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Active Flux Schemes for Advection Diffusion

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In this paper, we extend the third-order active-flux diffusion scheme introduced in Ref.[AIAA Paper 2014-2092] to advection diffusion problems. It is shown that a third-order active-flux advection-diffusion scheme can be constructed by adding the advective term as a source term to the diffusion scheme. The solution gradient, which is computed simultaneously to third-order accuracy by the diffusion scheme, is used to express the advective term as a scalar source term. To solve the residual equations efficiently, Newton's method is employed rather than explicit pseudo-time iterations, which requires a large number of residual evaluations. For unsteady computations, it leads to a third-order implicit time-stepping scheme with Newton's method. Numerical experiments show that the resulting advection-diffusion scheme achieves third-order accurate and the Newton solver converges very rapidly for both steady and unsteady problems.

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 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. 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, and approximately 3.5 in two and three dimensions. In order to make an impact on practical turbulent-flow simulations, however, the method needs to be extended to diffusion and viscous terms. It is, in fact, straightforward to construct an explicit active-flux diffusion scheme based on the Taylor expansion as shown in Ref.[4], which can actually be shown to be equivalent to the recovery approach in Ref.[5]. However, a severe stability restriction imposed on the explicit time step discourages the use for practical problems. To overcome the limitation, an implicit time-stepping scheme was constructed in Ref.[6]. The construction is made straightforward by the hyperbolic formulation of diffusion [7]. It has also been shown in Ref.[6] that the active-flux schemes lose third-order accuracy unless source terms are discretized in a compatible manner and that the scheme can become inconsistent unless the boundary condition is implemented correctly.

In this paper, we extend the implicit active-flux diffusion scheme 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 the third-order accuracy easily. This is a well-known issue for schemes that require compatible discretizations, including the residual-distribution method [8], the third-order edge-based finite-volume method [9], and the active-flux method. One way to ensure the compatibility is to formulate the advection-diffusion equation as a single hyperbolic system [10]. 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 [11]. 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

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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 work also aims at overcoming very slow convergence by the pseudo-time iterations employed in the previous work [6] for solving a system of globally coupled residual equations. It is shown that the convergence is significantly improved by Newton's method: five and two Newton iterations (i.e., only five and two residual evaluations) are sufficient for steady and unsteady problems, respectively.

2. Hyperbolic Advection-Diffusion System

2.1. Advection-Diffusion Equation

Consider the advection-diffusion equation:

$$\partial_\tau u + a\,\partial_x u = \nu\,\partial_{xx} u + s_1, \tag{2.1}$$

where τ denotes a pseudo time, a is a constant advection speed, ν is a constant diffusion coefficient, and $s_1 = s_1(x, u)$ is a source term. The source term includes forcing functions as well as a physical time derivative, e.g., the backward difference formula (BDF), for time accurate computations. In the discussion that follows, we focus on the pseudo steady state, but it is equivalent to advancing one time step in the physical time. Hence, the algorithm presented is equally applicable to steady and unsteady computations.

The active flux scheme is already available individually for the advective term [1] and the diffusive term [6]. In some methods, a third-order advection-diffusion scheme can be easily constructed by adding the advection and diffusion schemes. Examples include the finite-volume methods and the discontinuous Galerkin methods. However, in other methods, such a simple construction is known to destroy the formal accuracy of the individual schemes, for example, in the residual-distribution method [8] and in the third-order edge-based finite-volume method [9]. The active flux scheme is a mixture of both as it consists of two steps: the characteristic flux computation step and the finite-volume discretization step. The simple construction is applicable to the finite-volume discretization step, but not to the flux computation step. The latter requires a careful construction to preserve the accuracy as discussed in details for a hyperbolic system with source terms in Ref.[6]. In this paper, we propose a strategy for constructing active flux schemes for the advection-diffusion equation based on two alternative forms of the advection-diffusion equation.

