Final Report on the " New Directions in the Variational Multiscale Formulation of Large Eddy Simulation of Turbulence"

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1 Technical Progress

The work performed as part of this grant may be described in the context of developing numerical methods for solving the following variational problem: Find $u \in \mathcal{V}$, such that $\forall w \in \mathcal{V}$

$$B(w, u) = l(w), \tag{1}$$

where $l(\cdot)$ is an appropriate linear form and $B(\cdot, \cdot)$ is a semi-linear form (linear in the first slot). This represents the weak form for a system of partial differential equations. We assume that these equations are such that the straightforward Galerkin approximation of (1) on a space $\mathcal{V}^h \subset \mathcal{V}$ of reasonable dimension, is inaccurate. Target applications includes flows with turbulence and systems with shocks.

Modeled equations With this in mind, the following alternate finite dimensional problem is proposed: Find $u^h \in \mathcal{V}^h$, such that $\forall w^h \in \mathcal{V}^h$

$$B(w^h, u^h) + M(w^h, u^h; h, c) = l(w^h), \tag{2}$$

where $M(w^h, u^h; h, c)$ is a term added to the Galerkin approximation to improve its performance. It is a semi-linear form which depends upon the "mesh-size" h and a vector of parameters c. We refer to this term as the *model term*, as it can be shown to model the effect of the unresolved scales (outside of $\mathcal{V}^h$) on the resolved scales (inside $\mathcal{V}^h$). This term is to be selected so that the resulting solution u^h is close to a user-defined *optimal solution* $\mathbb{P}^h u$, where $\mathbb{P}^h$ is an appropriate restriction operator. That is

$$u^h \approx \mathbb{P}^h u. \tag{3}$$

Multiscale models Often the effect of the unresolved scales on the coarse and fine components of the resolved scales is distinct and must be modeled as such. To accommodate this we introduce the following finite dimensional problems with multiscale models: Find $u^h \in \mathcal{V}^h$, such that

$$\begin{aligned} B(\bar{w}^h, u^h) + \bar{M}(\bar{w}^h, u^h; h, \bar{c}) = l(\bar{w}^h), \forall \bar{w}^h \in \bar{\mathcal{V}}^h \\ B(\acute{w}^h, u^h) + \acute{M}(\acute{w}^h, u^h; h, \acute{c}) = l(\acute{w}^h), \forall \acute{w}^h \in \acute{\mathcal{V}}^h. \end{aligned} \tag{4}$$

In the equations above $\bar{\mathcal{V}}^h$ and $\acute{\mathcal{V}}^h$ represent the coarse and the fine scale resolved spaces (note $\mathcal{V}^h = \bar{\mathcal{V}}^h \oplus \acute{\mathcal{V}}^h$) and $\bar{M}$ and $\acute{M}$ represent the corresponding model terms.

Dynamic evaluation of parameters By requiring that (a) the solution of the modeled system above is optimal (that is (3) holds with an equality), and that (b) this holds not only on $\mathcal{V}^h$ but also on its subspaces, we have derived a consistency condition for the model term (dubbed as the variational counterpart of the Germano identity) which may be used to determine the parameters that appear in it. This leads to a dynamic evaluation of the parameters and in a sense to the closure of (2) or (4). It is remarkable that this identity does not require the exact solution u, but rather the numerical solution u^h and the form of the restriction operator $\mathbb{P}^h$.

As part of the current research grant we have considered the following extensions/applications of the framework described above.

1.1 A dynamic multiscale method for approximating conservation laws [1–3]

In this study we have developed a numerical method for the spectral approximation of non-linear conservation laws. These laws describe a broad range of physical phenomena which include the dynamics of gasses, the flow of traffic and the propagation of shallow water and nonlinear acoustic waves. In all these systems we have addressed the cases when the physical viscosity (or diffusivity) is small or zero. In the small viscosity case, the solution to such systems is known to develop local regions of large spatial and temporal gradients called shocks. The width of a shock reduces with reducing viscosity, and in the limit of zero viscosity the solution becomes discontinuous. In fact, in this limit in order to ensure unique solutions, the conservation law must be supplemented with an entropy production inequality and conditions that relate jumps in conserved quantities across the shock [9, 10].

