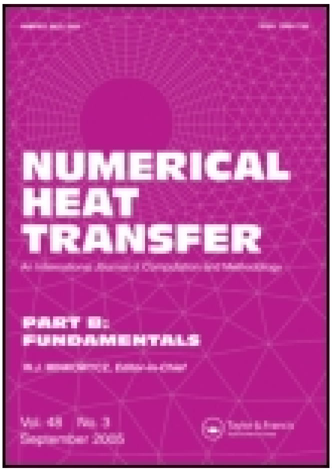

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On the Discretization of the Diffusion Term in Finite-Volume Continuum Mechanics

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ON THE DISCRETIZATION OF THE DIFFUSION TERM IN FINITE-VOLUME CONTINUUM MECHANICS

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The aim of this article is twofold: first, to present and analyze various practices for the finite-volume discretization of the diffusion term in continuum mechanics transport equations; and second, to illustrate the problems that scientific journal editors face with unscrupulous or ignorant contributors and incompetent or simply lazy and indifferent reviewers by analyzing several articles related to the finite-volume approximation of the diffusion term published by a group of authors in various refereed journals.

1. INTRODUCTION

The so-called diffusion term which describes the diffusion of the variable ϕ through the surface S,

$$\int_S \Gamma_\phi \ \mathrm{grad}\ \phi \cdot d\mathbf{s} \tag{1}$$

features in many equations of the mathematical physics. There ϕ stands for, e.g., the temperature, the species concentration, the fluid velocity component, the solid displacement component, the magnetic scalar potential, the magnetic vector potential component, etc., Γ_ϕ is the diffusion coefficient, and $\mathbf{s}$ is the surface vector.

In the finite-volume numerical methods that discretize the space with the grid lines coinciding with the coordinate lines, the discrete approximation of this term follows directly from its differential form. However, in the more recent methods that use arbitrary (polyhedral) control volumes with no reference to the coordinate lines, discretization of the diffusion term became somewhat arbitrary and attracted more attention.

In this article a review of the cell-centered finite-volume approximations of diffusive flux is presented, starting with early methods that use Cartesian meshes and finishing with contemporary methods that employ arbitrary polyhedral control volumes. Also, three publications by a group of authors published in three refereed

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Color versions of one or more of the figures in the article can be found online at www.tandfonline.com/unhb.

NOMENCLATURE

$\mathbf{d}$	distance vector
D	diffusion term
$\mathbf{e}_i$	covariant unit base vector
$\mathbf{e}^i$	contravariant base vector
$\mathbf{i}^i$	Cartesian unit base vector
$\mathbf{k}$	nonorthogonal part of the surface vector
N, P	computational points
$\mathbf{s}$	surface vector
S	surface area
x^i	Cartesian coordinate
Γ	diffusion coefficient
$\delta\xi^j$, $\delta\xi^k$	"dimensions" of the $\xi^i = \text{const.}$ cell face
Δ	orthogonal part of the surface vector
ξ^i	general curvilinear coordinate
ϕ	generic dependent variable
Subscripts	
f	cell face (center)
l, r, b, t	left, right, bottom, top
N, P	cell centers

journals claiming that they have developed a new formula for the discretization of diffusive flux are examined and it is found that they all present the same formula for the approximation of diffusive flux that has been known and used in both research and commercial codes and published in Ph.D. theses and journals for more than 30 years. This illustrates the problem of distinguishing original contributions from plagiarism in scientific journals.

2. APPROXIMATION OF DIFFUSIVE FLUX

2.1. Cartesian Mesh

In the early days of computational fluid dynamics (CFD), when Cartesian grids were used, the discretization of the diffusion term (1) was straightforward and the diffusive flux through the cell face f was approximated by

$$D_f = \int_{S_f} \Gamma_\phi \text{ grad } \phi \cdot d\mathbf{s} \approx \Gamma_\phi \left(\frac{\partial \phi}{\partial x^1}\right)_f S_f = \Gamma_\phi \frac{\phi_N - \phi_P}{d_f} S_f \tag{2}$$

where ϕ_N and ϕ_P are the values of dependent variable ϕ at the computational nodes N and P, respectively, $d_f = \overline{PN}$ is the distance between the points P and N, and S_f is the area of the face f (Figure 1).

