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On accurate discretization of turbulence transport equations in general coordinates

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Abstract

In this paper some discretization issues that arise in finite volume computations of turbulent flows in arbitrarily shaped domains are presented. Staggered grids are employed. Turbulence is modeled by the standard $k$-$\varepsilon$ model. Discretizations are discussed of a general transport equation which are exact for uniform and linear flow fields on irregular grids. A new higher-order monotone upwind scheme for the approximation of turbulence convection is formulated. A number of test problems show the utility of the present numerical method.

1 Introduction

In order to formulate the Reynolds-averaged Navier-Stokes equations with the $k$-$\varepsilon$ turbulence model in boundary-fitted coordinates, two methods can be adopted: staggered grids with grid-oriented velocity components as dependent variables, and Cartesian velocity components as primary unknowns on colocated grids. At present it is hard to say which approach is best to compute incompressible flows in arbitrary geometries. Nevertheless, since the 1980's, the latter method has received considerable attention, and commercial codes such as FLUENT and Flow3D have adopted this method.

During the past seven years, efforts have been made in Delft to make progress in numerical modeling of incompressible laminar and turbulent flows in general 2D and 3D geometries [6, 14, 9, 7, 16, 17]. These efforts have focussed on developing coordinate-invariant finite volume discretization of the Navier-Stokes equations on boundary-fitted structured grids, employing a staggered placement of the unknowns. Standard tensor notation is used. As a consequence, the formulation contains Christoffel symbols. In spite of that, discretization accuracy can be maintained if certain rules concerning the approximation of the geometric quantities are followed and the contravariant mass fluxes instead of velocity components are chosen as primitive variables, and the grid is not too non-smooth. The restriction to fairly non-smooth grids is in some cases undesirable. Therefore, a method has been developed which allows us to discretize the equations such that the discretization
is exact for uniform and linear flow fields on non-smooth grids [15]. It is expected that this discretization will retain accuracy near rapid changes in mesh size in the physical domain. This approach will be explained in Section 2 and its performance will be demonstrated.

Over the past two decades there have been many attempts to devise higher-order upwind schemes, which do not exhibit spurious oscillations. A monotonicity preserving property of these schemes is necessary when turbulence transport equations have to be accurately resolved. Otherwise, physically and numerically undesirable features such as negative turbulent kinetic energy may arise in high-gradient regions. In Section 2 a new TVD scheme - named ISNAS (Interpolation Scheme which is Nonoscillatory for Advected Scalars) - is proposed. This scheme is formally third-order accurate, free from numerical oscillations while keeping sharp gradients steep and is suitable for inclusion in general purpose finite volume codes. The ISNAS scheme is used to obtain higher-order accurate solutions of the $k$-$\varepsilon$ equations for the turbulent confined jet flow in 2D planar duct. These are compared with the solutions obtained with a hybrid central/upwind scheme.

## 2 Discretization in general coordinates

This section is concerned mainly with invariant discretizations of a general transport equation for any scalar $\phi$. We restrict ourselves to two dimensions; extension to three dimensions is straightforward. Details of the discretization of the momentum equations can be found e.g. in [9]. Using tensor notation in general coordinates [1], the transport equation for scalar $\phi$ is written as

$$\frac{\partial \rho \phi}{\partial t} + (\rho U^\alpha \phi)_{,\alpha} - (\kappa_\phi g^{\alpha\beta} \phi_{,\beta})_{,\alpha} = S_\phi$$  \hspace{1cm} (2.1)

where $\rho$ is the density, $U^\alpha$ is the contravariant velocity component, $S_\phi$ denotes a source term and $\kappa_\phi$ is a diffusion coefficient. The summation convention holds for Greek indices. The $k$-$\varepsilon$ model [4] can be represented by (2.1) as follows: for $\phi = k$ we have $\kappa_\phi = \mu_t/\sigma_k$ and $S_\phi = P_k - \rho \varepsilon$ and if $\phi = \varepsilon$ then $\kappa_\phi = \mu_t/\sigma_\varepsilon$ and $S_\phi = \frac{1}{2}(c_{e1} P_k - \rho c_{e2} \varepsilon)$, where

$$\begin{align*}
\mu_t &= \rho c_{\mu} \frac{k^2}{\varepsilon}, & P_k &= \mu_t g_{\alpha\beta}(g^{\alpha\gamma} U_{,\gamma}^\beta + g^{\beta\gamma} U_{,\gamma}^\alpha) U_{,\beta}^\varepsilon
\end{align*}$$  \hspace{1cm} (2.2)

