Computational Fluid Dynamics, Models, and The “Laws of Physics”

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Abstract

This post is an attempt to lay out in fairly complete detail some basic facts about Computational Fluid Dynamics (CFD) modeling. This technology is the core of all General Circulation Models (GCMs) of the atmosphere and has become widely used for numerical simulations in industry and government. We discuss some commonly believed erroneous and sometimes misleading statements about these models. In general, I believe that there is overconfidence in these simulations. This situation is related to the replication crisis in science generally.

1 Background

Numerical simulation over the last 60 years has come to play a larger and larger role in engineering design and scientific investigations. The level of detail and physical modeling varies greatly as do the accuracy requirements. For aerodynamic simulations accurate drag increments between configurations have high value. In climate simulations, a widely used figure of merit is temperature anomoly. Both drag increments and temperature anomoly are particularly difficult to compute accurately. The reason is simple: both output quantities are several orders of magnitude smaller than the overall absolute levels of momentum for drag or energy for temperature anomoly. This means that without tremendous effort, the output quantity is smaller than the numerical truncation error. Great care can sometimes provide processes that provide accurate results, but careful numerical control over all aspects of complex simulations is required. Contrast this with some fields of science where only general understanding is sought. In this case qualititatively interesting results can be easier to provide. This is known in the parlance of the field as “Colorful Fluid Dynamics.” While this is somewhat pejorative, these simulations do have their place. It cannot be stressed too strongly however that in turbulent simulations (and indeed in laminar simulations) even the broad ”patterns” can be quite wrong. Only after extensive validation, can such simulations be trusted qualitatively and even then only for the classes of problems used in the validation. This validation process for one aeronautical CFD code using full potential approximations with an integral boundary layer model consumed perhaps 50-100 man years of effort in a setting where high quality data was generally available. What is all too common among non-specialists is to conflate the two usage regimes or to make the assumption that realistic looking results imply quantitatively meaningful results.

2 Well Posed Problems – Electromagnetics and Linearly Elastic Structures

The first thing to discuss is that some fields of numerical simulation are very well founded on rigorous mathematical theory. Two that come to mind are electromagnetic scattering and linear structural dynamics.

*The opinions expressed are those of the author alone

Electromagnetic scattering is governed by Maxwell's equations which are linear. The theory is well understood, and very good numerical simulations are available [1, 2]. There are subtleties such as the interference of waves at long distances from their sources, which can cause rather large errors locally, for example at the bright spot on the back side of an illuminated sphere. Also exotic materials can be difficult to model accurately especially those with variable or non-isotropic material properties. However, generally, it is possible to develop accurate methods that provide high quality quantitative results.

Structural modeling in the linear elasticity range is also governed by well posed elliptic partial differential equations. There is very good theory for these problems and in fact there is the convenient St. Venant's principle, namely, the stresses and strains in a body at points that are sufficiently remote from points of application of load depends only on the static resultant of the loads and not on the distribution of loads. Here the practice can be quite good subject to the caveat that in some cases very dense finite element grids must be used and singularities resolved [2, 3]. Exotic materials can also be challenges here. This does not mean however that routine modeling is always adequate as costly industrial failures illustrate [4]. Engineering structures often result in problems that require very high resolution and great care with regard to details. There is some evidence that in many cases L2 norm errors in stress are on the order of 5% - 20% for commonly used models [2]. Fortunately, generous structural safety factors are employed where public health and safety are concerned. In any case, it is easy to become overconfident regarding the ease of generating finite element models and the accuracy of the results.

3 Computational Fluid Dynamics

The Earth system with its atmosphere and oceans is much more complex than most engineering simulations and thus the models are far more complex. However, the heart of any General Circulation Model (GCM) is a "dynamic core" that embodies the Navier-Stokes equations. Primarily, the added complexity is manifested in many subgrid models of high complexity. However, at some fundamental level it really is computational fluid dynamics. In fact GCM's were among the first efforts to solve the Navier-Stokes equations and many initial problems were solved by the pioneers in the field, such as the removal of sound waves. There is a positive feature of this history in that the methods and codes tend to be optimized quite well within the universe of methods and computers currently used. The downside is that there can be a very high cost to building a new code or inserting a new method into an existing code. In any such effort, even real improvements will at first appear to be inferior to the existing technology. This is pointed out for example in [5] and can really be a huge impediment to progress and the penetration of more modern methods into the codes.

The best technical argument I have heard in defense of GCM's is that Rossby waves are vastly easier to model than aeronautical flows where the pressure gradients and forcing can be a lot higher. There is some truth in this argument. The large scale vortex evolution in the atmosphere on shorter time scales is relatively unaffected by turbulence and viscous effects even though at finer scales, the problem is ill-posed. However, there are many other at least equally important components of the earth system. One important one is tropical convection, a classical ill-posed problem because of the large scale turbulent interfaces and shear layers. While usually neglected in aeronautical calculations, free air turbulence is in many cases very large in the atmosphere. It is typically neglected outside the boundary layer in GCM's. Thus, numerical viscosity determines the rate at which vortices break down. And of course there are clouds and precipitation. In addition some of these processes like clouds and convection have a very significant effect on overall energy balance. One must also bear in mind that aeronautical vehicles are designed to be stable and to minimize the effects of ill-posedness and in this sense are "easy" in that pathological nonlinear behaviors are avoided. In this sense they may be actually easier to model than the atmosphere. In any case aeronautical simulations are greatly simplified by a number of assumptions, for example that the onset flow is steady and essentially free of atmospheric turbulence. Aeronautical flows can often be assumed to be essentially isentropic outside the boundary layer.