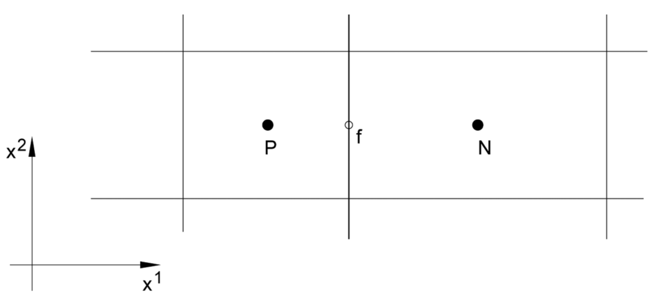

Figure 1. A section of Cartesian mesh.

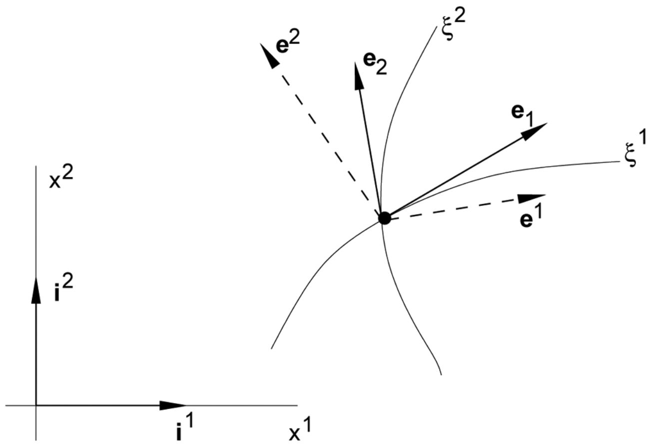

Figure 2. Curvilinear coordinates, natural and dual base vectors at a point in two dimensions.

2.2. Structured Body-Fitted Mesh

The next step in the development of the finite-volume method was the use of structured body-fitted curvilinear coordinates, Figure 2, and the discretization of the diffusive flux became more complicated.

Now, the gradient of dependent variable ϕ can be written as

$$\text{grad } \phi = \frac{\partial \phi}{\partial x^j}\mathbf{i}^j = \frac{\partial \phi}{\partial \xi^m}\frac{\partial \xi^m}{\partial x^j}\mathbf{i}^j = \frac{\partial \phi}{\partial \xi^m}\mathbf{e}^m \tag{3}$$

where $\mathbf{i}^j$ ($j = 1, 2, 3$) are the Cartesian base vectors and

$$\mathbf{e}^m = \frac{\partial \xi^m}{\partial x^j}\mathbf{i}^j \tag{4}$$

are the reciprocal (dual, contravariant) base vectors related to the unit (covariant) base vectors $\mathbf{e}_i$, tangential to the coordinate lines ξ^i ($i = 1, 2, 3$), by the relations

$$\mathbf{e}^i = \frac{\mathbf{e}_j \times \mathbf{e}_k}{\mathbf{e}_i \cdot (\mathbf{e}_j \times \mathbf{e}_k)} \tag{5}$$

where (i, j, k) is the cyclic permutation of (1, 2, 3). Note that $\mathbf{e}^i$ is orthogonal to the coordinate surface $\xi^i = \text{const}$. After multiplying both the numerator and the denominator by $\delta\xi^j\delta\xi^k$, where $\delta\xi^j$ and $\delta\xi^k$ are the "dimensions" of the cell face $\xi^i = \text{const.}$, the vector $\mathbf{e}^i$ can be written as

$$\mathbf{e}^i = \frac{\delta\xi^j\mathbf{e}_j \times \delta\xi^k\mathbf{e}_k}{\mathbf{e}_i \cdot (\delta\xi^j\mathbf{e}_j \times \delta\xi^k\mathbf{e}_k)} = \frac{\mathbf{s}^i}{\mathbf{e}_i \cdot \mathbf{s}^i} \quad (i = 1, 2, 3)\,(\text{no summation on}\, i) \tag{6}$$

where $\mathbf{s}^i = \delta\xi^j\,\mathbf{e}_j \times \delta\xi^k\,\mathbf{e}_k$ is the surface vector of the cell face $\xi^i = \text{const}$.

