Available online at www.sciencedirect.com
ScienceDirect
Comput. Methods Appl. Mech. Engrg. 337 (2018) 501–526
Computer methods in applied mechanics and engineering
www.elsevier.com/locate/cma

Variational multiscale error estimators for the adaptive mesh refinement of compressible flow simulations

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Received 27 November 2017; received in revised form 1 March 2018; accepted 7 March 2018
Available online 12 April 2018

Highlights

- The variational subscales are used as the error estimator.
- Subscales are defined as orthogonal, dynamic and non-linear.
- A scaled norm and an entropy measure compose a single error estimate.
- No additional differential equations are needed for the estimate.

Abstract

This article investigates an explicit a-posteriori error estimator for the finite element approximation of the compressible Navier–Stokes equations. The proposed methodology employs the Variational Multi-Scale framework, and specifically, the idea is to use the variational subscales to estimate the error. These subscales are defined to be orthogonal to the finite element space, dynamic and non-linear, and both the subscales in the interior of the element and on the element boundaries are considered. Another particularity of the model is that we define some norms that lead to a dimensionally consistent measure of the compressible flow solution error inside each element; a scaled L^2-norm, and the calculation of a physical entropy measure, are both studied in this work. The estimation of the error is used to drive the adaptive mesh refinement of several compressible flow simulations. Numerical results demonstrate good accuracy of the local error estimate and the ability to drive the adaptative mesh refinement to minimize the error through the computational domain.

Keywords: Compressible Navier–Stokes equations; Variational Multi-Scale (VMS) method; Orthogonal Sub-Grid Scales (OSGS); A-posteriori local error estimation; Adaptive Mesh Refinement (AMR)

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https://doi.org/10.1016/j.cma.2018.03.010

1. Introduction

The compressible Navier–Stokes equations, namely the conservation of mass, momentum, and energy, together with constitutive and thermodynamical relations, constitute a physical model that describes the compressible fluid flow phenomena. This model is able to represent the wide range of spatial and temporal flow scales typically encountered in engineering cases of interest. When numerically approximating these equations, the smallest flow scales (in turbulence or aeroacoustics, for example) must be modeled with a high level of accuracy by numerical means, but one major source of error is the discretization error: the solution obtained with coarse meshes is often too inaccurate, and calculating over fine meshes is impractical considering the amount of computational effort. Adaptive Mesh Refinement (AMR) methods deal with this issue by dynamically re-configuring the initial mesh and changing its structure employing some type of criteria. The AMR involves two main steps: first, the decision of which elements to modify (mainly the ones contributing the most to the global solution error), and then, the adaptation of those selected elements. The focus of the present work is to investigate a local estimate of the approximation error that can be suitable for driving the AMR of compressible flow simulations. To this end, we exploit the Variational Multi-Scale (VMS) framework introduced in [1], that is typically used to stabilize the fluid flow equations (see for instance the review of the VMS applied to fluid problems in [2]).

The VMS method decomposes the solution space into a resolved component, that is captured by the finite discretization, and a sub-grid part, which is the remainder that cannot be represented by the finite grid. The original discrete problem is therefore equivalent to two sub-problems: one for each scale. Although the variational sub-grid scales (or subscales) have been also adopted for turbulence modeling (see for example [3–5] and references therein), essentially, the role of the subscales is related to the error of the finite approximation. Indeed, the variational subscales vanish consistently as the discrete solution tends to the exact solution, so that, they have been identified with *residual-based* error estimators (e.g. in [6]). The recent literature on variational subscales error estimators is too vast to survey here, but we mention the early works of variational subscales as *a-posteriori* error estimates in [7,8], where a patch of the elements in the mesh was used to calculate the subscales by decoupling a global residual equation with a localization function, and the *element-residual* methods in [9,10], which were able to provide implicit estimations with the subscales inside each element of the mesh (and in some cases on the element boundaries). The application of the subscales as *explicit* a-posteriori estimators has been developed in [6,11,12] from the subscales in the interior and on the boundaries of the element using element Green's functions. In the case of incompressible flow simulations, the subscales have been used as error estimators for AMR in [13] by using a non-dimensional norm of the velocity subscales inside the element. However, the explicit a-posteriori error estimation given by the variational subscales has been less accurate than implicit goal-oriented methods for compressible flow problems in [14–18], or than energy norm estimates using implicit residual methods in [19,20], but cheaper, since the solution of additional differential equations is not required. We refer to the review article by [21] for a deeper understanding of the variational subscales as explicit a-posteriori error estimators.

