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Addressing the Challenges of Simulation-Based Design Optimization

Outstanding Issues in Simulation-Based Design Optimization

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http://mdob.larc.nasa.gov

Acknowledgments

(in chronological order)

- ASCoT/FAAST (Aerospace System Concept to Test / Fast Adaptive Aerospace Tools) project
- Eric Nielsen (NASA LaRC/CMSB)
  - CFD
- Jamshid Samareh (NASA LaRC/MDOB)
  - Geometry
- Mike Park (NASA LaRC/CMSB)
  - CFD, mesh adaptation
- David Darmofal and students (MIT)
  - CFD, error estimation, mesh adaptation, convergence acceleration

Outline

- Traditional optimization setting
- Features of realistic design problems
- Some approaches for dealing with increasingly realistic design problems
- Summary of outstanding issues

Traditional Simulation-Based Optimization Problem

- **Design ≠ Nonlinear Programming!!**
- Limit discussion to the subset of the total design problem that can be represented as NLP:

$$
\begin{aligned}
\text{minimize} \quad & f(x, u(x)) \\
\text{subject to} \quad & c_E(x, u(x)) = 0 \\
& c_I(x, u(x)) \le 0 \\
& x_L \le x \le x_U
\end{aligned}
$$

Given x, a simulation computes quantities u(x) of engineering or scientific interest by solving a system of differential equations $A(x,u(x)) = 0$

- $A=0$ may represent a system of coupled PDE, with each equation an aspect of the physical system

Traditional Optimization Approach

- Do until convergence:
  1. Build local models (usually Taylor series) of the objective and constraints based on information computed directly by the high-fidelity simulation
  2. Compute a trial step by solving a subproblem based on local models
  3. Use a globalization technique (e.g., line search, trust regions) to improve optimization convergence
- End do
- Assumptions:
  – Objectives, constraints, and associated derivatives are robust and affordable

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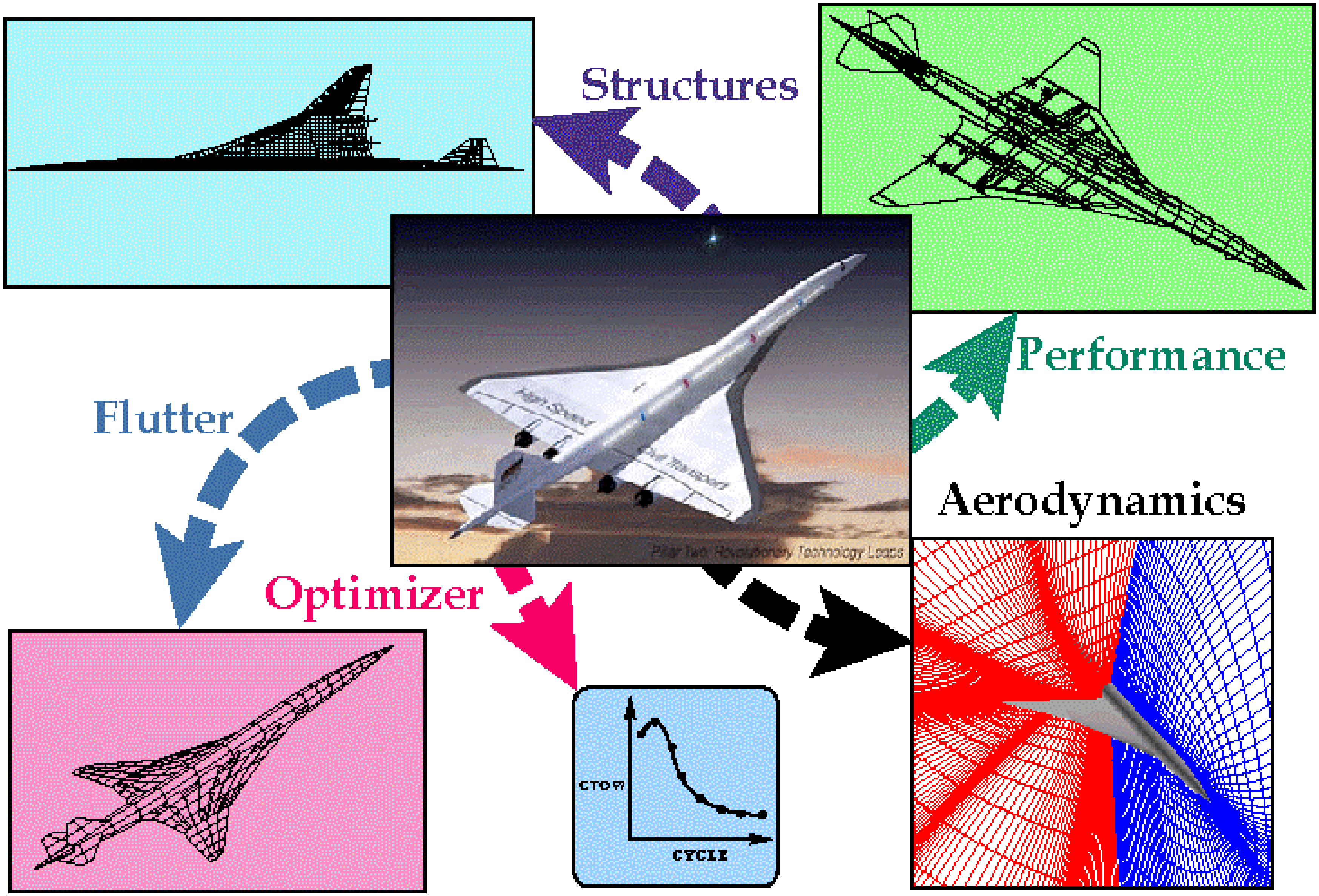
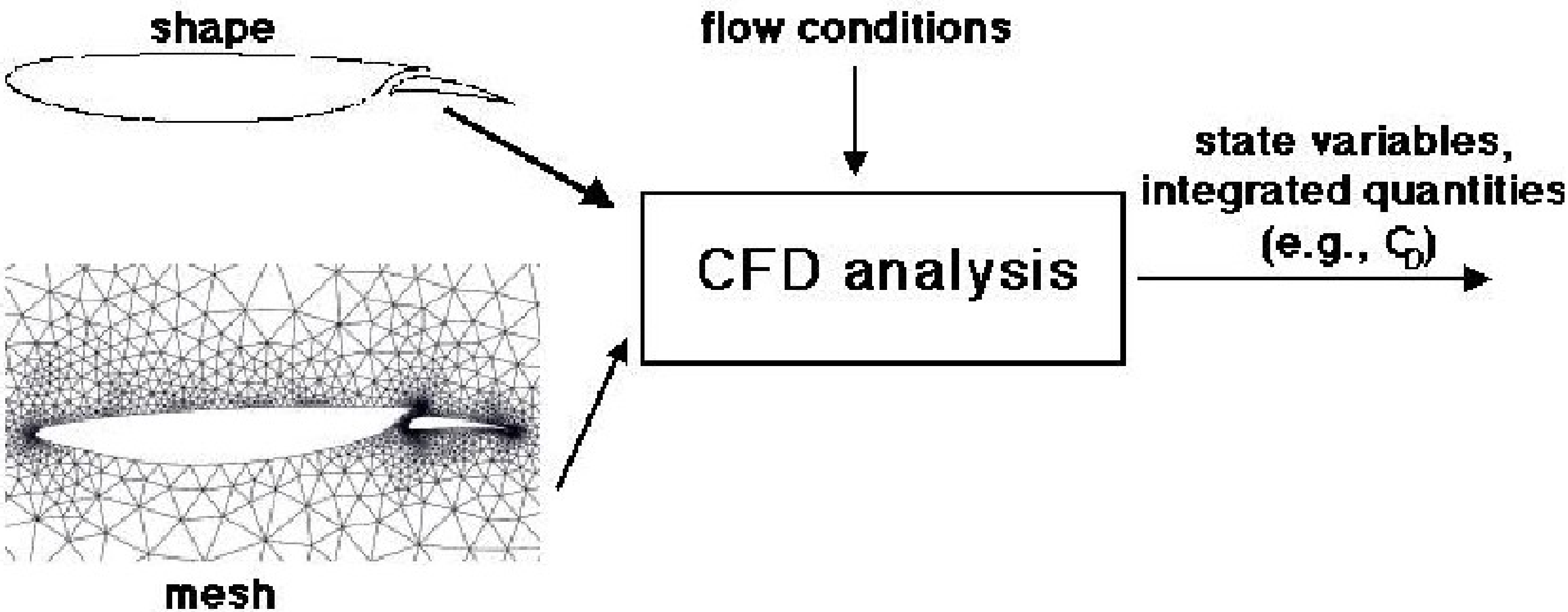
- Features of realistic design problems
  - Illustration: aerodynamic design
- Some approaches for dealing with increasingly realistic design problems
- Summary of outstanding issues

