Discrete Conservation Properties of Unstructured Mesh Schemes

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Abstract

Numerical methods with discrete conservation statements are useful because they cannot produce solutions that violate important physical constraints. A large number of numerical methods used in computational fluid dynamics (CFD) have either global or local conservation statements for some of the primary unknowns of the method. This review suggests that local conservation of primary unknowns often follows from global conservation of those quantities. Secondary conservation involves the conservation of derived quantities, such as kinetic energy, entropy, and vorticity, which are not directly unknowns of the numerical system. Secondary conservation can further improve physical fidelity of a numerical solution, but it is typically much harder to achieve. We consider current approaches to secondary conservation and techniques used outside of CFD that are potentially related. Finally, the review concludes with a discussion of how secondary conservation properties might be included automatically.

1. INTRODUCTION

Accuracy, stability, and consistency are the mathematical concepts that are typically used to analyze numerical methods for partial differential equations (PDEs). These important tools quantify how well the mathematics of a PDE is represented, but they fail to say anything about how well the physics of the system is represented by a particular numerical method. In practice, physical fidelity of a numerical solution can be just as important (perhaps even more important to a physicist) as these more traditional mathematical concepts. A numerical solution that violates the underlying physics (destroying mass or entropy, for example) is in many respects just as flawed as an unstable solution.

Unlike the issues of accuracy or instability, the violation of physical constraints by numerical methods tends to be a surreptitious problem that rarely causes outright failure of the method. As a result, physically incorrect numerical solutions can potentially go unnoticed. As numerical methods are applied to ever more complex physical systems such as magnetohydrodynamics, multiphase flows, hypersonics, or chemically reactive flows, the issue of the physical fidelity of numerical methods becomes ever more pressing. Relying on humans to catch the physical inconsistencies in numerical solutions to complex physical problems is becoming increasingly difficult. If possible, it is better to address the issue of physical fidelity at the numerical method design level. In fluid dynamics the physics of the system is often discussed in terms of conservation laws, and as a result discrete conservation laws are the focus of this review.

Section 2 starts with a review of global and local discrete conservation statements for primary variables (often mass, momentum, and total energy). Although finite-volume and discontinuous Galerkin methods are explicitly constructed to have local discrete conservation statements for the primary variables, the review highlights that many other numerical methods also have local discrete conservation statements for the primary solution variables, although the derivation is less obvious.

Far fewer numerical methods have discrete conservation statements for secondary or derived quantities. However, there is mounting evidence that secondary conservation significantly enhances the quality of numerical solutions. Entropy conservation is important in compressible flow situations. The classic carbuncle phenomena in shock simulations can be traced to entropy violation (Ismail et al. 2006). Kinetic energy conservation is important for large-eddy and direct numerical simulations of turbulent flows. Mittal & Moin (1997) show that kinetic energy conservation is critical for the turbulent energy cascade to be represented correctly. Vorticity conservation is important in turbulence (Zhang et al. 2001) and shallow-water simulations (Frank & Reich 2003). Dilatation conservation may be advantageous in acoustics simulations and in incompressible flow simulation (Chang et al. 2002). Section 3 discusses various approaches to obtaining secondary conservation statements.

It should be noted that there are other ways than discrete conservation statements to numerically quantify physical fidelity. Section 4 highlights some other possible approaches to capturing physics accurately when numerically solving PDEs. Recent work, discussed in Section 5, suggests that it may be possible to construct numerical methods so that secondary conservation statements are automatically achieved. This analysis suggests that secondary conservation properties are not directly related to any particular discretization method, but are more closely related to how the problem is formulated. As shown in **Figure 1**, it appears that most major discretization approaches have a certain subset of that approach, which possesses additional conservation properties.

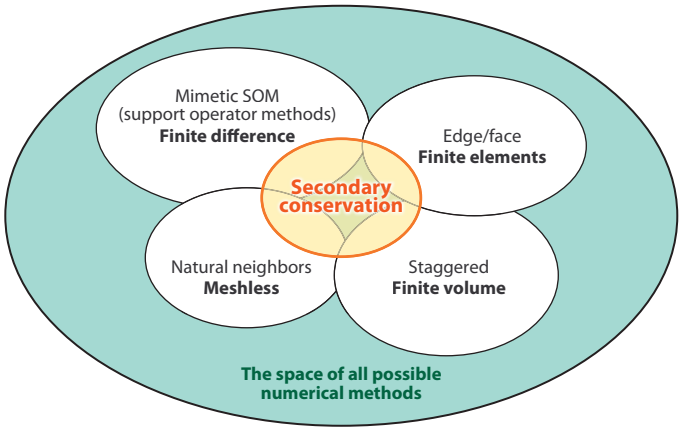

Figure 1

Secondary conservation properties are found in a subset of most discretization approaches. This Venn diagram is demonstrative and not a complete list of all possible CFD approaches.

2. CONSERVATION OF PRIMARY UNKNOWNS

2.1. Flux-Based Methods

Both finite-volume and discontinuous Galerkin finite-element methods use the idea of fluxes to ensure conservation of the mass density ρ, momentum density $\rho\mathbf{u}$, and (often) the total energy density ρe. In these methods, the Gauss divergence theorem is used to convert the divergence terms in the PDE into a sum of boundary fluxes (Mavriplis 1997). These types of methods locally conserve primary quantities irrespective of the approximation used for the fluxes. Any quantity leaving one subdomain must enter another subdomain or cross the global domain boundary.

One interesting extension of flux-based methods is that they can still maintain conservation properties even when the subdomains move and distort with time (Perot & Nallapati 2003). An example is shown in **Figure 2**. This type of formulation avoids the ALE (arbitrary Lagrangian-Eulerian) step of remapping the solution onto a new mesh at each time step. For example, the mass equation, $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$, on a moving subdomain Ω_i is

$$\frac{d}{dt}\left[\int_{\Omega_i(t)} w\rho d\mathbf{V}\right] + \int_{\partial\Omega_i(t)} w\rho(\mathbf{u}-\mathbf{u}_\Omega)\cdot\mathbf{n}dA = \int_{\Omega_i(t)} \rho\left[\frac{\partial w}{\partial t} + (\mathbf{u}-\mathbf{u}_\Omega)\cdot\nabla w\right]d\mathbf{V}, \qquad (1)$$

where $\mathbf{u}_\Omega$ is the speed at which the points in the subdomain Ω_i are moving, and w is the weighting function. When $w = 1$ in each moving subdomain (the finite-volume approach), the right-hand side of Equation 1 is zero, and conservation on a moving mesh is recovered. But conservation also occurs when the weight function is time independent and the mesh motion is Lagrangian ($\mathbf{u} = \mathbf{u}_\Omega$), or when a fixed mesh ($\mathbf{u}_\Omega = 0$) and a passive scalar (Lagrangian) weight function are used.

