Computational Challenges for Global Dynamics of Fully Developed Turbulence in the Context of Geophysical Flows

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Abstract. Geophysical turbulent flows posses a very large number of degrees of freedom, and no mechanism is presently known which can reduce this number to a manageable size. In order for numerical simulations to be of use in advancing our understanding of geophysical turbulence, they must complement and make use of experiments, observations and theoretical advances. One is thus compelled to tackle numerical simulations at the highest resolution possible today, using the most powerful computers available with a heavy reliance on advances in information technology. This implies the need for developing as well powerful graphical and analysis softwares that can handle data of the order of 10 Terabytes. Such computations are to be viewed either as *gedanken* experiments, or as models for turbulence, and potentially the most promising venue is to combine both approaches. This paper reviews a few of the problems associated with these considerations, while stressing the need to maintain close contact with theoretical tools which allow for the construction of subgrid–scale models to be used in Large Eddy Simulations.

1 Introduction

Turbulent flows are ubiquitous, and as manifestations of one of the last outstanding unsolved problems of classical physics, they form today the core picture of numerous scientific and engineering inquiries and are linked to many issues in the geosciences: for example, in geology (Earth interior and dynamo problem), meteorology (cloud physics), oceanography (the role of stratification), climatology (global warming), space weather (from the Sun through the solar wind to the magnetosphere and ionosphere of the Earth), and ecology. The study of turbulence is not limited to inquiries in geophysics; turbulence plays an equally prominent–often dual–role in the understanding of nonlinear processes in physics, as well as in industrial flows, through *e.g.* the presence of seed particles or bubbles, and in studies of combustive and chemically reactive flows, and an even more pragmatic role in the area of aeronautical engineering regarding aircraft safety or in epidemiology. This interest is inter-disciplinary, and the issue of universality (or not) of physical processes and scaling laws arises, as the modeling of such complex flows becomes more realistic, but is also in more demand because of the wide range of applicability.

Although no general theory of turbulence currently exists, progress has been made recently in answering some fundamental questions (see *e.g.* Frisch, 1995). Departure from normality in probability distribution functions (PDF) for a variety of flows is well documented, but the origin and dynamics of these "fat wings" are not understood. Such wings appear, in fact, in many nonlinear problems with a wide range of excited scales in geophysical flows (Sornette, 2000). Nonlinearities become important in turbulent flows and can overcome linear viscous dissipation when the Reynolds number, $R_e = U_o\ L_0/\nu$, is large, where U_0 and L_0 are characteristic velocity scale and length scale of the flow, and ν is the viscosity. This number is the control parameter that measures both the number of interacting modes and the ratio of active temporal or spatial scales in the problem. The number of degrees of freedom in turbulent fluids increases as $R_e^{9/4}$ for $Re \gg 1$ and for flows in nature, R_e often exceed $\approx 10^8$. It is clear that the ability to probe large R_e, and, hence, to examine details regarding the PDFs and structures of turbulent flows, depends critically on the ability to resolve a large number of spatial and temporal scales and understand the global dynamics as well as the local interactions between modes and structures.

Theory demands that computations of turbulent flows reflect a clear scale separation between the energy-containing, inertial (self–similar) and dissipative ranges. Numerical experiments allow for fully controlled testing of a variety of models both phenomenological and basic, and they attempt to follow directly as wide a range of scales as possible in order to compute the true behavior of the flow. Detailed convergence studies show that in order to achieve the desired scale separation between the energy–containing modes and the dissipation regime, it is necessary to compute on grids with regularly–spaced points of at least 2048^3 cells (see *e.g.* Sytine *et al.,* 2000 for the compressible case). Only today can such computations be accomplished, and the subsequent data handled, although with some difficulty. For a computation of velocity, density and pressure on such a grid of 8 billion degrees of freedom and with storage using 16-bit scaled integers, 80 gigabytes (GB) of compressed data per time frame is generated. To provide good temporal resolution in a run of 3,000 time steps, a snapshot may be required every 10 time steps. Since there is no proven reduction in the degrees of freedom in a turbulent system which is guaranteed to retain all of the important characteristics of the flow, *all* of the data generated by these computations must be kept. Thus a total of 20 terabytes (TB) of storage would be required. This amount of data is sizable even for a national center, and is entirely beyond the abilities of individuals to manage at university laboratories in the near future.

