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Divergence Formulation of Source Term

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Abstract

In this paper, we propose to write a source term in the divergence form. A conservation law with a source term can then be written as a single divergence form. We demonstrate that it enables to discretize both the conservation law and the source term in the same framework, and thus greatly simplifies the construction of numerical schemes. To illustrate the advantage of the divergence formulation, we apply the new formulation to construct a uniformly third-order accurate edge-based finite-volume scheme for conservation laws with a source term. Third-order accuracy is demonstrated for regular and irregular triangular grids for the linear advection and Burgers' equations with a source term.

1 Introduction

There is a class of numerical schemes that achieve a design order of accuracy based on vanishing residual. Examples are residual-based compact schemes [1], residual-distribution schemes [2], and the corrected scheme of Katz and Sankaran [3]. These schemes have a common property that the leading truncation error contains the derivatives of the target equations (or the residual), which may be called the residual property. These terms will vanish on convergence and the accuracy is upgraded to the next higher-order level. The order of accuracy of such schemes is typically one order higher (at least) than those of similar complexity. For example, for the advection equation, the residual-distribution schemes are second-order accurate within a compact stencil with no gradient reconstruction whereas the edge-based finite-volume scheme is essentially first-order accurate on such a stencil. Successful implementation of these schemes requires a careful construction to preserve the residual property for all terms in the target equations. If the residual property is not satisfied to the design order, the actual order of accuracy can be at least one order lower [4]. The technique to ensure the residual property typically depends on the discretization method and the type of equation. For example, the Galerkin-type discretization is proposed to preserve the third-order accuracy of the corrected scheme for equations with source terms [3, 5]. The residual-based compact schemes achieve the uniformly high-order accuracy by constructing a dissipation term based on the residual [6]. Alternatively, schemes independently constructed for different terms may be combined with a careful weighting function such as Peclet-number weighting for the advection-diffusion equation [7]. Although techniques are available for some specific schemes and equations, it is not straightforward in general to achieve the uniform accuracy for all terms present in a given target equation. To simplify the task of constructing uniformly accurate schemes for the advection-diffusion equation, a first-order hyperbolic formulation was proposed for diffusion in [8]. It enables to cast the advection-diffusion equation as a single hyperbolic system [9], thereby eliminating the need to develop two different schemes and carefully combine them to preserve the design accuracy. The hyperbolic formulation has recently been extended to the compressible Navier-Stokes equations [10]. In this paper, we introduce a similar idea for source terms in a conservation law. That is, we propose to cast a source term in the divergence form, and discretize it by the same type of scheme used for the conservation law. Naturally, then, the schemes will automatically have the residual

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property because the source term no longer appears. In this paper, we demonstrate the advantage of the proposed approach by constructing a third-order finite-volume scheme for conservation laws with a source term. However, the approach is quite general in that it applies to the differential equation rather than the numerical scheme. Therefore, it is generally applicable to other numerical schemes.

A similar approach exists in the well-balanced schemes. In [11], a wave-model-based source term discretization is proposed for the non-linear shallow water system of equations. Although our approach is somewhat similar to the the wave-model decomposition approach, there are distinctions. First, our main concern is the uniform accuracy while the wave-model decomposition is targeted at achieving a balance between the conservation law and the source term in the numerical scheme. Second, the wave-model decomposition is proposed for the source term involving the gradient of the solution variables [11] while the divergence formulation proposed herein applies to any source term. Third, the wave-model decomposition is closely tied with the physics of the conservation law whereas the divergence formulation is a purely mathematical manipulation and independent of the physics of the conservation law.

The paper is organized as follows. Section 2 describes the third-order finite-volume scheme, which is the main target discretization in this paper. Section 3 discusses the issue of uniform accuracy for the third-order scheme applied to conservation laws with source terms. Section 4 introduces the divergence formulation of source terms and illustrates the construction of the third-order scheme based on the new formulation. Sections 5 and 6 present simplified versions of the divergence formulation. Section 7 shows the numerical results obtained by the divergence formulations. Section 8 concludes the paper with remarks.

