1 Introduction. This paper deals with the problem of numerically determining a three dimensional vector field from its divergence and curl. The need to do this occurs in several fields including fluid dynamics and electromagnetics. The governing equations are often solved using indirect approaches including potential formulations or Biot–Savart type integrals [5] and least squares [1].

A good reason to be cautious about direct discretizations is that the equations are overdetermined, being a system of four equations in three unknowns, and it is not immediately evident what effect this will have at the discrete level. Nevertheless, since potential formulations can suffer from spurious mode problems [6] and the Biot–Savart approach requires special handling of boundaries, a direct treatment may be preferable. We present such a treatment in this paper.

The method we discuss is a generalization of that presented in [3] for planar systems. As in the planar case we use dual mesh systems made up of "complementary volumes" (or "covolumes") of which the prime examples are classical Voronoi-Delaunay mesh pairs. In the Voronoi–Delaunay approach the domain is suitably partitioned into tetrahedra which are considered to form a primal (Delaunay) mesh in the domain Ω. A dual (Voronoi) mesh is formed by connecting the circumcenters of the tetrahedra, giving a set of convex polygons each of which encloses a unique tetrahedral vertex. Combinatorial and topological properties of the primal and dual mesh systems play an important part in our analysis, allowing us to conclude, for example, that the solution of the discretized equations is exactly determined by the data if the same is true of the original system. On the other hand, the metric properties of the mesh system are used in deriving the error estimates. The interplay of topological and metric properties is a common feature of covolume discretizations.

The paper contains six sections. The second section deals with combinatorial properties of the mesh system. The third section shows how discrete vector fields are defined on the meshes and defines the basic integral operations for the discrete fields. These definitions are set up so that an important orthogonality property of vector fields is preserved (theorem 4). The discrete approximations and the basic error estimates are in section 4. In section 5 we specialize the results to rectangular meshes for which we are able to obtain improved convergence rates. The final section contains some basic numerical verifications.

2 Mesh notations and some basic results. We will prove our results for the case of a domain Ω which is a bounded polyhedron in R^3 with boundary Γ. The results we present are generally valid for multiply connected domains and domains with cutouts. The techniques for extending the results are similar to those used in [3] for the two dimensional case although there is greater variety in three dimensional cases depending on the genus of the surface(s) bounding the obstacle(s).

Assume that Ω has a *primal* family of finite element style tetrahedral partitions, parameterized by the maximum side length which is generically denoted by h. We will assume that the ratios of the radii of the circumscribing spheres and the inscribed spheres of all the individual tetrahedra are uniformly bounded above and below as h approaches 0. A dual mesh is formed by connecting adjacent tetrahedral circumcenters and, in the case of tetrahedra with a face on a boundary, by connecting their circumcenters with those of their boundary faces. By elementary geometry the connecting edges are perpendicular to the associated tetrahedral faces. These connections also form the edges of a set of polyhedra. It follows from elementary geometry that the edges of the tetrahedra are perpendicular to and in one–to–one correspondence with the faces of the dual polyhedra (covolumes) and dually. The reciprocal orthogonality between edges and faces is the key to the results which follow. A survey of algorithms for generating Voronoi–Delaunay meshes is given in [4].

For an entirely arbitrary tetrahedral partition the structure of the covolume partition can be complicated. To obtain a practical algorithm we will restrict the tetrahedral partition so that the dual partition has two (possibly dependent) properties. These properties are (1) interior covolumes have faces which are simple (planar) polygons and (2) each tetrahedral interior node lies in exactly one covolume. This does restrict the primal tesselation somewhat but not unduly. For instance the two conditions are certainly satisfied for a tetrahedral partition in which the dihedral angles are all acute. In that case, the two meshes form a Delaunay–Voronoi pair and the interior covolumes are convex. In addition the faces of the covolumes are not merely simple but convex as well. More generally any Delaunay–Voronoi pair will satisfy (1) and (2).

