Conducting and Reporting the Results of a CFD Simulation

Objective of a CFD Simulation

Objective is to achieve a high level of *credibility* and *confidence* in the results from CFD performed as part of the design and analysis of a propulsion system.

Credibility and confidence are obtained by demonstrating acceptable levels of error and uncertainty as assessed through *verification* and *validation*.

This discussion is focused on the question…

How good are your CFD results?

Determining this precisely is often difficult, but we can try to understand sources of error and ways to demonstrate quality CFD results.

Levels of the Use of CFD Results

1. Provide Qualitative Information.

Provide features of flow field (conceptual, rough estimates of quantities). Accuracy requirements are low.

2. Provide Incremental Quantities, ΔP.

- $P = P_{baseline} + \Delta P$
- Errors partially cancel for ΔP
- $\Delta P = (P_2 - P_1)_{actual} + (E_2 - E_1) = P_{actual} + \Delta E$
- Moderate accuracy requirement.

3. Provide Absolute Quantities, P.

Requires high level of accuracy.

Objectives of a CFD Analysis

The CFD analysis may provide:

- Steady-state flow at cruise conditions.
- Features of the shock system (positions, cowl stand-off).
- Features of the boundary layers (thickness, separation).
- Pressure recovery at throat and compressor face.
- Spillage (side walls, cowl).
- Bleed requirements (slots, bleed holes).
- Distortion at compressor face.
- Drag.
- Off-design flow features.
- Unsteady flow features (unstart, stability).
- Aerodynamic and thermal loads.

Aspects

Several aspects with regard to conducting and reporting the results of a CFD simulation:

- Uncertainty and Error
- Verification and Validation
- Iterative convergence
- Grid convergence
- When things go wrong

Uncertainty and Error

Uncertainty

"A potential deficiency in any phase or activity of the modeling process that is due to the lack of knowledge." (AIAA-G-077-1998).

The use of *potential* indicates that deficiencies may or may not exist.

Error

"A recognizable deficiency in any phase or activity and simulation that is not due to lack of knowledge." (AIAA-G-077-1998).

The deficiencies are knowable up examination. *Acknowledged* errors have procedures for identifying and removing them. U*nacknowledged* errors are undiscovered and no set procedures exist to find them.

Errors in CFD Results

Total Error = **Physical Modeling Error**
+ **Discretization Error**
+ **Programming Error**
+ **Computer Round-off Error**
+ **Usage Error**
+ **Post-Processing Error**

Physical modeling errors are usually acknowledged and may be quantified.

Discretization errors are grid dependent but a priori knowledge of the proper grid for a desired level of accuracy is generally lacking.

Programming errors should have been minimized by programmers.

Computer round-off errors are usually negligible or controllable.

Usage errors are minimized by proper training.

Post-processing errors are usually controllable.

Physical Modeling Errors

Many physical models are used in CFD and we must understand the limits and possible uncertainty and errors with each model:

- Spatial Dimensions. (2D, axisymmetric, 3D)
- Temporal Dimensions. (steady-state, unsteady)
- Equations. (Navier-Stokes, approximations)
- Turbulence Model.
- Thermodynamic and Transport Property model.
- Chemistry Model.
- Flow Boundary Conditions (inflow, outflow).
- Compressor Face Model.
- Bleed / Blowing Model.
- Vortex Generator Model.

Discretization Error

Errors that exist because continuum flow equations and physical models are represented in a discrete domain of space (grid) and time.

Level of error is function of interactions between the solution and the grid. Since solution is unknown before-hand, the grid generation may not produce the optimum grid.

Discretization error is quantified through **verification** methods that examine grid convergence.

Discretization error is controllable.

Verification and Validation

Verification

"The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model." (AIAA-G-077-1998).

Verification checks that there are no programming errors and that the coding correctly implements the equations and models. It also examines discretization errors in the CFD calculations.

Validation

"The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model." (AIAA-G-077-1998).

Validation checks that the CFD results agree with reality as observed in experiments, flight tests, or applications.