2 Third-Order Edge-Based Finite-Volume Scheme

Consider the conservation law with a source term.

$$\partial_x f + \partial_y g = s, \tag{1}$$

where (f, g) is a flux vector and s is a source term. The source term may include the discretized physical time derivative in the framework of the dual-time stepping scheme [12]. We assume that at least the numerical values of the source term are available at nodes on a computational grid. The node-centered edge-based finite-volume scheme for Equation (1) is given by

$$0 = -\frac{1}{V_j} \sum_{k \in \{K_j\}} \phi_{jk} A_{jk} + \frac{1}{V_j} \int_{\Omega_j} s \, dV, \tag{2}$$

where $\{K_j\}$ is a set of neighbors of j, ϕ_{jk} is a numerical flux, and A_{jk} is the magnitude of the directed area vector, $\mathbf{n}_{jk} = \mathbf{n}_{jk}^{\ell} + \mathbf{n}_{jk}^{r}$ (see Figure 1). The source term discretization is left open for the moment; it is the subject of the present paper and will be discussed in details later. We evaluate the numerical flux by the upwind flux:

$$\phi_{jk} = \frac{1}{2}(\mathbf{F}_L + \mathbf{F}_R) \cdot \hat{\mathbf{n}}_{jk} - \frac{1}{2}|\lambda|(u_R - u_L), \tag{3}$$

where $\mathbf{F} = (f, g)$, $\hat{\mathbf{n}}_{jk}$ is the unit directed area vector, and $\lambda = (\partial_u f, \partial_u g) \cdot \hat{\mathbf{n}}_{jk}$. The left and right fluxes and states are obtained by the linear extrapolation from the nodes:

$$\mathbf{F}_L = \mathbf{F}_j + \frac{1}{2}(\nabla \mathbf{F})_j \cdot \Delta \mathbf{l}_{jk}, \qquad \mathbf{F}_R = \mathbf{F}_k - \frac{1}{2}(\nabla \mathbf{F})_k \cdot \Delta \mathbf{l}_{jk}, \tag{4}$$

$$u_L = u_j + \frac{1}{2}(\nabla u)_j \cdot \Delta \mathbf{l}_{jk}, \qquad u_R = u_k - \frac{1}{2}(\nabla u)_k \cdot \Delta \mathbf{l}_{jk}, \tag{5}$$

where $\Delta \mathbf{l}_{jk} = (x_k - x_j, y_k - y_j)$. The scheme is second-order accurate if the nodal gradients, $(\nabla \mathbf{F})_j$ and $(\nabla u)_j$, are first-order accurate. It is third-order accurate on arbitrary triangular grids if the nodal gradients are second-order accurate. This third-order scheme was introduced and named the corrected scheme in Refs. [3, 13]. The third-order accuracy is confirmed also in [14]. It is emphasized that the third-order accuracy is achieved only on triangular grids (tetrahedral grids in three dimensions). The second-order accurate gradients can be computed by the least-squares method with a quadratic fit. Note that the quadratic fit will generate the gradient as well as the second derivatives, but the second derivatives are not used in the corrected scheme. As pointed out in Refs. [3, 13], the source term must be carefully discretized to achieve the third-order accuracy.

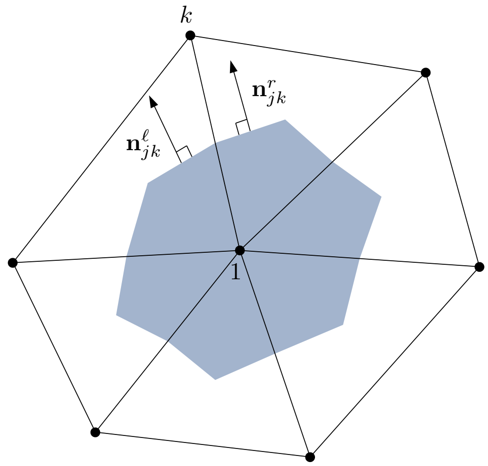


Figure 1: Dual control volume for node-centered finite-volume schemes with face normals associated with an edge, $\{j, k\}$.

