Numerical Uncertainty Analysis for Computational Fluid Dynamics using Student T Distribution – Application of CFD Uncertainty Analysis compared to Exact Analytical Solution

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Extended Abstract

Computational Fluid Dynamics (CFD) is the standard numerical tool used by Fluid Dynamists to estimate solutions to many problems in academia, government, and industry. CFD is known to have errors and uncertainties and there is no universally adopted method to estimate such quantities. This paper describes an approach to estimate CFD uncertainties strictly numerically using inputs and the Student-T distribution. The approach is compared to an exact analytical solution of fully developed, laminar flow between infinite, stationary plates. It is shown that treating all CFD input parameters as oscillatory uncertainty terms coupled with the Student-T distribution can encompass the exact solution.

Nomenclature

a	= channel width
δ_D	= experimental error
δ_{input}	= input error
δ_{model}	= modeling error
δ_{num}	= numerical error
δ_S	= simulated error
D	= experimental value
dp/dx	= pressure gradient
ε_{21}	= solution changes medium to fine grid

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ε_{32} = solution changes coarse to medium grid

e_a^{21} = extrapolated error

E = comparison 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 = simulated result

S_{k1} = solution variable for fine grid

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

u_{input} = input uncertainty

u_D = experimental uncertainty

u_{num} = numerical uncertainty

u_{val} = validation uncertainty

μ = viscosity

I. Introduction

CFD in many problems is the optimum balance between cost and accuracy. However, a comprehensive approach for verification using test data is needed for full validation. With shrinking budgets in all areas of aerospace industry, CFD is commonly used without proper verification and validation. This paper couples traditional uncertainty analysis with the Student-T distribution to estimate a numerical uncertainty without using test data. The results are compared to the exact analytical solution of fully developed, laminar flow between infinite, stationary plates.

A thorough literature review was performed by the authors in AIAA-2013-0258[1] and it was determined that the current state of the art for CFD uncertainty analysis is the ASME Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer [2]. The standard outlines a validation approach using experimental errors, modeling assumptions, simulation inputs, and numerical solutions of equations. The error, E, and validation standard uncertainty u_{val}, can be defined and conclusions drawn about whether the model is properly verified. This paper outlines a method to estimate the numerical uncertainty without using test data and shows the differences between the proposed methodology and the ASME Standard.

II. Methodology of ASME V&V 20-2009

A schematic showing the nomenclature and an overview of the validation process is shown in Figure 1[2]. The left side of the figure describes the terminology and the right side describes the validation process.

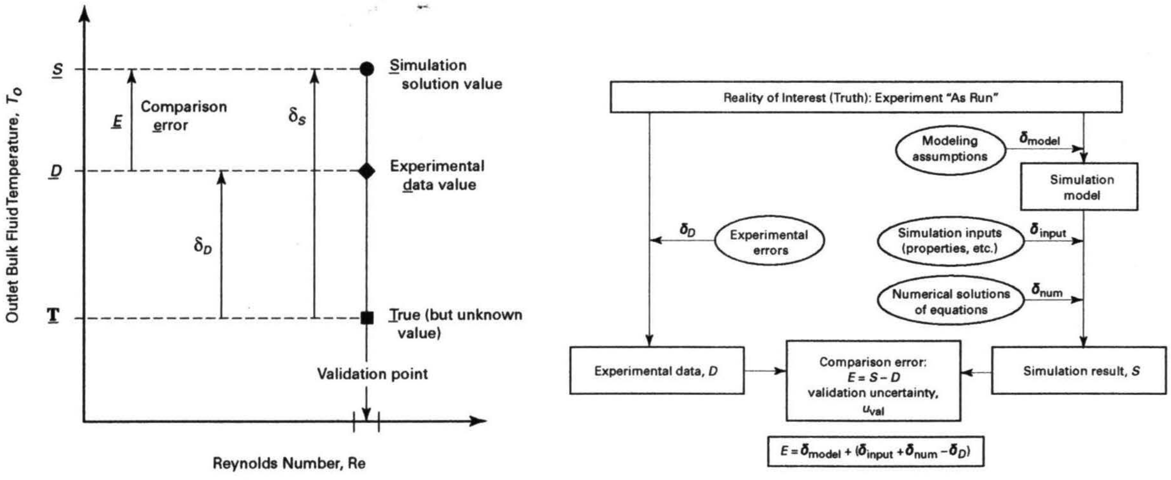

Figure 1: Schematic of nomenclature and Overview of Validation Process[2]

The methodology is as follows. The validation comparison error, E, is the difference between the simulated result, S, and the experimental value, D [2]. The goal is to characterize the interval modeling error, δ_{model}. The coverage factor, k, used to provide a given degree of confidence (ie 90% assuming a uniform distribution, k=1.65)[2].