Courtesy J.A. Samareh

High-fidelity design of an aerospace vehicle



Aerodynamic Optimization



minimize Integrated quantities, such as $-\frac{L}{D}$ $\left(\frac{\text{lift}}{\text{drag}}\right)$ or C_D (drag coefficient)

subject to constraints on, e.g., pitching and rolling moment coefficients, etc.

$x_l \leq x \leq x_u$

Aerodynamic Design Optimization

- CFD-based optimization is often viewed as a success story
  - CFD used regularly for point and multi-point design
    - E.g., Boeing TRANAIR code
  - But …
  - General success for “easy” problems
  - Many challenges remain for difficult problems
    - Reliability of physical models (transition, turbulence, gas-kinetic)
    - Some problems are ill-posed (e.g., transonic flow very sensitive to changes in geometry)
    - Long turnaround time of the simulations
    - Reliably available responses (objectives and constraints) and their derivatives
    - Integration of CFD into multidisciplinary optimization

Aerodynamic Optimization: Details of Limiting Factors

- Geometry
  - Inviscid grid generation is reliable
  - Viscous grid generation of good quality and mesh movement are difficult in 3D
  - Parametrization of shapes and their derivatives is difficult to obtain in 3D
  - Good optimization codes take long steps
    - Mesh movement breaks
    - Grid generation is not automated
    - Show stopper during design

Aerodynamic Optimization: Limiting Factors, cont.

- Computing sensitivity derivatives via
  - Finite-differences
  - Automatic differentiation (e.g., ADIFOR, ADIC)
  - Hand-coded adjoints
  - Complex variables

Objective or constraint

$$\partial f/\partial x = \boxed{\partial f/\partial G_v} \; \boxed{\partial G_v/\partial G_s} \; \boxed{\partial G_s/\partial g} \; \boxed{\partial g/\partial x}$$

Sensitivity of f wrt field volume grid point coordinates; to be computed by the analysis code

Field grid point sensitivities wrt surface grid points; to be computed by grid generator

Surface grid sensitivity wrt shape vectors; to be computed by surface grid generator

Geometry sensitivity wrt design variables; to be computed by geometry modeler (CAD) tools

- **Sensitivity analyses should be incorporated in grid tools and CAD**

Aerodynamic Optimization: Limiting Factors, cont.