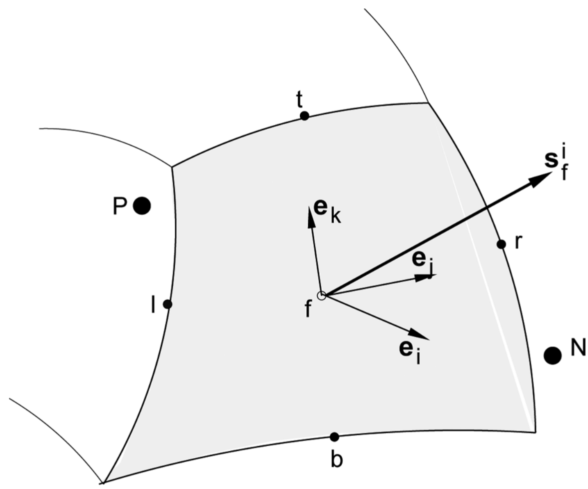

Figure 3. Curvilinear control volume.

Now the diffusive flux through the cell face f, lying in the coordinate surface $\xi^i = \text{const.}$ between points P and N (Figure 3),

$$D_f = \int_{S_f} \Gamma_\phi \text{ grad } \phi \cdot d\mathbf{s} = \int_{S_f} \Gamma_\phi \frac{\partial \phi}{\partial \xi^m} \mathbf{e}^m \cdot d\mathbf{s}$$
$$= \int_{S_f} \left(\Gamma_\phi \frac{\partial \phi}{\partial \xi^i} \mathbf{e}^i + \Gamma_\phi \frac{\partial \phi}{\partial \xi^j} \mathbf{e}^j + \Gamma_\phi \frac{\partial \phi}{\partial \xi^k} \mathbf{e}^k \right) \cdot d\mathbf{s} \tag{7}$$

can, by employing (6), be approximated by

$$D_f \approx \Gamma_\phi \frac{\phi_N - \phi_P}{\delta \xi^i} \frac{\mathbf{s}_f^i}{\mathbf{e}_i \cdot \mathbf{s}_f^i} \cdot \mathbf{s}_f^i + \Gamma_\phi \frac{\phi_r - \phi_l}{\delta \xi^j} \frac{\mathbf{s}_f^j}{\mathbf{e}_j \cdot \mathbf{s}_f^j} \cdot \mathbf{s}_f^i$$
$$+ \Gamma_\phi \frac{\phi_t - \phi_b}{\delta \xi^k} \frac{\mathbf{s}_f^k}{\mathbf{e}_k \cdot \mathbf{s}_f^k} \cdot \mathbf{s}_f^i \tag{8}$$

and, since $\delta \xi^i \mathbf{e}_i = \mathbf{d}_f^i$, where $\mathbf{d}_f^i = \overrightarrow{PN}$ is the distance vector, and similarly $\delta \xi^j \mathbf{e}_j = \mathbf{d}_f^j$ and $\delta \xi^k \mathbf{e}_k = \mathbf{d}_f^k$, where $\mathbf{d}_f^j = \overrightarrow{lr}$ and $\mathbf{d}_f^k = \overrightarrow{bt}$, the diffusive flux (8) gets the form

$$D_f \approx \Gamma_\phi \frac{\mathbf{s}_f^i \cdot \mathbf{s}_f^i}{\mathbf{d}_f^i \cdot \mathbf{s}_f^i} (\phi_N - \phi_P) + \Gamma_\phi \frac{\mathbf{s}_f^j \cdot \mathbf{s}_f^i}{\mathbf{d}_f^j \cdot \mathbf{s}_f^j} (\phi_r - \phi_l)$$
$$+ \Gamma_\phi \frac{\mathbf{s}_f^k \cdot \mathbf{s}_f^i}{\mathbf{d}_f^k \cdot \mathbf{s}_f^k} (\phi_t - \phi_b) \tag{9}$$

