VERIFICATION OF THE DISCRETIZATION ERROR OF NUMERICAL SOLUTIONS OF FLOWS USING UNSTRUCTURED MESHES

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Abstract: *The present work evaluates the discretization error estimator named Grid Convergence Index (GCI), which is based on the Richardson Extrapolation, taking into account: (1) a two-dimensional laminar flow inside a square cavity that has a known analytical solution; (2) unstructured meshes to discretize the problem domain; (3) The Element based Finite Volume Method (EbFVM); (4) The CFX CFD code to get the numerical solutions; and (5) two variables of interest, the mass flux in the cavity and the force applied by the top boundary on the fluid in the cavity. The error estimates obtained with GCI are reliable for all meshes and both variables but their accuracy can be considered satisfactory.*

Keywords: *numerical error; error estimator; finite volume; CFX.*

1. Introduction

The numerical error is defined as the difference between the exact analytical solution (Φ) of a variable of interest and its numerical solution (ϕ) (Ferziger and Peric, 2001):

$$E(\phi) = \Phi - \phi \tag{1}$$

The numerical error can be composed by four distinct parts (Marchi, 2001):

a) Truncation error is defined as a residual that comes from the substitution of the exact analytical solution of a variable on the discretized equation of the mathematical model;
b) Iteration error is the difference between the exact and the iterative solutions of the discretized equations;
c) Round-off error is due the finite representation of the real numbers used in computer calculations; and
d) Programming errors are caused by people in the implementation and use of a code.

Moreover, accordingly to Ferziger and Peric (2001), the discretization error (E) can be defined as the numerical error due only truncation error, *i.e.*, when all other three parts of the error (round-off, programming and iteration) are zero or negligible.

When the analytical solution of a desired problem is not known, the numerical error can not be calculated. In this case, it is used an estimative of the analytical solution (ϕ_∞) that give only an estimative of the error or uncertainty (U) of the numerical solution (Marchi, 2001), *i.e.*,

$$U(\phi) = \phi_\infty - \phi \tag{2}$$

The present work has as goal to evaluate the discretization error estimator named Grid Convergence Index – GCI (Roache, 1994), which is based on the Richardson Extrapolation, taking into account:

1) a two-dimensional laminar flow inside a square cavity that has a known analytical solution;
2) unstructured meshes to discretize the problem domain;
3) the Element based Finite Volume Method – EbFVM (Maliska, 2004);
4) the CFX (Ansys, 2004) CFD code to get the numerical solutions; and

5) two variables of interest, the mass flux in the cavity and the force applied by the top boundary on the fluid in the cavity.

This work was motivated by the fact that has few studies about the effects of the use of unstructured meshes on the numerical errors and on the performance of the error estimators (Marchi, 2001). More than that, it was found few studies about the numerical uncertainty for codes based on EbFVM. For example, the results of Souza (2000) do not bring any study about numerical uncertainty, even showing results on more than one mesh for the square cavity problem (Ghia *et. al.*, 1982). This work is focused on iteration errors. The present authors found only the works of Roache (1994) and Celik and Karatekin (1997) treating of error estimatives on unstructured meshes. These works show the effect of the use of two-dimensional meshes on error estimatives, however, only for the traditional form of the finite volume method, on a code created by the authors.

The present work is divided in the following way: in section 2 the mathematical and numerical models are presented; in section 3 it is presented the GCI error estimator; in section 4 it is defined the physical problem; and in sections 5 and 6, respectively, the results and the conclusion of the work are shown.

2. Mathematical and numerical models

2.1 Governing equations

Considering that the problems to be solved are two-dimensional, laminar, steady flows with negligible gravitational effects, incompressible fluid with constant properties, the mass and momentum equations are

$$\frac{\partial U_i}{\partial x_i} = 0 \tag{3}$$

$$\rho \frac{\partial (U_j U_i)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \mu \frac{\partial}{\partial x_j}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) + S_{U_i} \tag{4}$$

where U_i are the velocity components in i direction (for two-dimensional problems i represents u and v), x_i is the Cartesian coordinate in i direction (x and y, in this case), P is the pressure, ρ is the fluid density, μ is the viscosity and S_{Ui} is a source term associated with the velocity U_i.

