Comprehensive Approach to Verification and Validation of CFD Simulations Applied to Backward Facing Step – Application of CFD Uncertainty Analysis

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There are inherent uncertainties and errors associated with using Computational Fluid Dynamics (CFD) to predict the flow field and there is no standard method for evaluating uncertainty in the CFD community. This paper describes an approach to validate the uncertainty in using CFD. The method will use the state of the art uncertainty analysis applied to the ke-realizable turbulence model to predict the velocity uncertainty of a backward facing step.

Nomenclature

ε_{21}	= solution changes medium to fine grid
ε_{32}	= solution changes coarse to medium grid
e_a^{21}	= extrapolated error
GCI_{fine}^{21}	= grid convergence index
h	= representative grid size
p	= observed order
R_k	= convergence parameter
r_{21}	= ratio of grid sizes between grid 1 and 2
r_{32}	= ratio of grid sizes between grid 3 and 2
S_{k1}	= solution variable for fine grid

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S_{k2} = solution variable for medium grid

S_{k3} = solution variable for coarse grid

S_{ext}^{21} = extrapolated solution variable

S_L = lowest solution variable

S_U = highest solution variable

$U_{oscillatory}$ = uncertainty for oscillatory portion of the solution

$U_{monotonic}$ = uncertainty for monotonic portion of the solution

I. Introduction

CFD is the current state of the art and industry standard used for flow field predictions and analysis; however CFD has many challenges. There are inherent uncertainties and errors associated with using CFD to predict the flow field, and there is no standard method for evaluating uncertainty in the CFD community [1].

Some potentials errors include physical approximation error, computer round-off error, iterative convergence error, discretization errors, computer programming errors, and usage errors [2]. An uncertainty, as defined by the American Institute of Aeronautics and Astronautics (AIAA), is a potential deficiency in any phase or activity of modeling and simulation that is due to the lack of knowledge [3]. An example of an uncertainty in performing a CFD analysis is turbulence modeling [4]. There is a lot about turbulence modeling that is not understood [4]. There has been progress in estimating the uncertainty of CFD, but the approaches have not converged [1].

A thorough literature review has been performed to determine the best method to evaluate the uncertainty in CFD predictions. Both major journals in mechanical and aerospace engineering, AIAA and ASME, have published articles on this subject. The ASME method has been adopted by many researchers and provides a detailed approach to calculate uncertainty in CFD from different levels of grid refinement. The method published by the ASME Journal of Fluids Engineering is the state of the art for determining the uncertainty in CFD predictions and will be used for the proposed research problem.

A CFD model has been created of a backward facing step using ANSYS FLUENT and OpenFOAM. The backward facing step was solved previously for re-attachment length by Celik and Karatekin[5]. The backward facing step induces turbulence into the flow field and will provide adequate physics to compare the uncertainty of different turbulence models using the Comprehensive Approach to Verification and Validation of CFD Simulations [6]. This paper provides a detailed uncertainty analysis of the ke-realizable turbulence model for the backward facing step.

The structure of the paper is as follows. In section 2, the literature review is summarized for CFD uncertainty analysis. Section 3 presents the grid refinement study. Section 4 presents the numerical results of the backward facing step. Section 5 is the discussion. Section 6 is the conclusion.

II. Literature Review

A literature review was performed to determine the "State of the Art" method for calculating CFD uncertainties. CFD is extensively used in industry, government, and academia to design, investigate, operate, and improve understanding of fluid physics [3]. The rate of growth in using CFD as a research and engineering tool will be directly proportional to the level of credibility that the simulation can produce [3]. One needs to evaluate the uncertainty in the results of a CFD simulation to postulate a level of credibility. In 1986, The American Society of Mechanical Engineers (ASME) Journal of Fluids Engineering published a policy statement stating the need for quantification of numerical accuracy [1]. Other journals have issued similar statements [7]. These statements lead to research on the best method to determine numerical uncertainty. In 1995, Celik and Zhang published "Calculation of Numerical Uncertainty Using Richardson Extrapolation: Application to Some Turbulent Flow Calculations" which used Richardson's Extrapolation method to estimate the uncertainty in CFD [8]. In 1997, Ròache published "Quantification of Uncertainty in Computational Fluid Dynamics" [7]. Roaches research also used the Richardson Extrapolation method to quantify CFD uncertainties.

In 1998, the AIAA has published a "Guide for the Verification and Validation of Computational Fluid Dynamics Simulations" [3]. This document provides guidelines for assessing credibility via verification and validation [3]. The document does not recommend standards due to issues not yet resolved, but defines several terms [3]. "Uncertainty is defined as a potential deficiency in any phase or activity of the modeling process that is due to lack of knowledge [3]." "Error is defined as a recognizable deficiency in any phase or activity of modeling and simulation that is not due to lack of knowledge [3]." "Prediction is defined as the use of a CFD model to foretell the state of a physical system under conditions for which the CFD model has not been validated [3]." Uncertainty and error are normally linked to accuracy in modeling and simulation[3]. The guide defines four predominate error sources: insufficient spatial discretization convergence, insufficient temporal discretization convergence, lack of iterative convergence, and computer programming, but does not make claims about the accuracy of predictions [3]. The guide emphasizes that systematically refining the grid size and time step is the most important activity in verification [3]. Once the grid has been refined such that the discretization error is in the asymptotic region, Richardson's extrapolation can be used to estimate zero-grid spacing [3]. A sensitivity analysis and uncertainty analysis are two methods for determining the uncertainty in CFD [3]. The validation test compares a CFD solution to experimental data [3]. The guide has outlined the terms and an overall structure to performing validation, but does not offer a quantitative method.

In 1999, Stern, Wilson, Coleman, and Paterson, E. G., published Iowa Institute of Hydraulic Research (IIHR) Report No. 407 titled "Verification and Validation of CFD Simulations" [9]. In 2001, the American Society of Mechanical Engineers (ASME) Journal of Fluids Engineering published a "Comprehensive Approach to Verification and Validation of CFD Simulations" in an attempt to provide a comprehensive framework for overall procedures and methodology [6]. Two papers were published on the subject in Parts I [6] and Parts II [10] and used the methodology documented in IIHR Report 407. Numerical errors and uncertainties in CFD can be estimated using iterative and parameter convergence studies [6]. The method uses three convergence conditions as possible in estimating uncertainties; (1) monotonic convergence which uses Richardson's extrapolation, (2) oscillatory convergence which uses the upper and lower bounds to estimate uncertainty, (3) divergence in which errors and uncertainties cannot be estimated [6]. The literature provides an approach for estimating errors and uncertainties in CFD simulations for each of the three cases [9, 6, 10]. The approach uses Richardson's extrapolation, which is not new, however; the method has been extended to use input parameters and correction factors to estimate errors and uncertainties [9, 6, 10]. The method examines two sources for error and uncertainty: modeling and simulation. Examples of modeling errors include geometry, mathematical equations, boundary conditions, turbulence models, etc. [IVII]. Examples of numerical errors include discretization, artificial dissipations, incomplete iterative and grid convergence, lack of conservation of mass, momentum, energy, internal and external boundary non-continuity, computer round-off etc. [4]. The method lacks correlations among errors and assumes these are negligible, which may be inappropriate for some circumstances [6]. Additionally, the method provides a quantitative approach for determining the iterative convergence uncertainty [6]. Iterative Convergence must be evaluated and is typically done by monitoring the residuals order of magnitude drop graphically [6]. For oscillatory convergence, the deviation of a residual from the mean provides estimates of the iterative convergence [6]. This is based on the range of the maximum S_U and minimum S_L values [6]. For convergent iterative convergence, a curve-fit is used [6]. For a mixed convergent/oscillatory, iterative convergence is estimated using the amplitude and the maximum and minimum values [6]. A method for confirming validation is presented as compared to experimental data [6].

In 2008, the International Towing Tank Conference (ITTC) has published "Recommended Procedures and Guidelines – Uncertainty Analysis in CFD Verification and Validation Methodology and Procedures" [11]. The ITTC guide was largely based off of the methodology and procedures presented in the ASME Journal of Fluids Engineering a "Comprehensive Approach to Verification and Validation of CFD Simulations" [11]. Also in 2008, the ASME Journal of Fluids Engineering published a "Procedure for Estimating and Reporting of Uncertainty Due to Discretization in CFD Applications" [12].

In 2011, the National Energy Technology Laboratory (NETL) conference proceedings held a major section related to CFD Uncertainty Calculation [13]. Celik presented "Critical Issues with Quantification of Discretization Uncertainty in CFD" [13]. The proceedings were based off of the ASME "Comprehensive Approach to Verification and Validation of CFD Simulations" [6].

Summary of Literature Review: A thorough literature review has been performed to determine the best method to evaluate the uncertainty in CFD predictions. Both major journals in mechanical and aerospace engineering, AIAA and ASME, have published articles on this subject. The ASME method has been adopted by many researchers and provides a detailed approach to calculate uncertainty in CFD from different levels of grid refinement. The method published by the ASME Journal of Fluids Engineering is the state of the art for determining the uncertainty in CFD predictions and will be used for the proposed research problem.

III. Grid Refinement Study

Convergence studies require a minimum of three solutions to evaluate convergence with respect to an input parameter [2]. Consider the situation for 3 solutions corresponding to fine S_{k1}, medium S_{k2}, and coarse S_{k3} values for the *kth* input parameter [2]. Solution changes $\boldsymbol{\varepsilon}$ for medium-fine and coarse-medium solutions and their ratio R_k are defined by [2]:

$$\varepsilon_{21} = S_{k2} - S_{k1}$$

$$\varepsilon_{32} = S_{k3} - S_{k2}$$

$$R_k = \varepsilon_{21} / \varepsilon_{32} \quad (1)$$

Three convergence conditions are possible[2]:

(i) Monotonic convergence: $0 < R_k < 1$

(ii) Oscillatory convergence: $R_k < 0$[i]

(iii) Divergence: $R_k > 1$ **(2)**

The quantity of interest for the backward facing setup is velocity magnitude. Three grids were compared, and the convergence conditions were determined for every point in the computational domain. This is accomplished through interpolation between the medium to coarse grid and the fine to coarse grid. The velocity magnitude from the medium and fine grids are interpolated on to the coarse grid. Then the solutions changes, ε_{21}, ε_{32}, R_k, and convergence conditions are calculated for every point in the domain. Figure 1 shows the different convergence conditions inside the computational domain for the grid refinement study.