The N nodes of the tetrahedral mesh are assumed to be numbered sequentially in some convenient way, and likewise the T nodes of the dual mesh. Similarly, the F faces (edges) and E edges (faces) of the primal (dual) mesh are sequentially numbered. A subscript 1 on one of these quantities denotes the corresponding interior number. For example F_1 denotes the number of tetrahedral interior faces. The individual tetrahedra, faces, edges and nodes of the primal mesh are denoted by τ_i, μ_j, σ_k and ν_l respectively. Those of the covolume mesh are denoted by primed quantities such as σ'_j. A direction is assigned to each primal edge by the rule that the positive direction is from low to high node number. The dual edges are directed by the corresponding rule.

We will use the following standard results:

Lemma 1 *Let N, F, E and T denote the number of nodes, faces, edges and tetrahedra of a given tesselation of a polyhedral domain. Then*

$$N + F = E + T + 1 \tag{1}$$

$$N_1 + F_1 = E_1 + T - 1. \tag{2}$$

These can easily be proven by successive deletions of tetrahedra from the triangulation. ∎

3 Discrete vector fields. The main theorems in this section (theorems 3 and 4) are discrete analogs of theorems in vector field theory. Theorem 3 asserts the existence of a scalar potential when discrete circulation equations are satisfied and theorem 4 gives a discrete Helmholtz decomposition of a field of normal components.

Each boundary $\partial\mu_j$ ($\partial\mu'_k$) is assumed to be oriented by a right hand rule applied relative to the directed edge σ'_j (σ_k).

For each strictly interior dual edge σ'_j we can form a vector whose kth component is the sign of the orientation of the edge relative to the orientation of the kth strictly interior dual face. From these vectors we obtain the $F_1 \times E_1$ matrix G defined as follows:

$$(G)_{jk} := \begin{cases} +1 & \text{if } \sigma'_j \text{ is oriented positively along } \partial\mu'_k \\ -1 & \text{if } \sigma'_j \text{ is oriented negatively along } \partial\mu'_k \\ 0 & \text{if } \sigma'_j \text{ does not meet } \partial\mu'_k. \end{cases}$$

G has rank $E_1 - N_1$. To see the reason for this, note first that each column of G is associated with a dual face. Now take any interior covolume and sum the associated columns, each weighted ± 1 according to whether its normal points out of or into the covolume. Then the contributions from each dual edge appear twice in each sum with opposite signs. In this way we can form one null vector of G^t for each interior covolume. It is clear that there are no other vectors in the null space so the result follows.

In addition to G we will use another matrix B_1 containing the orientations of the tetrahedral faces relative to the outer normals of the tetrahedra. This matrix is defined for interior faces and has dimensions $F_1 \times T$. The definition of B_1 is:

$$(B_1)_{ji} := \begin{cases} +1 & \text{if } \mu_j \text{ is oriented with } \partial\tau_i \\ -1 & \text{if } \mu_j \text{ is oriented against } \partial\tau_i \\ 0 & \text{if } \mu_j \text{ does not meet } \partial\tau_i. \end{cases},$$

where "oriented with" means that the normal direction of μ_j is parallel to the outer normal of $\partial\tau_i$. The T dimensional vector with 1 in every position is in the null space of B_1 and is the only such vector, so that the rank of B is $T-1$.

In addition to B_1 we will also use the matrix B which is obtained from B_1 by augmenting it with rows corresponding to the dual edges which are normal to boundary faces. Recall that these edges pass through the circumcenters of the boundary faces. The additional values for the domain of B are associated with these circumcenters.

B_1 and G are related through $G^t B_1 = 0$. To see this, take a standard basis vector and multiply it by B. Then values ± 1 or 0 result on the dual edges the positive (negative) sign being associated with a dual edge directed out of (into) the node which carries the unit value. Multiplication by G^t corresponds to forming a signed sum of these values around the dual faces where the signs are precisely such as to effect a cancellation of the nonzero contributions. Transposing this result shows that $R(G) \subset N(B_1^t)$ where $N(\cdot)$ and $R(\cdot)$ denote the null space and range of their arguments.