2.2. Conservative Form

We write the advection-diffusion equation as a first-order hyperbolic system:

$$\partial_\tau \mathbf{u} + \partial_x \mathbf{f} = \mathbf{s}, \tag{2.2}$$

where

$$\mathbf{u} = \begin{bmatrix} u \\ p \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} au - \nu p \\ -u/T_r \end{bmatrix}, \quad \mathbf{s} = \begin{bmatrix} s_1 \\ s_2 \end{bmatrix}, \tag{2.3}$$

where $s_2 = -p/T_r$. Note that the system is equivalent to the advection-diffusion equation in the pseudo steady state for any nonzero value of the relaxation time, T_r. The equivalence in the steady state is the key idea first introduced in Ref.[7] for constructing diffusion schemes. Therefore, the relaxation time has no physical importance, and can be determined solely by numerical consideration, e.g., fast convergence to the steady state. A typical choice is the following:

$$T_r = \frac{L_r^2}{\nu}, \quad L_r = \frac{1}{2\pi}, \tag{2.4}$$

which can be derived for pure diffusion by requiring Fourier modes to propagate to enhance the iterative convergence as discussed in Ref.[10]. The same choice has been derived based on a similar argument applied to a first-order finite-volume scheme as described in Ref.[9].

2.3. Source Form

The conservative form (2.2) is suitable for the finite-volume discretization step of the active flux scheme. However, the flux computation step relies on the solution of the characteristic equations, and therefore requires the

complete eigen-structure for the hyperbolic advection-diffusion system (2.2). The complete eigen-structure is available for the advection-diffusion as described in Ref.[10], but currently not available for the compressible Navier-Stokes equations. To avoid the difficulty, we propose a method based on the following form of the advection-diffusion equation:

$$\partial_\tau u = \nu\,\partial_x p + s_1 - ap, \tag{2.5}$$

$$\partial_\tau p = \frac{1}{T_r}\left(\partial_x u - p\right), \tag{2.6}$$

where the advective term has been expressed by p, which will be equivalent to u_x in the pseudo steady state, and taken to the right hand side. A major advantage of this particular form is that it is exactly in the form of a hyperbolic system with source terms, for which the active flux scheme is already available [6]. The eigenvalues of the system are exactly the same as those of the hyperbolic diffusion system:

$$\lambda_1 = -\sqrt{\frac{\nu}{T_r}}, \quad \lambda_2 = \sqrt{\frac{\nu}{T_r}}, \tag{2.7}$$

and the eigenvectors are also the same [6]. Therefore, the flux computation step is exactly the same as described in Ref.[6] for pure diffusion problems, except that the source term includes the advective term as $-ap$. Note that since it requires only the eigen-structure of the diffusive term, it can be extended to the compressible Navier-Stokes equations for which a complete eigen-structure is known for a hyperbolized viscous term.

3. Active Flux Scheme for Advection-Diffusion Equation

To discretize the hyperbolic advection-diffusion system (2.2) by the active flux scheme, we begin by storing the cell-averages within each cell and the point-values at each face in a one-dimensional grid. In each cell, we construct quadratic polynomials, $u(x)$ and $p(x)$, by interpolating the face values and requiring that the cell-average of the polynomial reduces to the cell-averaged solution. Integrating the system (2.2) over a space-(pseudo-)time control volume of the cell j and the pseudo time interval $[k, k+1]$, we obtain

$$(\overline{\mathbf{u}}_j^{k+1} - \overline{\mathbf{u}}_j^k)h = -\Delta\tau\left[\mathbf{f}_{j+1/2} - \mathbf{f}_{j-1/2}\right] + \Delta\tau\int_{x_j-h/2}^{x_j+h/2}\mathbf{s}\,dx, \tag{3.1}$$

where $h = x_{j+1/2} - x_{j-1/2}$ is the mesh spacing and $\Delta\tau = \tau_{k+1} - \tau_k$ is the pseudo time step. Note that $\mathbf{f}_{j+1/2}$ and $\mathbf{f}_{j-1/2}$ are time-averaged fluxes, which can be evaluated by Trapezoidal rule without degrading accuracy [6], and that the source term is independent of pseudo time. It leads to the following pseudo-time marching scheme:

$$\overline{\mathbf{u}}_j^{k+1} = \overline{\mathbf{u}}_j^k - \frac{\Delta\tau}{h}\mathbf{Res}_j, \tag{3.2}$$

where

$$\mathbf{Res}_j = \mathbf{f}_{j+1/2} - \mathbf{f}_{j-1/2} - \int_{x_j-h/2}^{x_j+h/2}\mathbf{s}\,dx. \tag{3.3}$$

The source term discretization is performed exactly with the quadratic representation of the solution.