The present approach is similar to the one in [12], where an *explicit* a-posteriori estimation of the error for the Euler and Compressible Navier–Stokes equations was constructed. We also derive an explicit a-posteriori error estimator from the VMS framework, but our approach offers three different and novel ingredients. First, we define the space where the variational subscales live as the space orthogonal to the finite element space, contrary to the most common choice to define it equal to the space of the finite element residuals. This is the so-called *Orthogonal Sub-Grid Scales* (OSGS) method, first introduced in [22], and which has been recently applied as an explicit a-posteriori error estimator for the elastic problem of solids in [23]. We also include the temporal tracking of the subscales, to what is referred in [24] as the *dynamic* subscales, and account for including the subscales into all of the *non-linear* terms of the problem. In consequence, we refer to the subscales as to be orthogonal, dynamic and non-linear. Second, we model the effect of the subscales inside each element from the perspective of a Fourier analysis, as developed in [25,26], instead of using Green's functions in [1,6,11,12]. Third, we model the subscales on the boundaries of the elements, as first presented in [27], and calculate them as part of the error estimator.

In this article, the error estimation given by the variational multiscale is intended to drive the adaptive mesh refinement process of compressible flow simulations. The error estimate must be well constructed in a dimensional sense, so that, the contribution of the subscales of the different equations (i.e. the subscales of the mass, momentum and energy equations) into the estimation must be consistent. Several norms can be used in this regard. The L^1 and L^2 norms of the variational subscales of velocity in [13] and of the subscales of the separated compressible equations in [12], and the energy norm of the variational compressible problem in [20], have been previously applied to estimate the error inside each element. Since the error estimation given by each separated variational subscales (of the compressible equations) can vary greatly, and therefore, each refined mesh driven by the estimation of a single subscale may lead to unbalanced errors between the multiple variables of the problem, we propose to calculate the error estimation accounting for all the variational subscales. To this end, we propose two different approaches that provide dimensionally consistent measures of the solution error inside each element. The first approach is to calculate a scaled L^2-norm of the variational subscales inside the element, and on the element boundaries, as well. This approach goes in line to the one presented in [23]. The second approach is to compute the relative L^2 error norm of the physical entropy (for ideal gases) calculated using the variational subscales inside the element. The error estimation given by these two norms is used by the adaptive algorithm to drive the addition or removal of elements where the error is outside a given threshold. The *h-adaptive* method adopted here, including the refinement strategy and the data structures needed, has been presented in [28] and implemented in the `RefficientLib` software. Nevertheless, the proposed strategy is applicable to p, r, and hp adaptive mesh refinement techniques, although these are not explored in the present article. The AMR simulations demonstrate the ability of the variational subscales to lead an accurate approximation, provided the error estimation is kept always below the threshold inside the computational domain.

The paper is divided into the following parts. In Section 2, the compressible flow problem is presented. Next, the variational multi-scale finite element formulation of the problem is described in Section 3. The design of the variational subscales error estimator is presented in Section 4. Some numerical examples, including subsonic and supersonic problems in two and three dimensions, are demonstrated in Section 5. Finally, in Section 6 some conclusions close the article.

2. Problem definition

In this section, we present the governing equations for the compressible fluid flow problem, i.e., the compressible Navier–Stokes equations. For doing so, the strong form of the problem is described in the first part of the section. Then, we transform the strong form of the problem into a quasi-linear form that allows us to deal with the non-linearities of the problem. The weak form of the compressible problem is introduced at the last part of the section.

