Time-step sensitivity of nonlinear atmospheric models: numerical convergence, truncation error growth and ensemble design

João Teixeira(*,&), Carolyn Reynolds and Kevin Judd(#)  

Naval Research Laboratory, Monterey, CA, USA

(*) UCAR/VSP  

(&) Corresponding author. Address:  
Until April 1st 2005: Naval Research Laboratory, 7 Grace Hopper Ave, Monterey CA, 93943. Email: teixeira@nrlmry.navy.mil  
From May 1st 2005: NATO Undersea Research Centre, Viale San Bartolomeo 400 19138 La Spezia, Italy. Email: teixeira@saclantc.nato.int  

(#) On leave from the University of Western Australia, Perth, Australia

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Abstract

Computational models based on discrete dynamical equations are a successful way of approaching the problem of predicting or forecasting the future evolution of dynamical systems. For linear and mildly non-linear models, the solutions of the numerical algorithms in which they are based, converge to the analytic solutions of the underlying differential equations, for small time-steps and grid-sizes. In this paper, we investigate the time-step sensitivity of three non-linear atmospheric models of different levels of complexity: the Lorenz equations, a quasi-geostrophic (QG) model and a global weather prediction system (NOGAPS). We show that for chaotic systems, numerical convergence cannot be guaranteed forever. The decoupling of solutions for different time-steps follows a logarithmic rule similar for the three models. In regimes that are not fully chaotic, the Lorenz equations are used to show that different time-steps may lead to different model climates and even different regimes. We propose a simple model of truncation error growth in chaotic systems that reproduces the behavior of the QG model error growth for different time-steps. Experiments with NOGAPS suggest that truncation error is a substantial component of total forecast error of the model. Ensemble simulations with NOGAPS show that using different time-steps is a simple and natural way of introducing an important component of model error in ensemble design.
1. Introduction

Today, computational models of dynamical systems are quite common in fields as diverse as atmospheric and oceanic sciences, physics, biology and engineering (e.g. Potter 1973; Oran and Boris 1987; Murray 1989; Gershenfeld 1999). Weather and climate prediction models, which are based on relatively well-known non-linear partial differential equations, are probably the most remarkable and well-known examples of operational forecasting systems (e.g. Richardson 1922; Thompson 1961; Monin 1972; Marchuk 1974; Haltiner and Williams 1980; Daley 1989; Kalnay 2003). The Lorenz equations (Lorenz 1963) have been often used as a paradigm for the extreme sensitivity of some models to the initial conditions, which is the source of a major uncertainty in numerical weather prediction - NWP (e.g. Thompson 1957; Lorenz 1963; Leith 1974; Palmer 1995; Smith 2003).

It is also well known that chaotic systems such as the Lorenz equations are sensitive to model error. In section 2 of this paper, the Lorenz equations are used to explore this fact by testing the sensitivity of the model to time-steps considerably smaller than the one used originally by Lorenz (1963). This time-step sensitivity is often not referred to explicitly in recent general references on chaos and the Lorenz equations (e.g. Turcotte 1992; Strogatz 1994) or in recent studies of model error that make use of the Lorenz equations (e.g. Palmer 1993, 1995; Molteni 1994).

The time-step sensitivity of the Lorenz equations leads to some interesting consequences in terms of numerical convergence. In this paper it is shown that for fully chaotic systems numerical convergence cannot be guaranteed forever and that for
regimes that are not fully chaotic, different time-steps may lead to different model climates and even different regimes of the solution.

In order to study in more detail the consequences of the time-step sensitivity in a model with a dynamics that is closer to the real atmosphere but is still relatively simple, we use a quasi-geostrophic (QG) model. The model used is the QG potential vorticity model described in Marshall and Molteni (1993). The usefulness of this model for atmospheric predictability and ensemble prediction research has been well documented in previous studies (e.g., Molteni and Palmer 1993; Mureau et al. 1993; Buizza and Palmer 1995; Reynolds and Palmer 1998). The QG model is well suited for this type of study, since it is complex enough to capture baroclinic synoptic scale processes that are fundamental in forecast error growth, as well as being simple enough to allow for multiple extended integrations and complete linear stability analyses (e.g., Vannitsem and Nicolis 1997; Reynolds and Errico 1999).

The QG model study (section 3) shows results regarding the time-step sensitivity that are qualitatively similar to the results obtained with the Lorenz equations. We analyze in some detail the behavior of the error due to the different time-steps and we compare it with errors due to the initial conditions. An interesting behavior is apparent in its solutions and we develop a simple model for the evolution of the time truncation error.