- Modeling
  - Analysis-based functions are expensive and prone to failure away from the nominal design
  - Difficult to obtain reliable and affordable derivatives
- Optimization
  - Algorithms for analysis-based design are in their infancy
  - Derivative-free optimization is prohibitively expensive for large problems (although becoming more practical; see, e.g., APPS, Kolda, et al., Sandia CA)

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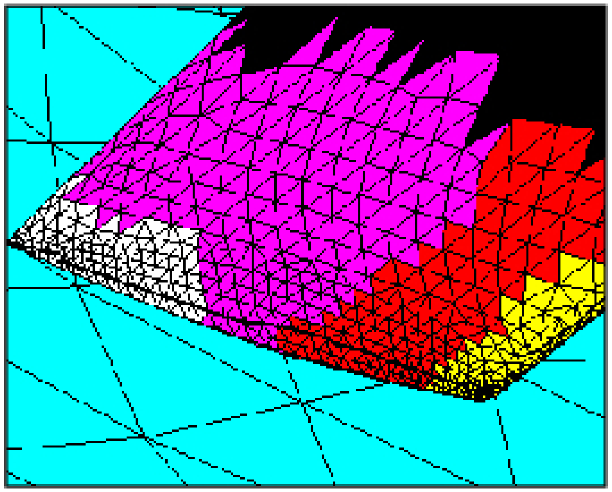
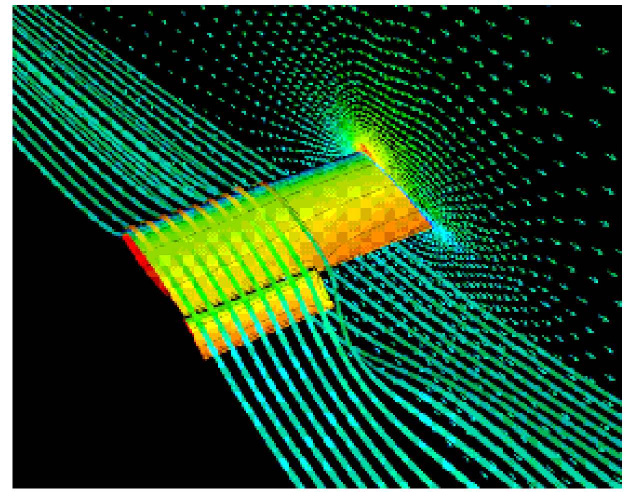
Components of Aerodynamic Design Environment

Domain Decomposition
(parallel processing)



Adjoint Solver

Flow Solvers

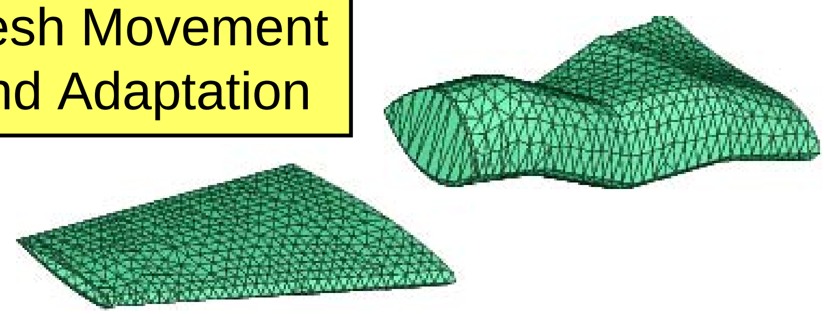


Optimization

Derivative Evaluation

Parametrization

Mesh Movement and Adaptation



Geometry/Parametrization

- Multidisciplinary Aerodynamic-Structural Shape Optimization Using Deformation (MASSOUD, Samareh, NASA LaRC)
  - Parametrizes changes in shape, not the shape itself (reduces the number of design variables)
  - Avoids manual grid re-generation
  - Uses advanced soft object animation algorithms for deforming grids
  - Analytical sensitivities are available
- GridEx – library of robust surface and volume grid generation software (Jones et al, NASA LaRC) under development
- Investigate mesh improvement techniques, e.g., mesh untangling (Freitag et al., Argonne)

Modeling

- Unstructured Navier-Stokes solvers FUN2/3D (Anderson & Nielsen, NASA LaRC)
  - Derivatives – hand-coded adjoint approach
- Adjoint methods for grid adaptation/error estimation (Darmofal & Venditti, MIT, following finite-element work of Patera & Peraire and Pierce & Giles)
  - Traditional grid adaptation relies on solution gradients; but what if the feature (e.g., shock) is in the wrong place
  - Adjoint-based adaptation avoids this problem and can be used to “tune” grids to accurately predict quantities of engineering interest, such as lift and drag
  - Can dramatically reduce the number of mesh points for a given application and produce the correct answer
  - Proof of concept in 2D; extensions to 3D in collaboration with Park (NASA LaRC)

Optimization Approaches

- Re-consider optimization problem formulation
  - Efficiency and ability to solve the problem very sensitive to problem formulation
  - Some alternatives
    - Simultaneous Analysis and Design (SAND)
      - Widely investigated (e.g., Ghattas et al.)
      - Fast, assumes the ability to manipulate simulation codes
    - Non-NLP formulations (Gurdal’s talk)
- Use of non-Taylor-series-based models
  - A variety of approximations and models available and used in engineering for a long time with heuristics
    - E.g., Variable Complexity Modeling, Reasonable Domain Approach (Va Tech group)
  - E.g., build the best possible data-fitting model (e.g., RSM) based on hi-fidelity simulations and use it for optimization

Approximation and Model Management Optimization (AMMO)

- AMMO (e.g., Alexandrov & Lewis, AIAA-96-4101/02
  - Use of engineering approximations and models
  - Provably convergent optimization techniques (trust-region globalization)
  - Can be used with any gradient-based algorithm
- Some related work
  - Sandia (Giunta's talk)
  - Data-fitting model management (0-order, Rice-Boeing group; IMB group; 1-order; Renaud et al.)

