DR. SCULPTOR®

Webinar

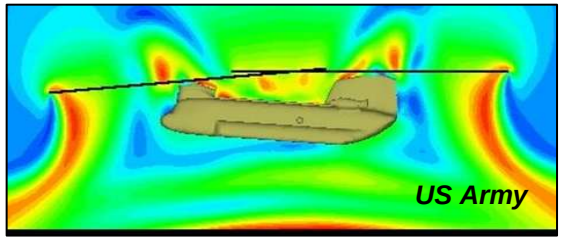
“Adjoint-Based Shape Optimization”

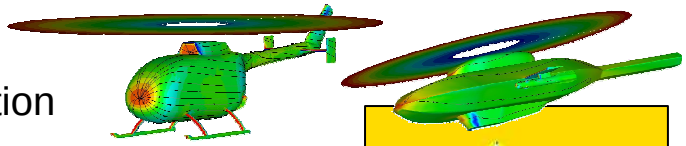
Dr. Eric Nielsen – e.j.nielsen@larc.nasa.gov
Dr. Mark Landon – mlandon@goSculptor.com
John Jenkins – jjenkins@goSculptor.com

FUN3D Core Capabilities

http://fun3d.larc.nasa.gov

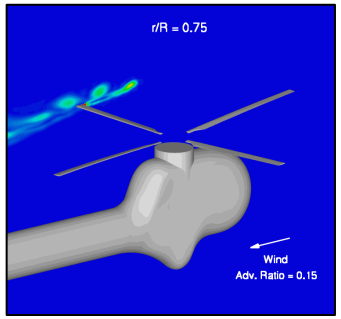
- Established as a research code in late 1980's; now supports numerous internal and external efforts across the speed range
- Solves 2D/3D steady/unsteady Euler/RANS equations on node-based mixed element grids for compressible/incompressible flows
- General dynamic mesh capability: any combination of rigid / overset / morphing grids, including 6-DOF effects
- Aeroelastic modeling using mode shapes, full FEM, CC, etc.
- Constrained / multipoint adjoint-based design and mesh adaptation
- Concurrent generation of visualization data: isosurfaces, slices, sampling surfaces, schlierens, etc.
- Distributed development team using agile/extreme software practices including 24/7 regression and performance testing
- Capabilities fully integrated, online documentation, training videos, tutorials

