Subgrid-scale mixing in climate models:
A novel look at diffusion, accuracy, stability and climate sensitivity

A proposal submitted to the
Department of Energy's Climate Change Prediction Program

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PROJECT NARRATIVE

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Abstract

We present the case for evaluating more fully the role of subscale diffusion in the dynamical core of atmospheric models. The study is justified from both theoretical and empirical points of view, and there is particular motivation because of current activities in the DoE-NCAR community to develop high resolution models and to understand the role of subscale mixing in atmosphere-ocean coupling. There is rich, but fragmented, material in the literature which can be productively brought together. To accomplish this integration we pose a set of numerical experiments across a hierarchy of models which, when bridged, offer a strategy for determining cause and effect. We then make the case that future development of dynamical cores and new computational grids will offer continuous challenges which must be evaluated.

Introduction

The modeling systems which are used to represent and predict weather and climate are constructed from modular subsystems that are quantitative expressions of physical, chemical, and biological processes (*e.g.* Collins *et al.* 2006a, Jacobson 2005, Trenberth 1992, IPCC 1997). Generally, natural processes and continuous equations which quantify these processes are cast onto a discrete grid and approximated with numerical techniques. This leads to two classes of processes: those which are explicitly resolved on the grid and those which take place on spatial scales smaller than the grid; that is, subgrid processes. Subgrid processes are represented by parameterizations, which are, in principle, representative on the spatial scale of the grid.

More specifically, the modules of the atmospheric component of a climate model are placed into two classes: the physical components and the dynamical components.

The physical components include radiation, clouds, and moist convection, and are parameterized, subgrid processes. The dynamical components represent the fluid mechanics of the atmosphere and include the resolved scales of motion. The dynamical components also include dynamical mixing on the subscale. Conceptually, one can imagine advection by the wind field shearing a constituent to the scale of the grid, at which point that feature is mixed into the background, the subgrid. This proposal will focus on the representation of the subgrid mixing in the dynamical component, the dynamical core, of atmospheric models.

The representation of the subgrid by the dynamical core is complicated by the fact that there are physical processes to be represented, numerical errors which manifest themselves as subscale mixing, and the use of mixing to assure numerical stability and to compensate for numerical dispersion errors. Numerical dispersion errors appear as unrealistic grid-scale structures, and diffusion is used as a remedy. Physically, subscale mixing is expected to account for the mixing associated with advective cascade, and it is also associated with turbulent mixing in the boundary layer, mixing by breaking gravity waves, and mixing due to shear instabilities. These later types of mixing are explicitly accounted for with parameterizations; however, their quantitative effect is conflated with the mixing associated with filtering and numerical errors.

The representation of subscale mixing in climate models has implications which extend far beyond the tailoring of numerical performance. It is straightforward to envision the impact of diffusion on tracer fields such as water vapor, ozone, and carbon monoxide. For instance, excessive diffusion smears out gradients near the tropopause and leads to the misrepresentation of stratosphere-troposphere exchange. More subtly, the subscale mixing has a profound effect on the general circulation in climate models. For instance, the work of Shaw and Shepherd (2007, and references therein) has established that the magnitude and the qualitative form of the mean meridional circulation are sensitive to the subscale mixing. One of the motivators for this proposal is experimentation done at the National Center for Atmospheric Research (NCAR) which shows sensitivity of the variability of the tropical ocean to the atmospheric diffusion (M. Jochum and W. Large, personal communication.) The sensitivity to the representation of the subgrid mixing in climate models stands, perhaps, in contradiction to the experience in weather prediction. In weather prediction diffusion and filtering have been used to remove small-scale features which corrupt the forecast of larger scale weather features. Since weather and climate models often share the same dynamical core, there are potentially conflicting requirements for the algorithms that represent subscale mixing.

This proposal will focus on the documenting and quantifying the role of subscale mixing in the dynamical core of climate models. We will not explicitly investigate turbulent mixing associated with either planetary boundary layer or gravity wave parameterizations. Therefore, from the point of view of physics, we will focus on the mixing that arises because of the cascade of structure to small spatial scales. In the field of meteorology this mixing is frequently represented as linear or nonlinear diffusion; hence, this is an investigation of diffusive processes in climate models. From the point of view of numerical methods, we will investigate the role of diffusion in both the stability and remediation of spurious small-scale structure. Since diffusion is also a consequence of numerical approximation, we will explicitly study the impact of this numerical error on model performance.

