FUN3D v13.1 Training

Session 5: Adjoint-Based Design for Steady Flows

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Learning Goals

- Introduction and basic approach taken in FUN3D
- Some lingo/nomenclature
- What is an adjoint, and what is it used for?
  - Error estimation and mesh adaptation
  - Sensitivity analysis for design optimization
- Design variables
- Objective/constraint functions
- Geometry parameterizations
- Setup and execution of a simple unconstrained problem
- Things to watch out for
- How to interpret results

What we will *not* cover

- Body transforms, body grouping
- Overset grid details
- Multipoint/multiobjective/constrained optimization
- Hooking in your own optimizer, parameterization tools
- Forward-mode differentiation using complex variables
- Design of unsteady flows
  - Later session

What to Expect

- Cost of design optimization is very problem-dependent, but in general you can expect to spend ~20 times the cost of a flow solution to get reasonable improvements, depending on how "good" the baseline is
- Generally see very rapid improvements initially, followed by diminishing returns
- We will cover the bare essentials here; also see the manual
  - There are many aspects we will not have time to cover here
- Hands-off design is challenging – be patient, send in questions, and we'll try to help you through
  - There are a lot of pieces involved, and getting things running smoothly always involves stumbling blocks along the way

Design Optimization Using FUN3D

- Based on a gradient-based approach
- FUN3D is distributed with support for several COTS gradient-based optimization packages
  - You must download and install your choice of these third-party libraries
    - DOT/BIGDOT (Vanderplaats R&D)
    - KSOPT (Greg Wrenn @ Langley)
    - PORT (Bell Labs)
    - NPSOL (Stanford)
    - SNOPT (Stanford)
    - Other packages are generally straightforward to hook up – couple of 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

Design Optimization Components

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 black-box 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

Notation and Governing Equations

We wish to perform rigorous adaptation and design optimization based on the steady-state Euler/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 $\quad$ $\mathbf{Q}$ = Dependent variables

$\mathbf{D}$ = Design variables $\quad$ $\mathbf{X}$ = 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 $\boldsymbol{\Lambda}$:

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

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

$\boldsymbol{\Lambda}_f$ = Flowfield adjoint variable

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

$\boldsymbol{\Lambda}_g$ = Grid adjoint variable

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

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

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

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

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:

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

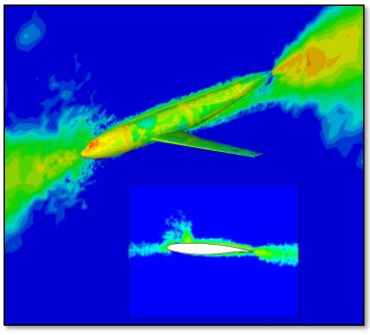
Direct relationship between local equation error and the output we are interested in

- 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?"

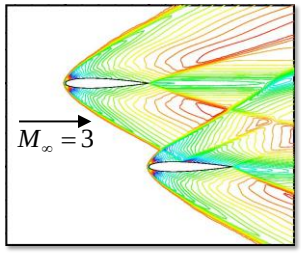


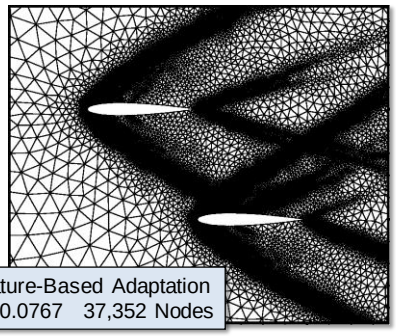
Blue=Sufficient Resolution
Red=Under-Resolved

Supersonic Adjoint-Based Mesh Adaptation

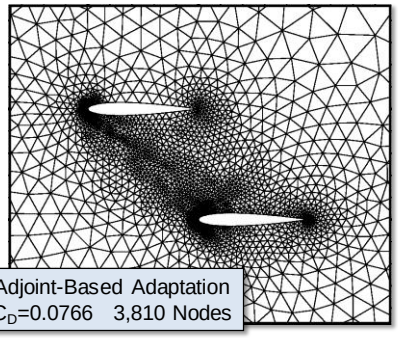
Collaboration with Venditti/Darmofal of MIT using FUN2D