The standard also outlines procedures to calculate numerical uncertainty, u_{num}, the uncertainty in the simulated result from input parameters, u_{input}, and the experimental uncertainty, u_D [2].

$$\delta_{model}\ \varepsilon [E - u_{val}, E + u_{val}] \quad \textbf{(1)}$$

$$E = S - D \quad \textbf{(2)}$$

$$u_{val} = k\left(\sqrt{{u_{num}}^2 + {u_{input}}^2 + {u_D}^2}\right) \quad \textbf{(3)}$$

U_{num} is calculated using a Richardson's Extrapolation approach and defined as a five-step procedure[2].

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[2].

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

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

Step 3 is to calculate the observed order, p, as shown in equation 6[2]. This equation must be solved iteratively.

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

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

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

Step 4 is to calculate the extrapolated values as shown in equation 7[2].

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

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

Step 5 is to calculate the fine grid convergence index and numerical uncertainty as shown in equation 8[2]. This approached used a factor of safety of 1.25 and assumed that the distribution is Gaussian about the fine grid, 90 % confidence.

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

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

U_{input} is calculated using a Taylor Series expansion in parameter space[2].

$$u_{input} = \sqrt{\sum_{i=1}^{n}\left(\frac{\vartheta S}{\vartheta X_i} u_{xi}\right)^2} \quad \textbf{(9)}$$

U_D is calculated using test uncertainty methodology as defied in the standard[2]. The purpose of this paper is to show an estimate of numerical uncertainty without test data. The reader is referred to the ASME standard for further information.

III. Proposed Methodology without Test Data

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

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

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

$$\boldsymbol{R_k = \varepsilon_{21} / \varepsilon_{32}} \quad \textbf{(10)}$$

Three convergence conditions are possible[3]:

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

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

(iii) Divergence: $R_k>1$ **(11)**

The methodology outlined in ASME V&V-2009[2] assumes monotonic convergence criteria for u_{num}. Further increasing the grid does not always provide a monotonically increasing result. This is shown in AIAA-2013-0258[1]. The proposed methodology is to treat all input parameters including the grid as an oscillatory convergence study. The uncertainty for cells with oscillatory convergence, using the following method outlined by Stern, Wilson, Coleman, and Paterson [3], can be calculated as follows in equation 12. ***S*** is the simulated result. For this case it is the upper velocity $\boldsymbol{S_U}$ and the lower velocity $\boldsymbol{S_L}$.

$$U_{Oscillatory} = \left|\frac{1}{2}(S_U - S_L)\right| \tag{12}$$

The proposed methodology as compared to the ASME Standard is as follows. If there is no experimental data, D=0, δ_D=0, and u_D=0.

$$E = S - D = S$$

$$\delta s = S - T$$

$$E = S - D = T + \delta s - (T + \delta_D) = \delta_S - \delta_D = \delta_S$$

$$u_{val} = k\left(\sqrt{u_{num}{}^2 + u_{input}{}^2 + u_D{}^2}\right) = u_{val} = k\left(\sqrt{u_{num}{}^2 + u_{input}{}^2}\right) \tag{13}$$

Report the simulated result, S as $$S \pm u_{val} \tag{14}$$

Also instead of assuming a gauss-normal distribution as in the standard when including test data, the k-value will come from the Student-T distribution as shown in Table 1.

