

MIMETIC RECONSTRUCTION OF VECTORS

J. BLAIR PEROT*, DRAGAN VIDOVIC†, AND PIETER WESSELING‡

Abstract. Compatible or mimetic numerical methods typically use vector components as the primary unknowns in the discretization. It is frequently necessary or useful to be able to recover vectors from these spatially dispersed vector components. In this paper we discuss the relationship between a number of low order vector reconstruction methods and some preliminary results on higher order vector reconstruction. We then proceed to demonstrate how explicit reconstruction can be used to define discrete Hodge star interpolation operators, and how some reconstruction approaches can lead to local conservation statements for vector derived quantities such as momentum and kinetic energy.

Key words. Vector, reconstruction, interpolation, conservation.

AMS(MOS) subject classifications. 65D05, 65N30, 65M60, 76M12, 76M10.

1. Background. Many numerical methods for the solution of Partial Differential Equations use point values or cell averages as the primary discrete unknowns. For scalar equations, such as the Poisson equation, the heat equation, or the scalar wave equation, this is a very appropriate starting point. However, for vector equations, such as Maxwell's equations or the Navier-Stokes equations, there is considerable evidence now suggesting that advantageous numerical properties can be obtained, by using integral averages of vector *components* as the primary discrete unknowns.

In Finite Elements these are often referred to as edge or face elements. They were originally discussed in 2D by Raviart and Thomas [1] and in 3D by Nédélec [2]. In the Finite Volume or Finite Difference context, this type of approach is often referred to as a staggered mesh method. The staggered mesh approach was first proposed for Cartesian meshes by Harlow and Welch [3] in 1965, and has since been generalized to unstructured and curvilinear meshes [4–7]. Face and edge elements are becoming increasingly popular in electromagnetic wave propagation. These methods appear to be the only way to capture difficult physical effects such as resonant frequencies (eigenmodes) [8]. Staggered mesh methods are attractive in incompressible fluid dynamics because they allow the exact satisfaction of the continuity constraint [9], and the satisfaction of a number of local conservation properties (conservation of kinetic energy being perhaps the most important) [10].

Having stated that vector components, not vectors themselves, should be the primary variables of interest when solving vector partial differential

*Department of Mechanical & Industrial Engineering, University of Massachusetts, Amherst, MA 01003 (perot@ecs.umass.edu).

†Applied Mathematics, TU Delft, Netherlands (D.Vidovic@ewi.tudelft.nl).

‡(P.Wesseling@ewi.tudelft.nl).

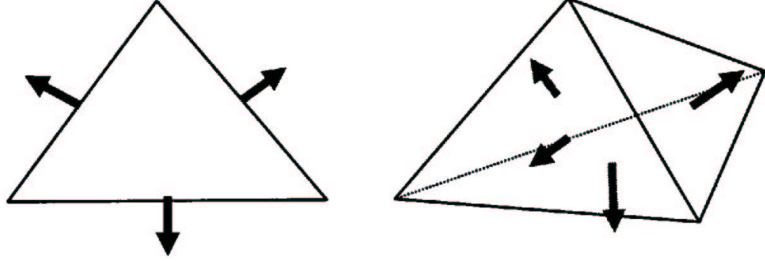


FIG. 1. *Representation of unknowns for low order face-based mimetic methods.*

equations, this paper will now proceed to discuss how vector quantities can be obtained in these schemes. In the case of the Navier-Stokes equations, the need for the velocity vector is obvious since the convective term requires a velocity vector. On the surface, it is far less clear why this might be a useful procedure for Maxwell's (or Stokes') equations. These equations can, and probably should, be discretized entirely in terms of vector components that are edge or face averages. Nevertheless, even in these discretization schemes there is the necessity to interpolate edge averages to face averages and vice-versa. Vector reconstruction can (though certainly does not have to) be used to construct numerically attractive interpolation schemes. Vector interpolation is also useful for graphical output.

We note that there is a more precise terminology emanating from Algebraic Topology for describing many of the concepts described in this paper. However, in order to keep the potential audience broad, and in order to discuss vectors (which fit less well in the formalism of differential forms), we will continue to use the more primitive vector calculus.

2. Lowest order face-based reconstruction methods. The lowest (first) order face-based mimetic methods all use $u_f = \frac{1}{A} \int \mathbf{v} \cdot \mathbf{n} dA$, the face-normal average vector component on element faces as the primary unknown (see Fig. 1). Throughout this paper the formulas and text refer to the three-dimensional case. This means that in two-dimensions 'cells' refers to 2D polygonal regions (often triangles in the figures), 'faces' are the boundaries of the cells and are actually 1D objects (frequently referred to in other texts as edges), and 'edges' coincide with faces in 2D.

The face-based FE method for simplices assumes a piecewise polynomial for the vector field of the form $\mathbf{v}(\mathbf{x}) = \mathbf{a} + b\mathbf{x}$ where \mathbf{a} is a constant vector and b a constant scalar in each element (or cell). For Cartesian grids, the polynomial is assumed to be $\mathbf{v}(\mathbf{x}) = \mathbf{a} + B\mathbf{x}$ where B is a diagonal matrix. Note that in both cases the normal component of the vector field is constant along each face of the element (or cell) and therefore also continuous across the face. This means that at lowest order the integral average of the normal vector component over the face, u_f , can also be associated

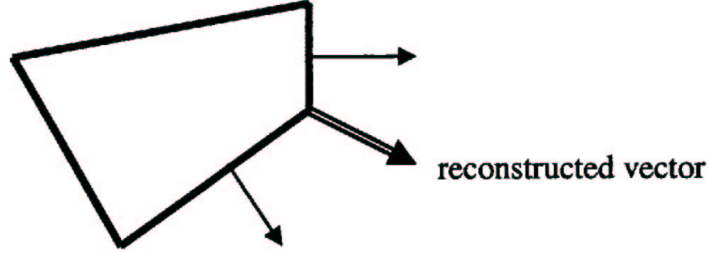


FIG. 2. *Reconstruction of corner vector from face normal components assuming no variation in the component values along each cell/element face.*

with a pointwise value on that face (often the midpoint value of the normal component is cited as the primary unknown). Also note that when the vector field is divergence free (which is frequently true in both the fluid dynamic and electromagnetic contexts), then the lowest order reconstruction on simplices assumes that the vector field is piecewise constant.