Due to inevitable uncertainties in initial conditions and to imperfect models, operational weather forecasts should also be viewed in a probabilistic sense, which means that forecasts should provide probabilities of the occurrence of specific events, as well as estimates of forecast skill (e.g. Leith 1974). A practical and computationally feasible approach to this problem is to perform an ensemble of forecasts from equally plausible
Ensembles of forecasts created by perturbing the initial state have been produced operationally at centers such as the European Centre for Medium-Range Weather Forecasts (ECMWF) and the National Centers for Environmental Prediction (NCEP) (e.g., Toth and Kalnay 1993; Buizza and Palmer 1998) since the early 1990s.

However, because forecast errors are due to both errors in the initial conditions and in the model formulation, ensemble techniques should include both initial condition and model error. A significant problem with many current ensemble schemes is that they are “under-dispersive”, that is, they often fail to include the verification state. This has been attributed in large part to the omission or inadequate treatment of model error in ensemble design. Recently, more attention has been turned to the inclusion of model error in ensemble design through, for example, the introduction of stochastic components in the physical parameterizations (e.g. Buizza et al. 1999). Also, more often than not, studies have associated model error with parameterization error and the non-linear effects in the predictability of a system due to discretization or truncation error have been basically neglected.

In section 4 of this paper we test the sensitivity of the Navy Operational Global Atmospheric Prediction System (NOGAPS) to different time-steps. We compare the sensitivity of NOGAPS with the QG model and discuss the differences in behavior. We also show that using different time-steps is a simple and potentially relevant way of introducing model uncertainty in ensembles.

As a summary we use this hierarchy of three models of different levels of complexity in order to answer the following three questions:
1) What are the consequences in terms of numerical convergence of using different time-steps in highly non-linear models such as the Lorenz equations?

2) What are the differences between error growth due to truncation error (time-step in this particular case) and initial condition error growth in simple but meteorologically relevant atmospheric models such as the QG model?

3) What is the impact of the truncation error in terms of the predictability of an operational system such as NOGAPS?

2. Lorenz equations and numerical convergence

The Lorenz equations,

\[
\begin{align*}
\frac{dX}{dt} &= \sigma(Y - X) \\
\frac{dY}{dt} &= rX - Y - XZ \\
\frac{dZ}{dt} &= XY - bZ
\end{align*}
\]

(with r=28, \(\sigma=10\), b=8/3) are integrated with a 2\textsuperscript{nd} order numerical scheme, as used by Lorenz (1963). To test the sensitivity to the time-step, the equations are integrated with 3 different time-steps: \(\Delta t=0.01\) (used in Lorenz (1963)), \(\Delta t=0.001\) and \(\Delta t=0.0001\) non-dimensional Lorenz time units (LTU). In fig.1 the time evolution of X during the first 15 LTU for the 3 different time-steps is shown. All solutions are apparently quite close to each other for some initial time, and at about 5 LTU the solution with time step 0.01 LTU starts to decouple from the other two solutions. At about 10 LTU the same happens with the solution obtained with time-step 0.001 LTU. Note that the initial state is situated at the attractor of a simulation performed with a much smaller time-step of \(10^{-7}\) LTU. The Y
and $Z$ evolution show a similar behavior, and the same general sensitivity to the time-step is present in simulations that start from other initial states.

These results suggest that there is no apparent convergence of the numerical algorithm used to solve the Lorenz equations. Convergence can be defined in the following sense. Let $\frac{d\Phi}{dt} = F(\Phi)$ be a system of ordinary differential equations (ODEs). Let $\Phi'_{\phi}$ represent the analytic solution of such a system given an initial state $\Phi^{0}_{\phi}$ and let $\Phi'_{n,\Delta t}$ represent a solution obtained from a numerical solver given an initial state $\Phi^{0}_{n}$ and using a time-step $\Delta t$. The numerical algorithm converges to the analytic solution if $\lim_{\Delta t \to 0} \Phi'_{n,\Delta t} = \Phi'_{\phi}$. Convergence of numerical solvers can be studied by comparing solutions for different time-steps.