The time-averaged flux is computed by Trapezoidal rule:

$$\mathbf{f}_{j+1/2} = \begin{bmatrix} a\dfrac{u_{j+1/2}^k + u_{j+1/2}^{k+1}}{2} - \nu\dfrac{p_{j+1/2}^k + p_{j+1/2}^{k+1}}{2} \\ -\dfrac{u_{j+1/2}^k + u_{j+1/2}^{k+1}}{2T_r} \end{bmatrix}, \tag{3.4}$$

and similarly for $\mathbf{f}_{j-1/2}$. The face values at $k+1$ are computed by solving the characteristic equations. Here, we employ the source form in Section 2.3. It is in the form of the hyperbolic diffusion system with source terms. Therefore, the algorithm developed in Ref.[6] is directly applicable. The solution to the characteristic equations

of the hyperbolic diffusion system with source terms is given by

$$u_{j+1/2}^{k+1} = \frac{1}{2}\left[u(x_R) + u(x_L) + L_r(p(x_R) - p(x_L)) + \frac{1}{\lambda_1}\int_{x_R}^{x_{j+1/2}} s_1^w \, dx + \frac{1}{\lambda_2}\int_{x_L}^{x_{j+1/2}} s_2^w \, dx \right], \tag{3.5}$$

$$p_{j+1/2}^{k+1} = \frac{1}{2}\left[p(x_R) + p(x_L) + \frac{1}{L_r}\left(u(x_R) - u(x_L) + \frac{1}{\lambda_1}\int_{x_R}^{x_{j+1/2}} s_1^w \, dx - \frac{1}{\lambda_2}\int_{x_L}^{x_{j+1/2}} s_2^w \, dx \right) \right], \tag{3.6}$$

where

$$x_L = \frac{x_{j+1/2} + x_{j-1/2}}{2}, \quad x_R = \frac{x_{j+3/2} + x_{j+1/2}}{2}, \tag{3.7}$$

$$s_1^w = L_r s_2 + (s_1 - ap), \quad s_2^w = L_r s_2 - (s_1 - ap). \tag{3.8}$$

Note that the pseudo-time step $\Delta\tau$ is taken locally with the CFL number 0.5 in the above formulas. The derivation of the above formulas is described in details in Ref.[6]. For unsteady computations, the physical time derivative discretized by the third-order backward difference formula (BDF3) is added to the source term s_1. See Ref.[6] for details.

4. Implicit Solver

For both steady or unsteady problems, it is necessary to solve the residual equation:

$$\mathbf{Res}(\mathbf{U}_h) = 0, \tag{4.1}$$

where $\mathbf{U}_h$ is a global numerical solution vector containing all cell-averages and face-values. The global residual vector $\mathbf{Res}(\mathbf{U}_h)$ is defined by a set of the cell-residuals (3.3) and the face-residuals. The face-residual is defined by

$$\mathbf{Res}_{j+1/2} = \begin{bmatrix} u_{j+1/2}^{k+1} - u_{j+1/2}^{k} \\ p_{j+1/2}^{k+1} - p_{j+1/2}^{k} \end{bmatrix}, \tag{4.2}$$

for the face $j + 1/2$. As in the previous study, the residual equation can be solved by the pseudo-time iteration (3.2) with the explicit face-value evaluation as in Equations (3.5) and (3.6). Thanks to the hyperbolic formulation for diffusion, the number of pseudo-time iterations exhibits linear increase with respect to the grid size, instead of quadratic that is typical for diffusion, as demonstrated in Ref.[6]. However, it still requires hundreds of residual evaluations for convergence and it is highly desirable to improve the solver convergence. To this end, we construct Newton's method:

$$\mathbf{U}_h^{k+1} = \mathbf{U}_h^k + \Delta\mathbf{U}_h, \tag{4.3}$$

where the correction $\Delta\mathbf{U}_h$ is obtained by solving the linearized system,

$$\frac{\partial \mathbf{Res}}{\partial \mathbf{U}_h}\Delta\mathbf{U}_h = -\mathbf{Res}(\mathbf{U}_h^k). \tag{4.4}$$

The residual Jacobian on the left hand side is constructed exactly, and the system is relaxed by the Gauss-Seidel relaxation with the under-relaxation parameter of 0.2 to reduce the linear residual by one order of magnitude in the L_∞ norm. Typically, we perform the Newton iteration to reduce the residual by six and two orders of magnitude for steady and unsteady problems, respectively. The advantage of the linear (instead of quadratic) increase in the number of iterations by the hyperbolic formulation is expected now in the number of linear relaxations. The implicit active-flux advection-diffusion scheme may be compared with the third-order residual-distribution scheme developed in Ref.[12]. Both schemes are based on the hyperbolic advection-diffusion system and third-order accurate for both the solution and the gradient on irregular grids. The implicit solver is not exactly Newton's method for the third-order residual-distribution scheme, but the residual Jacobian is block tri-diagonal and the convergence is as rapid as Newton's method in practice. On the other hand, our solver is exactly Newton's method, but the Jacobian is not compact having more than two off-diagonal blocks.

