Journal of Computational Physics 231 (2012) 7187–7213

Contents lists available at SciVerse ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Variational multiscale stabilization of high-order spectral elements for the advection–diffusion equation

S. Marras [a,*], J.F. Kelly [b], F.X. Giraldo [b], M. Vázquez [a,c]

[a] Barcelona Supercomputing Center (BSC-CNS), Barcelona, Spain
[b] Applied Mathematics, Naval Postgraduate School, Monterey, CA, USA
[c] IIIA-CSIC, Bellaterra, Spain

ARTICLE INFO

Article history:
Received 4 August 2011
Received in revised form 19 June 2012
Accepted 20 June 2012
Available online 4 July 2012

Keywords:
Spectral elements
High-order methods
Variational multiscale stabilization (VMS)
Advection–diffusion
Numerical weather prediction
First-Order Subcells (FOS) method
Monotonic schemes

ABSTRACT

One major issue in the accurate solution of advection-dominated problems by means of high-order methods is the ability of the solver to maintain monotonicity. This problem is critical for spectral elements, where Gibbs oscillations may pollute the solution. However, typical filter-based stabilization techniques used with spectral elements are not monotone. In this paper, residual-based stabilization methods originally derived for finite elements are constructed and applied to high-order spectral elements. In particular, we show that the use of the variational multiscale (VMS) method greatly improves the solution of the transport-diffusion equation by reducing over- and under-shoots, and can be therefore considered an alternative to filter-based schemes. We also combine these methods with discontinuity capturing schemes (DC) to suppress oscillations that may occur in proximity of boundaries or internal layers. Additional improvement in the solution is also obtained when a method that we call FOS (for First-Order Subcells) is used in combination with VMS and DC. In the regions where discontinuities occur, FOS subdivides a spectral element of order p into p^2 subcells and then uses 1st-order basis functions and integration rules on every subcell of the element. The algorithms are assessed with the solution of classical steady and transient 1D, 2D, and pseudo-3D problems using spectral elements up to order 16.

1. Introduction

A large number of physical applications relies on the accurate solution of the transport-diffusion equation

$$\frac{\partial q}{\partial t} + \mathcal{L}(q) = f, \tag{1}$$

where q is the concentration of the tracer, $\mathcal{L}(q) = \mathbf{u} \cdot \nabla q - \nabla \cdot (\nu \nabla q)$, $\nu > 0$ is a diffusion coefficient, $\mathbf{u}$ is a known velocity field, and f is a source term. The solution of (1) should respect two significant properties: (i) positivity should be preserved, and (ii) smearing at internal and boundary layers should not be excessive. These properties are extremely important in the context of transport in the atmosphere. Both limited-area and global atmospheric models for weather prediction need monotonic advection of tracers and moisture variables, otherwise the wrong amount of precipitation would be forecasted. Simple microphysics schemes, such as the Kessler parameterization [1], require three variables

* Corresponding author. Address: CASE, Barcelona Supercomputing Center, c. Jordi Girona 29, Barcelona 08034, Spain. Tel.: +34 93 4017295, fax: +34 93 4137721.
E-mail address: simone.marras@bsc.es (S. Marras).

0021-9991/$ - see front matter
http://dx.doi.org/10.1016/j.jcp.2012.06.028

(water vapor, cloud water, and rain), whereas more sophisticated parameterizations include additional variables such as ice and snow [2]. Similarly, climate models require transport of hundreds of tracers, each representing a different chemical species. Regardless of the physical scales of the model, tracers must remain positive since the physical parameterizations that govern sub-grid scale processes such as auto-conversion and sedimentation, implicitly assume such a condition. These issues have been addressed for both transient and stationary problems (see, e.g., [3]) and, in the context of finite element methods, so-called *stabilized* methods have been an active topic of research since their introduction in the early 1980s with the streamline-upwind method of Hughes and Brooks [4]. In this paper we address the problem of solving (1) by high-order spectral element methods (SEM) without losing the ability to approach a monotone solution of the problem. Higher-order accuracy, in fact, comes at the price of aliasing phenomena in the solution [5], but the anti-aliasing filters typically used to give a stable spectral element solution do not respect conditions (i) and (ii) described above. Therefore, to achieve monotonic results with high-order spectral elements, we consider stabilization schemes originally devised for finite elements, and focus on techniques that can be derived directly from *subgrid scale* considerations as originally defined in [6,7] in the context of variational multiscale methods. These schemes assure stability by designing a diffusion-type term that is added to the Galerkin formulation of the original problem.