As will be argued below and in [6, 7], the CFD literature is affected by positive results and selection bias. In the last 20 years, there has been increasing consciousness of and documentation of the strong influence biased work can have on the scientific literature. It is perhaps best documented in the medical literature where the scientific communities are very large and diverse [8–12]. These biases must be acknowledged by the community before they can be addressed. Of course, there are strong structural problems in modern science [8, 9] that make this a difficult thing to achieve.

Fluid Dynamics is a much more difficult problem than electromagnetic scattering or linear structures. First many of the problems are ill posed or nearly so, for example the inviscid transonic airfoil problem [13,14]. As is perhaps to be expected with nonlinear systems, there are also often multiple solutions, particulary in separated flows [15, 16]. Even in steady RANS (Reynolds Averaged Navier-Stokes) simulations there can be sensitivity to initial conditions or numerical details or gridding [17]. The AIAA Drag Prediction Workshop Series has shown the high levels of variability in CFD simulations even in attached mildly transonic and subsonic flows [18, 19]. These problems are far more common than reported in the literature. Perhaps even more disturbing, the phenomena of "pseudo-solutions" [16] seems to be common.

Another problem associated with nonlinearity in the equations is turbulence, basically defined as small scale fluctuations that have random statistical properties. There is still some debate about whether turbulence is completely represented by accurate solutions to the Navier-Stokes equations, even though most experts believe that it is. But the most critical element of difficulty is the fact that in most real life applications the Reynolds number is high or very high. An elementary description of the Reynolds' number is at

https://www.grc.nasa.gov/www/BGH/reynolds.html.

This reference is also a good elementary introduction to the critically important role of the boundary layer in fluid dynamics. The Reynolds number represents roughly the ratio of inertial forcing to viscous forcing. One would think if the viscous forcing was 5 to 7 orders of magnitude smaller than the inertial forcing (as it is for example in many aircraft and atmospheric simulations), it could be neglected. Nothing could be further from the truth. The inclusion of these viscous forces often results in an O(1) change in even total forces. Certainly, the effect on smaller quantities like drag is large and critical to successful simulations in most situations. Thus, most CFD simulations are inherently numerically difficult and simplifications and approximations are required. There is a truly vast literature on these subjects going back to the introduction of the digital computer and Von Neumann who made some of the first foreys into understanding the behaviour of discrete approximations. I can only go into a few of the aspects of this field that are particularly relevant here to understanding the place of such simulations in science.

The discrete problem sizes required for modeling fluid flows by resolving all the relevant scales grow as Reynolds number to the power 9/4 in the general case, assuming second order numerical discretizaitons. Computational effort grows at least linearly with discrete problem size multiplied by the number of time steps. Time steps must also decrease as the spacial grid is refined because of the stability requirements of the Courant-Freidrichs-Levy condition as well as to control time discretization errors. The number of time steps grows as Reynolds number to the power 3/4. Thus overall computational effort grows as Reynolds number to the power 3. Thus, for almost all problems of practical interest, it is computationally impossible (and will be for the forseeable future) to resolve all the important scales of the flow and so one must resort to subgrid models of fluctuations not resolved by the grid. For many idealized engineering problems, turbulence is the primary effect that must be so modeled. In GCM's there are many more, such as clouds. Below, several things will be argued. A good summary of some of the difficulties here is [15] for the design problem. See [20], [21], [22], [23], [24], and [25] for some other views that may not fully agree with the one presented here.

For modeling the atmosphere, the difficulties are immense. The Reynolds numbers are high and the turbulence levels are large but highly variable. Many of the supposedly small effects must be neglected based on scientific judgment. There are also large energy flows and evaporation and precipitation and clouds, which are all ignored in virtually all aerodynamic simulations for example. Ocean models require different methods as they are essentially incompressible. This in some sense simplifies the underlying Navier-Stokes equations but adds mathematical difficulties. Most incompressible methods are variants of Chorin's projection method [26]. Another good but mathematical introduction to fluid mechanics is [27].

3.1 The Role of Numerical Errors in CFD

In this section, I will briefly discuss the levels of numerical errors in engineering CFD RANS (Reynolds Averaged Navier-Stokes) codes and climate models because there is a stark disparity. Over the last 50 years, the practice of RANS simulations has improved dramatically.

1. Turbulence modeling has advanced from algebraic models to PDE based models with very significant improvements in accuracy.
2. Grid cell sizes are well adapted to generate only small levels of numerical truncation error at least in attached boundary layers. Generally, people tend to use 30-50 grid points in the boundary layer normal to the wall.
3. Solution methods have also improved with many codes able to achieve 6 digits of reduction of all the residuals.
4. Often via large numbers of iterations, the Navier-Stokes equations and the turbulence modeling equations are effectively solved simultaneously. This is required for model tuning to be meaningful and independent of numerical errors.
5. Very complex grid generation software allows confident gridding of new geometries with adequate grid resolution.
6. Advanced solver methods have allowed very large grids to be run routinely.
7. Modern numerical methods are well developed to be numerically stable by using upwinding and stabilization techniques. These are required to prevent unphysical wiggles that can become numerically unstable and make the discrete problem singular.