2.1. Compressible Navier–Stokes equations in strong form

Consider a spatial domain $\Omega \subset \mathbb{R}^d$, being d the number of space dimensions ($d = 2$ or 3), and the time interval $\left(0, t_f\right)$. Let $t \in \left(0, t_f\right)$ be a given time instant in the temporal domain, and $\boldsymbol{x} \in \Omega$ a given point in the spatial domain. Let Γ be the boundary of the domain Ω, and $\boldsymbol{n}$ the geometric unit outward normal vector on Γ. We split Γ into two sets: the *Dirichlet* boundary denoted as Γ_G, and the *Neumann* boundary denoted as Γ_N. The strong form of the initial and boundary-value problem consists of finding the solution vector $\boldsymbol{U} : \Omega \times (0, t_f) \to \mathbb{R}^{d+2}$, where $d + 2$ is the number of unknowns (the same as equations of the system), such that for the given Dirichlet boundary conditions $\boldsymbol{U}_G : \Gamma_G \times (0, t_f) \to \mathbb{R}^{d+2}$ and the Neumann boundary conditions $\boldsymbol{H} : \Gamma_N \times (0, t_f) \to \mathbb{R}^{d+2}$, the following compressible Navier–Stokes equations are satisfied:

$$\partial_t \boldsymbol{U} + \partial_j \boldsymbol{E}_j\left(\boldsymbol{U}\right) + \partial_j \boldsymbol{G}_j\left(\boldsymbol{U}\right) = \boldsymbol{F} \qquad \text{in} \quad \Omega \subset \mathbb{R}^d, \quad t \in \left(0, t_f\right), \tag{1}$$

$$\boldsymbol{D}\left(\boldsymbol{U}\right) = \boldsymbol{D}\left(\boldsymbol{U}_G\right) \qquad \text{on} \quad \Gamma_G, \quad t \in \left(0, t_f\right), \tag{2}$$

$$\boldsymbol{B}\left(\boldsymbol{U}\right) = \boldsymbol{H} \qquad \text{on} \quad \Gamma_N, \quad t \in \left(0, t_f\right), \tag{3}$$

$$\boldsymbol{U} = \boldsymbol{U}^0\left(\boldsymbol{x}\right) \qquad \text{in} \quad \Omega \subset \mathbb{R}^d, \quad t = 0. \tag{4}$$

The Eulerian time derivative and $\partial/\partial x_j$ are indicated in short notations ∂_t and ∂_j, respectively, and the usual summation convention is used over repeated indices. The Dirichlet boundary operator $\boldsymbol{D}\left(\cdot\right)$ is used to impose the components of $\boldsymbol{U}$ on different parts of Γ. The Neumann boundary conditions are given by the operator $\boldsymbol{B}\left(\cdot\right)$. Note that with our notation Γ_G and Γ_N may overlap.

The vector $\boldsymbol{U} = \left(\rho, \boldsymbol{m}, e_{\text{tot}}\right)^\top$ denotes a vector of conservative variables, density ρ, momentum $\boldsymbol{m} = \rho\boldsymbol{u}$, and total energy $e_{\text{tot}} = \rho\left(e + \boldsymbol{u} \cdot \boldsymbol{u}/2\right)$, where $\boldsymbol{u}$ stands for the velocity vector, and e is the internal energy. The *convective* flux in the jth-direction, $j = 1, \ldots, d$, is defined as

$$\boldsymbol{E}_j\left(\boldsymbol{U}\right) = \left(\rho u_j, \rho u_j u_1 + p\delta_{1j}, \rho u_j u_2 + p\delta_{2j}, \rho u_j u_3 + p\delta_{3j}, u_j\left(e_{\text{tot}} + p\right)\right)^\top, \tag{5}$$