We will focus on the numerical schemes used in NCAR's Community Atmosphere Model, version 3. (Collins *et al.* 2006b) This model has options for different dynamical cores, and we will focus on the spectral dynamical core and the finite volume dynamical core. Both of these methods are well established to propagate resolved, long-scale, structures. The spectral dynamical core is the current default configuration, and the finite volume dynamical core that is expected to be the default dynamical core of NCAR's next-generation Community Atmosphere Model, version 4 (CAM4). The two dynamical cores treat small-scales differently, from the perspective of both physical processes and numerical construction. We will perform a set of numerical experiments with suite of models of various degrees of complexity, with the goal of developing evaluation techniques which allow the determination in simple tests of predictors of the performance in more comprehensive models. Quantitative analysis of our numerical results will include explicit consideration of modeled spectra, statistical measures of spatial structure in modeled and observed tracer fields, sensitivity of the general circulation to model formulation, and stability and accuracy of the numerical schemes at high resolution.

The next section reviews the existing body of research and describes the motivation for our investigation. Then, the design and methodology of numerical experiments will be detailed. We will discuss the methods of analysis, and the extension of the results to comprehensive climate models.

Background and Motivation

The one dimensional advection-diffusion equation for a tracer will be used to develop the proposed research. For a scalar quantity A, with constant velocity u in the x direction, the advection-diffusion equation is

$$\frac{\partial A}{\partial t} + u\frac{\partial A}{\partial x} = D\frac{\partial^2 A}{\partial x^2} \qquad (1)$$

D is a diffusion coefficient which represents physical mixing; for instance, Fickian diffusion at molecular scales. When numerical approximation is made there are two conceptual changes to the mixing properties of Equation (1). First, the scale of the mixing moves to the scale of the grid.

The second conceptual change is the introduction of diffusive mixing due to the numerical formulation of the advection. That is, if *D* was formally set to zero, then the numerical approximation to the terms on the left hand side of (1) will usually have some characteristic of diffusion (see, for instance, Rood 1987). This numerical diffusion is a numerical artifact. In general numerical advection algorithms contain both diffusive errors and dispersion errors. Dispersion errors are those caused by the propagation of different wave lengths at different phase speeds; short waves propagate more slowly than they should. Often, the shortest resolved wave, one which requires two spatial grid cells to resolve, does not propagate at all. These dispersion errors lead to non-physical ripples in the approximate solution.

The artificial numerical diffusion is often used to remedy the ripples of the dispersion errors. In some cases, an explicit, but still non-physical, diffusion is added to numerical schemes to counter the non-physical rippling effect. In addition, diffusion is used either explicitly or implicitly to control numerical instability. Both linear and nonlinear formulations of diffusion are used in numerical approximation. Nonlinear diffusion algorithms trigger off of some attribute of the flow field such as spatial structure or velocity shear.

With the discussion above in mind, we write Equation (1) in the following form:

$$\begin{aligned} &\delta_t A + u\delta_x^A A = D_g \delta_x^2 A + D_f \delta_x^2 A \\ &\delta_t A + u(\delta'_x A + M_n \delta_x^2 A) = D_g \delta_x^2 A + D_f \delta_x^2 A \end{aligned} \quad (2)$$

This equation represents, heuristically, the actual implementation in a numerical model of Equation (1). In Equation (2) the δ represents some discrete approximation to the time (t) or the first or second spatial derivative (x). D_g is a diffusion coefficient at the scale of the grid which represents physical mixing in the discrete environment. D_f is a diffusion coefficient which represents the diffusive nature of filters that are added to control rippling or instability. δ^A is the symbolic representation for the discrete form of the advection algorithm. In the bottom equation this has been written as the sum of two operators. The term with the prime is non-diffusive, and uM_n is a diffusion coefficient associated with the numerical approximation of advection. In actual implementation, the diffusion may be linear or nonlinear, and the magnitude of some of the coefficients is not known. That is, they are flow dependent. There is an imprecise tuning towards some measure of credibility usually determined by the specific application of the numerical model. Equation (2) shows that physical and non-physical modes of mixing are entwined with each other. It also shows that the mixing is dependent upon the choice of numerical advection method as well as the spatial grid length. While not explicitly shown in Equation (2), in the atmosphere, the characteristics of diffusion in the vertical direction and in the horizontal plane are different.