In many respects, the data from numerical turbulence runs–particularly the size–is unique to turbulence studies. In the CONQUEST (CONcurrent QUErying Space and Time; Stolorz *et al.,* 1995) information system, for example, spatio-temporal features are extracted from large data sets. The features extracted may refer to cyclone tracks (or hurricanes) with distinct climatologic patterns, or they may be otherwise “indexable” (identifiable), and amenable to using learning algorithms that look for novel patterns or correlations. But in turbulence, one does not know yet *what* structures are key to our understanding the statistical properties of turbulent flows (*e.g.* vortex sheets, spiral or filaments, shocks or fronts, blobs, plumes or tetrads, knots, helices, tubes or arches) and their topology (see *e.g.* Kawahara *et al.,* 1997). Perhaps more importantly, turbulence data is 4-D because it is the spatio–temporal interactions between such structures–parallel or anti-parallel or orthogonal vortex filaments, single sheet or accumulations of such sheets embedded in a large-scale strain, kinking or intertwining of tubes; the latter is known to provide the elementary building blocks of turbulent transfer of energy to small scales in 3D and as such the source of our multi-scale problem. We note that in that light, an electronic data center for geophysical turbulent flows would be extremely useful, similar to the case of facilities for space physics observational data centers and theoretical physics experimental data centers.

Predictive models for geophysical flows require a unique synergy between computation and modeling, experiment and measurement. As an illustration, there is presently a world–wide effort to achieve an experimental dynamo with a small magnetic Prandtl number ($P_M = \nu/\eta$ where η is the magnetic diffusivity) similar to that of the Earth. Theoretical modeling (*e.g.* Pouquet, 1993; Nakayama, 2001), numerical computations (*e.g.* Nore *et al.,* 1997; Kageyama & Sato 1999) and experiments (Gailitis, 1993) must be inter–compared in order to define precisely the characteristics of the flow responsible for a viable dynamo.

Direct numerical simulations of turbulent flows can help elucidate the connection between multi–scale turbulent structures and the underlying non–Gaussian statistics. This link forms the basis of the notion of *intermittency* which plays a role in many geophysical phenomena, for example in droplet formation in clouds and in reactive flows where nonlinear interactions alter local chemical contact rates. However, intermittency is not yet included in models of these processes, nor is it clear how this should be done. A relatively new development, which may even demand new turbulence concepts, concerns the high resolution *in-situ* and remotely sensed geophysical data. These include lidar and radar measurements which can resolve turbulence structures throughout the atmospheric boundary layer to scales of a few meters, and data from such remote sensing platforms as Topex/Poseidon and QuikSCAT, which provide high resolution sea level and sea surface wind speed measurements, respectively. In principle, these data can be assimilated into global ocean and atmosphere circulation models. But the flows which these models address, and which the data represent, are non-Gaussian. An understanding of the role of intermittency will help determine how best to assimilate observational data into flow models for enhanced prediction capability, and long-term trending.

Indeed, beyond direct numerical simulations (DNS), research on parameterization of small scales for use in Large Eddy Simulations (LES) must be actively pursued as LES represents a strong link to theoretical approaches. Still, how do we proceed without being swamped by the complexity of closure schemes? Fast multi–processors enable us to compute turbulent flows at moderate Reynolds numbers in 3D and recently, a Taylor Reynolds number of $R_\lambda \sim 500$ (with $R_\lambda \sim R_e^{1/2}$) on a grid of 1024^3 points has been achieved (Kaneda, private communication). The vast amount of data associated with such a model must have its structures identified and be navigable in both space and time in order to be of use in parameterizing the small–scale behavior of the flow in LES models. For example, in the LANL-α model (Holm *et al.,* 1998), the small scales (which typically represent over 85% of the data) possess a dramatically reduced number of degrees of freedom when compared to conventional turbulence because it conserves the $\mathcal{H}_{1,\alpha}$ instead of the $\mathcal{L}_2$ norm: it correctly preserves the nonlinear structure of the Navier-Stokes equations for the dynamics of the large scales, but the dynamics of the small scales are limited to being swept by the larger scales. Although resolved in the computations, the information content of these scales is effectively small and we should be able to model them effectively.