where p is the pressure and $\boldsymbol{I} = [\delta_{ij}]$ is the identity or *Kronecker* tensor. The *diffusive* flux in the jth-direction, $j = 1, \ldots, d$, is

$$\boldsymbol{G}_j(\boldsymbol{U}) = \left(0, -\sigma_{j1}, -\sigma_{j2}, -\sigma_{j3}, -u_i\sigma_{ij} + q_j\right)^\top, \tag{6}$$

where $\boldsymbol{\sigma}$ is the viscous stress tensor, $\sigma_{ij} = \mu\left(\partial_j u_i + \partial_i u_j\right) - \frac{2}{3}\mu\left(\partial_l u_l\right)\delta_{ij}$, and $\boldsymbol{q}$ is the heat flux vector, $q_i = -\lambda\partial_i T$. Here μ is the viscosity, λ is the thermal conductivity and T is the temperature of the fluid. The vector of source terms is defined as

$$\boldsymbol{F}(\boldsymbol{U}) = (0, \rho\boldsymbol{f}, \rho\boldsymbol{f}\cdot\boldsymbol{u} + \rho r)^\top, \tag{7}$$

where $\boldsymbol{f}$ is a body force vector, and r is a heat source/sink term.

In the previous relations the caloric equation $e = c_v(T)\,T$ and the ideal law for gases $p = \rho RT$ are used to calculate the pressure and the acoustic speed $c = \sqrt{\gamma p/\rho}$, where the specific heat at constant volume $c_v(T)$ and the specific heat at constant pressure $c_p(T)$ are thermodynamic properties of the fluid, $\gamma = c_p/c_v$ is the ratio between the specific heats, and $R = c_p - c_v$ is the specific gas constant. The non-dimensional Mach number $M = |\boldsymbol{u}|/c$ is used to calculate the compressibility regime.

2.2. Quasi-linear form of the problem

Different formulations of the Navier–Stokes equations can be used, e.g. one can take $\boldsymbol{U}$ as the conservation variables, as done before, or one can also take $\boldsymbol{U} = (p, \boldsymbol{u}, T)^\top$, leading to the primitive variables formulation. Any of such formulations can be written in quasi-linear form as

$$\boldsymbol{A}_0(\boldsymbol{U})\,\partial_t\boldsymbol{U} + \boldsymbol{\mathcal{L}}(\boldsymbol{U};\boldsymbol{U}) = \boldsymbol{F} \qquad \text{in} \quad \Omega \subset \mathbb{R}^d, t \in \left(0, t_f\right), \tag{8}$$

together with appropriate boundary and initial conditions. Here we have introduced the non-linear operator $\boldsymbol{\mathcal{L}}$, which is defined as

$$\boldsymbol{\mathcal{L}}\left(\widehat{\boldsymbol{U}};\boldsymbol{U}\right) = \boldsymbol{A}_j\left(\widehat{\boldsymbol{U}}\right)\partial_j\boldsymbol{U} - \partial_k\left(\boldsymbol{K}_{kj}\left(\widehat{\boldsymbol{U}}\right)\partial_j\boldsymbol{U}\right). \tag{9}$$

Matrices $\boldsymbol{A}_0(\boldsymbol{U})$, $\boldsymbol{A}_j(\boldsymbol{U})$, and $\boldsymbol{K}_{kj}(\boldsymbol{U})$, for $k, j = 1, \ldots, d$, are $(d+2)\times(d+2)$ matrices that depend upon $\boldsymbol{U}$, and that are appropriately defined for each type of formulation, as described in the Appendix. Both the conservative and the primitive formulations will be applied in the next sections of the article.