For small viscosities, the standard Fourier-Galerkin approximation to non-linear conservation laws becomes unstable if the shock width is smaller than the grid size. For a large class of problems the computational cost of employing a grid which is fine enough to resolve a shock is prohibitive and as a result this method finds limited application. Further, in the limit of zero viscosity, even with sufficient grid refinement, the Fourier-Galerkin solution does not converge to the unique "physical" solution which satisfies the entropy production inequality. To overcome these difficulties associated with the Fourier-Galerkin method, several methods have been proposed. A large proportion of these methods involve appending to the Fourier-Galerkin formulation a numerical viscosity term (see [11] for example). These methods may be classified on the basis of the equations in which the viscosity appears. That is whether it appears in all the equations or only in the equations which govern the evolution of the fine resolved scales.

In several popular methods (such as the vanishing viscosity method [12]) that guarantee the convergence of the numerical solution to the unique entropy solution, the numerical viscosity is applied to both the coarse and the fine scale equations. On the other hand, in the vanishing spectral viscosity method proposed by Tadmor [13], the viscosity is applied only to the fine scale equations. As a result, this method retains the spectral accuracy of the coarse or the large scale modes while guaranteeing convergence to the entropy solution. It is interesting to note that in the context of the large eddy simulation (LES) of incompressible turbulent flows, the multiscale method of Hughes et al. [14, 15], also involves applying a numerical viscosity only to the fine scale equations.

Motivated by the class of methods where the viscosity appears only in the fine scale equations, we have proposed a method [2] where *different numerical viscosities appear in the large and the small scale equations*. In addition, in contrast to the methods described above, these viscosities are not determined *a-priori*, instead they are calculated as part of the solution (dynamically). The equations that are used to determine the viscosities are derived from the condition that the resulting numerical method be optimal in a certain user-defined sense. We have dubbed this method the *dynamic multiscale viscosity method*.

The equation used to dynamically determine the viscosities, is the variational counterpart of the Germano identity. The filtered part of this identity has found widespread use in determining model parameters in the LES of turbulent flows [16]. Recently, we have demonstrated how it may be used as a tool for determining unknown parameters in a

numerical method aimed at solving an abstract partial differential equation [1]. The present work is an application of this methodology to the spectral approximation of non-linear conservation laws. In particular we have used it to develop the dynamic multiscale method for a generic non-linear conservation law and then applied it to the model case of one-dimensional Burgers equation to study its properties. We have found that the dynamic multiscale method outperforms the vanishing spectral viscosity method. We have also applied it to the incompressible Navier Stokes equations in [3].

1.2 Analytical estimates of the subgrid model for Burgers equation with a shock [4]

We have developed analytical estimates for the exact subgrid model for Burgers equation when the solution is given by a shock. As described below, we have found that the form of the subgrid model is closely related to the definition of the optimal numerical solution.

For a Fourier-spectral method, when the optimal solution is defined to be the L^2 projection of the exact solution, we have demonstrated that the subgrid model can be interpreted as a wavenumber-dependent viscosity. This viscosity has a plateau for low wavenumbers (coarse resolved scales) and has a cusp described by a logarithmic singularity near the cutoff wavenumber (in the fine resolved scales). These results, which are obtained for Burgers equation, are remarkably similar to those obtained by Kraichnan [17] for three dimensional turbulence. In addition, they also motivate the use of different models at different scales.

