PROTECTION AGAINST MODELING AND SIMULATION UNCERTAINTIES IN DESIGN OPTIMIZATION

NSF GRANT DMI-9979711

Bernard Grossman, William H. Mason, Layne T. Watson, Serhat Hosder, and Hongman Kim
Virginia Polytechnic Institute and State University
Blacksburg, VA

Raphael T. Haftka
University of Florida
Gainesville, FL

Life-Cycle Engineering Program Meeting and Review
24-25 September 2002
Albuquerque, NM

Research Performed Under the Project

- Detection and Repair of Poorly Converged Optimization Runs
- Statistical Modeling of Structural Optimization Errors due to Incomplete Convergence
- Computational Fluid Dynamics (CFD) Simulation Uncertainties

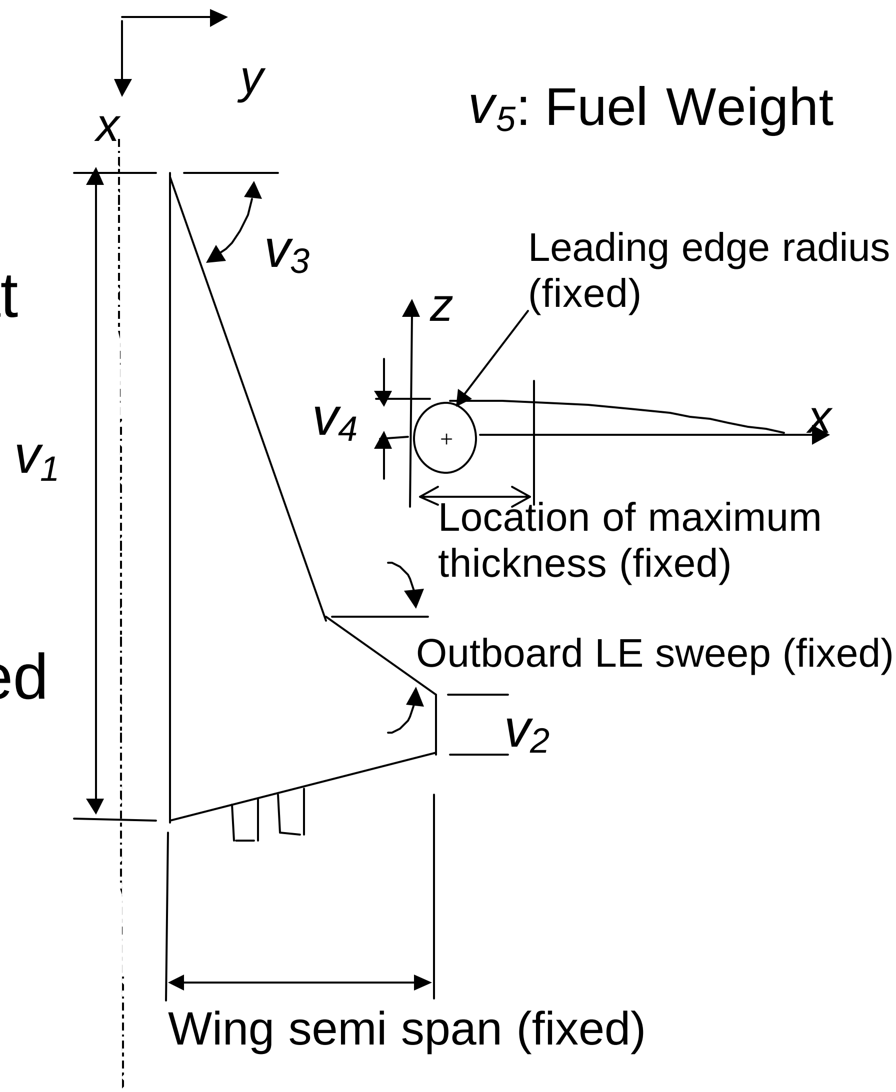
Statistical Modeling of Optimization Errors

Objective

- Estimate error level of the optimization procedure
  - Identify probabilistic distribution model of the optimization error
  - Estimate mean and standard deviation of errors **without expensive, accurate runs**

Test problem: High Speed Civil Transport (HSCT)

- 250 passenger aircraft, 5500 nm range, cruise at Mach 2.4
- Minimize take off gross weight (W_{TOGW})
- For this study, a simplified 5DV version is used



Structural Optimization and Modeling of Error

- Structural optimization performed *a priori* for many aircraft configurations to obtain optimum Wing Structural Weight (W_s)
- **Multiple optimization results** to construct response surface
- With multiple optimization results available, statistical techniques can be used to model the convergence error:

$$Error = W_s - \underbrace{(W_s)_t}_{\text{From high fidelity optimization}}$$

- Probabilistic model

  Error fit (expensive approach)
- Weibull Distribution

Previous Results

- **Weibull Distribution** models the convergence error of the optimization runs successfully
- **Difference fit** used to estimate the mean and standard deviation of errors **without expensive, high fidelity runs**

