On Hyperbolic Method for Diffusion with Discontinuous Coefficients

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Abstract

It is shown that the hyperbolic method, if formulated with diffusive fluxes as additional solution variables, works directly and naturally for diffusion problems with discontinuous coefficients as well as discontinuous tangential fluxes across a material interface. A suitable formulation is given, and numerical examples are shown to demonstrate that a hyperbolic scheme can produce exact non-differentiable piecewise-linear solutions for problems with discontinuous coefficients and tangential fluxes.

1 Introduction

A recent paper [1] published in Journal of Computational Physics presents high-order reconstruction-based cell-centered finite-volume schemes for the hyperbolic formulation of diffusion [2]. While it shows impressive results up to nearly fourth-order accuracy on unstructured triangular grids, the final numerical example presented in Ref.[1] indicates that all these hyperbolic diffusion schemes miserably fail for a diffusion problem with discontinuous coefficients. The authors conjecture that the failure is due to the lack of monotonicity preserving capability, and states that it opens up a new research direction towards monotonicity-preserving hyperbolic diffusion schemes. In this short note, I will show that the hyperbolic diffusion scheme, if suitably formulated, works directly and naturally for such problems. In fact, the hyperbolic method is well suited for diffusion problems with discontinuous coefficients, which arise quite typically in heat-conduction/transfer problems involving different properties/materials where the domains are connected via interface/boundary conditions [3, 4, 5]. In the next section, I will explain how the original hyperbolic formulation can fail for variable-coefficient or nonlinear diffusion equations, and then describe a hyperbolic formulation suitable for such problems. Finally, two numerical examples are shown to demonstrate that the hyperbolic scheme can produce exact non-differentiable piecewise linear solutions for problems with discontinuous coefficients.

2 Hyperbolic Formulations for Diffusion

2.1 Original Formulation

In the hyperbolic method [2], the diffusion equation,

$$\partial_t u = \nu(\partial_{xx} u + \partial_{yy} u), \tag{1}$$

where ν is a diffusion coefficient and u is a scalar solution variable, is solved in the following first-order system form:

$$\partial_\tau u = \nu(\partial_x p + \partial_y q) - \partial_t u, \quad \partial_\tau p = \frac{1}{T_r}(\partial_x u - p), \quad \partial_\tau q = \frac{1}{T_r}(\partial_y u - q), \tag{2}$$

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where τ is a pseudo time, and T_r is called the relaxation time. The system is equivalent to the original diffusion equation for any T_r in the pseudo steady state or as soon as the pseudo time derivatives are dropped; then $p = \partial_x u$ and $q = \partial_y u$, and thus $0 = \nu(\partial_x p + \partial_y q) - \partial_t u = \nu(\partial_{xx} u + \partial_{yy} u) - \partial_t u$. The first-order system is hyperbolic in the pseudo time τ, and therefore it can be discretized in space by methods for hyperbolic systems, e.g., upwind methods. The physical time derivative is discretized in time and treated as a source term [6, 7, 8]. Then, the pseudo time derivatives may be dropped to yield a consistent discretization of the diffusion equation in both time and space. The resulting discretization is known to possess special features: higher-order and higher quality gradients on unstructured grids, higher-order advective schemes for advection-diffusion equations, $O(1/h)$ convergence acceleration, where h is a mesh spacing, [9, 10]. The pseudo-time system (2) is similar to the classical hyperbolic heat equations of Cattaneo [11] and Vernotte [12], but fundamentally different in that T_r is a *free parameter* and it can be determined to optimize the properties of the discretization, e.g., faster iterative convergence and/or improved accuracy. The optimal formula derived in Refs.[2, 13] for fast iterative convergence is given by

$$T_r = \frac{L_r^2}{\nu}, \quad L_r = \frac{1}{2\pi}, \tag{3}$$

where L_r needs to be properly scaled for dimensional equations or general non-square domains [14]. In discussions that follow, we focus on steady problems, and therefore ignore the physical time derivative.

