Computers and Fluids 125 (2016) 71–81

Contents lists available at ScienceDirect

Computers and Fluids

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

Third-order active-flux scheme for advection diffusion: Hyperbolic diffusion, boundary condition, and Newton solver

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ARTICLE INFO

Article history:
Received 3 July 2015
Revised 29 October 2015
Accepted 30 October 2015
Available online 28 November 2015

Keywords:
Active flux
High-order
Advection diffusion
Unsteady
Newton
Boundary condition

ABSTRACT

In this paper, we construct active flux schemes for advection diffusion. Active flux schemes are efficient third-order finite-volume-type schemes developed thus far for hyperbolic systems. This paper extends the active flux schemes to advection diffusion problems based on a first-order hyperbolic system formulation that is equivalent to the advection–diffusion equation in pseudo-steady state. An active flux scheme is first developed for a generic hyperbolic system with source terms, applied then to a hyperbolized diffusion system, extended to advection diffusion by incorporating the advective term as a source term, and enabled for unsteady problems by implicit time integration. Boundary conditions are discussed in relation to a non-uniqueness issue, and a weak boundary condition is shown to resolve the issue. Both for steady problems and for sub-iterations within unsteady problems, a globally coupled system of residual equations is solved by Newton's method. Numerical results show that third-order accuracy is obtained in both the solution and the gradient on irregular grids with rapid convergence of Newton's method, i.e., four or five residual evaluations are sufficient to obtain the design accuracy in both space and time.

1. Introduction

Active flux schemes have been developed for hyperbolic systems of conservation laws in Refs. [1,2], built upon Scheme V of Van Leer [3], as a viable alternative to other high-order methods. Active flux schemes are finite-volume-based compact high-order schemes. These schemes are substantially different from other high-order schemes and have attractive features for a practical implementation. First, active flux schemes do not rely on a typical one-dimensional flux across a control-volume face, but incorporate multi-dimensional physics into the residual and do not introduce unphysical discontinuities into solution [4]. The numerical flux at a face is determined not by solving a one-dimensional Riemann problem, but calculated by the method of spherical mean, which is an exact solution to a multi-dimensional initial-value problem. It is equivalent to a solution to the characteristic equations in one dimension. Second, the memory requirement is much reduced compared with discontinuous Galerkin methods due to sharing of degrees of freedom among elements. In addition to cell-averages, active flux schemes carry point-values at faces; the latter are shared by adjacent cells, thus resulting in 2 degrees of freedom per cell for third-order accuracy in one dimension, 3 in two dimensions, and only 2.2 in three dimensions. The active flux methodology has been developed for systems of hyperbolic conservation laws in Refs. [1,2], but its extension to diffusive equations has not been well studied yet. Towards the development of practical third-order active-flux schemes for viscous flow simulations, in this paper, we focus on the construction of active-flux schemes for diffusion and advection diffusion problems.

One possible approach to the construction of active flux schemes for diffusion is the recovery approach proposed in Ref. [5]. Specifically, a quartic polynomial is constructed over two adjacent cells, based on a quadratic polynomial defined within each cell, and a diffusive flux is directly evaluated by differentiation at the face. However, our experience shows that the resulting explicit time-stepping scheme is subject to a severe stability restriction, and thus limiting its potential use (an analysis is given Ref. [6]). In order to develop high-order diffusion schemes while preserving the advantages of the active flux scheme, we consider the construction of diffusion schemes based on the first-order hyperbolic system method [7] where the diffusion equation is discretized in the form of a first-order hyperbolic system. One of the advantages of this method is that schemes developed for hyperbolic systems can be directly applied to diffusion. The method was first introduced for this purpose in Ref. [7], extended to the advection–diffusion equation in Ref. [8], to the Navier–Stokes equations in Ref. [9], to time-dependent advection–diffusion problems in Refs. [10,11]. At the same time, the method has also been

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http://dx.doi.org/10.1016/j.compfluid.2015.10.020
0045-7930/

employed for the development of first-, second-, and third-order edge-based finite-volume schemes as in Refs. [12–16], as well as high-order residual-distribution schemes in Refs. [10,11,17,18]. Through these papers, the method has been shown to offer a number of advantages over conventional methods, not only the drastic simplification in discretization (i.e., advection scheme for diffusion), but also significant acceleration in steady convergence by explicit and implicit solvers, providing an equal order of accuracy for the solution and the gradients (viscous/heat fluxes) and exceptionally high-quality gradients on fully irregular grids (see e.g., [17]).

This paper demonstrates that the active flux scheme for diffusion can be constructed by applying the active flux scheme developed for hyperbolic systems as presented in Refs. [1,2] in combination with the physical time integration by the backward difference formulas. In doing so, we have found that active flux schemes need a careful construction for hyperbolic systems with source terms, which include the hyperbolic diffusion system. This paper shows how to construct active flux schemes for hyperbolic systems with source terms, and then how the resulting schemes can be immediately turned into diffusion schemes. Boundary conditions are also discussed in relation to a non-uniqueness problem. Active-flux schemes are shown to allow infinitely many solutions if boundary fluxes are fixed by boundary conditions. We demonstrate that the issue is successfully resolved by a weak boundary procedure.