Models Amenable to AMMO

- Variable accuracy
  - Converge analyses to user-specified tolerance
- Variable resolution
  - Single physical model on meshes of varying degree of refinement
- Variable-fidelity physics
  - E.g., in CFD, physical models range from inviscid, irrotational, incompressible flow to Navier-Stokes equations for viscous flow
- Other
  - Data-fitting models, reduced-order models

Recall Traditional Optimization Setting

- Do until convergence:
  1. Build local models (usually Taylor series) of the objective and constraints based on information computed directly by the simulation
  2. Compute a trial step by solving a subproblem based on local models
  3. Check improvement in true responses
- End do

AMMO Setting

- Do until convergence:

1. Select a model from a suite of available models
2. Compute corrections based on high- and low-fidelity models
3. Compute a trial step by solving a subproblem based on corrected low-fidelity models, using standard techniques
4. Check improvement in true responses (globalization strategy)

- End do

Convergence vs. Performance

- **Convergence relies on ensuring local similarity of trends**
  - **Let $\tilde{f}$ be some lower-fidelity model of f. At each major iteration k, $\tilde{f}$ is required to satisfy**

    $$\tilde{f}(x_k) = f(x_k), \quad \nabla \tilde{f}(x_k) = \nabla f(x_k)$$

    Easily enforced when derivatives are available.

- **Enforcing first-order consistency: multiplicative β-correction,** **Haftka, 1991**
  - **Given $f(x)$ and $f_{lo}(x)$, define $\beta(x) \equiv \frac{f(x)}{f_{lo}(x)}$**
  - **Given x_k, build $\beta_k(x) = \beta(x_k) + \nabla \beta(x_k)^T (x - x_k)$**
  - **Then $\tilde{f}_k(x) = \beta_k(x) f_{lo}(x)$ satisfies the consistency conditions at x_k**

- **Practical efficiency is problem/model dependent and is influenced by the ability to transfer computational load onto low-fidelity computation; at worst, AMMO is conventional optimization.**

Managing Variable-Fidelity Physics Models: Multi-Element Airfoil

AIAA-2000-4886, Alexandrov, Nielsen, Lewis, Anderson

- A two-element airfoil designed to operate in transonic regime – inclusion of viscous effects is important
- Governing equations – time-dependent Reynolds-averaged Navier-Stokes (FUN2D)
- Conditions:
  - $M_\infty = 0.75$
  - $Re = 9 \times 10^6$
  - $\alpha = 1^o$ (global angle of attack)

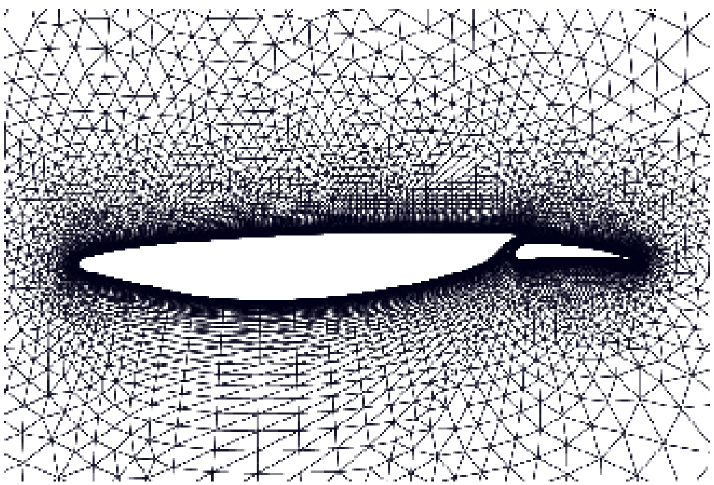
Multi-Element Airfoil, cont.

- **Hi-fi model – FUN2D analysis in RANS mode**
- **Lo-fi model – FUN2D analysis in Euler mode**
- **Computing on SGI Origin^{TM} 2000, 4 R1OK processors**

High-fidelity model

Viscous mesh:

10449 nodes and 20900 triangles



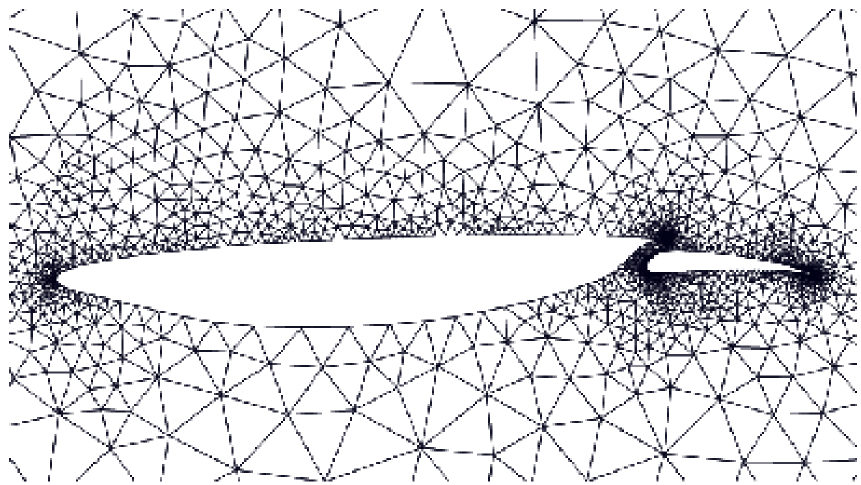
t/analysis $\approx$ 21 min

t/sensitivity $\approx$ 21 or 42 min

Low-fidelity model

Inviscid mesh:

1947 nodes and 3896 triangles

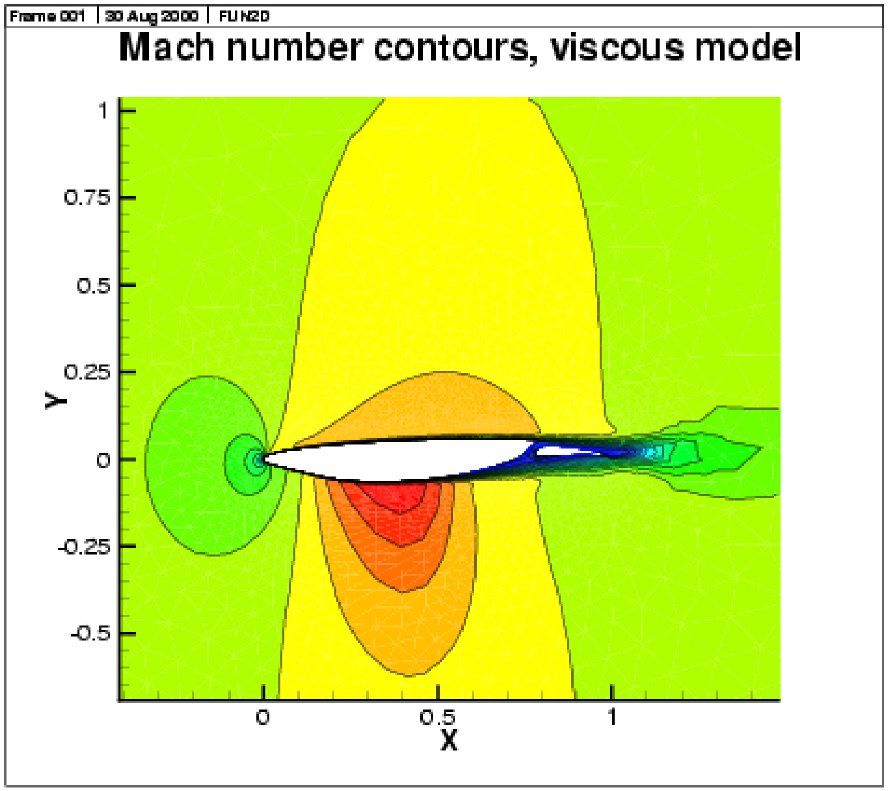


t/analysis $\approx$ 23 sec

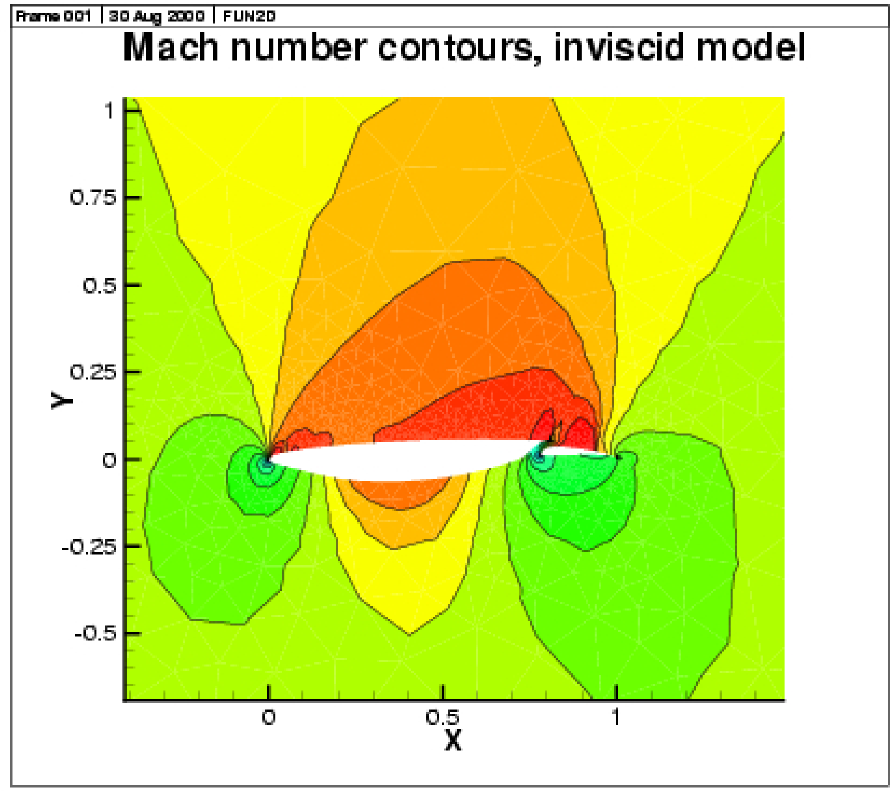
t/sensitivity $\approx$ 100 or 77 sec

Multi-Element Airfoil: Viscous Effects

High-fidelity model



Low-fidelity model



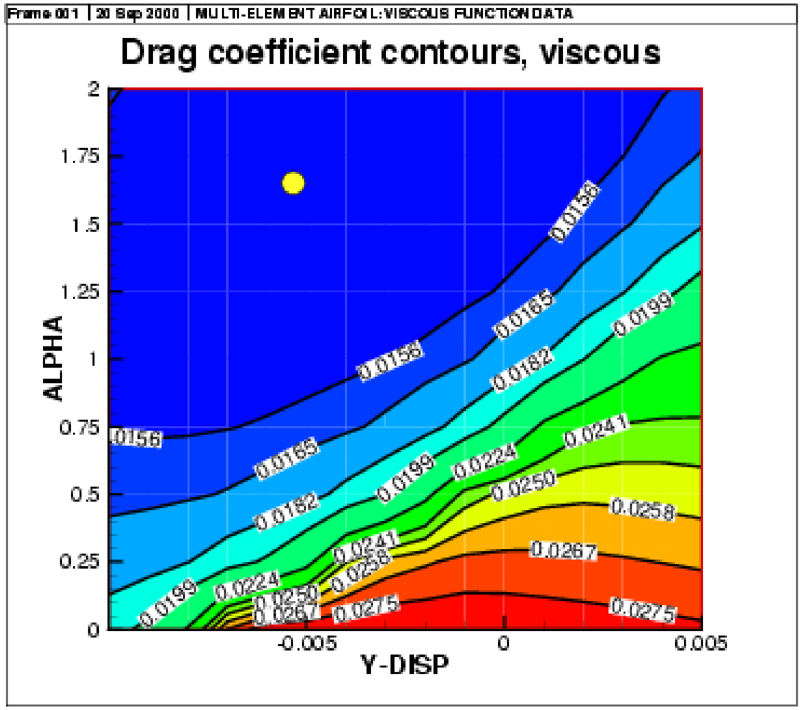
- **Boundary and shear layers are visible in the viscous case.**