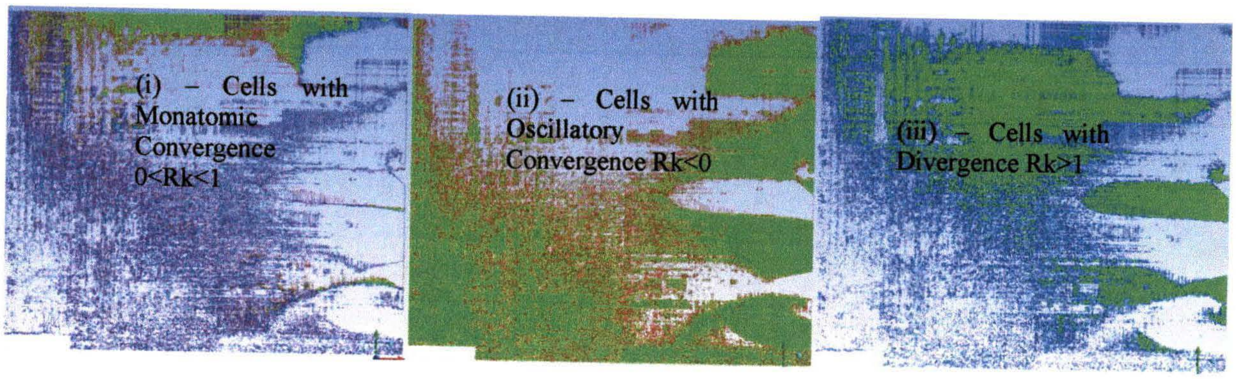
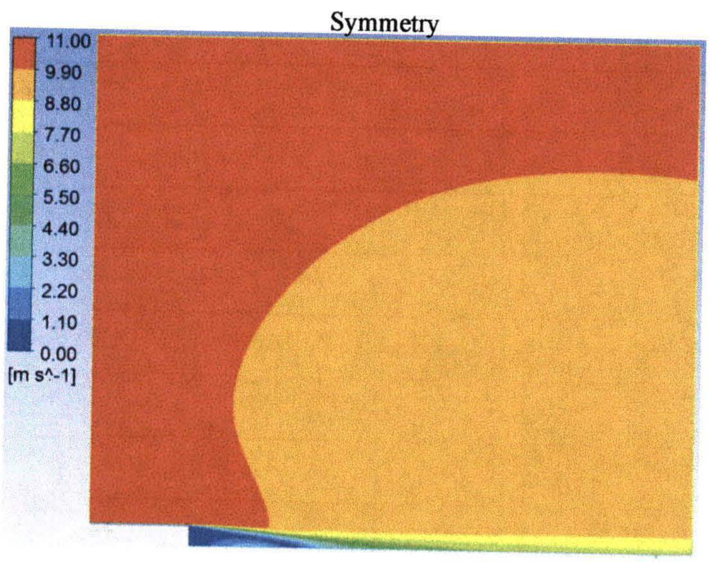


Figure 1: Convergence conditions for a Flat plate – Grid refinement 1

Uniform Velocity Inlet
U = 10 m/s



Pressure Outlet
Pgage = 0

Figure 2: Velocity Magnitude for Flow over Backward facing step – Coarsest Grid (Structured 1,192,000 cells)

IV. Numerical Results for Backward Facing Step

The uncertainty associated with the CFD calculation is the compilation of the elemental errors associated with each of the numerical, input, and solver errors. This uncertainty can be calculated using a Data Reduction equation the form $r = r(X_1, X_2, \ldots X_J)$ is shown in equation 3, below.

$$U_{CFD} = \left(\sum_{i=1}^{J}\left\{\left(\frac{\partial r}{\partial X_i}\right)^2 B_i^2\right\} + 2\sum_{i=1}^{J}\sum_{k=i+1}^{J}\left\{\left(\frac{\partial r}{\partial X_i}\right)\left(\frac{\partial r}{\partial X_k}\right)[B_i B_k]_{correlated}\right\} + \sum_{i=1}^{J}\left\{\left(\frac{\partial r}{\partial X_i}\right)^2 P_i^2\right\}\right)^{1/2} \quad (3)$$

Where,

B_i = the systematic (bias) error associated with variable X_i,

$(B_i B_k)_{correlated}$ = the correlated systematic error between variables X_i and X_k,

and P_i = the random error associated with variable X_i.

For the calculation, the correlated errors and random errors are neglected and the data reduction equation reduces to the following, as shown in equation 4.

$$U_{CFD} = \left(\sum_{i=1}^{J}\left\{\left(\frac{\partial r}{\partial X_i}\right)^2 B_i^2\right\}\right)^{1/2} \quad (4)$$

A list of variables for the k-e-realizable turbulence model analyzed is listed in Table 1.

Table 1: Uncertainty Variables, Xi

Type of Variable	Variables Xi	Value	Bias Error
Boundary Conditions	epsilion turbulent mixing length dissipation rate inlet (m2/s3)	0.5	0.5
	k turbulent intensity kinetic energy inlet (m2/s2)	0.05	0.05
	pressure outlet (Pa)	101325	2%
	velocity inlet (m/s)	10	0.5
Fluid Properties	kinematic viscosity nu represents air [0-50-100] deg C	1.79E-06	[13.6e-06 -> 23.06e-06]
Grid Size	Method - Uses Oscillatory Uncertainty	1,192,000 1,862,500 3,311,689	
Numerical	Method - Uses Richardson's Extrapolation (ASME 5 Step Procedure) – Calculated for Velocity at each Cell		
Solver	OpenFOAM (SimpleFoam) vs. Fluent		
Turbulence Models	ke-realiable, kwSST, and SpalartAllmaras		

Expanding the data reduction equation for the listed variables as shown in equation (5) in order from top to bottom.

$$U_{CFD-Velocity} = \left(\left(\left(\frac{\partial V}{\partial e}\right)^2 B_e^2\right) + \left(\left(\frac{\partial V}{\partial k}\right)^2 B_k^2\right) + \left(\left(\frac{\partial V}{\partial p}\right)^2 B_p^2\right) + \left(\left(\frac{\partial V}{\partial U}\right)^2 B_u^2\right) + \left(\left(\frac{\partial V}{\partial nu}\right)^2 B_{nu}^2\right) + \left(\left(\frac{\partial V}{\partial g}\right)^2 B_g^2\right) + \left(\left(\frac{\partial V}{\partial num}\right)^2 B_{num}^2\right) + \left(\left(\frac{\partial V}{\partial solver}\right)^2 B_{solver}^2\right) + \left(\left(\frac{\partial V}{\partial turb}\right)^2 B_{turb}^2\right)\right)^{1/2}$$

Each of the variables was analyzed separately for their elemental error sources. The following plots show the each variables and their corresponding uncertainty plot as a function of the percent uncertainty in the CFD Velocity prediction. The percent uncertainty is calculated by dividing by the local velocity (ie the uncertainty velocity in each cell divided by the velocity in each cell).

The uncertainty for each of the following was calculated as shown in equation 3 for each cell using the following method outlined by Stern, Wilson, Coleman, and Paterson [2]. $\boldsymbol{S}$ is the simulated result. For this case it is the upper velocity $\boldsymbol{S_U}$ and the lower velocity $\boldsymbol{S_L}$.

$$U_{Oscillatory} = \frac{1}{2}(S_U - S_L) \quad \textbf{(3)}$$

epsilion turbulent mixing length dissipation rate inlet (m²/s³)

For a value of 0.5 +/- 0.5 m^2/s^3, the uncertainty in the velocity prediction was 0 – 1.155 percent as shown in Figure 3.

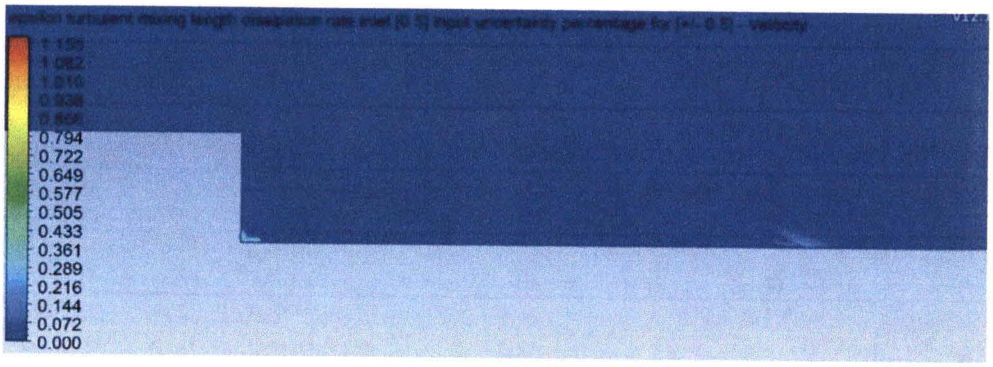


Figure 3: Epsilon Turbulent Mixing Length Dissipation Rate Inlet – Velocity Uncertainty Percentage

k turbulent intensity kinetic energy inlet (m²/s²)

For a value of 0.05 +/- 0.05 m^2/s^2, the uncertainty in the velocity prediction was 0 – 0.785 percent as shown in Figure 4.