Least squares reconstruction of the vector field was proposed by Nicolaides [4]. In that method one finds the constant vector field, \mathbf{v}_{cell} that best satisfies all the face equations $\mathbf{v}_{\text{cell}} \cdot \mathbf{n}_f = u_f$ for all the faces of a cell/element. For a divergence free field on a simplex, the result is the same as the FE reconstruction and $\mathbf{v}_{\text{cell}} = \mathbf{a}$.

Hyman and Shashkov [5] and Shashkov *et al.* [11] proposed reconstruction at the corners of each element using the immediately neighboring face unknowns (see Fig. 2). Because the low order FE approximation assumes the normal velocity is constant on faces, the corner velocities recovered by this method are identical to the low order FE reconstruction. To obtain the vector value at the cell center a simple average of the node velocities is suggested, $\mathbf{v}^{\text{CG}} = \frac{1}{NCN} \sum_{\text{nodes}} \mathbf{v}^n$ where NCN is the number of nodes in the cell or element.

Since $\mathbf{v}^n = \mathbf{v}^C + b(\mathbf{x}^n - \mathbf{x}^C)$ the simple average gives $\frac{1}{NCN} \sum_{\text{nodes}} \mathbf{v}^n = \mathbf{v}^C + b \frac{1}{NCN} \sum_{\text{nodes}} (\mathbf{x}^n - \mathbf{x}^C)$. If the cell center is defined to be the average of the cell corners the last term is zero, and we see that the simple average is the value at the cell center. For simplices and Cartesian meshes, the average of the cell corners equals the center of gravity (or centroid). Unlike the FE reconstruction, this approach is explicit and does not require a matrix inversion (which is as large as 6x6 for 3D Cartesian meshes). In addition, in contrast to the FE reconstruction this method can easily be generalized to arbitrary polygons, since no explicit piecewise polynomial form for the vector field is assumed.

Finally, Perot and Nallapati [12] suggest a reconstruction formula derived from Gauss' Divergence Theorem and the position vector, \mathbf{x} . In

particular it is noted that the exact relation

$$\int \mathbf{v} dV + \int \mathbf{x}(\nabla \cdot \mathbf{v}) dV = \sum_{\text{faces}} \int \mathbf{x} \mathbf{v} \cdot \mathbf{n} dA \quad (2.1)$$

applies in each element or cell. Making the same assumptions as the low order FE reconstruction (constant normal velocity along each face, constant dilatation, and a linear velocity field), gives the discrete interpolation formula

$$\mathbf{v}_c^{\text{CG}} = \frac{1}{V_c} \sum_{\text{cell faces}} \pm u_f A_f (\mathbf{x}_f^{\text{CG}} - \mathbf{x}_c^{\text{CG}}) \quad (2.2)$$

where CG stands for the (cell or face) center of gravity (or centroid) and the \pm is to account for the fact that u_f should point out of the cell in question. The cell volume is v_c and the face areas are A_f . This formula is directly equivalent to the low order FE reconstruction (since the assumptions are the same). However, like the method of Hyman and Shashkov it easily generalizes to arbitrary polygons.

We can see that the method of Hyman and Shashkov is fully equivalent to the FE interpolation but returns the vector value at the average of the element corner positions (which is not equal to the centroid position on arbitrary polygons). The method of Perot is also always equivalent to the FE method but returns the centroid value for the vector no matter what the element shape. The method of Perot is also a simple average of the primary unknowns, u_f , whereas the method of Hyman and Shashkov requires the intermediate step of corner velocity reconstruction. However, the corner reconstruction approach may be easier to generalize to higher order.

3. Higher order face-based reconstruction methods. For n^{th} order faced-based methods on simplices, the FE interpolation is generalized to $\mathbf{v}(\mathbf{x}) = \mathbf{a}(\mathbf{x}) + b(\mathbf{x})\mathbf{x}$, where \mathbf{a} and b are $n - 1$ order polynomials. The normal velocity component on each face is also an $n - 1$ order polynomial (and remains continuous across the face). For Cartesian meshes, the polynomial is assumed to be $\mathbf{v}(\mathbf{x}) = \mathbf{a}(\mathbf{x}) + B(\mathbf{x})\mathbf{x}$ where B is a diagonal matrix. As with all FE methods, the underlying interpolation changes for every possible element shape. The generalization to quads, hexahedra, prisms, and pyramids is non-trivial but possible [13, 14], and the FE generalization to arbitrary polygons appears to be extremely difficult.

At the next higher order, $\int \mathbf{v} dV$ and $\int \mathbf{x} \mathbf{v} \cdot \mathbf{n} dA$ are primary unknowns (along with u_f) of face-based mimetic methods. This means there is now a total of ND unknowns per face and ND unknowns per cell/element, where ND is the number of dimensions. The terminology face element is now less appropriate (since there are also cell unknowns), but it is still used. Staggered mesh and finite volume methods typically obtain higher order by enlarging the interpolation stencil rather than increasing the number of

unknowns within a cell. Higher order staggered mesh methods for Cartesian meshes using a larger stencil have been proposed [15, 16]. However, larger than nearest neighbor stencils on arbitrary 3D polygonal meshes are difficult to formulate and program, very difficult to implement efficiently on parallel computers, and create complex issues at domain boundaries. The common FE practice of more unknowns per cell is not commonly practiced in FV methods but is perfectly possible and is the approach discussed herein.