Finally, $c_{\mu}$, $c_{e1}$, $c_{e2}$, $\sigma_k$ and $\sigma_\varepsilon$ are dimensionless constants which, respectively, are taken to be 0.09, 1.44, 1.92, 1.0 and 1.3 according to [4].

The covariant and contravariant metric tensors are defined as

$$g_{\alpha\beta} = a_\alpha(\beta), \quad g^{\alpha\beta} = a^{(\alpha)} \cdot a^{(\beta)}$$  \hspace{1cm} (2.3)$$

with $a_\alpha(\beta) = \frac{\partial x}{\partial \xi}$ and $a^{(\alpha)} = \nabla x^\alpha$ the covariant and contravariant base vectors, respectively, with respect to the mapping $G \rightarrow \Omega : x = x(\xi)$. Here, $x$ are Cartesian coordinates and $\xi$ are general coordinates. The mapping is assumed to be regular, i.e. the Jacobian of the transformation, denoted as $\sqrt{g}$, does not vanish.

The mapping $x(\xi)$ is generated numerically. Because of practical considerations it is desirable to characterize a computational grid by the coordinates of the cell
vertices only, which are assumed to be joined by straight lines. Hence, we want to allow piecewise bilinear coordinate mappings. See Figure 2.1. As a consequence,

![Figure 2.1: Cell in computational domain $G$ and its image in the physical domain $\Omega$](image)

the grid lines need not to be smooth. All relevant geometric quantities can be subsequently calculated using central differences and bilinear interpolations in the obvious way. Owing to the piecewise bilinear mapping all these quantities are exact inside a cell. On the other hand, some of these quantities are discontinuous on cell faces - connections between the vertices of the cell. For instance, $a_{(\alpha)}$ is constant along $\xi^{\alpha}$-lines but the value of this constant changes from cell to cell since the grid lines need not to be smooth. Hence, across cell faces $\xi^{\alpha} = \text{constant} a_{(\alpha)}$ jumps. Furthermore, $a_{(\alpha)}$ is found to be continuous at $\xi^{\beta} = \text{constant} (\beta \neq \alpha)$. The smoothness properties of the other geometric quantities follow from those of the covariant base vectors. It appears, for example, that $\sqrt{g}$ and $a^{(\alpha)}$ are discontinuous at all cell faces, whereas $\sqrt{g} a^{(\alpha)}$ is continuous. For more details see [15].

The transport equation and the incompressible Reynolds-averaged Navier-Stokes equations will be solved using a finite volume technique on a staggered grid, as shown in Figure 2.1. The straightforward approach would be to discretize (2.1). This has been done in [17] for example. As already mentioned, this approach is restricted to more or less smooth grids. Moreover, the turbulent viscosity $\mu_t$ varies rapidly, so that $\mu_t$ has large jumps on cell faces. Hence, straightforward discretization of the diffusivity may results in large errors on non-smooth grids. Here we shall consider a discretization which is exact for uniform and linear scalar fields, regardless the smoothness of the grid and of the diffusion coefficient. For this purpose, the equation (2.1) will be rewritten in terms of partial Cartesian and general tensor notation, as follows

$$\frac{\partial \rho \phi}{\partial t} + \frac{1}{\sqrt{g}} \frac{\partial \rho V^\alpha \phi}{\partial \xi^\alpha} - \frac{1}{\sqrt{g}} \frac{\partial}{\partial \xi^\alpha} \left( \sqrt{g} a^{(\alpha)}_\beta k_\beta \frac{\partial \phi}{\partial x^\beta} \right) = S_\phi$$  \hspace{1cm} (2.4)