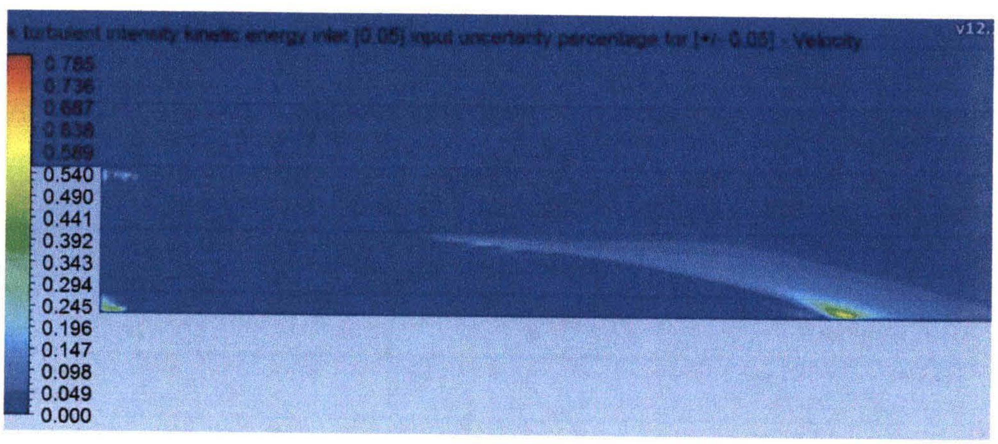


Figure 4: k Turbulent Intensity Kinetic Energy Inlet – Velocity Uncertainty Percentage

Pressure outlet (Pa)

For a value of 101325 +/- 2% Pa, the uncertainty in the velocity prediction was 0 – 20 percent as shown in Figure 5.

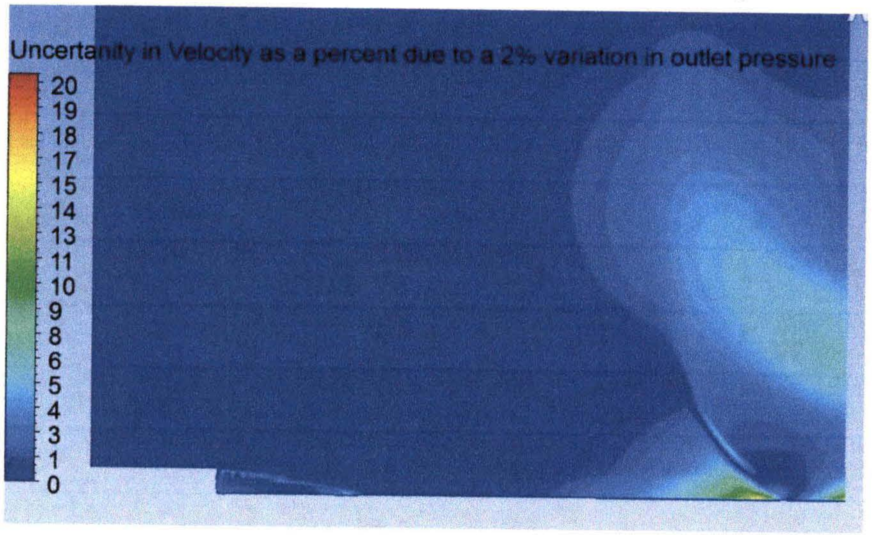


Figure 5: Pressure Outlet – Velocity Uncertainty Percentage

Velocity Inlet (m/s)

For a value of 10 +/- 0.5 m/s, the uncertainty in the velocity prediction was 0 – 6.558 percent as shown in Figure 6.

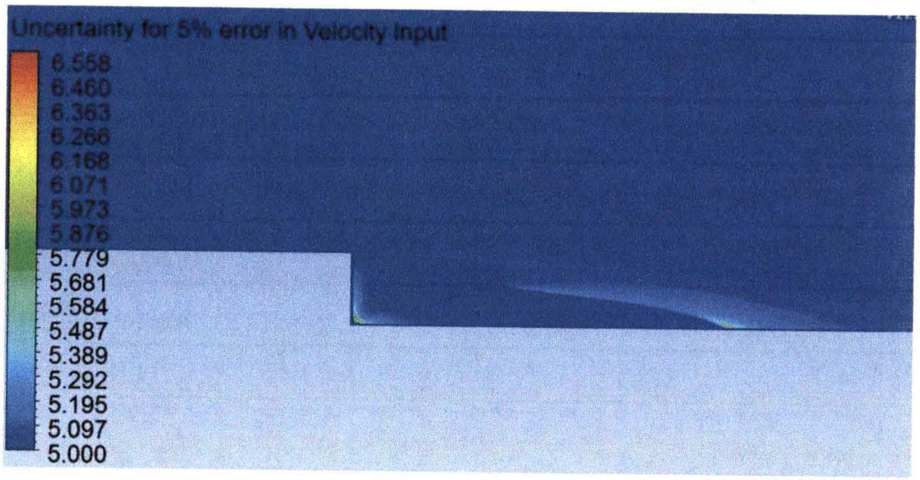


Figure 6: Velocity Inlet – Velocity Uncertainty Percentage

Kinematic viscosity nu=17.06e-06 [13.6e-06 -> 23.06e-06] (m^2/s) represents air [0-50-100] degrees C

For a value of nu=17.06e-06 [13.6e-06 -> 23.06e-06] (m^2/s), the uncertainty in the velocity prediction was 0 – 27.727 percent as shown in Figure 7.

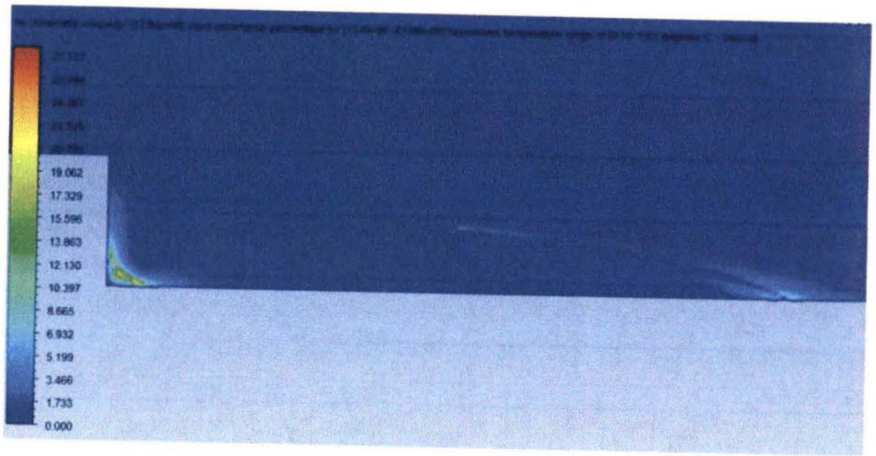


Figure 7: Kinematic Viscosity – Velocity Uncertainty Percentage

Grid size

For a grid size of 1,192,000 cells [grid 2 -1,862,500 cells], [grid3 - 3,311,689 cells], the uncertainty in the velocity prediction was 0 – 698 percent as shown in Figure 8.

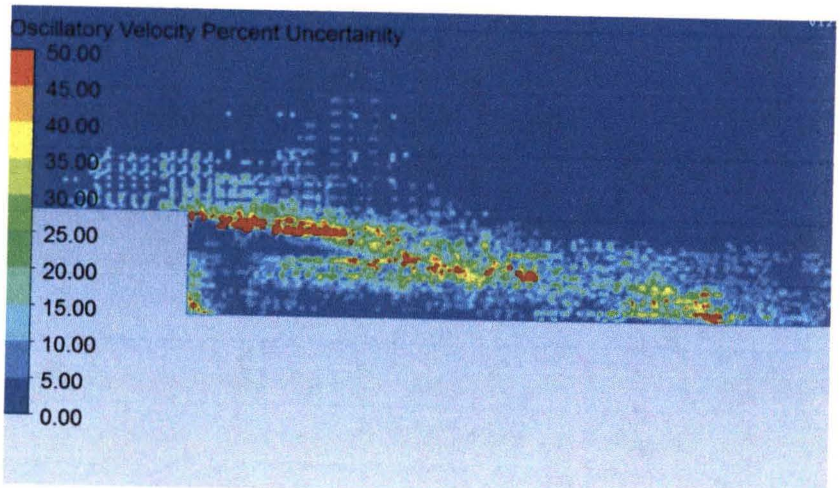


Figure 8: Grid Size – Velocity Uncertainty Percentage

Turbulence Models

The ke-realiable, kwSST, and SpalartAllmaras turbulence models converged using OpenFoam and the uncertainty was calculated as an oscillatory input parameter as shown in Figure 9.

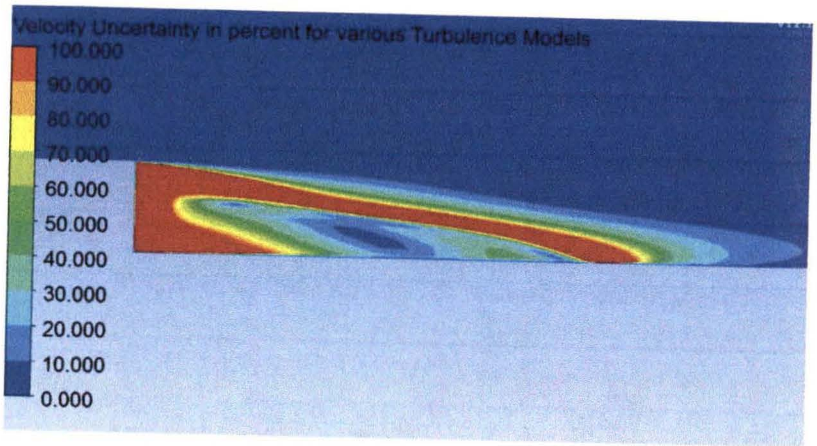


Figure 9: Turbulence Models – Velocity Uncertainty Percentage

Solver

OpenFoam and Fluent were used to calculate the velocity distribution on the backward facing step and the uncertainty was calculated as an oscillatory input parameter as shown in Figure 10.

