since they better cope with larger physical perturbations. He also pointed out that addressing nonlinear problems may require very large number of ensembles. Adam Algood [Department of Meteorology, FSU] applied the Analog Correction Method, based on using an archive of retrospective analyses, to statistical correction of NCEP ensemble precipitation forecasts. He pointed out the problems due to biases of precipitation forecasts, and the need to correct them. In particular, he mentioned the challenge and difficulty of properly representing diurnal cycle. Few other applications were presented as well. Arif Albayrak [CIRA/CSU] and Santha Akella [SCS/FSU] described uncertainty estimation in application to weather, and Jichun Wu [Department of Geology at FSU] in applications to geology. They indicated new possibilities for uncertainty estimation in application to geosciences.

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