Apparently, Ref.[1] uses the original hyperbolic formulation (2) in the conservative form:

$$\partial_\tau \mathbf{u} + \partial_x \mathbf{f} + \partial_y \mathbf{g} = \mathbf{s}, \tag{4}$$

where

$$\mathbf{u} = \begin{bmatrix} u \\ p \\ q \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} -\nu p \\ -u/T_r \\ 0 \end{bmatrix}, \quad \mathbf{g} = \begin{bmatrix} -\nu q \\ 0 \\ -u/T_r \end{bmatrix}, \quad \mathbf{s} = \begin{bmatrix} 0 \\ -p/T_r \\ -q/T_r \end{bmatrix}, \tag{5}$$

for solving a diffusion equation with a variable (and discontinuous) coefficient ν:

$$\partial_x(\nu \partial_x u) + \partial_y(\nu \partial_y u) = 0. \tag{6}$$

Suppose that the pseudo steady state is reached. Then, the first equation of the system (4) will reduce to

$$\partial_x(\nu p) + \partial_y(\nu q) = 0. \tag{7}$$

which is consistent with the target equation (6) if

$$p = \partial_x u, \quad q = \partial_y u. \tag{8}$$

But this is not true because the second and third equations of the system (4) will be

$$0 = \partial_x\left(\frac{u}{T_r}\right) - \frac{p}{T_r}, \quad 0 = \partial_y\left(\frac{u}{T_r}\right) - \frac{q}{T_r}, \tag{9}$$

and since $T_r = L_r^2/\nu$ is not constant,

$$p = T_r \partial_x\left(\frac{u}{T_r}\right) \neq \partial_x u, \quad q = T_r \partial_y\left(\frac{u}{T_r}\right) \neq \partial_y u. \tag{10}$$

Therefore, schemes based on the above conservative formulation are likely to be inconsistent for a non-constant coefficient diffusion equation. The consistency may be recovered by defining T_r as a global constant, e.g., by $T_r = L_r^2/\nu_\infty$, where ν_∞ is a global constant. However, then, a numerical scheme can suffer from a lack/excess of dissipation and may encounter instability and/or inaccuracy. Moreover, the variables p and q can be discontinuous for diffusion with discontinuous coefficients. Therefore, numerical schemes, which are designed based on the assumption that p and q are smooth, would encounter difficulties.

2.2 Preconditioned Formulation I

In Ref.[15], the hyperbolic method was extended to the compressible Navier-Stokes equations with the viscosity given by Sutherland's law. To deal with the solution-dependent viscosity, a preconditioned formulation was proposed, which, in the case of diffusion, corresponds to the following:

$$\partial_\tau u = \partial_x p + \partial_y q, \quad \frac{T_r}{\nu}\partial_\tau p = \partial_x u - \frac{p}{\nu}, \quad \frac{T_r}{\nu}\partial_\tau q = \partial_y u - \frac{q}{\nu}, \tag{11}$$

which is deliberately constructed as a preconditioned conservative system:

$$\mathbf{P}^{-1}\partial_\tau \mathbf{u} + \partial_x \mathbf{f} + \partial_y \mathbf{g} = \mathbf{s}, \tag{12}$$

where

$$\mathbf{P}^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & T_r/\nu & 0 \\ 0 & 0 & T_r/\nu \end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix} u \\ p \\ q \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} -p \\ -u \\ 0 \end{bmatrix}, \quad \mathbf{g} = \begin{bmatrix} -q \\ 0 \\ -u \end{bmatrix}, \quad \mathbf{s} = \begin{bmatrix} 0 \\ -p/\nu \\ -q/\nu \end{bmatrix}. \tag{13}$$

This formulation is directly applicable to variable-coefficient and nonlinear equations, and consistent with the target nonlinear diffusion equation (6). To see this, consider the pseudo steady state (or drop the pseudo time derivatives), where

$$\partial_x p + \partial_y q = 0, \quad 0 = \partial_x u - \frac{p}{\nu}, \quad 0 = \partial_y u - \frac{q}{\nu}, \tag{14}$$

which means

$$0 = \partial_x p + \partial_y q, \quad p = \nu\partial_x u, \quad q = \nu\partial_y u. \tag{15}$$

Therefore, it is consistent with the target nonlinear diffusion equation:

$$\partial_x(\nu\partial_x u) + \partial_y(\nu\partial_y u) = 0. \tag{16}$$

The system (12) is in the form typical in the local-preconditioning methods [16, 17, 18], and therefore discretization techniques are well known. Moreover, the flux Jacobian required to construct an upwind flux can be analytically obtained without differentiating the diffusion coefficient since the wave structure of the preconditioned system is determined by the preconditioned Jacobian:

$$\mathbf{P}\mathbf{A}_n = \mathbf{P}\left(\frac{\partial \mathbf{f}}{\partial \mathbf{u}}\hat{n}_x + \frac{\partial \mathbf{g}}{\partial \mathbf{u}}\hat{n}_y\right), \tag{17}$$

where $(\hat{n}_x, \hat{n}_y)$ is an arbitrary unit vector. Note that ν appears only in $\mathbf{P}$, and thus does not have to be differentiated with respect to $\mathbf{u}$. This greatly simplifies the eigen-structure analysis for complex nonlinear systems such as the compressible Navier-Stokes equations [19], not to mention nonlinear or variable-coefficient diffusion equations.