2.3. Weak form of the problem

Let $\boldsymbol{\mathcal{W}}$ be the space of functions where, for each $t \in (0, t_f)$, the unknowns are well defined, with the appropriate regularity that we will not analyze here. Let us also denote by $(\cdot,\cdot)_\omega$ the integral of the product of two functions (scalar or vector-valued) in a domain ω, omitting the subscript when $\omega = \Omega$. Introducing the form

$$A(\boldsymbol{U};\boldsymbol{V},\boldsymbol{W}) := \left(\boldsymbol{V}, \boldsymbol{A}_j(\boldsymbol{U})\,\partial_j\boldsymbol{W}\right) + \left(\partial_k\boldsymbol{V}, \boldsymbol{K}_{kj}(\boldsymbol{U})\,\partial_j\boldsymbol{W}\right), \tag{10}$$

the variational form of the problem can be written as: find $\boldsymbol{U} : (0, t_f) \to \boldsymbol{\mathcal{W}}$ such that

$$(\boldsymbol{V}, \boldsymbol{A}_0(\boldsymbol{U})\,\partial_t\boldsymbol{U}) + A(\boldsymbol{U};\boldsymbol{V},\boldsymbol{U}) = (\boldsymbol{V},\boldsymbol{F}) + (\boldsymbol{V},\boldsymbol{H})_{\Gamma_N}, \quad t \in \left(0, t_f\right), \tag{11}$$

$$(\boldsymbol{V},\boldsymbol{U}) = \left(\boldsymbol{V},\boldsymbol{U}^0\right), \qquad t = 0, \tag{12}$$

for all $\boldsymbol{V}$ in the adequate test functions space. The *Neumann* boundary operator is given by the diffusive fluxes

$$\boldsymbol{B}(\boldsymbol{U}) = -n_k\boldsymbol{K}_{kj}(\boldsymbol{U})\,\partial_j\boldsymbol{U}, \tag{13}$$

although part of the convective term could also be integrated by parts and contribute to the Neumann boundary conditions, in particular, the pressure term.

3. Finite element formulation

In this section, the finite element formulation of the compressible problem is described. The VMS formulation of the compressible problem that has been presented in [26,29] is recalled in the section. As it will be explained, the VMS framework is used for stabilizing the finite element approximation and allows us to use arbitrary interpolation spaces for the different variables of the problem. The finite element equation is described first. Then, we focus the attention on the solution of the subscales; we address the equation for the subscales in the interior of the element, and later, the approximation for the subscales on the element boundaries is addressed. Finally, we describe the time integration scheme that is used for advancing in time at the end of the section.

3.1. Variational multi-scale framework

Let us first consider a finite-element partition $\mathcal{T}_h = \{K\}$ of the domain Ω. The diameter of the element partition is denoted by h. We define the test functions space $\boldsymbol{\mathcal{W}}_h \subset \boldsymbol{\mathcal{W}}$ as made of continuous piecewise polynomial functions in space. The Galerkin approximation to problem (11)–(12) can be stated as follows: find $\boldsymbol{U}_h : (0, t_f) \to \boldsymbol{\mathcal{W}}_h$ such that

$$(\boldsymbol{V}_h, \boldsymbol{A}_0(\boldsymbol{U}_h)\,\partial_t \boldsymbol{U}_h) + A(\boldsymbol{U}_h; \boldsymbol{V}_h, \boldsymbol{U}_h) = (\boldsymbol{V}_h, \boldsymbol{F}) + (\boldsymbol{V}_h, \boldsymbol{H})_{\Gamma_N}, \quad t \in \left(0, t_f\right), \tag{14}$$

$$(\boldsymbol{V}_h, \boldsymbol{U}_h) = \left(\boldsymbol{V}_h, \boldsymbol{U}^0\right), \quad t = 0, \tag{15}$$

for all $\boldsymbol{V}_h \in \boldsymbol{\mathcal{W}}_h^0$, the discrete space of test functions (i.e., with components vanishing where Dirichlet conditions are prescribed on the boundary).

This approximation suffers from instability problems, which vary according to the way to construct $\boldsymbol{\mathcal{W}}_h$ (e.g. in the case of equally interpolating spaces).