3 Matching Truncation Error for Third-Order Accuracy

The truncation error of the edge-based scheme is obtained by substituting the exact solution into the right hand side of Equation (2). Without the source term ($s = 0$), the corrected scheme can be shown, by the Taylor expansion, to have the following truncation error on a regular symmetric stencil (e.g., see Figure 2(a)):

$$\mathcal{T}_j = C_1\,\partial_{xx}(\partial_x f + \partial_y g) + C_2\,\partial_{xy}(\partial_x f + \partial_y g) + C_3\,\partial_{yy}(\partial_x f + \partial_y g) + O(h^3), \tag{6}$$

where h is a typical mesh spacing, and the coefficients, C_1, C_2, and C_3, are geometrical constants of $O(h^2)$. These second-order error terms will vanish because $\partial_x f + \partial_y g = 0$ for the exact solution, and the truncation error is upgraded to third-order. Consequently, the discretization error is expected to be third-order. On the other hand, in order to achieve third-order accuracy for Equation (1) with $s \neq 0$, the source term must be discretized to produce the following truncation error:

$$\mathcal{T}_j = C_1\,\partial_{xx}(\partial_x f + \partial_y g - s) + C_2\,\partial_{xy}(\partial_x f + \partial_y g - s) + C_3\,\partial_{yy}(\partial_x f + \partial_y g - s) + O(h^3), \tag{7}$$

so that the second-order error terms will vanish for $\partial_x f + \partial_y g = s$. It is known that the one-point quadrature

$$\int_{\Omega_j} s\,dV = s_j V_j, \tag{8}$$

does not satisfy this requirement, and the Galerkin discretization,

$$\int_{\Omega_j} s\,dV = \sum_{k \in \{K_j\}} \frac{1}{2}(s_j + s_k) V_{jk}, \tag{9}$$

where $V_{jk} = \frac{1}{4}\Delta\mathbf{l}_{jk} \cdot \mathbf{n}_{jk}$, satisfies the requirement on a regular triangular grid of equilateral triangles [3]. For the regular grid as in Figure 2(a), the following edge-based discretization can be shown to satisfy the requirement:

$$\int_{\Omega_j} xs\,dV = \sum_{k \in \{K_j\}} \frac{1}{4}(5s_j - s_k) V_{jk}. \tag{10}$$

To achieve third-order accuracy on arbitrary triangular grids, an extended edge-based Galerkin source term discretization is proposed in [5]. In this paper, instead of proposing discretization schemes, we propose to rewrite the source term in the divergence form. Now that the whole equation is in the divergence form with virtually no source terms, the third-order accuracy can be achieved without any source-term discretization scheme such as above. The matching truncation error as in Equation (7) is no longer an issue. We emphasize that the central idea is to cast the source term in the divergence form and therefore it is generally applicable to virtually all discretization methods.

4 Divergence Formulation of Source Term

We propose to write Equation (1), locally around a node j, in the following divergence form:

$$\partial_x f + \partial_y g = \partial_x f^s + \partial_y g^s, \tag{11}$$

where

$$f^s = \frac{1}{2}(x - x_j)s - \frac{1}{4}(x - x_j)^2 \partial_x s + \frac{1}{12}(x - x_j)^3 \partial_{xx} s, \tag{12}$$

$$g^s = \frac{1}{2}(y - y_j)s - \frac{1}{4}(y - y_j)^2 \partial_y s + \frac{1}{12}(y - y_j)^3 \partial_{yy} s. \tag{13}$$

Then, the conservation law with the source term can be written as a single divergence form:

$$\partial_x \tilde{f} + \partial_y \tilde{g} = 0, \tag{14}$$

where $\tilde{f} = f - f^s$ and $\tilde{g} = g - g^s$. Note that the above equation is equivalent to

$$\partial_x f + \partial_y g = s + \frac{1}{12}(x - x_j)^3 \partial_{xxx} s + \frac{1}{12}(y - y_j)^3 \partial_{yyy} s. \tag{15}$$