For a system of ODEs, where $F$ is differentiable, Gronwall’s lemma can be used to show that (e.g. Henrici 1962; Gear 1971; Butcher 1987), if $\left|\frac{\partial F_i}{\partial \Phi_j}\right| < L$ (for all $i$ and $j$), then for $t \in [0, T]$ it is,

$$\left\|\Phi'_{n,\Delta t} - \Phi'_{\phi}\right\| \leq D\Delta t^{N} \frac{\left(e^{LT} - 1\right)}{L} + \left\|E_0\right\|e^{LT} \tag{2}$$

where $N$ is the order of accuracy of the solver, $D$ is a constant depending only on $F$, and $\|E_0\| = \|\Phi^{0}_{n} - \Phi^{0}_{\phi}\|$ is the error in the initial state. This implies that over finite forecasting windows $T < \infty$, the forecast is contained within an exponential error cone, and that as $\Delta t \to 0$ and $\|E_0\| \to 0$ the numerical solution converges to the analytic solution. Note however, that (2) does not imply uniform convergence on the infinite interval $[0, \infty)$, nor does it imply asymptotic convergence as $T \to \infty$. For chaotic systems, or systems that display sensitivity to initial conditions, convergence is not uniform, that is, as $T$ increases.
the values of $\|E_0\|$ and $\Delta t$ must be made exponentially smaller to attain the given accuracy. Sometimes (2) is too conservative, for example, for stable periodic motions numerical solutions can converge uniformly on $[0, \infty)$, or have less than exponential error growth.

It might be thought that what is usually referred to as Anosov-Bowen shadowing, implies a stronger result than (2), but this is not the case. Anosov-Bowen shadowing (Anosov 1967; Bowen 1975; Grebogi et al. 1990) implies that for suitably well-behaved systems and prescribed $\epsilon > 0$, there is a sufficiently small $\Delta t$ such that there exists $\Phi_n^0$ for any $\Phi_n^0$ with $\|\Phi_n^0 - \Phi_{n+1}^0\| < \epsilon$ for all $t \in [0, T]$. That is, there is a numerical solution that remains $\epsilon$-close to the analytic solution. This result is of little use for weather prediction purposes, since NWP models are almost certainly not suitably well-behaved, and $\Delta t$ would have to be prohibitively small.

Note that Lorenz (1989) tested the sensitivity of the Lorenz equations to time-steps larger than the one used originally in order to study non-linear numerical stability. In situations where the stability parameter is somewhere between a fully stable and a fully unstable regime, the solutions may exhibit a chaotic behavior. This issue should not be confused with what is being presented in the current paper that is about the loss of convergence after a certain amount of forecast time even for very small values of the stability parameter.

If the analytic solution is not known, convergence can be analyzed by computing an error that is the difference between numerical solutions obtained with the different time-steps on the one hand, and a numerical solution (that is considered to be the closest to the analytic solution) obtained with the smallest time-step possible.
In order to better understand the general behavior of the error, fig. 2 shows the time evolution of the logarithm (base 10) of the state vector L2 norm error between the results with time-steps $10^{-2}$, $10^{-3}$, $10^{-4}$, $10^{-5}$ and $10^{-6}$ LTU and the results obtained with time-step $10^{-7}$ LTU (considered the closest to the analytic solution). It shows, in general, a regime dominated by an average exponential growth until saturation is achieved. In the exponential growth regime, the error ($\delta$) behaves on average as $\delta \propto e^{at}$ where regressions give values that are consistent with the exponential growth of initial perturbations in the Lorenz system (e.g. Strogatz 1994). This shows similarities between the growth of errors created by (a) different initial conditions and (b) different time-steps. In fact, plots (not shown) of error growth caused by a certain time-step $\Delta t$ and by an initial condition error of the order of $\Delta t^2$ (note that the scheme is 2nd order accurate) illustrate well the general similarities between the two types of error. However, later on in this paper (when analyzing the QG model), it will be shown that there are some fundamental differences between the two types of error growth.

Also noticeable is an apparent regularity on the time that each of the curves saturates on the mean. In order to study this in more detail a critical time of decoupling ($T_c$) is defined as the first point in time after which the state vector L2 norm error corresponding to each time-step exceeds a certain threshold: 5 non-dimensional units in this case. It should be mentioned that the overall results are not particularly sensitive to this threshold value. Different decoupling times calculated for ten simulations (all starting from randomly selected initial states at the attractor of the smallest time-step experiment) as a function of the logarithm (base 10) of the time-step are shown in fig. 3. Also shown is the linear regression for the mean values of $T_c$ for each time-step. From the analysis of this
figure it can concluded that there is a certain degree of regularity in the way the solutions obtained with different time-steps decouple from the solution obtained with the smallest time-step. Linear regressions for each of the ten experiments lead to regression coefficients that vary between -5.1 and -5.8 and the regression coefficient for the mean values shown in fig. 3 is -5.5. These results suggest that the critical time of decoupling follows approximately

\[ T_c(\Delta t) \approx T_c(1) - 5.5 \log_{10}(\Delta t). \] (3)

