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AN UNCERTAINTY ESTIMATION EXAMPLE FOR BACKWARD FACING STEP CFD SIMULATION

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Abstract

Results uncertainty estimation has been computed for the fluid flow simulation of the incompressible turbulent flow in a Backward Facing Step, using the Grid Convergence Index method and the commercial CFD code ANSYS CFX. Results are shown both for the Shear Stress Transport turbulence model as well as for a variation of this model that incorporates a Reattachment Modification term.

INTRODUCTION

Uncertainty estimation of Computational Fluid Dynamics (CFD) results is becoming a necessary step in CFD studies, and a number of methods have been derived during the lat years in order to accomplish it. This paper presents an example of uncertainty estimation for a Backward Facing Step calculation, which corresponds to the ERCOFTAC database, case C-30.

NUMERICAL MODEL

The calculations have been performed with the commercial CFD code ANSYS CFX. The code is based on the Finite Volume method and vertex-centred.

Discretization Scheme

The Navier-Stokes conservation equations described below are discretized using an element-based finite volume method [1]. The mesh may consist of tetrahedral, prismatic, pyramid, and hexahedral elements. A control volume is constructed around each nodal point of the mesh, as illustrated in Figure 1. The subface between two control volumes within a particular element is called an integration point (ip); it is at integration points that the fluxes are discretized.
Integration point quantities such as pressure and velocity gradients are obtained from nodal values using finite element shape functions, with the exception of advected variables which are obtained using an upwind-biased discretization.

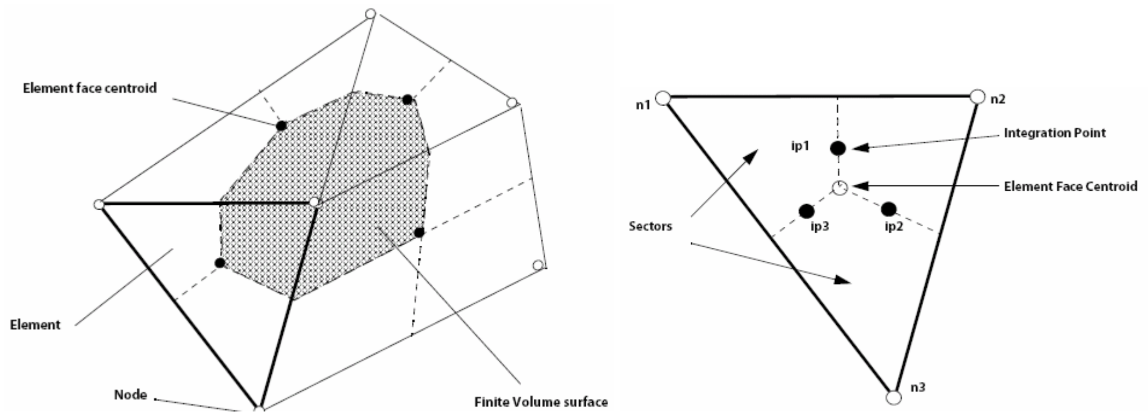

Figure 1: Finite Volume Surface and Mesh Element in the discretization

We now consider the discretization of the conservation equations at each control volume. The discretization is fully conservative and time-implicit. The conservation equations are integrated over each control volume, volume integrals are converted to surface integrals using Gauss' divergence theorem, and surface fluxes are evaluated in exactly the same manner for the two control volumes adjacent to an integration point.

The advection scheme used to evaluate the variable ϕ_{ip} in terms of neighbouring vertex values ϕ is extremely important for the solution accuracy. We write it in the form

$$\phi_{ip} = \phi_{up} + \beta \nabla\phi \cdot \Delta \vec{r} \tag{1}$$

Where ϕ_{up} is the upwind vertex value and Δr is the vector from the upwind vertex to the integration point. The quantity $\beta\nabla\phi.\Delta r$ is called Numerical Advection Correction. If $\beta = 0$, this scheme recovers the first-order upwind scheme, which is bounded but excessively diffusive. If $\beta = 1$, this scheme is a second-order upwind-biased scheme, but unbounded. A bounded high-resolution scheme can be obtained by making β as close to 1 as possible, but reducing where necessary to prevent overshoots and undershoots from occurring. For standard advection terms, CFX uses a method similar to that described by Barth and Jesperson [2].