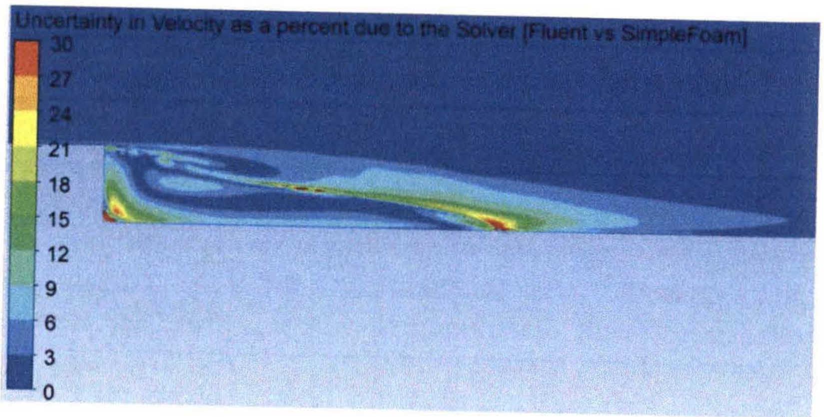


Figure 10: Solver – Velocity Uncertainty Percentage

The uncertainties of the variables with monotonic convergence (numerical) are calculated using Richardson's extrapolation as outlines by ASME V&V-2009 [14]. This is accomplished through the five-step procedure. Step 1, calculate representative grid size, ***h*** as shown in equation 4.

$$h_1 = \left(\frac{Total\ Volume}{total\ number\ of\ cells\ in\ fine\ grid}\right)^{\frac{1}{3}}$$

$$h_2 = \left(\frac{Total\ Volume}{total\ number\ of\ cells\ in\ medium\ grid}\right)^{\frac{1}{3}}$$

$$h_3 = \left(\frac{Total\ Volume}{total\ number\ of\ cells\ in\ coarse\ grid}\right)^{\frac{1}{3}} \quad \textbf{(4)}$$

Step 2 is to select three significantly (r>1.3) grid sizes and computer the ratio as shown in equation 5.

$$r_{21} = \frac{h_2}{h_1}$$

$$r_{32} = \frac{h_3}{h_2} \quad \textbf{(5)}$$

Step 3 is to calculate the observed order, p, as shown in equation 6. This equation must be solved iteratively.

$$p = \left[\frac{1}{\ln(r_{21})}\right] * [\ln\left(\frac{\varepsilon_{32}}{\varepsilon_{21}}\right) + ln\left(\frac{r_{21}{}^{p} - sign\left(\frac{\varepsilon_{32}}{\varepsilon_{21}}\right)}{r_{32}{}^{p} - sign\left(\frac{\varepsilon_{32}}{\varepsilon_{21}}\right)}\right) \quad \textbf{(6)}$$

Step 4 is to calculate the extrapolated values as shown in equation 7.

$$S_{ext}{}^{21} = \frac{(r_{21}{}^{p} * S_{k1} - S_{k2})}{(r_{21}{}^{p} - 1)}$$

$$e_a{}^{21} = \frac{(S_{k1} - S_{k2})}{(S_{k1})} \quad \textbf{(7)}$$

Step 5 is to calculate the fine grid convergence index and numerical uncertainty as shown in equation 8. This approached used a factor of safety of 1.25 and assumed that the distribution is Gaussian about the fine grid, 90 % confidence.

$$GCI_{fine}{}^{21} = \frac{1.25 * e_a{}^{21}}{(r_{21}{}^{p} - 1)}$$

$$U_{monotonic} = \frac{GCI_{fine}{}^{21}}{1.65} \quad \textbf{(8)}$$

Numerical

For a grid size of 1,192,000 cells [grid 2 -1,862,500 cells], [grid3 - 3,311,689 cells], the uncertainty in the velocity prediction was 0 – 5300 percent as shown in Figure 11 as estimated by Richardson's extrapolation method.

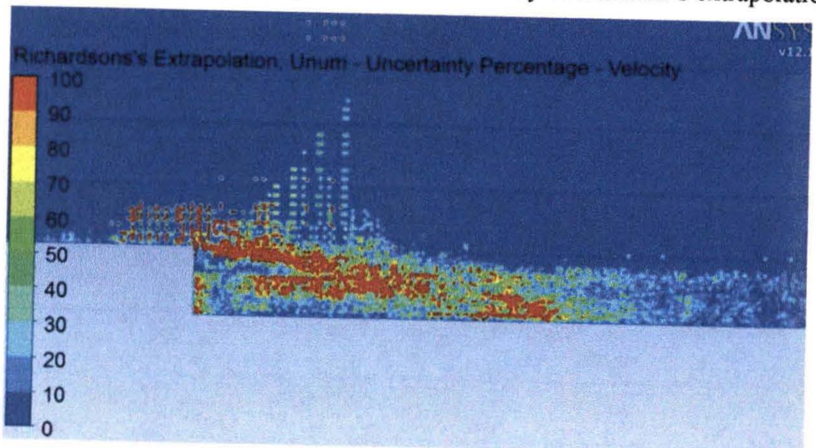


Figure 11: Numerical – Velocity Uncertainty Percentage

A root-sum-squared (rss) of the uncertainty variables was calculated (omitting Richardson's Extrapolation – see Discussion) and the velocity magnitude is shown in figure 12 with the corresponding uncertainty.

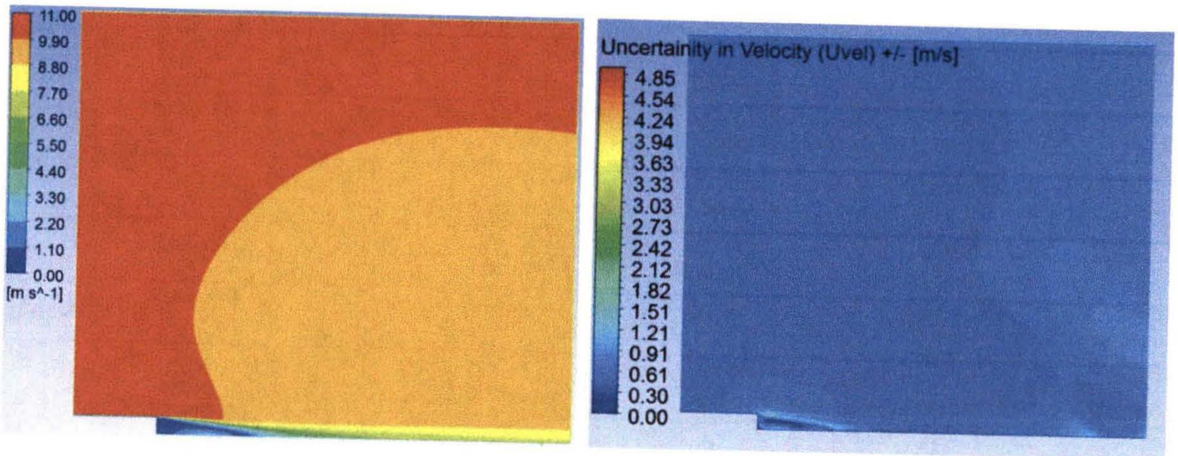


Figure 12: Velocity Prediction and Uncertainty Plot for ke-realizable Turbulence Model

The highest uncertainty is +/- 4.85 m/s. This occurs in the region shown in Figure 13 in red. Figure 13 is the same data presented on the right hand side of Figure 12, except zoomed in to the region near the backward step and a smaller scale is used.

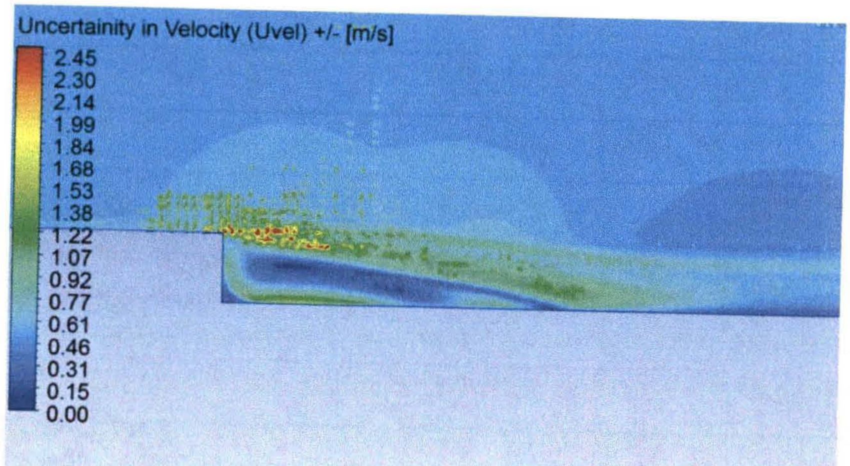


Figure 13: Velocity Uncertainty Plot for ke-realizable Turbulence Model

V. Discussion

The monotonic convergence uncertainty calculation (equations 4-8) was omitted in the rss uncertainty plot due to the values that were produced by using this method. The method produced uncertainty values that were on the order of 5000 percent of the localized velocity in the region near the backward step. It is believed this is due to the turbulence. Turbulence is calculated as a steady state value and fluctuations about that steady state. The fluctuations are inducing a non-linear result between the three grids and providing very large uncertainty bands in the localized region near the backward step. However, once you move approximately 5 lengths downstream of the backward step, the method begins producing reasonable results of 0 – 30 percent of the localized velocity. Treating the highly turbulent region behind the backward step as a monotonic case is in appropriate. It is believed that treating the grid as an input parameter with oscillatory convergence provides better results for a steady state, turbulent CFD simulation. This is evident in the R_k values shown in Figure 1. Most of the cells are exhibiting oscillatory convergence. It is believed all cells are exhibiting oscillatory convergence, however depending on when the sample takes place, one could misrule the results as monotonic or divergent.

During several preliminary cases of the grid convergence study, one case provided an excellent example of domain sizing. A CFD analyst is always troubled with trying to keep the domain size large enough to not affect the solution. Using the oscillatory method, one can see the solution differences between the three grids. In the case presented below, the domain size is too small. This is evident by calculating the uncertainty using an oscillatory convergence method as shown in Figure 14.