This relation establishes a clear limit for the predictability of the model with a particular time-step \( \Delta t \). Equation (3) can also be used to predict when the time of decoupling will occur for a certain time-step, without having to perform that particular simulation. Note that the results with \( \Delta t=10^{-6} \) LTU as the reference value (instead of \( 10^{-7} \) LTU) are basically the same as for the previous figure except of course for \( \Delta t=10^{-6} \) LTU which has now zero error. This confirms that the fundamental characteristics of these results are not sensitive to the reference value that is used to compute the error.

The logarithmic nature of eq. (3) is simply explained by the typical exponential growth of perturbations in chaotic systems. From the exponential growth relation \( \delta(t) \approx \delta_0 e^{\alpha t} \), an equation for a critical time \( T_c \), after which two trajectories initially separated by \( \delta_0 \) will decouple (at a threshold of \( \delta(T_c)=1 \)), can be obtained as, assuming \( \alpha \approx 0.9 \) (e.g. Strogatz 1994): \( T_c \approx -2.6 \log_{10}(\delta_0) \). This equation is similar to eq.(3) except for the fact that it includes a perturbation to the initial state instead of the time-step and that the proportionality coefficient is about half of the one from eq.(3). However, assuming that the perturbation is of the order of the truncation error and that the
The numerical scheme is 2\textsuperscript{nd} accurate leads to $\delta_0 \propto \Delta t^2$ and consequently to a relation close to eq.(3). This type of arguments allows for a generalization of eq.(3):

$$T_c \approx -2.6 \log_{10}(\Delta t^N),$$

where N is the order of the numerical scheme.

In order to explore the parameter space to understand the consequences of the time-step sensitivity for regimes that are not fully chaotic, the sensitivity to different values of $r$ is analyzed. The initial state for the following experiments is: X=5, Y=5 and Z=5). The value $r=28$ leads to the typical chaotic regime of the Lorenz equations. For $r=17$ however, the solution is quite regular and the time evolution of the L2 norm error for different time-steps indicates that in spite of oscillations the error is smaller for smaller time-steps (not shown) as expected for linear and mildly non-linear models.

Figure 4(a) shows the evolution of X for $r=19$ for 3 different time-steps ($10^{-2}$, $10^{-3}$ and $10^{-4}$ LTU). In this regime the solutions exhibit what is often referred to as transient chaotic behavior (Strogatz 1994), but after some time all solutions converge to a stable fixed point. Depending on the time-step used to integrate the equations, the values for the fixed points can be different, which means that the climate of the model is sensitive to the time-step. In this particular case the solution obtained with 0.01 LTU converges to a positive fixed point while the other two solutions converge to a negative value.

To conclude the analysis of the sensitivity to parameter $r$, fig. 4(b) shows the time evolution (with $r=21.3$) of X for 3 different time-steps. For time-steps 0.01 LTU and 0.0001 LTU the solution ceases to have a chaotic behavior and starts converging to a stable fixed point. However, for 0.001 LTU the solution stays chaotic, which shows that different time-steps may not only lead to uncertainty in the predictions after some time, but may also lead to fundamentally different regimes of the solution. These results
suggest that time-steps and grid-sizes may have an important impact in the statistics of climate models. Some more results regarding the time-step sensitivity of the Lorenz equations are discussed in Teixeira (2002), in particular with respect to higher-order numerical schemes.

3. Quasi-Geostrophic model and truncation error

In this section, results are presented based on experiments conducted with the quasi-geostrophic (QG) potential vorticity (PV) model described in Marshall and Molteni (1993). The resolution is a T21 spectral truncation and three levels in the vertical (corresponding to 800, 500 and 200 hPa). The model forcing is composed of specified source terms of PV that are spatially varying but temporally constant and correspond to northern winter climatology. The model has three types of dissipative forcing that are discussed in detail in Molteni (1994).

The QG model uses typically a 40 minute (min) time-step. To obtain the initial conditions for these experiments, the model is first integrated for 100 days using this time step. The last day of the integration is used as the starting point for multiple 100 day integrations with time-steps varying from 1.25 to 180 min. The integration with the highest temporal resolution (1.25 min) is taken as the control integration.