The exact integral relation (Eq. (2.1)) now provides the first order dilatation moments $\int \mathbf{x} \nabla \cdot \mathbf{v} dV$ immediately from the primary data. The zeroth order dilatation moment is also directly known $\int \nabla \cdot \mathbf{v} dV = \sum u_f A_f$. On a simplex the first order dilatation moments are enough to rapidly recover the centroid velocity vector. To see how, note that for a simplex the polynomial form is known and $\nabla \cdot \mathbf{v} = \nabla \cdot \mathbf{a} + \mathbf{x} \cdot \nabla b + bND$ where ND is the number of dimensions. Switching to index notation for clarity, this implies that $\int x_k v_{i,i} dV = (ND + 1)b_i \int x_k x_i dV$. In addition we can use the polynomial form to write $\int v_k dV = V v_k^{\text{CG}} + b_{,i} \int x_k x_i dV$. So in the case of simplices the point value of the vector at the center of gravity is given by the expression $\mathbf{v}_c^{\text{CG}} = \frac{1}{V_c} \int \mathbf{v} dV - \frac{1}{(ND+1)V_c} \int \mathbf{x} \nabla \cdot \mathbf{v} dV$ or in terms of primary variables

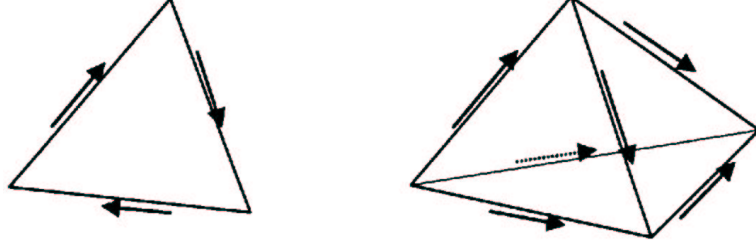
$$\mathbf{v}_c^{\text{CG}} = \frac{ND}{(ND + 1)V_c} \int \mathbf{v} dV - \frac{1}{(ND + 1)V_c} \sum_{\text{faces}} \int \mathbf{x} \mathbf{v} \cdot \mathbf{n} dA. \quad (3.1)$$

This is entirely equivalent to the FE reconstruction, though explicit and simpler than inverting an 8×8 matrix (in 2D) or a 15×15 matrix (in 3D). Note however, that this reconstruction expression for the centroid velocity vector does not appear to be general. It does not equal the FE reconstruction on Cartesian meshes.

Elements of the method of Hyman and Shashkov (in particular the corner velocity reconstruction) can be extended to higher order in 2D and 3D. Assuming linear variation of the normal vector component on a face, the primary variables u_f and $\int \mathbf{x} \mathbf{v} \cdot \mathbf{n} dA$ contain enough information to specify the face normal velocity at face corners and therefore the velocity vector at element corners.

Note that the reconstruction of the element corner velocities is straightforward only if the element corners only have ND faces meeting at every corner. The top corner of a pyramid is an instance that violates this condition. This type of corner is also degenerate for FE polynomial reconstructions. It is anticipated that a unique corner solution still exists even though the problem appears to be over specified.

Because the vector field is now piecewise quadratic, a simple average of the corner velocities is no longer sufficient to recover the centroid vector value. However, the cell value can be recovered from the corner velocities and the cell average value. For example, it can be shown that

FIG. 3. *Edge-based primary unknowns in 2D and 3D.*

$\mathbf{v}_c^{\text{CG}} = \frac{4}{3} \frac{1}{V_c} \int \mathbf{v} dV - \frac{1}{3} \frac{1}{3} \sum_{\text{nodes}} \mathbf{v}^n$ is satisfied on triangles, and on rectangles, $\mathbf{v}_c^{\text{CG}} = \frac{3}{2} \frac{1}{V_c} \int \mathbf{v} dV - \frac{1}{2} \frac{1}{4} \sum_{\text{nodes}} \mathbf{v}^n$ holds true. A general formula is not available at this time.

4. Lowest order edge-based reconstruction methods. The lowest (first) order edge-based mimetic methods use $u_e = \frac{1}{L_e} \int \mathbf{v} \cdot d\mathbf{l}$, the edge-tangential average vector component on element edges as the primary unknown (see Fig. 3). The edge-based FE method for simplices then assumes a piecewise polynomial for the vector field of the form $\mathbf{v}(\mathbf{x}) = \mathbf{a} + \mathbf{b} \times \mathbf{x}$ where \mathbf{a} and \mathbf{b} are constant vectors in each element. Whereas the lowest order face-elements are vorticity free (except between elements), the lowest order edge-based elements are divergence free (except between elements). The tangential velocity is constant along each edge and is therefore continuous. The velocity tangential to an element face is given by $\mathbf{v} \times \mathbf{n} = \mathbf{a} \times \mathbf{n} - (\mathbf{x} \cdot \mathbf{n})\mathbf{b} + (\mathbf{b} \cdot \mathbf{n})\mathbf{x}$ and varies linearly on the face in a fashion akin to a rotated face-based vector. The vorticity in the simplicital FE reconstruction is given by $\nabla \times \mathbf{v} = \mathbf{b}(ND - 1)$ where ND is the number of dimensions.

Edge elements have more degrees of freedom than face elements. In FE the choice of which element is appropriate depends on the physical nature of the vector in question and its inherent continuity requirements and natural boundary conditions. Because FE are restricted to certain element shapes, the primary mesh must define the elements/cells. However, in methods that handle arbitrary polygons, there is an additional choice because it is also possible for cells/elements to be associated with the dual mesh. This means edges could also be associated with the lines connecting the tetrahedra cell centers.

In the context of finite volume or finite difference methods there is far less published work on vector reconstruction of edge-based vectors. While it is not discussed in their papers the basic idea of Hyman & Shashkov of corner reconstruction is still valid. Again, some degeneracy may occur on cells that have more than three edges meeting at a corner (such as the top of a pyramid). And as before, the sum of the corner velocities equals the velocity at the cell center (defined to be the average of the corner positions).

On arbitrary polygonal meshes this is not equal to the cell center of gravity but is an equally well defined center.