It is well known that the L^2 projection of the exact solution (which has a discontinuity) on to a finite dimensional Fourier basis exhibits significant Gibb's phenomenon. Hence, in certain cases it may be preferable to define the optimal numerical solution to be close to the L^∞ projection. Solutions which approximate this projection are easily constructed by convolving the exact solution with exponential filters [18]. We have evaluated the exact subgrid term for these solutions and discovered that it may also be interpreted as a wavenumber dependent viscosity with a plateau at low wavenumbers and a cusp near the cutoff. However the magnitude of the viscosity is significantly greater than for the L^2 case. For example, for a the fourth order exponential filter it is about four times larger.

1.3 Two-Scale Dynamic VMS Method for LES [5]

We have developed a dynamic multiscale LES formulation and used it to solve the problem of sustained homogeneous isotropic turbulence [5]. The method employs two different Smagorinsky viscosities: one in all scales of the problem and another only in the fine scale equations. It is motivated by the fact that the exact eddy viscosity has a low plateau in the coarse resolved scales and a cusp in the fine resolved scales [17]. Our LES model is constructed to allow such a distribution. In addition, we do not prescribe the values of these viscosities *a-priori*, but rather evaluate them as part of the calculation (dynamically).

We have found that the variational Germano identity can be used to determine the two viscosities dynamically. In fact, in accordance with numerical and analytical results, it leads to a model with a lower value of the viscosity for the coarse scales and a higher value for the fine scales.

We have also observed that the performance of the dynamic multiscale model is better than both the dynamic single scale model [16] and the static multiscale model [15]. In fact this model appears to combine the advantages of both these approaches.

1.4 Generalized Smagorinsky Model in Physical Space [6]

In the large eddy simulation of turbulent flows the Smagorinsky eddy viscosity model [19] is among the most popular models. In this model the deviatoric part of subgrid scale tensor is represented by a nonlinear viscous term, wherein the eddy viscosity is constructed from the product of two terms. On of these terms, which provides the viscous time scale, is the magnitude of the rate of strain of the resolved velocity field. The other, which provides the viscous length scale, is usually the square of a measure of the filter width or the grid resolution.

When the grid spacing is uniform (or close to being uniform) in all directions, it is standard (following Deardorff [20]) to use the cube root of the volume of a finite volume cell or a finite element as the Smagorinsky length scale. Under these conditions, the only unknown that appears in the Smagorinsky model is a dimensionless parameter which may be determined analytically following Lilly's analysis [21] or as part of the simulation (dynamically) following the approach developed by Germano et al. [16]. In Lilly's analysis the numerical solution is represented using Fourier modes whose coefficients are set equal to that of an "exact" homogeneous isotropic field with the universal Kolmogorov spectrum. Thereafter the ensemble averaged numerical dissipation is evaluated and equated to the exact dissipation. This yields a relation from which the Smagorinsky parameter is obtained. While the results of this analysis are widely used, often in conjunction with finite volume/element/difference formulations, it is strictly applicable to a Fourier-spectral method as it assumes that the numerical solution is represented using Fourier modes. A more accurate version of Lilly's analysis would account for the precise form of the basis functions used in a numerical method.

When the grid spacing in each direction is different but regular, it is no longer clear that the Smagorinsky length scale is equal to cube root of the cell or element volume. In this case the appropriate value of the Smagorinsky length scale is obtained by extending Lilly's analysis [22]. In this approach, the cubical integration domain in wavenumber space which is used to evaluate the numerical dissipation is replaced by an appropriate regular hexahedron. While this approach successfully accounts for the anisotropy of the grid, it too is applicable only to Fourier-spectral methods. Further it cannot be applied to distorted or unstructured grids.

We have recently derived an extension of Lilly's analysis to physical space. Our expression for the Smagorinsky length scale accounts for the basis functions used in a numerical method. In particular, we consider methods such as the finite element and the finite volume method, where the basis functions interpolate the numerical solution in physical space. In our derivation of the Smagorinsky length scale, we require that the numerical solution be equal to the *nodal interpolant* of "exact" solution. Thereafter we evaluate the volume and ensemble averaged numerical subgrid dissipation in a cell (or an element) and set it equal to the exact subgrid dissipation. In addition, following Lilly, we assume that the exact solution is given by a homogenous isotropic field, and that the Kolmogorov hypotheses holds, so that an

analytical expression for the second order structure function is available. This allows us to derive an expression for the Smagorinsky length scale which takes into account the shape of the cell and the specific interpolation function used to represent the numerical solution. This expression is valid for distorted cells or elements and thus can be used for completely unstructured meshes.