2 Computational Issues in Geophysical Turbulence

2.1 A model of turbulence in one dimension, and adaptivity

The Burgers equation remains today a fertile ground for experimenting, both for numerical algorithms (Berger & Colella, 1989; Karniadakis *et al.,* 1991; Dietachmayer & Droegemeier, 1992; Gombosi *et al.,* 1994; Mavriplis, 1994) and for phenomenology for turbulence (Woyczynski, 1995; Frisch & Bec, 2000); it is also a model for many physical processes, from traffic fluctuations (Higuchi, 1978) to cosmology (Vergassola *et al.,* 1994). It reads:

$$\partial_t u + u\partial_x u = \nu \partial^2_{xx} u + f \tag{1}$$

where u is the velocity and f a forcing term which, in general, is taken to be concentrated in the large spatial scales and, for example, delta–correlated in time. When the forcing is identically zero, an exact solution is known through the Hopf–Cole transformation. Using the fact that the solution is a combination of ramps and shocks, one can show that the structure functions $\delta u(r) = u(x+r) - u(x)$ scale in the inertial range where dissipative processes can be ignored as $\langle \delta u(r)^p \rangle \sim r^{\zeta_p}$, with $\zeta_p = p$ for $p \leq 1$ and $\zeta_p = 1$ for $p \geq 1$. Furthermore, power laws for the wing of the PDFs of negative velocity gradients (the shocks) for (1) can be found analytically, but the index for such a law is in dispute (see Gotoh & Kraichnan (1998), and Frisch & Bec, *op.*

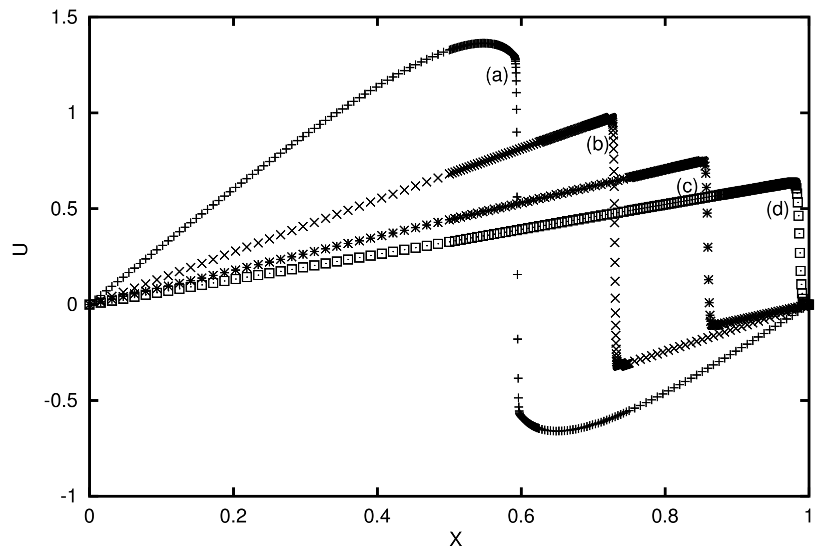

Fig. 1. 1D spectral element calculation of Burgers' equation with moving shock initial conditions (Huang, *et al.,* 1994) at $R_e = 5000$. The polynomial order is fixed at $N_p = 32$. The profiles are given at times (a) 0.2; (b) 0.6, (c) 1.0, and (c) 1.4. Note the clustering of points around the shock as the grid tracks the sharp velocity gradient there. The number of elements for each profile is 10, 8, 6, and 6, respectively. The grid is based on a binary tree, and adaptation occurs by binary splitting of an element (joining of two elements), if the velocity gradient is greater than (less than) some value.

cit.). The important point, though, is that such wings can now be computed analytically and thus lead to a better understanding of the role of structures in turbulent flows. Recently, it has also been shown, through an analogy with the XY spin model, that the tails of the Burgers velocity gradients can be recovered with Graner distributions (Noullez and Pinton, 2002).

Fast algorithms can be found that solve equation (1) with $L_0 \sim 1$, velocity $U_0 \sim 1$ and $\nu \sim 10^{-4}$ with only a few dozen nodal points. A criterion of choice of such points follows the concept of equidistribution according to a monitor function based in part on velocity gradients (see Figure 1; for a recent account see *e.g.* Huang & Russell (1997) and references therein). Is there a limitation on the achievable Reynolds number with grid adaptation at fixed number of points N? For a regular grid, and for Burgers equation, one can achieve $R_e \sim N^{3/2}$, a result that obtains by equating the characteristic time of nonlinear interactions based on the evaluation of the energy spectrum $E(k) \sim k^{-2}$, and of the diffusion time. This type of analysis is customary for Navier–Stokes flows using the concept of energy cascade, although for the Burgers equation the shock is a coherent structure and the time of formation of a shock is scale–independent. Let us now consider the extreme choice of taking all the available grid points in the vicinity of the shock with only a couple of points in the rarefaction wave (the ramp). Taking into account the fact that the local solution gives for the thickness of the shock a scaling $l_{min} \sim \nu^{1/2}$ because of the hyperbolic tangent profile, one now obtains $R_e \sim N^2$ (reminiscent of scaling when using irregularly spaced points with Chebychev polynomials).