Zhang *et al.* [17] presents an analog of Eqs. (2.1) and (2.2) for edge based vectors. This is based on the application of Stokes' Curl Theorem. Note that for each face the Curl Theorem states that

$$\begin{aligned} n_i \int (\varepsilon_{ijk} \nu_{k,j} x_m + \varepsilon_{imk} \nu_k) dA &= n_i \int \varepsilon_{ijk} (\nu_k x_m)_{,j} dA \\ &= \sum_{\text{edges}} \int x_n \nu_k dl_k. \end{aligned} \quad (4.1)$$

Index notation is used for clarity and ε_{ijk} is the standard permutation symbol. If we assume, consistent with the FE polynomials, that the vorticity is constant in each cell and the velocity component along each edge is constant and the tangential velocity varies linearly then this gives the formula,

$$\mathbf{v}_f^{\text{CG}} A_f = \int \mathbf{v} \times \mathbf{n} dA = \sum_{\text{edges}} \pm (\mathbf{x}_e^{\text{CG}} - \mathbf{x}_f^{\text{CG}}) u_e L_e \quad (4.2)$$

where L_e is the length of each edge and \pm indicates counterclockwise (right hand rule) integration around the edges of the face with respect to the face normal, \mathbf{n} . In this way the tangential velocity at the center of gravity of each face can be recovered. In 2D the reconstruction is complete since a face corresponds to a the cell/element. In 3D we note that sometimes the tangential velocity on faces is sufficient and the cell velocity vector is not actually required. This is the case for the rotational form of the convective term $(\nabla \times \mathbf{b}) \times \mathbf{v} + \nabla(\frac{1}{2} \mathbf{v} \cdot \mathbf{v})$ [11].

The face tangential velocity can be used to quickly recover the vorticity in the cell. Using the divergence theorem we note that,

$$\int \varepsilon_{ijk} \nu_{k,j} dV = \sum_{\text{faces}} \int \varepsilon_{ijk} \nu_k n_j dA. \quad (4.3)$$

Assuming the vorticity is constant in each cell we see that the sum of the face tangential velocities equals the cell vorticity.

$$\nabla \times \mathbf{v} = -\frac{1}{V_c} \sum_{\text{faces}} \int \mathbf{v} \times \mathbf{n} dA. \quad (4.4)$$

Remember that for the lowest order face-based reconstructions the cell vorticity is always zero and vorticity is confined to thin sheets between the elements/cells.

In 3D the cell velocity can be obtained from the relation,

$$\begin{aligned} \int (\varepsilon_{ijk} \nu_{k,j} x_m + \varepsilon_{imk} \nu_k) dV &= \int \varepsilon_{ijk} (\nu_k x_m)_{,j} dV \\ &= \sum_{\text{faces}} \int x_m \varepsilon_{ijk} \nu_k n_j dA. \end{aligned} \quad (4.5)$$

Assuming constant vorticity, and linear velocity we obtain

$$\varepsilon_{imk} \mathbf{v}_k^{\text{CG}} = -\frac{1}{V_c} \sum_{\text{faces}} \int x_m [\mathbf{v}_f^{\text{CG}} \times \mathbf{n} + (\mathbf{b} \cdot \mathbf{n})(\mathbf{x} - \mathbf{x}_f^{\text{CG}})]_i dA. \quad (4.6)$$

Note that $0 = \int (\delta_{ik} x_j + \delta_{jk} x_i) dV = \int (x_i x_j)_{,k} dV = \sum_{\text{faces}} \int x_i x_j n_k dA$ if we assume the position origin is at the cell center of gravity. Then the second term of (4.6) is seen to be zero and

$$\varepsilon_{imk} \nu_k^{\text{CG}} = -\frac{1}{V_c} \sum_{\text{faces}} A_f r_m^f (\mathbf{v}_f^{\text{CG}} \times \mathbf{n})_i - b_k \sum_{\text{faces}} A_f r_m^f r_m^f n_k \quad (4.7)$$

where $\mathbf{r}^f = (\mathbf{x}_f^{\text{CG}} - \mathbf{x}_c^{\text{CG}})$ is the distance between the face and cell center of gravities and $\mathbf{b} = \frac{\nabla \times \mathbf{v}}{ND-1}$. These formulas were developed for simplices but appear to generalize naturally to arbitrary polygons.

5. Higher order edge-based reconstruction methods. For n^{th} order edged-based methods on simplices, the FE interpolation is generalized to $\mathbf{v}(\mathbf{x}) = \mathbf{a}(\mathbf{x}) + \mathbf{b}(\mathbf{x}) \times \mathbf{x}$, where \mathbf{a} and \mathbf{b} are $n-1$ order polynomial vectors.

The primary unknowns for the next order edge-based discretizations are $\frac{1}{A_f} \int \mathbf{v} \times \mathbf{n} dA$ the average tangential velocity on faces, $\frac{1}{L_e} \int \mathbf{x} \mathbf{v} \cdot \mathbf{n} dl$ the moment of the tangential velocity component, as well as lowest order unknown $\frac{1}{L_e} \int \mathbf{v} \cdot \mathbf{n} dl$. Eqn. (4.1) now becomes an exact relation for the gradients or the face-normal vorticity (which are assumed constant) on each face,

$$\int \mathbf{x}(\mathbf{n} \cdot \nabla \times \mathbf{v}) dA = \sum_{\text{edges}} \int \mathbf{x} \mathbf{v} \cdot d\mathbf{l} - \int \mathbf{v} \times \mathbf{n} dA \quad (5.1)$$

and Eqn. (4.3) now becomes an exact expression for the average vorticity in the cell

$$\int \nabla \times \mathbf{v} dV = - \sum_{\text{faces}} \int \mathbf{v} \times \mathbf{n} dA \quad (5.2)$$

or its value at the center of gravity (since it is now assumed to vary linearly).

The corner reconstruction method still works for edge elements. The average tangential component and its first moment provide enough information to reconstruct the corner velocities exactly. However, as with the face-based elements, a simple average of the corner velocities is no longer sufficient to recover the vector at any cell center pointwise location, and a general averaging formula for arbitrary polygons is not known at this time. Corner velocities are discontinuous at the cell nodes and do not provide a unique output for the velocity at nodes (often desired for graphical output).

6. Mass matrices and the discrete Hodge star operator. In mimetic methods, it is frequently necessary to convert a face-based set of unknowns to edge-based or vice versa. This occurs because when primary unknowns are face-based the evolution equations are posed on a dual mesh that is edge-based. While mimetic FE methods avoid the explicit definition of a dual mesh, it is still present and implicitly defined by the functional form of the weighting functions in the weak statement of the equations. See Mattiussi [18] for a detailed explanation. This process of converting one type of vector field to another is sometimes referred to as a discrete Hodge star operator. This operator is symmetric and positive definite for Galerkin FE and for many low order mimetic methods, but it is not clear that symmetry is absolutely necessary. One possible method for explicitly converting a face-based vector structure to an edge based one is to reconstruct the piecewise polynomials in each cell/element based on existing face-based data and then use high enough order numerical quadrature on the piecewise polynomials to compute the necessary edge-based integrals. This is what implicitly happens in the Galerkin FE methods.