The above expression was first derived by Demirdžić [1] and later adopted by Perić in his Ph.D. thesis [2] and reported in their subsequent publications, e.g., [3, 4].

The first term on the right-hand side is treated implicitly, and the other two, the so-called cross-diffusion terms, explicitly in the deferred-correction manner.

2.3. General Unstructured Polyhedral Mesh

The finite-volume discretization which uses meshes made of arbitrary polyhedral control volumes, Figure 4 (Muzaferija [5] and Muzaferija and Gosman [6]) enabled one to discard with the complicated curvilinear coordinates. There, the diffusive flux of the variable ϕ through an internal cell face f is approximated as

$$D_f = \int_{S_f} \Gamma_\phi \text{ grad } \phi \cdot d\mathbf{s} \approx \Gamma_\phi (\text{grad } \phi)_f^* \cdot \mathbf{s}_f \tag{10}$$

and the gradient $(\text{grad } \phi)_f^*$ is constructed in the following manner:

$$(\text{grad } \phi)_f^* = (\text{grad } \phi)_f + \left[\frac{\phi_N - \phi_P}{|\mathbf{d}_f|} - \frac{(\text{grad } \phi)_f \cdot \mathbf{d}_f}{|\mathbf{d}_f|}\right] \frac{\mathbf{d}_f}{|\mathbf{d}_f|} \tag{11}$$

The second term on the right-hand side (the term in [ ] brackets) represents the difference between the central difference approximation of the derivative in the direction of vector $\mathbf{d}_f$ and the corresponding value obtained by interpolating the cell-center gradients. This correction term detects and smoothes out any unphysical oscillations that might occur in the iteration process. As a result, one gets

$$D_f \approx \Gamma_\phi \frac{\mathbf{d}_f \cdot \mathbf{s}_f}{\mathbf{d}_f \cdot \mathbf{d}_f} (\phi_N - \phi_P) + \Gamma_\phi \left[(\text{grad } \phi)_f \cdot \mathbf{s}_f - \frac{\mathbf{d}_f \cdot \mathbf{s}_f}{\mathbf{d}_f \cdot \mathbf{d}_f} (\text{grad } \phi)_f \cdot \mathbf{d}_f\right] \tag{12}$$

The first part of this term is treated implicitly, and the rest explicitly.

In a later publication, Demirdžić and Muzaferija [7] proposed a slightly different expression for $(\text{grad } \phi)_f^*$,

$$(\text{grad } \phi)_f^* = (\text{grad } \phi)_f + \left[\frac{\phi_N - \phi_P}{|\mathbf{d}_f|} - \frac{\overline{\text{grad } \phi} \cdot \mathbf{d}_f}{|\mathbf{d}_f|}\right] \frac{\mathbf{s}_f}{|\mathbf{s}_f|} \tag{13}$$

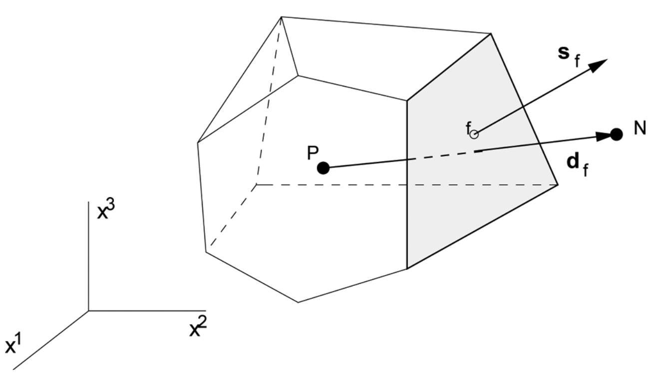

Figure 4. An arbitrary polyhedral control volume.