Verification Assessment

Verification assessment has two aspects:

Verification of a Code

Verifies that code has no programming errors and that the coding correctly implements the equations and models. The methods involve examining modules of code, checking basic assumptions (mass conservation), and comparing results to analytic results.

Verification of a Calculation

Verifies that a calculation (simulation) demonstrates a certain level of accuracy. The primary method for the verification of a calculation is the ***grid convergence study***.

Validation Assessment

- Validation assessment addresses if CFD code agrees with reality through comparison to experiments. Checks uncertainty in physical models.
- Experiment must also address its own errors.
- Unit ↑ Benchmark ↑ Subsystem ↑ Complete System.
- Set of validation cases are being collected and studied that cover the range of flow features present in inlets (turbulent boundary layers, shocks, shock / boundary layer interactions, subsonic ducts, supersonic diffusers).
- NPARC Alliance Validation Archive:

  www.grc.nasa.gov/www/wind/valid

Iterative and Grid Convergence

Convergence used in two ways:

Iterative Convergence

Simulations should demonstrate iterative convergence. As the algorithm iterates the solution, the simulation results approach a fixed value (residuals drop and level off). This applies to both steady and unsteady flow solutions. In the case of unsteady flows, the iterative convergence applies to iterations over a time step.

Grid Convergence

As the grid spacing is reduced, the simulation results become insensitive to the grid and approach the *continuum* results.

Iterative Convergence

Iterative Convergence can be demonstrated in several ways:

1. Value of the largest change in the solution over an iteration, δQ_{big}.
2. Iteration history of the L2 norm of the equation residual.
3. Examine conservative variables.
4. Iteration history of a local or global quantity of the flow.

Usually some measure of all of these are used to determine iterative convergence.

The largest change in the solution over an iteration is simply

$$\delta\hat{Q}_{Big} = \max\left(\delta\hat{Q}_{i,m}\right)$$

L2 Residual

The L2 norm of δQ is commonly called the *residual* of the equation solution and is computed as

$$L2 = \sqrt{\frac{\sum_{i=1}^{N}\sum_{m=1}^{M}\left(\delta\hat{Q}_{i,m}\right)^2}{M * N}}$$

where N, total number of grid points
M, number of elements in Q (5 for Navier-Stokes Equations)

- It represents the change in the solution over an iteration averaged over all the grid points and equations.
- The L2 residual is usually displayed and plotted as its log values, [log10(L2)].
- This shows the order-of-magnitude of the change in the solution.
- Generally desire the L2 residual to approach zero with iterations.