Global conservation: when the time rate of change of a quantity integrated over the entire domain is directly equal to the sum of the fluxes across the domain boundary

Local conservation: when the time rate of change of a quantity in a small region is directly equal to the sum of locally (pairwise) constructed fluxes, and the parity of those (pairwise) fluxes changes sign depending on the flux orientation

2.2. Partition-of-Unity Methods

Many numerical methods are known to be globally conservative (for the whole domain) but do not have an obvious local flux interpretation as described above and therefore are often considered not to be locally conservative. For example, it is often stated that classic Galerkin finite elements are globally conservative, but it is rarely asserted that they are locally conservative. However, with some additional analysis, it can be shown that local conservation statements are actually present for

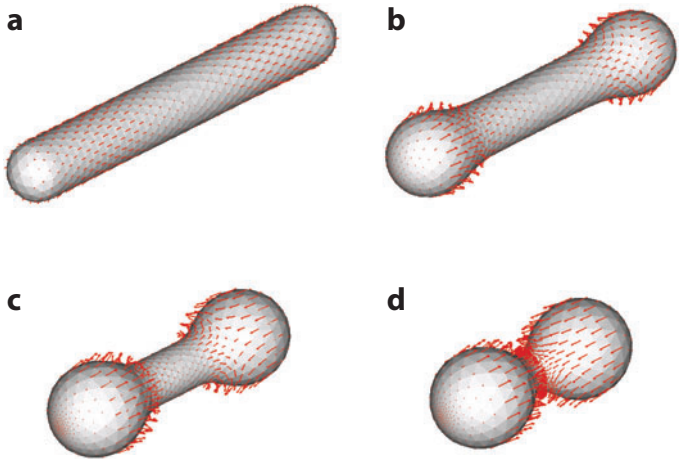

Figure 2

Calculation of droplet necking using conservative moving control volumes. Figure taken from Dai et al. (2002).

Galerkin finite-element methods (Oshima et al. 1998). A landmark paper by Hughes et al. (2000) explains in detail how Galerkin methods are locally conservative. Because the result is important, we reproduce it here using a completely different and slightly more general approach that only assumes the weight functions in the method are local and form a partition of unity.

In many numerical methods (including finite-element methods), a PDE is enforced in a weighted (or weak) sense. Integrating over the entire domain (rather than a subdomain as in Equation 1), the weak form of the mass equation becomes

$$\frac{d}{dt}\left[\int_\Omega w^i \rho d\mathbf{V}\right] + \int_{\partial\Omega} w^i \rho \mathbf{u}\cdot\mathbf{n} dA - \int_\Omega \rho \frac{Dw^i}{Dt} d\mathbf{V} = 0, \tag{2}$$

where w^i is the weight function for some location i, and $\frac{Dw^i}{Dt} = \frac{\partial w^i}{\partial t} + \mathbf{u}\cdot\nabla w^i$ is the total derivative of the weight function (which can be time dependent). For simplicity, we consider a compact weight function that is far from the boundary of the domain so that the second term in Equation 2 is zero. The last term does not look like a sum over boundary fluxes. Moreover, the various weight functions typically overlap, making it difficult to identify a definitive boundary (or flux) from one conservation region to another. Local conservation is therefore not immediately obvious.

However, if the weight functions are a partition of unity, then local conservation is still obtained. A weight function that is a partition of unity can always be written as $w^i = \frac{\phi^i}{\sum_k \phi^k}$, where $\phi^i(\mathbf{x}, t)$ is some function of space and time. Using this form for the weight function, the third term in Equation 2 becomes

$$\sum_j \int_\Omega \rho \frac{\left[\frac{D\phi^i}{Dt}\phi^j - \phi^i \frac{D\phi^j}{Dt}\right]}{\left(\sum_k \phi^k\right)^2} d\mathbf{V} = \sum_j \int_\Omega \rho \left[\frac{Dw^i}{Dt} w^j - w^i \frac{Dw^j}{Dt}\right] d\mathbf{V}. \tag{3}$$

The summation is over the whole domain, but if the partitions have local support, then the integral is nonzero only for the neighbors of w^i (where other partitions overlap with w^i). Note that each integral depends only on two weight functions, and it is antisymmetric in the i and j indices. Each integral is therefore essentially a flux into one partition and out of another. Because the support

is local, these fluxes are local, and this really is a local conservation statement. For the common case of time-independent weight functions, ($w^i = w^i(\mathbf{x})$), the flux between cell i and cell j in the last term in Equation 3 becomes $\int_\Omega \rho \mathbf{u} \cdot [(\nabla w^i) w^j - w^i (\nabla w^j)]\, d\mathbf{V}$. If this distributed flux integral is computed or approximated the same way for both cell i and for cell j, then the method is locally conservative. The quantity $[(\nabla w^i) w^j - w^i (\nabla w^j)] d\mathbf{V}$ acts like a distributed (or smeared) area.

The fluxes in partition-of-unity methods are volume integrals rather than area integrals because these methods can be thought of as an average over a set of finite-volume methods that differ only in how the control volume boundaries are defined. A partition-of-unity method can be thought of as the average of a single finite-volume method computed on a spectrum of different finite-volume meshes that have the same cell centers but different face (or flux) locations. Mattiussi (1997, 2000) discusses in detail this interpretation of finite-element methods as a weighted average of a finite-volume method over many different meshes. The arguments used here for the mass equation also hold for the momentum and total energy equations. The conservative pressure and stress terms are just like the advection term and also result in distributed local fluxes occurring between each pair of neighbors.

A large number of numerical methods (not just classic finite-element methods) use a partition of unity in their construction. Finite-volume and discontinuous Galerkin methods use a simple partition of unity with weight functions being one in a subdomain and zero outside that subdomain. Piecewise linear functions on simplices (triangles or tetrahedra) also easily form a partition of unity. Many meshless or particle methods use a partition of unity based on radial basis functions. When radial basis functions are used, the weight function becomes a rational polynomial, and the flux is difficult to integrate exactly. However, local conservation of the primary quantities still occurs as long as the integral approximation is consistently computed for each neighboring unknown.

