

The use of multiple parameterizations in ensembles

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Abstract

In an ensemble prediction system, using different physical parameterizations for different members samples the uncertainty in the description of the physical processes. Having independent algorithms of equal quality permits a reduction of the model error and improved probabilistic predictions.

The challenge is to arrive at an environment in which the ensemble of parameterizations gradually increases in quality while maintaining an appropriate amount of diversity. So far, unfortunately, multi-parameterization ensembles evolve in a fairly ad hoc manner based on what parameterizations happen to be available.

The Ensemble Kalman Filter and other data-assimilation methods can be used to evaluate the quality of multi-parameterization approaches. Multi-parameterization approaches are now used fairly commonly in both ensemble Kalman filters and short-range ensemble prediction systems.

1. Introduction

Since the beginning of numerical weather prediction, there has been a continuous encouraging improvement in the quality of forecasts. Since the early work in the sixties by e.g. Smagorinsky (1963, 1969), people have wondered about the closing gap between the practical quality of forecasts and the inherent theoretical predictability limit of the atmosphere.

Starting from a small error in the initial condition or analysis, forecast errors subsequently grow due to limitations of the weather prediction model and due to the chaotic nature of the atmosphere. Over the last decades, the initial conditions have become more accurate due to better analysis methods, better models and an improved observational network. Models have become better due to improved model dynamics, higher resolution and more realistic physical parameterizations. One would expect that the gap, which quantifies the improvement we can still hope to obtain, will close and become insignificant. This trend, however, is not born out by a long sequence of studies (Lorenz, 1982; Bengtsson and Hodges 2006). Thus, it would seem that we continue to live in an era in which weather forecasts can be improved substantially by our diligent work.

The precise description and simulation of forecast errors is the task of ensemble prediction systems (EPSs). Historically, it has been difficult to obtain a sufficient amount of spread in EPSs (Buizza et al. 2005). In recent years, however, the reliability of the EPSs has improved and it is not as evident as before that EPSs still suffer from under dispersion (e.g. Kipling et al. 2011). If an EPS contains accurate descriptions of all sources of error this informs us what we should work on to continue the improvement of our systems. On the other hand, an under dispersive ensemble suggests that we have unknown major sources of error in our system.

Modern EPSs often contain several methods to account for model error. The operational Canadian global EPS benefits from four different methods to account for model error (Houtekamer et al. 2009; Charron et al. 2010):

1. the addition of isotropic random perturbation fields,
2. the multi-parameterization method,
3. stochastic Physical Tendency Perturbations (denoted PTP, Buizza et al. 1999) and,
4. Stochastic Kinetic Energy Backscatter (denoted SKEB, Shutts 2005).

The first term, is a somewhat tuned description for sources of error of unknown origin and cannot directly be linked to a specific source of uncertainty. The second term samples among proposed physical parameterizations. The third term assigns a bulk uncertainty to all output of the model physics. It provides no insight into actual causes of the uncertainty. The fourth term relates to dissipation at the truncation limit and will become less important as model resolution increases.

Of the four terms listed and briefly discussed above, only the multi-parameterization method gives actual insight into weaknesses of the model that could be improved by further non-trivial work on the forecast model. It is the subject of the current paper.

2. Statistical considerations

The use of multiple competitive parameterizations for different members in an ensemble can be justified in a simple manner. Suppose the competent scientist Alex is able to estimate the impact of some physical process with mean zero and variance one. The lack of perfection may, for instance, be due to: the use of finite vertical resolution, the use of a limited number of iterations, the specific way of closing the set of equations and the undesirable impacts of strong gradients at the boundary.

Let us further assume that we have an equally competent scientist Bonnie who, in complete isolation of Alex, is working on a parametrization for the same process and produces an algorithm of the same quality. In her case, however, the error has different sources. She had access to a different set of observations and decided on a more accurate higher order closure. The performance of her scheme suffers, however, from an error in passing a parameter to a subroutine.

Suppose further that scientist Charley, in charge of the development of an operational EPS, can use the computer codes of both Alex and Bonnie. Taking the average output of the two codes will lead to an estimate with mean zero and variance 0.5. In addition, the difference between the two parameterizations is an estimate of the uncertainty. Reducing the variance by 50 % is evidently going to be very tempting for Charley.

This simple story is a big part of the motivation for using multi-parameterization ensembles or multi-model ensembles. The individual members of a multi-parameterization ensemble cannot to be seen as perturbations to an existing unperturbed model and consequently the mean estimate is better than anything one could otherwise obtain.