Table 1 – Student – T Distribution, k Values

Number of Cases	Degrees of Freedom	Confidence 90%
2	1	6.314
3	2	2.92
4	3	2.353
5	4	2.132
6	5	2.015
7	6	1.943
8	7	1.895
9	8	1.86
10	9	1.833
11	10	1.812
12	11	1.796
13	12	1.782
14	13	1.771
15	14	1.761
16	15	1.753
17	16	1.746
18	17	1.74
19	18	1.734
20	19	1.729
21	20	1.725
22	21	1.721
23	22	1.717
24	23	1.714
25	24	1.711
26	25	1.708
27	26	1.706
28	27	1.703
29	28	1.701
30	29	1.699
31	30	1.697
41	40	1.684
51	50	1.676
61	60	1.671
81	80	1.664
101	100	1.66
121	120	1.658
infty	infty	1.645

IV. Fully Developed Laminar Flow Between Stationary Parallel Plates

Fully developed laminar flow between stationary, parallel plates is an exact solution to the Navier-Stokes Equations as derived in "Introduction to Fluid Mechanics" [4]. The width of the channel is (a).

$$u = \frac{a^2}{2\mu}\left(\frac{\partial P}{\partial x}\right)\left[\left(\frac{y}{a}\right)^2 - \left(\frac{y}{a}\right)\right] \tag{14}$$

A CFD model of this problem was created in FLUENT. The fluid is air. Table 2 outlines the parameters used.

Table 2 – Parameters

a (m)	0.1
rho (kg/m3)	1.225
mu (Ns/m2)	0.00001789
dp/dx (N/m3)	-0.000400

The exact solution is shown in Figure 1.

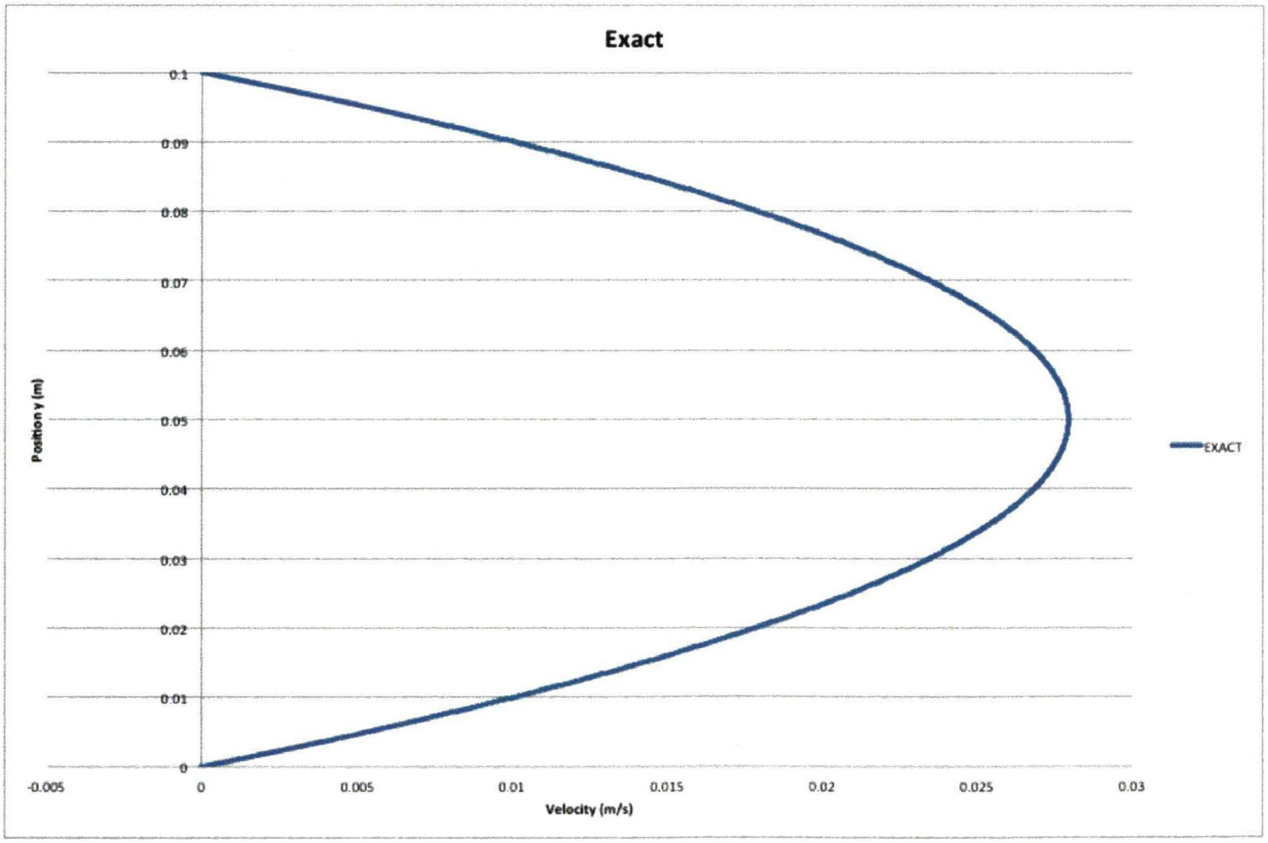

Figure 1 – Exact Solution

A CFD model was created for the same conditions and the uncertainty calculation performed as outlined in the next section.

