Stochastic Sub-grid Scale Models and the Spectral Kink

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ABSTRACT

The unresolved scales of motion in atmospheric general circulation models are typically modeled using the ensemble mean or Reynolds average within a grid-cell. Such schemes may not be capable of representing the true variability of the real atmosphere. According to the measurements of Nastrom and Gage [24], the observed kinetic energy spectrum of the atmosphere contains a kink, where the spectral slope changes from -3 at large scales to $-5/3$ in the mesoscale regime. Lindborg [20] and Waite and Bartello [31] present evidence that the large scale spectrum is dominated by rotational modes, whereas the ageostrophic or divergent modes are responsible for the $-5/3$ regime. To analyze the impact of stochastic parameterizations on the large scale dynamics, the tangent linear (TLM) and adjoint models can be applied. Our goal is to investigate how stochastic forcings project onto rotational and wave modes.

1 Introduction

Atmospheric processes are inherently multiscale as they involve a wide and often disparate range of spatial and temporal scales. For example, the dominant synoptic weather patterns encompass spatial scales spanning thousands of kilometers, whereas moist convective processes occur on length scales ranging down to a micron. For certain types of meteorological phenomena, such as tropical cyclones, it is important to accurately model both the local effects and the evolution of the ambient synoptic scale, where the time scale is typically on the order of a few days. However, for the numerical simulation of the Earth's climate, temporal scales range from several months to decades and even centuries, thus imposing formidable computational challenges. Despite the sophisticated numerical modeling techniques that have emerged over the past two decades, current models are not capable of resolving the full range of length and time scales. In particular, the unresolved physical processes within a grid cell are represented by bulk parameterizations which employ the ensemble mean or Reynolds average. These schemes are not capable of representing the full variability of the real atmosphere, preventing the climatological distribution from matching that of nature. Indeed, there are several factors contributing to this problem. Numerical approximation errors at resolved scales may change climate means. Improved numerical methods should reduce the discretization error, however, truncation errors are impossible to avoid. Furthermore, numerical models generally include unphysical dissipation or filters for stability. Recent mesoscale model implementations [27] restrict the amount of dissipation and encompass a broader range of the true mesoscale in the inertial sub-range. Turbulence closure schemes may not fully account for all scales below the truncation wavenumber k_T. One manifestation of these model deficiencies is the lack of a $k^{-5/3}$ scaling law in the mesoscale.

To date, the response of the resolved scales to random fluctuations has not been studied in a GCM that fully supports scales below the observed spectral kink. We review a few current approaches, and suggest that a new set of tools is required to address a critical question: how does subgrid-scale stochastic uncertainty propagate upscale to interact with flows distinctly possessing both large-scale rotational modes and mesoscale divergent modes?

2 The Spectral Kink

Nastrom and Gage [24] collected observational data indicating that the energy spectrum of the Earth's atmosphere contains a spectral kink separating large and small scales. Their spectra cover scales ranging from 3 km to nearly 10,000 km. The observed spectrum is characterized by an enstrophy cascade at large scales and an energy cascade at small scales. Charney attributes the -3 slope at scales above 1000 km to quasi-geostrophic turbulence. The mesoscale dynamics follow a Kolmogorov $-5/3$ spectral slope. Two different mechanisms have been proposed to explain the observed mesoscale spectra. The first is strongly nonlinear and based on quasi-2D turbulence. Lilly [17, 18] postulated that it is due to stratified turbulence at small scales. The second mechanism is based on a weakly nonlinear wave theory involving the spectrum of internal waves. At length scales below 1000 km, Lilly suggests that small scale sources of energy could be provided by thunderstorms and breaking internal waves. Small-scale shear instability may also contribute. He argues that only a small amount of this energy needs to inverse cascade in order to account for the observed mesoscale spectrum. Some of these types of atmospheric flows are nonhydrostatic, and therefore to reproduce the observed energy spectrum of the Earth's atmosphere might require running a global nonhydrostatic model with prescribed heat fluxes. The horizontal resolution of such a simulation would have to be on the order of 1 km in order to resolve the vertical convection leading to mesoscale storms or wave breaking.

The second mechanism is based on a weakly nonlinear wave theory involving the spectrum of internal waves. The latter has been explored by Garrett and Munk [10]. Indeed, there is evidence suggesting that this is the case in the ocean [7]. Dewan [4] and Van Zandt [30] have also suggested that the observed spectra are due to waves. This contribution is from modes not possessing potential vorticity, but not necessarily with high linear frequencies. If this is true for the atmosphere, then a 3D hydrostatic primitive equations model may be capable of correctly capturing the dynamics of the Earth's atmosphere. The length scales involved may be accessible at current weather model resolutions [27]. However, the time scales may be more restrictive as the explicit treatment of gravity waves could be important. Nevertheless, it would be extremely important to atmospheric modelers to determine whether or not the primitive equations are adequate for reproducing the observed dynamics of the global circulation. There is tentative evidence suggesting that the spectral kink is visible in results from the hydrostatic GFDL-Princeton SkyHi model, Koshyk et al [13]. Their approach is to use explicit methods and resolve as much as possible. Bartello [1] observes that it is important to respect the gravity wave Courant number in order to correctly capture the ageostrophic modes and thereby reproduce the spectral kink. Indeed, by varying the time step size, it may be possible to alter the location of the transition from a $-5/3$ to a -3 slope. The impact of stochastic sub-grid scale closures on the dynamics of the resolved scales and the resulting kinetic energy spectrum is an open question.