2.2 Problem domain discretization

In EbFVM the elements are created by joining points distributed on the domain, the nodes, and the control volumes are created surrounding these points with contributions of vary elements (Souza, 2000). In Fig. 1 is shown a triangular mesh with elements 123, 134, 145, 156, 167, 178 and 182, and also the volumes A and B. The nodes are identified by the black circles and the volumes by the hatched areas. A triangular element, for example the element 123, can be mapped on a triangular element on the reference plane (ξ,η) using interpolation functions $N(\xi,\eta)$ (Fig. 2).

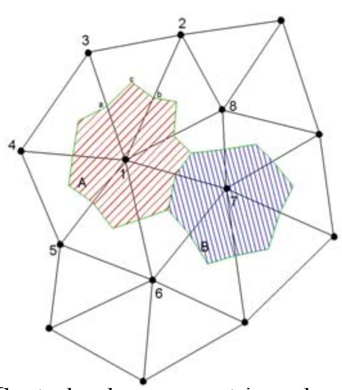

Figure 1. Control volumes on a triangular element unstructured mesh; adapted from Maliska (2004)

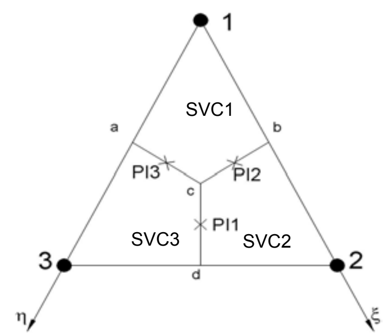

Figure 2. Mapped triangular element on (ξ,η) plane; adapted from Maliska (2004)

The properties balance on the control volume A are made by the sum of the elements 123, 134, 145, 156, 167, 178 and 182 contributions for each property. The discretization of the equations is quite similar to Finite Volume Method (Maliska, 2004; Ferziger and Peric, 2001). The difference is that the integrations are not made on the volume's central nodes, nor on the volume's boundary, but on the integration points, *PI* (Fig. 2), that are put on the middle of the median that forms the control volume. In Morais (2004) can be found a complete description of the calculus of a scalar property ϕ, and these derivatives, for a triangular element as well the interpolation functions for this element.

2.3 The CFX

The CFX-5 is a Computational Fluid Dynamics (CFD) code for general use. It combines a solver with pre and post-processing tool that allow the user to define, solve and analyze results of simulations with a very high degree of geometrical and physical complexity.

In CFX, the advection terms of the conservation equations are discretized accordingly to the following interpolation scheme (Ansys, 2004):

$$\phi_{pi} = \phi_m + \beta \nabla\phi \bullet \nabla r \tag{5}$$

where ϕ_m is the value of the variable of interest ϕ that is upwind the integration point pi; β is the blend factor. When β = 0, Eq. (5) gives a first order interpolation scheme (Ferziger and Peric, 2001), with its great robustness and numerical diffusion. But, with β = 1, Eq. (5) gives a second order scheme with its better accuracy, however with its numerical dispersion. In CFX is possible to choose β values between 0 and 1, but in this work only the schemes with blend factor equal one and zero were used for a better comparison between the results.

The CFX-5 has another discretization scheme, named Upwind. This scheme is also a first order scheme and gives identical results to scheme β = 0. So, in this work only the schemes blend factor = 1 and Upwind were used.

3. Discretization error estimators

The function of an error estimator is to calculate the uncertainty defined by Eq. (2), *i.e.*, to estimate the numerical error's value, defined in Eq. (1). The Richardson and GCI estimators are examples of *a posteriori* error estimator, *i.e.*, estimators that calculate the uncertainty based on the numerical solutions obtained with one or more meshes.