2.2 Data Analysis and Manipulation

Conventional statistical analysis methods, while simple to compute, may reduce data to a relatively few numbers, filtering out information that has been computed at great expense. Still-image visualizations may reveal important instantaneous features, difficult to detect using numerical methods, but fail to capture the dynamics of time-evolving phenomena. Only temporal animations may reveal the behavior of complex evolving features. To be most effective, these animations must be realized in a highly interactive manner, using tools that permit researchers to navigate data through both time and space (Clyne *et al.,* 1998). The computational demands for interactive visual data analysis on the scales discussed are staggering. Large data visualization systems exist, such as those developed by Parker (1999) and Painter (1999), but they rely on hardware costing millions of dollars. In many ways visualization systems such as these are brute force approaches and not entirely necessary for visual data exploration, particularly if the goal is to assist in discovery of large scale features. The efficient extraction of sub-regions of data in time and space also must be possible. The extraction of data may be preceded or followed by conversion to quantities (*e.g.* temperature, vorticity, or a component of the rate of strain tensor) that are derived from the raw model data.

Multiresolution data representation methods may offer a solution to these issues. The theory of wavelets offers a natural mathematical framework for such a representation. At each successive power-of-two resolution level the wavelet transformation yields a lower frequency approximation to the previous level along with higher frequency detail coefficients representing the loss of information between levels. The accuracy of these coarser approximations is dependent on the nature of the data itself and the choice of wavelet basis function used. Exploring optimal wavelet basis functions for various forms of scientific data is an active area of research (Tao, *et al.,* 1994; Kolarov & Lynch 1997; Wilson 2000), including in turbulence (Farge *et al.,* 1999). Wavelet transforms are invertible, and lossless reconstruction of the approximation to the next higher resolution is possible (Mallat 1989). The transformation to and from wavelet space can be accomplished in linear time. Using techniques such as lifting (Sweldens, 1996), reconstruction may be accomplished using only additions and subtractions of floating point numbers, making the inverse transformation exceptionally fast. Furthermore, the transformed data occupy no more space than the original data, making multiresolution representations possible without the use of additional data storage.

Applying 3D wavelet transforms directly to data volumes in the manner first proposed by Muraki (1993) allows the efficient construction of data at different scales but it does not enable the multiresolution data sub-setting that we seek. Partitioning the data into blocks and applying the 3D transform to the individual blocks may improve the situation (Ihm 1998; Rodler 1999). Block decomposition facilitates region extraction and improves cache performance on cache-based microprocessors. However, to our knowledge these block-based efforts have all assumed static data. Furthermore, current methods, primarily aimed at large medical data sets, assume the researcher knows *a priori* which sub-region is of interest. Organization strategies that do not make these assumptions and are more appropriate for turbulence data must be explored. Similarly, analysis tools that may exploit these multiresolution encodings must be developed.

2.3 Large Eddy Simulations (LES)

There are a variety of closure schemes that have been proposed for turbulence (see *e.g.* Kraichnan, 1976; Yoshizawa, 1985; Chasnov, 1991; Kaneda *et al.,* 1999). It is clear that, as the primitive equations become more complete, more forces being taken into account, the closures become more complex since they involve evaluating a large number of triple correlations between the various variables (velocity, density, pressure, entropy, magnetic field, ...). Such equations are difficult to solve analytically and resort to numerical solutions to analyze them is unavoidable. Economical and physically-motivated methods must be developed further as they represent the only reasonable hope for modeling turbulent flows. For example, a stochastic framework of the Langevin type (Bertoglio, 1984) or a combination with inviscid Burgers noise for the unresolved scales (Majda & Kramer, 1999), enhanced or real-space eddy viscosity (Métais & Lesieur, 1992), or closures based on a Lagrangian spectral theory (Kaneda, 1981; Yoshida *et al.,* , 2002; Gotoh *et al.,* , 2002) are promising venues. In particular in the latter case, there are no adjustable parameters and the Lagrangian approach removes the problem associated with the Direct Interaction Approximation (Kraichnan, 1977) and thus leads to a classical Kolmogorov $k^{-5/3}$ spectrum (see also Nakayama (2001) for the case of weak anisotropic MHD).