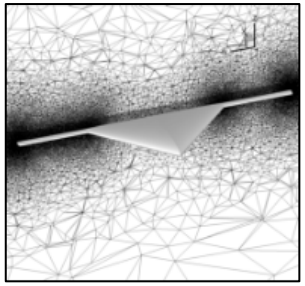




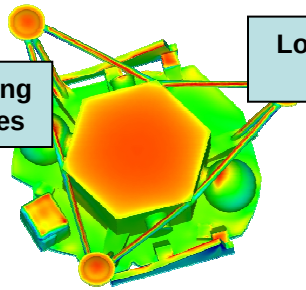
Rotorcraft

Ares

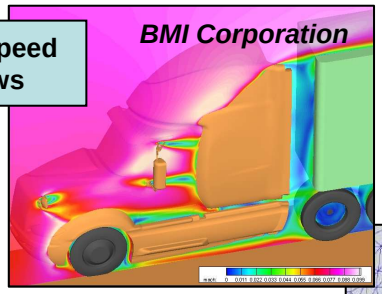




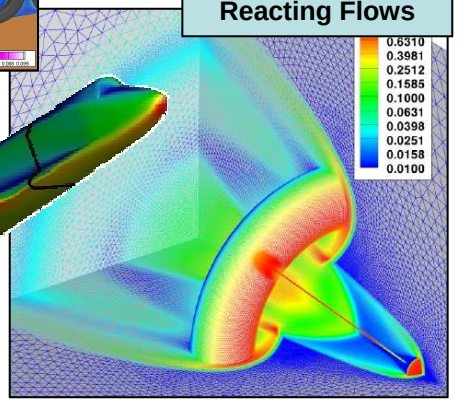
Morphing Vehicles

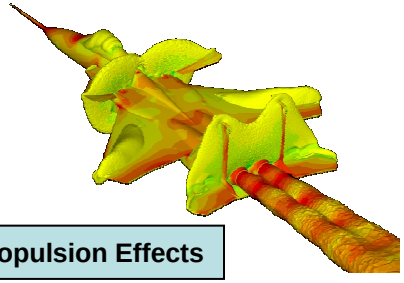


Low-Speed Flows

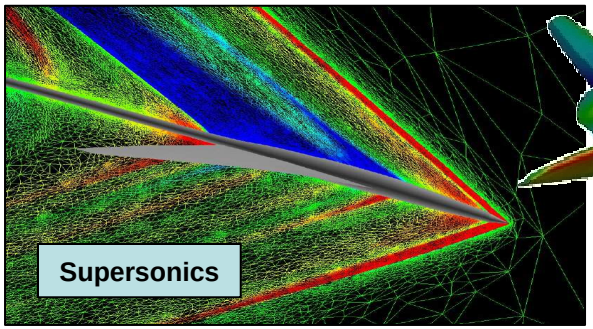


Reacting Flows



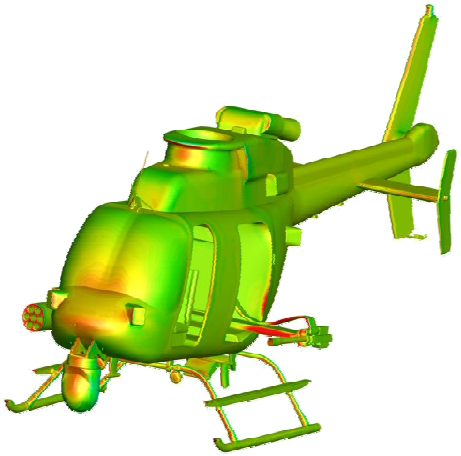


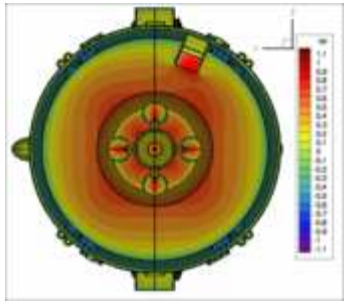
Propulsion Effects

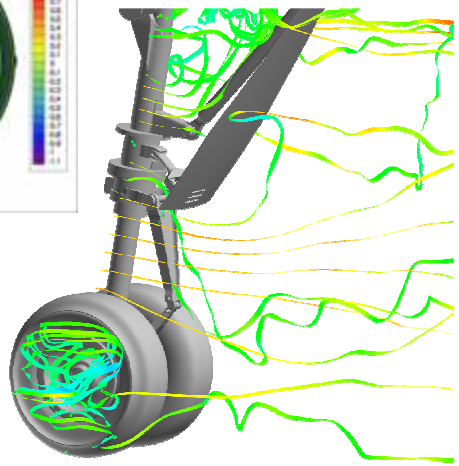


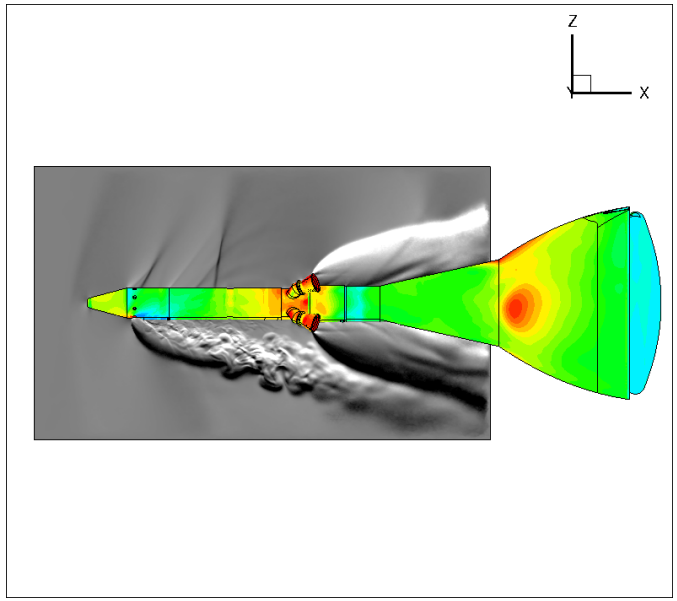
Supersonics

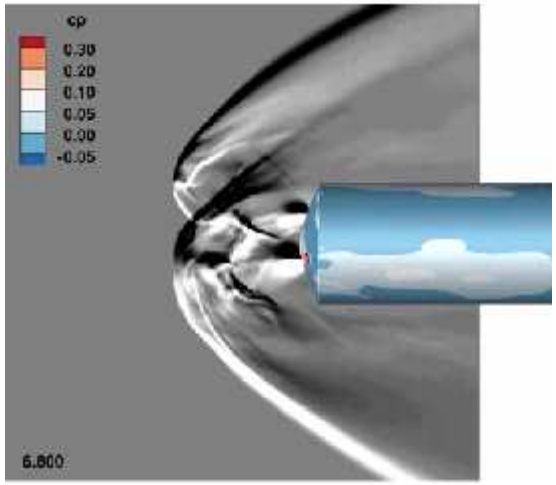
Some Recent FUN3D Applications

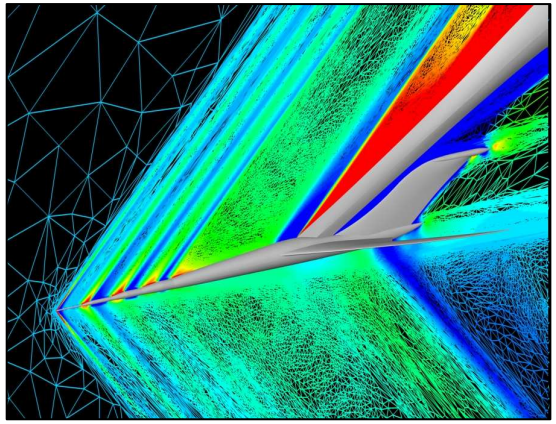


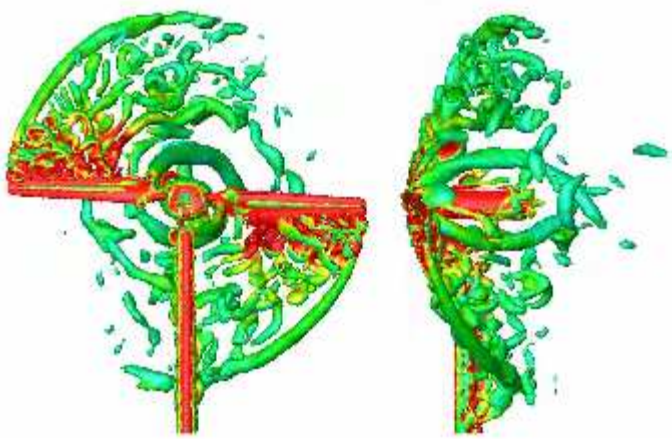


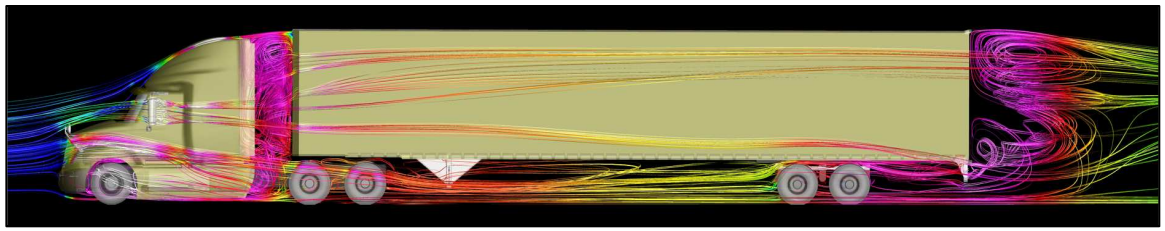












Design Optimization Using FUN3D

- Uses a gradient-based approach
- FUN3D is distributed with support for several COTS gradient-based optimization packages (user must obtain separately)
  - PORT (Bell Labs)
  - NPSOL (Stanford)
  - KSOPT (Greg Wrenn)
  - DOT/BIGDOT (Vanderplaats R&D)
  - SNOPT (Stanford) coming soon
  - Other packages generally straightforward to hook up (couple hours)
- These optimizers are based on the user supplying functions and gradients (and perhaps constraints and their gradients also)
  - Optimizers know nothing about CFD, all they see are f and ∇f
- In CFD, objective/constraint functions are generally based on things like lift, drag, pitching moment, etc.
  - But can be anything you code up, generally speaking

Some Terminology

Functions

- When the optimizer requests a function value, it requires a flow solution with inputs and a grid corresponding to the current design variables

Gradients

- When the optimizer requests a gradient value, it requires a sensitivity analysis with inputs and a grid corresponding to the current design variables
  - The most straightforward way to generate sensitivity information is to perturb each design variable independently and run the CFD solver as a black-box to generate finite differences
    - This is prohibitively expensive when each finite difference requires a new CFD simulation (or two): *cost scales linearly with the number of design variables*
  - The most efficient sensitivity analysis approach for CFD simulations based on large numbers of design variables (hundreds or thousands) is the adjoint method: *cost is independent of the number of design variables*

Notation and Governing Equations

We wish to perform rigorous adaptation and design optimization based on the Euler and Navier-Stokes equations, ***without requiring any a priori knowledge of the problem***:

$$\frac{\partial \mathbf{Q}}{\partial t} + \mathbf{R}(\mathbf{D}, \mathbf{Q}, \mathbf{X}) = 0$$

$\mathbf{R}$ = Spatial residual

$\mathbf{Q}$ = Dependent variables

$\mathbf{D}$ = Design variables

$\mathbf{X}$ = Computational grid

- Incompressible through hypersonic flows
- May include turbulence models and various physical models from perfect gas through thermochemical nonequilibrium

What is an Adjoint?

Combine cost function with Lagrange multipliers Λ:

$$L(\mathbf{D},\mathbf{Q},\mathbf{X},\Lambda_f,\Lambda_g) = \underbrace{f(\mathbf{D},\mathbf{Q},\mathbf{X})}_{\text{Cost Function}} + \Lambda_f^T \underbrace{\mathbf{R}(\mathbf{D},\mathbf{Q},\mathbf{X})}_{\text{Flowfield Equations}} + \Lambda_g^T \underbrace{(\mathbf{K}\mathbf{X} - \mathbf{X}_{surf})}_{\text{Mesh Movement Equations}}$$

f = Cost function (lift/drag/boom/etc)

$\mathbf{K}$ = Mesh movement elasticity matrix

Λ_f = Flowfield adjoint variable

Λ_g = Grid adjoint variable

Differentiate with respect to $\mathbf{D}$:

$$\frac{dL}{d\mathbf{D}} = \frac{\partial f}{\partial \mathbf{D}} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{D}}\right]^T \Lambda_f + \left[\frac{\partial \mathbf{Q}}{\partial \mathbf{D}}\right]^T \left\{\frac{\partial f}{\partial \mathbf{Q}} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right]^T \Lambda_f\right\}$$

$$+ \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \left\{\frac{\partial f}{\partial \mathbf{X}} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{X}}\right]^T \Lambda_f + \Lambda_g^T \mathbf{K}\right\} - \Lambda_g^T \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]_{surf}$$

$$\longrightarrow \underbrace{\left[\frac{\partial \mathbf{R}}{\partial \mathbf{Q}}\right]^T}_{\text{Governing Eqns}} \Lambda_f = \underbrace{-\frac{\partial f}{\partial \mathbf{Q}}}_{\text{Engineering Output}}$$

This adjoint equation for the flowfield has powerful implications for:

- Error estimation & mesh adaptation
- Sensitivity analysis

Adjoints for Error Estimation and Mesh Adaptation

It is apparent that:

$$\mathbf{\Lambda}_f \equiv \frac{\partial f}{\partial \mathbf{R}} \longrightarrow$$