1.5 The adjoint weighted equation for steady advection in a compressible fluid [7]

Our analysis for the multiscale problem lead to this new weak formulation for advective systems.

Two common approaches to computing transport phenomena are based on least-squares and stabilized formulations. The former are robust and stable, but may require sophisticated techniques to retain desired accuracy in some cases. On the other hand, the performance of stabilized methods is determined by the choice of the mesh-dependent stabilization parameters that are inherent in their formulation .

The adjoint weighted equation (AWE) formulation, which is an alternative variational framework suitable for pure advection, may be viewed as a combination of the two. Work on the related nearly optimal PetrovGalerkin method prompted the observation motivating this concept, that in the advective limit certain stabilized methods, including the streamline upwind PetrovGalerkin method, perform well for arbitrarily large values of the stabilization parameter, so that the Galerkin part may be discarded. The resulting scheme is similar to the least-squares approach, but employs the adjoint operator in the weighting slot.

The adjoint weighted equation is not restricted to solenoidal (i.e. divergence free) velocities. Preliminary analysis indicates that the adjoint weighted equation shares the robustness of the least-squares approach, yet in computational tests provides superior numerical performance on the problems considered.

1.6 Adjoint weighted variational formulation for direct computational solution of an inverse heat conduction problem [8]

A direct extension of the AWE formulation can be applied for solving the inverse heat conduction problem. This development is described below.

It is more and more common to encounter an inverse problem in which interior data, as opposed to exterior data only, is available. This is true to varying degrees of approximation and in a variety of contexts. Aquifer permeability, for example, may be inferred by local measurements of the water pressure head. Inverse problems in coastal evolution also involve interior data, representing the position of the coastline. In magnetic resonance (MR) electrical impedance tomography, the electrical current flux vector within a body can be remotely measured. In MR and ultrasound (US) thermometry, the temperature distribution within the body can be measured (or inferred) by remote measurements. In acousto-optic imaging, the measured signal is proportional to the local photon intensity, but the constant of proportionality is spatially varying and unknown *a priori*. And finally, both MR and

US can be used to measure interior particle displacement associated with tissue mechanical deformation. When combined with other data, such measurements can be used to reconstruct the elastic modulus distribution within the tissue. These are all examples where interior measurements of a field variable can be remotely measured.

With the exception of the elasticity inverse problem, all the cases described above can be accurately modeled by a scalar potential problem. Even in the case of elasticity imaging, several authors have obtained practically useful results using a scalar model equation to reconstruct material properties. Therefore we consider the following field equation:

$$\nabla \cdot (u(x)\nabla\phi) = \sigma(x)\partial_t^{(n)}\phi. \tag{5}$$

In the context of heat conduction, for example, the transient heat equation has $n = 1$ (a first order partial derivative in time), $\phi(x,t)$ represents the (measured) temperature field, $u(x)$ represents the unknown thermal conductivity, and $\sigma(x)$ represents the heat capacity. In the case of scalar models for inverse elasticity, on the other hand, $\phi(x,t)$ represents the measured displacement component, $n = 2$, $\sigma(x)$ represents the mass density of the tissue, and $u(x)$ the unknown tissue stiffness. In both the thermal or elastic contexts, the right hand side of the above equation may be regarded as known. In the simplest case, for example, quasistatic measurements lead to $\partial_t\phi \equiv 0$, and so the right hand side vanishes.