with $V^\alpha = \sqrt{g} a^{(\alpha)}_\beta \mathbf{u}$ the contravariant mass flux component and $\mathbf{u}$ the velocity field. Because $\sqrt{g} a^{(\alpha)}_\beta$ is smooth at cell face $\xi^\alpha = \text{constant}$, so is $V^\alpha$. Discretization of (2.4) is obtained by integration over a finite volume $G_{ij}$ with center $(i, j)$ as indicated in Figure 2.1. In $G$ we choose a uniform grid such that the mesh-size $\delta \xi^\alpha = 1$. Hence,
we have
\[ \int_{G_{ij}} \frac{\partial \rho V^2 \phi}{\partial \xi^\alpha} d\xi^1 d\xi^2 \approx \rho V^1 \phi_{(i+1/2,j)} - \rho V^2 \phi_{(i-1/2,j)} + \rho V^2 \phi_{(i,j-1/2)} \tag{2.5} \]
whereas the time derivative and the source term are integrated using the midpoint rule:
\[ \int_{G_{ij}} \frac{\partial \rho \phi}{\partial t} dG \approx \sqrt{g} \frac{\partial \rho \phi}{\partial t}_{(i,j)}, \quad \int_{G_{ij}} S_{\phi} dG \approx \sqrt{g} S_{\phi}_{(i,j)} \tag{2.6} \]
So far, no difficulties arose because none of the quantities used in the above formulae are discontinuous. Furthermore, these discretizations are exact for constant \( \rho \) and \( \phi \).

The cell-face values have to be approximated in terms of values of \( \phi \) in neighbouring cell centers. This will be explained later. The only point left to discuss is the approximation of the diffusion term. First, the diffusion term is rewritten as follows:
\[ \frac{1}{\sqrt{g}} \frac{\partial}{\partial \xi^\alpha} (\sqrt{g} a^{(a)}_{\phi} \frac{\partial \phi}{\partial \xi^\alpha}) = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \xi^\alpha} (\sqrt{g} a^{(a)} \cdot \kappa_{\phi} \nabla \phi) \tag{2.7} \]
with \( \nabla \phi = (\frac{\partial \phi}{\partial x^1}, \frac{\partial \phi}{\partial x^2})^T \). Integration over \( G_{ij} \) yields:
\[ -\int_{G_{ij}} \frac{\partial}{\partial \xi^\alpha} (\sqrt{g} a^{(a)} \cdot \kappa_{\phi} \nabla \phi) d\xi^1 d\xi^2 \approx \]
\[ -\sqrt{g} a^{(1)} \cdot \kappa_{\phi} \nabla \phi_{(i+1/2,j)} - \sqrt{g} a^{(2)} \cdot \kappa_{\phi} \nabla \phi_{(i,j-1/2)} \tag{2.8} \]
At cell faces, \( \kappa_{\phi} \nabla \phi \) is smooth. Hence, when \( \kappa_{\phi} \) is discontinuous, \( \nabla \phi \) is discontinuous. Thus, approximation of \( \nabla \phi \) using central differences is inaccurate. We now discuss a method to approximate \( \kappa_{\phi} \nabla \phi \) accurately. Using smoothness of \( \kappa_{\phi} \nabla \phi \) at point \((i+1/2,j)\), for example, we have
\[ \phi_{(i+1,j)} = \int_{x_{(i,j)}}^{x_{(i+1,j)}} \frac{1}{\kappa_{\phi}} \kappa_{\phi} \nabla \phi \, dx \approx \kappa_{\phi} \nabla \phi_{(i+1/2,j)} \int_{x_{(i,j)}}^{x_{(i+1,j)}} \frac{1}{\kappa_{\phi}} \, dx \tag{2.9} \]
The latter integral can be approximated as follows:
\[ c_{(1)} = \int_{x_{(i,j)}}^{x_{(i+1,j)}} \frac{1}{\kappa_{\phi}} \, dx = \frac{1}{2} \left( a^{(1)}_{\phi} \big|_{(i,j)} + a^{(1)}_{\phi} \big|_{(i+1,j)} \right) \tag{2.10} \]
In order to find a second equation for \( \kappa_{\phi} \nabla \phi \) we choose another integration path through point \((i+1/2,j)\). An obvious choice is by taking the average of two paths, as follows:
\[ \frac{1}{4} \phi_{(i+1/2,j)} = \frac{1}{4} \left( \int_{x_{(i,j-1)}}^{x_{(i+1,j+1)}} \nabla \phi \, dx \right) \approx \kappa_{\phi} \nabla \phi_{(i+1/2,j)} \cdot c_{(2)} \tag{2.11} \]
with
\[ c_{(2)} = \frac{1}{8} a^{(2)}_{\phi} \big|_{(i,j-1)} + \frac{1}{4} a^{(2)}_{\phi} \big|_{(i,j)} + \frac{1}{8} a^{(2)}_{\phi} \big|_{(i,j+1)} + \]
\[ \frac{1}{4} c^{(2)}_{\phi} \big|_{(i+1,j-1)} + \frac{1}{4} a^{(2)}_{\phi} \big|_{(i+1,j)} + \frac{1}{8} c^{(2)}_{\phi} \big|_{(i+1,j+1)} \tag{2.12} \]
Solving (2.9) and (2.11) for $\kappa_\phi \nabla \phi_{(i+1/2,j)}$ results in