In practice, it is not evident that one can find N equally competent scientists working independently on the same process. In fact, for a multi-parameterization ensemble using a single modeling environment, perhaps only the US and Europe have the necessary critical size. For smaller centers, even maintaining $N=1$ may be a challenge and the operational exchange of ensemble forecasts with other operational centers may be an alternative to an in-house multi-parameterization approach.

From the sources of error mentioned above, some are legitimate in the sense that they reflect an existing choice or uncertainty on how to best model a process. If, for instance, the process is like the throwing of a die, there is a natural range of possibilities one always has to consider and coming up with a unique answer would be suboptimal in the context of an EPS. Other sources of error, such as coding errors, are not legitimate in the sense that they do not correspond to any inherent uncertainty in nature and they can likely be reduced when more people work together on exactly the same code.

3. The absence of a perfect model

By using pairs of integrations, it is possible to quantify the difference between two models or two parameterizations. It is more difficult to make statements about the magnitude of model error that is legitimate and inevitable. It has been argued on more theoretical grounds, however, that some level of approximation is an inherent part of model development.

As expressed by experts, a substantial amount of uncertainty is related to closure and turbulence.

It is, for instance, noted in the textbook by Tennekes and Lumley (1972) on page 4 that:

Statistical studies of the equations of motion always lead to a situation in which there are more unknowns than equations. This is called the closure problem of turbulence theory: one has to make (very often ad hoc) assumptions to make the number of equations equal to the number of unknowns. Efforts to construct viable formal perturbation schemes have not been very successful so far. The success of attempts to solve problems in turbulence depends strongly on the inspiration involved in making the crucial assumption.

An overview of turbulence closure techniques is given in chapter 6 of the book by Stull (1988). It is seen that one may want to select different closure schemes for the atmospheric boundary layer in different applications. According to Stull the closure problem is one of the unsolved problems of classical physics.

The same type of consideration also arises in the context of the parameterization of deep convection as described by Arakawa (1993, page 1, left-hand side column):

“Physical processes associated with condensation of water vapor are inherently nonlinear and, therefore, their collective effects can directly interact with larger-scale circulations. But most individual clouds, in which condensation takes place, are subgrid-scale for the conventional grid size of general circulation and numerical weather prediction models. Then, for a set of model equations to be closed, we must formulate the collective effects of subgrid-scale clouds in terms of the prognostic variables of grid scale. This is the problem of cumulus parameterization in numerical modeling of the atmosphere.”

As stated again by Arakawa (1993, page 1, right-hand side column), cumulus parameterization is a closure problem:

“Since cumulus parameterization is an attempt to formulate the collective effect of cumulus clouds without predicting individual clouds, it is a closure problem in which we seek a limited number of equations that govern the statistics of a system with huge dimensions. The core of the parameterization problem is, therefore, in the choice of appropriate closure assumptions.”

Finally, according to Arakawa (1993, page 14), different legitimate parameterizations of cumulus convection do exist:

“It is also emphasized that cumulus parameterization is a closure problem, in which the choice of appropriate closures is crucial. The conceptual framework for cumulus parameterization, however, is still in its developing stage, and there exist great uncertainties in choosing appropriate closures. Correspondingly, a number of parameterization schemes with different closures have been proposed.”

In the work by Grell and Dévényi (2002), a number of different closure hypotheses is made available in the same deep convection subroutine. Thus one is, for instance, able to mimic closure as in Arakawa and Schubert (1974), as in Kain and Fritsch (1992) or as in Kuo (1974). The available 16 different closures can interact with any of the other closures giving a potential total of 13824 ($16 \times 6 \times 4 \times 6 \times 6$) different schemes. Grell and Dévényi propose to use a Bayesian assimilation method to determine the likelihood that a particular closure is correct. One could imagine that different closures would be selected for different characteristic atmospheric conditions. For the Arctic one might, for instance, end up using different closures than for the Intertropical Convergence Zone. Estimating the likelihood of all the possible closures in different locations and seasons will evidently be a complex estimation problem.

In spite of the great potential of this approach, it is more common to select available parameterizations for deep convection to form an EPS.

4. Operational use of multi-parameterization ensembles.

At operational centers, the development of a set of physical parameterizations is historically only weakly connected with the improvement of the EPS. Have an expert in medium-range ensemble forecasting develop, for instance, a new alternative parameterization for deep convection, to better sample the uncertainty in convection, is unlikely to lead to an algorithm with a strong foundation in either observations or atmospheric physics. Conversely, a specialist in convective processes may not fully appreciate the amplitude of the uncertainty and be reluctant to introduce structural changes. To arrive at an appropriate description of uncertainty in a well working parameterization for deep convection it would seem that model development and probabilistic forecasting should be combined.