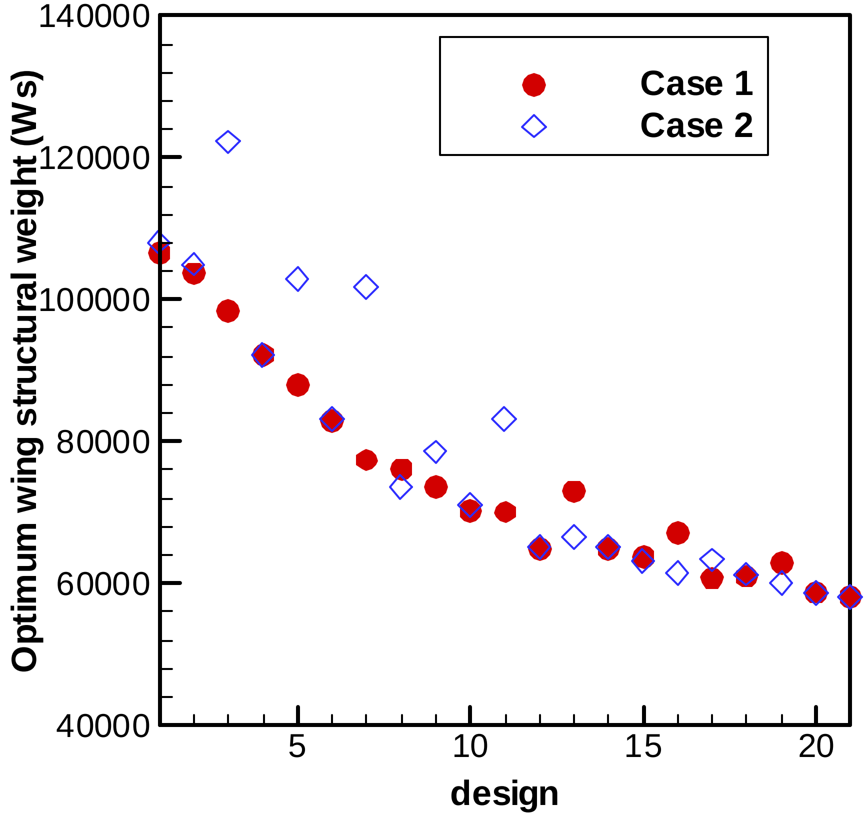
Multiple sets of low fidelity optimization results required for Difference Fit

Changing convergence criteria (previous results)

Changing initial design points (current results)

Change of the Initial Design Point

	Case 1	Case 2
Average error in W_s	5.51%	5.34%



- For Case 2, the initial design points perturbed from that of Case 1, by random factors between 0.1 ~ 1.9
- High fidelity runs used in error calculations
- In average, Case 2 has the same level of error as Case 1

Difference fit to estimate statistics of optimization errors

Errors of two optimization runs of different initial design point

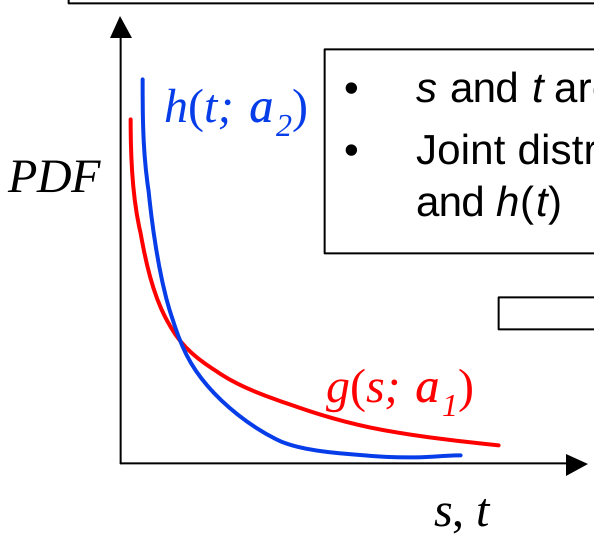
$s = W_1 - W_t$

$t = W_2 - W_t$, (W_t: unknown true optimum, **<u>expensive to calculate</u>**)

The difference of s and t is equal to $W_1 - W_2$

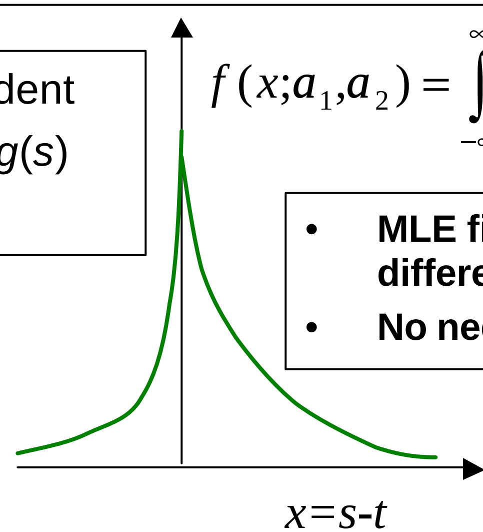
$x = s - t = (W_1 - W_t) - (W_2 - W_t) = W_1 - W_2$

We can fit distribution to x instead of s or t.