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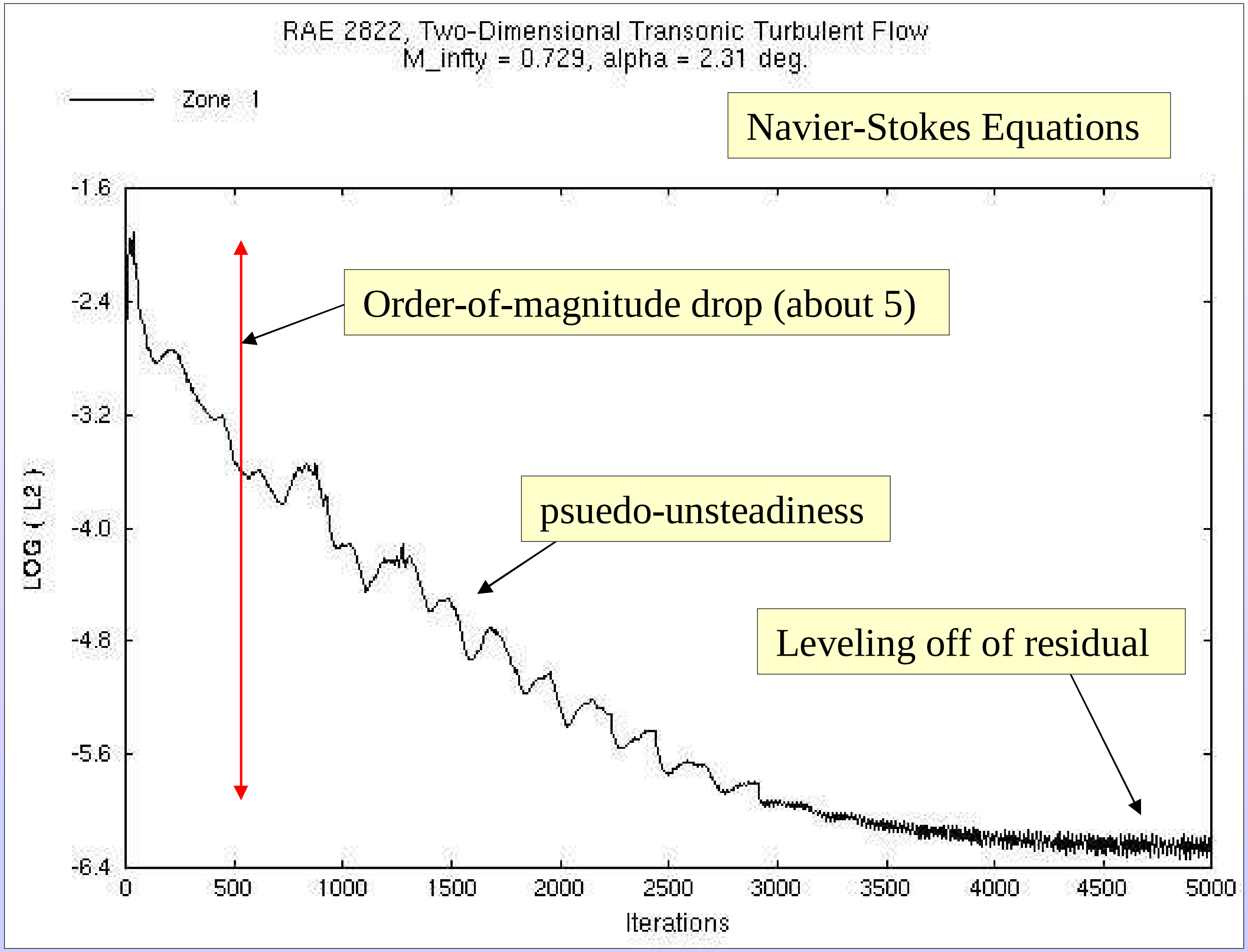
L2 Residual Plots