Theorem 1 *Let $v \in R^{F_1}$. Then $\exists\ \phi \in R^T$ such that $v = B_1\phi$ if $G^t v = 0$.*

Proof. Since B_1 is $F_1 \times T$ and of rank $T-1$ and using lemma 1 we have

$$\begin{aligned} \dim N(B_1^t) &= F_1 - T + 1 \\ &= E_1 - N_1. \end{aligned}$$

Recalling that $R(G) \subset N(B_1^t)$ and since $\dim R(G) = E_1 - N_1$ we have $N(B_1^t) = R(G)$. Solvability of the equation

$$B_1\phi = v$$

holds if

$$(v, z) = 0 \quad \forall z \in N(B_1^t),$$

where (,) denotes the standard Euclidean inner product. From above this is equivalent to

$$(v, G\psi) \;=\; 0 \quad \forall \psi \in R^{N_1}$$

and these are equivalent to the theorem. ■

The covolume algorithm for the div-curl equations provides approximations to the quantities $\mathbf{u}\cdot\mathbf{n}$, where $\mathbf{u}$ denotes the exact solution vector at the center of a primal face and $\mathbf{n}$ denotes a normal to the face. The corresponding approximate quantities are denoted by u_j where j indexes the faces.

Any set of normal components defined on faces can be identified with R^F. We will introduce an inner product into R^F by

$$(u, v)_W := \sum_{\mu_j \in \bar{\Omega}} u_j v_j s_j h'_j,$$

where s_j is the area of μ_j and h'_j is the length of σ'_j. The resulting inner product space is denoted by $\mathcal{U}$, and $\mathcal{U}_0$ denotes the space

$$\mathcal{U}_0 := \{u \in \mathcal{U}; u\mid_\Gamma = 0\}.$$

The associated norm is denoted by $\|\cdot\|_W$. Clearly, this is three times a discrete L^2 norm.

For each tetrahedron τ_i discrete flux and divergence operators are defined on $\mathcal{U}$ by

$$(\hat{D}u)_i := \sum_{\mu_j \in \partial\tau_i} u_j \tilde{s}_j$$

and

$$(Du)_i := (\hat{D}u)_i / A_i.$$

By $\tilde{s}_j$ we mean s_j negatively signed if the corresponding velocity component is directed towards the inside of τ_i and positively signed otherwise.

For each interior covolume face μ'_k discrete circulation and curl operators are defined by

$$(\hat{C}u)_k := \sum_{\sigma'_j \in \partial\mu'_k} u_j \tilde{h}'_j$$

and

$$(Cu)_k := (\hat{C}u)_k / s'_k.$$

The tilde on h'_j means that this quantity is to be taken with a negative sign if the dual edge is directed against the positive sense of description of $\partial\mu'_k$ and a positive sign otherwise.

Denote by S and H'_b the diagonal matrices $S := \mathrm{diag}(s_j)$ and $H'_b := \mathrm{diag}(h'_j)$. It can be checked directly that

$$\begin{aligned} \hat{D} &= B^t S \\ \hat{C} &= G^t H', \end{aligned}$$

where H' denotes the restriction of H'_b to interior dual edges. We also define difference operators

$$\begin{aligned} P_b\phi &:= (H'_b)^{-1} B\phi \quad \forall \phi \in R^T \\ P\phi &:= (H')^{-1} B_1\phi \quad \forall \phi \in R^T. \end{aligned}$$

Corresponding to theorem 1 we have

Theorem 2 *Let $v \in R^{F_1}$. Then $\exists\ \phi \in R^T$ such that $v = P\phi$ if $Cv = 0$.* ■

Now introduce two subspaces of $\mathcal{U}_0$:

$$\begin{aligned} \mathcal{Z}_0 &= \{u \in \mathcal{U}_0; \hat{D}u = 0\} \\ \mathcal{W}_0 &= \{u \in \mathcal{U}_0; \hat{C}u = 0\}. \end{aligned}$$

Then we have

Theorem 3 *Let $u \in \mathcal{Z}_0$, $v \in \mathcal{W}_0$, then*

$$(u, v)_W = 0.$$

Proof. From theorem 2 and using summation by parts we have

$$(u, v)_W = (u, P\phi)_W = (u, P_b\phi)_W = (\hat{D}u, \phi) \quad \forall \phi \in R^T.$$

Since $u \in \mathcal{Z}_0$ we have $\hat{D}u = 0$ and the theorem follows. ∎

4 Div-curl systems. In this section we formulate the discrete approximations for div-curl equations and show that they have a unique solution (theorem 5). The basic error estimate is given in theorem 6.