- **Objective:** Adapt grid to compute drag on lower airfoil as accurately as possible
- **Result of adjoint-based adaptation:**
  - Uniformly-resolved shocks are not required
  - Drag is computed accurately with a 90% smaller grid





Feature-Based Adaptation
C_D=0.0767 37,352 Nodes

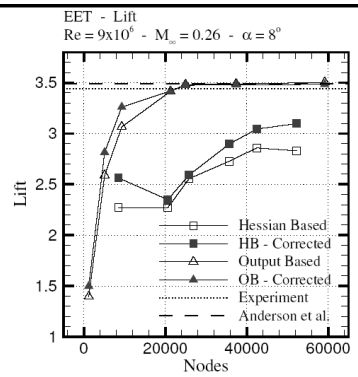


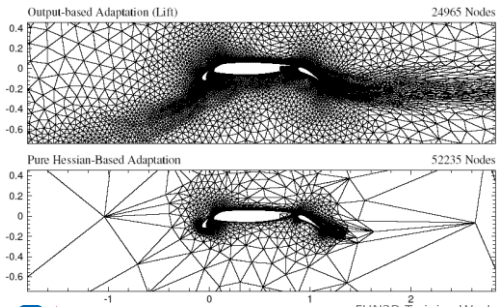
Adjoint-Based Adaptation
C_D=0.0766 3,810 Nodes

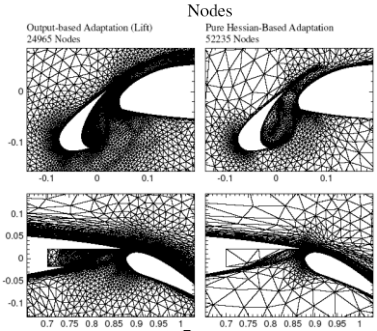
Adjoint-Based Mesh Adaptation for High Lift

Collaboration with Venditti/Darmofal of MIT using FUN2D

- Initial grid was coarse Euler mesh
- Pressure-based indicator only resolves strong flow curvature
- Adjoint-based indicator also includes important smooth regions, stagnation streamline and wakes







Adjoints for Sensitivity Analysis

Examine the remaining terms in the linearization:

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

$$\mathbf{K}^T \boldsymbol{\Lambda}_g = -\left\{\frac{\partial f}{\partial \mathbf{X}} + \left[\frac{\partial \mathbf{R}}{\partial \mathbf{X}}\right]^T \boldsymbol{\Lambda}_f\right\}$$ Discrete adjoint equation for mesh movement

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

Function Evaluation	**Sensitivity Evaluation**
1. Compute surface mesh at current D	3. Solve flowfield adjoint equations
2. Solve mesh movement equations	2. Solve mesh adjoint equations
3. Solve flowfield equations	1. Matrix-vector product over surface

Analysis Cost = Sensitivity Analysis Cost

Even for *1000s* of design variables

Design Variables in FUN3D

- Global flowfield variables
  - Mach number, angle of attack, sideslip, noninertial rates
- Shape variables
  - These depend entirely on the geometric parameterization being supplied to FUN3D
  - FUN3D has no native shape variables, other than the grid points themselves
- Additional variables related to unsteady simulations

Objective/Constraint Functions 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

- We call each term in the summation a *component* function and the summation f_i a *composite* function
- User may specify which boundary patch in the grid (or all) to which each component 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 pose them accordingly
- This general form leads to numerous ways to pose an optimization problem; each optimizer has its own limitations though
  - Extensive discussion in manual