The error (difference) between the control integration and the integrations with coarser time steps is shown as a function of forecast time for the first 50 days in Figure 5. For the QG model the error is defined as the length of the vector difference between the control state vector and the state vector from the longer time step integration. The state
vector, in this case, is the non-dimensional streamfunction, although results using a kinetic energy metric are similar. The integration with the coarsest temporal resolution (180 min) diverges significantly from the control integration after 10 days and this difference reaches saturation at around 20 days. For the integration with the 2.5 min time-step, divergence from the control occurs much later, after approximately 40 days, reaching saturation at around 50 days. Apparent in Fig. 5 is the regular interval between the “decoupling times” for the different time steps. In fact, the evolution of the decoupling time (chosen as when the error becomes greater than $2 \times 10^{-3}$) exhibits a log relationship with the time-step in qualitative agreement with eq. (3). This relationship will be discussed in some detail when analyzing fig. 8, which also shows the decoupling time evolution for NOGAPS.

In order to analyze in detail the evolution of the truncation error, the logarithm of the error for the different time-steps is shown in fig. 6. Also shown are two examples of errors caused by initial conditions, to allow for a comparison between truncation error and initial condition error. In general, the initial condition error grows exponentially as expected. The truncation error, however, shows a fundamentally different behavior: an initially rapid growth during the first 2 days is followed by a period (between about days 2 and 10) of relatively slow growth and then only after that is the error growing exponentially until saturation is attained. Note that there is significant uniformity in the growth rates for the different perturbations (i.e., all the curves have similar shape).

In order to try to understand these differences between the initial error growth and truncation error growth it should be taken into account that because each of the integrations is computed with a different time-step, they correspond to slightly different
model climatologies or attractors. The initial rapid growth phase is consistent with the idea that at first, each model integration moves rapidly toward its own attractor, away from the attractor of the control.

A simple model of error growth can be constructed, by considering the relative error growth rates in the stable and unstable directions. In here, the essential idea behind the generalized Hartman-Grobman theorem (Pugh 1969, Shub 1987) is utilized, which implies that there is a nonlinear change of coordinates so that the dynamics of the nonlinear system is equivalent to that of a linear system with the same positive and negative eigenvalues. Hence, it can be assumed after linearization that the error growth obeys

\[
\frac{ds}{dt} = a\varepsilon_{\Delta t} - \sigma s + au
\]

\[
\frac{du}{dt} = \beta\varepsilon_{\Delta t} + bs + \lambda u
\]  

(4)

where \(s\) represents the error in the direction of the stable modes, \(u\) the error in the direction of the unstable modes, \(\sigma\) is the rate of decay of stable modes, \(\lambda\) is the sensitivity to the initial conditions, \(a\) and \(b\) are coupling constants, \(\varepsilon_{\Delta t}\) is the typical one-step integration (truncation) error given the time-step \(\Delta t\), and \((a, \beta)\) are the relative projection of the one-step integration error onto the stable and unstable directions.

If the coupling between stable and unstable modes is relatively weak, which means \(|\sigma\lambda| > |ab|\), we can solve analytically an approximate version of these equations that neglects the coupling terms and obtain
Figure 7 shows the error growth for the stable and unstable modes and the total error \( \sqrt{s^2 + u^2} \) based on eq. (5) with the following values: \( \sigma = 0.01, \lambda = 0.5, \alpha = 0.5, \beta = 0.01 \) and \( \varepsilon_\lambda = 10^{-12} \Delta t^4 \) (with \( \Delta t \) in minutes), for time-steps of 10, 20 and 40 minutes. The constants were chosen in such a way as to be able to loosely reproduce some of the results shown in fig.6. Note that it is important that \( \alpha > \beta \) to obtain the plateau in the growth rate between rapid initial error growth as the solution moves onto the attractor, and the stage at which the error growth due to the sensitivity to the initial conditions becomes dominant.

Figure 7 illustrates a few relevant properties of this model of error growth. The total error is dominated during the first couple of days by the rapid movement of the trajectory towards its own attractor (away from the control attractor). This is represented by the stable mode exponentially decaying towards its asymptotic value. After about 10 days the unstable mode becomes the dominant component leading to a steady exponential growth of the error. The perturbations eventually become saturated (not included in fig.7). For \( t \) larger than a certain value, say \( \sigma t > 2 \), the stable error reaches a plateau: \( s(t) \approx \frac{\alpha \varepsilon_\lambda}{\sigma} \). The error growth model shows that this asymptotic value becomes, as expected, larger with larger time-steps. This is indeed the case in fig.6 and the different plateau values, for the different time-steps, can actually be used in order to confirm that the time integration scheme of the QG model is of fourth order, a fact that is used to estimate the “linear” one-step truncation error in fig. 7.
The fact that the duration of the plateau in the total error is independent of the time-step is another interesting feature that the simple model is able to reproduce. In fact, assuming that the plateau period is over when the stable and the unstable errors become equal, it is straightforward to see from eq. (5) that such a value is independent of the time-step. Overall, this simple model is able to explain the evolution of the truncation error growth in the QG model in a very satisfactory manner.