We consider the three dimensional div-curl problem for $\mathbf{u}$,

$$\begin{aligned} \operatorname{div} \mathbf{u} &= \rho && (3) \\ \mathbf{curl}\, \mathbf{u} &= \boldsymbol{\omega} && (4) \\ \mathbf{u} \cdot \mathbf{n} \,|_\Gamma &= f \quad . && (5) \end{aligned}$$

We will assume that the following compatibility conditions hold:

$$\begin{aligned} \operatorname{div} \boldsymbol{\omega} &= 0 && (6) \\ \int_\Omega \rho dv &= \int_\Gamma f ds. && (7) \end{aligned}$$

See [2] for the mathematical background to this problem.

Equations (3)-(5) are discretized by

$$\begin{aligned} Du &= \bar{\rho} && (8) \\ Cu &= \bar{\omega}_{\mu'} && (9) \\ u \,|_\Gamma &= \bar{f}, && (10) \end{aligned}$$

where

$$\begin{aligned} \bar{\rho}_i &= \frac{1}{A_i} \int_{\tau_i} \rho dv \\ (\bar{\omega}_{\mu'})_k &= \frac{1}{s'_k} \int_{\mu'_k} \boldsymbol{\omega} \cdot \mathbf{t} ds \\ \bar{f} &= \frac{1}{s_j} \int_{\mu_j} f ds \qquad \mu_j \in \Gamma. \end{aligned}$$

The equations (8)-(10) are not all independent. In fact, there are at least E_1 relations between the equations (9) corresponding to the fact that the area weighted sums of the data over covolumes is zero (corresponding to the compatibility condition (7)) as well as a further relation which is equivalent to (7). The discrete equations do have a unique solution as we prove next.

Theorem 4 *Equations (8)-(10) have a unique solution.*

Proof. Consider the homogeneous equations with $\bar{\omega}_{\mu'} = 0$ and $f = 0$ in (8)-(10). These equations have at least one solution u, and this solution satisfies $u \in \mathcal{Z}_0$ and $u \in \mathcal{W}_0$. But then theorem 3 implies $u = 0$ which implies the uniqueness part of the result. Let K denote the $(T + F_1 \times F_1$ coefficient matrix of the linear system; then it follows that K has rank F_1.

For the existence, we consider the linear system generated by (8)-(10). and let K' denote the corresponding augmented matrix of K of order $(T + E_1) \times (F_1 + 1)$. It follows from the compatibility conditions that this matrix has rank at most $T - 1 + E_1 - N_1 = F_1$ and existence follows from this. ∎

Next, we introduce two functions $u^{(1)}$ and $u^{(2)}$ defined by

$$\begin{aligned} u_j^{(1)} &:= \frac{1}{s_j} \int_{\mu_j} \mathbf{u} \cdot \mathbf{n} ds \quad \mu_j \in \bar{\Omega} \\ u_j^{(2)} &:= \frac{1}{h'_j} \int_{\sigma'_j} \mathbf{u} \cdot \mathbf{n} ds \quad \sigma'_j \in \Omega. \end{aligned}$$

If σ'_j is connected to the boundary Γ, $u_j^{(2)} := u_j^{(1)}$.