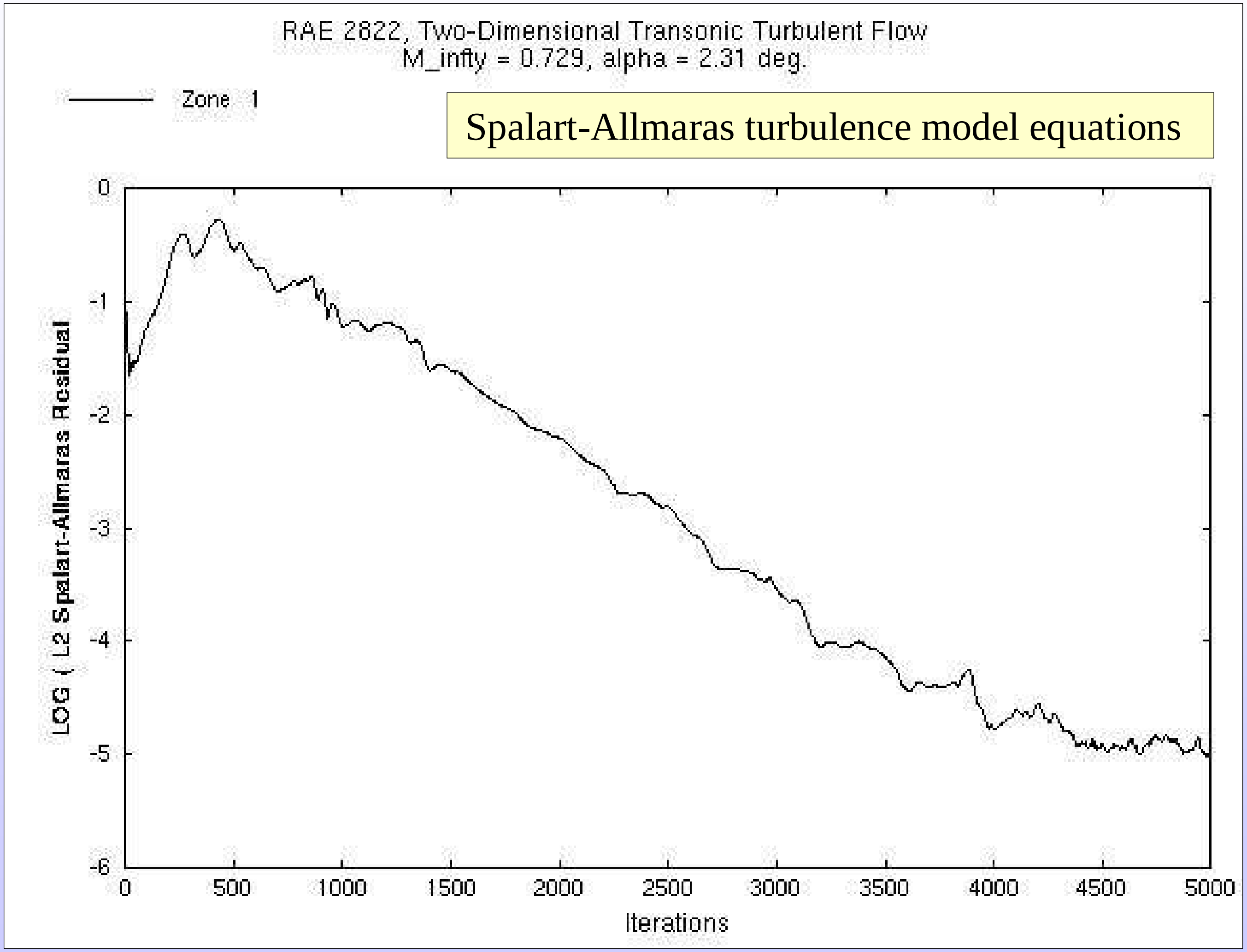
The behavior of the residual is not always so smooth.

Unsteadiness (real or pseudo) in the solution (typical of turbulent and separated flows) may limit how far the residual drops.

Often a couple of orders-of-magnitude drop is all one achieves.



L2 Residual Plots (continued)



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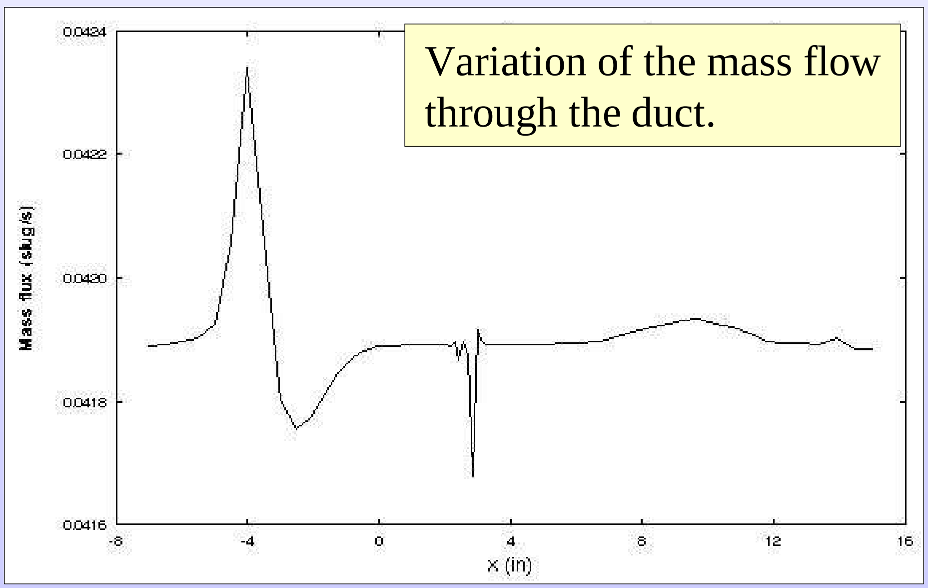
Examine Conservative Variables

The solution of the conservation equations must satisfy those conservative principles. Iterative convergence can be demonstrated through examination of the conservative variables:

For example, one can examine the conservation of mass through a duct:



Variation of the mass flow through the duct.