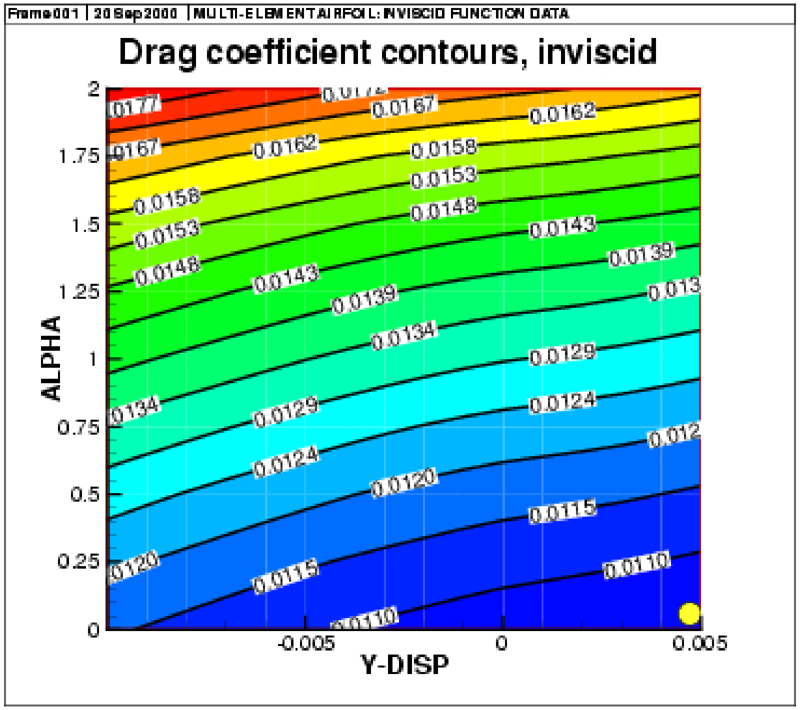
Multi-Element Airfoil: Computational Experiments

- **Objective function:** minimize drag coefficient subject to bounds on variables
- **Case 1:** (for visualization)
  - Variables: angle of attack, y-displacement of the flap
  - Solve problem with hi-fi models alone using a commercial optimization code (PORT, Bell Labs)
  - Solve the problem with AMMO, PORT used for lo-fi subproblems
- **Case 2:**
  - Variables: angle of attack, y-displacement of the flap, geometry description of the airfoil; 84 variables total
  - Same experiment

Multi-Element Airfoil: Models

- Time/function for inviscid model negligible compared to viscous model
- Descent trends are reversed — unusual but a good test