Consider the transpose of the low order Perot interpolation method for determining the cell centroid vector value (Eq. (2.2)). The transpose operation applied to those centroid values is $\sum_{\text{face cells}} \pm \mathbf{v}^{\text{CG}} \cdot (\mathbf{x}_f^{\text{CG}} - \mathbf{x}_c^{\text{CG}})$. This is a first order accurate (like the reconstruction itself) integration along the median dual edge connecting two cell centroids. Note that the median dual edge consists of two line segments each joining the face centroid to the neighboring cell centroids. We can therefore write to first order

$$\int \mathbf{v} \cdot d\mathbf{l} \approx \mathbf{R}^T \frac{1}{V_c} \mathbf{R} \int \mathbf{v} \cdot \mathbf{n} dA \quad (6.1)$$

where the line integral is along the median dual edge and the area integral over the corresponding face. The reconstruction operator is defined as $\mathbf{R}\nu_f = \sum_{\text{cell faces}} (\mathbf{x}_f^{\text{CG}} - \mathbf{x}_c^{\text{CG}}) \nu_f$. On uniform (or nearly uniform) meshes, errors cancel out during the integration and despite the first order nature of the reconstruction and integration, this approximation is found to be second order accurate. The discrete Hodge star operator that converts from face-based to edge based vectors is $\mathbf{R}^T \frac{1}{V_c} \mathbf{R}$.

Exact (rather than approximate) integration over a simplex median dual mesh and the low order piecewise approximation $\mathbf{v} = \mathbf{a} + \mathbf{b}\mathbf{x}$ gives a slightly modified formula

$$\int \mathbf{v} \cdot d\mathbf{l} = \sum_{\text{face cells}} \pm \mathbf{v}^{\text{CG}} \cdot (\mathbf{x}_f^{\text{CG}} - \mathbf{x}_c^{\text{CG}}) \pm \frac{(\nabla \cdot \mathbf{v})}{2ND} (\mathbf{x}_f^{\text{CG}} - \mathbf{x}_c^{\text{CG}})^2 \quad (6.2)$$

which is only symmetric on a uniform mesh, but which is probably always positive definite.

The distributed two-step nature of the low order corner reconstruction approaches makes it difficult to evaluate the properties of their effective discrete Hodge star operators. However, due to the demonstrated equivalence

of these methods with the reconstruction method of Perot, it can be demonstrated that for simplices and Cartesian grids, these methods also produce symmetric positive definite discrete Hodge star operators.

7. Conservation properties of the Navier-Stokes equations.

The attractive conservation properties of Cartesian staggered mesh methods have been known for some time [19]. On Cartesian meshes the orthogonal structure of the mesh allows non-overlapping staggered control volumes to be defined in which conservation is relatively easy to demonstrate. However, on general unstructured meshes demonstrating that local conservation properties (such as those obtained in standard Finite Volume methods) exist is extremely difficult. The problem lies in the fact that only velocity components and transport equations for velocity components exist so it is difficult to make conservation statements about vector quantities.

Two conservation statements of particular interest are conservation of momentum and conservation of kinetic energy (in the incompressible limit). Conservation of vorticity or circulation (the curl of the momentum) is also possible and is discussed in Perot et al. in Refs. [7, 10, 17]. Finite Element methods frequently have a global conservation statement that can be associated with them, but one attraction of mimetic methods is their ability to correctly represent physics at the local (cell) level as well.

In the following sections we focus on the conservation properties of low order face-based discretization schemes of the Navier-Stokes equations. Integrating along the two line segments connecting the cell centers and the face center (a dual mesh edge) gives a discrete equation for each dual edge.

$$\frac{\partial}{\partial t}[\mathbf{R}^T \mathbf{m}_c] + \mathbf{R}^T \mathbf{a}_c = -\mathbf{G}p_c \quad (7.1)$$

where $\mathbf{m}_c = \frac{p_c}{V} \sum_{\text{faces}} (\mathbf{x}_f^{\text{CG}} - \mathbf{x}_c^{\text{CG}}) u_f A_f$ is the cell momentum, and $\mathbf{a}_c = \frac{1}{V_c} \sum_{\text{faces}} \{ \mathbf{u} u_f - \mu (\nabla \mathbf{u} + \mathbf{u} \nabla) \cdot \mathbf{n} - \lambda (\nabla \cdot \mathbf{u}) \mathbf{n} \}_f A_f$ is a standard finite volume flux representation of the advection-diffusion term in each cell. The term with the second coefficient of viscosity, λ can also be directly absorbed into the pressure term instead of into \mathbf{a} . The exact operator \mathbf{G} is the difference between the pressure at the two end points of the line segment.

On Dirichlet boundaries the normal velocity is fixed and this equation does not exist. On variable-boundaries (such as an outflow), the pressure on the boundary is fixed and only one segment of the dual mesh edge has non-zero length.

8. Conservation of momentum. In order to show conservation of momentum, we must be able to show that linear combinations of the existing discrete edge based equations can be constructed such that those combinations look like a local discrete vector conservation statement.

Consider a single cell. We have update equations for the normal component on each face of that cell. Let us associate each line segment of the dual edge equation with the cell in which it resides. Ultimately we will

multiply both line segments by the same scaling factor, so this splitting is really for accounting purposes only. If the cell face is also a domain boundary the associated dual edge only has a single segment (associated with the interior cell).