Statistical analysis of the variation. This indicates the level of iterative convergence error in determining the mass flow through the duct.

```
--- mflux ---

Number of Data Points (nd) =           81

Average mass flux     =   4.1896842E-02
Minimum mass flux     =   4.1679405E-02
Maximum mass flux     =   4.2340528E-02
Inflow  mass flux     =   4.1888103E-02
Outflow mass flux     =   4.1885339E-02
Error #1 (max-min)    =   0.000661   [   1.58%]
Error #2 (in-out)     =  -0.000003   [ -0.01%]
Standard deviation    =   6.7133369E-05
Stand deviation (pct) =   0.1602349    %
```

Change in Local or Global Quantity

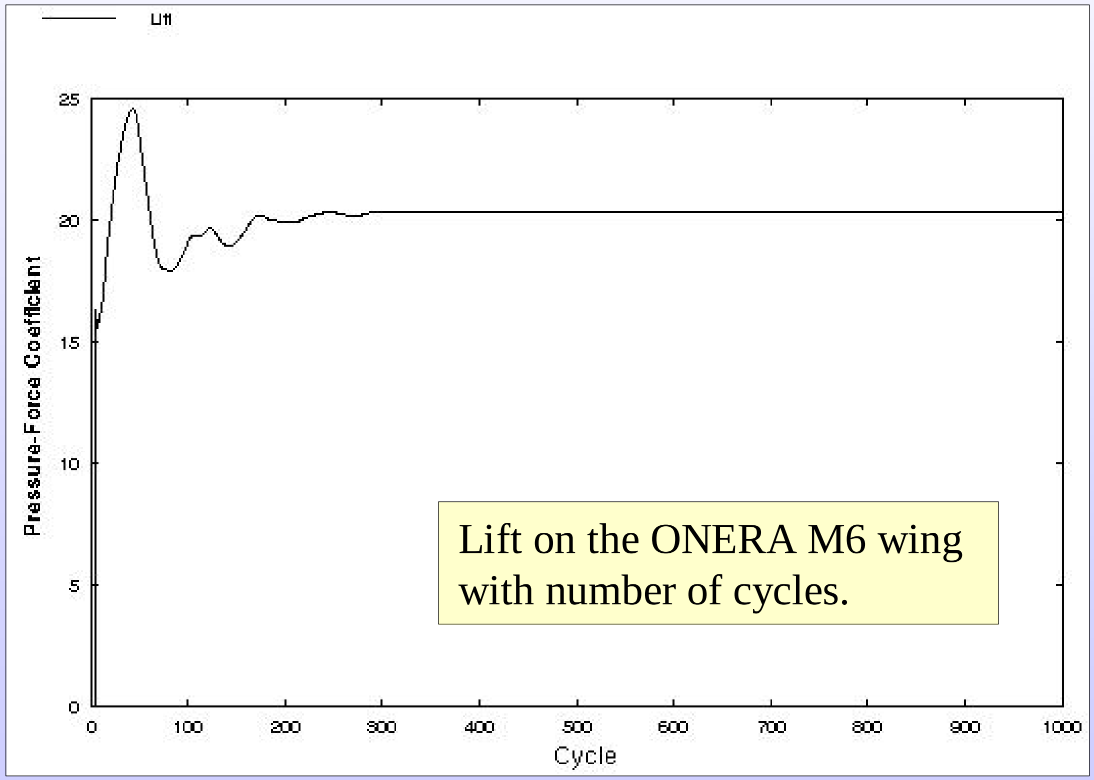
The change in a local or global property is perhaps the best measure of iterative convergence since it typically directly monitors the quantity that is important for the engineering analysis.