V. Uncertainty Calculation

The uncertainty can be calculated by expanding equation 13 for pressure, density, numerical (grid), and solver.

$$u_{val} = k * \left(\left(\left(\frac{\partial V}{\partial pressure} \right)^2 B_{pressure}^2 \right) + \left(\left(\frac{\partial V}{\partial rho} \right)^2 B_{rho}^2 \right) + \left(\left(\frac{\partial V}{\partial num} \right)^2 B_{num}^2 \right) + \left(\left(\frac{\partial V}{\partial solver} \right)^2 B_{solver}^2 \right) + \right.$$

$$\left. + \left(\left(\frac{\partial V}{\partial velocity} \right)^2 B_{velocity}^2 \right) \right)^{1/2} \qquad \textbf{(15)}$$

The proposed method is to calculate the uncertainty as an oscillatory input parameter and multiply by the appropriate Student-T k-factor.

For Numerical, three grids were used and the t value of 2.92.

$$u_{val} = 2.92 * \left(\left(\left(\frac{\partial V}{\partial num} \right)^2 B_{num}^2 \right) \right)^{1/2} \qquad \textbf{(16)}$$

$$u_{val} = 2.92 * \left| \frac{1}{2} (S_U - S_L) \right| \qquad \textbf{(17)}$$

The centerline velocity was chosen as an example to plot, however at all points the uncertainty bands always encompass the exact solution.

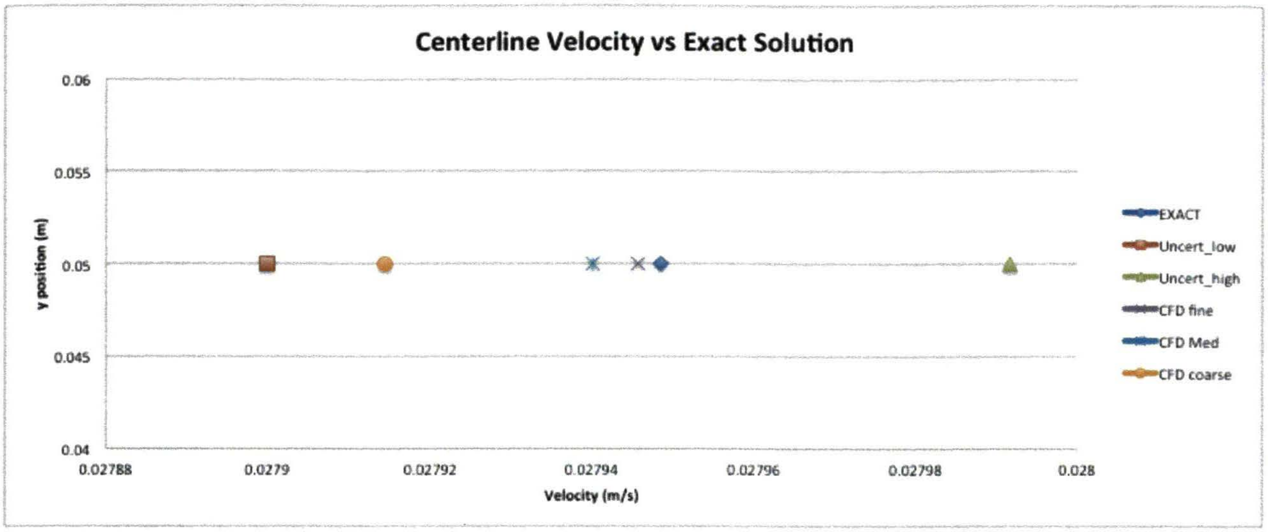

Figure 2 – Exact Solution vs. CFD with Uncertainty (Centerline Velocity) - Grid

If there is also a variation in the inlet velocity due to a tolerance or known bias, run the model at the low and high limits and use a new t-value of 2.132, which corresponds to five cases. The five cases would be three for grids and two for flow rates. A five percent variation in inlet velocity was chosen for this example.