The hyperbolic formulation of diffusion employed here and in Ref. [7] is related, as mentioned in Ref. [7], from the pioneering work of Cattaneo [19] and Vernotte [20]. In these references, the hyperbolic model for diffusion was introduced as an alternative model to resolve the paradox of the infinite propagation speed associated with the classical diffusion equation expressed by second-order derivatives. The equivalence between the hyperbolic model and the diffusion equation is established in the limit of vanishing relaxation time [21]. Therefore, in order to employ the hyperbolic model to solve the diffusion equation, the relaxation time needs to be very small, often leading to a hyperbolic system with stiff source terms. There have been efforts in constructing numerical schemes for such a model [22], and for a particular generalization to advection diffusion [22–25], focusing on the treatment of the stiff source terms. Also, there has been a series of works [26–30] concerning the use of Cattaneo's model for advection–diffusion problems targeting at applications in which the finite propagation speed has a physical importance. As stated in Ref. [30], their advection–diffusion system is not equivalent to the classical advection–diffusion equation with a second-derivative diffusion term in the steady state. In contrast, the hyperbolic method considered here deliberately designs a first-order hyperbolic system to recover the classical advection–diffusion equation in the steady state [8]; and the same for the Navier–Stokes equations [9,15,16]. In this context, the 'relaxation time' is a free parameter that can be chosen to enhance convergence to the steady state

Recently, high-order explicit time-integration schemes have been developed for advection–diffusion-reaction problems [31–33] based on a hyperbolic formulation similar to the one considered in Ref. [8]. In their work, the relaxation time is carefully defined to retain time accuracy with explicit time integration schemes. As a consequence, the explicit time step is subject to a typical $O(h^2)$-type restriction, (where h is a mesh spacing) although a larger time step is allowed compared with conventional schemes. In the hyperbolic method considered here, we choose an artificial relaxation time, so that explicit time-stepping schemes (used to reach the steady state) allow $O(h)$ time steps, or equivalently the condition number of a linearized system associated with implicit solvers becomes $O(1/h)$, not $O(1/h^2)$, and thus significantly improved convergence is achieved in iterative solvers. When a time-accurate solution is needed, we prefer to employ "sub-cycling", where each (large) time step is executed as the solution to a pseudo-steady problem, as discussed further below.

Given a successful construction of active-flux diffusion schemes, we discuss an extension to advection diffusion problems. It should be pointed out that the extension is not as straightforward as adding the diffusion scheme to the advection scheme. Such a naive extension will destroy third-order accuracy easily. This is a well-known issue for schemes that require compatible discretizations, including the residual-distribution method [34], the third-order edge-based finite-volume method [13], and the active-flux method. One way to ensure the compatibility is to formulate the advection–diffusion equation as a single hyperbolic system [8]. Then, the construction of the active-flux scheme will be trivially simple for the advection–diffusion equation. However, this strategy is currently not applicable to the compressible Navier-Stokes equations because a complete characteristic decomposition has not been discovered yet for hyperbolic formulations of the compressible Navier-Stokes equations [9,15,16]. As a practical alternative, we propose a strategy of adding the advective term to the diffusion scheme as a source term. The idea is applied to the computation of the face values, and the cell-averages are updated by the usual finite-volume method with the sum of advective and diffusive fluxes to guarantee discrete conservation. We demonstrate that the resulting advection–diffusion scheme yields third-order accurate solution and gradients for both steady and unsteady advection diffusion problems.

This paper also presents a highly efficient Newton solver for a system of globally coupled residual equations, which needs to be solved both for steady problems and for sub-iterations within unsteady problems. It is shown that the convergence is significantly improved by Newton's method: four or five Newton iterations (i.e., only four or five residual evaluations) are sufficient both for steady problems and for the sub-iterations within unsteady problems that were mentioned above.

The present study focuses on linear advection–diffusion problems in one dimension to illustrate the basic ideas on extending the active flux method to diffusion and advection diffusion. All numerical results are therefore presented for linear problems. Essential ideas are applicable to nonlinear problems as well as higher dimensions, but algorithmic details remain a subject for future research and beyond the scope of the paper.

The paper is organized as follows. In Section 2, we present a hyperbolic diffusion system and its characteristic form. In Section 3, we construct an active-flux scheme for a generic hyperbolic system with source terms. In Section 4, we apply the developed active-flux scheme to the hyperbolic diffusion system. In Section 5, we extend the scheme to unsteady problems. In Section 6, we discuss an extension to advection diffusion problems. In Section 7, we describe a Newton solver used to solve the residual equations. In Section 8, we present numerical results for steady and unsteady advection diffusion problems. Finally, in Section 9, concluding remarks are given.

2. Hyperbolic diffusion system

Consider the diffusion equation:

$$\partial_\tau u = \nu\, \partial_{xx} u + s_1, \tag{1}$$

where ν is a constant diffusion coefficient and $s_1 = s_1(x, u)$ is a source term. In this Section, and also in Sections 3 and 4, we focus on steady problems, and thus the variable τ is a pseudo-time. Steady solutions can be obtained by solving, instead of the diffusion equation, the following first-order hyperbolic system:

$$\partial_\tau \mathbf{u} + \partial_x \mathbf{f} = \mathbf{s}, \tag{2}$$

where

$$\mathbf{u} = \begin{bmatrix} u \\ p \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} -\nu p \\ -u/T_r \end{bmatrix}, \quad \mathbf{s} = \begin{bmatrix} s_1 \\ s_2 \end{bmatrix}, \tag{3}$$

where $p = \partial_x u$, $s_1 = s$, $s_2 = -p/T_r$, and T_r is a relaxation time that remains to be chosen.