Local quantity is point value. Global quantity is integrated over a portion of the flow field.

Examples include:

- Lift on a wing
- Drag on a wing
- Inlet recovery
- Heat flux

Global quantities usually show a smooth convergence.



Lift on the ONERA M6 wing with number of cycles.

Grid Convergence Study

Quantifies:

1. "*ordered*" discretization error band (related to grid size by order ***p***)
2. ***p***, order of grid convergence (order-of-accuracy)
3. continuum or "zero grid spacing'' value of observed quantity

Approach:

- Assumed or demonstrated that all other error terms are negligible, minimized, accepted, or under control.
- Perform CFD solution on two or more grids of increased refinement.
- Solutions must be in the "asymptotic range of convergence''.
- If three solutions, can then compute order of convergence, ***p***.
- Use Richardson extrapolation to compute continuum value.
- Compute Grid Convergence Indices (**GCI**) as discretization error band.

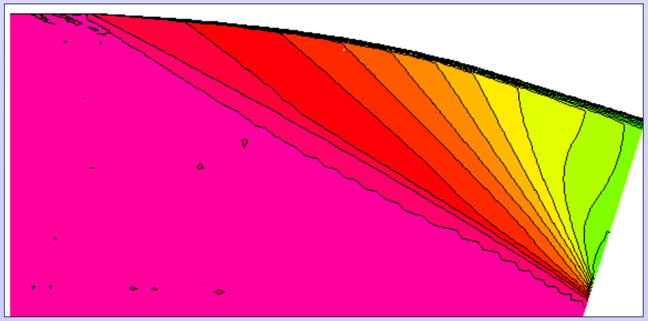
Grid Generation Considerations

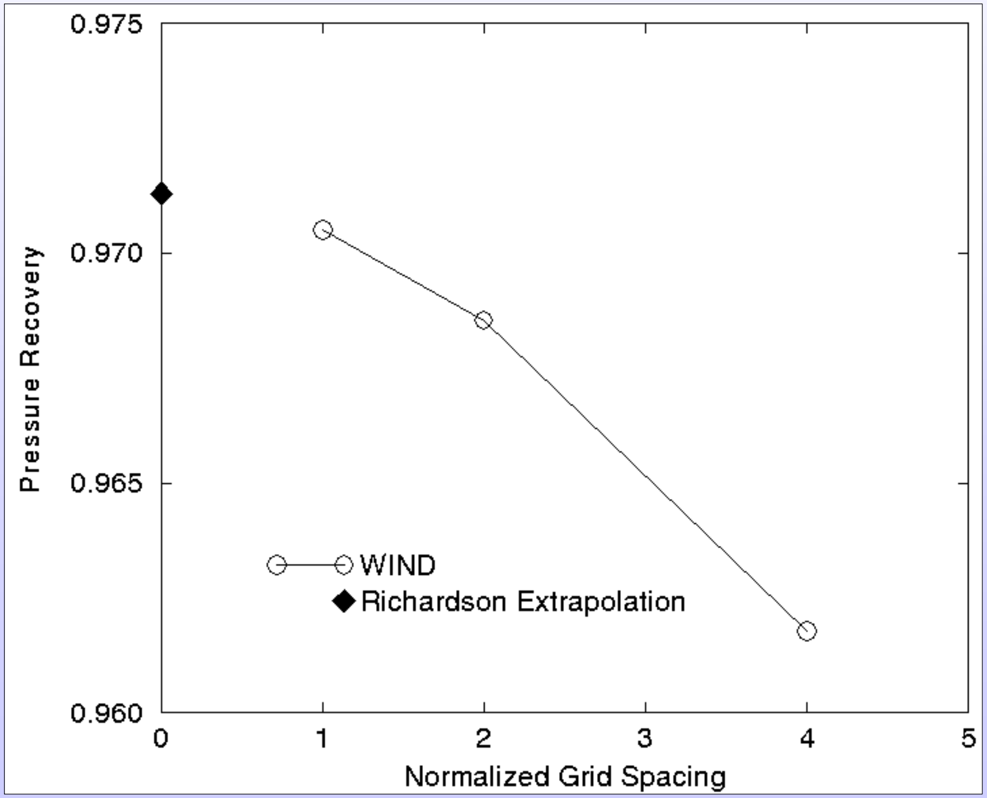
- Viscous wall spacing set for y+ < 1.0 for fine grid.
- Flow field resolution set to resolve shock system.
- Grid density to keep grid spacing ratio below 15%.
- Use ICEM CFD to construct and GRIDGEN to improve.
- Subset grid to remove some sub-layer grid points for wall function.
- Best if grid refinement ratio, $r = h_2 / h_1 = 2.0$
- h is grid spacing.
- Minimum, $r > 1.1$
- WIND allows for grid sequencing ($r = 2$).