This somewhat expanded definition of local conservation (to include distributed fluxes) implies that any method that is globally conservative, and that has weight functions with local support, must also be locally conservative. This is because it is not possible to obtain global conservation (total cancellation in the interior of the domain) from a method with a small (local) stencil unless the various local contributions cancel out internally when the local equations are summed together. These local cancellations can then invariably be identified with local fluxes.

2.3. Staggered Mesh Methods

Staggered mesh methods distribute pressure and velocity components to different locations on a mesh. They were first introduced by Harlow & Welch (1965) for Cartesian meshes. The method was generalized to mapped Cartesian meshes by Wesseling et al. (1992) and later to unstructured meshes by Hall et al. (1985, 1991) and Nicolaides (1993). Generalizations from Voronoi meshes to general (median dual) meshes were proposed by Perot & Nallapati (2003). Unstructured mesh versions of the method have proven versatile and have been applied to a wide variety of flow situations (Dai et al. 2002, Perot & Gadebusch 2007, Martell et al. 2009).

Staggered mesh methods are notable in this work because it was discovered early on by Lilly (1965) that they have secondary conservation properties, which are discussed extensively in Section 3. On Cartesian meshes, staggered mesh methods can enforce local conservation of the primary variables by staggering control volumes. However, this approach of shifting control volumes is only possible when the mesh is Cartesian. It is difficult to show that unstructured staggered mesh methods conserve momentum. For unstructured staggered mesh methods, the face normal velocity component is the primary variable. The velocity vector itself (or the momentum vector) is not directly defined. Local conservation is proved on unstructured staggered mesh systems by showing that certain combinations of the discrete equations result in discrete statements of

momentum conservation within each mass control volume (Perot & Zhang 1999). Additional details and the proof for local conservation are found in Zhang et al. (2001).

As with all secondary conservation statements, the correct discrete representation for the derived quantity (momentum in this case) is as important as the discrete conservation statement itself. Any arbitrary interpolation for the momentum (from the unknown normal velocity, U_f, on the faces) will probably not be conserved. So far it has only been shown that the discrete momentum defined by $\int \mathbf{u} dV \approx \sum(\mathbf{x}_f^{CG} - \mathbf{x}_c)U_f$, where $\mathbf{x}_f^{CG}$ is the face center of gravity, is a locally conserved quantity for unstructured staggered mesh methods.

Higher-order staggered mesh methods that are conservative can be formulated two different ways. On Cartesian meshes, Richardson extrapolation is frequently used (Verstappen & Veldman 1996, Morinishi et al. 1998, Vasilyev 2000). The lowest-order discrete equations are formulated on the fine mesh, and on a coarser mesh consisting of every other mesh point. These two systems are then combined with the appropriate weights that remove additional truncation error terms. Because each method is locally conservative, a weighted average of the two methods is also conservative. Richardson extrapolation is difficult (possibly impossible) to apply to an unstructured mesh method. Higher-order unstructured staggered mesh methods are discussed by Subramanian & Perot (2007), who use more unknowns per cell to achieve higher-order interpolation. This approach to higher order is reminiscent of the discontinuous Galerkin approach to higher order, but unlike the discontinuous Galerkin approach (and similar to a finite-volume method), basis functions are implicit and the interpolation procedure is explicit. The higher-order unstructured staggered mesh methods of Subramanian & Perot use interpolation assumptions that are nearly identical to face elements that are used extensively in numerical methods for Maxwell's equations in electromagnetism. The connection between unstructured staggered mesh methods and these remarkable finite-element methods is further discussed in Section 4.

2.4. Other Approaches

Many other methods used in computational fluid dynamics (CFD) are provably globally conservative and are often also locally conservative. Particle methods typically conserve mass by construction and often conserve momentum. Particle exchange arguments are used to prove conservation of momentum in smooth particle hydrodynamics (SPH) methods. However, we note that the most popular corrections to SPH methods that improve their consistency also destroy momentum conservation (Vaughan et al. 2008). Some SPH and particle methods can be given a Hamiltonian structure. If symplectic time integrators are used, then a discrete approximation for the energy can be conserved by these methods.

Lattice Boltzmann methods conserve mass and momentum by construction, but conservation of energy typically requires at least two lattice speeds (McNamara et al. 1997). Two-speed implementations require careful construction to retain stability. The large number of different numerical methods developed for CFD over the past decades makes it impossible for us to discuss primary conservation in all possible methods here.

3. SECONDARY CONSERVATION STATEMENTS

Secondary conservation properties are an indirect indication that a numerical method is well formulated to capture the physics of the system. Unlike primary conservation, secondary conservation statements cannot be directly imposed during the construction of the numerical method. There is also some indication that secondary conservation leads often (but not always) to enhanced accuracy. This is shown in **Figure 3** for two different kinetic energy–conserving schemes

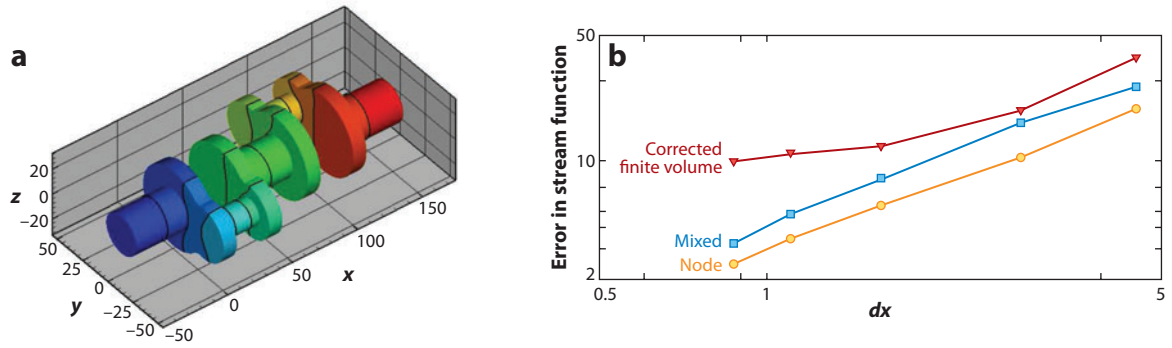

Figure 3

Comparison of kinetic energy–conserving schemes and a classic finite-volume method on an unstructured tetrahedral mesh: (*a*) solution domain and (*b*) discrete L2 error versus average mesh size. Further details can be found in Perot & Subramanian (2007b).

and a classic finite-volume method. This figure shows a computation of Darcy flow (porous media flow) through a complex conduit. **Figure 3*a*** shows the computational domain used and pressure contours, and **Figure 3*b*** shows there is roughly an order-of-magnitude improvement in the L2 stream-function error for most of the energy-conserving schemes.