Generally the results are reproducible and reliable for thin boundary and shear layer dominated flows assuming little flow separation and subsonic flow. There are now a few codes that are capable of demonstrating grid convergence for the simpler geometries or lower Reynoldss numbers. However, almost all these simulations make a number of simplifying assumptions, for example that the onset flow is steady and essentially free of turbulence, and of constant pressure and temperature. However, as discussed elsewhere in this paper, these methods and codes all flounder when confronted with separated flows. Despite a massive effort over the last 30 years, results are not skillful and in many cases not reproducible.

The contrast with climate models speaks for itself. Typical grid spacings in climate models are often 50km and the vertical resolution is almost certainly inadequate. Further many of the models use spectral methods that are not fully stable. Various forms of filtering are used to remove undesirable oscillations. Modern upwinding methods and stabilized finite element methods are more reliable. Further, the many subgrid models are solved sequentially adding another source of numerical errors and making tuning problematic.

3.2 Some Basic Mathematics

It is important to come to grips with some mathematics fundamentals that at least partially explain why the Navier-Stokes equations are so difficult to solve accurately for separated flows. The Euler equations can be reformulated to show that the Total Pressure and Total Temperature are constant along streamlines. So long as the flow is attached, every point can be traced upstream to the inflow boundary and so these quantities are uniquely determined. However, if there is a closed streamline as there is usually in the separated flow case, the problem is singular because Total Pressure is undetermined on that steamline. In a practical Euler inviscid simulation, that level will be set by any crosswind numerical dissipation and will be an artifact of the details of the numerical methods used. Despite this one can regularize the Euler equations to be nonsingular even in this case by adding dissipation to the formulation. That dissipation necessarily degrades accuracy and leads to spurious total pressure loss for example.

In the case of the Navier-Stokes equations there is always cross wind diffusion present due to the molecular viscosity. However this is quite small in the high Reynolds' number case. In fact in many RANS simulations numerical dissipation and eddy viscosity are vastly larger, implying that the real viscosity plays no role in setting the total pressure loss in a separation bubble. It is an artifact of the numerical methods used and in some cases (if the grid is fine enough) the eddy viscosity. Unfortunately turbulence models are tuned independent of their role in separation modeling, so there is no expectation that they will generate the "right" result.

3.3 The Role of Turbulence and Chaos in Fluid Mechanics, Some Science Basics

In this section I will describe some well verified science from fluid mechanics that govern all Navier-Stokes simulations and that must inform any non-trivial discussion of weather or climate models. One of the problems in climate science is lack of fundamental understanding of these basic conclusions of fluid mechanics or (as perhaps the case may be for some) a reluctance to discuss the consequences of this science.

1. Virtually all real world flows have turbulent features and chaotic features such as large scale vortical flow.

2. Turbulent fluid has an effectively higher viscosity than laminar fluid. The generation, destruction, and transport of turbulence is critical to advanced fluid simulations and has a large impact on the global features and forces. This is equally true in 2D and 3D.

3. PDE transport models are vastly more accurate than local algebraic models of turbulence.

4. There is a problem here in that if a separation becomes large enough, a vortex street (in 2D) or a complex vortex pattern (in 3D) can develop. Turbulence models do not do a sterling job with these situations.

5. Without modeling the turbulence (and other chaotic features) in some way, results will be pretty badly wrong even in very simple cases.

6. Rossby waves are similar to a vortex street in their physics and must be resolved in detail to get good results. They are chaotic too.

7. Even in 2D, the proper rate of decay of vortices is critically dependent on modeling the level of turbulence and properly transporting it.

8. Climate is chaotic too and there is only weak evidence on whether it is predictable. There is even less evidence about its computability.

9. Just to give one fundamental problem that is a showstopper at the moment is how to control numerical error in any time accurate eddy resolving simulation. Classical methods fail. How can one tune such a model then? You can tune it for a given grid and initial condition, but that tuning might fail on a finer grid or with different initial conditions. This problem is just now beginning to be explored and is of critical importance for predicting climate or any other chaotic flow.

10. When truncation errors are significant (as they are in most practical fluid dynamics simulations particularly climate simulations), there is a constant danger of "overtuning" subgrid models or indeed discretization parameters or the hunderds of other parameters. The problem here is that tuning a simulation for a few particular cases too accuately is really just getting large errors to cancel for these

cases. Thus skill will be actually worse for cases outside the tuning set. In climate models the truncation errors are particularly large and computation costs too high to permit systematic study of the size of the various errors. Thus tuning is problematic.

In some cases, it may be possible to use Navier-Stokes to generate features like Rossby waves or a vortex street without modeling turbulence though the results are suspect. The problem here is that this helps us little in predicting the weather where chaos will overcome any skill at about 5-7 days. It also helps us little with predicting ENSO for example because quantitatively skillful predictions generally require modeling turbulence and other chaotic features of the flow. Isolated "successes" of this type are misleading outliers and offer us very little insight.