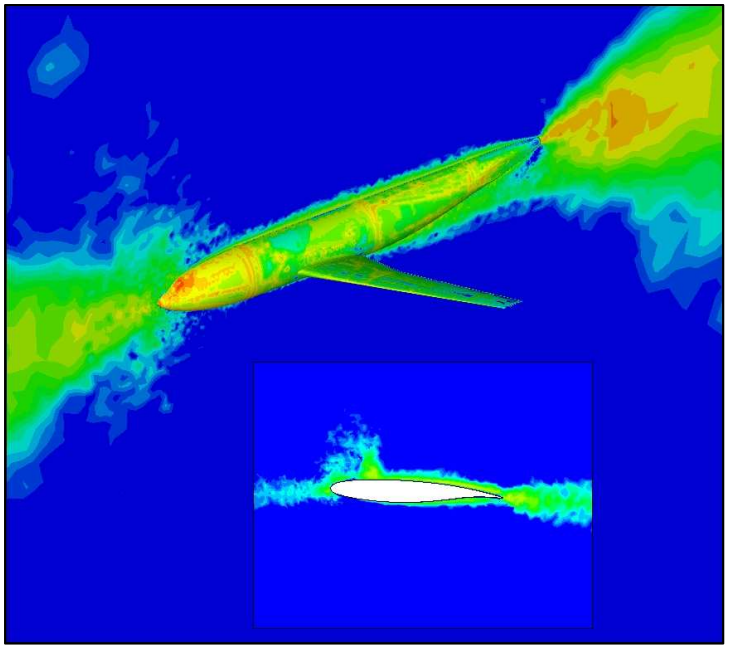
Direct relationship between local equation error and the output we are interested in!

- These relationships can be used to get error estimates on f
- Also used to compute a scalar field explicitly relating local point spacing requirements to output accuracy for a user-specified error tolerance
- Often yields non-intuitive insight into gridding requirements
- Relies on underlying mathematics to adapt, rather than heuristics such as solution gradients

User no longer required to be a CFD expert to get the right answer

Transonic Wing-Body:

"Where do I need to put grid points to get 10 drag counts of accuracy?"



Blue=Sufficient Resolution
Red=Under-Resolved

Adjoints for Sensitivity Analysis

Examine the remaining terms in the linearization:

$$\frac{dL}{d\mathbf{D}} = \frac{\partial f}{\partial \mathbf{D}} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{D}}\right]^T \mathbf{\Lambda}_f + \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]^T \left\{\frac{\partial f}{\partial \mathbf{X}} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{X}}\right]^T \mathbf{\Lambda}_f + \mathbf{\Lambda}_g^T \mathbf{K}\right\} - \mathbf{\Lambda}_g^T \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]_{surf}$$

$$\longrightarrow \quad \mathbf{K}^T \mathbf{\Lambda}_g = -\left\{\frac{\partial f}{\partial \mathbf{X}} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{X}}\right]^T \mathbf{\Lambda}_f\right\}$$

Discrete adjoint equation for mesh movement

$$\longrightarrow \quad \frac{dL}{d\mathbf{D}} = \frac{\partial f}{\partial \mathbf{D}} + \mathbf{\Lambda}_f^T \frac{\partial \mathbf{R}}{\partial \mathbf{D}} - \mathbf{\Lambda}_g^T \left[\frac{\partial \mathbf{X}}{\partial \mathbf{D}}\right]_{surf}$$

Sensitivity equation

Function Evaluation

1. Compute surface mesh at current D
2. Solve mesh movement equations
3. Solve flowfield equations

Sensitivity Evaluation

3. Solve flowfield adjoint equations
2. Solve mesh adjoint equations
1. Matrix-vector product over surface

Analysis Cost = Sensitivity Analysis Cost

Even for *1000's* of design variables

Design Variables in FUN3D

- Global flowfield parameters
  - Mach number, angle of attack
- Shape variables: ***Sculptor's role***
  - FUN3D relies on a pre-defined relationship between a set of parameters, or design variables, and the discrete surface mesh coordinates
  - Given current values of design variables, surface parameterization determines discrete surface mesh
  - This narrows down the number of design variables from hundreds of thousands (raw grid points) to dozens or hundreds
    - Optimizers will perform more efficiently
    - Smoother design space
  - However: parameterization package must also provide Jacobian of the surface mesh with respect to the design variables
- Additional variables related to unsteady simulations

Objectives/Constraints in FUN3D

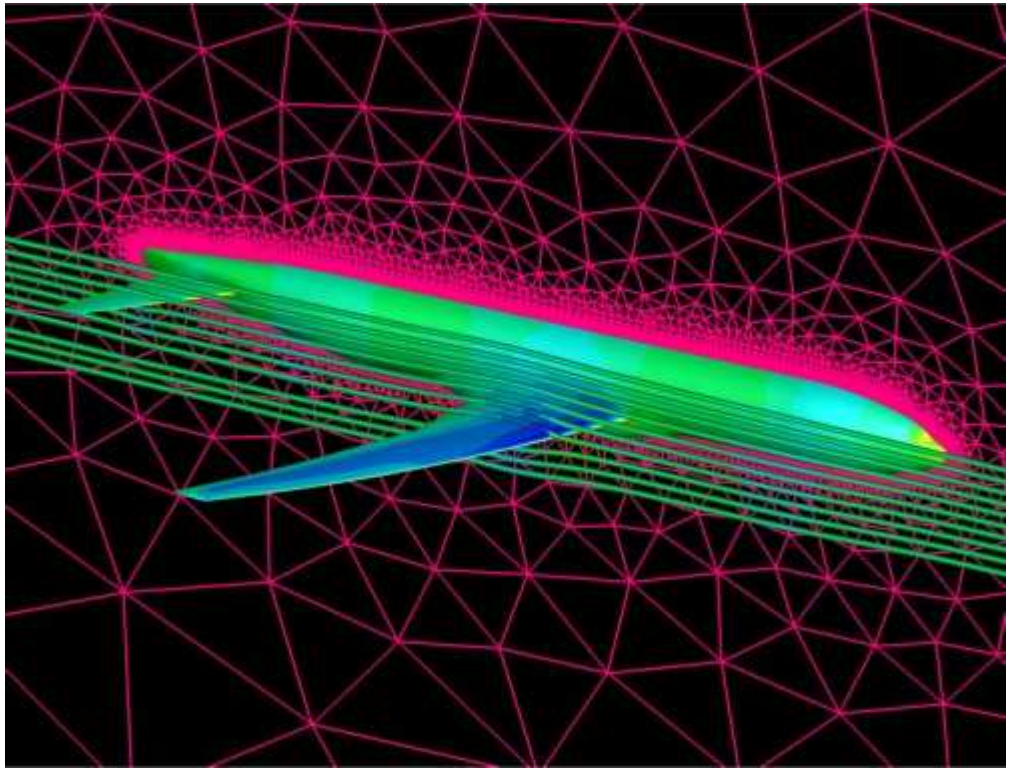
$$f_i = \sum_{j=1}^{J_i} \omega_j (C_j - C_j^*)^{p_j}$$

ω = weight C = aero coeff
p = power C^*= target aero coeff

- User may specify which boundary patch in the grid (or all) to which each function applies
- Constraints may be explicit or added as “penalties”
- Multipoint/multiobjective: as many composite functions/constraints as desired
  - Only limited by particular optimization package
  - Adjoints for multiple functions/constraints computed simultaneously
- The optimization always seeks to *minimize* the objective function(s), so they should be posed accordingly

Demonstration Problem

Turbulent Transonic Flow Over Wing-Body-Tail Configuration



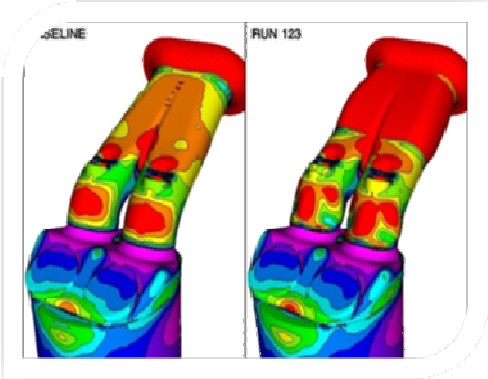
- Geometry, conditions from 4th AIAA Drag Prediction Workshop (June 2009)
  - Geometry, grids available on DPW-4 website
- M_∞=0.85, α=1°, Re_{MAC}=3.5 million
- Mesh consists of 672,235 nodes / 3,935,055 tetrahedra
  - Too coarse to adequately resolve all flow physics; solely intended as a demonstration case (full tutorial available for download on FUN3D website)
- Each flow/adjoint solution takes 2-4 minutes on 128 cores (commodity hardware)