Note that we have completely ignored the pseudo-time derivative, and thus no pseudo-time stepping is performed. Therefore, the resulting unsteady scheme is not a dual time-stepping scheme. It is an implicit time-stepping scheme with the unsteady residual equation solved by Newton's method.

5. Results

5.1. Steady Problem

We consider a steady advection-diffusion problem taken from Refs.[10, 12, 13]:

$$a\,\partial_x u = \nu\,\partial_{xx} u + s_1, \tag{5.1}$$

with the boundary conditions $u(0) = 0$ and $u(1) = 1$, and the forcing term,

$$s_1 = \frac{\nu\pi}{a}[a\cos(\pi x) + \nu\pi\sin(\pi x)]. \tag{5.2}$$

The exact solution is given by

$$u(x) = \frac{exp(-a/\nu) - exp(ax/\nu - a/\nu)}{exp(-a/\nu) - 1} + \frac{\nu}{a}\sin(\pi x). \tag{5.3}$$

The parameters are set as $a/\nu = 0.01, 0.1, 1.0, 10, 100$. The Dirichlet boundary condition is imposed weakly at both ends as described in Ref.[6]. Therefore, the solution values are determined by the numerical scheme for all cells and faces, including the boundary faces. Steady convergence is taken to be achieved when the L_1 norm of the residual is reduced by six orders of magnitude. The initial solution is set by a randomly perturbed exact solution. Computations have been performed for a series of grids: 16, 32, 64, and 128 cells. The grids are uniformly spaced for $a/\nu = 0.01, 0.1, 1.0$, and slightly stretched for $a/\nu = 10, 100$.

Results are shown in Figures 1-10. As shown in Figures 1, 3, 5, 7, and 9, the numerical solutions are very accurate throughout he boundaries even on the coarsest grid of 16 cells. Figures 2, 4, 6, 8, 10 show that third-order accuracy has been verified for both the solution and the gradient for all cases. In the case of $a/\nu = 100$, Figure 10 shows that fourth-order accuracy is achieved for the solution and the gradient at faces and the gradient in the cells. Although one order higher order of accuracy has been known to occur for a finite-volume hyperbolic advection-diffusion scheme when advection dominates [9], it is not immediately clear how it happens to the active-flux scheme. These results show that the implicit solver converged within five Newton iterations and the number of linear relaxations increases linearly with the number of nodes, not quadratically which is typical for diffusion problems. Note that these results demonstrate significant improvements over the explicit pseudo-time stepping scheme as it only requires about five residual evaluations to obtain the solution, rather than hundreds of residual evaluations [9].

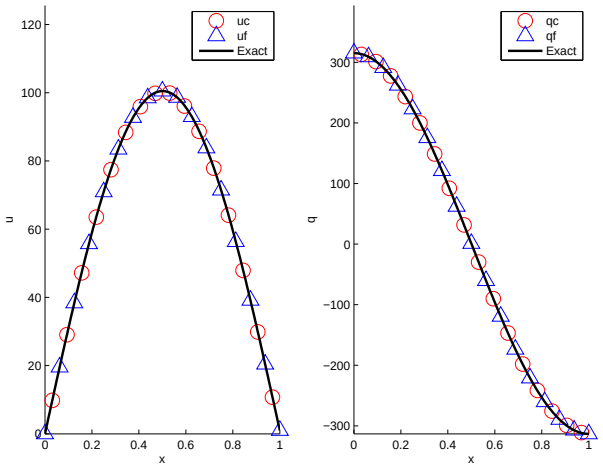

Figure 1. $a/\nu = 0.01$: **Steady solution on the 16-cell grid.** (uc, pc) **are the cell-averaged values, and** (uf, pf) **are the point values at the face.**