It has been suggested (Houtekamer and Lefaiivre, 1997) that a global multi-parameterization ensemble can actually be used as a tool to improve the model physical parameterizations. In practice, there are a number of problems, however, that will have to be addressed:

1. The global EPS is at lower resolution than the deterministic model. The latter model may permit the use of more state-of-the-art physical parameterizations and is thus a more attractive tool for model development.
2. The global EPS is fairly heavy to run and only a fraction of the available information may be of relevance to the study of a particular process. Additional assumptions, such as linearity, may be necessary to relate the response of the ensemble to a specific physical parameterization. In a deterministic context, it is easier to extract information that can be compared with the available observations of a measurement campaign.
3. It is fairly rare that a single person is interested in the simultaneous development of multiple physical parameterizations.

Over the last 15 years, the improvement of the model physics in the Canadian experimental and operational global EPS has been largely driven by external factors as indicated schematically in Figure 1. Similar dynamics likely drive the evolution of other multi-parameterization ensembles.

For a given physical process, at the initial time (say 1995) a center uses parameterization A for the operational forecasts and two persons are responsible for it. From time to time they are made aware of cases where forecast errors were unusually large and subsequent investigations often lead to improvements of the system. Oddly, they often find that an actual “bust” was due to some other component of the model which does not behave in an optimal manner. Always comparing their

Darwinism in the evolution of a multi-parameterization ensemble

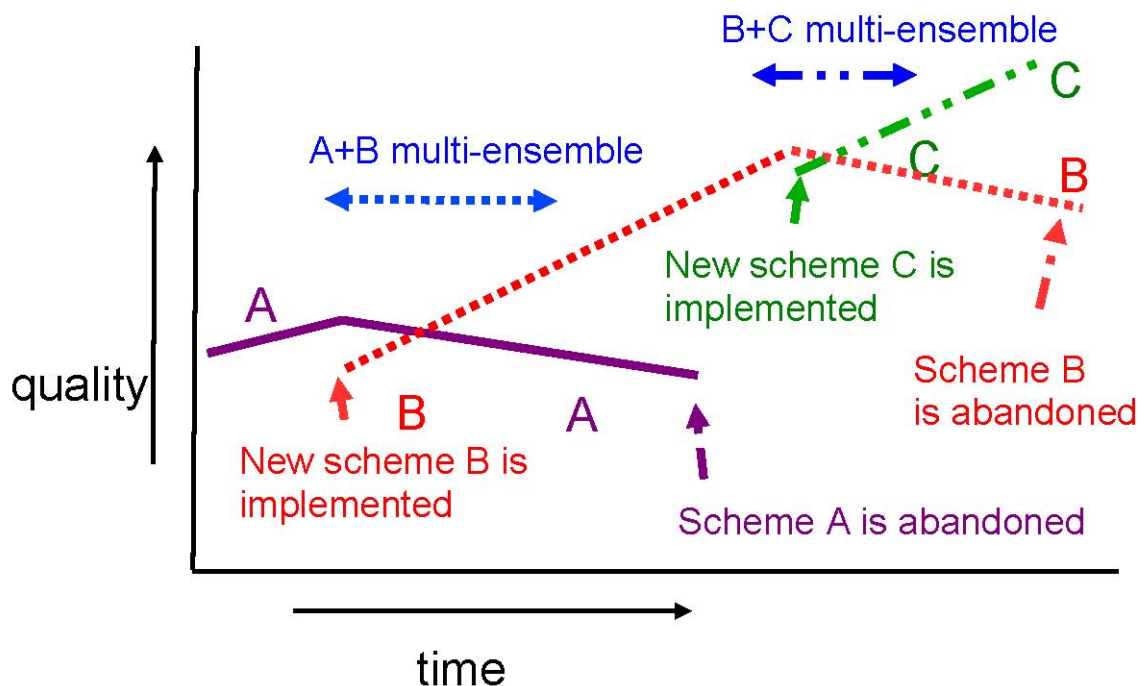


Figure 1. Schematic evolution over a period of $O(10)$ years of the model configurations that are used.

proposed modifications against verifying observations, they steadily improve the quality of the system. This small team is, however, aware of the fundamental limitations of the parameterization and decides to import a more modern parameterization B from another center. The initial results with the new parameterization are somewhat disappointing, but, with its entire attention on parameterization B, the team soon manages to equal the quality of scheme A. In fact, continuing the good work, the new parameterization soon outperforms the old one. In part, this is due, however, to parameterization A no longer being optimally adjusted to changes in the environment such as the use of a higher horizontal resolution. In this picture, there is some period in which schemes A and B are of similar quality suggesting they both be used in the operational EPS. At some stage, however, it becomes questionable if the inferior parameterization A still has a positive contribution to the overall quality of the EPS and it might be decided not to port the parameterization to a new computational environment. A few years later, say in 2005, the story may repeat itself with the arrival of parameterization C. Oddly, this new parameterization may conceptually be closer to the original parameterization A than to the parameterization B it now will come to replace.