3.4 Numerical Dissipation, A Necessary Evil

Because the Navier-Stokes equations have a hyperbolic component, all discretization methods must employ numerical dissipation to be fully stable. There is a huge literature on these methods which goes back to the dawn of numerical analysis and methods have improved tremendously. A good but old reference is Richtmyer and Morton's excellent book [28]. In some sense all these methods are equivalent to increasing the effective viscosity beyond the real fluid viscosity. This issue is one of the very important choices method and code developers must make. Too little dissipation results in spurious "wiggles" in the solution or sometimes exponential growth and too much causes disturbances to be reduced too quickly. The natural tendency is to err on the side of too much dissipation and just use a finer grid. Since turbulence models augment the viscosity, they can also damp disturbances too quickly. In fact this is one of the important research topics in CFD. Once again the literature is vast and many of the issues too subtle to go into in any detail here. A good summary of some of the problems in selecting numerical methods for CFD modeling is contained in [25].

3.5 Time Accurate Calculations – A Panacea?

All turbulent flows are time dependent and there is no true steady state. However, using Reynolds averaging as discussed in Wilcox [29], one can separate the flow field into a steady component and a hopefully small component consisting of the unsteady fluctuations. The unsteady component can then be modeled in various ways so that the steady component can be computed. I won't go into technical detail here as the details are clearly given in Wilcox's book. As one would guess, the larger the truly unsteady component is, the more challenging the modeling problem becomes.

One might be tempted to just always treat the problem as a time dependent problem. This has several challenges however. At least in principle (but not always in practice) one should be able to use conventional numerical consistency checks in the steady state case. For example, one can check grid convergence, calculate sensitivities for parameters cheaply using linearizations, and use the residual as a measure of reliability. For the Navier-Stokes or Euler equations, these things can be very challenging, especially the grid convergence one, where there is no rigorous proof that the infinite grid limit exists or is unique. In fact, there is strong evidence for multiple solutions, some corresponding to states seen in testing, and other not. However, in practice, one can often show convincing evidence of grid convergence within some basin of attraction of that solution. One can hope to use finite element methods with all their attractive properties, solution adaptive grids, etc. All these conveniences are either inapplicable to time accurate simulations or are much more difficult to assess.

Time accurate simulations are also challenging because the numerical errors are in some sense cumulative, i.e., an error at a given time step will be propagated to all subsequent time steps. There is a well developed theory and practice for controling these errors for ordinary differential equations (ODEs) [30,31]. Generally, some kind of stability of the underlying continuous problem is required to achieve convergence. Likewise a stable numerical scheme is helpful. Backward differentiation methods are computationally more expensive than explicit schemes but offer superior stability properties. Of course, modern methods are vastly superior to the best methods of the 1960's, such as the leapfrog scheme, which has been well known since the 1970's to suffer from nonlinear instability.

For any chaotic time accurate simulation, classical methods of numerical error control fail. Because the initial value problem is ill-posed, the adjoint diverges. This is a truly daunting problem. We know numerical errors are cumulative and can grow nonlinearly, but our usual methods are completely inapplicable. This is a very serious problem if the output of the simulation is to be assessed for uncertainty or used as evidence in any issue involving public safety.

One often hears that "the climate of the attractor is a boundary value problem" and therefore it is predictable. Aside from the abuse of the technical term "boundary value problem" involved, this is nothing but an assertion with little to back it up. And of course, even assuming that the attractor is regular enough to be predictable there is the separate question of whether it is computable with finite computing time. It is similar to the folk doctrine that turbulence models convert an ill-posed time dependent problem into a well posed steady state one. This doctrine has been proven to be wrong - as the prevalence of multiple solutions discussed above shows. However, those who are engaged in selling CFD have found it attractive despite its unscientific and effectively unverifiable nature.

In the setting of choatic systems, the main argument that time accurate simulations are meaningful that I have heard (that is honest and worth further research) is "at least there is an attractor." The thinking is that if the attractor is sufficiently attractive, then errors in the solution will die off or at least remain bounded and not materially affect the time average solution or even the "climate" of the solution. The solution at any given time may be wildly inaccurate in detail as Lorenz discovered [32], but the climate will (according to this argument) be right. At least this is an argument that can be developed and eventually quantified and proven or disproven. My intuition is that a discretization of a complex problem can actually exhibit an attractor whose statistics differ a lot from the continuous one. Paul Williams has a very good example of this [33] for the Lorentz attractor showing that the "climate" of the attractor can be a strong function of the time step. Evidence is emerging of a similar effect due to spatial grid resolution for time accurate Large Eddy Simulations and a disturbing lack of grid convergence [34]. Further, the attractor may be only slightly attractive and there will be bifurcation points and saddle points as well. And, the attractor can be of very high dimension, meaning that tracing out all its parts could be computationally a monumental if not impossible task. So far, the bounds on attractor dimension are very large. My suggestion would be to develop and fund a large long term research effort in this area with the best minds in the field of nonlinear theory. Theoretical understanding may not be adequate at the present time to address it computationally. There is some interesting work by Wang at MIT for example that may eventually be computationally feasible [35] that could address some of the stability issues for the long term climate of the attractor. For the special case of periodic or nearly periodic flows, another approach that is more computationally tractable is discussed by Darmofal and Krakos [36]. This problem of time accurate simulations of chaotic systems it seems to me is a very important unsolved question in fundamental science and mathematics and one with tremendous potential impact across many fields.