$$
\kappa_\phi \nabla \phi_{(i+1/2,j)} = c^{(1)}(\phi_{(i+1,j)}^{(i+1,j)}) + c^{(2)}(\phi_{(i,j+1)}^{(i,j+1)} + \phi_{(i+1,j+1)}^{(i+1,j+1)})
$$

(2.13)

where

$$
c^{(1)} = \frac{1}{C}(c_2^2, -c_2^1)^T, \quad c^{(2)} = \frac{1}{C}(-c_1^2, c_1^1)^T,
$$

$$
C = c_2^2 c_1^1 - c_1^2 c_2^1
$$

(2.14)

Substitution of (2.13) in (2.8) gives a discretization which is exact when $\nabla \phi$ is constant, and hence exact for linear scalar fields. The other cell-face fluxes can be derived in exactly the same way. The total number of variables linked together is 9.

The cell-face values in (2.5) will be approximated with a higher-order TVD scheme called ISNAS. We assumed $\rho$ = constant. The method to construct this scheme is based on the fact that the normalized variable diagram proposed in [5] can be reformulated in terms of Sweby's TVD diagram [11]. We shall give a brief description. We consider the control volume surrounding point $(i,j)$ as shown in Figure 2.1 and assume that $V_{(i+1/2,j)}^1 > 0$. A normalized variable $\hat{\phi}$ at point $(i+m,j)$ is defined as

$$
\hat{\phi}_{(i+m,j)} = \frac{\phi_{(i+m,j)} - \phi_{(i-1,j)}}{\phi_{(i+1,j)} - \phi_{(i-1,j)}}, \quad m = -1, \frac{1}{2}, 0, \frac{1}{2}, 1
$$

(2.15)

Hence, $\hat{\phi}_{(i-1,j)} = 0$ and $\hat{\phi}_{(i+1,j)} = 1$. Several upwind schemes can be reformulated in terms of normalized variables. For example, QUICK may be written as

$$
\hat{\phi}_{(i+1/2,j)} = \frac{3}{4} \hat{\phi}_{(i,j)} + \frac{3}{8}
$$

According to [2], a scheme $\hat{\phi}_{(i+1/2,j)} = f(\hat{\phi}_{(i,j)})$, with $f$ a continuous or piecewise continuous function, is monotone if and only if

1. $\forall \hat{\phi}_{(i,j)} \in [0,1], \quad \hat{\phi}_{(i,j)} \leq f(\hat{\phi}_{(i,j)}) \leq 1$

2. $\forall \hat{\phi}_{(i,j)} \notin [0,1], \quad \hat{\phi}_{(i+1/2,j)} = f(\hat{\phi}_{(i,j)}) = \hat{\phi}_{(i,j)}$