- s and t are independent
- Joint distribution of $g(s)$ and $h(t)$

$$f(x; a_1, a_2) = \int_{-\infty}^{\infty} g(s) h(s - x) ds$$



- **MLE fit for optimization difference x using $f(x)$**
- **No need to estimate W_t**

Estimated distribution parameters

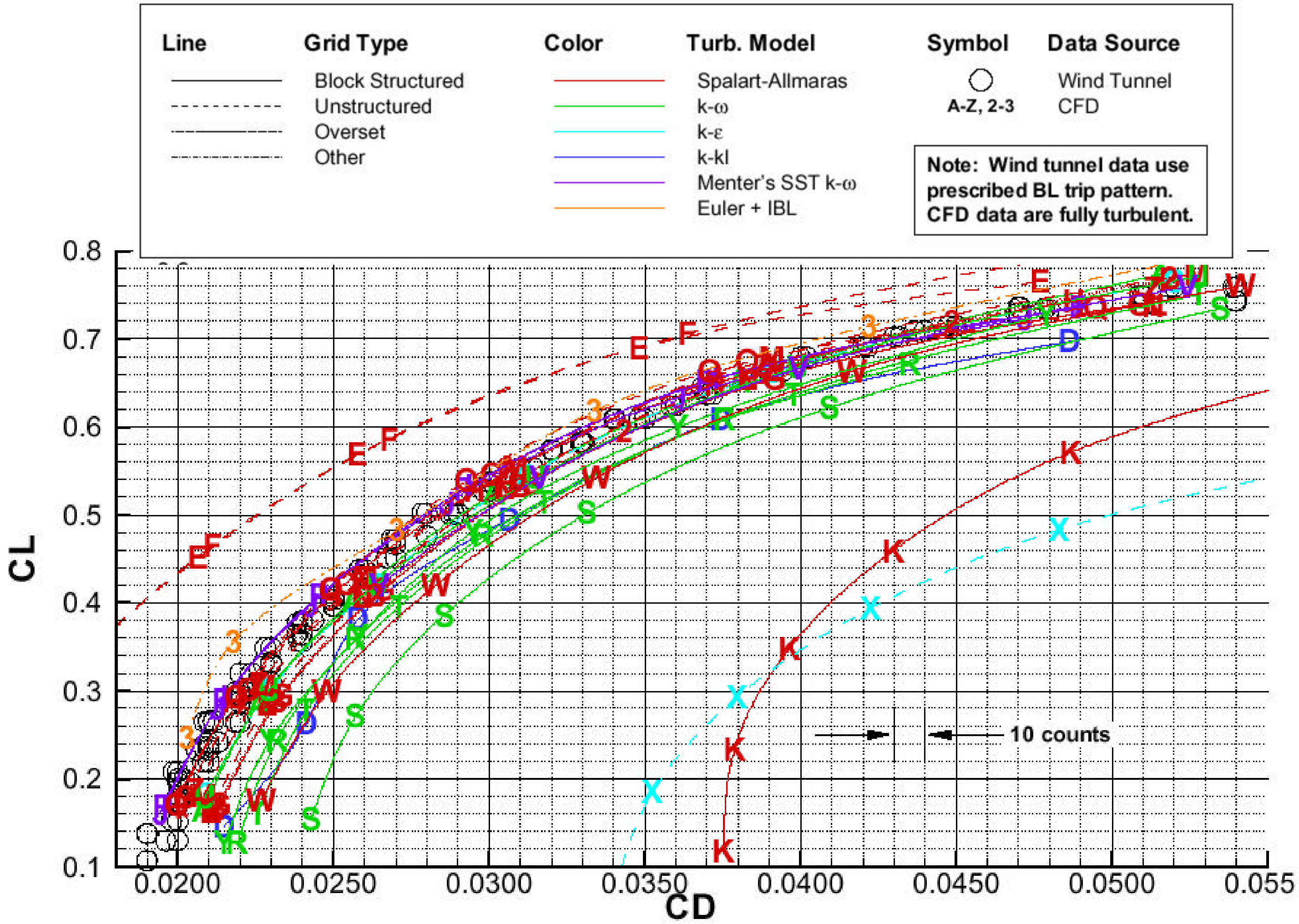
Cases		Case 1	Case 2
Average of Abs(W_1-W_2)		5941	
Estimate of mean, *lb*.	From data	4458	4321
	Error fit (discrepancy)	4207 (-5.63%)	3952 (-8.54%)
	Difference fit (discrepancy)	3804 (-14.7%)	3481 (-19.4%)
Estimate of STD, *lb*.	From data	8383	9799
	Error fit (discrepancy)	7157 (-14.6%)	7505 (-23.4%)
	Difference fit (discrepancy)	9393 (12.0%)	9868 (0.704%)
p-value of χ^2 test		0.5494	

Conclusions for Statistical Modeling of Optimization Errors

- Multiple simulation results enable statistical techniques to estimate the uncertainty level of the simulation error
- “Weibull distribution” successfully used to model the convergence error of the optimization runs
- Multiple starting points used to construct two sets of low fidelity optimizations
- “Difference fit” allowed the estimation of average errors without performing high fidelity optimizations