There are a number of approaches to obtaining secondary conservation statements. Each approach tends to focus on a particular secondary quantity. Some of the more common secondary conservation statements that are useful in CFD are discussed below.

3.1. Kinetic Energy

Discrete kinetic energy conservation is important in direct numerical and large-eddy simulations of incompressible turbulence. This is discussed by Moin & Mahesh (1998) for finite-volume and staggered mesh methods. Benhamadouche & Laurence (2002) come to the same conclusion using finite-element methods. The energy cascade is a critical physical process in turbulence simulations. Even in compressible turbulence simulations it has been observed that discrete kinetic energy conservation of the nonlinear advection terms significantly enhances the accuracy of the simulation (Subbareddy & Candler 2009). The kinetic energy equation is

$$\frac{\partial\left(\frac{\rho}{2}\mathbf{u}^2\right)}{\partial t}+\nabla\cdot\left(\frac{\rho}{2}\mathbf{u}^2\mathbf{u}\right)=-\nabla\cdot(\mathbf{u}p)+\nabla\cdot(\mathbf{u}\sigma)+p(\nabla\cdot\mathbf{u})-\sigma:\nabla\mathbf{u}. \tag{4}$$

The final term (the dissipation) is negative definite and proportional to the viscosity. The penultimate source term is zero for incompressible flow. In the limit of inviscid incompressible flow, the kinetic energy is an exactly conserved quantity. Practically, in the limit of high–Reynolds number incompressible flow (turbulence), the dissipation term is extremely small and the kinetic energy is very nearly conserved. Artificial dissipation, if it exists, is a problem because it is likely to completely overwhelm the small physical dissipation.

Kinetic energy conservation can usually be achieved by using a discrete approximation for the skew-symmetric form of the advection term (Feiereisen et al. 1981). For incompressible flow, the conservative (or divergence) form of the momentum advection term is $\nabla\cdot(\mathbf{uu})$, the advective form is $\mathbf{u}\cdot(\nabla\mathbf{u})$, and the skew-symmetric form of the equations is one-half of each, $\frac{1}{2}\nabla\cdot(\mathbf{uu})+\frac{1}{2}\mathbf{u}\cdot(\nabla\mathbf{u})$. Analytically these forms are identical when $\nabla\cdot\mathbf{u}=0$, but their numerical implementations may behave differently. Multiplying the discrete skew-symmetric form by the discrete velocity and

using a discrete chain rule produces the discrete conservative form of the kinetic energy advection term, which looks like a discrete version of $\nabla \cdot (\mathbf{u}\frac{1}{2}\mathbf{u}^2)$. On Cartesian meshes, discrete chain rules are available for both staggered and collocated meshes (Strand 1994). On unstructured meshes, discrete chain rules can be found for staggered mesh methods and are explicitly imposed for mimetic methods (described in Section 4).

We note that the skew-symmetric form of the advection terms typically does not conserve momentum, so one conservation property has often been traded for another in this approach. In addition, the advection term is quite important, but is not the only piece of the kinetic energy conservation equation. True kinetic energy conservation also requires that the pressure and stress terms behave conservatively (Felten & Lund 2006).

The idea of using skew symmetry for kinetic energy conservation has been generalized a number of different ways. For Cartesian mesh compressible flows, Morinishi (2010) discusses 16 possible skew-symmetric forms for the advection term and their respective conservation properties. Other works concerning kinetic energy conservation in compressible flows include Honein & Moin (2004) and Subbareddy & Chandler (2009), and references therein. Mahesh et al. (2004) discuss a large-eddy-simulation implementation that conserves kinetic energy using collocated variables, which has been highly imitated.

Staggered mesh methods are interesting because they can conserve both momentum and kinetic energy. The proof on Cartesian meshes was provided by Lilly (1965) early in the development of these methods. The extension to unstructured meshes is detailed in Perot (2000) for two dimensions and Zhang et al. (2001) for three dimensions. These papers show that kinetic energy conservation is possible for both the divergence form of the advection term (which conserves momentum) and the rotational form, $\boldsymbol{\omega} \times \mathbf{u} + \nabla(\frac{1}{2}\mathbf{u}^2)$, of the advection term (which conserves vorticity). The advection term in the derived discrete kinetic energy equation becomes $\sum_{cells} \boldsymbol{D} U_f (\frac{1}{2}\mathbf{u}_{c1}^{n+1/2} \cdot \mathbf{u}_{c2}^{n+1/2})$ if the momentum advection flux uses a central (one-half) weighting of the two neighboring cells, such as $F_f = U_f \frac{1}{2}(\mathbf{u}_{c1}^{n+1/2} + \mathbf{u}_{c2}^{n+1/2})$. This kinetic energy flux is not exactly intuitive. Whereas the momentum flux uses a simple average of the velocity in the two neighboring cells, the kinetic energy does not use a simple average of the cell kinetic energy. It uses a face kinetic energy value that is really only defined for that face. Note that within the unstructured staggered mesh framework, strict kinetic energy conservation imposes a constraint on both the time-advancement scheme (trapezoidal) and the momentum flux (simple average). The trapezoidal method is a low-order example of a symplectic time-marching scheme. It is likely that other symplectic time-advancement schemes might also conserve kinetic energy. With regard to the issue of secondary conservation, prior investigators have focused almost exclusively on the spatial discretization scheme. However, unstructured staggered mesh schemes and multisymplectic methods (discussed in Section 4) indicate that time advancement is also an important issue. Classical stabilized time-advancement schemes such as Runge-Kutta or Adams-Bashforth methods will always add some artificial dissipation to the system. This can be advantageous in certain situations because kinetic energy–conserving methods can display aliasing issues in a numerical method that is poorly resolved spatially. If the physical (or turbulence model) dissipation is not sufficient due to numerical resolution issues, the method does not add artificial dissipation to the system, and the solution will look noisy without some form of stabilization.