$$u_{val} = 2.132 * \left(\left(\left(\frac{\partial V}{\partial num}\right)^2 B_{num}^2\right) + \left(\left(\frac{\partial V}{\partial velocity}\right)^2 B_{velocity}^2\right)\right)^{1/2} \quad \textbf{(18)}$$

$$u_{val} = 2.132 * \left|\frac{1}{2}(S_U - S_L)\right| \quad \textbf{(19)}$$

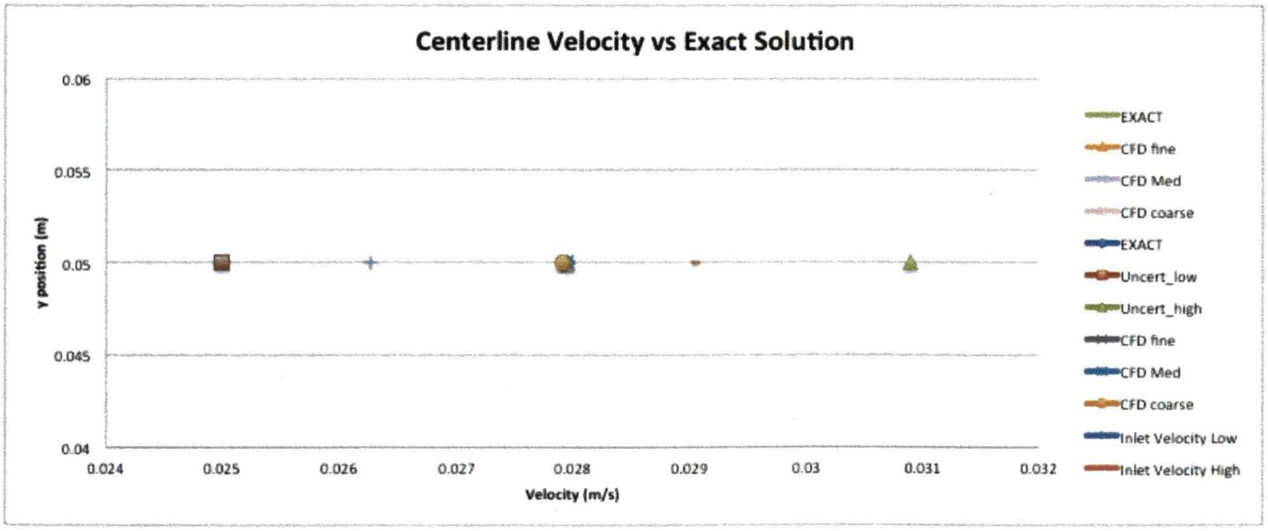

Figure 3 – Exact Solution vs. CFD with Uncertainty (Centerline Velocity) – Grid and Inlet Velocity

Also to include the outlet pressure boundary condition, run the model at the low and high known bias or tolerances and use a new t-value of 1.943, which corresponds to seven cases. The seven cases would be three for grid, two for flow rate, and two for pressure outlet boundary condition.

$$u_{val} = 1.943 * \left(\left(\left(\frac{\partial V}{\partial num}\right)^2 B_{num}^2\right) + \left(\left(\frac{\partial V}{\partial velocity}\right)^2 B_{velocity}^2\right) + \left(\left(\frac{\partial V}{\partial pressure}\right)^2 B_{pressure}^2\right)\right)^{1/2} \quad \textbf{(20)}$$