The Richardson estimator estimates the value of the analytical solution (ϕ_∞) by the generalized Richardson extrapolation (Roache, 1994), given by

$$\phi_\infty = \phi_1 + \frac{(\phi_1 - \phi_2)}{(q_{ef}^{p_L} - 1)} \tag{6}$$

where ϕ_1 and ϕ_2 are, respectively, the numerical solutions obtained with fine and coarse meshes, p_L is the asymptotic order of the discretization error (Marchi, 2001) and q_{ef} is the effective mesh refinement ratio, defined as (Roache, 1994)

$$q_{ef_{21}} = \left(\frac{N_1}{N_2}\right)^{\frac{1}{D}} \tag{7}$$

being N_1 and N_2 the number of elements on the fine and coarse meshes, respectively, and D is the dimensionality of the problem. In this work, D = 2.

Introducing Eq. (6) into Eq. (2), the numerical uncertainty of the solution obtained with fine mesh is given by

$$U_{Ri}^{p_L}(\phi_1) = \frac{(\phi_1 - \phi_2)}{(q_{ef_{21}}^{p_L} - 1)} \tag{8}$$

When the asymptotic order (p_L) is unknown, the apparent order (p_U) can be calculated. This order is obtained with numerical solutions on three different meshes: fine (ϕ_1), coarse (ϕ_2) and supercoarse (ϕ_3), with $N_1 > N_2 > N_3$ elements, respectively. Considering that any effective mesh refinement ratio between the pairs of meshes 1-2 and 2-3, defined in Eq. (7), it is possible to demonstrate that (Marchi, 2001)

$$p_U = \frac{\log\left[\left(\frac{\phi_2 - \phi_3}{\phi_1 - \phi_2}\right)\left(\frac{q_{ef_{21}}^{p_U} - 1}{q_{ef_{32}}^{p_U} - 1}\right)\right]}{\log(q_{ef_{21}})} \tag{9}$$

So, the Richardson estimator based on the apparent order (p_U) results in

$$U_{Ri}^{p_U}(\phi_1) = \frac{(\phi_1 - \phi_2)}{(q_{ef_{21}}^{p_U} - 1)} \tag{10}$$

The GCI estimator (Roache, 1994) is an extension of Richardson estimator. It is obtained with the application of a safety factor (F_S) and considering an interval where the true error is statistically hoped to be found. Mathematically, one gets

$$U_{GCI}^{p}(\phi_1) = F_S \left| U_{Ri}^{p}(\phi_1) \right| \tag{11}$$

where p represents p_L or p_U. In this work, $F_s = 3$ as recommended by Roache (1994).

4. Problem definition

As proposed by Shih *et al.* (1989), the fluid inside a square cavity is moved circularly due a boundary condition of velocity, $u(x,1)$, prescribed on superior boundary (see Fig. 3 for more details). The mathematical description of these boundary conditions and the source term $B(x,y,\text{Re})$ can be found in Shih *et al.* (1989), as well as the analytical solution of the problem for u, v and P. The circulation center is at $x = 0.5$ m and $y = \cos 45° \approx 0.707$ m.

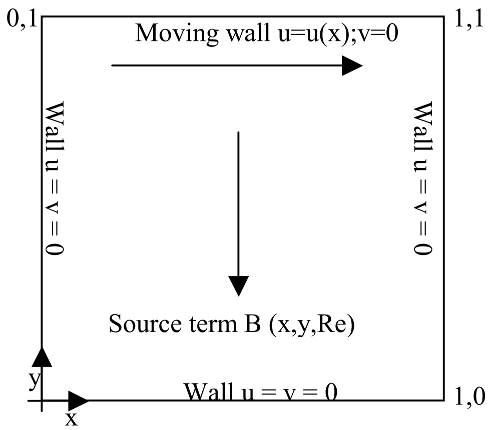

Figure 3. Problem domain and boundary conditions; adapted from Shih *et al.* (1989)

The variables of interest of this problem are the mass flux (FM) inside the cavity and the force (FP) applied by the upper plate on the fluid, defined by

$$FM = \int_{\cos 45°}^{1} \rho\, u(0.5, y)\, W\, dy \tag{12}$$

$$FP = \int_{0}^{1} \mu \left(\frac{\partial u}{\partial y} \right)_{y=1} W\, dx \tag{13}$$

where $\rho = 1$ kg/m^3, $\mu = 1$ Pa.s and W is the cavity deepness in z direction that is equal to 1 m. The analytical solutions of Eqs. (12) and (13) are: $FM = 1/8 = 0.125$ kg/s; e $FP = 8/3 \approx 2.6667$ N.