For a single cell, multiplying each segment equation by the face normal vector and face area and summing over the cell faces gives (assuming outward normals for convenience).

$$\sum_{\text{faces}} \mathbf{n}_f A_f \left\{ \frac{\partial}{\partial t} \mathbf{m}_c + \mathbf{a}_c \right\} \cdot (\mathbf{x}_f^{\text{CG}} - \mathbf{x}_c^{\text{CG}}) = - \sum_{\text{faces}} \mathbf{n}_f A_f (p_f - p_c). \quad (8.1)$$

A number of geometric identities allow this equation to be simplified. In particular,

$$\sum_{\text{faces}} \mathbf{n}_f A_f = 0 \quad \text{and} \quad \mathbf{I} = \frac{1}{V} \sum_{\text{faces}} (\mathbf{x}_f^{\text{CG}} - \mathbf{x}_c^{\text{CG}}) \mathbf{n}_f A_f. \quad (8.2)$$

These expressions (like many of the paper's formulas) are a result of Gauss' Divergence Theorem. They both start from the exact expression, $\int a_{i,j} dV = \sum_{\text{faces}} \int a_i n_j dA$. If a_i is constant and the faces are planar then $0 = \sum_{\text{faces}} \int n_j dA = \sum_{\text{faces}} \mathbf{n}_f A_f$. If $a_i = x_i$ then $\int_V \delta_{ij} dV = \sum_{\text{faces}} \int x_i n_j dA$ and if the faces are planar the second relation is derived. These expression simplify the previous momentum vector equation on each cell to,

$$V_c \left(\frac{\partial}{\partial t} \mathbf{m}_c + \mathbf{a}_c \right) = - \sum_{\text{faces}} \mathbf{n}_f A_f p_f. \quad (8.3)$$

Since the advection diffusion term is also represented as a sum of fluxes we see that this is a statement of local momentum conservation for the discrete momentum, \mathbf{m}_c . One key distinction with standard finite volume methods is that the conserved quantity is a derived, not a primary variable. Conservation of momentum places restrictions on the form of the advection-diffusion term but does not restrict how the discrete momentum \mathbf{m}_c must be defined.

The derivation of momentum conservation is possible because the integration operator (the square root of the discrete Hodge star operator) \mathbf{R}^T , has an explicit geometric inverse. Global conservation is a result of the traditional telescoping property where internal fluxes cancel out.

9. Conservation of kinetic energy. Taking the dot product of the incompressible momentum equation with the velocity (and assuming constant viscosity for simplicity) gives the kinetic energy equation,

$$\frac{\partial(\frac{1}{2}u^2)}{\partial t} + \nabla \cdot \left(\mathbf{u} \frac{1}{2}u^2 \right) = -\nabla \cdot (\mathbf{u}p) + \nabla \cdot \nu \nabla \left(\frac{1}{2}u^2 \right) - \nu u_{i,j} u_{i,j}. \quad (9.1)$$

This equation shows that in the incompressible limit kinetic energy is convected and diffused. It is also transported by pressure and removed by velocity gradients, but it is never created. In the inviscid, incompressible limit, kinetic energy is a conserved variable. In the viscous limit, we would like the total kinetic energy to decrease at the correct rate (and never increase).

Numerical methods with numerical diffusion decrease kinetic energy more quickly than the physics would suggest ($\nu u_{i,j} u_{i,j}$). Numerical diffusion excessively smears solutions and can be detrimental in some situations, such as DNS and LES simulations of turbulence where energy dissipation is a critical physical process controlling the turbulence. Kinetic energy conservation is a statement that numerical diffusion is not present in the method. It is also a statement of stability.

To demonstrate kinetic energy conservation, each segment of the dual-edge equation within a cell is multiplied by the area weighted normal velocity component and summed over the cell faces to obtain

$$\sum_{\text{faces}} u_f A_f \mathbf{R}^T \left\{ \frac{1}{V_c} \mathbf{R} A_f \frac{\partial u_f}{\partial t} + \mathbf{a}_c \right\} = - \sum_{\text{faces}} u_f A_f (p_f - p_c). \quad (9.2)$$

Focusing first on the time derivative term we see that this is an approximation for the cell average kinetic energy because

$$u_f A_f \mathbf{R}^T \frac{1}{V_c} \mathbf{R} A_f \frac{\partial u_f}{\partial t} = V_c \mathbf{v}_c \cdot \frac{\partial \mathbf{v}_c}{\partial t} = V_c \frac{\partial \frac{1}{2} (\mathbf{v}_c)^2}{\partial t}. \quad (9.3)$$

If the system is fully discrete, this result still holds as long as we multiply each equation by the half-time velocity $u_f^{n+1/2} = \frac{1}{2}(u_f^n + u_f^{n+1})$. Then,

$$\begin{aligned} \frac{u_f^{n+1} + u_f^n}{2} A_f \mathbf{R}^T \frac{1}{V_c} \mathbf{R} A_f \frac{u_f^{n+1} - u_f^n}{\Delta t} &= V_c \frac{\mathbf{v}_c^{n+1} + \mathbf{v}_c^n}{2} \cdot \frac{\mathbf{v}_c^{n+1} - \mathbf{v}_c^n}{\Delta t} \\ &= V_c \frac{\frac{1}{2} (\mathbf{v}_c^{n+1})^2 - \frac{1}{2} (\mathbf{v}_c^n)^2}{\Delta t}. \end{aligned} \quad (9.4)$$

Due to incompressibility $\sum_{\text{faces}} u_f A_f = 0$ the second part of the pressure term is zero and the pressure term becomes a faced based conservative flux term, $-\sum_{\text{faces}} u_f^{n+1/2} A_f p_f$.

The advection-diffusion term becomes,

$$\sum_{\text{faces}} u_f^{n+1/2} A_f \mathbf{R}^T \mathbf{a}_c = \mathbf{a}_c \sum_{\text{faces}} u_f^{n+1/2} A_f \mathbf{R}^T = \mathbf{a}_c \cdot \mathbf{v}_c^{n+1/2} V_c. \quad (9.5)$$

Expanding the advection-diffusion term gives,

$$V_c \mathbf{v}_c^{n+1/2} \cdot \mathbf{a}_c = \mathbf{v}_c^{n+1/2} \cdot \sum_{\text{faces}} \{ \mathbf{u} u_f - \nu (\nabla \mathbf{u}) \cdot \mathbf{n} \}_f A_f. \quad (9.6)$$

Considering the convective term first,

$$\mathbf{v}_c^{n+1/2} \cdot \sum_{\text{faces}} \mathbf{u} u_f A_f = \mathbf{v}_c^{n+1/2} \cdot \sum_{\text{faces}} \frac{1}{2} (\mathbf{v}_c + \mathbf{v}_{c-n}) u_f A_f. \quad (9.7)$$

Here we have assumed that the velocity vector in the advective flux calculation is the simple average of the neighboring two cell velocities. One cell is the cell in question and the other is the nearest neighbor. The velocity in the first term can come out of the summation leaving the incompressibility condition (which is zero), so finally the advective term becomes $\sum_{\text{faces}} (\frac{1}{2} \mathbf{v}_c^{n+1/2} \cdot \mathbf{v}_{c-n}) u_f A_f$. This is also a flux term. Note that the kinetic energy fluxing through the cell faces is quite specific. It is one half of the dot-product of the two neighboring cell velocities. To obtain correct symmetry conservation also requires that the advection velocity be the half-time velocity. This implies that true conservation (in unsteady flows) occurs only if the advection term is semi implicit. The normal flux can be time lagged. This is an example of the implicit midpoint rule which is known to be a symplectic integrator. Other symplectic time integration schemes may also be possible. There appears to be a close connection between mimetic discretization schemes and symplectic time integration which should be explored more fully.