$$u_{val} = 1.943 * \left|\frac{1}{2}(S_U - S_L)\right| \quad \textbf{(21)}$$

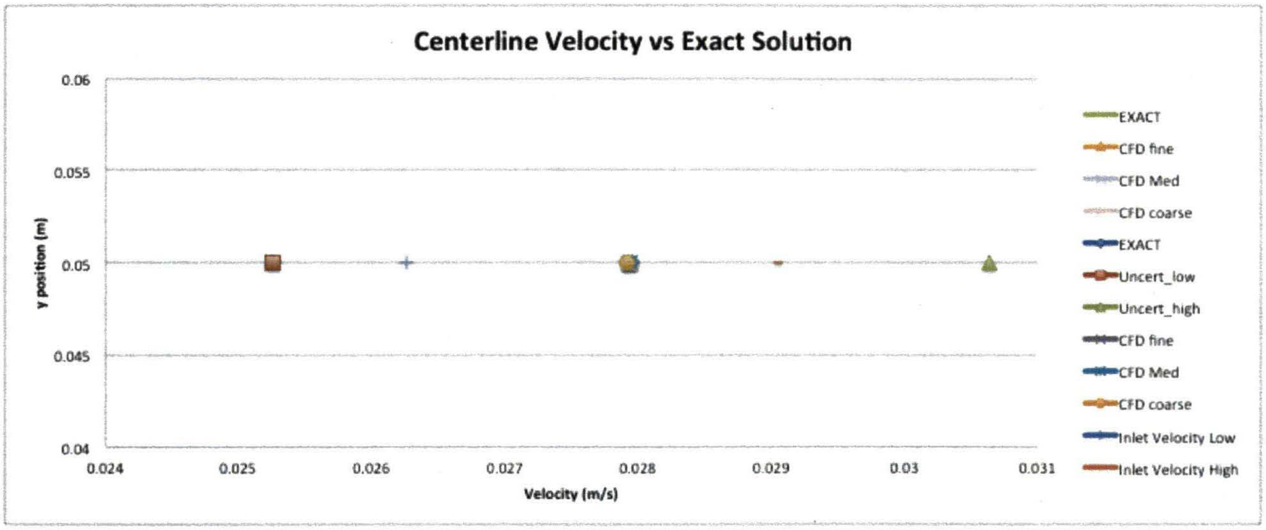

Figure 4 – Exact Solution vs. CFD with Uncertainty (Centerline Velocity) – Grid, Inlet Velocity, and Outlet Pressure

To account for the variation in fluid properties, the kinematic viscosity for air between 0 and 100 degrees Celsius is $13.6X10^{-6}$ to $23.06X10^{-6}$. The model was run at these limits to account for the possible variation in fluid properties and a new value of t= 1.86 was chosen, which corresponds to the nine cases.

$$u_{val} = 1.86 * \left(\left(\left(\frac{\partial V}{\partial num}\right)^2 B_{num}^2\right) + \left(\left(\frac{\partial V}{\partial velocity}\right)^2 B_{velocity}^2\right) + \left(\left(\frac{\partial V}{\partial pressure}\right)^2 B_{pressure}^2\right) + + \left(\left(\frac{\partial V}{\partial rho}\right)^2 B_{rho}^2\right)\right)^{1/2}$$

(22)