3.2. Entropy

Entropy conservation and creation are significant concerns in compressible flow calculations (Thornber et al. 2008). The transport equation for the entropy (assuming Fourier heat

conduction) is

$$\frac{\partial(\rho s)}{\partial t} + \nabla \cdot (\rho s) = \frac{1}{T}\sigma : \nabla \mathbf{u} + \nabla \cdot (k \nabla \ln T) + k \frac{\nabla T}{T} \cdot \frac{\nabla T}{T}. \quad (5)$$

This equation states that entropy is conserved, except when it is generated by positive definite source terms that depend on molecular processes (proportional to viscosity and conductivity). If mass, momentum, and energy are the primary transport quantities in a numerical simulation, then the discrete entropy is a derived quantity that is determined via a table or an equation of state. Entropy conservation is difficult to enforce because Equation 5 is not discretized. However, if a discrete form of Equation 5 can be derived from the primary transport equations, then the numerical solutions cannot violate the second law of thermodynamics.

The solution to entropy conservation is not as simple as adding a discrete entropy transport equation to the numerical system. This just results in the equation of state being violated. Some methods replace the discrete energy equation with a discrete entropy equation. This conserves entropy, but the problem has simply been shifted to the first law of thermodynamics—the total energy is no longer discretely conserved. Wenneker et al. (2003) address the trade-offs of using the entropy equation instead of the total or the internal energy equations in the discrete system.

Entropy variables are a set of variables that symmetrize the coupling in the Navier-Stokes equations between the primary variables (Harten 1983). Entropy variables are derived from an entropy function that is not necessarily the physical entropy. Tadmor (1984) then showed that this transformation can be extended to make the equation system skew-self-adjoint. In this form, the equations discretely conserve total energy as well as entropy. Hughes et al. (1986) use this idea in the finite-element context. Jameson (2008) uses this approach to develop an entropy-conserving finite-volume scheme.

The use of entropy variables is similar to the use of skew symmetry in the advection term to obtain kinetic energy conservation. It is also related to the idea of Hamiltonian PDEs (or multi-symplectic PDEs), which are addressed in the next section. Hamiltonian systems also rely heavily on skew symmetry. Although the entropy is conserved in this approach, mass and momentum may no longer be. When transformed in this way, the primary variables of the discretization are entropy variables, so it is not always clear that mass and momentum are still discretely locally conserved quantities.

Serrano & Espanol (2001) describe an interesting particle method that uses a dynamical Voronoi Lagrangian mesh. This method uses a discrete entropy transport equation. However, total energy (which is obtained from an equation of state) is shown to be discretely conserved when a near-zero term is added to the flux in the momentum equation. This extra term is a discrete form of the Gibbs-Duhem equality ($dP - s dT = 0$), which is not satisfied discretely. The resulting method discretely conserves mass, momentum, entropy, and total energy.

3.3. Vorticity

The evolution equation for the vorticity in an incompressible constant viscosity flow is

$$\frac{\partial \boldsymbol{\omega}}{\partial t} + \nabla \times (\boldsymbol{\omega} \times \mathbf{u}) = \nabla \cdot \nu \nabla \boldsymbol{\omega}. \quad (6)$$

Because of the curl, this equation is often not immediately recognized as a conservation statement. Integrating the equation over a control volume makes the conservation clearer because the advection (second) term becomes two flux terms, $\int_{\partial\Omega} \boldsymbol{\omega}\mathbf{u} \cdot \mathbf{n} dA$ and $\int_{\partial\Omega} \mathbf{u}\boldsymbol{\omega} \cdot \mathbf{n} dA$. The second flux term happens to be zero in two dimensions. Therefore, vorticity (sometimes called circulation) is also a locally conserved quantity even in three dimensions. In a two-dimensional (2D) incompressible

inviscid flow, all the moments of the vorticity are also conserved quantities because vorticity is then just a passive scalar. The vorticity equation has some similarity with Maxwell's equations for electromagnetism as those equations are also more simply written in terms of curls rather than divergences.

Vorticity is a critical physical quantity in turbulent flows, which are governed by vortex stretching, and in very low–Reynolds number flows (the Stokes flow regime). When the momentum advection term is written in rotational form, $\boldsymbol{\omega} \times \mathbf{u} + \nabla(\frac{1}{2}\mathbf{u}^2)$, unstructured staggered mesh methods have been shown to conserve vorticity as well as kinetic energy (Perot 2000). However, this form of unstructured staggered mesh methods has not been proven to conserve momentum. On a Cartesian mesh, the rotational form of the advection term can be shown to be equivalent to the divergence form, and the staggered mesh method has been shown to locally conserve momentum, kinetic energy, and vorticity (Lilly 1965). Frank & Reich (2003) show that certain SPH methods conserve vorticity in the shallow-water equations. This is an example of a 2D, incompressible, inviscid limit in which vorticity is a passive scalar.

4. OTHER PHYSICS-CAPTURING METHODS

Other fields in science and engineering have discovered completely different approaches to capturing PDE physics within a numerical method. These fields have different and potentially useful analysis methods that are worth mentioning within this review. Further developments in CFD conservation might use at least one of these ideas.

4.1. Face and Edge Elements

Face and edge elements are the generic name often applied to 2D Raviart-Thomas (Raviart & Thomas 1977) and 3D Nedelec (1980) finite elements. When used on simplices (triangles, tetrahedra, and their higher-dimensional analogs), these elements are also known as Whitney (1957) elements. These elements are also closely related to a series of 3D incompressible elements derived by Griffiths (1981). Edge and face elements are widely used for numerical solutions in electromagnetics (Maxwell's equations) to represent electric and magnetic vector fields and their evolution (see White 1998, Rodrigue & White 2001, and references therein). Edge and face elements recognize that vector quantities (such as velocity and vorticity in the CFD case) need to be treated fundamentally differently than simple scalar or cell-averaged scalar unknowns. These methods always represent vectors in terms of distributed vector components (somewhat like the staggered mesh representation). **Figure 4** shows an example of a low-order face element basis function. These elements are useful for enforcing the divergence constraint $\nabla \cdot \mathbf{B} = 0$ on the magnetic field. We note that staggered mesh methods were largely developed to enforce $\nabla \cdot \mathbf{u} = 0$ and that face elements and unstructured staggered mesh methods have many similarities.

The remarkable properties of edge and face elements are typically discussed in the terminology of algebraic topology. This is a field of mathematics developed to discuss calculus in a dimension-independent way. The relation of these elements (and their scalar counterparts) to algebraic topology concepts such as Whitney (1957) forms and the de Rham (1931) complex is well documented (Bossavit & Mayergoyz 1989, Hiptmair 2001). Although the theoretical concepts of algebraic topology do not generalize well to the nonlinear (advection) terms in the Navier-Stokes equations, the elements themselves can of course still be used.