The VMS framework introduced in [1], has been established for overcoming this issue. The idea of the VMS framework is to decompose the space of the unknowns into a finite-dimensional space $\boldsymbol{\mathcal{W}}_h$, and an infinite-dimensional one, $\widetilde{\boldsymbol{\mathcal{W}}}$, so that $\boldsymbol{\mathcal{W}} = \boldsymbol{\mathcal{W}}_h \oplus \widetilde{\boldsymbol{\mathcal{W}}}$. The unknown and the test functions are accordingly split as $\boldsymbol{U} = \boldsymbol{U}_h + \widetilde{\boldsymbol{U}}$ and $\boldsymbol{V} = \boldsymbol{V}_h + \widetilde{\boldsymbol{V}}$, respectively. We shall refer to functions in $\boldsymbol{\mathcal{W}}_h$ as the *resolved* scales and to functions in $\widetilde{\boldsymbol{\mathcal{W}}}$ as the *error* or *subscales*.

Eq. (11) can be equivalently written as the system of equations

$$(\boldsymbol{V}_h, \boldsymbol{A}_0(\boldsymbol{U})\,\partial_t \boldsymbol{U}) + A(\boldsymbol{U}; \boldsymbol{V}_h, \boldsymbol{U}) = (\boldsymbol{V}_h, \boldsymbol{F}) + (\boldsymbol{V}_h, \boldsymbol{H})_{\Gamma_N}, \tag{16}$$

for all $\boldsymbol{V}_h \in \boldsymbol{\mathcal{W}}_h^0,\ t \in (0, t_f)$, and

$$\left(\widetilde{\boldsymbol{V}}, \boldsymbol{A}_0(\boldsymbol{U})\,\partial_t \boldsymbol{U}\right) + A(\boldsymbol{U}; \widetilde{\boldsymbol{V}}, \boldsymbol{U}) = (\widetilde{\boldsymbol{V}}, \boldsymbol{F}) + \left(\widetilde{\boldsymbol{V}}, \boldsymbol{H}\right)_{\Gamma_N}, \tag{17}$$

for all $\widetilde{\boldsymbol{V}} \in \widetilde{\boldsymbol{\mathcal{W}}}^0,\ t \in (0, t_f)$, and likewise for the initial condition, Eq. (12). In Eq. (17), $\widetilde{\boldsymbol{\mathcal{W}}}^0$ is the space of subscale test functions.

The finite element part in (16) can be resolved, but the effect of the subscales on the finite element solution (or resolved scales) needs to be modeled somehow. It has been extensively surveyed that including the effect of the subscales in the finite element formulation has turned out to be a very good strategy to solve many of the intrinsic drawbacks of the standard Galerkin method for finite elements: the VMS method is capable of providing stable solutions for convective problems, saddle point problems, and solving many other problems related to the finite element approximation of computational physics problems, see for instance the reviews in [2,4].

3.1.1. Finite element equation

We first analyze the equation for the finite element scale (16). The *time-dependent* terms involving the temporal derivatives in the Left-Hand-Side (LHS) of Eq. (16) can be split as

$$(\boldsymbol{V}_h, \boldsymbol{A}_0(\boldsymbol{U})\,\partial_t \boldsymbol{U}) = (\boldsymbol{V}_h, \boldsymbol{A}_0(\boldsymbol{U})\,\partial_t \boldsymbol{U}_h) + \left(\boldsymbol{V}_h, \boldsymbol{A}_0(\boldsymbol{U})\,\partial_t \widetilde{\boldsymbol{U}}\right). \tag{18}$$

Similarly, the second term in the LHS of Eq. (16) can be split as

$$A(\boldsymbol{U}; \boldsymbol{V}_h, \boldsymbol{U}) = A\left(\boldsymbol{U}; \boldsymbol{V}_h, \boldsymbol{U}_h\right) + A\left(\boldsymbol{U}; \boldsymbol{V}_h, \widetilde{\boldsymbol{U}}\right). \tag{19}$$