This work focuses on a novel robust and stable computational method to solve the following model problem: Given measured temperature field(s) $\phi^{(j)}(x)$ and source field(s) $f^{(j)}(x)(j = 1, 2, \ldots, N)$ defined in $\Omega \subset \mathbb{R}^2$, find $u(x)$ such that

$$\nabla \cdot (u(x)\nabla\phi^{(j)}) = f^{(j)}(x) \qquad j = 1, 2, \ldots N. \tag{6}$$

Traditional computational formulations to solve this equation are challenged by two key aspects of this problem. First of all, it is well known that for $N = 1$ (a single measured field), a standard Galerkin discretization of this purely advection equation is unstable. Therefore, even with enough boundary data to render a unique reconstruction from a single measured field, the Galerkin method will break down. Secondly, for $N \geq 2$, the problem is to find a single unknown field that satisfies simultaneously several partial differential equations. In this case, the problem is overdetermined, unless a solvability condition is satisfied by the data (we derive this solvability condition in the appendix.) These conditions to yield a well-posed problem are relatively restrictive.

A natural approach to address the overdetermined nature of the above equation when $N \geq 2$ is to use least squares. It is clear, however, that using least squares in the discrete context, that is using discrete equations derived from the Galerkin condition, leads to an unstable method. Using least squares in the continuous context and then discretizing via Galerkin, is a viable option. We show in examples below, however, that least squares tends to be overly dissipative, and thus tends to damp out the solution.

We have derived a novel variational formulation, the Adjoint Weighted variational Equation (AWE), of the two-field problem. We find that the conditions to yield a well-posed problem in the AWE formulation are relatively mild, and the AWE formulation is always well-posed when the strong form is well-posed. Further, when both problems are well posed, they give identical solutions. The Galerkin discretization of the AWE formulation leads to a stable and convergent numerical method. We prove an optimal rate of convergence, demonstrate

optimal rates of convergence computationally (and sometimes superconvergence), and show good computational performance on examples with both smooth and rough coefficients and solutions.

2 List of Publications

The work performed during this grant has been documented in the following publications:

1. A.A. Oberai and J. Wanderer. A Dynamic Approach for Evaluating Parameters in a Numerical Method. International Journal for Numerical Methods in Engineering, 62:5071, 2005.

2. A.A. Oberai and J. Wanderer. A Dynamic Diffusivity Method for the Spectral Approximation of Conservation Laws. Computer Methods in Applied Mechanics and Engineering, 195(13-16):17781792, 2006.

3. A.A. Oberai and J. Wanderer. Variational Formulation of the Germano Identity for the Navier-Stokes Equations. Journal of Turbulence, 6, 2005.

4. A.A. Oberai, C. E. Colosqui, and J. Wanderer. Analytical Estimates of the exact Subgrid Model for a Burgers Shock. In preparation, 2007.

5. J. Wanderer and A.A. Oberai. Two-Scale Dynamic VMS formulation of LES. In preparation, 2007.

6. C.E. Colosqui and A.A. Oberai. Generalized Smagorinsky Model in Physical Space. Computers and Fluids, submitted, 2007.

7. A.A. Oberai, P.E. Barbone, and I. Harari. The adjoint weighted equation for steady advection in a compressible fluid . International Journal for Numerical Methods in Fluids, 54:683695, 2007.

8. P.E. Barbone, I. Harari, and A.A. Oberai. Adjoint weighted variational formulation for direct computational solution of an inverse heat conduction problem . Inverse Problems, submitted, 2007.

3 Plans for future research

During the period this grant the PI moved from Boston University to Rensselaer Polytechnic Institute. In order to accommodate this move, the ECPI grant at BU was terminated and the PI was awarded a new grant for RPI. This report is the final report for the grant that was active while the PI was at Boston University.

As part of the new grant at RPI the PI proposes to continue to work on multiscale problem in fluid mechanics. This work is described in the new grant proposal that the PI had submitted to DOE. The progress of this work will be communicated to DOE via standard annual progress reports and a final report.

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