Comment on "Modifications to the gradient schemes on unstructured cell centered grids for the accurate determination of gradients near conductivity changes" [Phys. Fluids 31, 047104 (2019)]

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In a very recent article, Trautmann et al.¹ proposed a modified gradient computation technique for problems involving conductivity jumps. Referred to as the Flux Conservative Divergence Theorem (FC-DT), the modified approach computes the face values of electric potential by accounting for the nonlinear behavior in cells across which the conductivity jumps occur. The authors showed that the FC-DT approach could accurately compute the gradients (electric field) and the current density on Cartesian meshes but led to large errors on distorted meshes when a cross-gradient was imposed. The goal of this comment is to highlight further shortcomings of the FC-DT approach on arbitrary polygonal meshes by effecting comparison with the Modified Green Gauss (MGG) reconstruction, which is also a gradient scheme based on the divergence theorem and to probe the role of grid quality in this context.

The FC-DT technique computes the face values of electric potential using conductivity-weighted linear interpolation with a correction for grid skewness by the following equation:

$$
\phi_f = \frac{\beta \sigma_P \phi_P + (1-\beta) \sigma_N \phi_N}{\beta \sigma_P + (1-\beta) \sigma_N} + (\beta \nabla \phi_P + (1-\beta) \nabla \phi_N) \cdot (\mathbf{f} - \mathbf{f}').
$$

These face values are used to compute the electric field ∇*ϕ* and hence the current density $\mathbf{j} = \sigma \nabla \phi$ in each cell. On skewed meshes where $f \neq f'$, the FC-DT approach involves an iterative process since the

correction depends on the gradients. The Modified Green Gauss (MGG) reconstruction, derived from a variant of the divergence theorem, 2 reconstructs the current density at the cell centers for problems with conductivity jumps by the following equation:³

$$
\mathbf{j}_P = \frac{1}{\Omega} \sum_f \sigma_f \left(\frac{\delta \phi}{\delta n} \right)_f (\mathbf{f} - \mathbf{c}) \Delta s_f,
$$

where **f** and **c** are the position vectors of the centers of the face and cell, respectively; Δs_f is the face area; Ω is the cell volume; and the summation is over all faces of the cell. The conductivity at face σ_f is obtained from the values at cells using harmonic averaging, 1 while the normal derivative at the face is computed using Zwart's approach with nonorthogonality correction by the following equation:²

$$
\bigg(\frac{\delta \phi}{\delta n}\bigg)_{f} = \alpha \frac{\phi_{N} - \phi_{P}}{r_{NP}} + \big(\mathbf{n}_{f} - \alpha \mathbf{r}_{f}\big) \cdot \bigg(\frac{\nabla \phi_{P} + \nabla \phi_{N}}{2}\bigg),
$$

where \mathbf{n}_f is the unit normal to the face, \mathbf{r}_f is the unit vector along the line joining P and N , and r_{NP} is the distance between the cell centers along that line. The value of $\alpha = \mathbf{n}_f \cdot \mathbf{r}_f$ is a measure of nonorthogonality, and it must be emphasized that MGG reconstruction becomes iterative on nonorthogonal meshes. The electric field at the cell center can be calculated from the reconstructed current density, and this

FIG. 1. Meshes used in the study: (a) uniform Cartesian triangulated mesh, (b) nonuniform Cartesian triangulated mesh, (c) randomly triangulated mesh, and (d) distorted structured mesh. The highlighted horizontal line is the interface at $y = 1$ across which the conductivity jump takes place, and only the zoomed-in view of the meshes are shown for clarity.

approach has been employed previously for electrohydrodynamic simulations with property jumps.³

We investigate the role of mesh topology on the performance of FC-DT and MGG approaches for the two test cases discussed in the work by Trautmann et al , where a piece-wise linear variation for the electric potential is considered. Studies are conducted on four different meshes, as shown in Fig. 1, in addition to a uniform Cartesian mesh with a conductivity ratio of 1000. The two test cases have a constant current density of 10 A/m² in the vertical direction (y-direction) with case 1 considering no cross gradient (in the x-direction), while case 2 has a constant additional cross-gradient of 10 V/m. The maximum error in current density j_y in the domain obtained for case 1 and case 2 are presented in Table I. It may be remarked that we employ the same definition of error as employed in the work by Trautmann et al ¹

From Table I, we infer the following:

- 1. On the uniform Cartesian mesh, which is orthogonal $(\alpha = 1)$ and nonskewed, it is easy to see that the current density errors from both approaches are close to machine precision, independent of the cross-gradient. This is not surprising because it is easy to show that the expression for current density using MGG and FC-DT approaches are identical on this mesh where the computation is noniterative as well.
- 2. On the uniform Cartesian triangulated mesh, the FC-DT approach computes the current density exactly for case 1 but incurs a significant error for case 2. This mesh, which is obtained by dividing the uniform Cartesian mesh along the

diagonal in all cells, has no skewness but is nonorthogonal $(f = f', \beta = 1/2$ and $\alpha < 1$). One can see with a little effort that the computed value using the FC-DT approach of the electric potential at the interface differs from its true value by an amount proportional to the product of $(x_P - x_N)$ and the additional cross-gradient. The cross-gradient is zero for case 1 and nonzero for case 2, which explains why the FC-DT approach has no current density errors in the former case but larger errors in the latter case. The FC-DT approach clearly fails to preserve constant current density j_y , as can be seen from Fig. $2(a)$, which also depicts significant errors near the interface. On the nonuniform Cartesian triangulated mesh, we observe that the FC-DT approach fails to exactly compute the current density even when there are no cross-gradients, and the errors are accentuated when a cross-gradient is imposed. This is due to the combined effects of skewness and nonorthogonality at the interface because of which the correction term strongly depends on the y-gradients, and the iterative process converges quickly (in 6 iterations) to an erroneous electric field. MGG reconstruction computes the current density accurately for both test cases on uniform [see Fig. $2(a)$] as well as nonuniform Cartesian triangulated meshes but requires 22 and 135 iterations, respectively.

3. On the randomly triangulated mesh, both the gradient techniques lead to machine precision errors in the current density for the two test cases. This is attributed to the perfect symmetry near the interface owing to the construction of the mesh (which is by reflection about $y = 1$), resulting in zero

skewness and complete orthogonality at the interface although the mesh is skewed and nonorthogonal elsewhere in the domain.

4. The distorted structured mesh has asymmetry near the interface, resulting in varying amounts of skewness and nonorthogonality along it. While the FC-DT approach which converges in 6 iterations unsurprisingly fails to preserve the exact current density for both test cases (with errors of 70% for case 1 and 4500% for case 2), MGG reconstruction requires 35 iterations to converge but does not result in machine-precision errors either for both the test cases on this mesh. This is also reflected in the centerline current density profile shown in Fig. 2(b) as well as the error contours shown in Fig. 3, which clearly indicate that the errors are concentrated in the vicinity of the interface. The location of maximum errors depends upon the nonorthogonality and skewness of the mesh at the interface. Nevertheless, the errors from MGG reconstruction

are significantly smaller (less than 0.2%) compared to those from the FC-DT approach and are expectedly unaffected by the cross-gradient. Interestingly, the errors in current density j_y do not diminish with progressive grid refinement for both approaches, as shown in Table II. However, the errors in electric field E_x due to the constant cross-gradient (see Table II) decrease with increasing grid resolution for MGG reconstruction, while the FC-DT approach exhibits an inconsistent behavior.

The FC-DT approach accurately computes the electric field and current density to machine precision only in cases where the grid is orthogonal and nonskewed in the vicinity of the interface. The modification proposed by the authors $^{\rm l}$ is based on one-dimensional considerations and does not recognize the tangential jump in the current density when a constant cross-gradient is imposed on grids that are skewed and/or nonorthogonal at the vicinity of the

FIG. 3. Contours of errors in current density *j^y* on the distorted structured mesh for case 2: (a) FC-DT approach and (b) MGG reconstruction. The horizontal line denotes the interface, and only the part of the domain in the vicinity of the interface is shown for clarity.

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conductivity jump. MGG reconstruction, which is a vector interpolation based on the divergence theorem, is advantageous because it directly reconstructs the conserved current density from its normal component at the faces. The methodology thus remains transparent to the tangential jump at the interface, thereby resulting in current density estimates with acceptable errors on arbitrary polygonal meshes, independent of the magnitude of the cross-gradient. However, on Cartesian meshes and those derived from it (triangulated meshes), the electric field and current density errors from MGG reconstruction are close to machine precision. The ability of MGG reconstruction to compute the gradients with reasonable accuracy on arbitrary polygonal meshes necessitates 10–150 iterations depending on the extent of nonorthogonality. Nevertheless, these computations are inherent to finite volume solvers that involve time-marching, and it is possible to devise a noniterative variant of MGG reconstruction that is both inexpensive and accurate in that context.²

We believe that MGG reconstruction^{2,3} as well as a recent gradient scheme based on the hyperbolic treatment of diffusion⁴ could provide ideas to further improve the FC-DT scheme on generic unstructured meshes for problems with discontinuous coefficients.

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