Lemma 2 *Assume that $\mathbf{u} \in W^{1,p}(\Omega), p > 2$, then we have*

$$\left\| u^{(1)} - u^{(2)} \right\|_W \leq Ch|\mathbf{u}|_{1,p,\Omega}.$$

Proof. Let κ_j denote the polyhedron associated with the face μ_j and the dual edge σ'_j which is obtained by connecting the circumcenters of the primal cells which share μ_j to its vertices. By a Sobolev embedding theorem we have

$$W^{1,p}(\kappa_j) \hookrightarrow L^1(\kappa_j^r) \quad p > 2 \quad r = 1, 2,$$

where $\kappa_j^1 = \sigma'_j$ and $\kappa_j^2 = \mu_j$. It follows that $V : \mathbf{u} \to u_j^{(1)} - u_j^{(2)}$ defines a bounded linear functional on $W^{1,p}(\kappa_j)$. Clearly, $u_j^{(1)} - u_j^{(2)}$ is zero for constant $\mathbf{u}$ so we have

$$\left| u_j^{(1)} - u_j^{(2)} \right| \leq C_1(h, p)|\mathbf{u}|_{1,p,\kappa_j}$$

and a standard rescaling argument then shows that the right side is

$$\leq Ch^{1-3/p}|\mathbf{u}|_{1,p,\kappa_j}.$$

where C is independent of h and u. Summing over the domain we obtain

$$\begin{aligned} \sum_{\mu_j \in \bar{\Omega}} |u_j^{(1)} - u_j^{(2)}|^2 s_j h'_j &\leq C \sum_{\mu_j \in \bar{\Omega}} h^{2-6/p} |\mathbf{u}|^2_{1,p,\kappa_j} s_j h'_j \\ &\leq Ch^{5-6/p} \sum_{\mu_j \in \bar{\Omega}} |\mathbf{u}|^2_{1,p,\kappa_j}. \end{aligned}$$

Then by Hölder's inequality and taking C such that $h^3 F \leq C$ we have

$$\begin{aligned}\left\|u^{(1)} - u^{(2)}\right\|_W^2 &= Ch^{5-6/p}\left(\sum_{\mu_j \in \bar{\Omega}} |\mathbf{u}|_{1,p,\kappa_j}^p\right)^{2/p}\left(\sum_{\mu_j \in \bar{\Omega}} 1\right)^{(p-2)/p} \\ &\leq Ch^{5-6/p} F^{(p-2)/p} |\mathbf{u}|_{1,p,\Omega}^2 \\ &\leq Ch^2 |\mathbf{u}|_{1,p,\Omega}^2\end{aligned}$$

which we wanted to show. ∎

From this lemma we can obtain the error basic estimate for the approximate solution:

Theorem 5 *Assume that* $\mathbf{u} \in W^{1,p}(\Omega), p > 2$. *Then we have*

$$\left\|u - u^{(1)}\right\|_W \leq Ch|\mathbf{u}|_{1,p,\Omega}.$$

Proof. Define $v^{(i)} = u - u^{(i)}, i = 1, 2$, clearly, $v^{(1)} \in \mathcal{Z}_0$ and $v^{(2)} \in \mathcal{W}_0$. Let $\bar{u} = (u^{(1)} + u^{(2)})/2$. A calculation using Theorem 3 shows that

$$\|u - \bar{u}\|_W = \frac{1}{4}\left\|u^{(1)} - u^{(2)}\right\|_W.$$

On the other hand, we have

$$u - \bar{u} = u - u^{(1)} - (u^{(2)} - u^{(1)})/2.$$

Then

$$\left\|u - u^{(1)}\right\|_W \leq \|u - \bar{u}\|_W + \frac{1}{2}\left\|u^{(2)} - u^{(1)}\right\|_W$$

and the result follows from lemma 2. ∎

5 Uniform meshes. In this section we will look more closely at the situation in which the domain Ω is a cube and the mesh is a uniform cubic mesh. For this case the dual mesh is also uniform cubic, being shifted by one half the mesh spacing in each coordinate direction from the primal mesh.

For this uniform mesh case the basic error estimate can be improved. The difference in the uniform mesh case arises from the improved approximation theory which is possible. Apart from approximation theory the earlier results have obvious analogs which it is unnecessary to spell out in detail. The new approximation results correspond to lemma 2 and theorem 5.