The mass flows must be discretized in a careful manner to avoid pressure-velocity decoupling. This is performed by generalizing the interpolation scheme proposed by Rhie and Chow [3], such that the advecting velocity is evaluated as follows:

$$u^i_{ip} = \overline{u^i}_{ip} + d_{ip}\left(\left(\frac{\partial P}{\partial x^i} - \rho_m g^i\right) - \left(\overline{\frac{\partial P}{\partial x^i} - \rho_m g^i}\right)\right)_{ip} \tag{2}$$

where

$$d_{ip} \propto -V/a$$
$$a \propto \rho_m V/\delta t + b \tag{3}$$

and b represents the sum of advection and viscous coefficients in the discretized momentum equation. The overbar denotes the average of the control volume values adjacent to the integration point.

Solution Strategy

Segregated solvers employ a solution strategy where the momentum equations are first solved, using a guessed pressure, and an equation for a pressure correction is obtained.
Because of the ‘guess-and-correct’ nature of the linear system, a large number of iterations are typically required in addition to the need for judiciously selecting relaxation parameters for the variables.
ANSYS CFX uses a coupled solver, which solves the hydrodynamic equations (for *u*, *v*, *w*, *p*) as a single system. This solution approach uses a fully implicit discretisation of the equations at any given time step. For steady state problems, the time-step behaves like an ‘acceleration parameter’, to guide the approximate solutions in a physically based manner to a steady-state solution. This reduces the number of iterations required for convergence to a steady state, or to calculate the solution for each time step in a time dependent analysis.

The linear system of equations is solved using a coupled algebraic multigrid technique [4].

SIMULATION DETAILS

The example corresponds to a Backward Facing Step geometry, from the ERCOFTAC Test Case C-30. The step size H is 0.0127 m, the tunnel height is 8H and the tunnel span is 12H.
The origin of the coordinate system is located at the low corner of the step, with the inlet boundary located at x = -4H, the outlet boundary at x = 40 H and the top boundary at y = 9H.

A set of three grids has been used in the calculations, with the mesh parameters given in Table 1.

	Nodes A	Nodes B	Nodes C	Nodes D	Nodes E
Grid1	40	17	20	135	20
Grid2	60	25	30	200	20
Grid3	90	40	45	300	20

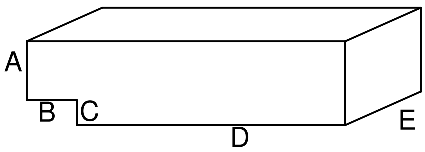

Table 1: mesh parameters for the three grids used in the calculation

Although not necessary for the simulation or results accuracy, the tunnel span has also been discretized in space with 20 nodes in order to preserve the geometry width.
Mesh nodes have been refined towards the walls with a geometric law of ratio 1.25, where the first node has been set at 0.1 mm from the wall.

The flow Reynolds number is 50000, defined as $Re = U_{ref} L_{ref} / \nu$ where U_{ref} is 44.2 m/s and L_{ref} is H. That means the flow kinematic viscosity ν is 1.1227e-5 m^2/s.

The definition of the Boundary Conditions is as follows:

- Inlet: velocity and turbulence profiles for fully developed turbulent flow, provided from Dr. Eça from IST Lisbon, with U_{ref} = 44.2 m/s.
- Outlet: average relative static pressure = 0 Pa.
- Tunnel top and bottom surfaces: walls with u=v=0.0 m/s.
- Tunnel side walls: symmetry condition.

The Shear Stress Transport turbulence model with Automatic wall treatment by Menter [5] has been used for the simulation, as well as a modification of this model that incorporates a term for accurate boundary layer reattachment prediction. The reattachment modification term accounts for an additional production of the kinetic energy k in separated shear layers, as standard RANS and RSM models underpredicts the Reynolds stresses in this area.

UNCERTAINTY ESTIMATION PROCEDURE

The uncertainty estimation has been calculated by means of the Grid Convergence Index (GCI) method [6]. The method defines the numerical uncertainty U for any local or integral variable as

$$U = F_s |\gamma_{RE}| \tag{3}$$

where F_s is a safety factor and γ_{RE} is the error estimation resulting from the Richardson extrapolation [6]. Richardson extrapolation defines the error γ_{RE} as

$$\gamma_{RE} = \phi_i - \phi_0 = \alpha h_i^{\,p} \tag{4}$$

Where ϕ_i is the numerical solution on a given grid i, ϕ_0 is the exact solution, α is a constant, h_i is a measure of the representative mesh cell size and p is the observed order of accuracy of the numerical method.