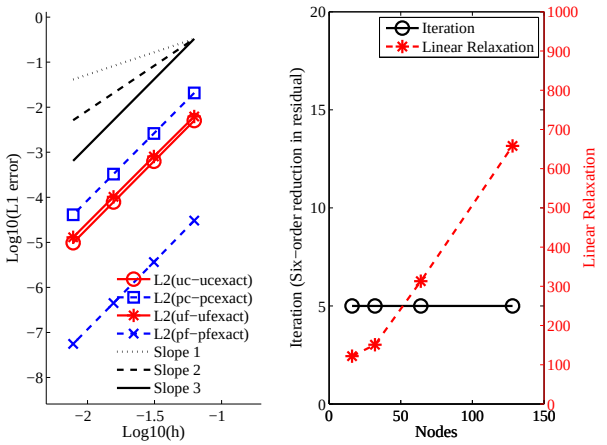

Figure 2. $a/\nu = 0.01$: L_1 **Error and iterative convergence results for a steady problem.**

5.2. Unsteady Problem

We consider the following unsteady advection-diffusion problem,

$$\partial_t u + a\,\partial_x u = \nu\,\partial_{xx} u, \tag{5.4}$$

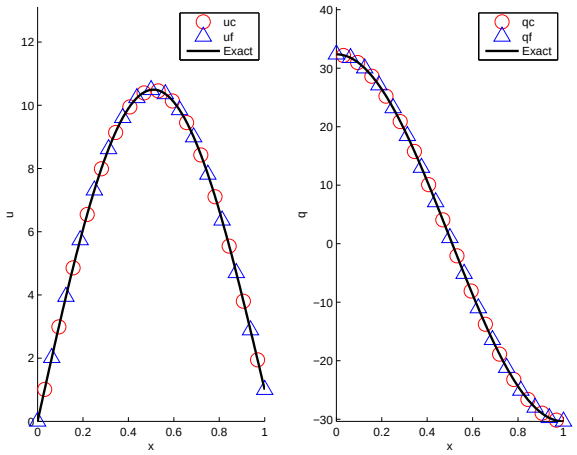

Figure 3. $a/\nu = 0.1$**: Steady solution on the 16-cell grid.** (uc, pc) **are the cell-averaged values, and** (uf, pf) **are the point values at the face.**

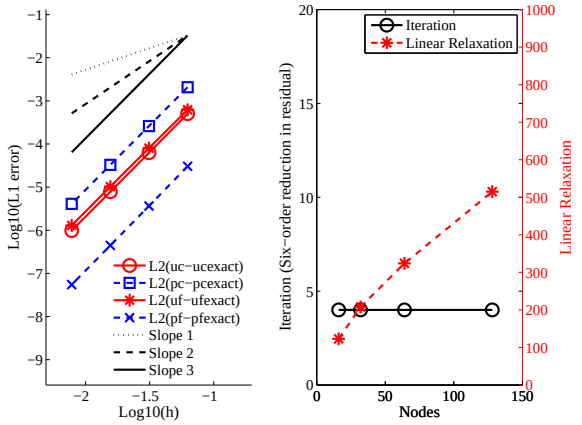

Figure 4. $a/\nu = 0.1$**:** L_1 **Error and iterative convergence results for a steady problem.**

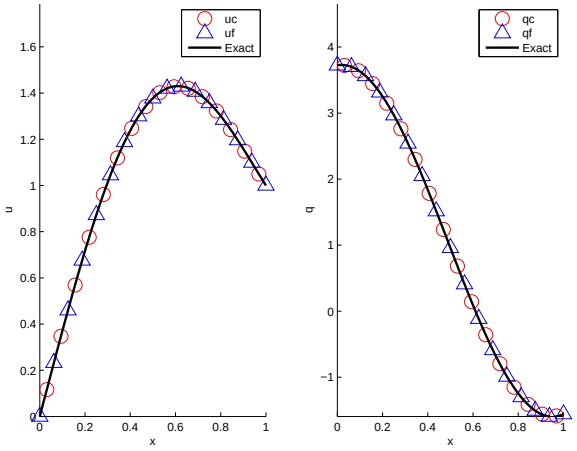

Figure 5. $a/\nu = 1.0$**: Steady solution on the 16-cell grid.** (uc, pc) **are the cell-averaged values, and** (uf, pf) **are the point values at the face.**