Sculptor® provides:

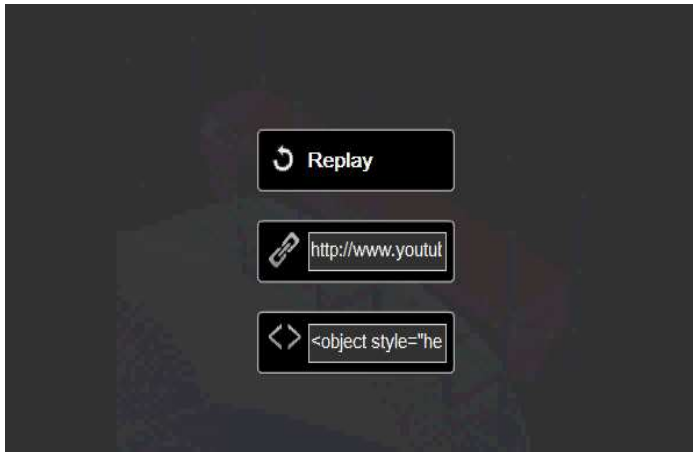
- Arbitrary Shape Deformation (ASD)
- Smooth, Accurate, Volumetric, Real-time deformation (morphing)
- Tri-variate relationship between "ASD Control points" and the model's geometry (FEA mesh, CFD mesh, and/or CAD geometry)
- Control points' are grouped together to define shape change design variables for optimization (translation, rotation, scaling)
- Helps find the shape changes (often times subtle and non-intuitive) that produce large gains in performance
- Interfaced with most all CFD, FEA, CAD formats
- Internal optimization tools, or it can be run in Batchmode within external optimization tools

OPTIMAL SOLUTIONS

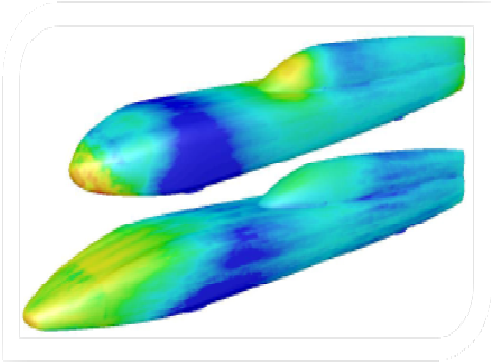
Sculptor examples:



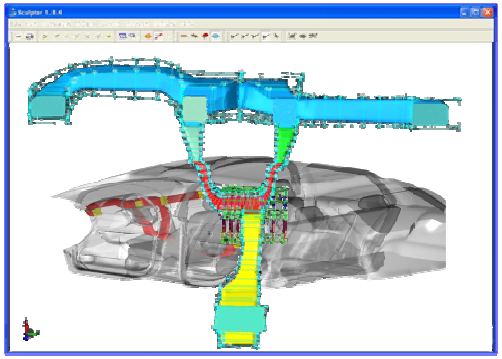
Intake valve port



Racecar

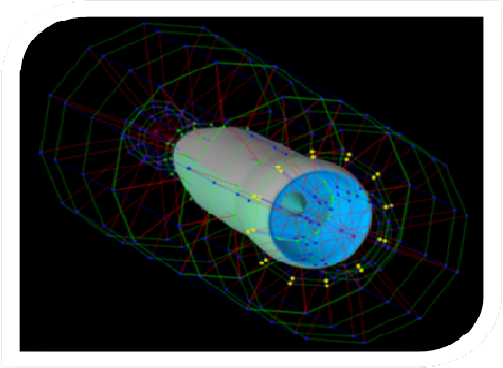


Electric Streamliner

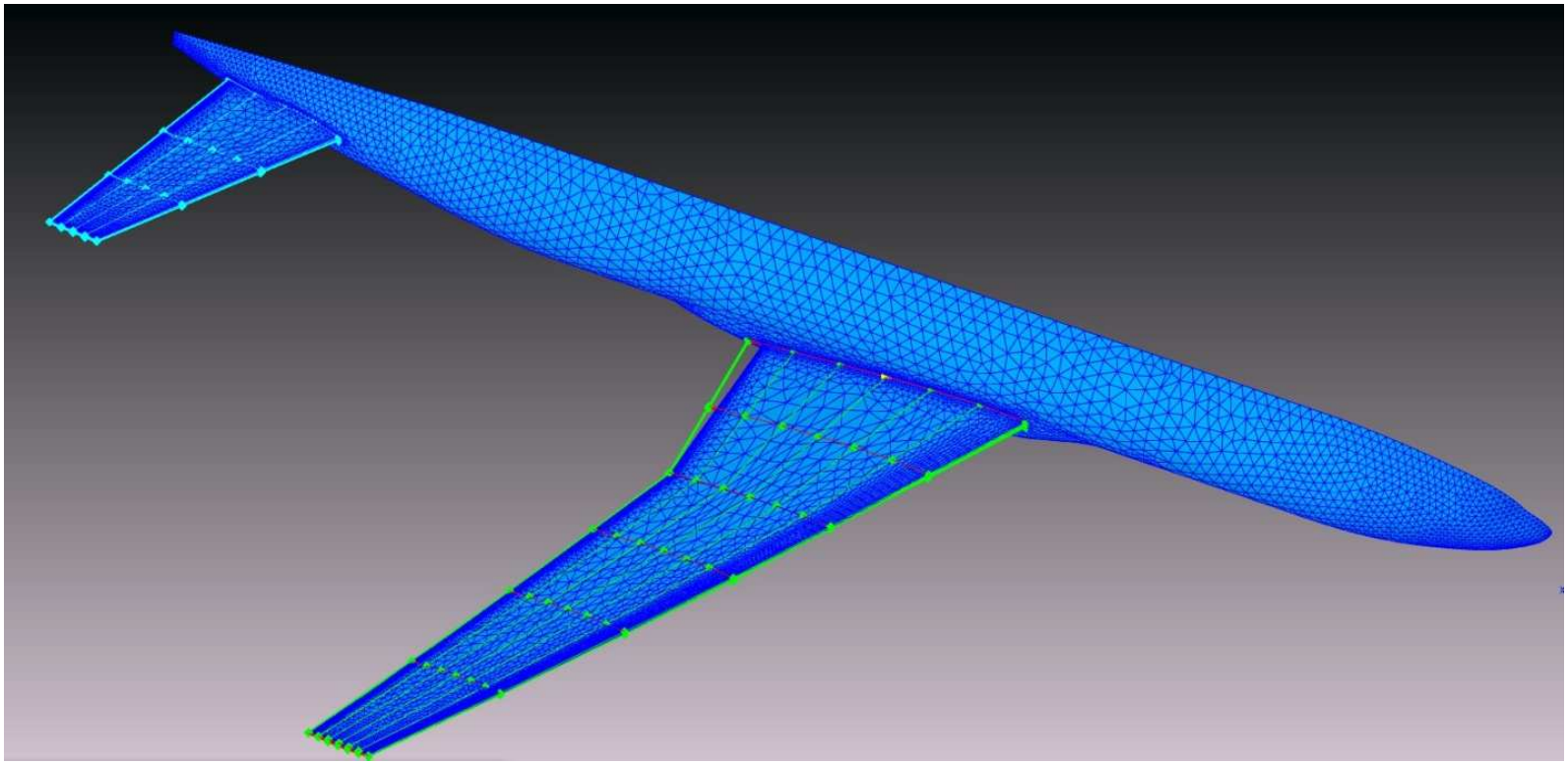


HVAC Ducts

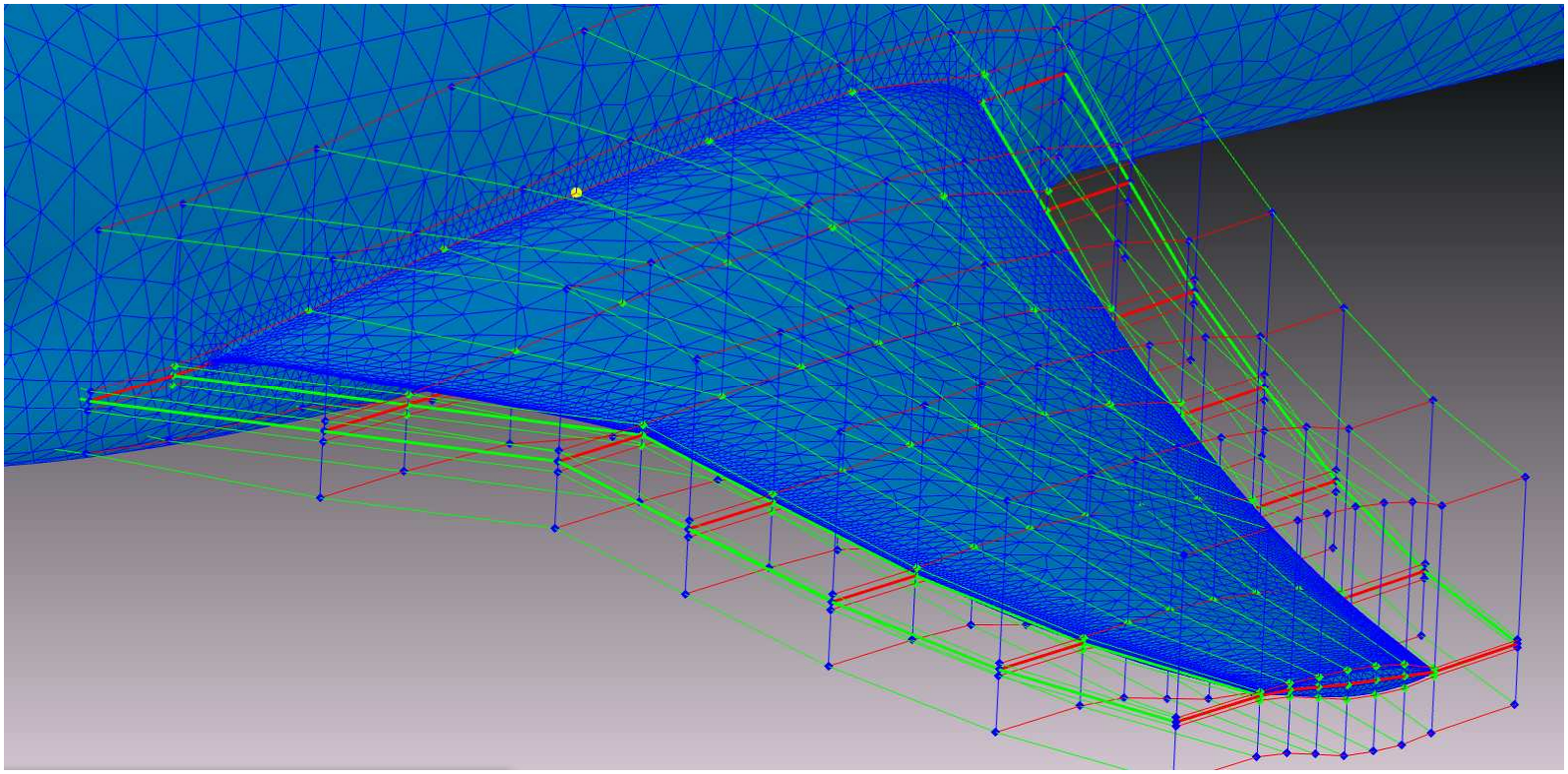
F1 Racecar



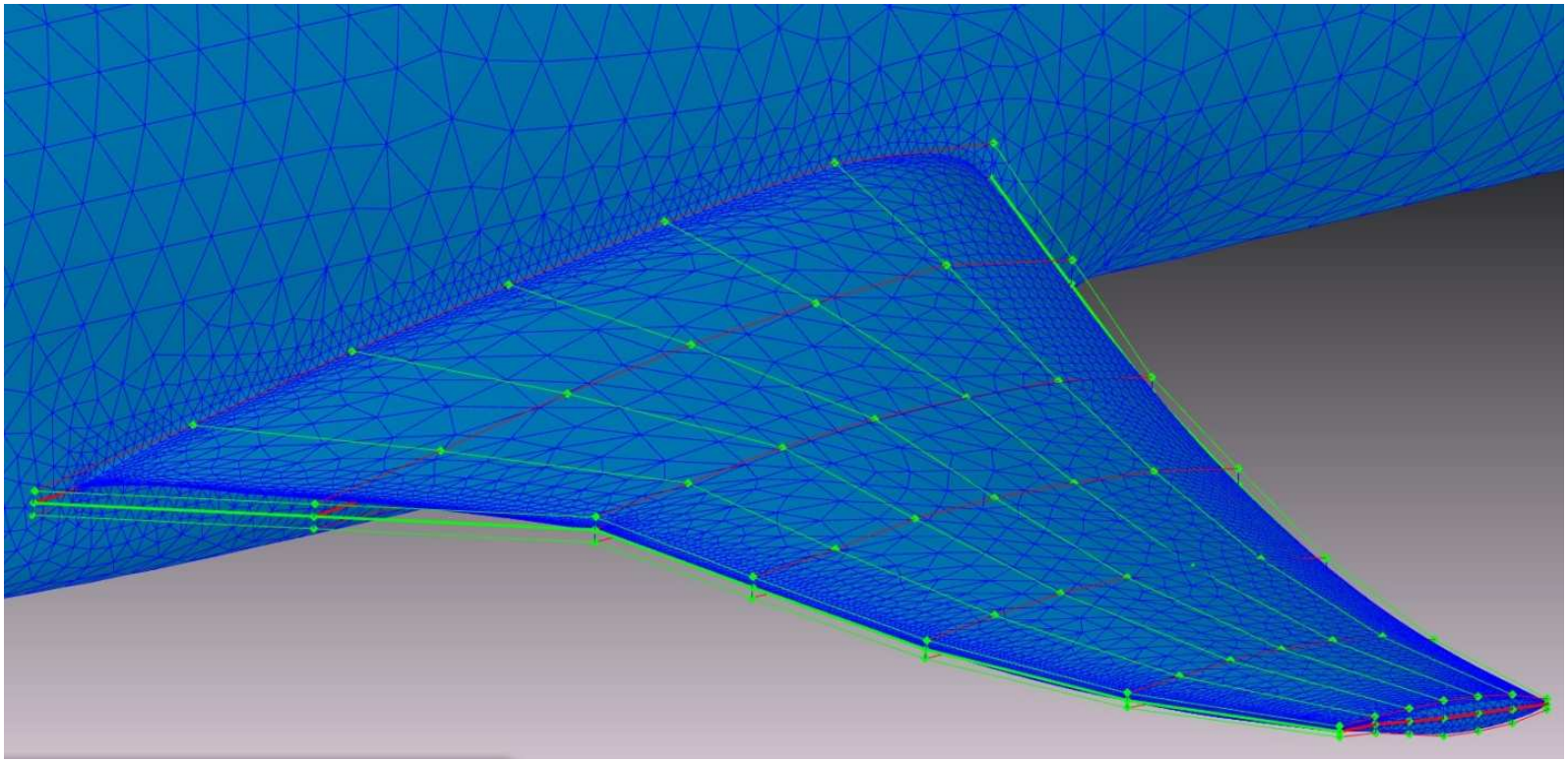
Nacelle



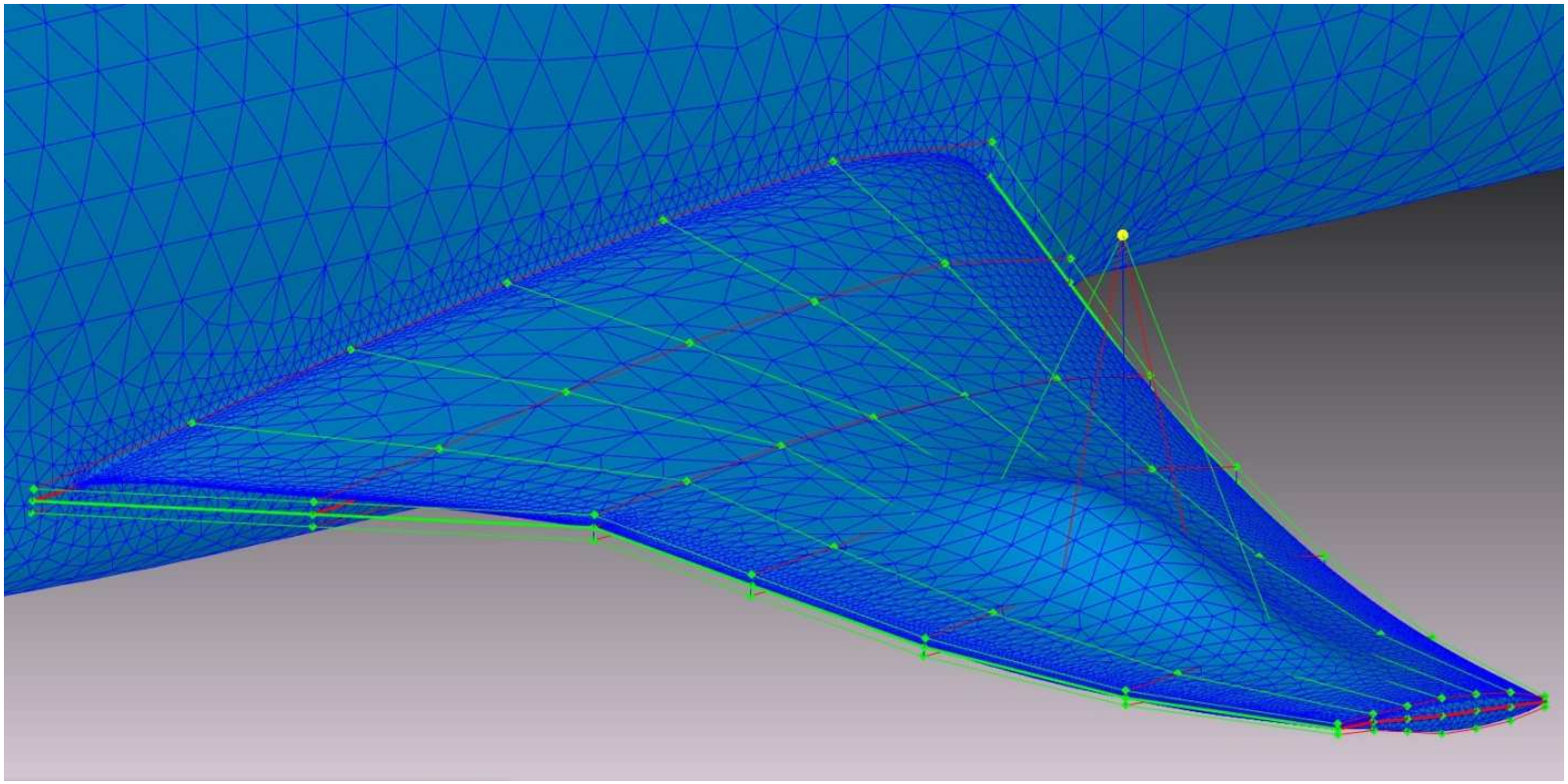