The last two terms on the right hand side vanish precisely at the node j. Therefore, it is consistent with the target equation (1) at the node j. Also, they are $O(h^3)$ in the neighborhood of j, and will not affect the accuracy of the third-order scheme. In other words, the divergence form behaves like the original source term up to the truncation error order. Note that the divergence form of the source term is not a conservative form (as it should not be) because it is defined locally around each node. The divergence formulation of the source term (14) brings a dramatic simplification in the construction of the third-order corrected scheme. As it has virtually no source terms, it can be discretized by the third-order corrected scheme with no special source term discretization schemes. The accuracy of the third-order corrected scheme for equations with no source terms has already been demonstrated for regular and irregular triangular grids in [3, 13, 14]. We thus expect the same for the third-order corrected scheme applied to Equation (14). To construct the third-order scheme for Equation (1), therefore , we propose to discretize Equation (14) instead. The third-order corrected scheme for Equation (14) is then given by

$$0 = -\frac{1}{V_j} \sum_{k \in \{K_j\}} (\phi_{jk} + \psi_{jk}) A_{jk}. \tag{16}$$

We evaluate the source term flux, ψ_{jk}, by the central flux:

$$\psi_{jk} = \frac{1}{2}(\mathbf{F}^s_L + \mathbf{F}^s_R) \cdot \hat{\mathbf{n}}_{jk}, \tag{17}$$

where $\mathbf{F}^s = (f^s, g^s)$. The left and right fluxes are obtained by the linear extrapolation from the nodes:

$$\mathbf{F}^s_L = \mathbf{F}^s_j + \frac{1}{2}(\nabla \mathbf{F}^s)_j \cdot \Delta \mathbf{l}_{jk}, \qquad \mathbf{F}^s_R = \mathbf{F}^s_k - \frac{1}{2}(\nabla \mathbf{F}^s)_k \cdot \Delta \mathbf{l}_{jk}. \tag{18}$$

Note that the third derivatives of the source term that arise in the flux gradients, $(\nabla \mathbf{F}^s)_j$ and $(\nabla \mathbf{F}^s)_k$, are $O(h^3)$, and therefore can be ignored. The method requires the gradient as well as the second derivatives of the source term. They may be obtained analytically if possible, or numerically by the quadratic reconstruction used in the corrected scheme. Here, the second derivatives of the source term computed by the quadratic fit need to be stored. Note that the flux added to j does not necessarily balance with the flux added to k over the edge jk, i.e. $\psi_{jk} \neq -\psi_{kj}$. It means that the local discrete conservation does not hold for the source term and the source term is evaluated independently at each node as it should be.

5 One-Component Divergence Formulation

It is possible to formulate the divergence form by

$$f^s = (x - x_j)s - \frac{1}{2}(x - x_j)^2 \partial_x s + \frac{1}{6}(x - x_j)^3 \partial_{xx} s, \tag{19}$$

$$g^s = 0, \tag{20}$$

or

$$f^s = 0, \tag{21}$$

$$g^s = (y - y_j)s - \frac{1}{2}(y - y_j)^2 \partial_y s + \frac{1}{6}(y - y_j)^3 \partial_{yy} s. \tag{22}$$

In either case, third-order accuracy can be achieved. These formulations are more economical than the symmetric formulation in the previous section because only one flux component needs to be computed. Numerical experiments show that the results obtained by these fluxes are nearly identical to those obtained by the symmetric formulation for the problems tested in this study.

6 Exact Divergence Formulation

If the source term is simple enough, we can define the fluxes, (f^s, g^s), analytically. Consider the following equation:

$$\partial_x f + \partial_y g = \cos(x - y). \tag{23}$$

This equation can be written as

$$\partial_x f + \partial_y g = \partial_x f^s + \partial_y g^s, \tag{24}$$

where the source term fluxes may be defined as (the choice is not unique)

$$f^s = \sin(x - y), \quad g^s = 0. \tag{25}$$

By discretizing the divergence form (24), which is exactly equivalent to the original equation (23), by the corrected scheme with the central flux, we expect to achieve the third-order accuracy on arbitrary triangular grids. The flux gradients required in the corrected scheme may be computed by the quadratic fit, or can be computed analytically. In this approach, only the gradient of the fluxes are required; the second derivatives are not required.