From a management viewpoint, figure 1 presents solid evidence that scientists did a good job in improving the quality of the forecast model. The team working on the parameterization of the physical process can also be happy because, as a result of their work on new algorithms, the agreement with nature has much improved.

The main problem with the picture in figure 1 and the above story is its ad hoc character. This is in particular apparent to the person responsible for the development of the EPS. At the initial time (in 1995), the EPS was under dispersive. During a short period, there were two very different competitive parameterizations for the same process and the ensemble enjoyed an improved reliability. At some stage, however, this reliability had to be sacrificed to improve the statistical resolution of the ensemble and the ensemble again became under dispersive.

At least on a conceptual level, one could imagine a different situation in which the parameterization of the process is entirely based on first principles. Where there is uncertainty about a principle, for instance on the choice of a closure approximation, alternative branches in the algorithm are available for sampling by the members of the ensemble. As knowledge about the process improves, branches are either modified, abandoned or created. Gradually the parameterization will improve and the associated simulated uncertainty will decrease.

Schemes such as the one proposed by Grell and Dévényi (2002) seem to offer this natural link between quality and simulation of uncertainty.

5. The standard package

It would be impossible for a small team to maintain alternative codes for all aspects of the model which have uncertainty. Suppose that one has a nicely modular physics library in which N different subroutines correspond to N different physical processes. If the center has exactly one subroutine for any particular process it is virtually guaranteed that weaknesses in the library will be found sooner or later by any of the many persons using the model and its output. When a change in the computational environment occurs only one configuration will have to be migrated.

Alternatively, one could imagine having a much richer library with 2 subroutines for every individual process. Naively, one could think that it will take just twice as much effort to maintain and develop this library. However, there are now 2^N different combinations of the subroutines that, since different components of the model may interact non-linearly, ideally would all have to be tested. For a small team of non-experts, such a task will be very challenging.

For this reason, it is important to only seek out alternatives for aspects of the model where the choices made have a substantial impact on the forecasts.

Over the years different groups have experimented with the multi-parameterization approach and in order of decreasing impact on short to medium-range forecasts, we can identify substantial uncertainty in the handling of:

1. deep convection,
2. the planetary boundary layer,
3. the surface.

Examples of multi-parameterization ensembles are given in Mullen and Baumhefner (1988), Houtekamer and Lefaiivre (1997), Stensrud et al. (2000), Pellerin et al. (2003), Fujita et al. (2007), Meng and Zhang (2007), Charron et al. (2010) and Berner et al. (2011).

In general, it would seem that the multi-parameterization approach is relatively popular for short-range EPSs. This may be because selecting a different parameterization will quickly lead to weather systems that have a different structure and look different to users of the EPS.

6. The Ensemble Kalman Filter

Eventually evolving errors project onto large-scale growing modes (Toth and Kalnay 1993). This observation led to the development of the breeding and singular vector methods for ensemble prediction.

It has long been common in medium-range EPSs to somehow add amplitude to the initial perturbation in order to arrive at a sufficiently large spread in the medium-range. In the Canadian system, we used to have a special procedure named “the kick” to correct the analysis for some members towards and beyond a higher quality operational analysis (Houtekamer and Lefaiivre, 1997, option 7 in section 2). This ad hoc procedure would increase the initial spread as desired.

After an adjustment period of a few days all perturbations evolve towards and come to project upon growing modes of the system. Thus, whatever perturbation strategy is used, medium-range EPSs have fairly similar spread characteristics after a few days (Buizza et al. 2005). This observation makes medium-range ensembles ill-suited to discriminate between different strategies to account for and sample model error. One would really like to validate the model error component before it changes nature and transforms into a regular growing mode of the system.

In an ensemble Kalman filter (EnKF), it is of crucial importance to have high-quality error statistics for short-range forecasts and unjustifiable methods, such as described above, are likely to degrade

performance. In the context of a global EnKF, such as used in Canada with interpolation towards observation times in the 6h assimilation window, the error statistics are used between forecast times of 3 and 9h. For a regional-scale EnKF, the assimilation window may be shorter and consequently the error statistics need to be of high quality at an even shorter forecast range. This requirement makes the EnKF a candidate tool for the evaluation of different methods to account for model error.