3 Stochastic Parameterizations

Typically, closure is achieved by assuming a scale separation and Reynolds averaging the Navier-Stokes equations. Sub-grid scale (SGS) processes are represented by empirical results (e.g. planetary boundary layer and surface-atmosphere interactions) or physical arguments (e.g moisture-flux based deep convection) that suggest relationships between large-scale and perturbation quantities. The sub-grid scale mean effect is included as a tendency of resolved variables and simultaneously acts in a dissipative fashion to remove energy from the truncation scale. Despite the remarkable success of this approach, increased computational power is enabling GCMs to simulate and forecast finer scales, below which these schemes remain valid. The inclusion of stochastic terms has emerged as an alternative and tacitly admits the fact that it may not be possible to deterministically represent processes below the truncation scale. In general, plausible classes of stochastic SGS closures include a random component that responds to resolved conditions.

It is widely recognized among the atmospheric sciences community that atmospheric GCMs underestimate the variability of tropical moist convection [19]. Stochastic sub-grid scale models have been suggested as an alternative [19, 25, 26, 32, 22, 12] to represent the variability of the unresolved scales. While in most cases the stochasticity is introduced by adding a white or red noise into the deterministic small scale forcing in an ad hoc fashion, Majda and his collaborators [22, 12] have proposed a systematic coarse graining procedure of Ising type–Markov jump processes modeling the underlying microscopic dynamics of the physical phenomenon being parameterized, i.e. in their case, convective inhibition (CIN). Nevertheless, the procedure can be easily expanded and generalized to account for many other sub-grid effects such as cloud radiative feedback, gravity wave activity, sea ice, etc. The results obtained in [12] for the case of an idealized tropical climate convective parameterization are very promising. It is demonstrated that, under some parameter regimes, the stochastic parameterization affects a great deal the climatology as well as the large scale variability. More importantly, their results are very sensitive to the strength of the microscopic interactions and to the characteristic time scale of the microscopic model. One of the goals of our work is to examine how the coarse grained stochastic models of Majda and his collaborators influence the large scale dynamics of a realistic GCM.

4 Tangent Linear and Adjoint Models

A novel use of the TLM and adjoint is to determine leading finite-time sensitivities to stochastic SGS closure schemes in the GCM. Stochastic schemes are intended to represent the unavoidable uncertainty in unresolved scales. Individual realizations of that uncertainty can also be considered perturbations to the resolved flow, analogous to perturbations intended to represent uncertainty in initial conditions. The most viable technique available to quantify the sensitivity to small perturbations is the singular vector method, which requires a TLM and its adjoint. The technique has been used extensively at synoptic scales, where the flow is dominated by rotational modes. Ehrendorfer and colleagues [5, 6] also used singular vectors to study optimal perturbations in both a dry and moist mesoscale TLM, and their work is perhaps the seminal study in the mesoscale predictability literature. Here we distinguish between intrinsic predictability, which is a property of the system, and extrinsic predictability, which is more akin to the maximum achievable predictive skill [28] [29] because it includes flaws in our models and observing capability. Optimal perturbation analysis, via identification of the leading singular vectors, is the study of intrinsic predictability relative to a chosen uncertainty norm.

Lorenz [21] first recognized the importance of singular vectors in examining finite-time perturbation growth. The leading singular vectors are optimal finite-time perturbations and finding them is a linear optimization problem. Farrell [9] demonstrated their utility in identifying optimal perturbations for cyclogenesis. In reference [5] the problem was generalized for atmospheric predictability studies, and here we summarize the important concepts. The maximization, over the time interval τ, leading to the definition of the singular vectors can be written as:

$$\mathscr{J}(\mathbf{a}) = (\mathbf{B}^{\tau}\mathbf{a})^{\mathbf{T}}\,\mathbf{C}\,(\mathbf{B}^{\tau}\mathbf{a}) \;, \tag{1}$$

subject to the constraint $\mathbf{a}^{\mathbf{T}}\mathbf{C}\mathbf{a}$. Matrix $\mathbf{B}$ contains the linearization of operators B^{n}, the superscript $\mathbf{T}$ represents the transpose, and matrix $\mathbf{C}$ is the norm definition. Defining

$$\mathbf{S} \equiv \mathbf{C}^{-1}(\mathbf{B}^{\tau})^{\mathbf{T}}\mathbf{C}\mathbf{B}^{\tau} \;,$$

the solution to the maximization problem (1) is the first eigenvector of $\mathbf{S}$. The complete set of eigenvectors are also the singular vectors.