While [37] is an excellent contribution by two unusually honest scientists, there is in my opinion reason for skepticism about their proposal to make climate models into eddy resolving simulations. Their assessment of climate models is in my view mostly correct and agrees with the thrust of this post, but there are a host of theoretical issues to be resolved before casting our lot with largely unexplored simulation methods that face serious theoretical challenges. Dramatic increases in resolution are obviously sorely needed in climate models and dramatic improvements may be possible in subgrid models once resolution is improved. Just as an example, modern PDE based models may make a significant difference. I don't think anyone knows the outcomes of these various steps toward improvement.

3.6 The "Impossibility" of Code Improvement?

This is mentioned in [5], but has been a well known feature of CFD for a very long time. Because existing codes have typically been around for a long time and have had an extensive history of tuning of subgrid model parameters, algorithmic parameters, and computing efficiency work; any initial attempt to show "improvement" over the current capability is very difficult. The problem has several facets. There is synergy between different subgrid model choices and the many algorithmic choices. Many more modern algorithmic methods are improvements to robustness and reliability but actually increase computer time. Since the original capability is incapable of running robustly the most challenging cases the new method may be able to model, there is pressure to exclude these from the test suite. And of course the test suite was often developed for testing software changes to the existing code and so the test suite is often limited to cases for which the current code provides meaningful answers. Indeed this issue of code and/or model selection is always an extremely controversial one with everyone having their own opinion and their own axe to grind. The way to deal with this in my opinion is to be able to show the improvements in robustness and reliability to customers of the codes directly. This issue is in some sense the flip side of the overselling so typical of the CFD literature of new methods or in many cases slight tweaks of existing methods. Much of what is shown in the literature is in fact not really very useful to customers of the codes. What is actually used in practice is often older codes and methods that draw scant attention in the literature. This is another source of subtle bias that may mislead outsiders.

4 The "Laws of Physics"

The "laws of physics" are usually thought of as conservation laws, the most important being conservation of mass, momentum, and energy. Usually when people say a quantity is conserved, they mean its total divergence is zero. Thus conservation of mass is expressed as

$$\vec{\nabla} \cdot (\rho \vec{v}) = 0 \tag{1}$$

where ρ is the local fluid density and $\vec{v}$ is the local fluid velocity. Momentum and energy are more complex stories. Assuming there are no net sources in a given flux box, the divergence of momentum should be zero for that box and any discrete violation of this conservation law is cause for concern. However, technically, most important simulation problems have sources for momentum, energy, and/or mass, i.e., the mass, momentum, and energy are not strictly speaking conserved. If the sources can be cast in divergence form, then we can speak of conservation of the modified mass, momentum, or energy. The momentum sources can be either kinematic such as imposed pressure gradients, viscous stresses, or externally imposed forces. One example is the mass source from an engine converting fuel to exahust gases.

The conservation laws with appropriate source terms for fluids are the Navier-Stokes equations. These equations correctly represent the local conservation laws and offer the possibility of numerical simulations. I'm not going to state these equations here because of the technical detail and resulting length. You can find a very complete version in [38]. Also included in this paper is a complete mathematical description of the Spalart Allmaras (SA) turbulence model which is almost as complex as the Navier-Stokes equations themselves. It turns out that this model seems to exhibits better stability properties than many of its competetors. Unfortunately turbulence models are not based on the conservation laws themselves but on complex relationships derived mostly from 2D simple sets of test data. This will be discussed below.

4.1 Initial Value Problem or Boundary Value Problem?

It is worth some space trying to clarify this issue because much of the commentary on it is confused and too vague to be useful. Basically, it is often argued that even though the initial value problem for any chaotic system is ill-posed, in the long term the "climate of the attractor" is stable and predictable so climate is a boundary value problem. This is quite confused. Basically, the problem here is that the details of the chaotic dynamics of the system help determine the long term statistical quantities we really want to know. Also, there is evidence of structural instability for the attractor in simple systems. Further there is very little we know for sure about the mythical attractor, not its dimension and not the Lyopanov constants involved (how attractive it is), and not where to expect bifurcations or "regime" changes. Without this information statements about computability are speculative at best.

A simple analogy for the climate system might be a wing as Nick Stokes has suggested. As pointed out above, the drag for a well designed wing is in some ways a good analogy for the temperature anomaly of the climate system. A few facts:

1. In general the overall forces on the wing are often very close to linear as a function of the angle of attack (the forcing here). This is "predicted" by very simple models like linear potential flow theory.

2. This observation is of little practical importance for predicting anything useful. Useful predictions require us to know the slope of the linear function and its intercept. To be useful linear potential theory must have both its slope and intercept adjusted based on some other source of data. Simple linear models of climate must have their effective forcings given from outside sources of data.

3. To compute the intercept and slope, linear potential flow is useless. One MUST take account of all the chaos of turbulence and other nonlinear behaviours which have a large effect on the forces.

4. The uncertainty in such computations is often high precisely because of the chaos and nonlinearity.

In the climate, the same thing is roughly true. The climate may respond linearly to changes in forcings over a narrow range. But that tells us little. To be useful, one must know the rate of response and the value (the value of temperature is important for example for ice sheet response). These are strongly dependent on details of the dynamics of the climate system through nonlinear feedbacks.

I would argue that the whole conceptual distinction between "forced" responses and "internal variability" while containing an element of truth, is often used as a fig leaf to cover uncertainties or ignorance. There is no good way to distinguish these two types of response except using complex climate models whose skill at doing so is unvalidated.