The diffusion term becomes

$$\mathbf{v}_c^{n+1/2} \cdot \sum_{\text{faces}} \nu (\nabla \mathbf{u}) \cdot \mathbf{n} A_f = \mathbf{v}_c^{n+1/2} \cdot \sum_{\text{faces}} \nu \frac{\partial \mathbf{u}}{\partial \mathbf{n}} A_f. \quad (9.8)$$

Using a very simple approximation for the normal derivative gives, $\sum_{\text{faces}} \nu \mathbf{v}_c^{n+1/2} \cdot (\mathbf{v}_{c-n} - \mathbf{v}_c) \frac{A_f}{L_f}$ which can be expanded in two parts as

$$\begin{aligned} &= \sum_{\text{faces}} \nu \frac{1}{2} (\mathbf{v}_{c-n}^{n+1/2} + \mathbf{v}_c^{n+1/2}) \cdot (\mathbf{v}_{c-n} - \mathbf{v}_c) \frac{A_f}{L_f} \\ &\quad - \sum_{\text{faces}} \nu \frac{1}{2} (\mathbf{v}_{c-n}^{n+1/2} - \mathbf{v}_c^{n+1/2}) \cdot (\mathbf{v}_{c-n} - \mathbf{v}_c) \frac{A_f}{L_f} \end{aligned} \quad (9.9)$$

this simplifies to a viscous diffusion of kinetic energy term and a negative definite dissipation term.

$$\begin{aligned} &= \sum_{\text{faces}} \nu \left(\frac{1}{2} \mathbf{v}_{c-n}^{n+1/2} \cdot \mathbf{v}_{c-n} - \frac{1}{2} \mathbf{v}_c^{n+1/2} \cdot \mathbf{v}_c \right) \frac{A_f}{L_f} \\ &\quad - \sum_{\text{faces}} \nu \frac{1}{2} (\mathbf{v}_{c-n}^{n+1/2} - \mathbf{v}_c^{n+1/2}) \cdot (\mathbf{v}_{c-n} - \mathbf{v}_c) \frac{A_f}{L_f}. \end{aligned} \quad (9.10)$$

To see that this latter term is an approximation of the dissipation term consider the divergence theorem applied to $\int (x_n \nu_{i,n} \nu_{i,m})_{,m} dV =$

$\sum_{\text{faces}} \int x_n \nu_{i,n} \nu_{i,m} n_m dA$. Then assuming the velocity gradients are constant in the volume gives

$$\nu_{i,m} \nu_{i,m} V_c = \sum_{\text{faces}} (x_f - x_c)_n \nu_{i,n} \nu_{i,m} n_m A_f. \quad (9.11)$$

With the approximation $(\mathbf{v}_f - \mathbf{v}_c) \approx \frac{1}{2}(\mathbf{v}_{c-n} - \mathbf{v}_c)$ this becomes the dissipation in a cell,

$$= \sum_{\text{faces}} \frac{1}{2} (\mathbf{v}_{c-n} - \mathbf{v}_c) \cdot \frac{(\mathbf{v}_{c-n} - \mathbf{v}_c)}{L_f} A_f. \quad (9.12)$$

The final statement of local energy conservation is,

$$\begin{aligned} & V_c \frac{\frac{1}{2}(\mathbf{v}_c^{n+1})^2 - \frac{1}{2}(\mathbf{v}_c^n)^2}{\Delta t} + \sum_{\text{faces}} \left(\frac{1}{2} \mathbf{v}_c^{n+1/2} \cdot \mathbf{v}_{c-n} \right) u_f A_f \\ &= - \sum_{\text{faces}} u_f^{n+1/2} A_f p_f + \sum_{\text{faces}} \nu \frac{\partial}{\partial n} \left(\frac{1}{2} \mathbf{v}_{c-n}^{n+1/2} \cdot \mathbf{v}_{c-n} \right) A_f \\ & \quad - \sum_{\text{faces}} \nu \frac{1}{2} (\mathbf{v}_{c-n}^{n+1/2} - \mathbf{v}_c^{n+1/2}) \cdot (\mathbf{v}_{c-n} - \mathbf{v}_c) \frac{A_f}{L_f}. \end{aligned} \quad (9.13)$$

For strict negative definite dissipation, the viscous diffusion term should use the half-time velocity (implicit midpoint rule) as well. Note that this equation is not solved in the numerical code. It is a rearrangement of the numerical equations that demonstrates that a discrete analog of kinetic energy conservation holds under certain fairly strict assumptions about the form of the advection and diffusion terms.

Global kinetic energy conservation follows from the internal cancellation of fluxes. The symmetry of the discrete Hodge star operator is useful for deriving kinetic energy conservation. However, a positive definite discrete Hodge star would be sufficient to formulate a strictly positive kinetic energy.

In order to test the kinetic energy conservation property a problem was chosen that has zero mass flux at the boundaries, but is inherently unsteady. The initial flow field of this problem involves a Rankine vortex located in the bottom left quadrant of a box. Although the problem is tested in a 3D domain (1.0m \times 1.0m \times 0.1m) and using an unstructured tetrahedral mesh, it is a two-dimensional flow since the motion only occurs in X - Y plane and only the Z component of the vorticity vector is nonzero. The domain is meshed with 7578 tetrahedra. The viscosity of the fluid is 0.01m²/s and the maximum initial velocity magnitude is 0.16m/s. The initial tangential velocity reaches its maximum at radius $R = 0.01$ m for an initial circulation Reynolds number of 1.