The practical utility of face and edge elements can be more convincing than the advanced mathematics. **Figure 5** reproduces results from Costabel & Dauge (2003). This figure shows the resonant modes in an electromagnetic waveguide computed with a standard Lagrangian polynomial finite-element method (**Figure 5*a***) and those computed with Raviart-Thomas elements

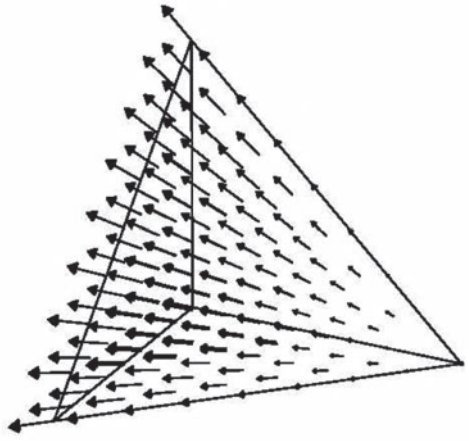

Figure 4

The basis function for the lowest-order Nedelec face element on a tetrahedron. The normal velocity component is constant on one face and zero on the others.

(**Figure 5*b***). The Raviart-Thomas modes are not exact, but they are very close and have been shown to converge exponentially (Coyle & Ledger 2003). Similar problems arise in fluid dynamics in acoustics. The continuous spectrum produced by the classic finite-element method is not physically correct. In particular, the classic finite-element method misses the first 193 zero modes that result from the divergence-free constraint on the magnetic field.

The basis functions used in unstructured staggered mesh methods are equivalent to using the lowest-order face element reconstruction. Higher-order unstructured staggered mesh methods also use the same unknowns as higher-order face elements for the case of simplictical elements. On Cartesian meshes, the higher-order reconstructions can differ slightly from face elements.

Even though the reconstruction/interpolation is often the same, staggered mesh methods and face elements are not the same numerical method because the weight functions used to discretize

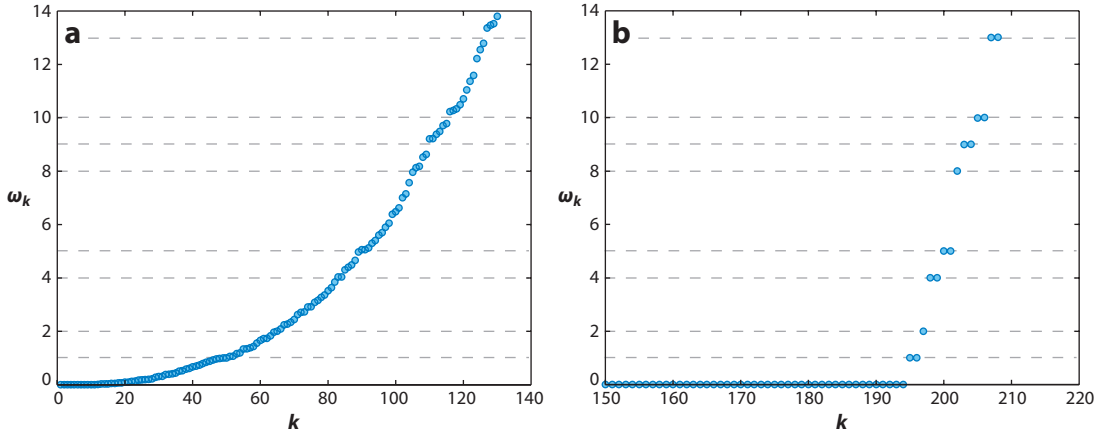

Figure 5

Eigenfrequency versus rank *k* for a waveguide from Costabel & Dauge (2003), with numerical results from Boffi et al. (1999). Horizontal gray lines are the exact modes that resonate. (*a*) A standard 15-point triangle element. (*b*) A 15-point Raviart-Thomas element.

the equations are different. In the development of methods that capture physics well, it appears that the weighting of the equations (e.g., finite element, finite volume, finite difference, particle) is far less important than the underlying interpolation assumptions (basis functions).

4.2. Multisymplectic Schemes

Keller (1971) box schemes and Preissman (1961) box schemes are an entirely different type of numerical method. In these methods the space and time discretization are intimately coupled. They were popularized for the solution of the boundary layer equations by Cebeci et al. (1980) and Bradshaw et al. (1981). More recently, these methods have become popular for solving complex wave equations such as the Korteweg de Vries equation (Ascher & McLachlan 2005). It has been shown that these methods always propagate waves in the correct direction (Frank 2006). In this sense, their dispersion relations, while containing some errors related to the mesh spacing, are at least never physically unrealistic. This is not true of many classic methods for solving wave equations. Furthermore, the Keller box scheme was shown by Frank et al. (2006) to be multisymplectic, which is the PDE equivalent of a symplectic time-marching scheme for an ordinary differential equation (ODE) (Bridges & Reich 2001). Box schemes have been applied to the Euler equations by Chattot (1999) and to convection-diffusion equations by Croisille & Greff (2005).

Like many particle methods, the analysis of box schemes focuses on the Hamiltonian (rather than a Newtonian) representation of the dynamics/physics. Symplectic integrators are loosely related to variational integration methods for ODEs, which use the slightly different discrete Lagrangian (rather than a discrete Hamiltonian) to derive the discrete equation system.

Multisymplectic schemes are applied to PDEs, which have a Hamiltonian representation (symplectic schemes are for Hamiltonian ODEs). The discrete Hamiltonian can very often be associated with the total energy of the system, and therefore the energy is typically conserved by box methods. This implies that at least one secondary conservation property (conservation of energy) is present and may imply that primary conservation (such as conservation of mass and momentum) is present as well because a discrete Hamiltonian structure to the discrete equations is likely to produce the necessary symmetries for additional conservation properties. Entropy is always conserved in a Hamiltonian system.

Recent work (Perot & Subramanian 2007a) shows that the Keller box schemes are loosely related to unstructured staggered mesh methods and discrete calculus methods (presented in Section 5). A multisymplectic partial differential equation (Hamiltonian PDE) has the form $\mathbf{K}\frac{\partial \mathbf{u}}{\partial t} + \mathbf{L}\frac{\partial \mathbf{u}}{\partial x} = \nabla_{\mathbf{u}} H(\mathbf{u})$, where $\mathbf{K}$ and $\mathbf{L}$ are skew-symmetric constant matrices. This suggests a close connection between this approach and the skew-self-adjoint approach Tadmor (1984) used in CFD.