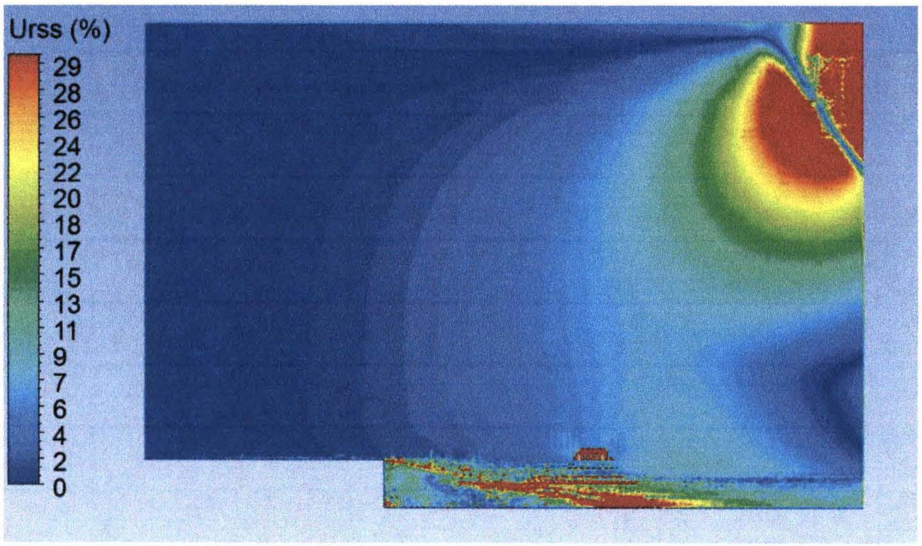


Figure 14: Example of (3) Grids with a Domain not large enough for the calculation

The uncertainty is high near the boundary conditions; this shows the domain is not sized appropriately.

It is computationally time consuming to run all of the different input parameters. It is suggested that the community compile a list of input parameters for each of the turbulence models and estimated uncertainty values for each of the parameters. The code used for this study was OpenFOAM and Table 2 of the Appendix is a list of all the input parameters for a ke-realizable case. Table 2 includes the input parameters and estimated uncertainties for the backward facing step. All values presented are in the form of a percent of the localized velocity.

VI. Conclusion

This paper outlines an uncertainty analysis for the ke realizable turbulence model for a backward facing step. The velocity magnitude was predicted using CFD. The uncertainty parameters listed in Table1 were analyzed using an oscillatory convergence calculation or a monotonic convergence calculation. Plots of the velocity magnitude can be combined with a corresponding uncertainty plot for an accurate velocity prediction.

There are other variables that would influence the uncertainty calculation. Examples of these other parameters include solution schemes, other turbulence models, and time accurate solutions. Future work will include analyzing each of these items.

It is suggested that the CFD community begin to compile a list of the many variables associated with each uncertainty calculation for different problems and output variables. Ideally, an analyst could assemble a table of all uncertainty variables and estimate a number based on historical data rather than running separate CFD cases for each variable. The procedure above has been scripted and future work will include other geometries and turbulence models.

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[14] An American National Standard., "Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer", The American Society of Mechanical Engineers. ASME V&V 20-2009

Table 2: Table of Input Parameters for ke-realizable OpenFOAM Turbulence Model

ke Inputs:					Default Values	Recommended Uncertainty
Boundary Conditions:						
	epsilon	inlet	turbulentMixingLengthDissipationRateInlet	mixing length	0.5	1.20%
				value	1	
		wall	epsilonWallFunction	value	0	
		outlet	type	value	1	
	k	inlet	turbulentIntensityKineticEnergyInlet	intensity	0.05	0.80%
				value	1	
		wall	kqRWallFunction	value	0	
		outlet	type	value	1	
	nut	inlet	type	value	1	
		wall	nutWallFunction	value	0	
		outlet	type	uniform	0	
	nuTilda	inlet	zeroGradient			
		wall	zeroGradient			
		outlet	zeroGradient			
	p	inlet	zeroGradient			10x the variation
		wall	zeroGradient			
		outlet	type	fixed value	0	
	U	inlet	type	x	10	1.3x the variation
				y	0	
				z	0	
		wall	type	x	0	
				y	0	
				z	0	
		outlet	type	x	1	
				y	0	
				z	0	
Turbulence	Turbulence Tranport Model	**nu**	Newtonian	[0 2 -1 0 0 0 0]	1.00E-06	[0-100 deg C] -> 28%
	Turbulence Propoerties	simulationType	RASModel			
	RAS Properties		RASModel	realizableKE		
ControlDict	End Time				150000	
	timestep (or CFL)				1	
	write percision				6	
	timePrecision				6	

Table 2: Table of Input Parameters for ke-realizable OpenFOAM Turbulence Model - continued

SolutionSchemes	gradSchemes	p	Gauss linear			
		U	Gauss Linear			
	divSchemes	phi, U	Gauss limitedLinearV			
		phi,k	Gauss limitedLinear			
		phi,epsilon	Gauss limitedLinear			
		phi,R	Gauss limitedLinear			
		R	Gauss linear			
		phi, nuTilda	Gauss limitedLinear			
		nuEff*dev(T(grad(U)))	Gauss linear			
	laplacianSchemes	nuEff,U	Gauss linear corrected			
		1|A(U)),p	Gauss linear corrected			
		DkEff,k	Gauss linear corrected			
		DepsilonEff,epsilon	Gauss linear corrected			
		DREff,R	Gauss linear corrected			
		DnuTildaEff,nuTilda	Gauss linear corrected			
	interpolationSchemes	interpolate(U)	linear			
	snGradSchemes	default	corrected			
	fluxRequired	default no	p			
Solvers	p	solver	GAMG;			30%
		smoother	GaussSeidel;			
		cacheAgglomeration	true;			
		nCellsInCoarsestLevel	10;			
		agglomerator	faceAreaPair;			
		mergeLevels	1;			
		tolerance	1e-06;			
		relTol	0.05;			
	pFinal	solver	GAMG;			
		smoother	GaussSeidel;			
		cacheAgglomeration	true;			
		nCellsInCoarsestLevel	10;			
		agglomerator	faceAreaPair;			
		mergeLevels	1;			
		tolerance	1e-06;			
		relTol	0;			
	(U|k|epsilon)Final	solver	PBiCG;			
		preconditioner	DILU;			
		tolerance	1e-05;			
		relTol	0;			
	PIMPLE	nOuterCorrectors	4;			
		nCorrectors	1;			
		nNonOrthogonalCorrectors	0;			
		pRefCell	0;			
		pRefValue	0;			
	SIMPLE	nNonOrthogonalCorrectors	0;			
		residualControl	p	1e-2;		
			U	1e-3;		
			(k|epsilon)	1e-3;		
	relaxationFactors	p	0.3;			
		U	0.7;			
		k	0.7;			
		epsilon.*	0.7;			
	cache	grad(U);				
Mesh Size	number of cells					Case Specific - Use Oscillatory Method

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Comprehensive Approach to Verification and Validation of CFD Simulations Applied to Backward Facing Step – Application of CFD Uncertainty Analysis

Curtis E. Groves and Marcel Ilie, PhD

University of Central Florida, Orlando, FL 32816

Paul A. Schallhorn, PhD

National Aeronautics and Space Administration, Kennedy Space Center, FL, 32899

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Background

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- **How good is CFD?**

- There are uncertainties and errors in using CFD
  - No standard method for evaluating uncertainty in CFD
  - Potential Errors include:
    - physical approximation error
    - computer round-off error
    - iterative convergence error
    - discretization errors
    - computer programming errors
    - usage errors
    - turbulence induced errors

http://www.cfd4aircraft.com/int_conf/IC3/welcome/welcome.html

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Background

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- **This presentation describes an approach to validate the uncertainty in using CFD. The method will use the state of the art uncertainty analysis applied to the ke-realizable turbulence model to predict the velocity uncertainty of a backward facing step.**

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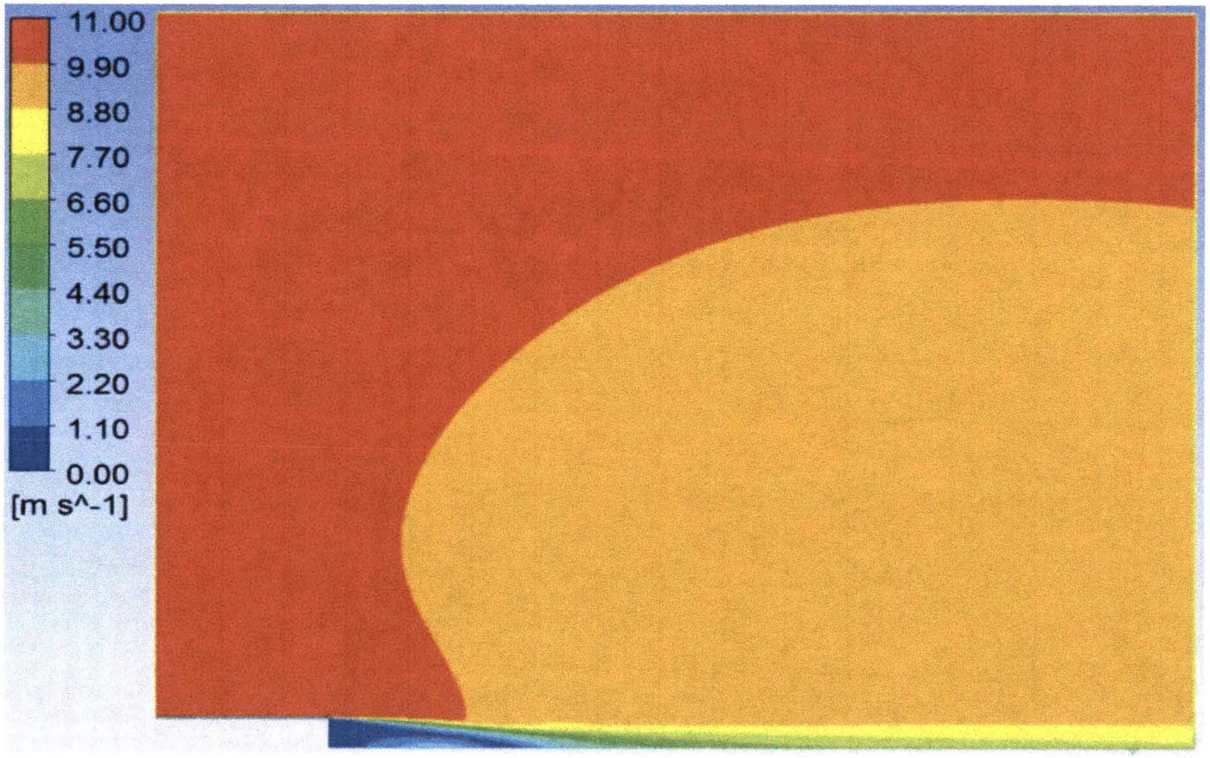
Velocity Magnitude Prediction – Backward Facing Step

