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Advances in Turbulence IX
Proceedings of the Ninth European Turbulence Conference
I.P. Castro, P.E. Hancock & T.G.Thomas (Eds.)

Regularization opportunities in the adjoint analysis of multiscale systems

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The purpose of this abstract is to summarize the taxonomy of regularization opportunities available in the adjoint analysis of multiscale fluid systems. Adjoint analysis has a broad range of important applications in fluid mechanics, including:

A) transonic airfoil shape optimization [1],

B) optimization of open-loop control distributions for transitional and turbulent flow systems [2], [3], [4], [5], and

C) state reconstruction and parameter estimation in numerical weather prediction (known operationally as "4D-VAR") [6].

In order to apply adjoint analysis, a cost functional is first defined which represents mathematically the physical objective in performing the computational optimization. In problem A, this objective is typically to maximize the lift/drag ratio of the airfoil for a range of different cruise configurations while respecting a variety of practical "feasibility" constraints related to the construction of the airfoil. In problem B, the objective is typically to reduce drag or to reduce TKE in order to inhibit transition to turbulence, though in combustion applications the objective is typically the opposite—that is, to excite the flow with minimal control input in order to enhance turbulent mixing. In problem C, the objective is typically to reconcile the numerical weather model with recent weather measurements in order to obtain accurate weather forecasts. Once the control objective is defined mathematically as a cost functional, adjoint analysis may be used as a tool to determine an appropriately-defined *gradient* of the cost functional with respect to the unknown parameters; the adjoint field calculation is thus a central component of high-dimensional gradient-based control optimization strategies. Refs. [5], [7] contain a brief review of our perspective on a few of the relevant issues related to such problems.

Even though the mathematical framework for adjoint-based optimization is fairly mature and has already been used successfully in a broad range of applications in fluid mechanics, many flow systems still present fundamental challenges to this approach. These challenges are often related to the multiscale complexity of fluid systems. Turbulent flows are dominated by a nonlinear cascade of energy over a broad range of length scales and times scales. Adjoint analyses of such flows must be crafted with care in order to be well behaved over this full range of scales. In numerical weather prediction, the problem of finding the current state of the model based on past measurements is effectively ill-posed, as it does not necessarily depend smoothly on the measurements taken. Even in laminar flows, adjoint field calculations can be exponentially unstable in thin shear layers unless the optimization problem is formulated properly.

The issues of "well-posedness" and "regularization" are not simply mathematical curiosities. Far from it, these issues are central to the efficient and accurate solution of high-dimensional optimization problems. If a particular optimization problem does not have a smooth dependence on the unknown variables (as is the case in ill-posed problems), gradient-based solution approaches are essentially rendered useless. Without leveraging gradient information, adaptive strategies which attempt to solve a high-dimensional optimization problem based on function evaluations alone typically require an excessive number of function evaluations to converge, thereby making them impractical. Even in problems which are mathematically well posed, numerical resolution of the adjoint field can be exceedingly difficult to obtain, or the extraction of the gradient of the cost functional from the adjoint field exceedingly prone to amplification of numerical error, unless the proper care is taken in the definition of the adjoint field. There is quite a bit of flexibility in how an adjoint-based optimization problem is defined, and the choices made in this definition have an enormous impact on the rate of convergence of the resulting numerical algorithm.

The objective of the present research effort is to develop a uniform framework for understanding these well-posedness and regularization issues. In the adjoint-based optimization of PDE systems in general, there are three spatial domains of interest: the domain on which cost functional is defined, which we denote Ω_1, the domain over which the state of the system modeled, which we denote Ω_2, and the domain on which the "control" is applied, which we denote Ω_3. Typically, the system model, and the cost functional which measures this model, are defined over a time interval $[0,T]$. The "control" can also be defined over $[0,T]$, as in true control problems, or can be defined at a particular instant of time, as done in the forecasting problem. In the process of adjoint-based optimization, inner products are used (or implied, if not explicitly stated) on all three of these space-time domains.