The solution depends on the norm, which we choose in order to identify the upscale "error cascade" associated with stochastic SGS parameterizations in multiscale flow. We propose uncertainty norms appropriate for separately measuring the influence of SGS uncertainty on mesoscale divergent modes and large-scale rotational modes. Ehrendorfer and Errico [5] compared the spectrum of singular values and the associated singular vectors computed with the oft-used total energy (TE) norm to those computed with a derived "rotational" norm (called the **R** norm), which included energy in only the rotational modes. The TE norm included contributions from gravity waves and thus resulted in many more growing modes than the rotational norm. They concluded that much of the growth in the TE optimal perturbations is due to gravity waves introduced by geostrophic adjustment, and they are either damped or rapidly propagate out of the limited-area domain, leaving potential energy behind. The spatially-white noise perturbations they employed had a small likelihood of projecting onto the rotational modes that grew over the short time scales. Those results are compelling, but are limited in two fundamental ways: relatively short residence time of gravity waves owing to lateral boundary conditions, and the lack of gravity-wave breaking that may produce a $k^{-5/3}$ spectrum. Removal of these limitations will enable a more complete picture of unstable perturbations.

We envision a global rotational norm similar to [5], and separately derive a global divergent-mode norm (hereafter the **D** norm). These global norms are relatively easy to compute and we do not have to resort to an explicit normal-mode initialization to isolate gravity waves. We can then compute the leading singular vectors and the associated spectrum of singular values of each to determine their responses to plausible classes of SGS uncertainty. The optimization time for those norms, which is constrained by the validity of the tangent-linear approximation, is somewhat of a research problem itself, but published results provide guidance. For the large-scale rotational norm, an optimization time of 24 h should be useful. Gilmour et. al. [11] showed that the linear approximation is sometimes valid for that length in the European Centre for Medium-Range Weather Forecasting operational GCM. Ehrendorfer and collaborators [5, 6] used a 24 h optimization time successfully. Optimization times as long as 72 hours have also been used for large-scale flow problems [14].

The concept of instantaneous optimals suggests that a very short optimization time will be effective and appropriate for the **D** norm. Recently, DelSole [3] clarified the role of instantaneous optimals, which are perturbations that maximize instantaneous growth rates of energy (or potential enstrophy) in turbulent dynamics. At the short-time limit, these are indistinguishable from finite time optimal perturbations based on an energy (or potential enstrophy) norm. As noted by the author, this implies that at least one finite optimal perturbation will grow in all turbulent systems. DelSole [3] derived these properties with a generic nonlinear discretized forced-dissipative system, and noted that in typical implementations the dissipation results in more decaying modes than growing modes. He also noted that mesoscale models are typically not of that generic form because of high-order nonlinearities in parameterizations of radiation and convection as well as contravariant vertical velocity terms in terrain-following coordinate systems. Strong nonlinearity in the stochastic parameterizations will be avoided for these reasons, but weak nonlinearity can be retained and results will still apply to a wide range of SGS stochastic processes. The nonlinearity associated with divergent modes is also retained and handled by using short optimization times in the singular-vector computations.

To ensure that our stochastic schemes do not affect the scaling laws intrinsic to the nonlinear model, optimal perturbations can be computed for the **R** and **D** norms with zero optimization time. The tangent-linear approximation will also be verified by perturbing the full nonlinear model at t_0 with the linear combination of the singular vectors. The **R** and **D** norms are computed to measure the phase-space distance between perturbed and unperturbed solutions as a function of time. The linearity assumption is violated when the norms begin to grow nonlinearly. These experiments also provide for examination of the upscale error cascade in spectral space through both the $k^{-5/3}$ and k^{-3} spectral regimes. The typical view of constant upscale error energy flux in spectral space [16, 29] for the k^{-3} regime can be verified, and a picture consistent with the $k^{-5/3}$ regime will emerge.

The analysis described above is suitable for time scales shorter than typical weather forecasts because of the requirements for linearity to be valid. We propose to extend the validity of our results, perhaps to climate time scales, by investigating recently developed techniques that show potential to avoid the constraint of linearity. An ensemble-adjoint method [15, 8] uses an average of adjoint sensitivity computed over a range of perturbations, over a relatively short time scale, to approximate the nonlinear sensitivity in climate limit. Mu et. al. [23] proposed a conditional nonlinear optimal perturbation (CNOP) approach to solve the nonlinear problem analogous to the singular-vector approach described above. The results are promising, but the optimization problem may be difficult to solve for a GCM. These techniques can be verified with selective identical twin experiments utilizing the full nonlinear stochastic-dynamic GCM.

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