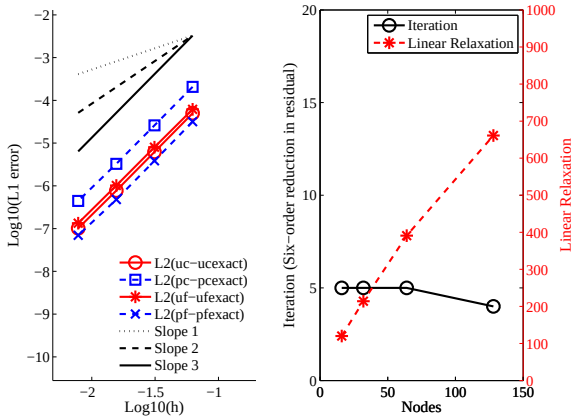

Figure 6. $a/\nu = 1.0$**:** L_1 **Error and iterative convergence results for a steady problem.**

with the following boundary conditions:

$$u(0) = 0, \tag{5.5}$$
$$u(1) = U\cos(\omega t), \tag{5.6}$$

where U and ω are arbitrary constants. The exact solution exists to this problem; it can be found in Ref.[14]. For numerical results, the parameters have been set as follows:

$$a = 4.246, \quad \nu = 2.123, \quad U = 2.0, \quad \omega = 2\pi. \tag{5.7}$$

Again, the boundary condition is imposed weakly and thus the solutions are computed by the numerical scheme at all cells and faces. At every physical time step, the initial solution is set as the solution at the previous physical time step, and the Newton sub-iteration is taken to be converged when the L_1 norm of the unsteady residual is reduced by two orders of magnitude. To start up the computation, we use BDF1 over the first step, BDF2 in the next step, and BDF3 thereafter. Ideally, it would be best to perform the first two steps with a small enough time step not to introduce large errors, but numerical results show that the low-order errors in the first two steps do not greatly impact the accuracy of the solution at a later time.

We tested the scheme for a given grid of 20 cells with randomly distributed nodes by refining the time step: $0.4/2^m$, where $m = 0, 1, 2, 3$. The final time is 6.0, i.e., six periods in the unsteady boundary condition. Results

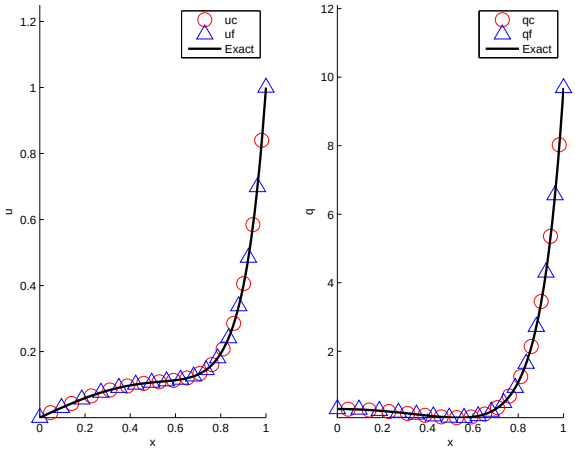

Figure 7. $a/\nu = 10$**: Steady solution on the 16-cell grid.** (uc, pc) **are the cell-averaged values, and** (uf, pf) **are the point values at the face.**

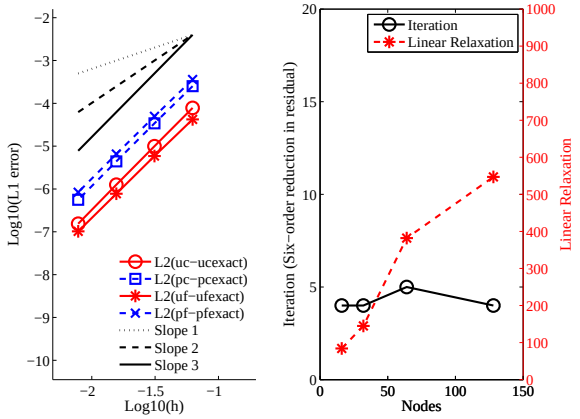

Figure 8. $a/\nu = 10$**:** L_1 **Error and iterative convergence results for a steady problem.**