There are three unknowns in equation (4): ϕ_0, α and p, so in theory three grids are necessary in order to obtain the uncertainty estimation of a given local or integral variable.

Eça and Hoekstra [7] observed that more than a grid triplet is usually necessary to estimate the uncertainty as the estimation may vary a lot among different grid triplets. However, for the example presented in this paper, only one grid triplet have been used.

During the grid convergence study with three grids, the solution is convergent if

$$(\phi_2 - \phi_1) \cdot (\phi_3 - \phi_2) > 0 \tag{5}$$

$$p > 0 \tag{6}$$

Conditions (5) and (6) are necessary to ensure that ϕ changes monotically and that converges to a finite value for grid cell size zero.

If for a variable computed on three grids, conditions (5) and (6) are fulfilled, and

$$\frac{h_3}{h_2} = \frac{h_2}{h_1} \tag{7}$$

Then p can be obtained from

$$p = \frac{\log\left(\dfrac{\phi_3 - \phi_2}{\phi_2 - \phi_1}\right)}{\log\left(\dfrac{h_2}{h_1}\right)} \tag{8}$$

and $\gamma_{RE} = \phi_1 - \phi_0$ from

$$\gamma_{RE} = \frac{\phi_2 - \phi_1}{\log\left(\dfrac{h_2}{h_1}\right)^p - 1} \tag{9}$$

As only one grid triplet is used for a relatively complex turbulent flow, Roache [8] recommends using a safety factor F_s in order to estimate the uncertainty U, as shown in equation (3). The proposed values for F_s are:

If $0.5 < p < 3.5$, $F_s = 1.25$
If $3.5 < p < 4.5$, $F_s = 3.00$
If $p < 0.5$ or $p > 4.50$, the uncertainty U is calculated as the maximum difference between the solutions obtained on the calculation grids multiplied by a safety factor $F_s = 3.00$ for $p < 0.5$ or $F_s = 1.35$ for $p > 4.50$.

RESULTS

All simulations have been performed using double precision. Results quantities ϕ_1,ϕ_2 and ϕ_3 are shown in tables 3 and 4, together with the observed order of convergence p and the uncertainty U. Values of h_i are shown in table 2, and have been calculated as L_{ref} / number of nodes in the step.

	h = Lref/C
Grid1	0.006350
Grid2	0.000423
Grid3	0.000282

Table 2: Values of h_i

The studied quantities are the following local variables: u, v, Cp defined as $(p-p_{outlet})/(½\rho U^2)$, eddy viscosity ν_t, all of them being monitored at x=0,y=1.1h, x=h,y=0.1h and x=4h,y=0.1h, and the following integral variables: friction resistance coefficient at the top and bottom walls and pressure resistance coefficient at the bottom wall.

	x=0,y=1.1H			x=0,y=1.1H		
	SST Grid1	SST Grid2	SST Grid3	SSTrm Grid1	SSTrm Grid2	SSTrm Grid3
u	0.57151	0.53566	0.51808	0.60176	0.56328	0.54321
p u	0.263058071			0.240292141		
U u	0.16029	0.16029		0.17565	0.17565	
v	-0.0091355	-0.0087869	-0.0085967	-0.011966	-0.011274	-0.01082
p v	1.494207444			0.155597629		
U v	0.000443496	0.00024197		0.003438	0.003438	
Cp	-0.50731	-0.57796	-0.61629	-0.48197	-0.55116	-0.59111
p Cp	1.508157465			0.202753981		
U Cp	0.089823071	0.048732036		0.32742	0.32742	
νt	5.05180E-06	3.57700E-06	2.9218E-06	6.89790E-06	4.74730E-06	3.79010E-06
p νt	2.001003582			0.298832866		
U νt	1.85169E-06	8.22641E-07		9.3234E-06	9.3234E-06	