The Fun3D aircraft model with ASD volumes on around the wing and tail.



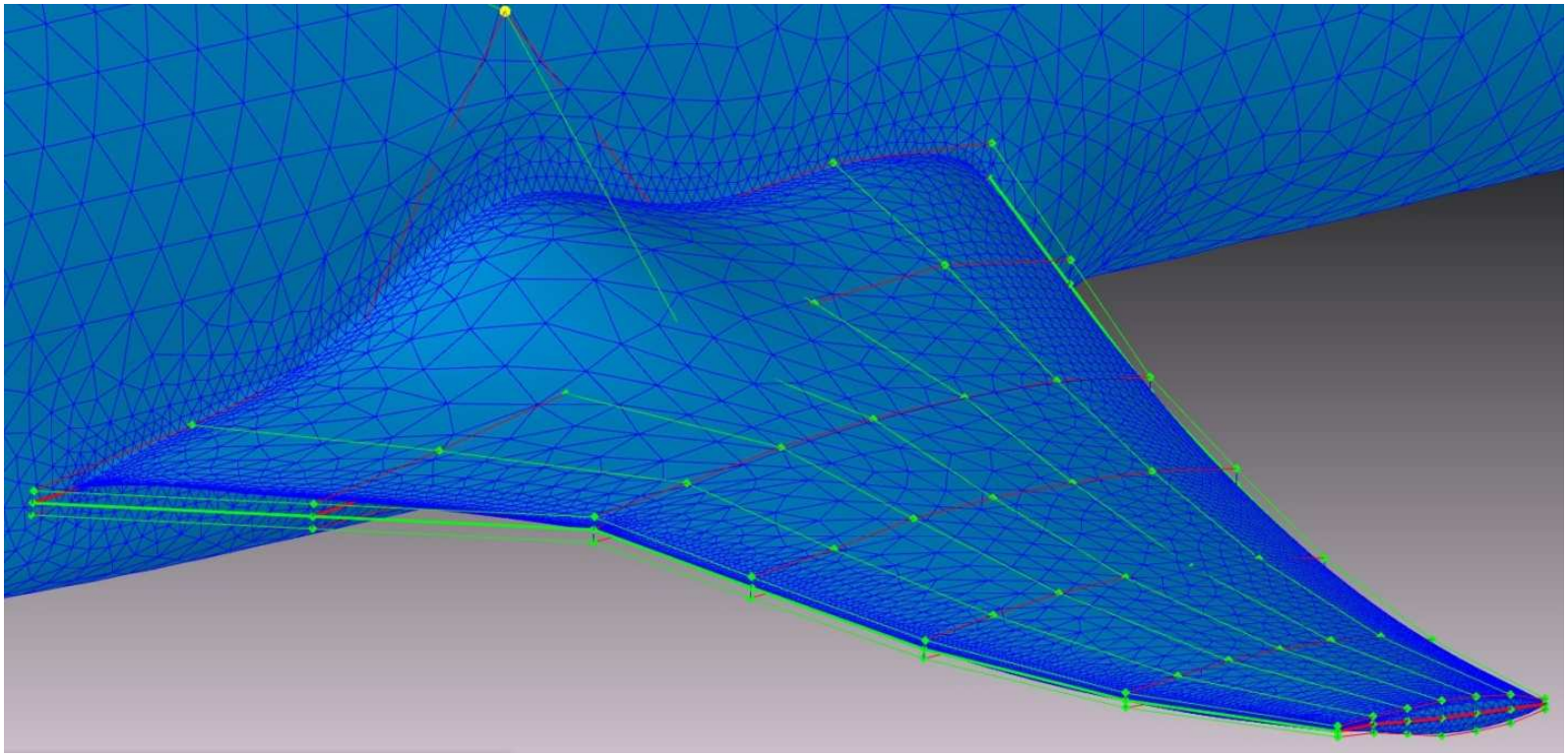
The complete ASD volume around the wing shown here with the external (inactive) control points. The inactive control points are necessary to define the ASD volumetric deformation out into the flow domain.