Equation (2) is also a symbolic representation of the dynamical core of a model. There is advection, physical mixing, numerical mixing, and filtering. Whether stated or not, all dynamical cores used in climate and weather models have these components. Their discussion is relegated to the art of model building. To understand diffusive processes in dynamical cores is difficult; quantification is evasive. We know it could be important, but it is difficult to develop a satisfying, scientific approach to the problem.

The quality of simulations, the quality of observations, and the ever increasing demands derived from the problems faced by atmospheric scientists motivates our proposal to investigate, with some rigor, subscale mixing in climate models. Below we establish the importance of the representation of diffusive processes to both geophysical and numerical performance.

Numerical methods for atmospheric models were originally developed for numerical weather prediction. Since explicit small-scale waves, *e.g.* gravity waves from model initialization, harm weather forecasts, dissipative numerical schemes and filters were used to damp short waves. From the perspective of climate modeling, an intriguing paper, Mahlman and Umscheid (1987), showed that the mean temperature of the wintertime high latitude stratosphere was strongly sensitive to resolution. In short, for higher resolution the mean state was further away from radiative equilibrium and in better agreement with observations. The analysis of this behavior pointed to the generation and dissipation of small-scale waves, gravity waves, as being the cause for the difference of the mean temperature at different resolutions. The mechanism for generation of the waves in this model was strongly related to the numerical methods and the grid used in the model. The mechanism for dissipation was the nonlinear diffusion of Smagorinsky (1963). More theoretical work, such as reviewed in Holton *et al.* (1995), exposed the link between dissipative processes and the general circulation. Physically, this is interpreted as the dissipation of gravity waves and Rossby waves. In models, these effects are represented as parameterization as well as implicitly in the treatment of the smallest scales by the numerical algorithm (see Equation (2)).

Work with the finite difference model used by Mahlman and Umscheid (1987) has continued until recently. This work, along with a large independent body of theoretical study and numerical simulation, established the role of small scale mixing in the maintenance of the quasi-biennial oscillation, the mean meridional circulation, and tracer distributions. Of notable relevance to this proposal is the paper by Koshyk and Hamilton (2001), which investigates the energy spectra of the Mahlman and Umscheid (1987) model at different resolutions. They conclude that subgrid parameterization does not properly represent the effects of unresolved mixing at most altitudes. While the characteristics of the numerical scheme are not discussed at length in Koshyk and Hamilton, the finite difference method used in the model is known to be noisy both because of dispersion errors and the generation of noise at the grid scale. Therefore, it is reasonable to assert that some of the deficiencies and non-physical behavior noted by Koshyk and Hamilton might be directly related to artifacts in the numerical scheme. Ultimately, they advocate a critical re-evaluation of subgrid processes.

More recently Shepherd and Shaw (2004) and Shaw and Shepherd (2007) have shown that mean meridional circulation is sensitive to both the spatial structure of the mixing, conceptually diffusion, as well as the magnitude of the diffusion coefficient. This work reiterates the importance of subscale mixing in climate simulation. Of direct relevance, it demonstrates the need to understand both the physical and the numerical source of small-scale waves as well as the dissipation of these waves.

The modeling of trace constituents in the atmosphere brings the treatment of subscale mixing to the front. Constituent distributions which are determined by advective processes, *i.e.* those with long chemical lifetimes, contain small scale structures. There are high quality tracer observations from both aircraft and satellite instruments which provide insight into the dynamics of the atmosphere, including mixing. A consideration of subscale mixing in constituent modeling was essential in developing the models used to investigate polar ozone depletion; there was the need to quantify the mixing associated with planetary waves at the edge of the polar vortex. Observations showed isolation of the air in the polar vortex, with episodic shredding of air from the vortex and mixing into middle latitudes. This mixing mechanism is not well modeled by diffusion; it is a shearing process, followed by advective cascade, and, ultimately, small scale mixing.