Yet another advantage, which is directly relevant to the scope of this short note, lies in the extra variables, which now correspond to the diffusive fluxes:

$$p = \nu\partial_x u, \quad q = \nu\partial_y u. \tag{18}$$

Diffusion equations can have discontinuous coefficients as well as gradients, but the diffusive fluxes are continuous, at least in the direction normal to the interface of discontinuous coefficients. Numerically, it is easier to work with continuous variables rather than discontinuous variables. For example, any special averaging for a discontinuous coefficient such as the well-known harmonic mean, which ensures the continuity of the diffusive flux across a material interface [3], is not required.

This formulation has been successfully employed for the compressible Navier-Stokes equations in two [10, 15, 20] and three dimensions [6, 19, 21, 22], where the extra variables represent the viscous stresses and the heat fluxes. This is the formulation suitable for solving a variable-coefficient or nonlinear diffusion equation with discontinuous coefficients.

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2.3   Preconditioned Formulation II

In some cases, we may wish to have $(p, q) = (\partial_x u, \partial_y u)$ for nonlinear problems. For example, in the efficient construction of the discontinuous Galerkin method for the hyperbolic diffusion [23, 24], the variables p and q are used to replace high-order moments in the polynomial for the primary variable u. The process can be complicated if $(p, q) = (\nu \partial_x u, \nu \partial_y u)$ since the derivatives of (p, q) used to represent high-order derivatives of u will involve high-order derivatives of ν. To avoid this complication, one can consider the following formulation [14, 25]:

$$\partial_\tau u = \partial_x(\nu p) + \partial_y(\nu q), \quad T_r \partial_\tau p = \partial_x u - p, \quad T_r \partial_\tau q = \partial_y u - q, \tag{19}$$

so that the system is still formulated to be consistent with the target nonlinear diffusion equation, and yields $(p, q) = (\partial_x u, \partial_y u)$ at convergence. This is, again, in the preconditioned conservative form, and a numerical flux can be constructed with a dissipation matrix based on a frozen ν as described in Refs.[14, 25]. For the problem and the discretization considered in this short note, however, Formulation I is more suitable, and therefore this formulation will not be discussed further. We mention it because it is also a useful formulation for nonlinear diffusion problems.

3   Numerical Results

We demonstrate Formulation I for two examples of discontinuous-coefficient problems. The discretization is a cell-centered finite-volume discretization, where the residual is defined as an approximation to the system (12) integrated over a computational cell j by the midpoint rule, and then multiplied by $\mathbf{P}$:

$$\mathbf{Res}_j = \mathbf{P}_j \sum_{k \in \{k_j\}} [\mathbf{\Phi}_{jk} A_{jk} - \mathbf{s}_j V_j], \tag{20}$$

where $\{k_j\}$ is a set of neighbors of the cell j, A_{jk} is the length of the face across j and k, V_j is the area of the cell j, $\mathbf{P}_j$ and $\mathbf{s}_j$ are evaluated by the solution stored in the cell j. See Figure 1. Note that the pseudo time derivatives have been dropped. The numerical flux $\mathbf{\Phi}_{jk}$ is constructed by following a common practice in the local-preconditioning technique (see Ref.[26]):

$$
\begin{aligned}
\mathbf{\Phi}_{jk} &= \frac{1}{2}[\mathbf{f}_n(\mathbf{u}_L) + \mathbf{f}_n(\mathbf{u}_R)] - \frac{1}{2}\mathbf{P}^{-1}|\mathbf{P}\mathbf{A}_n|(\mathbf{u}_R - \mathbf{u}_L) \\[2mm]
&= \frac{1}{2}\begin{bmatrix} -(p_{nL} + p_{nR}) \\ -(u_L + u_R)\hat{n}_x \\ -(u_L + u_R)\hat{n}_y \end{bmatrix} - \frac{L_r}{2\overline{\nu}}\begin{bmatrix} u_R - u_L \\ (p_{nR} - p_{nL})\hat{n}_x \\ (p_{nR} - p_{nL})\hat{n}_y \end{bmatrix},
\end{aligned} \tag{21}
$$