CFD Uncertainties

Motivation



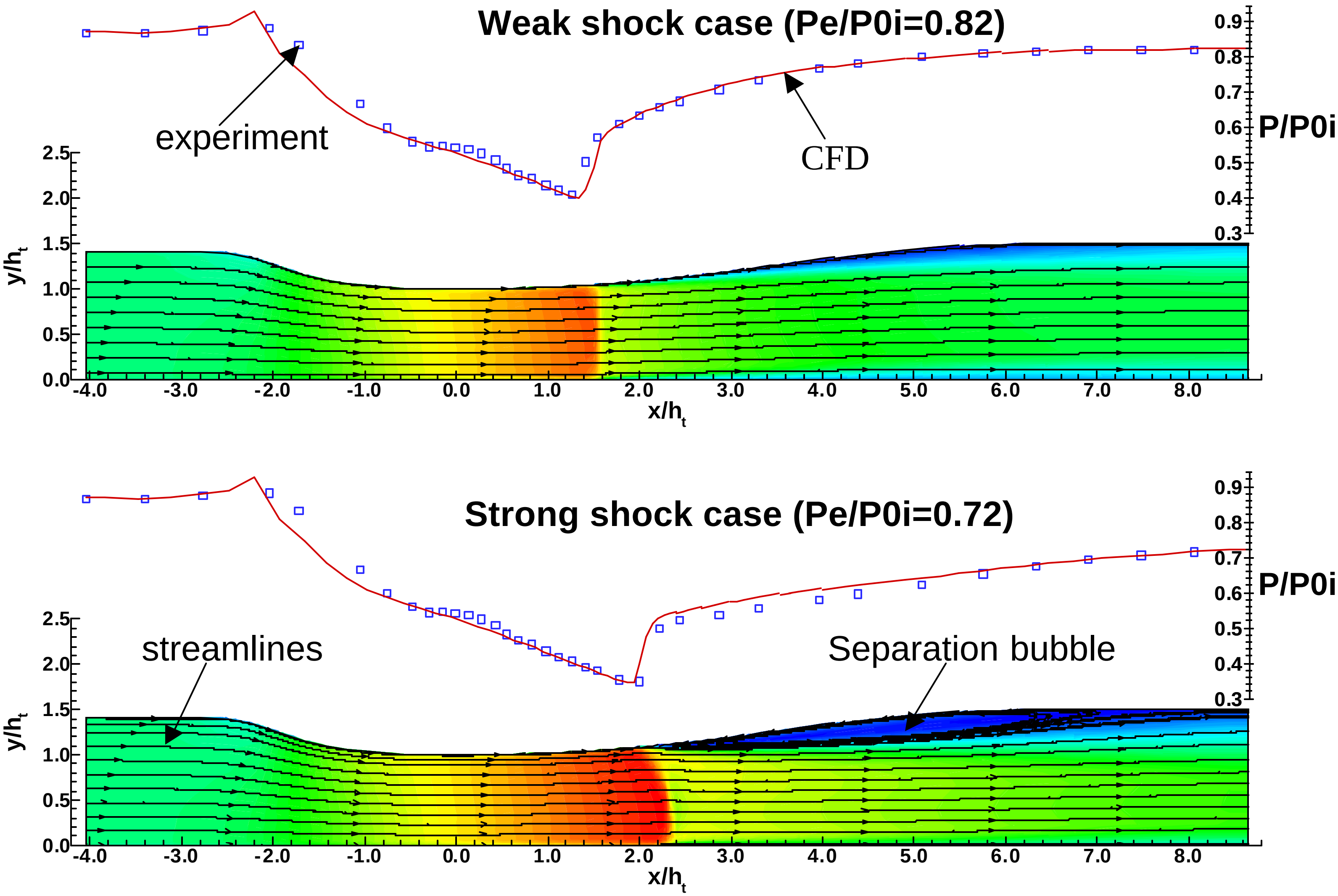
Drag polar results from 1st AIAA Drag Prediction Workshop (Hemsch, 2001)

Objective

- **Finding the magnitude of CFD simulation uncertainties that a well informed user may encounter and analyzing their sources**

- We study 2-D, turbulent, transonic flow in a converging-diverging channel
  - complex fluid dynamics problem
  - affordable for making multiple runs
  - known as “Sajben Transonic Diffuser” in CFD validation studies

Transonic Diffuser Problem



Contour variable: velocity magnitude

Uncertainty Sources (following *Oberkampf and Blottner*)

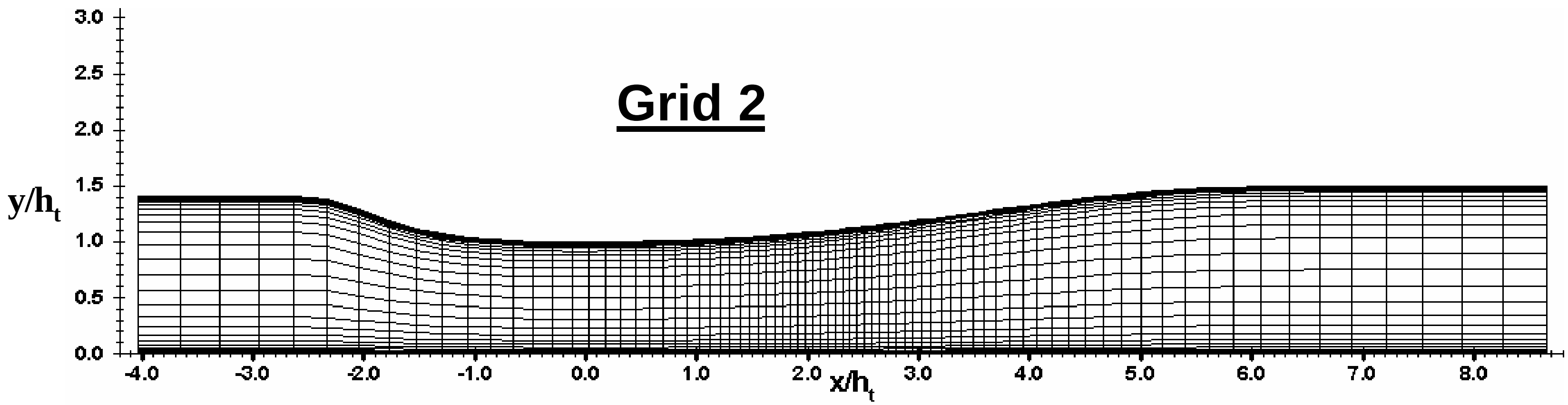
- **Physical Modeling Uncertainty**
  - PDEs describing the flow
    - Euler, Thin-Layer N-S, Full N-S, etc.
  - ***boundary conditions*** and initial conditions
  - ***geometry representation***
  - auxiliary physical models
    - ***turbulence models***, thermodynamic models, etc.
- **Discretization Error**
- Iterative Convergence Error
- Programming Errors