$$u_{val} = 1.86 * \left|\frac{1}{2}(S_U - S_L)\right| \quad \textbf{(23)}$$

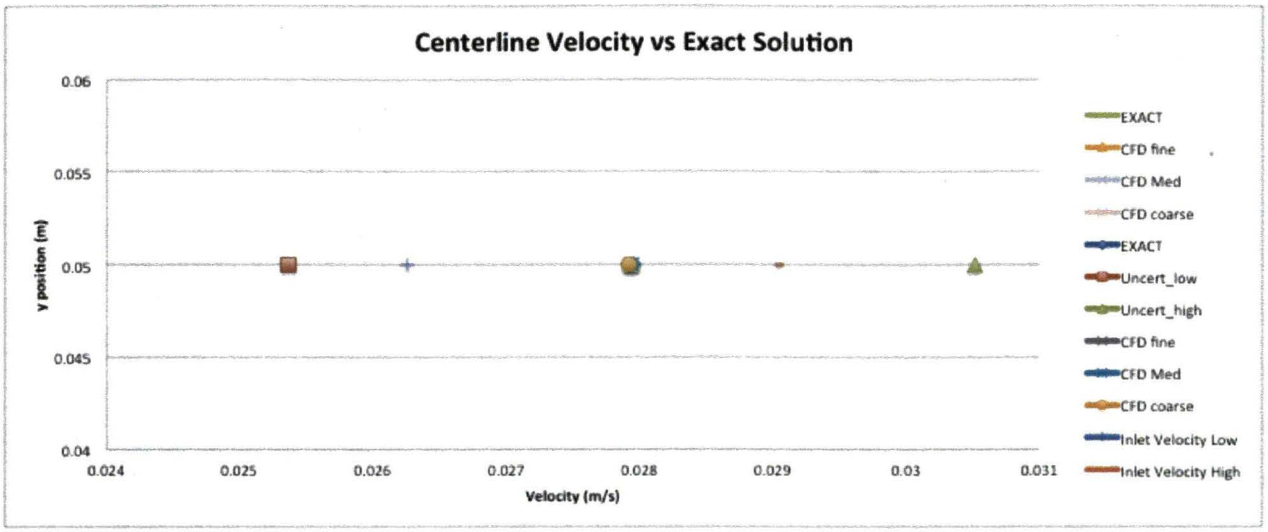

Figure 5 – Exact Solution vs. CFD with Uncertainty (Centerline Velocity) – Grid, Inlet Velocity, Outlet Pressure, and Density

Fluent has been used to calculate the results above; we also consider the solver as an input to the model. To account for the variation in the solver, the model was run in OpenFOAM. The t value was updated to 1.833 because the numbers of cases are ten.

$$u_{val} = 1.833 * \left(\left(\left(\frac{\partial V}{\partial num}\right)^2 B_{num}^2\right) + \left(\left(\frac{\partial V}{\partial velocity}\right)^2 B_{velocity}^2\right) + \left(\left(\frac{\partial V}{\partial pressure}\right)^2 B_{pressure}^2\right) + + \left(\left(\frac{\partial V}{\partial rho}\right)^2 B_{rho}^2\right) + \left(\frac{\partial V}{\partial solver}\right)^2 B_{solver}^2 \right)^{1/2} \quad \textbf{(22)}$$

$$u_{val} = 1.833 * \left|\frac{1}{2}(S_U - S_L)\right| \quad \textbf{(23)}$$

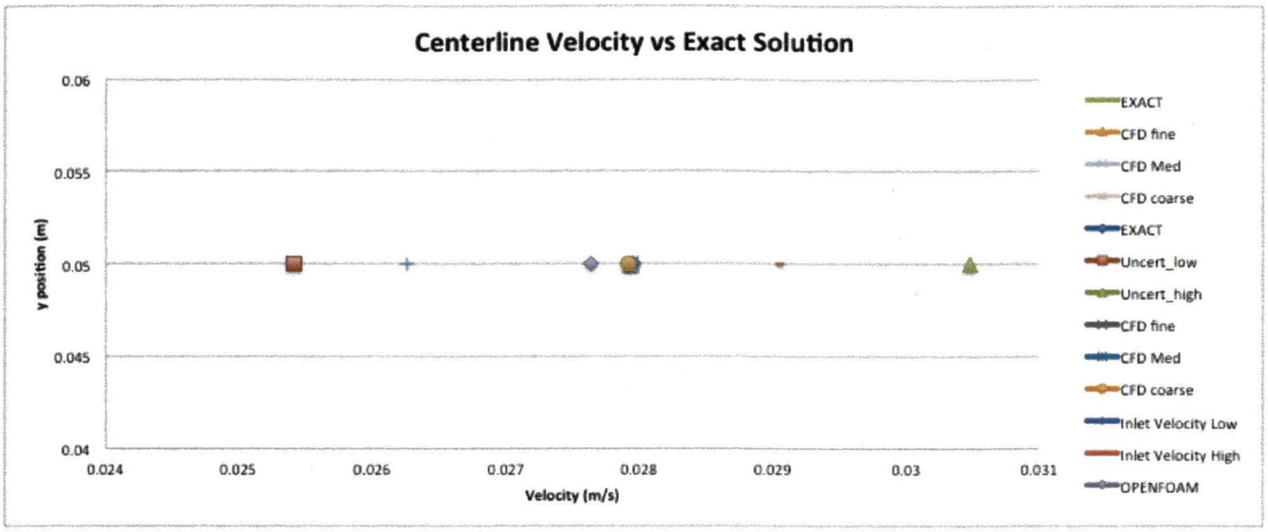

Figure 6 – Exact Solution vs. CFD with Uncertainty (Centerline Velocity) – Grid, Inlet Velocity, Outlet Pressure, Density, and Solver

Figure 7 is a plot of all the CFD cases, uncertainty, and an exact comparison.