5. Results

5.1 Meshes

The domain's discretization was done in way to get meshes with elements distributed as more uniformly as possible, *i.e.*, with small differences on element size and volume, as recommended by Celik (2005). The number of divisions on the domain sides (boundaries) indicates, to mesh generator, the number of nodes that must be put between the points that generate this side of the mesh.

All meshes were generated using tetrahedrical elements, because CFX-5 always uses three-dimensional meshes. To get a two-dimensional flow simulation, symmetry boundary conditions were applied at the domain faces, as indicated by Ansys (2004). The number of elements on the face was got to calculate the grid refinement ratio with Eq. (7). These elements were generated using only the nodes on domain face.

For the six meshes used at the simulations, the following variables are presented in Tab. 1: the number of divisions used on each domain side; the number of elements used to discretize the two-dimensional domain shown in Fig. 3 (the face elements explained above); the average size of elements (it will be defined ahead); and the effective mesh refinement ratio calculated with Eq. (7). The lines of this column in Tab. 1 are not aligned to other lines to show that the grid refinement ratio, q_{ef}, are between meshes A-B; B-C; C-D; D-E and E-F.

Table 1. Meshes used in this work.

Mesh	# Divisions of each boundary	# Elements of 2D domain	$\overline{h}$	q_{ef}
A	5	50	1.414×10^{-1}	
				q_{ef} (AB) = 2.2000
B	10	242	6.428×10^{-2}	
				q_{ef} (BC) = 1.9091
C	20	882	3.367×10^{-2}	
				q_{ef} (CD) = 2.0443
D	40	3686	1.647×10^{-2}	
				q_{ef} (DE) = 1.9779
E	80	14420	8.328×10^{-3}	
				q_{ef} (EF) = 1.9885
F	160	57021	4.188×10^{-3}	

5.2 Numerical solutions

To calculate the variables of interest (*FM* and *FP*) were got two lines on domain. The first one, to calculate *FM*, is vertical (constant x) at the middle of the cavity (x = 0.5 m) and with y-coordinate varying between 0.707 m (cos 45°) and the upper boundary (y = 1 m). The beginning of the line was got at the theoretical center of the rotational flow just for facility, because the CFX post processor gives results at any point of the domains using interpolation of nodal results.

The second line, used to calculate *FP*, is horizontal (y constant) at y = 0.99375 m and with the x-coordinate varying between 0 and 1 m. This y value is equal to 1-1/160 m, where 160 is the number of the divisions on each boundary of the finest grid. The number of points used to get the results at each line is equal to the number of the divisions on the boundary side that this line intersects.

To calculate *FP*, the second line and the upper boundary velocities are used. Moreover, to calculate the y-direction velocity gradient is mandatory (see Eq. 13). The approximation of this derivative is done by the difference between two consecutive points of the simulation results:

$$\left.\frac{\partial u}{\partial y}\right|_i = \frac{\Delta u_i}{\Delta y_i} = \frac{u_i - u_{i-1}}{y_i - y_{i-1}} \tag{14}$$

With the approximation used in Eq. (14), the asymptotic order (p_L) of *FP* is one and it is not dependent of the discretization scheme used for advection terms, because this is the smallest order of all used approximations. For the variable *FM*, the asymptotic order is 2 and 1 for, respectively, blend factor = 1 and Upwind schemes. The necessary integrations on both variables, see Eqs. (12) and (13), were made using the trapezoidal rule (Kreyszig, 1999). The results obtained for both variables of interest are shown in Tab. 2. These results should be compared to those analytical ones shown above.