On the other hand, it has been proposed that numerical methods themselves represent a closure of the primitive equations. In particular, the ability of non-oscillatory advection schemes to represent the effects of the unresolved scales of motion has already been explored (Oran and Boris, 1993, Porter *et al.,* 1994). For example, such a solver can accurately reproduce the dynamics of an atmospheric convective boundary layer. When an explicit turbulence model is implemented, the solver does not add any significant numerical diffusion and thus appears to include an effective subgrid scale model. Are the conservation/symmetry properties of the underlying equations sufficient to lead to that effect? Can such methods recover the law of the wall in channel flows? Similarly, the MPDATA methods (Smolarkiewicz and Margolin, 1998) developed for studying precipitation over mountains or forest fires can be studied to assess/quantify its LES properties exploiting a set of benchmark problems in the large R_e limit. A recent study of Burgers equation using such a code (Margolin and Rider, 2002) shows that the equivalent equation for the cell-averaged velocity $\bar{u}$ reads:

$$\partial_t \bar{u} + \bar{u}\partial_x \bar{u} - \nu_0 \partial^2_{xx} \bar{u} = \delta x^2 [\alpha \partial_x \bar{u} + \beta |\partial_x \bar{u}|] \partial^2_{xx} \bar{u} + \delta x^2 \zeta \bar{u} \bar{u}_{xxx} + \delta x^2 \eta \frac{\bar{u}^3_x}{\bar{u}} + \delta x^3 \gamma \bar{u}_{xxxx} \tag{2}$$

with δx the grid spacing, and where α, β, γ, ζ and η vary according to the numerical method used. Indeed, the first term on the *r.h.s.* acts as a numerical/physical nonlinear turbulent viscosity. However, this approach remains empirical and must be backed by strong closure schemes. Furthermore, the adaptive-mesh-refinement capabilities of codes developed for turbulence studies should also be assessed in the same fashion, thereby trying to link numerically–based and physically–based parameterization schemes.

3 Can we Learn from Fully Developed Turbulence?

The hallmark of turbulence is the creation of fluid motions at ever smaller scale and faster time scales, until the energy finally has cascaded down to the microscopic scales at which it can be dissipated as heat by viscosity. This turbulent cascade process is a successive loss of stability that occurs with increasing rapidity as the Reynolds number is increased. Fully-developed turbulence at high R_e is known to be "intermittent." This means, for example, that in the decay of turbulence the correlations in the flow at different scales do not follow a simple geometric relation between scales. Instead it comes in intermittent "gusts" and the cascade of energy has fractal properties. Thus, the heart of the problem of analyzing turbulence data, *i.e.* the statistical description of many interacting degrees of freedom (infinitely so in the limit $R_e \to \infty$) is fundamentally an information technology problem. The complexity is so rich that attacking this problem will require advances in IT research that should serve many other purposes and will go hand in hand with the development of computational power for the foreseeable future.

The seminal paper of R.H. Kraichnan (1994) on intermittency for a passive scalar such as a non-reactive pollutant, has led several teams to show that there are intermittency corrections to the scaling laws stemming from dimensional analysis, even though the velocity field in that model is well behaved (Gaussian with power-law spatial correlation and delta correlated in time). Such laws can be linked to the dynamics of structures, ramps or fronts, highly concentrated in space/time (Sreenivasan *et al.,* 1997; Warhaft, 2000; Shraiman & Siggia, 2000; Falkovich *et al.,* 2001). The corrections these authors find to a linear variation of scaling exponents with order is a signature of the persistence of the dynamical influence of the large scales of the turbulent flow; it arises, as a memory of initial conditions, through the existence of statistical Lagrangian invariants (with time). An example of such an invariant involves, in the isotropic case, the one–time three–point correlation function $C_3(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)$: even though, through Richardson law of dispersion, the average distance between the three points increases in time as $t^{3/2}$, there exists a function of the *shape* of the triangle formed by the three points at positions $(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3)$ as they evolve temporally, such that C_3 indeed remain constant (see Pumir, 1998). These invariants have physical consequences, for example concerning the problem of return to isotropy in the small scales, which is slower than thought previously and which is associated with intermittency.