There is some important literature on simple models of error growth that considers the general effects of model error (e.g. Leith 1978; Dalcher and Kalnay 1987; Toth and Kalnay 1993; Reynolds et al 1994; Simmons and Hollingsworth 2002; Vannitsem and Toth 2002; Kalnay 2003), although in slightly different contexts than on the present paper. The simple model introduced in here considers the numerical (time) truncation error explicitly and divides the error in its stable and unstable components.

4. Time-step sensitivity in NOGAPS

In this section we analyze the impact of using different time-steps in the context of the Navy Operational Global Atmospheric Prediction System (NOGAPS). NOGAPS (Hogan and Rosmond 1991) is a global spectral model in the horizontal and energy conserving finite difference (hybrid-sigma coordinate) in the vertical. The model uses vorticity and divergence, virtual potential temperature, specific humidity, and terrain pressure as the dynamic variables, with a semi-implicit treatment of gravity wave propagation. The physical parameterizations include boundary layer turbulence (Louis et al. 1982), moist convection (Emanuel and Zivkovic-Rothman 1999), convective and
stratiform clouds (Teixeira and Hogan 2002), and solar and longwave radiation (Harshvardhan et al. 1987). NOGAPS is the global NWP model of the US Navy, and drives several applications such as the Coupled Ocean Atmosphere Mesoscale Prediction System (COAMPS™) (Hodur 1997; Hodur and Doyle 1998) and the Navy aerosol prediction model.

The results shown here correspond to a spatial resolution of T79L30. As with the simpler models, experiments are conducted by integrating NOGAPS using different time-steps, starting from the same initial state. A control 10 day integration is performed using a small time-step of 60 s. A series of integrations are then performed using larger time-steps of 120, 240, 480 and 960 s (a typical operational time-step for this resolution would be 900 s). Figure 8 is analogous to Fig. 6 but based on NOGAPS 10 day forecasts starting from January 28th 2004 at 00 UTC. Figure 8 shows the logarithm (base 10) of the L2 norm error in dry total energy, integrated over the globe and from the surface to 150 hPa. As a reference, the forecast error (based on the difference between the forecasts and the analysis) from the operational (T239L30) forecast for the same day truncated to T79, is also shown.

As with the QG model, there is an initial rapid perturbation growth within the first day, followed by a period of slower growth. This initial rapid growth may be a manifestation of the model integrations with different time steps moving toward their own climatologies, or attractors as discussed in section 3. However, the overall behavior of the error is quite different from the QG model. The difference between the errors due to the different time-steps is smaller in NOGAPS. See for example that in fig. 6, close to the start of the simulation, the error difference between the version with 180 s and the
version with 20 s (9 times smaller) is about four orders of magnitude. In contrast, in NOGAPS the difference between the error with 960 s and the error with 120 s (8 times smaller) is only about one order of magnitude. The immediate implication of this result is that while in the QG model the time integration scheme is of fourth order, in NOGAPS the time integration appears to be of order one.

Another relevant difference is that all errors plotted in fig. 8 are starting to feel the effects of saturation after just a few days of simulation, which is in contrast to the behavior of the errors in the QG model. An important outcome of the analysis of fig. 8 is the fact that the magnitude of the truncation error is significant, when compared with the total forecast error of NOGAPS (forecasts minus analysis). See for example, that the difference between the 960 s integration and the 60 s integration ranges between 40-60% of the total forecast error. This fact helps to reiterate the importance of model error in the predictability of NWP models, supporting some recent studies that have raised this issue (e.g. Orrel et al 2001), although in different contexts.