resulting in the following approximation for the diffusive flux:

$$D_f \approx \Gamma_\phi \frac{|\mathbf{s}_f|}{|\mathbf{d}_f|} (\phi_N - \phi_P) + \Gamma_\phi \left[(\text{grad } \phi)_f \cdot \mathbf{s}_f - \frac{|\mathbf{s}_f|}{|\mathbf{d}_f|} \overline{\text{grad } \phi} \cdot \mathbf{d}_f \right] \tag{14}$$

where the overbar indicates the arithmetic average of the gradients calculated at nodes P and N. The use of the arithmetic average in Eq. (13), instead of the linear interpolation as in Eq. (11), makes the added term (the term in [ ] brackets) equal exactly to zero in the case of linear and quadratic variation of ϕ, even on a nonuniform mesh.

In order to discretize the diffusion term on a 2-D polyhedral mesh, Davidson [8] constructs a quadrilateral around the cell face, applies the Gauss theorem to calculate the gradient of the dependent variable, and arrives at the 2-D version of Eq. (9), which is identical to the formula used in, e.g., [3].

Finally, Mathur and Murthy [9] re-derived Eq. (9) for the 2-D curvilinear mesh and used it to modify Eq. (12) or (14) to obtain

$$D_f \approx \Gamma_\phi \frac{\mathbf{s}_f \cdot \mathbf{s}_f}{\mathbf{d}_f \cdot \mathbf{s}_f} (\phi_N - \phi_P) + \Gamma_\phi \left(\overline{\text{grad } \phi} \cdot \mathbf{s}_f - \frac{\mathbf{s}_f \cdot \mathbf{s}_f}{\mathbf{d}_f \cdot \mathbf{s}_f} \overline{\text{grad } \phi} \cdot \mathbf{d}_f \right) \tag{15}$$

Similarly, based on experience from the directly derived Eq. (9), Demirdžić and Muzaferija and co-workers used the following approximation in their subsequent publications, e.g., [10–17], which deal with various physical problems, including fluid flow, solid body deformation, phase change, and electrostatics:

$$D_f \approx \Gamma_\phi \frac{\mathbf{s}_f \cdot \mathbf{s}_f}{\mathbf{d}_f \cdot \mathbf{s}_f} (\phi_N - \phi_P) + \Gamma_\phi \left[(\text{grad } \phi)_f \cdot \mathbf{s}_f - \frac{\mathbf{s}_f \cdot \mathbf{s}_f}{\mathbf{d}_f \cdot \mathbf{s}_f} \overline{\text{grad } \phi} \cdot \mathbf{d}_f \right] \tag{16}$$

In their renowned book [18], Ferziger and Perić refer to the Muzaferija thesis [5], implying the use of (12), but they actually use (14), giving it a geometric interpretation (Figure 5, top right):

$$D_f \approx \Gamma_\phi |\mathbf{s}_f| \frac{\phi_N - \phi_P}{|\mathbf{d}_f|} + \Gamma_\phi |\mathbf{s}_f| \overline{\text{grad } \phi} \cdot \left(\frac{\mathbf{s}_f}{|\mathbf{s}_f|} - \frac{\mathbf{d}_f}{|\mathbf{d}_f|} \right) \tag{17}$$