4.3. Mimetic Schemes

Mimetic schemes or support operator methods (Shashkov & Steinberg 1995, Hyman & Shashkov 1999) attempt to construct discrete differential operators (e.g., for the gradient, divergence) that satisfy the properties of the continuous differential operators. In particular, a discrete integration by parts statement is sought. The discrete operators should obey a discrete property that is equivalent to

$$\int_{\Omega} w \nabla \cdot \mathbf{u} dV = -\int_{\Omega} \mathbf{u} \cdot \nabla w dV + \int_{\partial\Omega} w \mathbf{u} \cdot \mathbf{n} dA. \tag{7}$$

One of the discrete operators in the pair (gradient or divergence) is usually defined by the discrete integration by parts statement. Having this discrete property allows the methods to display

attractive properties. The approach has been used extensively for the heat equation and Darcy flow. These methods can handle highly distorted (even concave) polygonal meshes and highly discontinuous or anisotropic material properties (see Margolin & Shashkov 2007, Lipnikov et al. 2009, and references therein).

Discrete calculus methods: numerical methods in which all discretization (transformation to a finite system) is performed exactly

4.4. Natural-Neighbor Methods

The natural-neighbor method is a meshless method that is popular in solid mechanics for crack propagation and the analysis of stress singularities. These methods come in a number of flavors with both the original Sibson and several newer non-Sibsonian shape functions (Sukumar 2003) being used. All natural-neighbor methods shape functions form a partition of unity and therefore have the ability to conserve primary variables. In addition, the Voronoi construction of the shape functions means that these methods have discrete divergence and gradient operators that are closely related to unstructured staggered mesh methods on polygonal cell domains. They are likely to have secondary conservation properties similar to staggered mesh methods.

5. DISCRETE CALCULUS METHODS

Many of the methods described above that have secondary conservation properties can be derived as discrete calculus methods (Perot & Subramanian 2007b). The key to discrete calculus methods is that they explicitly separate the discretization and the approximation processes that are necessary to solve a PDE on a computer. The most important aspect of discrete calculus methods is that the discretization process, which involves turning a PDE into a finite-dimensional algebraic system of equations, is performed exactly. The resulting exact discrete system is always overdetermined with more unknowns than equations so it cannot be solved. The approximation step that is necessary to solve the equations involves relating some of the discrete unknowns to each other via certain algebraic relations, and these relations are invariably material constitutive relationships.

This two-step approach to solving PDE systems numerically (exact discretization, followed by approximation of an overdetermined algebraic system) has a number of advantages. First, the discretization process is exact. The discrete version of calculus (e.g., gradients, divergences) is therefore exact. It obeys integration by parts statements, and every other property of the continuous operators, because it has to; no approximation has been introduced. The presence of these discrete properties is extremely useful because it means that the resulting discrete equations can often be manipulated into discrete kinetic energy, entropy, and vorticity statements in the same way that the continuous equations are manipulated.

It is also important that the approximation in discrete calculus methods invariably occurs in the constitutive equations involving material properties. Constitutive equations are physical approximations hypothesized by humans to represent certain macroscopic material states. It is therefore consistent to place all the numerical approximation in the same place as the physical approximation. The precise nature of the approximation determines if the discrete calculus method has the flavor of a finite-element method, a finite-volume method, a finite-difference method, a particle method, etc. Discrete calculus methods are a small subset of each discretization approach (see **Figure 1**). The idea of splitting discretization and approximation is somewhat novel, so a brief example is presented below.

5.1. Example

One of the simplest PDEs, Laplace's equation, $\nabla \cdot k \nabla T = 0$, occurs in many areas of science and engineering. It is discussed here in the context of steady-state heat conduction. In heat conduction,

T is the unknown temperature and k is a material property—the conductivity. The equation can be written more generally as

$$\nabla \cdot \mathbf{q} = 0, \tag{8a}$$

$$\mathbf{g} = \nabla T, \tag{8b}$$

$$\mathbf{q} = -k\mathbf{g}, \tag{8c}$$

where $\mathbf{q}$ is the heat flux and $\mathbf{g}$ is the temperature gradient. We note that Equation 8a, involving the heat flux, can be considered to be an exact statement of physics, and Equation 8b is just a definition of the gradient operator (mathematics), but Equation 8c is a constitutive relation (Fourier's law). Equation 8c is a physical approximation that is reasonably valid for many materials, whereas Equations 8a and 8b should be inviolate. The utility of breaking up PDEs in this way into their smaller constitutive parts (with different roles) is extensively discussed for a wide variety of PDE equation systems by Tonti (1975, 1976).

One possible exact discretization of the physics (Equation 8a) and calculus (Equation 8b) is

$$\sum_{\substack{cell\\faces}} \int_{A_i} \mathbf{q} \cdot \mathbf{n}\, dA = \mathbf{D} Q_f = 0, \tag{9a}$$

$$g_e = \int_{C1}^{C2} \nabla T \cdot d\mathbf{l} = T_{C2} - T_{C1} = \mathbf{G} T_c. \tag{9b}$$

Exact discretization often results in unknowns that are integral quantities, such as the heat flux $Q_f = \int_{A_i} \mathbf{q} \cdot \mathbf{n}\, dA$. The control volume approach given in Equation 9a to discretization is not the only way to make an equation discrete in an exact way, but it is a well-understood technique so it is used in this simple example. The second exact discretization given in Equation 9b is just as important (and far more neglected in practice).

The system involving Equations 9a and 9b is exact and discrete (finite). It only requires a relation between g_e and Q_f to be solvable, so the discrete equivalent of Equation 8c must be formulated. In most methods the number of elements in the unknown vectors g_e and Q_f is the same, so they can be related by a square matrix, $Q_f = \mathbf{M} g_e$. For a stable method, $\mathbf{M}$ should be positive definite (a negative eigenvalue is like having a negative conductivity), and for computational efficiency it is convenient if $\mathbf{M}$, or its inverse, is sparse.