A summary of the differences and similarities between the behavior of the QG and NOGAPS models is depicted in fig. 9 that shows a similar qualitative log relationship between the decoupling time and the time-step of the integration, in both NOGAPS and the QG model. These are also qualitatively similar to eq.(3), obtained for the Lorenz equations, that was explained based on the typical exponential growth of errors in chaotic systems. It is important to note that, as expected from the analysis of fig. 6 and fig.8, the slopes for the two models are quite different: -16.7 for the QG model and -2.9 for NOGAPS.
The differences between the behavior of the QG model and NOGAPS can be, at least, partly explained by taking into account that NOGAPS is a much more complex model that includes a full set of physical parameterizations to represent subgrid-scale physical processes such as radiation, turbulence, clouds and moist convection. These parameterizations can introduce non-linearities and have several specific numerical problems that are not necessarily present in a simpler (dynamics only) model such as the QG model.

The accuracy of the time integration discussed above is a good example of such issues. Although the dynamics of NOGAPS is integrated with a second order scheme, the fact that the parameterizations are integrated with a first order scheme leads to the effective accuracy of the scheme to be of order one as shown in fig. 8. A problematic issue is that some of these parameterizations are not numerically convergent in terms of vertical resolution. Another important problem is non-linear numerical stability that can constrain (for numerical reasons) the values of some of the parameterization terms. Reviews on some of these numerical issues related to parameterizations can be found in Beljaars (1991), for example. Physical parameterizations lead to numerical intricacies that are often difficult to isolate, making the interpretation of NOGAPS results much more complicated than with the QG model.

After the realization of the relevant role of the time truncation error in terms of the total forecast error as shown in fig. 8 it is worth mentioning that although spatial resolution has been increasing during the last few years (decreasing the spatial truncation error), temporal resolution has not. Actually, due to improvements in numerical methods (e.g. Semi-lagrangian advection), time-steps have increased in some operational models,
leading to an increase in the time truncation error. This quest for stable numerical methods with large time-steps, due to efficiency concerns, may well have its price in terms of the truncation error, both in the expected traditional linear sense and in the more non-linear sense that we explore in this paper.

In terms of ensemble design these results suggest that ensemble spread may be enhanced by using different temporal resolutions for different ensemble members. Preliminary experiments seem to indicate that this is indeed the case. One example is shown in fig. 10 where the ensemble spread (RMS 500 hPa height) for the globe, the NH extra-tropics and the SH extra-tropics, based on a 10 day T79L30 (900 s time-step), 20-member ensemble is given by the solid lines. The dashed lines indicate the ensemble spread when ten of the members are integrated with the time-step reduced by half (from 900 to 450 s). Changing the time step of 50% of the ensemble members results in increased spread, particularly in the northern hemisphere extratropics. These preliminary experiments suggest that varying temporal resolution may be a natural way to introduce more variability due to model uncertainty into ensemble formulation.

5. Summary

This paper explores the time-step sensitivity of non-linear atmospheric models and shows that solutions with small but different time-steps will decouple from each other after a certain finite amount of simulation time. The decoupling time depends on the time-step in a logarithmic way (due to the exponential growth of perturbations), which means that the decoupling time can be predicted. The logarithmic nature of decoupling
time also implies that however small the time-step may be, there is always a finite point in time after which the numerical solution diverges, which means that for chaotic systems uniform numerical convergence can only be guaranteed for a finite amount of time.

The logarithmic relation is present in simulations using three models of different levels of complexity: the Lorenz equations, a quasi-geostrophic (QG) model and the Navy’s operational global weather prediction model NOGAPS. In the Lorenz equations, for regimes that are not fully chaotic, the sensitivity to the time-step is more complex and different time-steps can lead to different model climates or even different regimes. These results suggest that the statistics of climate models may be affected by the time-step and grid-size.

Using a QG model we show that truncation errors caused by different time-steps evolve in a substantially different manner when compared to initial condition errors. Initial condition errors grow exponentially as expected while truncation errors show an initially rapid growth followed by a plateau (slow error growth) and then only after that, exponential error growth until saturation is achieved.

We propose a simple analytic model of truncation error growth that considers the relative error growth rates in the stable and unstable directions. This simple model suggests that time-step truncation error in non-linear models is a combination of two errors: (i) a stable error with an initially rapid growth caused by the fact that each model simulation moves rapidly toward its own attractor, away from the attractor of the control, exponentially decaying towards a saturation value that is a function of the time-step; and (ii) an unstable error with a mean exponential growth similar to initial condition error.
We use the Navy Operational Global Atmospheric Prediction System (NOGAPS) in order to study the sensitivity to the time-step of a fully developed operational weather prediction model. Our analysis shows that the overall behavior of the truncation error is different from the QG model, with an initially rapid truncation error growth during the first day or so followed by a period of slower growth towards saturation. The results show that although the dynamics of NOGAPS is second-order accurate in time, the numerical solvers of the parameterizations lead to a first-order overall accuracy in the time integration.