Among many choices for the fluxes, there is a trivial choice. For example, for the linear advection equation,

$$\partial_x f + \partial_y g = (a - b)\cos(x - y), \tag{26}$$

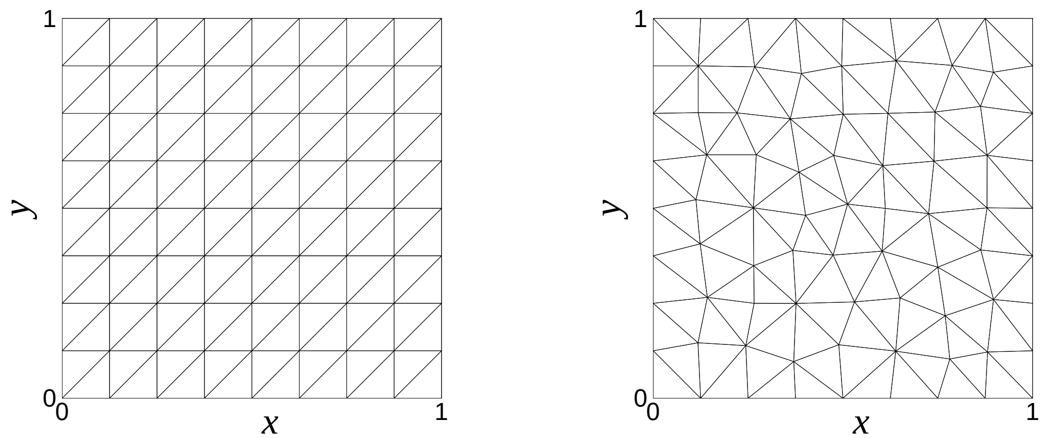
where $(f, g) = (au, bu)$, the following choice,

$$f^s = a\sin(x - y), \quad g^s = b\sin(x - y), \tag{27}$$

which is obtained by substituting the exact solution into (f, g), will make the flux source term discretization the truncation error. In this case, any numerical scheme will produce the exact solution.

7 Results

We present numerical results for linear and nonlinear problems on regular and irregular triangular grids with 9×9, 17×17, 33×33, 65×65, 129×129, and 257×257 nodes. The coarsest grids are shown in Figure 2. For all problems, we compute the numerical solution by marching in time with the two-stage TVD Runge-Kutta scheme [15] until the solution change becomes less than 10^{-12} in the L_1 norm. The initial solution is the exact solution with random perturbation. The quadratic fit for the gradient is performed with the nearest neighbors on the regular grids (with stencil extensions for the boundary nodes), and with 10 neighbors (including neighbors of neighbors) on the irregular grids. Note that five neighbors are typically sufficient for the quadratic fit, but the neighbors must be selected carefully to avoid ill-conditioning of the least-squares matrix. In this study, for the irregular grids, we avoid ill-conditioning simply by increasing the number of neighbors up to 10. It should be possible to make the third-order scheme nearly as compact as the second-order scheme by a more sophisticated selection of neighbors. The Dirichlet boundary condition is applied everywhere on the boundary for all problems.



(a) Regular grid

(b) Irregular grid

Figure 2: 9×9 *regular and irregular grids. The irregular grid is generated from the regular grid by random diagonal swapping and smoothing.*

7.1 Linear Advection

We consider the linear advection equation

$$\partial_x f + \partial_y g = (a - b)\cos(x - y), \tag{28}$$

where $(f, g) = (au, bu)$ and $(a, b) = (2.31, 1.12)$. The exact solution is given by