Similarly, Jasak, in his Ph.D. thesis [19], and in less detail in the subsequent publication [20], gives the geometric interpretation to (12), (14), and (16), naming them the minimum correction, the orthogonal correction, and the overrelaxed approach, respectively (Figure 5). He approximates the diffusive flux as

$$D_f \approx \Gamma_\phi (\text{grad } \phi)_f^* \cdot \mathbf{s}_f = \Gamma_\phi \left[\frac{\phi_N - \phi_P}{|\mathbf{d}_f|} |\Delta_f| + (\text{grad } \phi)_f \cdot \mathbf{k}_f \right] \tag{18}$$

where vectors Δ_f and $\mathbf{k}_f$ satisfy the condition

$$\mathbf{k}_f = \mathbf{s}_f - \Delta_f \tag{19}$$

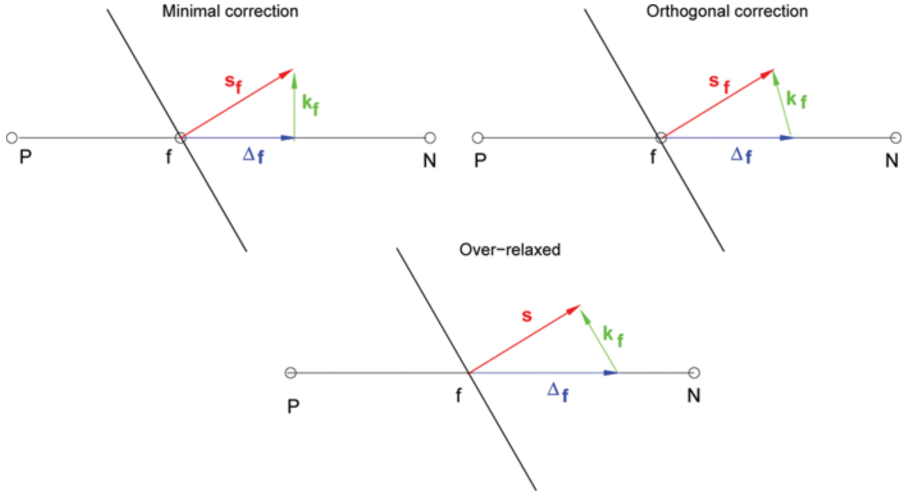

Figure 5. Geometric interpretation of the diffusion term approximation [19].

For the minimum correction approach, Eq. (12),

$$\Delta_f = \frac{\mathbf{d}_f \cdot \mathbf{s}_f}{\mathbf{d}_f \cdot \mathbf{d}_f} \cdot \mathbf{d}_f \tag{20}$$

for the orthogonal correction approach, Eqs. (14) and (17),

$$\Delta_f = \frac{|\mathbf{s}_f|}{|\mathbf{d}_f|} \cdot \mathbf{d}_f \tag{21}$$

and for the overrelaxed approach, Eq. (16),

$$\Delta_f = \frac{\mathbf{s}_f \cdot \mathbf{s}_f}{\mathbf{d}_f \cdot \mathbf{s}_f} \cdot \mathbf{d}_f \tag{22}$$

Jasak compared the performance of these three approaches and found that the overrelaxed approach is more robust and more efficient than the other two, expecially in case of highly nonorthogonal meshes. This is expected because, unlike the other approaches, which are somewhat arbitrary, the overrelaxed approach comes as a result of a direct discretization of the transport equations.

3. "ORIGINAL" CONTRIBUTION BY A GROUP OF AUTHORS

In addition to the references mentioned in the previous section which point to the original contributions toward discretization of the diffusion term, the above-mentioned formulas have been reproduced in many other publications and theses. This is especially the case when commercial or public-domain codes are employed in research, since most of them use (and have been using for decades) the overrelaxed approach, first Eq. (9) in conjunction with block-structured grids based on body-fitted general curvilinear coordinates and later Eq. (16) in conjunction with arbitrary polyhedral meshes (e.g., STAR-CD, FLUENT, Open-FOAM, and STAR-CCM+).