	x=H,y=0.1H			X=H,y=0.1H		
	SST Grid1	SST Grid2	SST Grid3	SSTrm Grid1	SSTrm Grid2	SSTrm Grid3
u	-0.0028959	-0.0014233	-0.001011	-0.006768	-0.0024567	-0.001929
p u	0.469955614			0.775412516		
U u	0.0056547	0.0056547		0.006140748	0.000751623	
v	0.00062348	0.00047929	0.00038371	0.0026972	0.0017821	0.0015279
p v	1.014065755			0.472864022		
U v	0.000192587	0.000127661		0.0035079	0.0035079	
Cp	-18744	-72436	-140180	-3299.8	-28836	-18868
p Cp	Divergence			Divergence		
U Cp	Divergence	Divergence		Divergence	Divergence	
νt	1.97900E-08	6.00600E-09	7.4106E-09	8.61350E-08	2.75260E-08	2.39930E-08
p νt	Divergence			1.036880386		
U νt	Divergence	Divergence		7.79608E-08	4.69954E-09	
	x=4H,y=0.1H			x=4H,y=0.1H		
	SST Grid1	SST Grid2	SST Grid3	SSTrm Grid1	SSTrm Grid2	SSTrm Grid3
u	-0.15983	-0.15798	-0.1577	-0.11031	-0.11425	-0.11463
p u	0.697033701			0.863383054		
U u	0.00272492	0.00340615		0.005450702	0.000525702	
v	-0.001954	-0.0015929	-0.00135	-0.0073963	-0.005698	-0.0052601
p v	0.977901882			0.500359379		
U v	0.000485727	0.00060716		0.002860424	0.00073755	
Cp	-4.4128	-4.4486	-4.4652	-4.7701	-4.4483	-4.7555
p Cp	1.895465683			Divergence		
U Cp	0.045015136	0.056268921		Divergence	Divergence	
νt	9.73480E-06	7.48560E-06	5.1453E-06	1.95750E-05	1.07000E-05	1.43110E-05
p νt	Divergence			Divergence		
U νt	Divergence	Divergence		Divergence	Divergence	

Table 3: Local variables results for SST model and SST model with Reattachment Modification

	SST			SSTrm		
	Grid1	Grid2	Grid3	Grid1	Grid2	Grid3
*$C_{f\ BW}$	0.35428143	0.35648442	0.357478807	0.396169909	0.395262797	0.393742128
p $C_{f\ BW}$	0.294			-0.191		
U $C_{f\ BW}$	0.00959211	0.00959211		Divergence	Divergence	
*$C_{f\ TW}$	0.68257927	0.68129133	0.680590501	0.682579271	0.681291331	0.680590501
p $C_{f\ TW}$	0.225			0.812		
U $C_{f\ TW}$	0.00596631	0.00596631		0.008685323	0.00096297	
*$C_{p\ BW}$	0.39900496	0.4641372	0.534270432	0.961980333	0.964609107	0.991248579
p $C_{p\ BW}$	-0.0273096			-0.855		
U $C_{p\ BW}$	Divergence	Divergence		Divergence	Divergence	
**X_r	6.792	6.689	6.653	5.748	5.736	5.756
p X_r	0.388			Divergence		
U X_r	0.354	0.354		Divergence	Divergence	

** x 1E-04,adimensionalised with $\rho * U_{ref}^2 *$Lref∗Span,   ** adimensionalized with H*

Table 4: Integral quantities results for SST model and SST model with Reattachment Modification

DISCUSSION

From the results presented above, it is observed that the order of convergence is in general low and it strongly depends on the variable selected, ranging from p $C_{f\ TW}$ = 0.225 to p Cp at x=H,y=0.1H = 1.895 for SST, and from p νt at x=0,y=0.1H = 1.036 to p v at x=0,y=0.1H = 0.155 for SST with Reattachment Modification.

In addition to the previous issue, it is also observed that in general the level of uncertainty decreases with grid refinement.

It is also observed that the level of uncertainty is typically smaller than the differences between results using different turbulence models, which mean that in the example discussed model uncertainties is larger than discretization uncertainties.

CONCLUSSIONS

This paper presents an example of CFD results uncertainty estimation using the Grid Convergence Index method and the commercial CFD code ANSYS CFX. The test case models an incompressible turbulent flow in a Backward Facing Step. Results are shown both for the Shear Stress Transport turbulence model as well as for a variation of this model that incorporates a Reattachment Modification term.
It has been observed that turbulence model uncertainties are typically larger than discretization uncertainties, and that the observed order of convergence may vary significantly depending on the variable selected for the uncertainty estimation.

Immediate future work is the analysis of different grid triplets in order to obtain better estimations for the solution uncertainties.

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