Many use this analogy of climate modeling with simplified engineering modeling to try to transfer the credibility [not fully deserved] from CFD simulations of simple systems to climate models or other complex separated flow simulations. This is not a correct implication. In any case, even simple aeronautical simulations can have very high uncertainty when used to simulate challenging flows.

4.2 Turbulence and SubGrid Models

The Spalart Allmaras turbulence model is an example of subgrid models giving rise to sources and in some cases additional terms in the equations [39]. There are many other competing models, each with its strengths and weaknesses [29]. The subgrid models must modify the Navier-Stokes equations if they are to have the needed effect. Turbulence models typically modify the true fluid viscosity by dramatically increasing it in certain parts of the flow, e.g., a boundary layer. The problem here is that these changes are not really based on the "laws of physics", and certainly not on the conservation laws. The models are typically based on assumed relationships that are suggested by limited sets of test data or by simply fitting available test data. They tend to be very highly nonlinear and typically make an O(1) difference in the total forces. As one might guess, this area is one where controversy is rife. An example of this is [40] in which the weaknesses of eddy viscosity models are discussed. Another is [41]. Most would characterize this as a very challenging problem, in fact one that will probably never be completely solved, so further research and controversy is a good thing.

However, turbulence modeling has advanced termendously over the last 50 years as computers have gotten more powerful. Practical turbulence models in the 1980's were algebraic, i.e., the turbulence variables were determined by simple local algebraic relationships. These models were not very accurate. More modern turbulence models such as the Spalart Allmaras or the Shear Stress Transport models solve global partial differential equations for the eddy viscosity. These equations are usually solved with the Navier-Stokes equations iteratively with many cycles between the two sets of equations. A few more modern codes actually solve the two equation sets fully coupled using Newton's method. These more modern models are often much more accurate than the older albegraic models. That is intuitively clear in that the evolution of turbulence in one grid cell is influenced by the turbulence in neighboring cells particularly those upstream of the cell in question. Many climate model subgrid models are algebraic in nature. This is required by the huge computing requirements. It is reasonable however to assume that these quantities are actually influenced by neighboring grid cells and so better accuracy could be acheived by solving global PDE's for them. Given the very large grid cells used, state of the art turbulence models are probably not going to give meaningful results.

For those who want to see all the details of how one successful integral method was developed, the Ph. D. thesis of Mark Drela [42] is honest and direct. Chapter 6 discusses the boundary layer method and its lag entrainment turbulence model. On page 86, we find that "This formula for the dissipation coefficient, despite having been derived solely from a special class of equilibrium flows, is now assumed to apply to all turbulent flows in general. As with the majority of useful statements about turbulent flow, this is mostly a leap of faith, justified primarily by the argument that in the laminar formulation decoupling the local disipation coefficient from the local pressure gradient led to substantial accuracy gains." This type of statement is not unusual among the specialists who develop the models, who seem to be pretty honest about their limitations. However, outsiders and particularly those who run codes developed by others can develop an unwarranted faith in them. This is encouraged by the nature of the biases in the literature and the "marketing" of CFD to laymen, which is a dark pseudo-science in its own right usually dominated by Colorful Fluid Dynamics.

Indeed negative results about subgrid models have begun to appear with Zhao et al 2016 [43] being one important example. This paper shows that cloud microphysics models have parameters that are not well constrained by data. Using plausible values, ECS (equilibrium climate sensitivity) can be "engineered" over a significant range. Another interesting result is [44] showing that model results can depend strongly on the order chosen to solve the numerous subgrid models in a given cell. In fact the models should be solved simultaneously so that any tuning is more independent of numerical details of the methods used. This is a fundamental principle of using such models and is the only way to ensure that tuning is meaningful. Indeed, many metrics for skill are poorly replicated by current generation climate models, particularly regional precipitation changes, cloud fraction as a function of lattitude, Total Lower Troposphere temperature changes compared to radiosondes and satellite derived values, tropical convection aggregation and Sea Surface Temperature changes just to name a few. This lack of skill for SST changes seems to be a reason why model ECS is often inconsistent with observationally constrained energy balance methods.

Given the large grid spacings used in climate models this is not surprising. Truncation errors are almost certianly larger than the changes in energy flows that are being modeled. In this situation, skill is to be expected only on those metrics involved in tuning (either conscious or subconscious) or metrics closely associated with them. In layman's terms, those metrics used in tuning come into alignment with the data only because of cancellation of errors.

One can make a plausible argument for why models do a reasonable job of replicating the global average surface temperature anomoly. The models are mostly tuned to match top of atmosphere radiation balance. If their ocean heat uptake is also consistent with reality (and it seems to be pretty close) and if the models conserve energy, one would expect the average temperature to be roughly right even if it is not explicitly used for tuning. However, this apparent skill does not mean that other outputs will also be skillful.

This problem of inadequate tuning and unconscious bias plagues all application areas of CFD. A typical situation involves a decades long campaign of attempts to apply a customer's favorite code to an application problem (or small class of problems). Over the course of this campaign many many combinations of gridding and other parameters are "tried" until an acceptable result is acheived. The more challenging issue of establishing the limitations of this acceptable "accuracy" for different types of flows is often neglected because of lack of resources. Thus, the cancellation of large numerical errors is never quantified and remains hidden waiting to emerge when a more challenging problem is attempted.

4.3 Overconfidence and Bias

As time passes, the seriousness of the bias issue in science continues to be better documented and understood. One recent example is [10] which quotes one researcher as saying "Loose scientific methods are leading to a massive false positive bias in the literature." It is worth quoting the abstract from [45] at length.