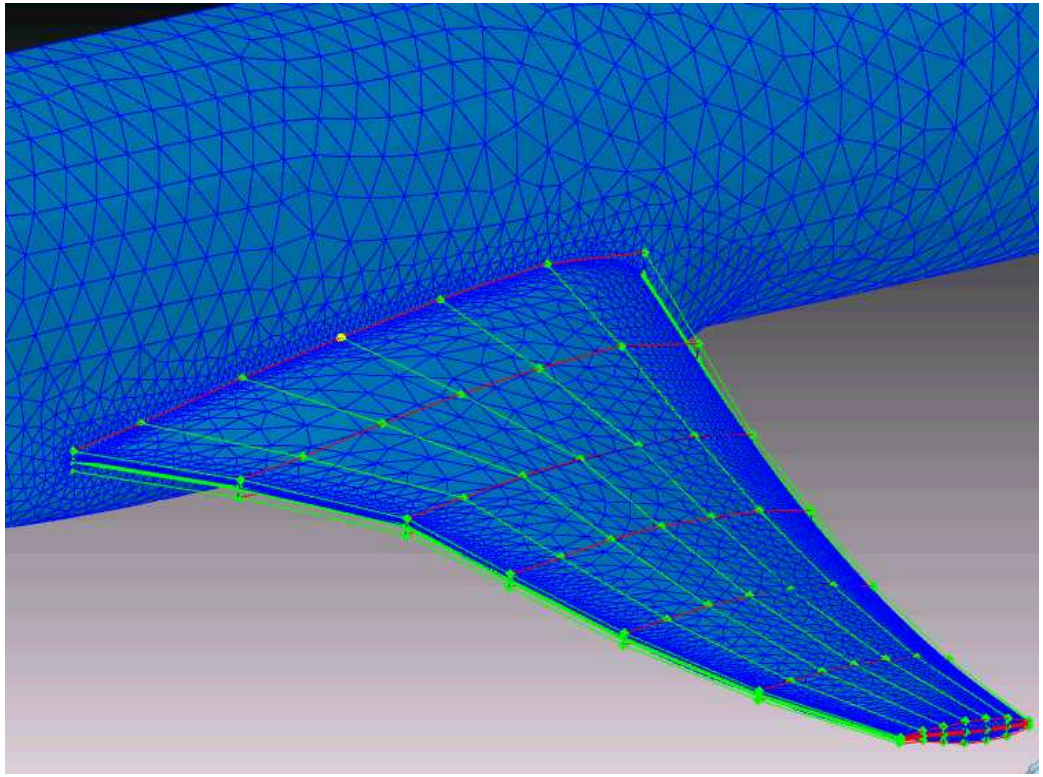
Close up view of the wing's ASD volume without the external 'inactive' control points.



A top surface DV (control point) is moved in the upward Z-direction resulting in a smooth deformation of the wing's top surface, localized near the control point.



A top surface DV is moved in the upward Z-direction resulting in a smooth 'volumetric' deformation at the wing-fuselage intersection maintaining high cell quality at the intersection's vicinity.



Movie of real-time deformation in Sculptor GUI.

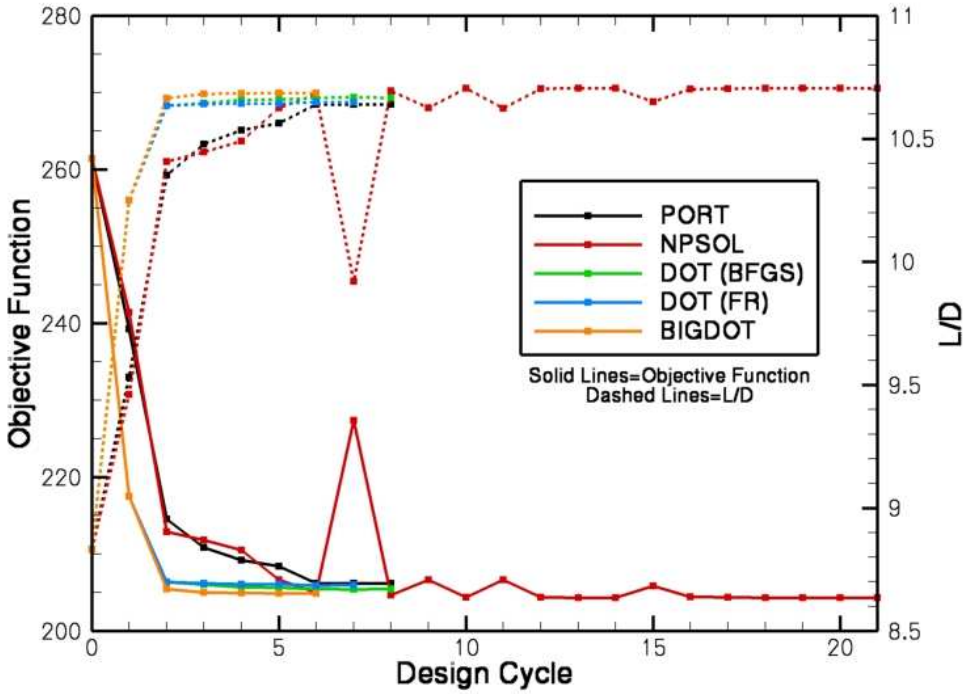
- Other possible DVs that could be defined:
  - deform the leading and trailing edges
  - perform rigid body movements of the wing and tail in the Z-direction and/or the X-direction
  - rigid body rotations of an airfoil about a hinge line vector
  - all of these deformations/movements can be performed and still maintain smooth accurate cell quality at the wing-or-tail to fuselage intersection
- Sculptor provides the sensitivity of each of the model's nodes with respect to the value of each shape change DV that is defined. This gradient information is calculated for the X, Y, and Z-directions of each node
- These sensitivities (Jacobian) are provided to FUN3D via a text file
- FUN3D's adjoints provide the sensitivities of the CFD functions with respect to the model's nodes movement

Example 1: Maximize Lift-to-Drag Ratio

- 94 active design variables
- Objective function seeks to minimize difference between current and target L/D values:

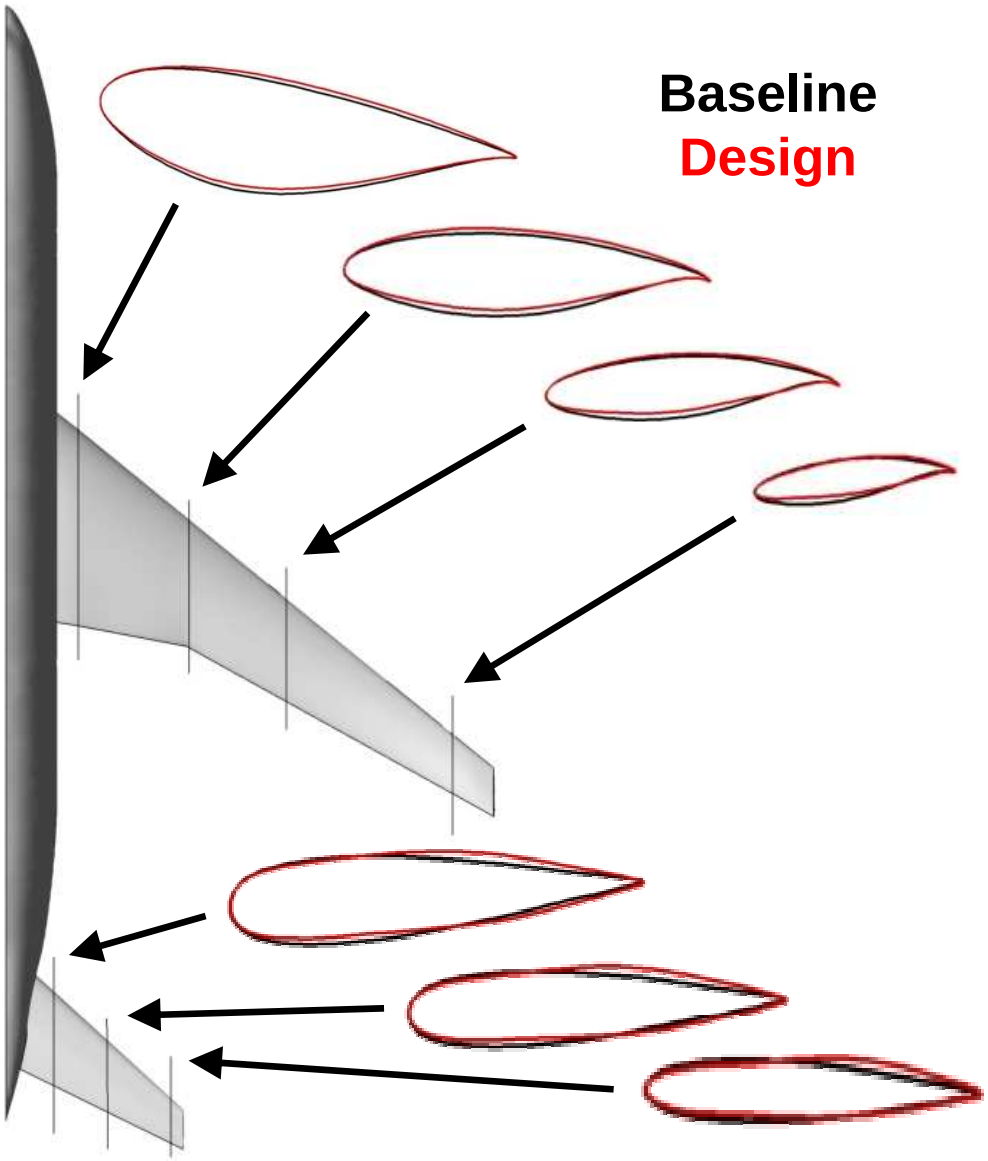
$$\min f = (L/D - 25)^2$$

- Baseline L/D is 8.83; target value of 25 chosen arbitrarily large

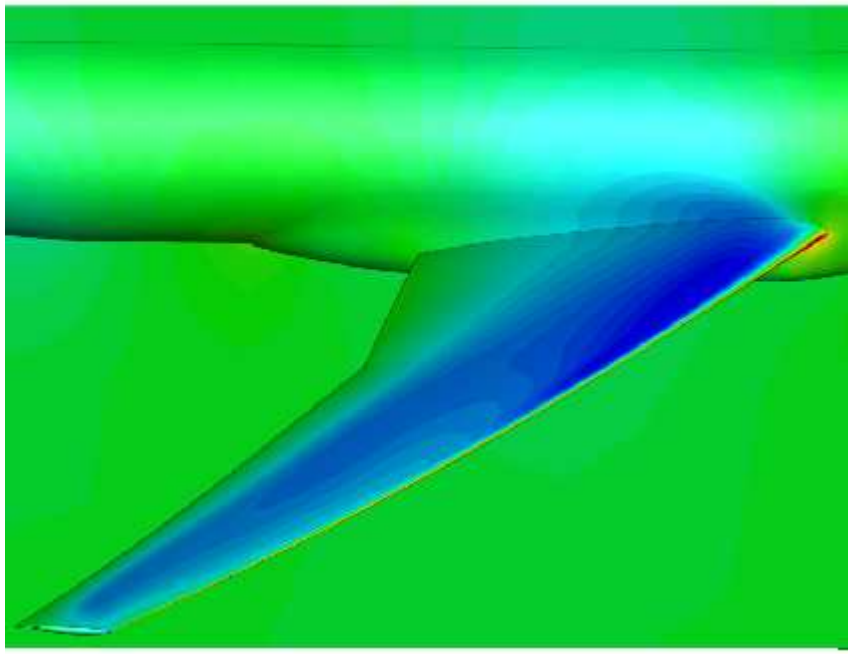


Optimizer	Design L/D	Function Calls	Gradient Calls
PORT	10.64	30	8
NPSOL	10.70	22	21
DOT (BFGS)	10.67	45	8
DOT (FR)	10.65	41	7
BIGDOT	10.69	40	6

Example 1: Final Design



Pressure field during design



- Results based on PORT optimization shown
- Wing and tail camber increased across the span

Example 1: Solution Efficiency

Optimizer, Sensitivity Analysis	Flow Solves	Adjoint Solves	Execution Time (hrs)
PORT			
Adjoint	30	8	**1.6**
Central Differences	1534	N/A	**76.7***
NPSOL			
Adjoint	22	21	**2.3**
Central Differences	3970	N/A	**198.5***
DOT (BFGS)			
Adjoint	45	8	**2.6**
Central Differences	1549	N/A	**77.5***
DOT (FR)			
Adjoint	41	7	**2.1**
Central Differences	1357	N/A	**67.9***
BIGDOT			
Adjoint	40	6	**1.9**
Central Differences	1168	N/A	**58.4***

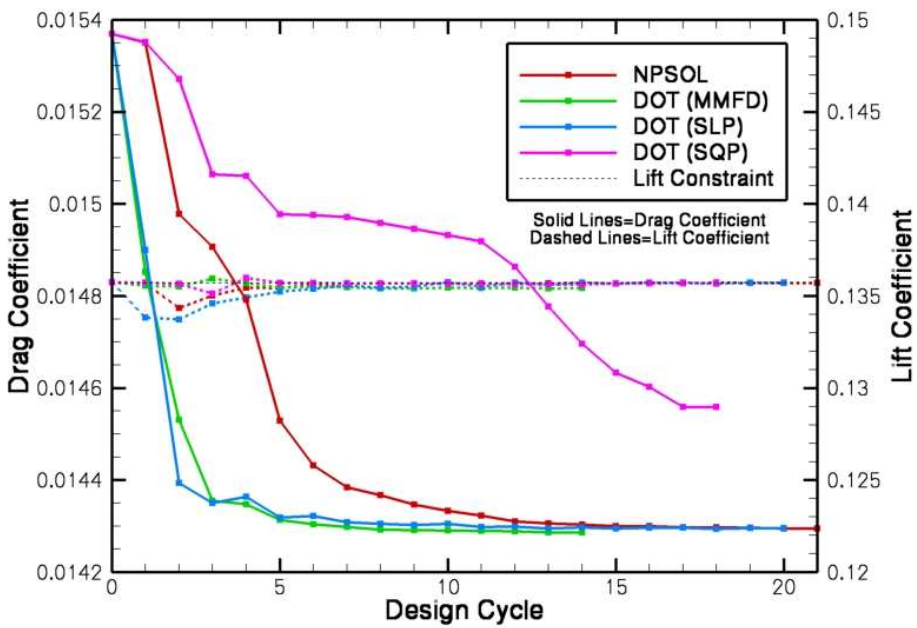
- *Central difference timings are estimates based on 3 minutes per solution (would likely be longer due to convergence requirements for accurate differencing)
- Adjoint is 1-2 orders of magnitude faster than conventional approach

Example 2: Min Drag with Constraint on Lift

- 94 active design variables
- Objective function seeks to minimize drag by setting a zero target:

$$\min\ f = 10000(C_D - 0)^2$$

- Baseline drag is 153.7 counts
- Factor of 10000 added to scale function to O(1) quantity
- Lift explicitly constrained to baseline value of 0.1357 $\pm\ \varepsilon$
- FUN3D performs 2 simultaneous adjoint solutions; one for lift, one for drag



Optimizer	Design Drag Counts	Function Calls	Gradient Calls
NPSOL	143.0	22	21
DOT (MMFD)	142.9	133	14
DOT (SLP)	143.0	23	20
DOT (SQP)	145.6	36	18

Example 2: Solution Efficiency

Optimizer, Sensitivity Analysis	Flow Solves	Adjoint Solves	Execution Time (hrs)
NPSOL			
Adjoint	22	21	**2.3**
Central Differences	3970	N/A	**198.5***
DOT (MMFD)			
Adjoint	133	14	**6.4**
Central Differences	2765	N/A	**138.3***
DOT (SLP)			
Adjoint	23	20	**2.5**
Central Differences	3783	N/A	**189.2***
DOT (SQP)			
Adjoint	36	18	**2.5**
Central Differences	3420	N/A	**171.0***

- *Central difference timings are estimates based on 3 minutes per solution (would likely be longer due to convergence requirements for accurate differencing)
- Adjoint is 1-2 orders of magnitude faster than conventional approach

Q/A

“Adjoint-Based Shape Optimization”

Dr. Eric Nielsen – e.j.nielsen@larc.nasa.gov
Dr. Mark Landon – mlandon@goSculptor.com
John Jenkins – jjenkins@goSculptor.com

Thank You

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