We show that uncertainties from different sources interact

Computational Modeling

- General Aerodynamic Simulation Program (GASP)
  - A commercial, Reynolds-averaged, 3-D, finite volume Navier-Stokes (N-S) code
  - Has different solution and modeling options. An informed CFD user still "uncertain" about which one to choose
- For inviscid fluxes (commonly used options in CFD)
  - Upwind-biased 3rd order accurate Roe-Flux scheme
  - Flux-limiters: Min-Mod and Van Albada
- Turbulence models (typical for turbulent flows)
  - Spalart-Allmaras (Sp-Al)
  - k-ω (Wilcox, 1998 version) with Sarkar's compressibility correction

Grids Used in the Computations

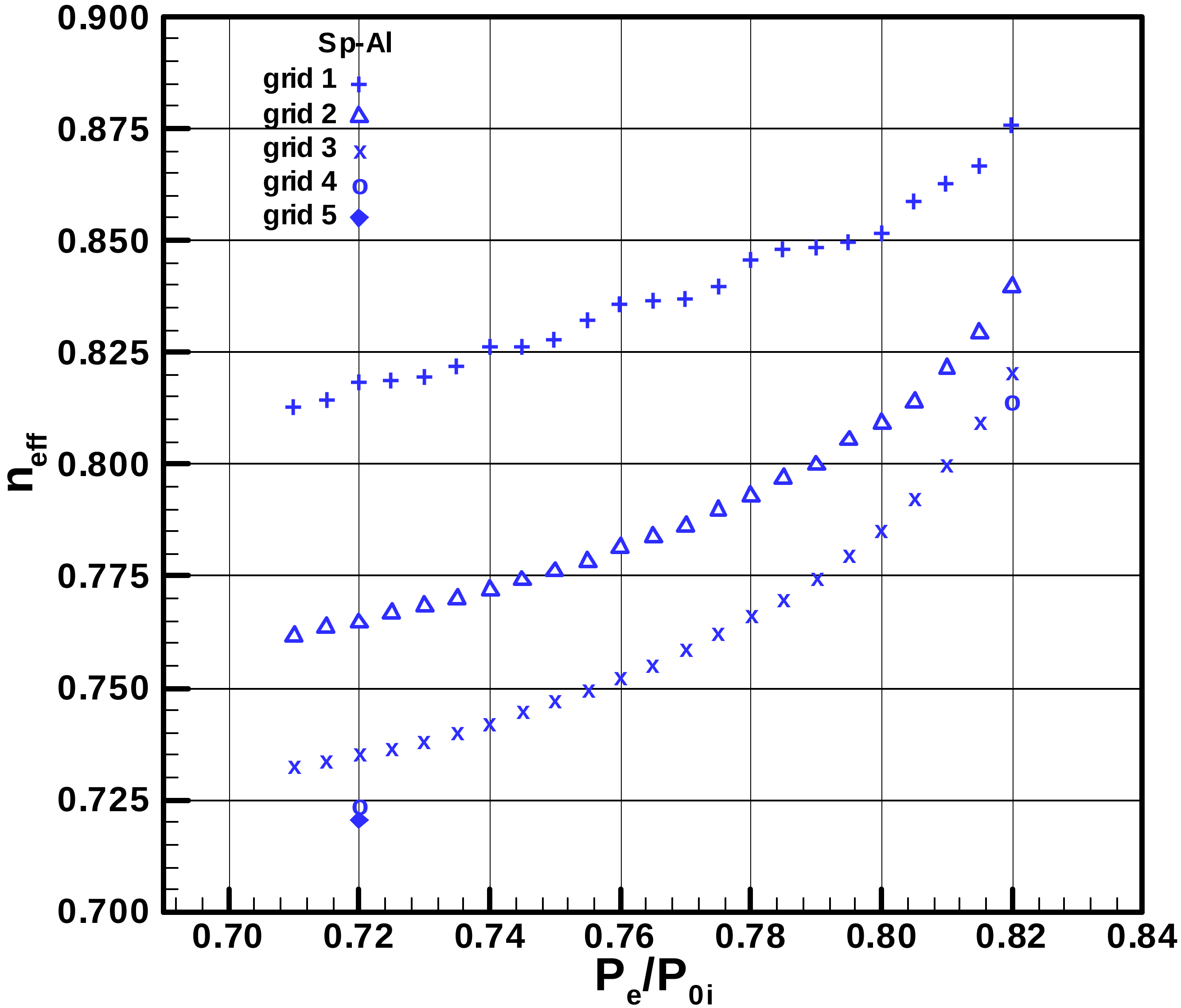


Grid level	Mesh Size (number of cells)
1	40 x 25
2	80 x 50
3	160 x 100
4	320 x 200
5	640 x 400