> **Poor research design and data analysis encourage false-positive findings. Such poor methods persist despite perennial calls for improvement, suggesting that they result from something more than just misunderstanding. The persistence of poor methods results partly from incentives that favour them, leading to the natural selection of bad science.**

In less scholarly settings, these results are typically met with various forms of rationalization. Often we are told that"the fundamantels are secure" or "my field is different" or "this affects only the medical fields." To those in the field, however, it is obvious that strong positive bias affects the Computational Fluid Dynamics literature for the reasons described above and that practitioners are often overconfident.

This overconfidence in the codes and methods suits the perceived self-interest of those applying the codes (and for a while suited the interests of the code developers and researchers) as it provides funding to continue development and application of the models to ever more challenging problems. Recently, this confluence of interests has been altered by an unforseen consequence, namely, laymen who determine funding have come to believe that CFD is a solved problem and hence have dramatically reduced the funding stream for fundamental development of new methods and also for new theoretical research. This conclusion is an easy one for outsiders to reach given the CFD literature, where positive results predominate even though we know the models are just wrong both locally and globally for large classes of flows, for example strongly separated flows. We have attempted to show a broader class of problems in our recent work [6, 7, 15]. Unfortunately, this problem of bias is not limited to CFD, but I believe is common in many other fields that use CFD modeling as well.

Another rationalization used to justify confidence in models are appeals to the "laws of physics" as discussed above. These appeals however omit a very important source of uncertainty and seem to provide a patena of certainty covering a far more complex reality. Such pronouncements are far more applicable to electromagnetic or linearly elastic structural modeling, even though even there a host of caveats must be added. In fluid dynamics, the story is different. Such appeals are perhaps convenient for those who like a particular set of model results, but not really completely honest. In fact, all computationally feasible models of high Reynolds' number flows resort to critical models that are in a fundamentally different category than the "laws of physics" as defined here.

Another corollary of the doctrine of the "laws of physics" is the idea that "more physics" must be better. Thus, simple models that ignore some feedbacks or terms in the equations are often maligned. This doctrine also suits the interest of some in the community, i.e., those working on more complex and costly simulations. It is also a favored tactic of Colorful Fluid Dynamics to portray the ultimately accurate simulation as just around the corner if we get all the "physics" included and use a sufficiently massive parallel computer. As we have argued in [6], this view is not an obvious one when critically examined. It is widely held however among both people who run and use CFD results and those who fund CFD.

4.4 Further Research

So what is the future of such simulations and GCM's? As attempts are made to use them in areas where public health and safety are at stake, estimating uncertainty will become increasingly important. Items deserving attention in my opinion are:

- One popular method for estimating uncertainty is to simply run a range of credible models and observe the spread of the outcomes. This method has limitations and can only provide an optimistic lower bound on the uncertainty. A variant of this approach is to assess the sensitivity of results to changes in subgrid model parameters. An example of this method is [46]. This latter method is just beginning to be applied in a rigorous way, but also has significant limitations.

- There are many many other parameters in such simulations other than the turbulence and other subgrid models. Parameters controling the computational grid are an important one as are parameters of the numerical discretization. In GCM's there are more. Sensitivity of the results to these parameters has been an implicit (but rarely discussed as such except in connection with design optimization) feature of much of the CFD literature. Unfortunately, much of it is very unsystematic and subject to biased reporting. There is a lot of important work to be done in this area.

- One measure that builds confidence is to show that in the limit of fine grid, the method's results converge in some meaningful way. This is also a desirable property of any subgrid models used. Unfortunately, once one starts down the Large Eddy Simulation road, it becomes impossible. For GCM's this grid convergence issue is probably impossible to reliably assess. It is hard enough for the Navier-Stokes equations where it is still a subject of controversy and research.

- There are well understood adjoint methods for estimating sensitivity to small changes to parameters and effective eigenvalue methods for determining stability, at least on a given grid. However, these methods are computationally challenging and usually absent from codes. They require careful attention to all aspects of code development to generate derivatives in addition to residuals. In old codes, it may be easier to start over rather than trying to retrofit the needed technology. Unfortunately, for eddy resolving time accurate simulations, the adjoint diverges, a consequence of the ill-posed nature of the initial value problem. With sufficient effort, both theoretical and computational, this difficulty might be overcome in the future [35].

- As mentioned above, developing and implementing better methods is often neglected in favor of "more physics" (or as may be the case pseudo-physics), i.e., including more terms in the model equations which invariably results in higher computing requirements and a resort to less reliable numerical methods. Adding more parameters seems superficially to be an advantage in that more classes of phenomena can be modeled. However, it can make the task of deriving parameter values and empirical relationships much more difficult. This is argued for example in [6]. It is also often argued as well in support of eddy viscosity turbulence models against Reynolds stress models. There is an argument to be made that lower or intermediate complexity models deserve more attention.

- Getting some reliable information about stability, Lyapunov constants, or even linearized stability information is simply very rare in practice but can have tremendous value in new situations, for example at bifurcation points or points where multiple solutions exist. Bear in mind these multiple solutions can be very close together. There are algorithms to estimate this information but they are almost never available in the codes, and when available are almost never relied on because of weak solvers and other larger errors.