Analysis of numerical models with tracer observations gives insight into the spatial and temporal characteristics of diffusion. For a scheme such as the Lin and Rood (1996), which has implicit, nonlinear, scale dependent diffusion, it was found that at resolution of 1-2 degrees of latitude in the horizontal plane, credible simulations where obtained. The Lin and Rood scheme is an elemental part of the finite volume dynamical core to be discussed below. At much higher resolutions, it becomes necessary to add an additional grid scale mixing to, for instance, simulate the tracer gradients at the edge of the polar vortex. As a function of resolution the scheme changes from being over diffused to being under diffused. Again, this is numerical diffusion; though, there is a physical interpretation for the form of the diffusion in this scheme.

McKenna *et al.* (2002) investigate, explicitly, the formulation of the subscale mixing. In this paper a diffusion-free Lagrangian trajectory calculation is used calculate tracer advection. The geometry of the particles, their nearness, is used to develop a mixing algorithm. Under the assumption of quasi-isentropic flow, McKenna *et al.* show that with a reasonable set of mixing length assumptions they can generate tracer fields that are clearly over mixed or under mixed. More recently, Wild and Prather (2006) have studied tropospheric ozone distributions as a function of model resolution and found significant changes in, for instance, ozone production in polluted environments. These studies use the advection scheme of Prather (1986), which has very little numerical diffusion. Prather (personal communication) has done preliminary experiments of the same design with the Lin and Rood (1996) scheme. These experiments show that numerical diffusion in the Lin and Rood scheme causes significant differences at the resolutions that have been studied. The question arises: do the two numerical schemes converge, and do they converge to the same the solution?

We have established both through our own experience and with some highlights from the literature that the algorithm chosen for subscale mixing has significant consequences on the geophysical performance of a model. The impact is sometimes intuitive, for example, structure in tracer fields or variability across frontal boundaries. Other times, for example, the impact of the mixing of small scales on the mean temperature or the mean meridional circulation is less intuitive. We have established that the physics of subgrid processes and the numerical formulation are conflated.

As discussed with regard to Equation (2), there is numerical diffusion in models and diffusion is used to remedy numerical errors and tailor the performance of numerical schemes. These numerical uses are discussed more fully.

In both finite difference and spectral schemes there is rippling where there are strong gradients of the advected field. This rippling can be viewed as either dispersion errors, with the shortest wave lengths being non-propagating, or in the case of the spectral model as the Gibbs phenomenon. In either case, the ripples are a manifestation of discrete approximations to highly varying, continuous fields. These ripples are non-physical; for instance they produce values of scalars that are higher or lower, even negative, that supported by a physical solution to the advection equation. Many strategies have been used to address these problems. They include borrowing from neighboring grid cells, filling of negative values (and ignoring overshoots), both global and local diffusion, and limiting of advective fluxes to keep the rippling from occurring (see, Rood 1987). Most of the methods are diffusive; some do not conserve mass and momentum. Other strategies have included the use of different formulations for different equations; for instance, one technique is used for the momentum equation, another for temperature, and another for water vapor. This approach introduces inconsistencies in the model manifested by the lack of correlated behavior between different parameters.

Related to this rippling effect, is the phenomenon of accumulation of too much "energy" in the smallest resolved scales. This comes from cascade of energy from large scales to small scales by advection, then the trapping of energy in these scales by non-propagation. The same sort of trapping of “energy” can be realized if there is a physical or numerical source at small spatial scales. In order to counter this accumulation in small scales, again, diffusion is added to the model. Diffusion is, by default, second order. In many applications fourth or higher order diffusion, hyper-diffusion, is added to the model because of the scale dependency of diffusion (see below). Again, this use of diffusion as a remedy or filter to counter rippling mixes both physical and numerical needs.