An important point that stands out from this study is that truncation error (with operational time-steps) can be a substantial (40 to 60 %) part of the total forecast error of NOGAPS (forecast minus analysis). It is also shown that the decoupling between forecasts with different time-steps in NOGAPS also follows a logarithmic relation (as in the Lorenz equations and the QG model) but occurs much earlier than in the QG model.

Finally, preliminary NOGAPS ensemble experiments are performed using two different time-steps. The results show an increase in the ensemble spread of the root-mean-square (RMS) error of 500 hPa geopotential height. This suggests that different time-steps may well be a natural and simple way of introducing model error in weather prediction ensemble design.

In the weather and climate prediction community, when thinking in terms of model predictability, there is a tendency of often associating model error with the physical parameterizations. In this paper, it is shown that time truncation error in non-linear models behaves in a more complex way than in linear or mildly non-linear models and that it can be a substantial part of the total forecast error. The fact that it is relatively
simple to test the sensitivity of a model to the time-step, allowed us to study the implications of time-step sensitivity in terms of numerical convergence and error growth in some depth. The simple analytic model proposed in this paper helped in showing that the evolution of truncation error in non-linear models can be understood as a combination of the typical linear truncation error and of the initial condition error associated with the error committed in the first time-step integration (proportional to some power of the time-step).

An interesting question is how much of this simple study of the truncation error could help in understanding the behavior of more complex forms of model error associated with the parameterizations in weather and climate prediction models, and its interplay with initial condition error.

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References


Figure captions

FIG. 1. Time evolution of variable X during the first 15 LTU (for 3 different time-steps).

FIG. 2. Time evolution of the logarithm (base 10) of the state vector L2 norm error based on the difference between results with time-steps $10^{-2}$, $10^{-3}$, $10^{-4}$, $10^{-5}$ and $10^{-6}$ LTU and results obtained with time-step $10^{-7}$ LTU (considered the closest to the analytic solution).

FIG.3 - Decoupling time (in LTU) as a function of the logarithm (base 10) of the time-step for ten simulations from randomly selected initial states. Also shown is the linear regression corresponding to the mean values of decoupling time at each time-step.

FIG. 4. Sensitivity to different values of parameter r. The time evolution of (a) X for r=19 (for 3 different time-steps) and (b), X for r=21.3 (for 3 different time-steps).

FIG. 5. Time evolution of the L2 norm error in the non-dimensional stream function state vector of the QG model based on the difference between results with time-steps of 180, 80, 40, 20, 10, 5 and 2.5 minutes, and the results obtained with the control time-step of 1.25 minutes (considered the closest to the analytic solution).

FIG. 6. As in Fig.5, but for the evolution of the logarithm (base 10) of the error. Also shown are errors corresponding to two simulations with perturbed initial conditions of different magnitudes that use the control time-step (thin solid grey lines).
FIG. 7. Time evolution of the logarithm (base 10) of the error based on the simple model for error growth proposed in eqs. (4) and (5), showing the stable, unstable and total error for an equivalent time step of 10 minutes, and the total error for 20 and 40 minutes.

FIG. 8. Time evolution of the logarithm (base 10) of the L2 norm error in dry total energy (J kg$^{-1}$) of NOGAPS (integrated over the globe and from the surface to 150 hPa) starting on January 28th 2004 at 00 UTC, based on the difference between results with time-steps of 960, 480, 240 and 120 s, and the results obtained with the control time-step of 60 s. Also shown for reference is the operational (T239L30 with a time-step of 300 s) forecast error (forecast minus analysis) for the same day truncated to T79.

FIG. 9. Decoupling time for NOGAPS (time at which the error in Fig.8 becomes greater than 2) and the QG model (time at which the error in Fig.5 becomes greater than 2x10$^{-3}$) as a function of time-step. Also shown are logarithmic-regression lines fitted to each series of points.

FIG. 10. Time evolution of the ensemble spread of the geopotential height (m) at 500 hPa for a T79L30 NOGAPS 20-member ensemble. Solid lines refer to an ensemble with varying initial conditions but the same time-step of 900 s. Dashed lines refer to an ensemble with varying initial conditions and two different time-steps: 10 members have a time-step of 900 s and the other 10 a time-step of 450 s. Results shown are for the entire globe, the northern hemisphere extra-tropics (NHX - 30N to 90N), and southern hemisphere extra-tropics (SHX- 30S to 90S).
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