In numerical tests of the vortex motion in the absence of viscosity, the total discrete kinetic energy remained constant to within six significant

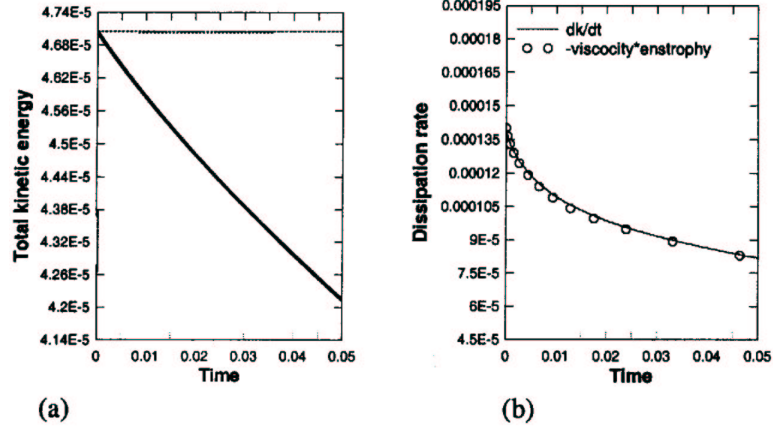


FIG. 4. Kinetic energy conservation test. (a) Total kinetic energy vs. time. (b) Rate of change of kinetic energy versus time (solid line) and total physical dissipation versus time (circles).

digits after 5000 time steps (0.05 Seconds). This is about as constant as can be expected given the tolerance prescribed for the iterative solver and is shown as the dotted line in Fig. 4(a). When viscosity is present ($0.01 \text{ m}^2/\text{s}$), the total discrete kinetic energy as a function of time is also shown in Fig. 4(a). The rate of change of the kinetic energy obtained by differentiating this curve is compared with the calculated physical dissipation. A perfect match is shown in Fig. 4(b). This test indicates that the theoretical analysis of this section is well founded and that there is no artificial dissipation in the method.

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REFERENCES

- [1] P.A. RAVIART AND J.M. THOMAS, *A mixed finite element method for second order elliptic problems*, Springer Lecture Notes in Mathematics Vol. **606**, Springer-Verlag, 292–315, 1977.
- [2] J.-C. NEDELEC, *Mixed finite elements in R^3* , Numer. Math., **50**, 315–341, 1980.
- [3] F.H. HARLOW AND J.E. WELCH, *Numerical calculations of time dependent viscous incompressible flow of fluid with a free surface*, Phys. Fluids, **8** (12), 2182–2189, 1965.
- [4] R.A. NICOLAIDES, *The covolume approach to computing incompressible flow*, Incompressible Computational Fluid Dynamics, M.D. Gunzburger & R.A. Nicolaides, eds., Cambridge University Press, 295–234, 1993.
- [5] J.M. HYMAN AND M. SHASHKOV, *The orthogonal decomposition theorems for*

- mimetic finite difference methods*, SIAM J. on Num. Anal., **36** (3), 788–818, 1999.
- [6] P. WESSELING, A. SEGAL, C.G.M. KASSELS, AND H. BIJL, *Computing flows on general two-dimensional nonsmooth staggered grids*, J. of Engin. Math., **34**, 21–44, 1998.
 - [7] J.B. PEROT, *Conservation properties of unstructured staggered mesh schemes*, J. Comput. Phys., **159**, 58–89, 2000.
 - [8] D. WHITE, *Orthogonal vector basis functions for time domain finite element solution of the vector wave equation*, 8th Biennial IEEE Conference on Electromagnetic Field Computation, Tucson, AZ. UCRL-JC-129188, 1998.
 - [9] W. CHANG, F. GIRALDO AND J.B. PEROT, *Analysis of an Exact Fractional Step Method*, J. Comput. Phys., **179**, 1–17, 2002.
 - [10] J.B. PEROT AND X. ZHANG, *Reformulation of the unstructured staggered mesh method as a classic finite volume method*, Finite Volumes for Complex Applications II, Hermes Science Publications, pp. 263–270, 1999.
 - [11] M. SHASHKOV, B. SWARTZ, AND B. WENDROFF, *Local reconstruction of a vector field from its normal components on the faces of grid cells*, J. Comput. Phys., **139**, 406–409, 1998.
 - [12] J.B. PEROT AND R. NALLAPATI, *A Moving Unstructured Staggered Mesh Method for the Simulation of Incompressible Free-Surface Flows*, J. Comput. Phys., **184**, 192–214, 2003.
 - [13] P. CASTILLO, J. KONING, R. RIEBEN, M. STOWELL, AND D. WHITE, *Discrete Differential Forms: A Novel Methodology for Robust Computational Electromagnetics*, LLNL report UCRL-ID-151522, January 2003.
 - [14] R. RIEBEN, *A Novel High Order Time Domain Vector Finite Element Method for the Simulation of Electromagnetic Device*, Ph.D. dissertation, University of California at Davis, Livermore, CA, 2004 UCRL-TH-205466.
 - [15] Y. MORINISHI, T.S. LUND, O.V. VASILYEV, AND P. MOIN, *Fully Conservative Higher Order Finite Difference Schemes for Incompressible Flow*, J. Comput. Phys., **143**, 90–124, 1998.
 - [16] O.V. VASILYEV, *High Order Finite Difference Schemes on Non-uniform Meshes with Good Conservation Properties*, J. Comput. Phys., **157**, 746–761, 2000.
 - [17] X. ZHANG, D. SCHMIDT, AND J. B. PEROT, *Accuracy and Conservation Properties of a Three-Dimensional Unstructured Staggered Mesh Scheme for Fluid Dynamics*, J. Comput. Phys., **175**, 764–791, 2002.
 - [18] C. MATTIUSI, *An analysis of finite volume, finite element, and finite difference methods using some concepts from algebraic topology*, J. Comput. Phys., **133**, 289–309, 1997.
 - [19] D.K. LILLY, *On the computational stability of numerical solutions of time-dependent non-linear geophysical fluid dynamics problems*, Mon. Weather Rev., **93** (1), 11–26, 1965.