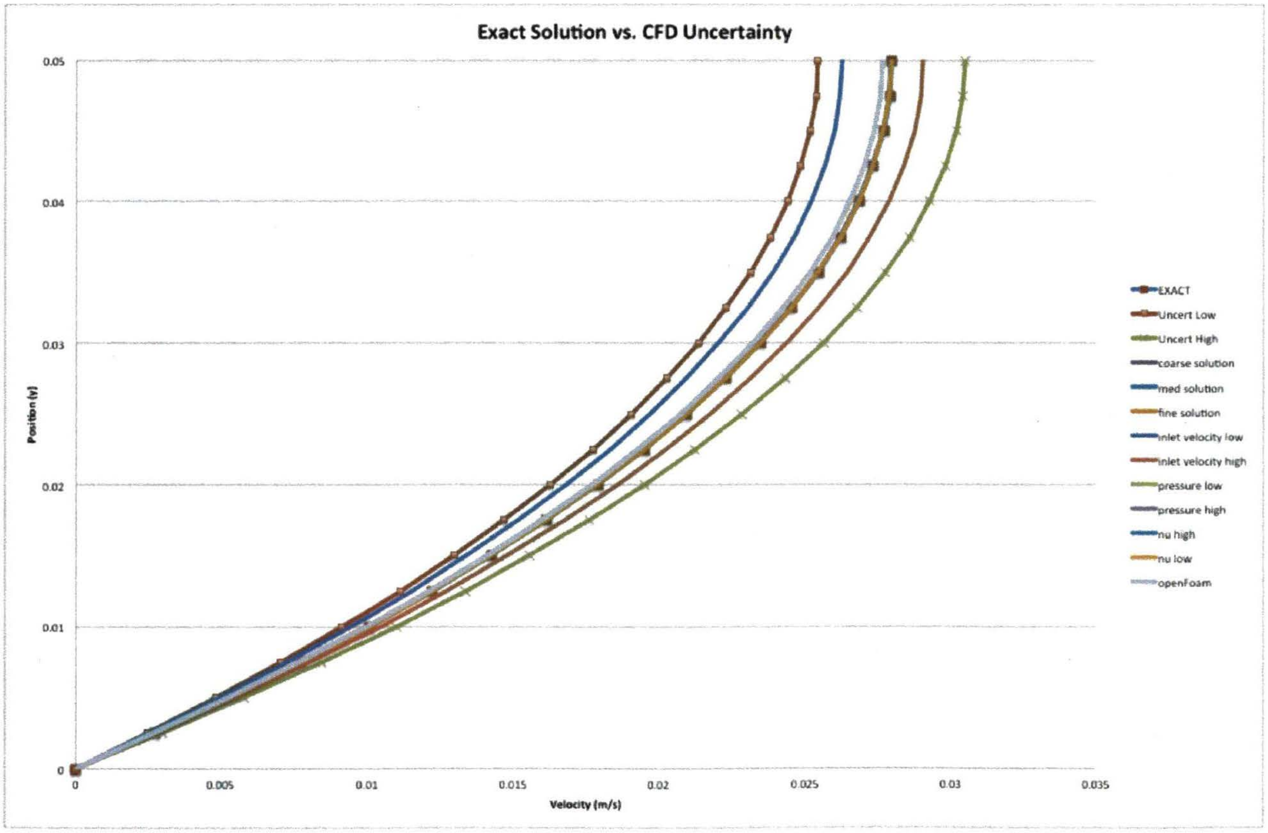

Figure 7 – Exact Solution vs. CFD with Uncertainty (Parallel Plates – Half of Domain) – Grid, Inlet Velocity, Outlet Pressure, Density, and Solver

VI. Conclusion

It can be concluded that treating all inputs to a CFD model as oscillatory uncertainty parameters coupled with the Student-T distribution can supply an uncertainty estimate that encompasses the exact solution for the case considered above (fully developed, laminar, flow between stationary parallel plates). To summarize the approach and general idea, there is a standard[2] for calculating verification and validation of CFD using a combined numerical and experimental data. The approach described above is a way to estimate the uncertainty of a model if test data is not available. An analyst should make use of all test data that is available or able to be funded and use the ASME standard. However, if test data is missing or not attainable, the method described makes assumptions that each CFD solution belongs to an underlying Student-T distribution and a corresponding uncertainty can be estimated for a selected confidence interval.

References

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[4] Fox, Robert., McDonald, Alan, "Introduction to Fluid Mechanics" 3rd Edition. John Wiley & Sons, 1985