Figure 6 shows that the flux and line integral are near each other but involve different geometric regions (a line integral and an area integral in three dimensions). The simplest possible Hodge

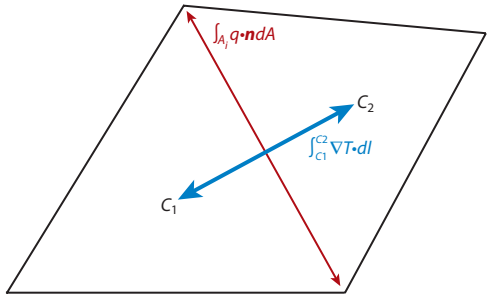

Figure 6

Interpolation problem for the discrete calculus method applied to steady heat conduction.

star operator, **M**, is a diagonal matrix such that

$$Q_f \simeq \left(-k\frac{A_f}{L_{c1-c2}}\right) g_e. \tag{9c}$$

This approximation is second-order accurate on Cartesian meshes or unstructured meshes when the cell circumcenter is used for the location of the temperature unknowns.

Note that this discrete system has a maximum principle (like the original PDE) that guarantees that the maximum (and minimum) value of the solution will lie on the domain boundary. In addition, the discrete divergence **D** and discrete gradient operator **G** can be shown to be adjoint matrices. Perhaps most importantly for this review, a secondary conservation statement that is the discrete version of the equation $\nabla \cdot k \nabla T^2 = \frac{k}{2T^2}(\nabla T^2) \cdot (\nabla T^2)$ can be derived for the variable T^2 [which is closely related to the total variation of importance in TVD (total variation diminishing) schemes].

Other approximations for Fourier's law (Equation 8c) are certainly possible. Mattiussi (1997) describes the interpolation leading to a finite-element method. Perot & Subramanian (2007a) discuss the interpolation leading to Keller-Box methods. A finite-volume approach that is node based (like a finite-element method) rather than cell based (like this finite-volume example) is discussed in Subramanian & Perot (2007).

The relationship that exists between certain physical variables and certain topologies in the mesh (points, lines, faces, or volumes) is the reason that the field of algebraic topology is useful for analyzing discrete calculus methods. This topology information actually exists in the physics but is hidden when we write PDE equations for the physics using infinitesimals. When a PDE is discretized and returned to the finite realm, the topologic information invariably returns in the form of the integral unknowns, and this topological information must be respected. The observation that the equation for 3D inviscid vorticity evolution is the same as that for the evolution of a small line segment is not a coincidence; vorticity (like g_e in the example above) should be discretized as a line integral quantity. Similarly, velocity should be discretized as a flux (like Q_f in the example above) as is the case for staggered mesh methods and face elements.

The simple example shown above is for a scalar quantity (the temperature), but discrete calculus discretization methods become much more powerful when they are used on vector equation systems such as Maxwell's equations for electromagnetism or the Navier-Stokes equations for fluid dynamics. The discrete calculus approach demands that only certain components of vectors (normal to a face, or tangential to a line) be used as unknowns. Vectors, in the more traditional sense of two or three associated quantities at a certain location, are unknown in algebraic topology (or in discrete calculus methods). Traditional vector fields can be recovered using consistent interpolation schemes (Shashkov et al. 1998, Perot et al. 2006).

6. CONCLUSION

This work is based on the premise that capturing the physics inherent in a PDE is as important as, or perhaps even more important than, capturing the mathematical properties. Although this idea pervades this presentation, it is only fair to point out that this is a philosophical bias of the author's, not a golden rule. It could be, and has been, argued that methods with secondary conservation properties are more difficult to implement. In addition, conservative methods can be quite unforgiving computationally. Nonlinear equation systems such as Navier-Stokes always generate modes that cannot be precisely represented by the discretization. Energy-conserving methods keep unresolved mode energy within that system (in the resolved modes). Perhaps it is actually better to remove that energy with some numerical diffusion or dealiasing rule. In

concrete terms, the simulation of an inviscid vortex with a fully conservative method will result in a stable solution in which the velocity never grows exponentially. However, if the vortex is not well resolved, that solution can also be very noisy and essentially useless at long times because of aliasing errors. Many conservative methods avoid this issue in practice by adding small amounts of numerical dissipation via the time-stepping scheme. One can view these aliasing effects either as a helpful hint from the method that the resolution is inadequate, or alternatively as a lack of robustness in the methodology.

In the past, there has been a great distinction made between local conservation and global conservation. We hope this review has narrowed that divide. The article suggests that a method that is globally conservative and that uses local basis functions must also be locally conservative. Although many methods lack an obvious flux calculation, we have demonstrated that many methods implicitly are indeed calculating fluxes. This articles dodges the issue of boundary conditions and conservation, but this detail is addressed in the provided references.

Secondary conservation is the focus of current research, but the terminology may be deceptive. In practice, kinetic energy conservation is often more important than momentum conservation. And particularly when solving compressible flows, satisfaction of both the first and second law of dynamics would seem to be of equal importance. When developing methods with secondary conservation statements, two approaches appear to have significant merit. The discretization of Hamiltonian dynamics (rather than Newtonian) appears to often lead to discrete systems with the necessary symmetries. One difficulty with Hamiltonian dynamics is that this approach to physics really only applies to the inviscid situation (Euler equations). Serrano & Espanol (2001) show one way to generalize the Hamiltonian approach to the full Navier-Stokes equations. Tadmor (1984) shows another. The second approach to secondary conservation is the discrete calculus approach in which the method is constructed so that there are no approximations in the discrete version of the calculus. All approximation is in the constitutive equations. The discrete calculus approach leads to existing numerical methods (such as face-edge elements, staggered mesh methods, multisymplectic box schemes, and mimetic methods), but it also has led to the development of new solution methods with good conservation properties (Subramanian & Perot 2007).

One important physical fidelity issue that conservation statements do not address is the issue of spurious (unphysical or unmathematical) solutions to the equations. For example, if a gradient of a variable is equal to zero, that variable should be spatially constant throughout the domain. Similarly if a discrete curl of a vector field is zero, that vector field should be equal to the gradient of a scalar field (this is an application of Helmholtz decomposition). Most discrete gradients (and discrete curls) violate this principle. Methods based on algebraic topology (face/edge elements) explicitly address this issue. Discrete calculus methods address it indirectly.

SUMMARY POINTS

1. Many methods are locally conservative for primary variables.
2. Secondary conservation is important for physically realistic solutions.
3. Secondary conservation results from how the system is set up.
4. Most discretization approaches have a subset that conserves secondary quantities.
5. It is possible to a priori construct numerical methods that have secondary conservation properties.

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