In the continuous setting, the form of each of these inner products may incorporate either derivatives or "anti-derivatives" in both space and time. Mathematically, these inner products are related to the natural measures for functions defined in the Sobolev space $H^p(0,T;H^q(\Omega_i))$, where q is the differentiability order in space, p is the differentiability order in time, and Ω_i denotes the spatial domain. Note that Sobolev spaces with negative differentiability indices can also be considered in this framework by taking p and/or q negative. Such inner products are natural alternatives to the L_2 inner product when considering functions

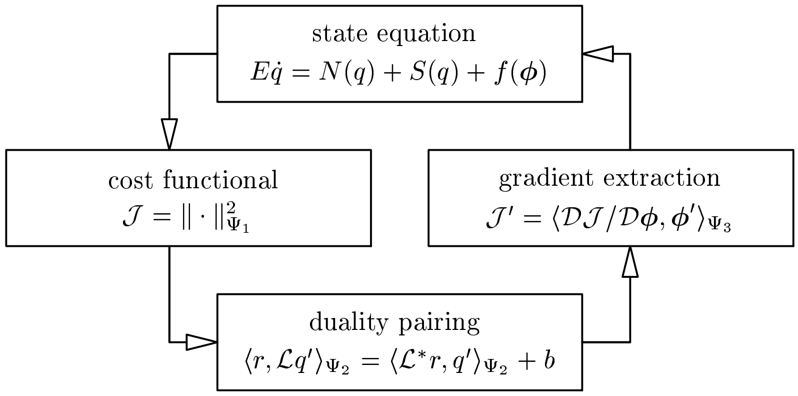

Figure 1: The four essential components of the adjoint-based optimization process. As outlined in the text, each component of this process is associated with a distinct opportunity for regularization.

of different degrees of regularity in both space and time. How each of these inner products is defined, in addition to any smoothing that might be applied to the state equation itself, has important consequences on the smoothness of the several variables in this problem, as summarized in Figure 1. As a shorthand, we use Ψ_1, Ψ_2, and Ψ_3 to identify the appropriate inner products on the three space-time domains of interest in this problem.

The first regularization opportunity is given by adding an artificial (but well-motivated) term to the discretized state equation itself. Two common examples are dynamic subgrid-scale models (in turbulence research) and hyperviscosity (in numerical weather prediction). Addition of such a term to the numerical model is useful for tuning the behavior of the numerical model at the unresolvable scales, and can be used to make a problem well-posed if it is not otherwise. In addition to modifying the actual governing equation, we can also consider its different derived forms (e.g., the vorticity form instead of the velocity-pressure form of the Navier-Stokes equation). These different yet equivalent forms may serve to focus on different aspects of the dynamics in numerical simulations and adjoint analyses thereof.

The second regularization opportunity is given by the definition of the cost functional. As mentioned previously, the cost functional in adjoint analysis of fluid systems can take any of a wide variety of forms depending on the problem under consideration. However, in most such formulations, the cost functional involves the norm of a flow quantity taken over some subdomain of the space-time domain under consideration, which we have denoted Ψ_1. In most optimization studies performed in the existing literature, L_2 norms are used in the definition of the cost functional. However, selecting norms which incorporate either derivatives or anti-derivatives effectively builds in a "filter" into the definition of the cost functional, thereby allowing extra emphasis to be placed on certain scales of interest in the multiscale problem.

The third regularization opportunity is given by the form of the duality pairing used to define the adjoint state and the adjoint operator; incorporating derivatives or anti-derivatives into the definition of the duality pairing can help to obtain better behaved, and therefore numerically tractable, adjoint operators.

Finally, the fourth regularization opportunity is the definition of the inner product used to extract the cost functional gradient. Incorporating derivatives into this inner product allows us to extract smoother gradients, thereby preconditioning the optimization process.

In the present paper, we have presented a comprehensive framework for regularizing various aspects of the adjoint-based optimization process. Though adjoint-based optimization has already seen a broad range of applications in fluid mechanics, exploitation of these regularization opportunities appears to be very important when applying such techniques to difficult problems of both physical and engineering interest, such as high-Reynolds number turbulence. Further discussion of the these issues, including analysis of the various types of regularization in the context of the data assimilation problem applied to the Kuramoto-Sivashinsky equation, will be discussed in a forthcoming paper [8].

Acknowledgments

Generous funding from Prof. Belinda King's program at AFOSR is gratefully acknowledged.

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