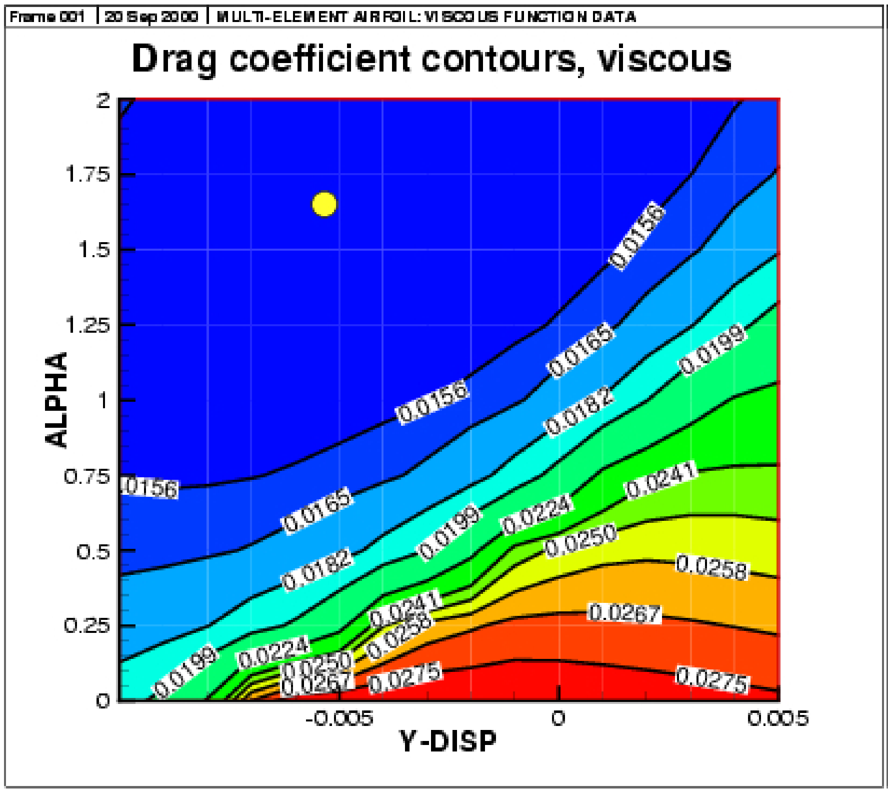


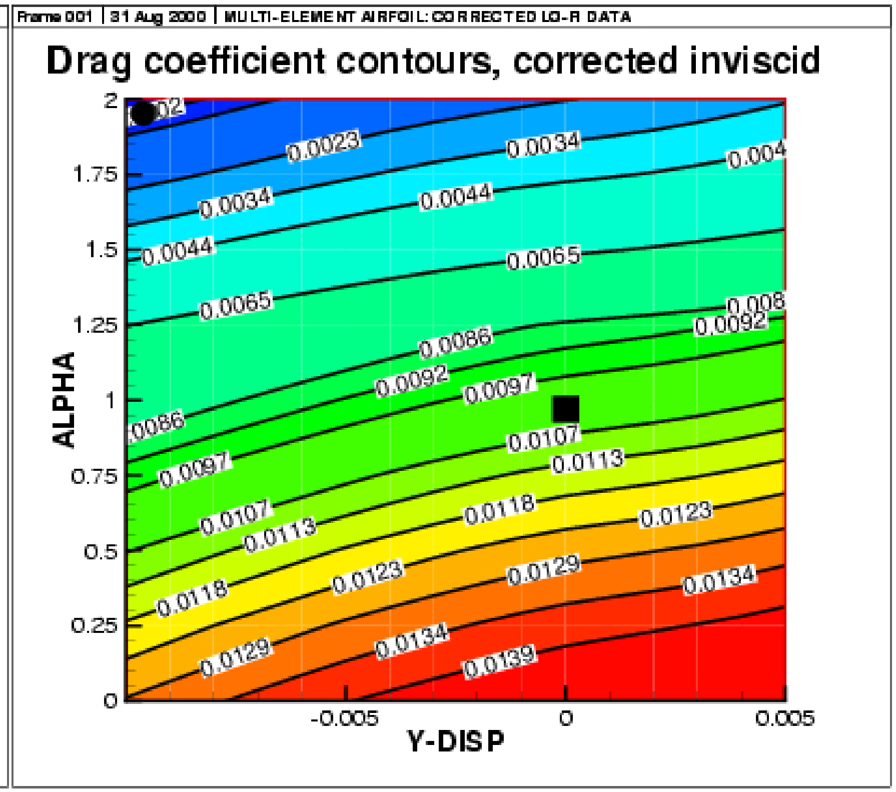


Multi-Element Airfoil: AMMO Iterations with 2 Variables

Iteration 1. Starting point: $\alpha = 1.0$, y-disp $= 0.0$

High-fidelity objective vs. corrected low-fidelity objective





New point: $\alpha = 2.0$, y-disp $= -0.01$

Multi-Element Airfoil: Performance Summary

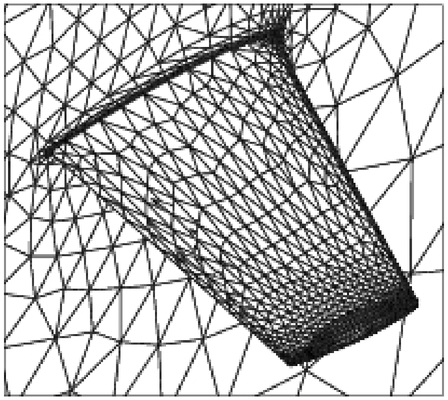
Notation: No. functions / No. Gradients

Test	hi-fi eval	lo-fi eval	total t	factor
PORT with hi-fi analyses, 2 var	14/13		$\approx$ 12 hrs	
AMMO, 2 var	3/3	19/9	$\approx$ 2.41hrs	$\approx$ 5
PORT with hi-fi analyses, 84 var	19/19		$\approx$ 35 hrs	
AMMO, 84 var	4/4	23/8	$\approx$ 7.2hrs	$\approx$ 5

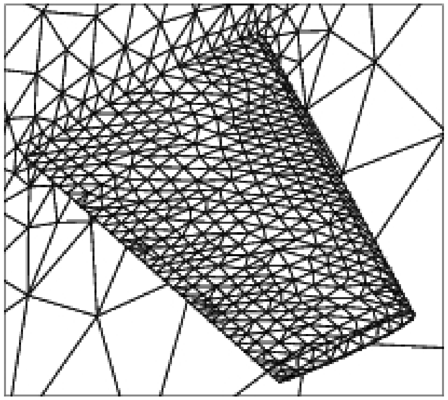
$C_D^{initial}$ = 0.0171 at α=1°, flap y-displacement=0
C_D^{final} = 0.0148 at α=1.6305°, flap y-displacement=-0.0048
a decrease of ≈ 13.45%

3D Aerodynamic Design with AMMO

Hi-fi: FUN3D N-S on a finer mesh



Lo-fi: FUN3D Euler on a coarse mesh



$$\min_x \quad 5C_D^2 + \tfrac{1}{2}(C_L - 0.12303)^2$$
$$s.t. \quad x_l \le x \le x_u$$

α_0=3.06°, M_∞=0.84, Re=5x10^6

Lift_0 = 0.12302, Drag_0 = 0.01713, Objective_0 = 0.0014670

Cost Reduction with AMMO
(No. functions / No. gradients)

Test	Hi-fi eval	Lo-fi eval	Final Lift	Final Drag	f
PORT/hi-fi	13/11		0.11146	0.01532	0.0012793
AMMO	3/3	22/15	0.10657	0.01511	0.0012796

- Factor 2 savings in terms of wall-clock time
- Area of further study – optimal termination for low-fidelity computations

Why Is This Working?