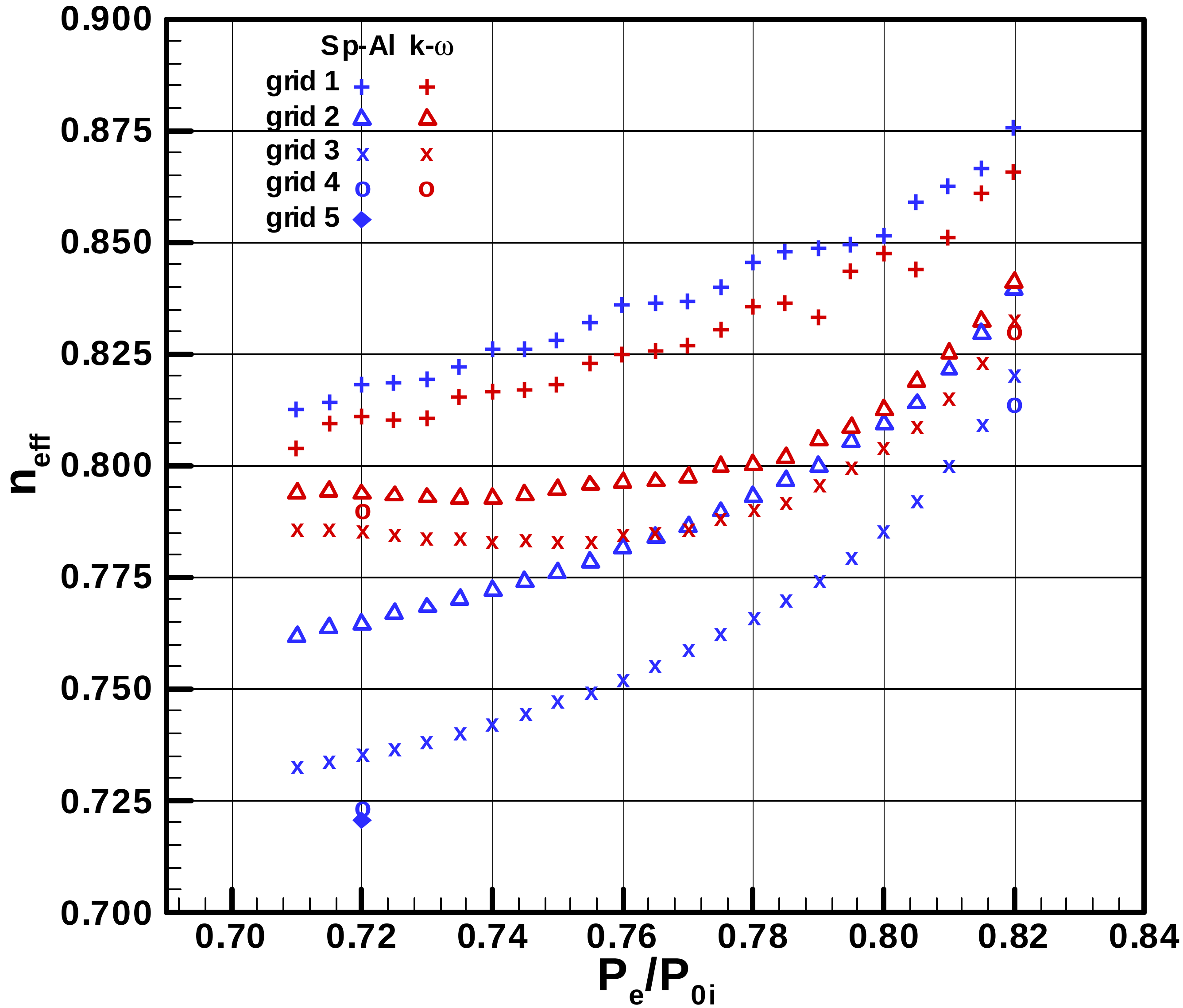
A single solution on grid 5 requires approximately 1170 hours of total node CPU time on a SGI Origin2000 with six processors (10000 cycles)