Table 2. Numerical results for mass flux (*FM*) and force of plate (*FP*).

Mesh	Mass flux (kg/s)		Force of plate (N)	
	Blend Factor = 1	Upwind	Blend Factor = 1	Upwind
A	0.088731233	0.083781846	18.141249567	19.870826006
B	0.114103463	0.112583208	4.285552285	4.888788220
C	0.122242379	0.121814640	3.115642582	3.331372810
D	0.124483571	0.124370775	2.609222026	2.813162603
E	0.124905337	0.124861074	2.579033834	2.684809871
F	0.124995705	0.124953565	2.630198032	2.654268843

The computation times to get the numerical solutions of Tab. 2 are presented in Tab. 3. All computations were made using double precision. As convergence criteria for iterative process it was used nondimensional residual smaller than 10^{-10} for all conservation equations. All simulations were done using a PC type microcomputer, with AMD Athlon 1500+ processor and 256 MB of RAM. The operational system used was the Windows 2000 SP3.

Table 3. Computational time necessary to get the numerical solutions.

Mesh	CPU time (seconds)	
	Blend Factor = 1	Upwind
A	13.0	12.9
B	32.6	31.0
C	70.7	64.4
D	426.0	451.8
E	1776.0	1861.0
F	8097.0	8843.0

5.3 Verification of the discretization error

The behavior of the discretization error for the two variables of interest with the mesh size can be seen in Figs. 4 and 5. In Figs. 4 to 7, the results are presented for a mean size of elements, shown in Tab. 1, and defined as (adapted of Celik, 2005):

$$\bar{h} = \left(\frac{S}{N}\right)^{\frac{1}{D}} \tag{15}$$

where S represents the problem domain (in two-dimensional domains S is equal to domain area); N is the number of elements on domain and D is the dimensionality of the problem, 2 in this work.

For the mass flux, the discretization error is reduced monotonically when $\bar{h}$ is reduced, as shown in Fig. 4. This also happens for the force of plate, Fig. 5, but with an oscillation for the solutions obtained with Blend Factor = 1. This oscillation disables the calculus of the apparent order and, as a consequence, to apply the error estimator based on this order. It is observed also that the numerical results of each variable and their errors are very close between both the discretization schemes.

5.4 Performance of the GCI estimator

The apparent order (p_U) for both variables of interest is presented in Tab. 4. It is observed that the values of the apparent order are quite different of the asymptotic order for both variables. The performance of GCI estimator is shown in Figs. 6 and 7 for both variables of interest. In these figures, the results are presented as a ratio between the GCI (Eq. 11) and the true error (Eq. 1). As demonstrated by Marchi and Silva (2002), the uncertainty must be calculated based on the smallest value between the asymptotic and apparent orders (since the last one exists and is positive). Considering this, the GCI estimator is reliable on all meshes for both variables of interest. By definition, a reliable error estimative is when $U_{GCI} / E \geq 1$. The error estimative accuracy can be considered just satisfactory, because the ratio between U_{GCI} and E is fairly far from one.