$$u(x, y) = \sin(x - y). \tag{29}$$

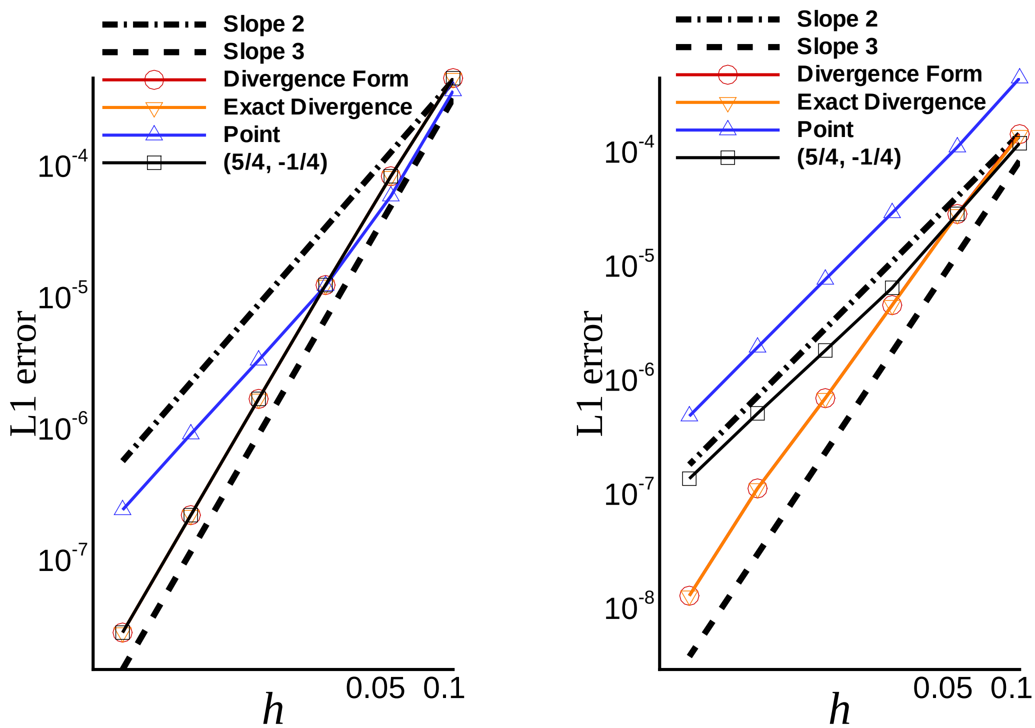
Error convergence results for the regular grids are shown in Figure 3(a). As expected, the solution is only second-order accurate with the point source discretization. The solution is third-order accurate with the discretization (10) indicated by $(5/4, -1/4)$ in the plot, the divergence formulation, and the exact divergence formulation with $f^s = (a-b)\sin(x-y)$ and $g^s = 0$. The third-order results are nearly identical. For the divergence formulation, the gradient and the second derivatives were obtained from the quadratic fit. Results for the irregular grids are shown in Figure 3(b). For the irregular grids, h is determined as the L_1 norm of the square root of the control volume. The solution is second-order accurate with the point source discretization as well as the discretization (10). On the other hand, the divergence formulation and the exact divergence formulation lead to third-order accuracy on irregular grids. Results obtained by the one-component divergence formulation described in Section 5 are almost identical to those of the divergence formulation (the results overlap one another), and therefore not plotted.

7.2 Burgers' Equation

We consider Burgers' equation:

$$\partial_x f + \partial_y g = \cos(x - y)\sin(x - y) - \cos(x - y), \tag{30}$$

where $(f, g) = (u^2/2, u)$. The exact solution is given by Equation (29). The numerical results are very similar to those for the linear problem. Error convergence results for the regular grids are shown in Figure 4(a). The solution is second-order accurate with the point source discretization. Third-order accuracy is obtained with the discretization (10), the divergence formulation, and the exact divergence formulation with $f^s = -\sin(x-y) + \frac{1}{2}\sin^2(x-y)$ and $g^s = 0$. The third-order results are almost identical. For the divergence formulation, again, the gradient and the second derivatives were obtained from the quadratic fit. Results for the irregular grids are shown in Figure 4(b). The solution is second-order accurate with the point source discretization and the discretization (10). The divergence formulation and the exact divergence formulation lead to third-order accuracy on irregular grids. Again, results obtained by the one-component divergence formulation described in Section 5 overlap with those of the divergence formulation, and therefore not plotted.