Lemma 3 *Assume that* $\mathbf{u} \in H^2(\Omega)$. *Then we have*

$$\left\|u^{(1)} - u^{(2)}\right\|_W \leq Ch^2|\mathbf{u}|_{2,\Omega}.$$

Proof. As previously,let κ_j denote the polyhedron associated with the face μ_j and the dual edge σ'_j. By a Sobolev embedding theorem we have

$$H^2(\kappa_j) \hookrightarrow L^1(\kappa_j^r) \quad r = 1, 2,$$

where $\kappa_j^1 = \sigma'_j$ and $\kappa_2^2 = \mu_j$. Hence $V : \mathbf{u} \rightarrow u_j^{(1)} - u_j^{(2)}$ is a bounded linear functional on $H^2(\kappa_j)$. For uniform meshes it is easy to verify that $u_j^{(1)} - u_j^{(2)}$ vanishes for linear $\mathbf{u}$ so it follows that

$$\left| u_j^{(1)} - u_j^{(2)} \right| \leq C(h)|\mathbf{u}|_{2,\kappa_j}$$

and the usual rescaling argument gives that the right side is

$$\leq Ch^{1/2}|\mathbf{u}|_{2,\kappa_j}.$$

Then it follows that

$$\begin{aligned} \sum_{\mu_j \in \bar{\Omega}} |u_j^{(1)} - u_j^{(2)}|^2 s_j h'_j &\leq C \sum_{\mu_j \in \bar{\Omega}} h|\mathbf{u}|^2_{2,\kappa_j} s_j h'_j \\ &\leq Ch^4 \sum_{\mu_j \in \bar{\Omega}} |\mathbf{u}|^2_{2,\kappa_j}. \end{aligned}$$

which gives the result. ∎

Theorem 6 *Assume that* $\mathbf{u} \in H^2(\Omega)$,, *then we have*

$$\left\| u - u^{(1)} \right\|_W \leq Ch^2|\mathbf{u}|_{2,\Omega}.$$

Proof. The proof is similar to the proof of theorem 5. ∎

6 Numerical test. To confirm the rate of convergence given by the previous theorem we computed a numerical example. The domain of computation is the unit cube. The domain was first divided into equal small cubes with dimension $h \times h \times h$. Then a dual mesh was generated (dual cubes). We consider the following problem

$$\begin{aligned} \mathrm{div}\, \mathbf{u} &= 0 \\ \mathbf{curl}\, \mathbf{u} &= \boldsymbol{\omega} \\ u_x \mid_{x=0} &= u_y \mid_{y=0} = u_z \mid_{z=0} = 0 \\ u_x \mid_{x=1} &= \sin(1)\cos(y)\cos(z) \\ u_y \mid_{y=1} &= -2\cos(x)\sin(1)\cos(z) \\ u_z \mid_{z=1} &= \cos(x)\cos(y)\sin(1) \end{aligned}$$

where $\mathbf{u} = (u_x, u_y, u_z)$ and

$$\boldsymbol{\omega} = \begin{pmatrix} \cos(x)\sin(y)\sin(z) \\ -2\sin(x)\cos(y)\sin(z) \\ \sin(x)\sin(y)\cos(z) \end{pmatrix}.$$

The exact solution of this problem is

$$\mathbf{u} = \begin{pmatrix} \sin(x)\cos(y)\cos(z) \\ -2\cos(x)\sin(y)\cos(z) \\ \cos(x)\cos(y)\sin(z) \end{pmatrix}.$$

Four meshes were used in the computation, $h = 0.5$ for the coarsest mesh and $h = 0.0625$ for the finest mesh. The results are shown in the table.

Table 1. Errors Between u and $u^{(1)}$.

h	0.5	0.25	0.125	0.0625
$\|u-u^{(1)}\|_W$	0.26d-01	0.56d-02	0.13d-02	0.31d-03

The average rate of convergence for this example is about $h^{2.1}$ which is slightly better than the rate given by the theorem.

Conclusions. We have presented an algorithm for discretizing three dimensional div-curl systems in three dimensions. We proved uniqueness of the solution to the discretized equations and an error estimate showing first order convergence in general and second order for regular meshes. A basic numerical example was also shown.

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