where $\mathbf{f}_n = [-(p, q) \cdot \hat{\mathbf{n}}_{jk}, -u\hat{n}_x, -u\hat{n}_y]$, $\overline{\nu} = (\nu_L + \nu_R)/2$, $p_{nL} = (p_L, q_L) \cdot \hat{\mathbf{n}}_{jk}$, $p_{nR} = (p_R, q_R) \cdot \hat{\mathbf{n}}_{jk}$, and $\hat{\mathbf{n}}_{jk} = (\hat{n}_x, \hat{n}_y)$ is the unit vector normal to the face pointing from the cell j to the neighbor cell k. The left and right states are evaluated by

$$
\begin{aligned}
u_L &= u_j + \left(\frac{p_j}{\nu_j}, \frac{q_j}{\nu_j}\right) \cdot (\mathbf{x}_m - \mathbf{x}_j), & u_R &= u_k + \left(\frac{p_k}{\nu_k}, \frac{q_k}{\nu_k}\right) \cdot (\mathbf{x}_m - \mathbf{x}_k), \\
p_L &= p_j, & p_R &= p_k, \\
q_L &= q_j, & q_R &= q_k, \\
\nu_L &= \nu(\mathbf{x}_m^-), & \nu_R &= \nu(\mathbf{x}_m^+),
\end{aligned} \tag{22}
$$

where $\mathbf{x}_m$ is the face-midpoint location, $\mathbf{x}_m^-$ and $\mathbf{x}_m^+$ indicate evaluations from within the cells j and k, respectively, $\mathbf{x}_j$ and $\mathbf{x}_k$ are the centroid coordinates of the cells j and k, respectively, u_j and u_k are the solution values stored at the cells j and k, respectively (similarly for p and q), $\nu_j = \nu(\mathbf{x}_j)$, and $\nu_k = \nu(\mathbf{x}_k)$. The above face reconstruction corresponds, for linear diffusion equations, to the

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first-order version of Scheme II in Refs.[13, 26], DG(P0P1)+DG(P0) in Ref.[23], and Hybrid P1+P0 in Ref.[1]. Note that the residual depends only on the face-neighbors (see Figure 1) and gradient computations such as least-squares fits are not needed, and therefore the discretization is compact. By construction, the residual will vanish if the exact solution u is a linear function. Refs.[1, 23] show that second-order accuracy is obtained in u for smooth solutions. Observe also that only the normal diffusive flux p_n appears in the upwind flux. Therefore, the discretization is transparent to the tangential diffusive flux, accurately inheriting the property of the diffusion equation.
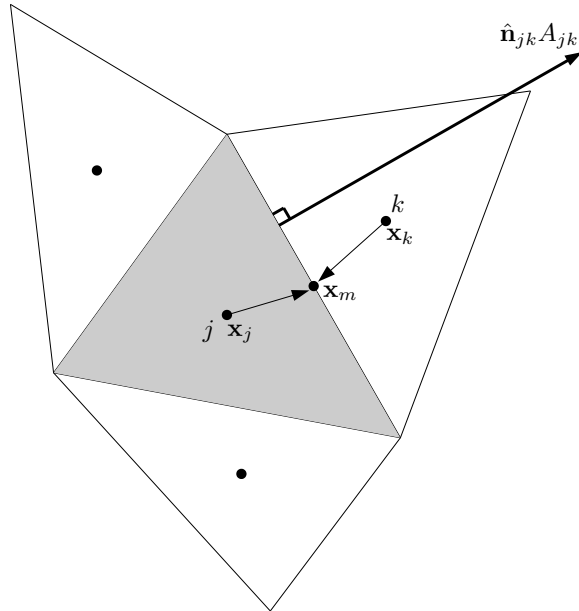

Figure 1: Residual stencil for the cell-centered hyperbolic scheme (Scheme II).