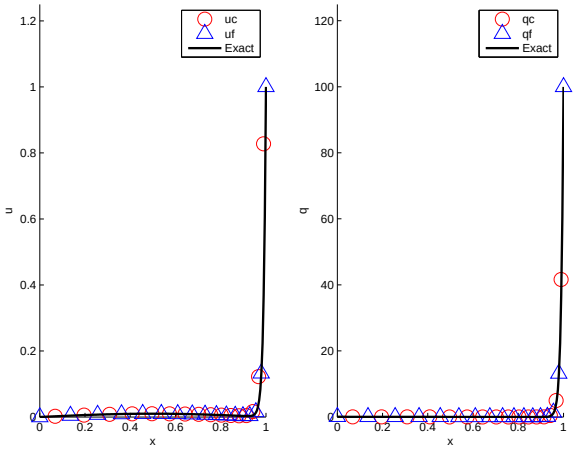

Figure 9. $a/\nu = 100$**: Steady solution on the 16-cell grid.** (uc, pc) **are the cell-averaged values, and** (uf, pf) **are the point values at the face.**

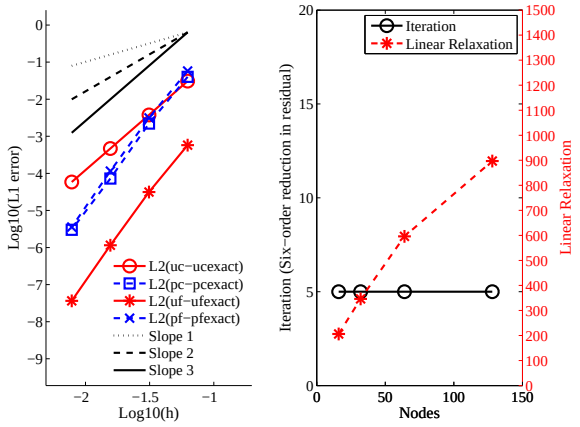

Figure 10. $a/\nu = 100$**:** L_1 **Error and iterative convergence results for a steady problem.**

are shown in Figure 11, which confirms the formal third-order time accuracy. The accuracy deteriorates in the finest grid apparently because the spatial error begins to dominate. Also shown is the iterative convergence for the Newton sub-iteration. Only two iterations, thus two residual evaluations, are required at every physical time step. This is a tremendous improvement over the explicit pseudo-time stepping scheme in Ref.[6], which requires hundreds of residual evaluations per physical time step. The cell-averaged solution and gradient at $t = 5.0, 5.25, 5.5, 5.75$ are plotted in Figures 12, 13, 14, 15, respectively. These results show that the active-flux advection-diffusion scheme enables highly accurate unsteady simulations on a rather coarse grid even for irregular grids.

6. Concluding Remarks

In this paper, we have extend the third-order active-flux diffusion scheme introduced in Ref.[6] to advection-diffusion problems. We constructed a third-order active-flux advection-diffusion scheme by adding the advective term as a source term to the diffusion scheme. The solution gradient, which is computed simultaneously to third-order accuracy by the diffusion scheme, is used to express the advective term as a scalar source term. For unsteady computations, we employ a third-order implicit time-stepping scheme with the unsteady residual equations solved by Newton's method. Third-order accuracy in the solution as well as in the gradient, and rapid

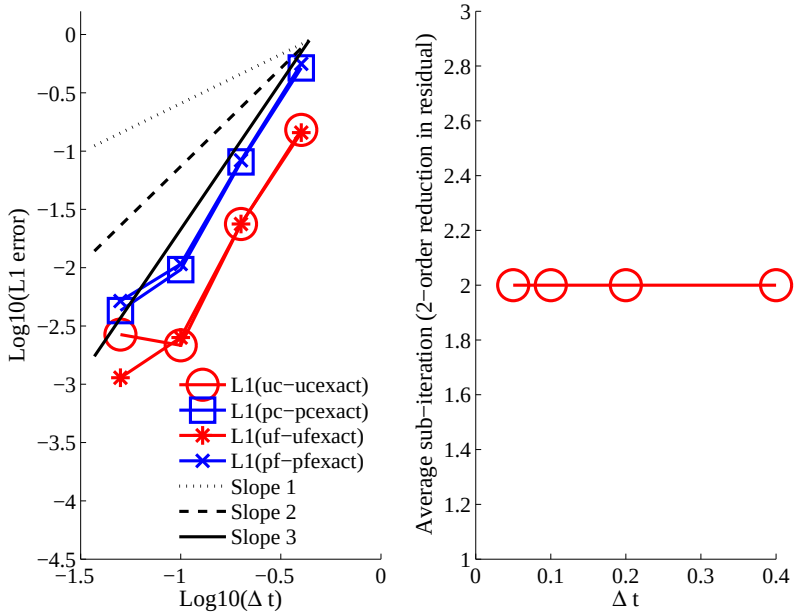

Figure 11. Numerical results for BDF3. Time accuracy on the left and the number of sub-iterations on the right.

convergence by Newton's method have been demonstrated for steady and unsteady problems.