The determination of the exponents ζ_p is an open problem for Navier–Stokes and MHD turbulence, and such exponents differ from the Burgers values mentioned in §2.1; however, one can also observe with both experiments and numerical simulations a saturation – Burgers being an extreme case – whereby the exponents, as p grows, tend to a limit for a passive scalar; this phenomenon is attributed to the presence of sharp fronts in the spatial distribution of the scalar density. Intermittency deals with the localization of sharp structures in space/time. Their signature is felt in the existence of fat wings in PDFs with strong events highly more probable than for the Gaussian with the same mean and variance and, as stated before, in the departure from a linear law with order of the scaling exponents of structure functions. Beyond Navier–Stokes, intermittency has been quantified in this manner in the Solar Wind (Burlaga *et al.,* 1990; Ruzmaikin *et al.,* 1995; Tu & Marsch, 1995) and in DNS for MHD (Politano *et al.,* 1998; Gomez *et al.,* 1999; Müller & Biskamp, 2000). It has been modeled successfully for Navier–Stokes flows (Castaing *et al.,* 1993; She & Leveque, 1994), as shown by numerous laboratory experiments starting with Anselmet *et al.,* (1984), and direct numerical simulations (Vincent and Meneguzzi, 1994), including in the compressible case at *r.m.s.* Mach numbers of unity (Porter *et al.,* 1999).

How much can we learn from these considerations when examining realistic flows, such as when considering anisotropy due to rotation, stratification or a uniform magnetic field, as well as in the vicinity of interfaces, or a combination of such effects, as they occur in geophysical flows? In the case of coupling to a magnetic field, in the kinematic regime where the magnetic field remains passive, anomalous scaling appears already at second order (Vergassola, 1996), and a comparison with standard two–point closures would thus be of great interest; in the case of a passive vector with pressure included, similarly corrections arise (Yoshida & Kaneda, 2001). What is the energy spectrum in anisotropic flows (see *e.g.* Ishihara *et al.,* 2002)? Is there return to isotropy at small scale for anisotropic forcing such as shear waves? Finally, the way that intermittency can be incorporated in Large-Eddy Simulations and its effects on small–scale physics is largely unknown today, although Lagrangian techniques that allow us to follow the flow locally may prove useful. The challenge is thus to retain simple modeling approaches (the only viable ones for realistic flows of industrial or geophysical interests) yet incorporating some of this knowledge recently uncovered in specific cases.

4 Conclusion

Computations should be selected to provide data sets of archetypal geophysical turbulent flows which would then enable a variety of physical conditions to be explored with as few actual runs as possible, but at the highest resolution feasible today. This kind of data would allow controlled testing of models developed in the geosciences community, and appropriate scaling laws for sub-grid scale models could then be derived from it. Such an approach could also be used to facilitate data assimilation in geophysical models from observations in order to enhance predictive capabilities. The societal impacts, with the direct effect of turbulence on geophysical flows is clear. The broader impact on education can also be mentioned, at the graduate and undergraduate levels and for the involvement of high–school teachers with exciting scientific developments at the frontier of what is possible today. An example is atmospheric turbulence and oceanic circulation, and their interaction at the air–sea interface. At intermediate scales, strong stable stratification (together with rotation) structures the flow and impedes mixing in the vertical direction (Kaneda & Ishida, 2000), destroys – at least partially – statistical isotropy, and affects variability. Questions such as whether a quasi–two dimensional approach is sufficient, or the hydrostatic approximation at the planetary scale, are wide open (see *e.g.* Danilov & Gurarie (2000) for a recent review; also, Kimura and Herring, 1996). In a broader sense, the interaction of turbulence and waves (*e.g.* here, internal gravity waves; in MHD, Alfvén and magneto-acoustic waves) remains an open problem, in some cases in part because of the non–uniformity of the weak turbulence approximation (Newell *et al.,* 2001); this approach which allows for a theoretical evaluation of scaling laws for fluxless and constant flux solutions of the equations is of great interest and has huge potential applications.

Because of the vast demands inherent to research areas in the geosciences, only a concerted effort will allow in due time for a possible breakthrough on some of the important and difficult questions remaining in the field of geophysical turbulence involving global scale dynamics. A process must be put together whereby, if successful, it would provide access to and dissemination of turbulence data with demonstrated scale separation; it would be not only immediately valuable to the geosciences community, but would also benefit industrial and commercial interests.

AP wishes to thank Aimé Fournier, Sébastien Galtier, Thomas Gomez, Steve Hammond, Jack Herring, Darryl Holm, Yoshi Kimura, Don Lenschow, Rich Loft, Sasha Madronitz, Len Margolin, Don Middleton, Hélène Politano, Yannick Ponty, David Porter, Piotr Smolarkiewicz, Paul Swarztrauber, Steve Thomas, Joe Tribbia, and Paul Woodward for useful discussions.

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