(a) Regular grids

(b) Irregular grids

Figure 3: *Error convergence results for the linear advection equation.*

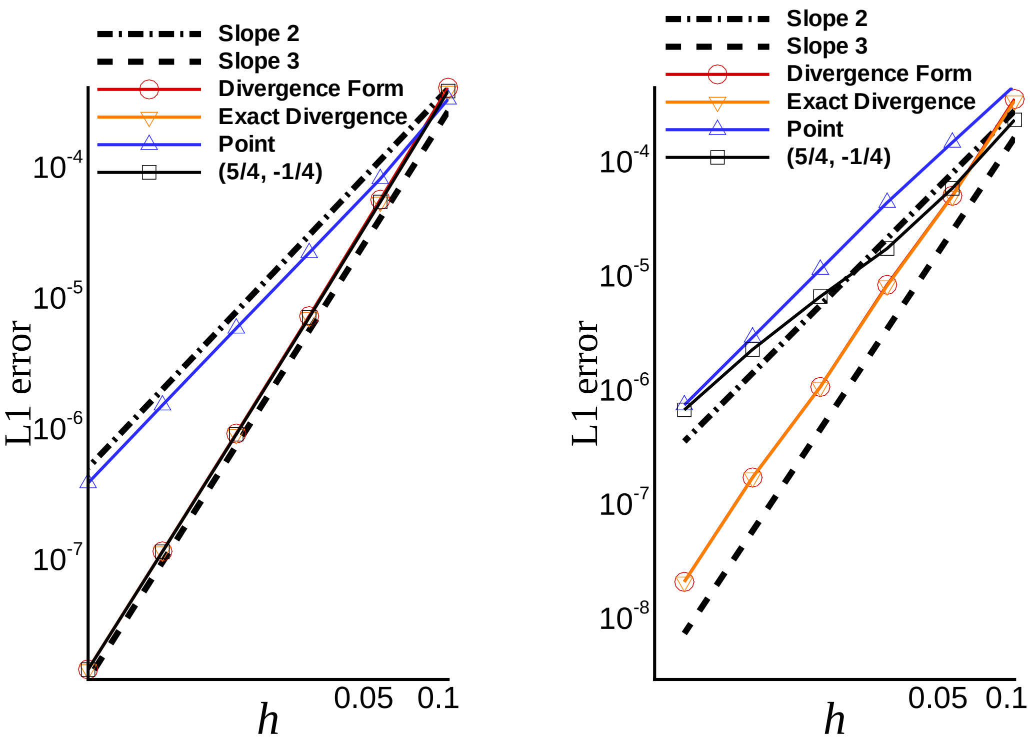
8 Concluding Remarks

We have introduced a general divergence formulation of source terms. It enables to write a conservation law with a source term in a single divergence form, and discretize the conservation law and the source term in the same numerical framework. Two divergence formulations have been proposed. One is to define the fluxes locally up to the truncation error, either by a symmetric formulation or one-component formulations. The other is to define the fluxes analytically by integrating the source term, which is possible if the source term is analytically integrable. In either case, the source term can be expressed in the divergence form, and can be discretized by the same numerical scheme used for the conservation law. We have shown that it greatly simplifies the construction of uniformly accurate schemes for the third-order finite-volume scheme as an example. Numerical results obtained for the linear advection and Burgers' equation confirmed third-order accuracy with the divergence formulations for arbitrary triangular grids.

For the third-order edge-based scheme, unless the exact divergence formulation is possible, the divergence formulation requires the second derivatives of the source term in addition to the gradient. They can be obtained directly from the least-squares gradient reconstruction by a quadratic fit. Note that the source term discretization can be performed in two steps: (1) the quadratic reconstruction of the source term, (2) the edge-based residual computation for the divergence form of the source term. If the quadratic reconstruction can be performed within a compact stencil, each step involves the nearest neighbors only. For time-accurate computations, the physical time derivative is discretized at each node and treated as a source term. Then, the divergence formulation can be applied to the physical time derivative for achieving third-order accuracy in time-accurate computations.

For first and second order schemes, the divergence formulation may not be required for preserving the accuracy, but can be employed if needed or if the unified discretization is desirable. In that case, the second-derivative terms in Equations (12) and (13) can be ignored for second-order schemes, which makes the error term in Equation (15) of second order. For first-order schemes, the first- and second-derivative terms in Equations (12) and (13) can be ignored, which makes the error term of first order.

For special differential systems, the divergence formulation will not require the gradient nor the second derivatives of the source term. For example, the divergence formulation can be designed to yield



(a) Regular grids (b) Irregular grids

Figure 4: *Error convergence results for Burgers' equation.*

a *hyperbolic* formulation of the source terms for the hyperbolic diffusion system [8]. The details on the application to the hyperbolic diffusion system will be reported elsewhere.

Finally, the core idea of the divergence formulation is to discretize the conservation law and the source term in the same numerical framework by unifying the form of the equation. Therefore, it is generally applicable to virtually all discretization methods.

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