Example: Supersonic Diffuser

- Example grid convergence study with three grids.
- Mach 2.35.
- $r = h_2 / h_1 = 2$.
- Asymptotic range observed in plot.
- Richardson extrapolation.

Grid	Normalized Grid Spacing	P_2/P_0
1	1	0.97050
2	2	0.96854
3	4	0.96178





Order of Convergence

- Order of grid convergence, *p*.
- Errors reduce as grid is refined.

$$E = f(h) - f_{exact} = Ch^{p} + H.O.T.$$

- *h* is the grid spacing.
- *C* is a constant.
- Use three values to solve for order of convergence.

$$p = \ln\left(\frac{f_3 - f_2}{f_2 - f_1}\right) \Big/ \ln(r)$$

- For this example, p = 1.786

Richardson Extrapolation

- Extrapolation of two quantities to continuum value at "zero grid spacing".
- Provides estimate of error.
- Extrapolate is of higher order.

$$f_{h=0} \cong f_1 + \frac{f_1 - f_2}{r^p - 1}$$

- For this example, $(p2/p0)_{h=0} = 0.97130$

Grid Convergence Index (GCI)

- Standardized method for reporting discretization error.
- Based on Richardson extrapolation.
- Error band on fine grid solution.
- Expressed as percentage.

$$GCI_{fine} = \frac{F_s \left|\varepsilon\right|}{\left(r^p - 1\right)} \qquad \varepsilon = \frac{f_2 - f_1}{f_1}$$

- FS is factor of safety (FS = 1.25 if three or more grids)
- For this example,
  - GCI_{12} = 0.1031% (0.0010)
  - GCI_{23} = 0.3562% (0.0035)
- "Pressure recovery is 0.971 with grid error of 0.001."

Asymptotic Range of Convergence

- Solutions are in range in which errors decrease at rate denoted by order of convergence, *p*.
- Check that constant *C* is indeed constant over solutions,

$$C = \frac{E}{h^p}$$

- Check with GCI values over three solutions,

$$GCI_{23} = r^p \, GCI_{12}$$

- For this example, ratio = 1.002

Summary: Reporting CFD Results

In summary, for a CFD analysis, report the following:

- Objective of CFD analysis
- Geometry simplifications
- Grid resolution
- Boundary and initial conditions
- Equations and physical models
- Algorithm settings
- Iterative convergence criteria
- Grid convergence criteria
- Results (values, plots, visualizations)
- Errors that can be quantified
- Sensitivity to models and parameters (turbulence, chemistry)

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Further Information on CFD

A sample of books and resources for learning more on CFD:

Anderson, D.A., Tannehill, J.C., and Pletcher, R.H., Computational Fluid Mechanics and Heat Transfer, McGraw-Hill, 1984.

Anderson, J.D., Computational Fluid Dynamics, McGraw-Hill, 1995.

Hirsch, C., Numerical Computation of Internal and External Flows (2 Volumes), John Wiley & Sons, 1988 & 1990.

Hoffmann, K.A. and S.T. Chiang, Computational Fluid Dynamics (3 Volumes), EES Books, 2000. (also AIAA coarse).

Wilcox, D.C., Turbulence Modeling for CFD, DCW Industries, 1998.

AIAA Courses (CFD, Turbulence)

Grid Generation training (ICEM, Pointwise, VGRID)