- I would argue that the most important elements needing attention, both in CFD and in climate and weather modeling, are new theoretical work and insights and the development of more accurate data. The latter work is not glamorous and the former can entail career risks. These are hard problems and in many cases, a particular line of enquiry will not yield anything really new.

And what are some of the dangers to be combated?

- It is critical to realize that the literature is biased and that replication failures are often not published.

- We really need to escape from the elliptic boundary value problem (well posed) mental model that so many with a passing familiarty with the issues continue to hold. A variant of this mental model one encounters in the climate world is the doctrine of "converting an initial value problem to a boundary value problem." Aside from being technical nonsense and misleading, this just confuses the issue, which is really about the attractor and its properties. The methods developed for well-posed elliptic problems have been pursued about as far as they will take us. However, this mental model can result in dramatic overconfidence in models in CFD.

- A corollary of the "boundary value problem" misnomer is the idea that "If I run the model right, the answer will be right" mental model. This is patently false and even dangerous, however, it gratifies egos and aids in marketing.

5 Conclusion

I have tried to lay out in summary form some of the issues with high Reynolds number fluid simulations and to highlight the problem of overconfidence as well as some avenues to try to fundamentally advance our understanding. Laymen need to be aware of the typical tactics of the dark arts of "Colorful Fluid Dynamics" and "science communication." It is critical to realize that much of the literature is affected by selection and positive results bias. This is something that most will admit privately, but is almost never publicly discussed.

How does this bias come about? An all too common scenario is for a researcher to have developed a new code or a new feature of an old code or to be trying to apply an existing code or method to a particular test case of interest to a customer. The first step is to find some data that is publicly available or obtain customer supplied data. Much of the older and well documented experiments involve flows that are not tremendously challenging. One then runs the code or model (adjusting grid strategies, discretization and solver methodologies, and turbulence model parameters or methods) until the results match the data reasonably well. Then the work often stops (in many cases because of lack of funding or lack of incentives to draw more scientifically balanced conclusions) and is published. The often large number of runs with different parameters that provided less convincing results are explained as due to "bad gridding," "inadequate parameter tuning," "my inexperience in running the code," etc. The supply of witches to be burned is seemingly endless. These rationalizations are usually quite honest and sincerely believed, but biased. They are based on a cultural bias that if the model is "run right" then the results will be right, if not quantitatively, then at least qualitatively. As we saw above, those who develop the models themselves know this to be incorrect as do those responsible for using the simulations where public safety is at stake. As a last resort one can always point to any deficiencies in the data or for the more brazen, simply claim the data is wrong since it disagrees with the simulation. The far more interesting and valuable questions about robustness and uncertainty or even structural instability in the results are often neglected. One logical conclusion to be drawn from [5] and [37] is that the world of GCM's is little better. However, these papers are a hopeful sign of a desire to improve and are to be strongly commended. Some will find it disconcerting that it took decades for people to weakly acknowledge what the best people in fluid dynamics have known for a long time. And there is some excellent fundamental work being done by some of the leaders in turbulence modeling [47].

This may seem a cynical view, but it is unfortunately based on practices in the pressure filled research environment that are all too common. There is tremendous pressure to produce "good" results to keep the funding stream alive as those in the field well know. Just as reported in medically related fields, replication efforts for CFD have often been unsuccessful, but almost always go unpublished because of the lack of incentives to do so. It is sad to have to add that in some cases, senior people in the field can supress negative results. Some way needs to be found to provide incentives for honest and objective replication efforts and publishing those findings regardless of the opinions of the authors of the method. Priorities somehow need to be realigned toward more scientifically valuable information about robustness and stability of results and addressing uncertainty.

However, I believe there are some promising signs of progress in science. In medicine, [11] shows that reforms can have dramatic effects in improving the quality of the literature. There is a growing recognition of the replication crisis generally and the need to take action to prevent science's reputation with the public from being irreparably damaged. As simulations move into the arena affecting public safety and health, there will be hopefully increasing scrutiny, healthy skepticism, and more honesty. [5] and [37] are important (and difficult in the politically charged climate field) steps forward on a long and difficult road to improved science. [22] is also a step forward.

In my opinion those who can retard progress in CFD are often involved in "science communication" and "Colorful Fluid Dynamics." They sometimes view their job as justifying political outcomes by whitewashing high levels of uncertainty and bias or making the story good click bait by exaggerating. Worse still, many act as apologists for "science" or senior researchers and tend to minimize any problems. Nothing could be more certain to produce the exact opposite of the desired outcome, viz., a cynical and disallusioned public already tired of the seemingly endless scary stories about dire consequences often based on nothing more than the pseudo-science of "science communication" of politically motivated narratives. This effect has already played out in medicine where the public and many physicians are already quite skeptical of health advice based on retrospective studies, biased reporting, or slick advertising claiming vague but huge benefits for products or procedures [48]. Unfortunately, bad medical science continues to affect the health of millions and wastes untold billions of dollars. The mechanisms for quantifying the state of the science on any topic and particularly estimating the often high uncertainties are very weak. As always in human affairs, complete honesty and directness is the best long term strategy. Particularly for science, which tends to hold itself up as having high authority, the danger is in my view worth addressing urgently. In my view, this response is demanded not just by concerns about public perceptions, but also by ethical considerations and simple honesty as well as a regard for the lives and well-being of the consumers of our work who deserve the best information available.

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