The first stabilized schemes based on the addition of a diffusive stabilization term to the Galerkin equation are the *Artificial Viscosity* methods (AV) [8] and the *streamline-upwind* method (SU) [4]. AV, or *hyper-viscosity* (HV), is often used in atmospheric and ocean modeling due to the property of preserving the correct energy cascade in simulations that involve turbulence. The SU scheme uses the information in the direction of the flow to add viscosity only in the streamline direction. Both methods use a constant diffusion coefficient that does not typically change from element to element. A major improvement came by introducing the residual of the governing equation in the definition of the stabilization term. When the computed solution approaches the exact solution, the stabilization term should vanish. This strategy is known as residual weighting and generates a family of stabilization methods used mostly in FEM-based Computational Fluid Dynamics (CFD). These schemes, which are *consistent* in that the stabilization terms goes to zero as the numerical solution approaches the exact solution, are considered in this paper. The most commonly used are the *streamline-upwind/Petrov–Galerkin* (SUPG) and the *Galerkin/Least-Squares* (GLS), devised in 1982 [9] and 1989 [10], respectively, as a consistent counterpart to SU. GLS was designed as a generalization of SUPG, but in the limit of pure advection, or for piece-wise linear elements, the GLS and SUPG methods are equivalent. Stability analysis for these two methods is detailed in [11,12,10]. The *Gradient Galerkin/Least-Squares* [13] for advection–diffusion with a reaction term, or the *Unusual Stabilized Finite Element Method* (USFEM) [14,15] are a few examples. In the framework of high-order methods, Petrov–Galerkin stabilization was applied by Pasquarelli and Quarteroni [16] to stabilize the advection–diffusion equation with the spectral method. Canuto used bubble functions to address the same issue [17] (see also [18,19]).

The analyses of Hughes [6], Hughes and Stewart [20], and Hughes et al. [7] form the unifying theory of all stabilized finite element methods. According to this theory, stabilized methods are subgrid scale models where the unresolved scales are intimately related to the instabilities at the level of the resolved scales, and thus should be used in the construction of the stabilization term. These schemes are known as *variational multiscale (VMS)* methods. Details are given in Section 2.2.2. VMS methods are all residual-based methods that improve the stability properties of the solution, and preserve the accuracy of the underlying numerical scheme [21]. However, Godunov's theorem [22] implies that the latter property may be violated in the proximity of discontinuities or strong gradients. To the authors' knowledge, the only application of VMS to spectral elements is the work of Wasberg et al. [23] in the context of large eddy simulation.

Neither SUPG, GLS, nor VMS, however, preclude the formation of over- and under-shoots in the proximity of sharp gradients of the solution. For this reason, *discontinuity capturing* (DC) techniques, also referred to as *spurious oscillations at layers diminishing* (SOLD) methods are used in combination with SUPG and VMS to introduce an additional term to the stabilized form of the equation. This issue was treated for the first time in [24], where details on how to build the stabilization parameter are also given, and in [25] for non-linear problems. A detailed review of most existing SOLD schemes can be found in a two-part paper by John and Knobloch [26,27], where a modification of the *discontinuity-capturing* of Codina [28] is presented and is shown to be a promising option for FE solutions characterized by boundary layers.

All these methods strongly depend on a parameter that will be identified by τ throughout the paper. It will be also referred to as *intrinsic time*. A classical result for τ was obtained by Franca et al. in [29] by error analysis. Their result was reproduced by other authors using different approaches. Additional expressions for τ were found by Codina in [30,31], by Codina et al. in [32], by Harari and Hughes in [13], and by Shakib et al. in [33], who based the derivation on the (discrete) maximum principle. Another expression is due to Franca and Valentin [15] who based their derivation on convergence and stability analysis. Starting with the formalization of VMS methods by Hughes [6], τ has often been derived using Green's functions, a thorough analysis of which is done by Hughes and Sangalli in [34]. Recently, Houzeaux et al. [35] proposed a new way to derive the approximate subgrid scale solution, with results that are comparable to those of Hauke and García-Olivares in [36]. In [37], Codina builds τ using the Fourier analysis of the problem; however, determining τ remains open. For this reason, we propose τ for higher-order spectral elements and use it to construct an appropriate stabilization method. To further improve the solution, we combine VMS and DC with a method that we here call FOS (for First-Order Subcells). This technique subdivides a tensor product spectral element of order p and dimension d into p^d subcells, and then uses 1st-order basis functions and integration rules on every subcell of the element.