Grid 2 is the typical grid level used in CFD applications

Uncertainty in Nozzle Efficiency



Uncertainty in Nozzle Efficiency



Discretization Error by Richardson's Extrapolation

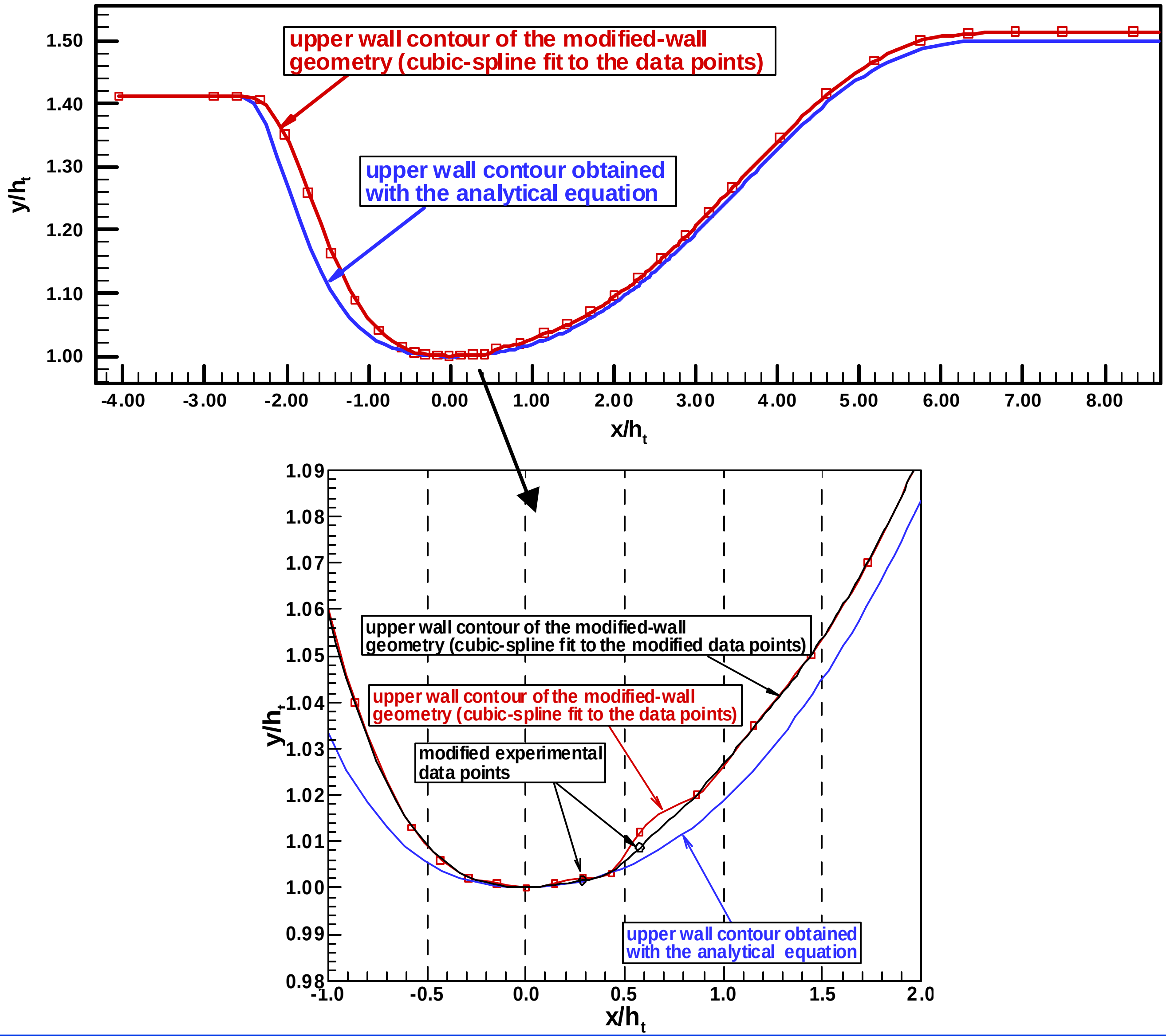
error coefficient ← a; order of the method → p

$$f_k = f_{exact} + a\,h^p + O(h^{p+1})$$

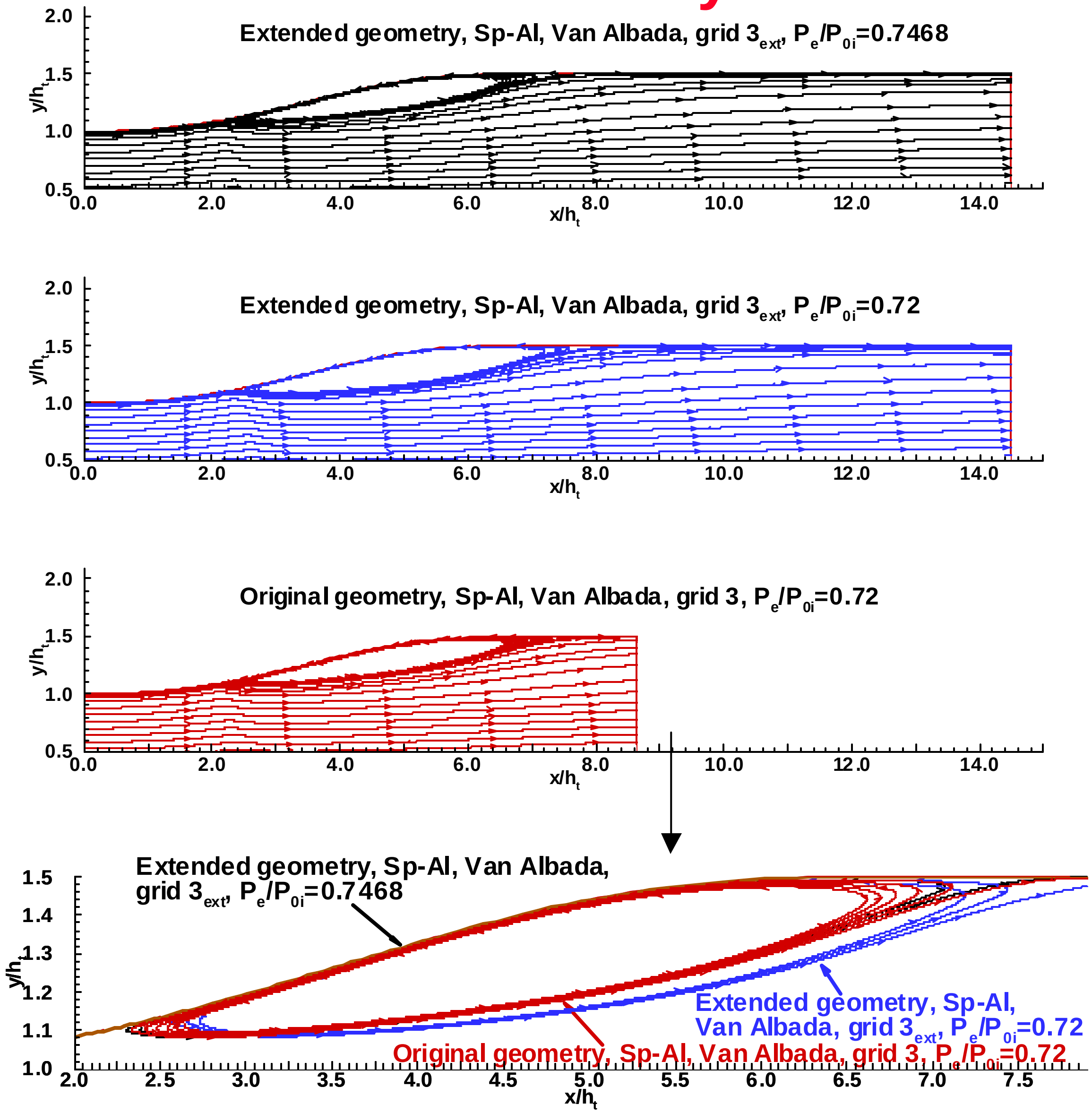
grid level ← k; a measure of grid spacing → h