- Replaced local Taylor-series approximations with variable-fidelity physics models by assuring local consistency of models via 1st order corrections
- Why expectations of better performance than Taylor series?
  - More global behavior of the models
  - When data-fitting models are affordable, they can be used as well
- Derivative information crucial

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Outstanding Issues in Single-Discipline Optimization

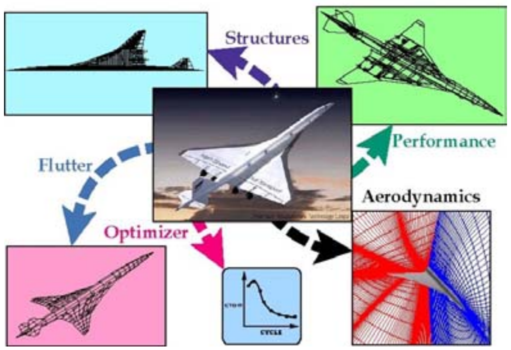
- Geometry/Grid
  - Grid generation is not automatic, is expensive, introduces discontinuities; can handle large changes in design variables
  - Deformation can handle only small changes in variables, but is faster
  - Need sensitivities built into grid/CAD tools
- Simulations
  - Need to improve confidence in analysis codes
    - Better reliability of physical models (e.g., turbulence)
    - Uncertainty quantification associated with simulation fidelity (risk associated with a choice of fidelity)
    - …

Outstanding Issues in Single-Discipline Optimization

- Optimization
  - Continue reducing cost algorithmically
  - Recover from failed evaluations
  - Advertise the need for interfaces to optimization and uncertainty-based design (requirements)
  - Investigate techniques for affordable multipoint and robust design
  - Keep designer in the loop (avoid tendencies for push-button optimization)

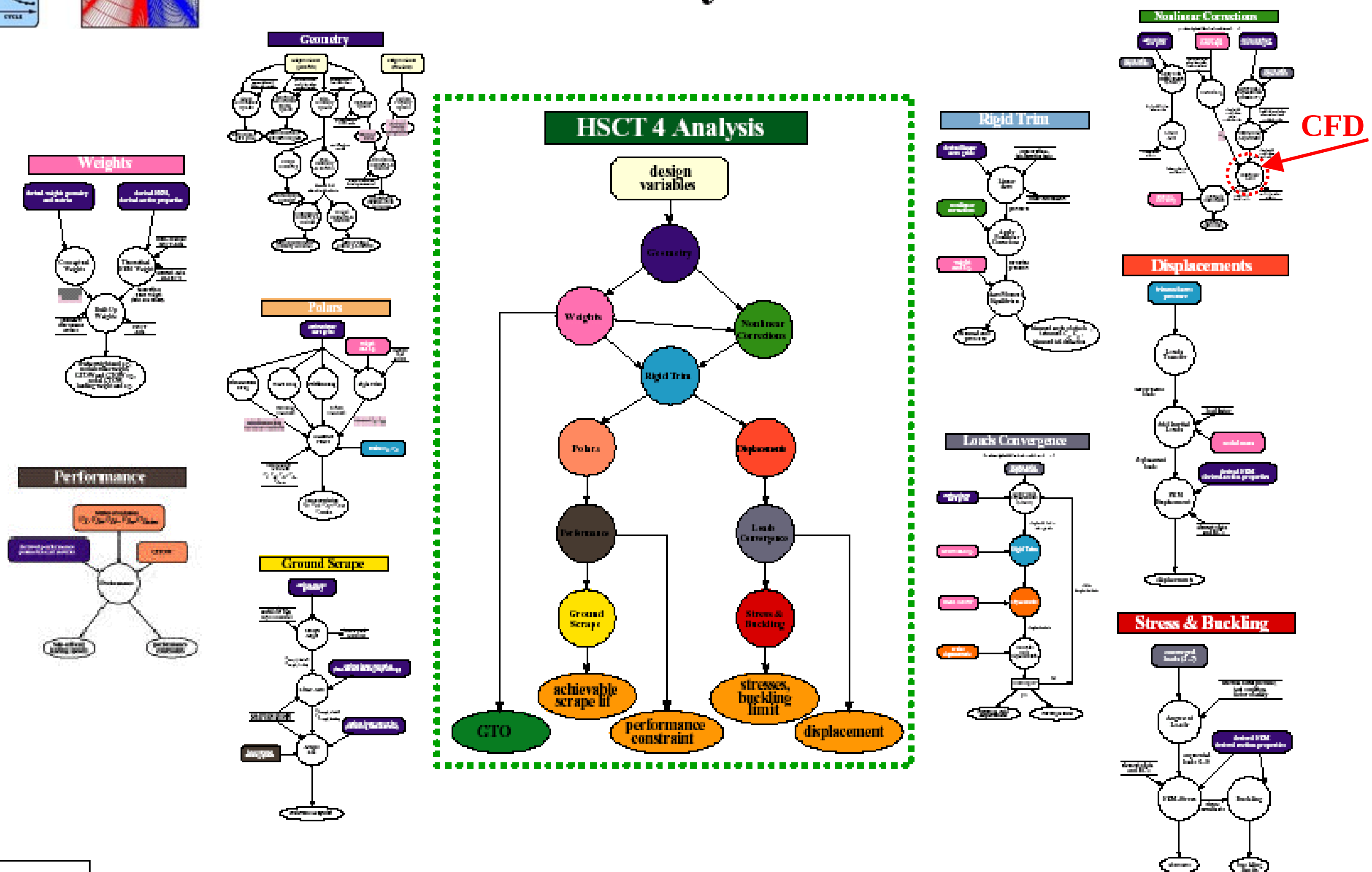
Context

- Multidisciplinary design optimization (Lewis' talk)



Small design problem extracted from

Full HSCT 4 Analysis Procedures



Courtesy J.A. Samareh

Outstanding Issues

- Integration of disciplinary simulation tools into complex environment
  - Hi-fi analyses impossible for MDO for now
  - Computational frameworks (e.g., DAKOTA (Sandia))
  - Different geometry models
  - Sensitivity information needed
- Analytical features of MDO problem formulation strongly influence the practical ability of optimization algorithms to solve the MDO problem reliably and efficiently (next talk)
- …