3. $f(0) = 0$ and $f(1) = 1$

Moreover, according to [5], a scheme $\hat{\phi}_{(i+1/2,j)} = f(\hat{\phi}_{(i,j)})$ that passes through the point $f(\frac{1}{2}) = \frac{3}{4}$ while having a slope of $\frac{3}{4}$ at $(\frac{1}{2}, \frac{3}{4})$ is third-order accurate. It appears that a good choice would be to derive a third-order polynomial which passes through the points $(0,0), (1,1)$ and $(\frac{1}{2}, \frac{3}{4})$, while having a slope of $\frac{3}{4}$ at $(\frac{1}{2}, \frac{3}{4})$. We find the following scheme

$$
\hat{\phi}_{(i+1/2,j)} = \begin{cases} 
\hat{\phi}_{(i,j)}, & \hat{\phi}_{(i,j)} < 0 \\
\frac{3}{2} \hat{\phi}_{(i,j)} - \frac{5}{2} \hat{\phi}_{(i,j)}^2 + \frac{3}{2} \hat{\phi}_{(i,j)} & 0 \leq \hat{\phi}_{(i,j)} \leq 1 \\
\hat{\phi}_{(i,j)}, & \hat{\phi}_{(i,j)} > 1 
\end{cases}
$$

(2.16)

The corresponding TVD scheme with a limiter in terms of Sweby’s flux limiter function is derived as follows. First, (2.16) is rewritten as

$$
\hat{\phi}_{(i+1/2,j)} = \hat{\phi}_{(i,j)} + \frac{1}{2} (3 \hat{\phi}_{(i,j)} - 2 \hat{\phi}_{(i,j)}^2)(1 - \hat{\phi}_{(i,j)})
$$

(2.17)
In terms of un-normalized variables, this equation (2.17) simply reads

\[ \phi_{(i+1/2,j)} = \phi_{(i,j)} + \frac{1}{2} \Psi(r_{(i+1/2,j)})(\phi_{(i+1,j)} - \phi_{(i,j)}) \]  \hspace{1cm} (2.18)

where \( \Psi \) is a flux limiter to be derived and the limiter argument \( r_{(i+1/2,j)} \) is the ratio of two consecutive solution gradients defined by

\[ r_{(i+1/2,j)} = \frac{\phi_{(i,j)} - \phi_{(i-1,j)}}{\phi_{(i+1,j)} - \phi_{(i,j)}} \]  \hspace{1cm} (2.19)

Using (2.15), this ratio can be expressed in terms of normalized variables

\[ r_{(i+1/2,j)} = \frac{\hat{\phi}_{(i,j)}}{1 - \hat{\phi}_{(i,j)}} \]  \hspace{1cm} (2.20)

From (2.17) and (2.20), we deduce the following flux limiter used in what we call the ISNAS scheme:

\[ \Psi(r) = \frac{r^2 + 3r}{(1 + r)^2}, \quad r \geq 0 \]  \hspace{1cm} (2.21)

With (2.16), (2.18) and (2.20) it follows that for all \( r < 0 \), \( \Psi(r) = 0 \). We note that \( \Psi(1) = 1 \), which is necessary for a scheme to be at least second-order accurate [11]. Moreover, it can be shown for an arbitrary limiter \( \Psi \) that \( \Psi'(1) = \frac{1}{3} \) is necessary and sufficient for third-order accuracy, which is true for the ISNAS limiter. The implementation of this scheme is as follows: the convective terms are approximated by the first-order upwind scheme including the third-order accurate terms as a deferred correction, as suggested by [3]. This ensures diagonal dominance for the resulting algebraic equations, thus enhancing iterative rate of convergence while restoring third-order accuracy at steady-state convergence. To ensure monotonicity the correction terms are limited by (2.21).

3 Numerical framework

The overall solution algorithm can be summarized as follows: in every time step first the momentum and continuity equations are solved and then each turbulence equation. The whole process is repeated until convergence to a stationary solution is achieved. Time discretization is done by the implicit Euler method and linearization is carried out with the Newton method. A second-order pressure-correction scheme [12] is used to obtain a divergence-free velocity field. The three linear systems, namely momentum, pressure and transport equations, are solved in each time step by a preconditioned GMRES solver [8]. For preconditioners we use incomplete LU factorizations. For details we refer to [13].