Turbulence model	Pe/P0i	estimate of p (observed order of accuracy)	estimate of $(n_{eff})_{exact}$	Grid level	Discretization error (%)
Sp-Al	0.72 (strong shock)	1.32	0.720	1	14.30
				2	6.79
				3	2.72
				4	1.09
Sp-Al	0.82 (weak shock)	1.58	0.811	1	8.00
				2	3.54
				3	1.12
				4	0.40
k- ω	0.82 (weak shock)	1.66	0.829	1	4.43
				2	1.45
				3	0.46
				4	0.15

Error in Geometry Representation



Downstream Boundary Condition



Uncertainty Comparison in Nozzle Efficiency

Maximum value of	Strong Shock	Weak Shock
the total variation in nozzle efficiency	10%	4%
the difference between grid level 2 and grid level 4	6% (Sp-Al)	3.5% (Sp-Al)
the relative uncertainty due to the selection of turbulence model	9% (grid 4)	2% (grid 2)
the uncertainty due to the error in geometry representation	0.5% (grid 3, k-ω)	1.4% (grid 3, k-ω)
the uncertainty due to the change in exit boundary location	0.8% (grid 3, Sp-Al)	1.1% (grid 2, Sp-Al)

Conclusions for CFD Uncertainties

- Based on the results obtained from this study,
    - Informed users may get large errors for the cases with strong shocks and substantial separation
- Systematic uncertainty (discretization error and turbulence models) large compared to numerical noise
- Grid convergence not achieved with grid levels that have moderate mesh sizes
- Uncertainties from different sources interact, especially in the simulation of flows with separation
- We should asses the contribution of CFD uncertainties to design problems that include the simulation of complex flows

Publications

1. Hosder, S., Grossman, B., Haftka, R. T., Mason, W. H., and Watson, L. T., “Observations on CFD Simulation Uncertainties,” Proceedings of the 9th AIAA/ISSMO Symposium on Multidisciplinary Analysis and Optimization, Paper No. AIAA-2002-5531, Atlanta, GA, Sept. 2002.
2. Kim, H., Papila M., Haftka, R. T., Mason, W. H., Watson, L. T., and Grossman, B., “Estimating Optimization Error Statistics via Optimization Runs From Multiple Starting Points,” Proceedings of the 9th AIAA/ISSMO Symposium on Multidisciplinary Analysis and Optimization, Paper No. AIAA-2002-5576, Atlanta, GA, Sept. 2002.
3. Kim, H., Mason, W. H., Watson, L. T., Grossman, B., Papila, M., and Haftka, R. T., "Protection Against Modeling and Uncertainties in Design Optimization," in *Modeling and Simulation-Based Life Cycle Engineering*, eds.: K. Chung, S.Saigal, S. Thynell and H. Morgan, Spon Press, London and New York, 2002, pp. 231-246.
4. Hosder, S., Watson, L. T., Grossman, B., Mason, W. H., Kim, H., Haftka, R. T., and Cox, S. E., “Polynomial Response Surface Approximations for the Multidisciplinary Design Optimization of a High Speed Civil Transport,” *Optimization and Engineering*, Vol. 2, No. 4, December 2001, pp.431-452.
5. Kim, H., Papila M., Mason, W. H., Haftka, R. T., Watson, L. T., and Grossman, B., “Detection and Repair of Poorly Converged Optimization Runs,” *AIAA Journal*, Vol. 39, No. 12, 2001, pp. 2242-2249.
6. Kim H., “Statistical Modeling of Simulation Errors and Their Reduction via Response Surface Techniques,” Ph.D Dissertation, Virginia Tech., July 2001.
7. Kim, H., Haftka, R. T., Mason, W. H., Watson, L. T., and Grossman, B., “A Study of the Statistical Description of Errors from Structural Optimization,” Proceedings of the 8th AIAA/NASA/ISSMO Symposium on Multidisciplinary Analysis and Optimization, Paper No. AIAA-2000-4840-CP, Long Beach, CA, Sept. 2000.

Publications (continued)

8. Kim, H., Papila M., Mason, W. H., Haftka, R. T., Watson, L. T., and Grossman, B., "Detection and Correction of Poorly Converged Optimizations by Iteratively Re-weighted Least Squares," Paper AIAA-2000-1525, 41st AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, Atlanta, GA, April 3-6, 2000.