Another important feature relevant to the application considered here is that the residual vanishes even for a non-differentiable continuous piecewise linear exact solution, provided the domain is discretized into a set of regions where the solution is differentiable within each region. This is not a typical feature in conventional diffusion schemes because many conventional diffusion schemes involve the computation of the solution gradients, and this step often uses a linear fit across such regions, where the solution is continuous but not differentiable, and thus fails to be exact for piecewise linear functions. It is also worth pointing out that no special averaging is necessary for ν to enforce the continuity of the diffusive flux at the face [3] simply because we directly work with the diffusive flux variables, p and q, and their face-normal component can be assumed to be continuous. For $\bar{\nu}$ in the dissipation coefficient, it suffices to use the arithmetic average since the dissipation term has the order property and it merely provides stability. For nonlinear problems, ν_L and ν_R should be evaluated by u_L and u_R, respectively [14, 25].

For all problems considered below, the Dirichlet boundary condition is imposed weakly through the numerical flux with the right state specified based on a given boundary condition. More specifically, we set $u_R = u_b$, where u_b is the given boundary value, and $(p_R, q_R) = (p_L, q_L)$ since there are no boundary conditions for the gradient [14]. Numerical solutions are obtained by solving the residual equations by an implicit solver with the initial solution given by an exact solution with random perturbations. The residual Jacobian is constructed by exactly differentiating the residual with respect to the discrete unknowns, and approximately inverted by the Gauss-Seidel relaxation until the linear residual is reduced by four orders of magnitude. The implicit iteration rapidly converges to machine zero within five iterations for the problems considered. Further algorithmic details can be found in Ref.[14].

Example 1: We first consider the following example [27]:

$$0 = \partial_x(\nu u) + \partial_y(\nu u), \quad \text{in } (x, y) \in (0, 1) \times (0, 1), \tag{23}$$

where ν is discontinuous:

$$\nu = \begin{cases} \nu_1 & x \le 0.5, \\ \nu_2 & x > 0.5, \end{cases} \tag{24}$$

with $\nu_1 = 1/30$ and $\nu_2 = 1/15$. The exact solution is given by

$$u = \begin{cases} \dfrac{\nu_2 x + 2\nu_1\nu_2}{0.5(\nu_1 + \nu_2) + 4\nu_1\nu_2} & x \le 0.5, \\[4mm] \dfrac{\nu_1 x + 2\nu_1\nu_2 + 0.5(\nu_2 - \nu_1)}{0.5(\nu_1 + \nu_2) + 4\nu_1\nu_2} & x > 0.5, \end{cases} \tag{25}$$

which is continuous throughout the domain, but not differentiable at $x = 0.5$. It can be easily confirmed that the solution gradient is discontinuous at $x = 0.5$ in the x-direction, but the diffusive fluxes are continuous everywhere. This is the problem that the failure of hyperbolic schemes based on the original formulation is reported for in Ref.[1]. The domain is randomly triangulated with 81 nodes and 128 triangles, except that the line at $x = 0.5$ is kept straight to represent the interface between the regions with different coefficients. The implicit solver converged rapidly, and produced numerical solutions with errors at a machine-zero level. The solutions are plotted in Figure 2. These plots are based on the nodal solutions computed by averaging the values given by the solution polynomials defined over each cell: linear u and constant (p, q). Note that the averaging has no effect since the numerical solution u is linear and exact, and the variables p and q are constant and exact. The results confirm the linear exactness of the residual. The same problem was solved on different sizes of grids, but the numerical solutions are, again, exact within machine zero, and look exactly the same as those in Figure 2 (except for the mesh).

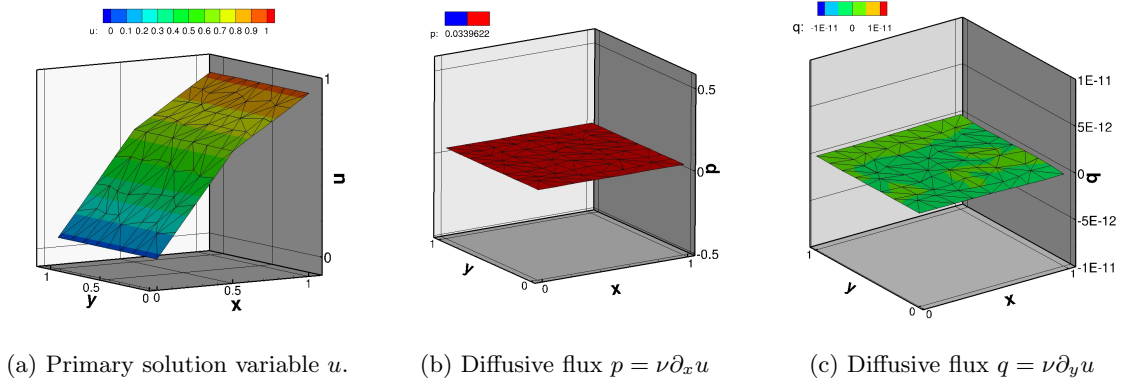| (a) Primary solution variable u. | (b) Diffusive flux $p = \nu\partial_x u$ | (c) Diffusive flux $q = \nu\partial_y u$ |

Figure 2: Example 1. Numerical solutions and the computational grid.