In spite of the above evidence, a group of authors first published the article, "Nouvelle approche pour la discrétisation de flux diffusifs en volumes finis a forte obliquité" [21], then its slightly extended translation from French [22], and at same time another very similar article [23], and claim that they have developed a new Improved Deferred Correction (IDC) scheme which performs much better than the Standard Deferred Correction (SDC) scheme. The fact is that their "new" IDC scheme is identical to the overrelaxed approach, e.g., [4, 8, 19], and the SDC scheme is the orthogonal correction scheme [7, 18]. They also claim that the SDC is still widely used, which is not true; even its originators, Demirdžić and Muzaferija, have abandoned it in favor of the overrelaxed approach, as evident from their later publications, e.g., [10–17].

At the time when this article was practically finished, there appeared yet another (fourth!) paper by Wu and Traoré [24] dealing with the diffusive flux. In it, the authors suddenly discovered the article by Mathur and Murthy [9] and Jasak's thesis [19] and practically copied parts of them, with addition of a method from Ferziger and Perić 's book [18]. Strikingly, they still do not admit their plagiarism or ignorance, but say that the overrelaxed approach "was revisited recently by Traoré et al. [22, 23]," forgetting that they have claimed in their earlier publications that "A new approach for diffusive flux . . . is proposed" [22] or "In this article, a new IDC scheme . . . is developed" [23], etc.!

Even the name they gave to their "new" scheme, "Improved Deferred Correction scheme," shows the authors' (and reviewers'?) ignorance. Namely, they do not distinguish between two distinct processes, the discretization and the solution algorithm. They claim that they have improved the discretization of the diffusion term while the deferred correction is a part of the solution algorithm.

4. SUMMARY AND CONCLUSIONS

In this article a chronological review of various approaches to discretization of the diffusion term by the cell-centered finite-volume methods for the solution of various continuum mechanics problems, including heat transfer, fluid flow, solid-body deformation, and electrostatics, is presented. It is also illustrated that not everything that is published has undergone an honest, professional peer review.

1. It is shown that:

    a. The most successful overrelaxed approach steams from the direct discretization of the scalar transport equation written in terms of Cartesian vector components and the curvilinear body-fitted numerical mesh, first derived in 1983 [1] and used in, e.g., 1985, 1990, and 1993 [2–4].
    b. When discarding the limitations and the complications of the curvilinear grids, Muzaferija et al. used the minimal correction in 1994 and 1997 [5, 6] and the orthogonal correction in 1995 [7]. However, in all subsequent publications from 2000 to 2011, e.g., [10–17], they used the overrelaxed method.
    c. In the meantime, Davidson in 1996 [8] and Mathur and Murthy in 1997 [9] arrived at the overrelaxed approximation, the former considering 2-D unstructured and the latter 2-D curvilinear structured meshes.

d. In 1996 Jasak [19] gave the names and a geometric interpretation to the three above-mentioned approximations, compared their performance, and concluded that the overrelaxed approach is better than the other two, especially in case of highly skewed meshes. This should not be a surprising outcome, bearing in mind that the overrelaxed approach is the result of a direct discretization of the transport equations, while the other two are more *ad hoc*, intuitive approaches.

2. In the above original publications, the discretization of the diffusion term was only a small part of the total contribution. Many other researchers, especially those using the public code OpenFOAM and the major commercial codes FLUENT, STAR-CD, and STAR-CCM+, have also been using the over-relaxed approach for many years. In spite of this, several publications dedicated to discretization of the diffusion term were published by a group of authors between 2006 and 2009 [21–23], in which they claimed to have developed a new, robust, and efficient scheme for discretizing the diffusion term, while presenting the long-known overrelaxed approach.

Five years after their "original" contribution, in 2014, the researchers from the same group published another article dedicated to the discretization of the diffusion term [24], in which the publications by Jasak [19] and Mathur and Murthy [9] (but not the others) were referenced without admitting that their "new, robust, efficient" scheme was not quite new.

Whatever those authors' motives in submitting such manuscripts, they would not have been published if the reviewers did their job. Here, we are talking about articles in four journals, which means at least eight reviewers. The fact is that a thorough article review can take anything between a couple of days and a couple of weeks, but it is only fair to decline to review a manuscript if that effort cannot be invested, instead of ticking it off as publishable.

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