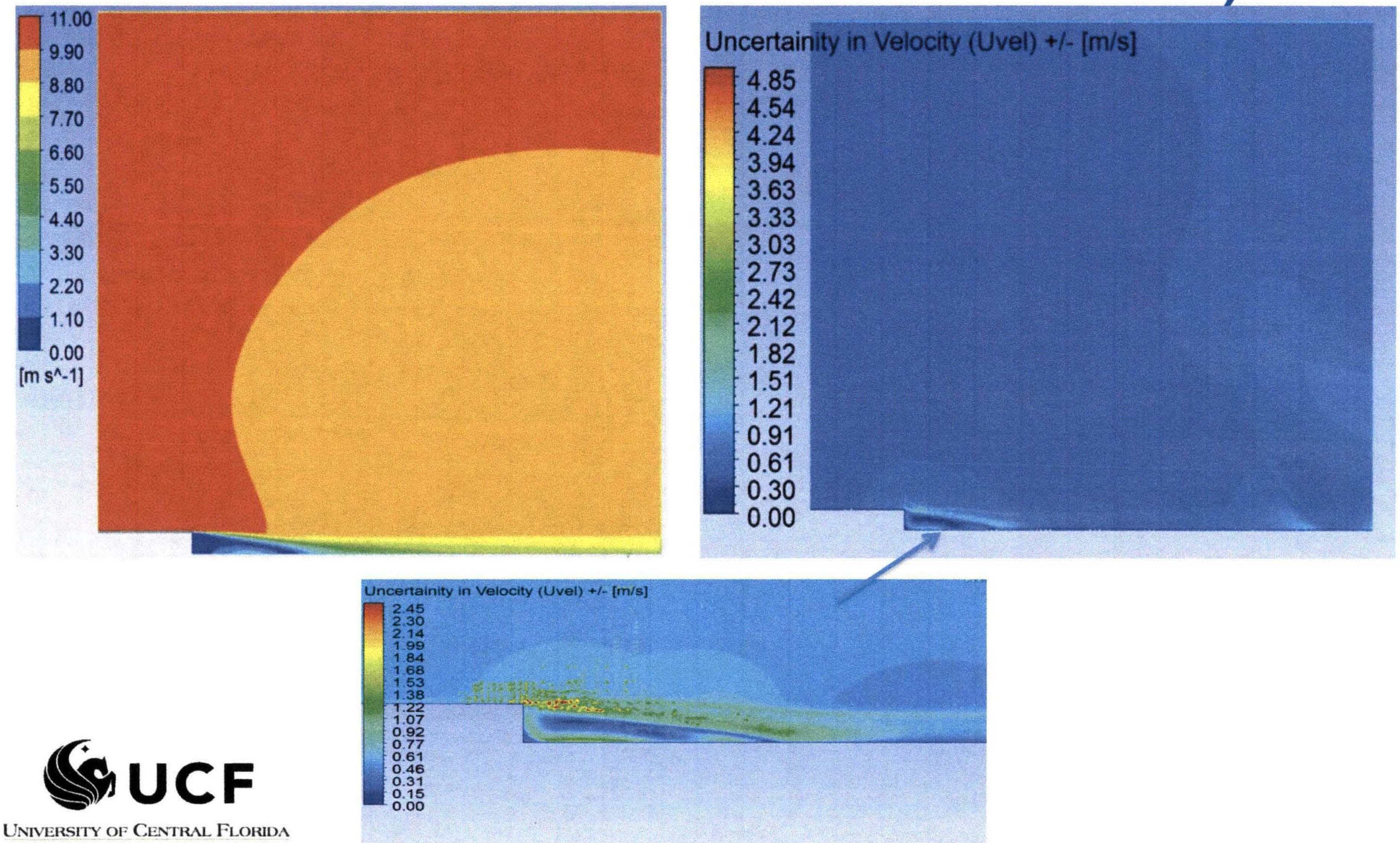
Symmetry

Uniform Velocity Inlet
U = 10 m/s



Pressure Outlet
Pgage = 0

Velocity Prediction with Uncertainty



Method

- To estimate the uncertainty, the following ASME Standard was used.

ASME V&V 20-2009 "**Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer**"

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Summary of Method

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- Convergence studies require a minimum of three solutions to evaluate convergence with respect to an input parameter. Consider the situation for 3 solutions corresponding to fine S_{k1}, medium S_{k2}, and coarse S_{k3} values for the *kth* input parameter. Solution changes **ε** for medium-fine and coarse-medium solutions and their ratio R_k are defined by:

$$\varepsilon_{21} = S_{k2} - S_{k1}$$
$$\varepsilon_{32} = S_{k3} - S_{k2}$$
$$R_k = \varepsilon_{21} / \varepsilon_{32}$$

- Three convergence conditions are possible:

Monotonic convergence: $0 < R_k < 1$

Oscillatory convergence: $R_k < 0$[i]

Divergence: $R_k > 1$

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Summary of Method –cont.

- The uncertainty associated with the CFD calculation is the compilation of the elemental errors associated with each of the numerical, input, and solver errors. This uncertainty can be calculated using a Data Reduction equation the form $r = r(X_1, X_2, \ldots X_J)$ as shown,

$$U_{CFD} = \left(\sum_{i=1}^{J}\left\{\left(\frac{\partial r}{\partial X_i}\right)^2 B_i^2\right\} + 2\sum_{i=1}^{J}\sum_{k=i+1}^{J}\left\{\left(\frac{\partial r}{\partial X_i}\right)\left(\frac{\partial r}{\partial X_k}\right)[B_i B_k]_{correlated}\right\} + \sum_{i=1}^{J}\left\{\left(\frac{\partial r}{\partial X_i}\right)^2 P_i^2\right\}\right)^{1/2}$$

- Where,

B_i = the systematic (bias) error associated with variable X_i,
$(B_i B_k)_{correlated}$ = the correlated systematic error between variables X_i and X_k,
and P_i = the random error associated with variable X_i.

For the calculation, the correlated errors and random errors are neglected and the data reduction equation reduces to the following, as shown

$$U_{CFD} = \left(\sum_{i=1}^{J}\left\{\left(\frac{\partial r}{\partial X_i}\right)^2 B_i^2\right\}\right)^{1/2}$$

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Uncertainty Variables ke-realizable (OPENFOAM – SimpleFoam)

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- There are 87 Different Input Parameters for the ke-realizable model in SimpleFoam
  - These include:
    - Boundary Conditions
    - Wall Functions
    - Fluid Properties
    - Turbulence Parameters
    - Solution Schemes
    - Solvers
    - Mesh
    - ect.

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Uncertainty Variables Considered

Type of Variable	Variables Xi	Value	Bias Error
Boundary Conditions	epsilion turbulent mixing length dissipation rate inlet (m2/s3)	0.5	0.5
	k turbulent intensity kinetic energy inlet (m2/s2)	0.05	0.05
	pressure outlet (Pa)	101325	2%
	velocity inlet (m/s)	10	0.5
Fluid Properties	kinematic viscosity nu represents air [0-50-100] deg C	1.79E-06	[13.6e-06 -> 23.06e-06]
Grid Size	Method - Uses Oscillatory Uncertainty	1,192,000 1,862,500 3,311,689	
Numerical	Method - Uses Richardson's Extrapolation (ASME 5 Step Procedure) – Calculated for Velocity at each Cell		
Solver	OpenFOAM (SimpleFoam) vs. Fluent		
Turbulence Models	ke-realiable, kwSST, and SpalartAllmaras		

Expanding the data reduction equation for the listed variables in order from top to bottom.

$$U_{CFD-Velocity} = \left(\left(\left(\frac{\partial V}{\partial e} \right)^2 B_e^2 \right) + \left(\left(\frac{\partial V}{\partial k} \right)^2 B_k^2 \right) + \left(\left(\frac{\partial V}{\partial p} \right)^2 B_p^2 \right) + \left(\left(\frac{\partial V}{\partial U} \right)^2 B_u^2 \right) + \left(\left(\frac{\partial V}{\partial nu} \right)^2 B_{nu}^2 \right) + \left(\left(\frac{\partial V}{\partial g} \right)^2 B_g^2 \right) + \left(\left(\frac{\partial V}{\partial num} \right)^2 B_{num}^2 \right) + \left(\left(\frac{\partial V}{\partial solver} \right)^2 B_{solver}^2 \right) + \left(\left(\frac{\partial V}{\partial turb} \right)^2 B_{turb}^2 \right) \right)^{1/2}$$

Oscillatory Variables

- The uncertainty for each of the following was calculated for each cell using the following method outlined by Stern, Wilson, Coleman, and Paterson. ***S*** is the simulated result. For this case it is the upper velocity S_U and the lower velocity S_L.
  - **epsilion turbulent mixing length dissipation rate inlet (m^2/s^3)**
  - **k turbulent intensity kinetic energy inlet (m^2/s^2)**
  - **Pressure outlet (Pa)**
  - **Velocity Inlet (m/s)**
  - **Kinematic viscosity nu=17.06e-06 [13.6e-06 -> 23.06e-06] (m^2/s) represents air [0-50-100] degrees C**
  - **Grid size**
  - **Turbulence Models**
  - **Solver**

$$U_{Oscillatory} = \frac{1}{2}(S_U - S_L)$$

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Results (Oscillatory Variables)

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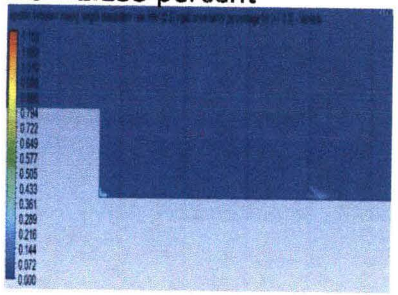
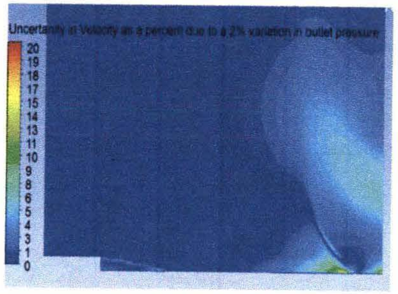
epsilion turbulent mixing length dissipation rate inlet (m^2/s^3)