Example 2: Next, we consider another example from Ref.[27], which is based on the same diffusion equation as in Example 1, but with the following exact solution:

$$u = \begin{cases} 1 + x + y & x \le 0.5, \\[3mm] 1 + \dfrac{\nu_2 - \nu_1}{2\nu_2} + \dfrac{\nu_1}{\nu_2} x + y & x > 0.5, \end{cases} \tag{26}$$

where $\nu_1 = 1/30$ and $\nu_2 = 1/300$. The solution is again continuous, but not differentiable at $x = 0.5$. The x-component of the diffusive flux $\nu\partial_x u$ is continuous, but this time the y-component, i.e., the tangential flux $\nu\partial_y u$, is discontinuous across the interface at $x = 0.5$. The problem is solved on the same grid as in Example 1. Again, the implicit solver converged in five iterations to machine zero, and produced numerical solutions with errors in the order of machine zero. The solutions are shown in Figure 3. These plots are based on the nodal values as before, except that q is plotted by the cell

values to emphasize that the discontinuous diffusive flux has been produced exactly by the numerical scheme. As expected, the hyperbolic scheme can produce, without any special technique such as limiters, the exact piecewise linear solution even in the presence of a discontinuous tangential flux.

(a) Primary solution variable u.   (b) Diffusive flux $p = \nu \partial_x u$ (c) Diffusive flux $q = \nu \partial_y u$
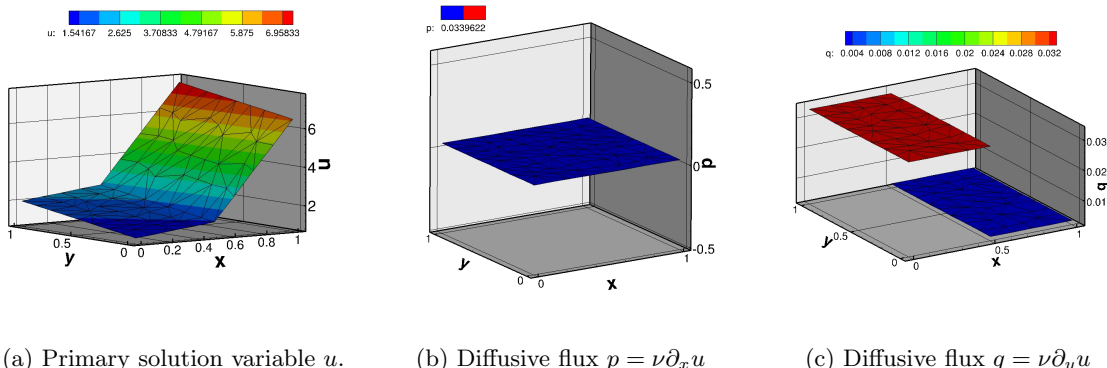
Figure 3: Example 2. Numerical solutions and the computational grid.

These examples show that the hyperbolic scheme works directly and naturally for diffusion problems with discontinuous coefficients and tangential fluxes if constructed based on the preconditioned formulation with the diffusive fluxes employed as the additional solution variables. High-order hyperbolic finite-volume schemes developed in Ref.[1] have a great potential for generating highly-accurate and practical methods for variable-coefficient and nonlinear diffusion equations if applied to the preconditioned formulation. Care must be taken, however, not to perform the high-order reconstruction across the interface of two different properties/materials: each state, $\mathbf{u}_L$ or $\mathbf{u}_R$, must be evaluated with least-squares derivatives computed within its own domain. Otherwise, as mentioned earlier, the scheme will lose the exactness for a designed order of polynomials in each domain. Such a reconstruction procedure is straightforward, by compactness, in the hyperbolic discontinuous Galerkin method [23, 24, 25].

Acknowledgments

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