Future work should focus on extensions to two and three dimensions as well as to the Navier-Stokes equations. The idea of treating the advective term as a source term can be extended to the compressible Navier-Stokes equations by a new hyperbolic formulation for the Navier-Stokes equations proposed in Ref.[15].

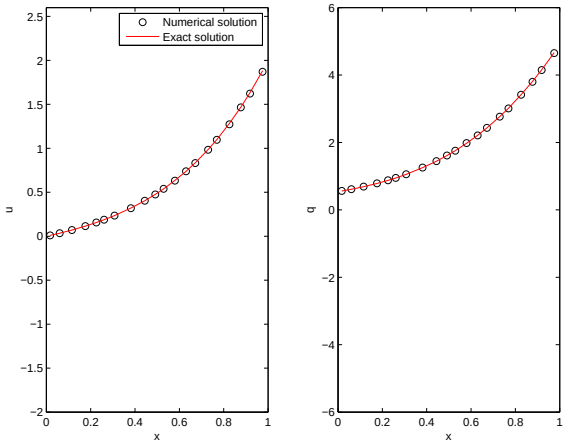

Figure 12. Unsteady solution at $t = 5.0$. $\Delta t = 0.1$ and 20 cells.

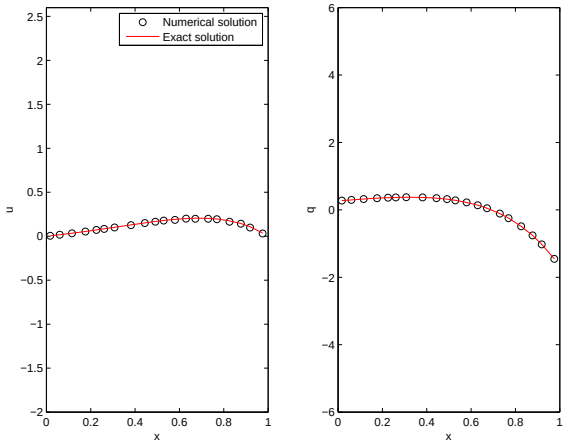

Figure 13. Unsteady solution at $t = 5.25$. $\Delta t = 0.1$ and 20 cells.

Acknowledgments

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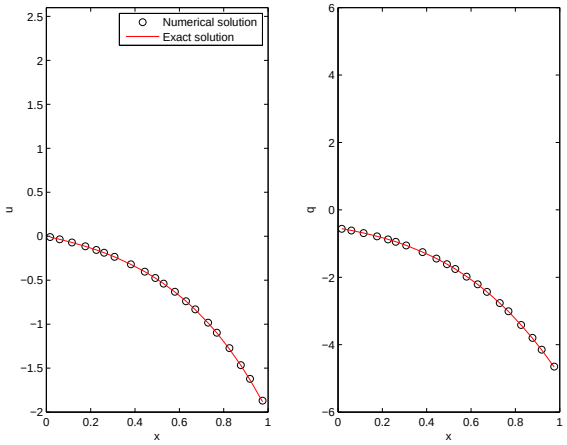

Figure 14. Unsteady solution at $t = 5.5$. $\Delta t = 0.1$ and 20 cells.

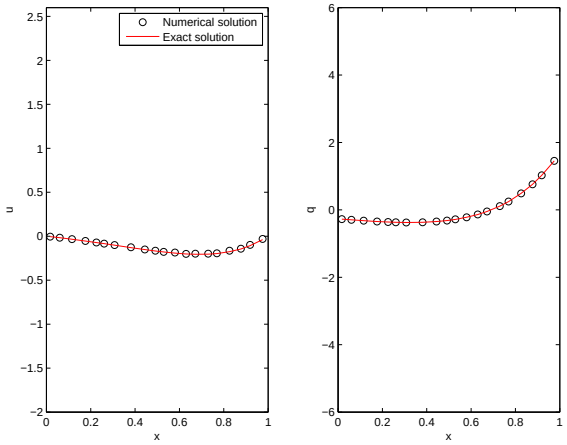

Figure 15. Unsteady solution at $t = 5.75$. $\Delta t = 0.1$ and 20 cells.

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