Finally, diffusion is used in numerical schemes to achieve or enhance numerical stability. Indeed many of the first finite difference schemes used in numerical models in the 1960s are productively interpreted as unstable schemes stabilized by diffusion (Rood 1987). In more modern schemes stabilization provided by diffusion is more subtle. Often the diffusion appears as a damping on the divergent component of the wind. The target of this diffusion is, for example, some inconsistencies that might arise from treating the advection in two dimensions as the sum of one-dimensional advection operations. In a well formulated scheme, this diffusion should be small. However, it may not be insignificant, and it may require reconsideration as resolution is changed.

Above we have provided the scientific background and motivation to study subscale mixing in climate models. We have deconstructed the geophysical and numerical aspects of the problem and established that better knowledge of subscale mixing is important to climate modeling. The problem remains complex, and multiple strategies for studying the problem are necessary. There is a conflation of geophysical and numerical dissipative processes. Further, there is a conflation of mixing due to several geophysical mechanisms, *e.g.* gravity wave drag, boundary level turbulence, and advective cascade. Dissipative processes accumulate over time; they are non-local. It is, therefore, difficult to design quantitative methods of analysis that link cause and effect. Below we outline our approach to the problem.

<u>Experiment Design, Method, and Analysis</u>

Below we describe our approach to explore the role of diffusive processes in climate models. We propose a novel, integrating approach which uses a hierarchy of models and an array of analysis techniques. There have been studies in many fields which investigate turbulence and mixing processes in numerical models. Within the field of atmospheric science, studies range from investigations of constant velocity tracer advection to sensitivity studies in comprehensive general circulation models. We will focus on the representation of dissipative processes in the dynamical core, and we intend to use tracer fields to probe dynamical processes. The study is a balance of reduction-based investigation and unification of results. It is beyond the limits of this proposal to present all of the possible experiments and analysis techniques which might be productive. Our initial investigations will utilize a suite of tests which range from an idealized baroclinic instability test case to an aqua-planet configuration.

The idealized baroclinic instability test case is fully described in Jablonowski and Williamson (2006a, b). This deterministic initial value test case for dry dynamical cores assesses the evolution of an idealized baroclinic wave in the Northern Hemisphere. The initial state is quasi-realistic and completely defined by analytic expressions which are a steady-state solution of the adiabatic inviscid *primitive equations* with pressure-based vertical coordinates. An overlaid perturbation then triggers the growth of a baroclinic disturbance over the course of several days.

This is in contrast to long-term aqua-planet simulations that retain the full complexity of the atmosphere with physical parameterizations, but simplify the surface conditions and radiative forcing (Neale and Hoskins 2001a,b). In particular, a flat ocean surface with analytically prescribed sea surface temperatures (SSTs) is used that eliminates the complexities with respect to sea-ice, land, orography and land-ocean contrasts. Furthermore, the equinoctial symmetric insolation is fixed but includes the diurnal cycle. The well-mixed CO_2 concentration is prescribed and ozone is specified. Such aqua-planet simulations have already been applied at NCAR to assess the impact of different dynamical cores on climate simulations (Williamson and Olson 2003). Meanwhile, an aqua-planet intercomparison project under the guidance of David L. Williamson (NCAR) is under way.

Other tests with intermediate complexities are also suggested. Besides the long-term idealized climate assessments by Held and Suarez (1994) we target dynamical core test cases like 3D Rossby-Haurwitz waves (Monaco and Williams 1975, Giraldo and Rosmond 2004) and mountain-induced Rossby wave trains (Qian *et al.* 1998, Tomita and Satoh 2004). These latter two deterministic test cases belong to the class of the baroclinic instability wave test, but add new aspects to the investigation of subgrid-scale mixing processes. The mountain induced wave motions explore the impact of orographic features on the subgrid-scale diffusion, the Rossby-Haurwitz wave will be used to address the stability of traveling wave packets. In particular, wavenumber 4 simulations will be assessed that were discussed in detail for the shallow water equations by Thuburn and Li (2000). In general, these tests can be considered 3D extensions of the Williamson *et al.* (1992) shallow water test suite.

In addition, our investigations will be complemented by idealized tracer experiments that shed light on both the diffusive characteristics of the dynamics and transport processes. Among them are the tracer transport simulations by Zubov *et al.* (1999), Schär *et al.* (2002) and Galewsky *et al.* (2005).