To the author's knowledge, the experience with the multi-parameterization method in EnKF systems has invariably been positive.

As noted by Fujita et al. (2007), the ability of the multi-parameterization method to account for structural model error directly translates into improved results for meteorologically relevant features:

Particularly important are the improvements in the location and structure of mesoscale features that are seen when using the ensemble Kalman filter. The ICPH ensemble shows considerable improvement in the placement and intensity of the dryline, dryline bulges, frontal boundary, PBL depth and structure and rainbands that form during both days studied.

Note that ICPH refers to having perturbations in both the initial conditions and the physics.

It has been confirmed by Meng and Zhang (2007) that the EnKF framework benefits from having an appropriate sample of parameterizations:

Through various observing system simulation experiments, the performance of an ensemble Kalman filter is explored in the presence of significant model error caused by physical parameterization. The EnKF is implemented in the mesoscale model MM5 to assimilate synthetic sounding and surface data derived from the truth simulations at typical temporal and spatial resolutions for the cold-season snowstorm event that occurred 24-26 January 2000 and the warm-season MCV event that occurred on 10-13 June 2003.

Results show that although the performance of the EnKF is degraded by different degrees when a perfect model is not used, the EnKF can work fairly well in different kinds of imperfect scenario experiments.

Using a global EnKF, Houtekamer et al. (2009) concluded that:

1. The use of the multimodel option improves assimilation results in particular for temperature in the lower troposphere.
2. The multimodel and PTP (Physical Tendency Perturbation) option both sample uncertainty in the physical tendencies but, by selecting alternative legitimate configurations of the model physics, the multimodel option samples the uncertainty in a more appropriate manner.
3. The SKEB (Stochastic Kinetic Energy Backscatter) algorithm that had been adjusted for optimal performance in the medium-range EPS could not be used to improve EnKF performance.

In EnKF implementations using real observations, we need a model error forcing much bigger than can currently be obtained from any of the popular approaches to account for model error in EPSs.

Using the multi-parameterization approach, SKEB and/or PTP does not provide nearly enough spread to the EnKF system. Houtekamer et al. (2009) had to add random isotropic perturbation fields, reflecting error sources of unknown origin, to obtain a realistic amount of spread in their EnKF. Possibly these error sources correspond with specific data-assimilation problems.

The need for large-amplitude components reflecting error sources of unknown origin may cast some doubt on the validity of EnKF-based statements on the validity of specific ways to simulate weaknesses in the forecast model. To eliminate the unknown component, one could consider using an OSSE (Observation System Simulation Experiment) with an EnKF and a nature run obtained with a different model. In such an environment, all unexplained error would truly be model error and one can investigate how to best sample this model error.

In any experimental environment, negative conclusions with respect to certain algorithms may always be associated with the specifics of a local implementation. There is, for instance, no general agreement on the parameters that need to be used in the SKEB and PTP algorithms. Perhaps the EnKF framework can be used to tune some of the parameters in these schemes.

7. Discussion and conclusion

Use of multiple parameterizations in an EPS amounts to sampling the model uncertainty in a realistic manner. This leads to improved statistical resolution and reliability of the EPS and provides users with possible scenarios with different meteorological structure.

In numerical weather prediction, due to the finite resolution of the forecast model, ad hoc assumptions are often necessary to make the number of equations equal to the number of unknowns. This is known as the closure problem and justifies having multiple algorithms for a single process. Having multiple parameterizations gives a lower limit to the uncertainty due to the process. This uncertainty can possibly be reduced by further model development.

Eventually, remaining stochasticity could perhaps be simulated in a natural way in parameterizations (Houtekamer and Lefaiivre, 1997, page 2425; Charron et al. 2010, page 1900). A specific example for deep convection is described by Plant and Craig (2008).

In theory, one can use a multiple parameterization system, in combination with data assimilation, towards model improvement. This possibility has been little exploited in practice. This is partly due to the low resolution of EPSs and partly due to the difficulty of extracting specific information on a specific process.

The EnKF can be used to validate a system with multiple parameterizations. It has generally been found to be of interest to have multiple algorithms for deep convection, for the planetary boundary layer and for surface processes. This suggests that, at least for short-range forecasts, these are the areas where the most significant improvements can be made. It should be noted, however, that with current EnKF systems one is only able to explain a fraction of the forecast error. Houtekamer et al. (2009) report that for winds, temperature and surface pressure the ensemble spread more than doubles due to the simulation of model error. It would be very important to perform OSSEs to better understand the error dynamics in a data-assimilation cycle.

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