4 Results and discussions

A comparative test performed on standard and the more accurate discretizations as explained in [17] and Section 2, respectively, concerns a pure diffusion equation

\[ \frac{d}{dy} \left( D \frac{d\phi}{dy} \right) = 0 \]  \hspace{1cm} (4.1)
solved on a rectangle domain $[0, 1] \times [0, 4]$. In the domain a non-smooth grid of $20 \times 20$ cells is generated, as shown in Figure 4.1. The diffusion coefficient $D$ is piecewise constant, as follows: $D = 3$ in $0 \leq y \leq 2$ and $D = 6$ elsewhere. The boundary conditions are chosen such that the solution has the following form

$$
\phi(y) = \begin{cases} 
-\frac{1}{3}y + 1, & 0 \leq y \leq 2 \\
-\frac{1}{3}y + \frac{2}{3}, & 2 < y \leq 4
\end{cases}
$$  \hspace{1cm} (4.2)

Figure 4.1 shows the results of both discretizations. As expected, the straightforward approach does not give the correct solution, whereas in the case of new discretization the linear field as given by (4.2) is recovered.

![Figure 4.1: (a): the non-smooth grid; (b): wrong solution obtained with standard approach; (c): correct solution obtained with new discretization](image)

The second test problem is a turbulent co-flow jet in a planar duct. The flow involves several interesting features such as the presence of recirculation with unknown reattachment and separation points and the coexistence of both strong and weak shear regions. The geometry considered here is a symmetric planar duct with height $D_0 = 0.16$ m and a nozzle diameter $d_0 = 0.012$ m, as shown in Figure 4.2. Furthermore, $U_j = 12.538$ m/s and $U_a = 0.3981$ m/s are the jet and ambient flow

![Figure 4.2: Flow configuration](image)
velocities, respectively. Computations were performed with the standard high-Re $\kappa$-$\varepsilon$ model in conjunction with wall functions on three different uniform grids, namely $50 \times 40$, $70 \times 50$ and $90 \times 60$ cells. Because of symmetry, computations are performed in half the domain only. Figures 4.3, 4.4 and 4.5 provide a comparison of turbulent viscosity profiles arising from the hybrid central/upwind [10] and the IS-

![Graph showing turbulent viscosity profiles](image)

**Figure 4.3: Turbulent viscosity profile at $z = 0.3$ m**

![Graph showing turbulent viscosity profiles](image)

**Figure 4.4: Turbulent viscosity profile at $z = 0.3$ m**

NAS schemes, all at location $z/D_0 = 1.875$. Figure 4.3 shows that in going from a coarse to a refined grid the level of turbulent viscosity calculated using the IS-NAS scheme does not change much and that grid-independence has already been achieved on the $70 \times 50$ grid. As shown in Figure 4.4, the change is large, however, for the hybrid scheme. In that case the turbulent viscosity is underestimated on both $70 \times 50$ and $90 \times 60$ grids. Figure 4.5 demonstrates that $\mu_t$ is rather sensitive to
the convection scheme adopted. This can be explained as follows. In regions where shear stress is small, the production of turbulent energy and its dissipation rate are negligible. However, the dissipation terms in the transport equations of both $k$ and $\varepsilon$ remain nonzero. These terms must be in balance with the transport mechanism, in particular the convective transport. Hence, it is important to approximate the convection of turbulence quantities accurately. When any numerical diffusion is introduced in the convection term (by the hybrid scheme, for example), this leads to a too high dissipation rate $\varepsilon$ and, since $\varepsilon$ is a sink term in the $k$-equation, to too low levels of turbulent energy. As a consequence, since $\mu_t$ is proportional to $k^2/\varepsilon$, this double-edged effect causes $\mu_t$ to become significantly too low.

5 Conclusions

A new discretization of the general transport equations as proposed in [15] has been presented which shows good results for non-smooth grids and discontinuous diffusion coefficient. A formally third-order accurate TVD scheme for the approximation of convective transport in the finite volume context has been formulated, using Leonard's variable normalization technique. This scheme appears to be satisfactory. In the computation of confined co-flow jet in a 2D planar duct, the discretization of convection in the turbulence transport equations is shown to be of primary importance to the numerical accuracy of the solution for the $k$-$\varepsilon$ turbulence model. Monotone higher-order schemes for the discretization of convective transport of turbulence can significantly reduce the grid size necessary for an error-free solution.
References