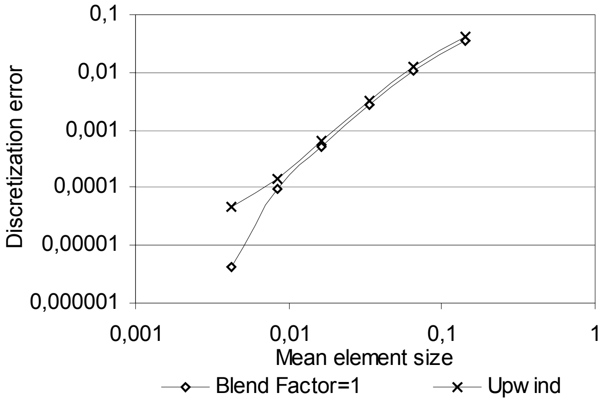

Figure 4. Absolute value of discretization error for *FM*

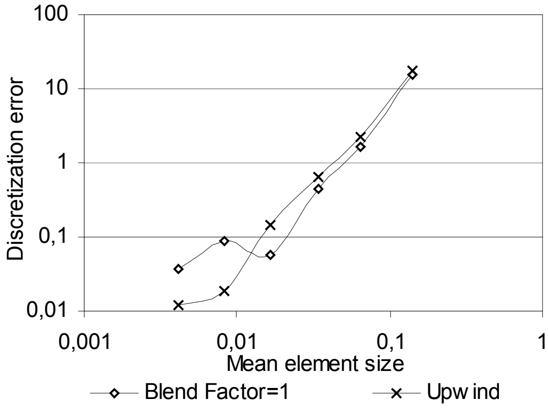

Figure 5. Absolute value of discretization error for *FP*

Table 4. Apparent order (p_U) for mass flux (*FM*) and force of plate (*FP*).

Mesh	Mass flux		Force of plate	
	Blend Factor=1	Upwind	Blend Factor=1	Upwind
C-B-A	1.289	1.290	3.065	2.792
D-C-B	2.066	2.053	1.388	1.782
E-D-C	2.309	2.282	3.931	1.920
F-E-D	2.281	2.469	Inexistent	2.127

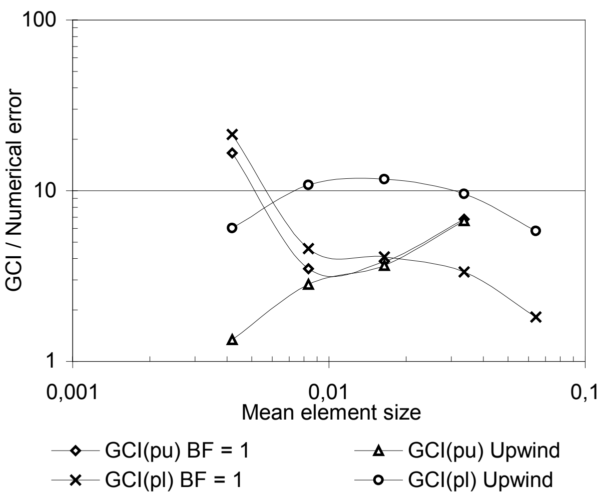

Figure 6. Ratio U_{GCI}/E for *FM*

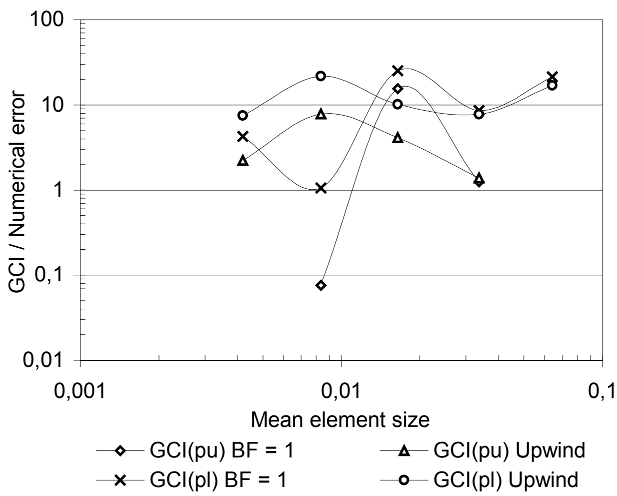

Figure 7. Ratio U_{GCI}/E for *FP*

6. Conclusion

The present work had as main goal to analyze the performance of the GCI estimator for discretization errors of unstructured meshes. The numerical solutions were obtained with the CFX code that employs the Element based Finite Volume Method. A two-dimensional laminar flow inside a square cavity was solved. The variables of interest were the mass flux in the cavity and the force applied by the top boundary on the fluid in the cavity. The error estimates obtained with GCI are reliable for all meshes and both variables but their accuracy can be considered satisfactory.

7. Acknowledgements

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