0 – 1.155 percent



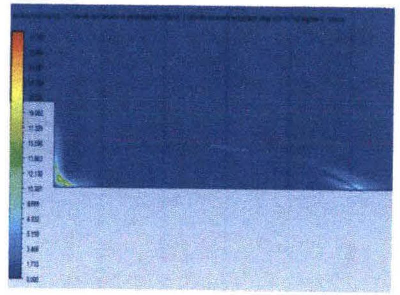
Pressure outlet (Pa)

0 – 20 percent



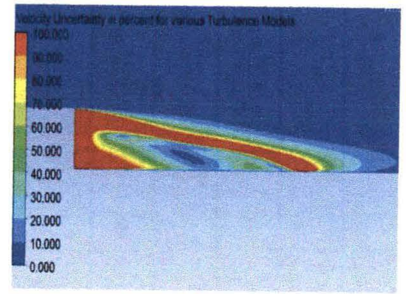
Kinematic viscosity nu=17.06e-06 [13.6e-06 -> 23.06e-06] (m^2/s) represents air [0-50-100] degrees C

0 – 27.727 percent



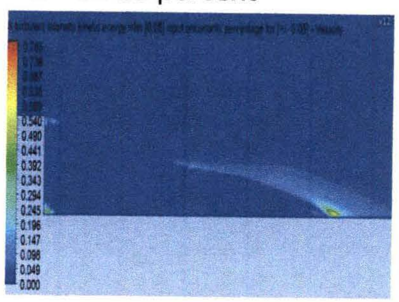
Turbulence Models

> 100 %



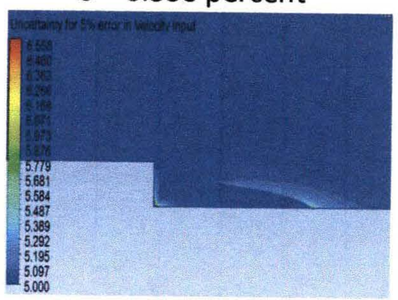
k turbulent intensity kinetic energy inlet (m^2/s^2)

0 – 0.785 percent



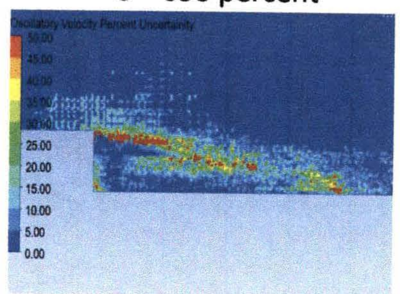
Velocity Inlet (m/s)

0 – 6.558 percent



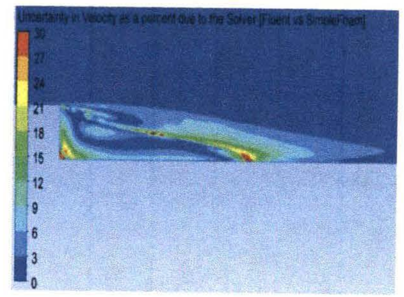
Grid size

0 – 698 percent



Solver

> 30 %



Percent – is the percentage change in local velocity

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Monotonic Convergence Variables (Numerical)

- The uncertainties of the variables with monotonic convergence (numerical) are calculated using Richardson's extrapolation as outlines by ASME V&V-2009. This is accomplished through the five-step procedure.
- Step 1, calculate representative grid size, ***h*** as shown

$$h_1 = \left(\frac{Total\ Volume}{total\ number\ of\ cells\ in\ fine\ grid}\right)^{\frac{1}{3}}$$

$$h_2 = \left(\frac{Total\ Volume}{total\ number\ of\ cells\ in\ medium\ grid}\right)^{\frac{1}{3}}$$

$$h_3 = \left(\frac{Total\ Volume}{total\ number\ of\ cells\ in\ coarse\ grid}\right)^{\frac{1}{3}}$$

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Monotonic Convergence Variables (Numerical)

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- Step 2, calculate representative grid ratio, ***r*** as shown

$$r_{21} = \frac{h_2}{h_1}$$

$$r_{32} = \frac{h_3}{h_2}$$

- Step 3 is to calculate the observed order, p, as shown. This equation must be solved iteratively.

$$p = \left[\frac{1}{\ln(r_{21})}\right] * [\ln\left(\frac{\varepsilon_{32}}{\varepsilon_{21}}\right) + ln\left(\frac{{r_{21}}^{p} - sign\left(\frac{\varepsilon_{32}}{\varepsilon_{21}}\right)}{{r_{32}}^{p} - sign\left(\frac{\varepsilon_{32}}{\varepsilon_{21}}\right)}\right)$$

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Monotonic Convergence Variables (Numerical)

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- Step 4 is to calculate the extrapolated values as shown

$$S_{ext}^{21} = \frac{(r_{21}^{p} * S_{k1} - S_{k2})}{(r_{21}^{p} - 1)}$$

$$e_a^{21} = \frac{(S_{k1} - S_{k2})}{(S_{k1})}$$

- Step 5 is to calculate the fine grid convergence index and numerical uncertainty as shown. This approached used a factor of safety of 1.25 and assumed that the distribution is Gaussian about the fine grid, 90 % confidence.

$$GCI_{fine}^{21} = \frac{1.25 * e_a^{21}}{(r_{21}^{p} - 1)}$$

$$U_{monotonic} = \frac{GCI_{fine}^{21}}{1.65}$$

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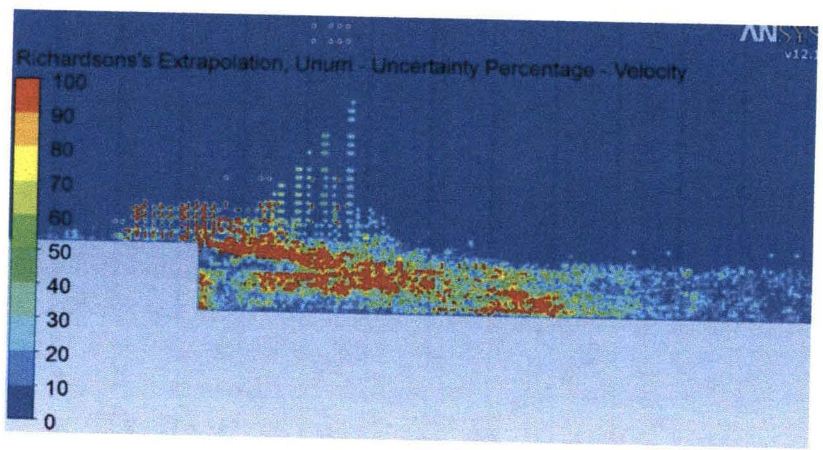
Results (Monotonic Convergence)

Numerical

For a grid size of 1,192,000 cells [grid 2 -1,862,500 cells], [grid3 - 3,311,689 cells], the uncertainty in the velocity prediction was 0 – 5300 percent as shown in Figure 11 as estimated by Richardson's extrapolation method.



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Results (Monotonic Convergence)

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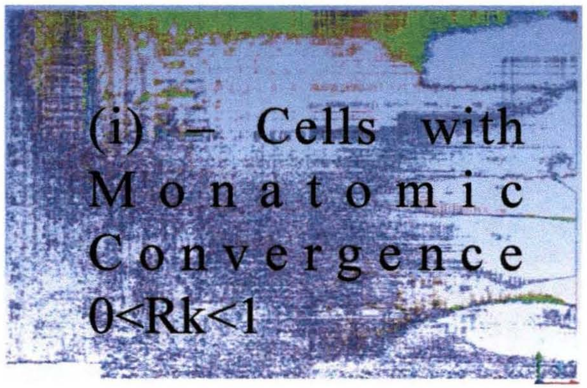
Numerical

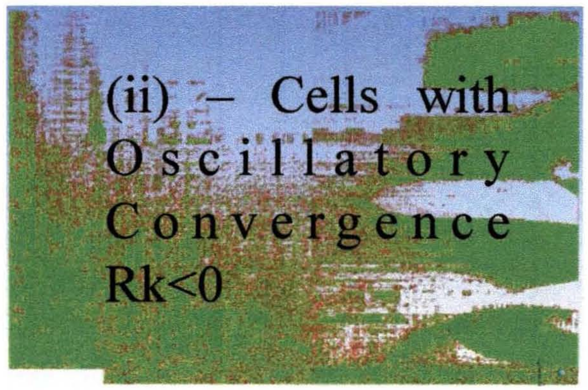
Three convergence conditions are possible:

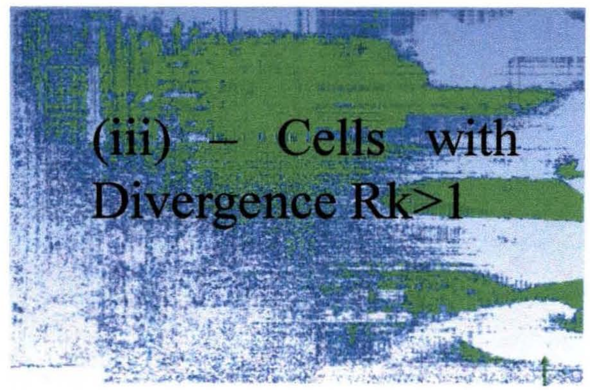
Monotonic convergence: $0 < R_k < 1$

Oscillatory convergence: $R_k < 0$[i]

Divergence: $R_k > 1$







It is believed the errors in this method is due to the turbulence. Turbulence is calculated as a steady state value and fluctuations about that steady state. The fluctuations are inducing a non-linear result between the three grids and providing very large uncertainty bands in the localized region near the backward step. Treating the highly turbulent region behind the backward step as a monotonic case is in appropriate.

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Results

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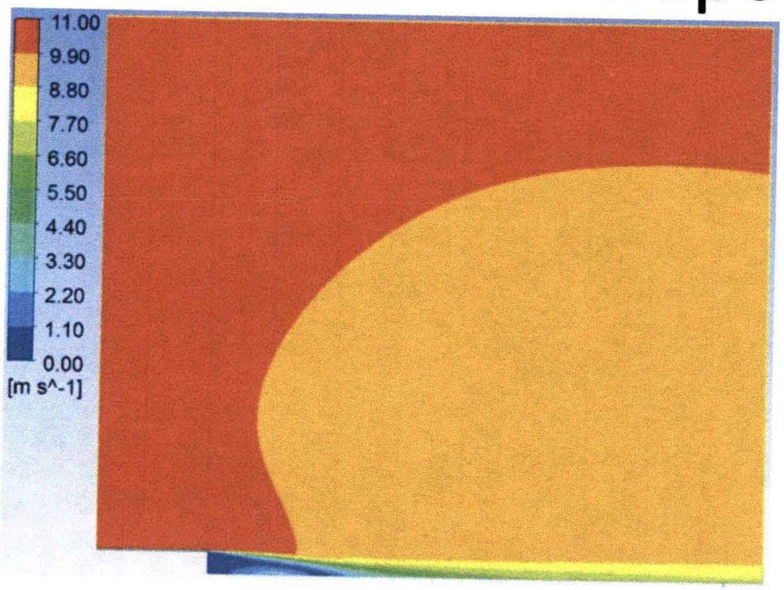
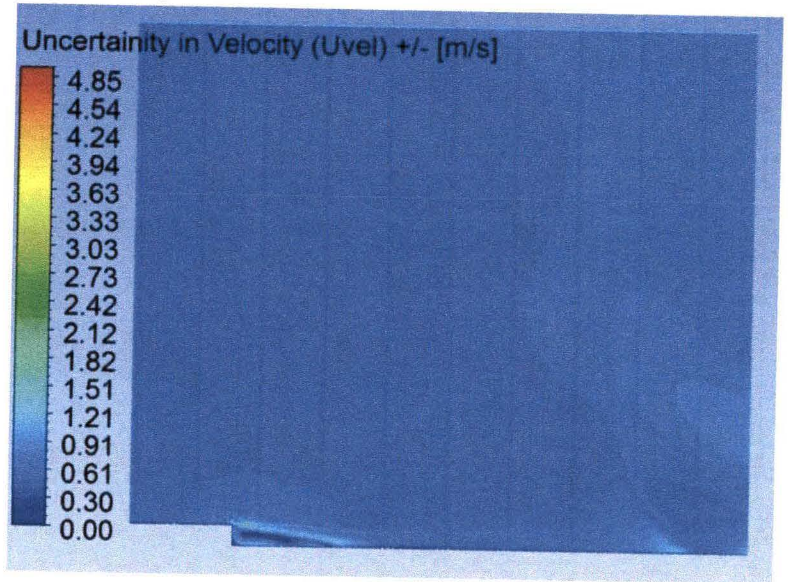
- A root-sum-squared (rss) of the uncertainty variables was calculated (omitting Richardson's Extrapolation)





The highest uncertainty is +/- 4.85 m/s.

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Note on Domain Sizing

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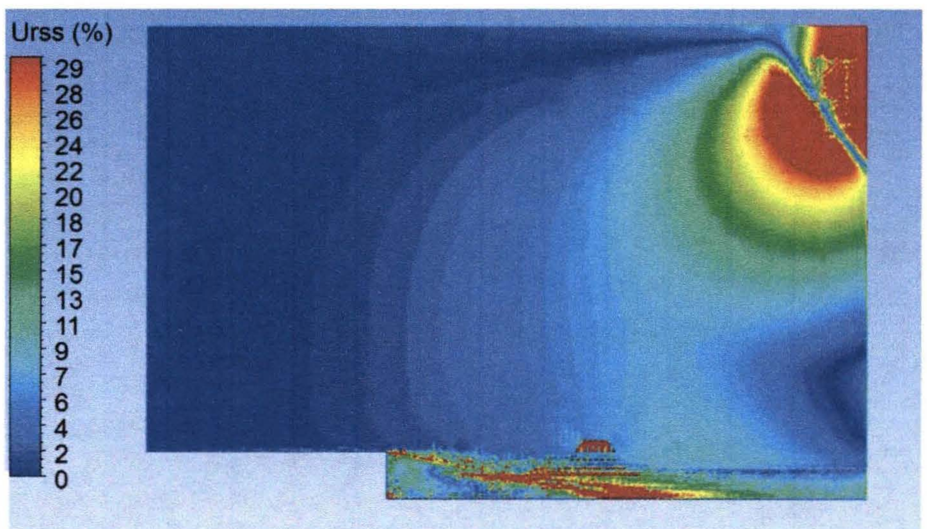
- During several preliminary cases of the grid convergence study, one case provided an excellent example of domain sizing.
  - A CFD analyst is always troubled with trying to keep the domain size large enough to not affect the solution.
    - Using the oscillatory method, one can see the solution differences between the three grids. In the case presented below, the domain size is too small.



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Conclusion

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- This paper outlines an uncertainty analysis for the ke realizable turbulence model for a backward facing step.
- The velocity magnitude was predicted using CFD.
- The uncertainty parameters listed in Table1 were analyzed using an oscillatory convergence calculation or a monotonic convergence calculation.
- Plots of the velocity magnitude can be combined with a corresponding uncertainty plot for an accurate velocity prediction.
- There are other variables that would influence the uncertainty calculation. Examples of these other parameters include solution schemes, other turbulence models, and time accurate solutions. Future work will include analyzing each of these items.

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Conclusion /Recommendation

- The following input uncertainty's are recommended

Type of Variable	Variables Xi	Value	Bias Error	Uncertainity
Boundary Conditions	epsilion turbulent mixing length dissipation rate inlet (m2/s3)	0.5	0.5	1.2% of local velocity
	k turbulent intensity kinetic energy inlet (m2/s2)	0.05	0.05	0.8 % of local velocity
	pressure outlet (Pa)	101325	2%	10x the variation
	velocity inlet (m/s)	10	0.5	1.3x the variation
Fluid Properties	kinematic viscosity nu represents air [0-50-100] deg C	1.79E-06	[13.6e-06 -> 23.06e-06]	28% of the local velocity
Grid Size	Method - Uses Oscillatory Uncertainty	1,192,000 1,862,500		grid specific
		3,311,689		
Numerical	Method - Uses Richardson's Extrapolation (ASME 5 Step Procedure) – Calculated for Velocity at each Cell			
Solver	OpenFOAM (SimpleFoam) vs. Fluent			30% of the local velocity
Turbulence Models	ke-realiable, kwSST, and SpalartAllmaras			Future work will consider more turbulence models

Recommendation / Future Work

- It is suggested that the CFD community begin to compile a list of the many input parameters associated with each uncertainty calculation for different problems and output variables.
- Ideally, an analyst could assemble a table of all uncertainty variables and estimate a number based on historical data rather than running separate CFD cases for each variable.

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Backup

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Uncertainty Variables ke-realizable (OPENFOAM – SimpleFoam)

ke Inputs:					Default Values
Boundary Conditions:					
	epsilon	inlet	turbulentMixingLengthDissipationRateInlet	mixing length	0.5
				value	1
		wall	epsilonWallFunction	value	0
		outlet	type	value	1
	k	inlet	turbulentIntensityKineticEnergyInlet	intensity	0.05
				value	1
		wall	kqRWallFunction	value	0
		outlet	type	value	1
	nut	inlet	type	value	1
		wall	nutWallFunction	value	0
		outlet	type	uniform	0
	nuTilda	inlet	zeroGradient		
		wall	zeroGradient		
		outlet	zeroGradient		
	p	inlet	zeroGradient		
		wall	zeroGradient		
		outlet	type	fixed value	0
	U	inlet	type	x	10
				y	0
				z	0
		wall	type	x	0
				y	0
				z	0
		outlet	type	x	1
				y	0
				z	0
Turbulence	Turbulence Tranport Model	**nu**	Newtonian	[0 2 -1 0 0 0 0]	1.00E-06
	Turbulence Propoerties	simulationType	RASModel		
	RAS Properties		RASModel	realizableKE	
ControlDict	End Time				150000
	timestep (or CFL)				1
	write percision				6
	timePrecision				6

SolutionSchemes	gradSchemes	p	Gauss linear	
		U	Gauss Linear	
	divSchemes	phi, U	Gauss limitedLinearV	
		phi,k	Gauss limitedLinear	
		phi,epsilon	Gauss limitedLinear	
		phi,R	Gauss limitedLinear	
		R	Gauss linear	
		phi, nuTilda	Gauss limitedLinear	
		nuEff*dev(T(grad(U)))	Gauss linear	
	laplacianSchemes	nuEff,U	Gauss linear corrected	
		1|A(U)),p	Gauss linear corrected	
		DkEff,k	Gauss linear corrected	
		DepsilonEff,epsilon	Gauss linear corrected	
		DREff,R	Gauss linear corrected	
		DnuTildaEff,nuTilda	Gauss linear corrected	
	interpolationSchemes	interpolate(U)	linear	
	snGradSchemes	default	corrected	
	fluxRequired	default no	p	
Solvers	p	solver	GAMG;	
		smoother	GaussSeidel;	
		cacheAgglomeration	true;	
		nCellsInCoarsestLevel	10;	
		agglomerator	faceAreaPair;	
		mergeLevels	1;	
		tolerance	1e-06;	
		relTol	0.05;	
	pFinal	solver	GAMG;	
		smoother	GaussSeidel;	
		cacheAgglomeration	true;	
		nCellsInCoarsestLevel	10;	
		agglomerator	faceAreaPair;	
		mergeLevels	1;	
		tolerance	1e-06;	
		relTol	0;	
	(U|k|epsilon)Final	solver	PBiCG;	
		preconditioner	DILU;	
		tolerance	1e-05;	
		relTol	0;	
	PIMPLE	nOuterCorrectors	4;	
		nCorrectors	1;	
		nNonOrthogonalCorrectors	0;	
		pRefCell	0;	
		pRefValue	0;	
	SIMPLE	nNonOrthogonalCorrectors	0;	
		residualControl	p	1e-2;
			U	1e-3;
			(k|epsilon)	1e-3;
	relaxationFactors	p	0.3;	
		U	0.7;	
		k	0.7;	
		epsilon.*	0.7;	
	cache	grad(U);		
Mesh Size	number of cells			