Objective/Constraint Functions Examples

Unconstrained Drag Minimization

$$f = C_D^2$$

Drag Minimization with C_L=0.5 Lift Penalty

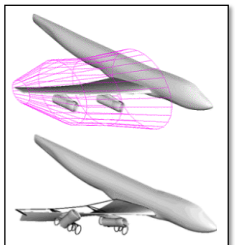
$$f = 10C_D^2 + (C_L - 0.5)^2$$

Drag Minimization with Explicit C_L=0.5 Lift Constraint

$$f_1 = C_D^2 \qquad f_2 = C_L$$

Geometry Parameterizations

- FUN3D relies on a predefined relationship between a set of parameters, or design variables, and the discrete surface mesh coordinates
- Given $\mathbf{D}$, surface parameterization determines $\mathbf{X}_{surf}$ (surface mesh)
- For example, given the current value of wing thickness at a location, what are the corresponding xyz-coordinates of the 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
- The other requirement of the parameterization package is that it provides the Jacobian of the relationship between the design variables and the surface mesh, $\partial \mathbf{X}_{surf}/\partial \mathbf{D}$
- While users may provide their own parameterization scheme, FUN3D is set up to handle three common packages:
  - MASSOUD: Aircraft-centric design variables (thickness, camber, planform, twist, etc.)
  - Bandaids: General patching tool to handle fillets, winglets, and other odd shapes
  - Sculptor: Commercial package from Optimal Solutions
- To dump out the surface grids in the Tecplot format necessary for these tools, run the flow solver with `'--write_massoud_file'`
  - This procedure generates a `[project]_massoud_bndryN.dat` file for the i^{th} solid boundary



Wing Twist via MASSOUD

Directory Tree for FUN3D-Based Design

`Design`
- Main directory for design execution
- The only directory here without a hardwired name

`Design/ammo`
- Design is executed from here using the `opt_driver` executable
- `design.nml` resides here

`Design/description.i`
- `i` suffix is an integer referring to the design point (to accommodate multipoint design)
- Contains all of the baseline files describing this design point (CFD model and all input decks specific to it)
- **The optimization never changes anything in here**; this is where the optimizer can always find the problem definition
- **You provide the problem description for the i^{th} design point here**

`Design/model.i`
- `i` suffix is an integer referring to the design point (to accommodate multipoint design)
- All CFD runs are performed here
- **You never change anything in here**; it only contains outputs

`Design/model.i/Flow`
- All flow solutions are performed here

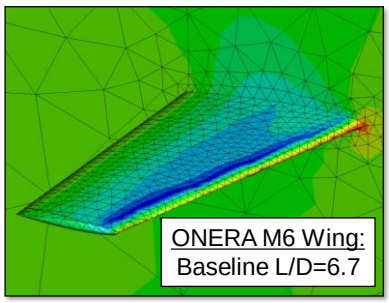
`Design/model.i/Adjoint`
- All adjoint solutions are performed here

`Design/model.i/Rubberize`
- All parameterization evaluations are performed here

`Design/model.i/Rubberize/surface_history`
- A Tecplot file for every surface grid evaluated during the design is stored here

You need not set up this tree manually; the code will do it for you, provided some basic pathnames

Maximize L/D for Transonic Flow Over a Wing



- To create the directory structure necessary for performing the optimization, issue the following command:

```
'/path/to/your/FUN3D/installation/Design/opt_driver --setup_design 1'
```

- The trailing integer represents the number of design points desired
- This command will prompt you for several paths and then will set up the required directory structure
- First we will discuss the files that must be provided in the `description.1` directory

Maximize L/D for Transonic Flow Over a Wing

Files Required in `description.1` Directory

`command_line.options`

```
3
0 flow
1 adjoint
'--rmstol 1.e-3'
0 mpirun
```

- This file is used to specify any command line options (CLOs) required by the FUN3D executables, as well as MPI
- The first line specifies the number of executables for which you are providing CLOs
- This is followed by a line containing an integer and a keyword
  - The integer specifies the number of CLOs you are providing for the code identified by the keyword
- This is followed by the actual CLOs for the current executable
- Note 'mpirun' is an available keyword: this provides a mechanism to feed your `mpirun` executable any options it may require (`-nolocal`, `-machinefile filename`, etc.)
  - Depends on your environment, queue structure, etc.

Maximize L/D for Transonic Flow Over a Wing

Files Required in `description.1` Directory

We are assuming the use of a MASSOUD parameterization for this example

`design.1, design.gp.1`

- These files are input files for MASSOUD for the 1st body; the MASSOUD setup tool provides these when you set up your parameterization
- Do not change these files

`design.usd.1`

- This file is an input file for MASSOUD for the 1st body; the MASSOUD setup tool provides this template when you set up your parameterization
- Depending on how you choose to "link" raw MASSOUD variables to create new variables, this defines the linking weights (see MASSOUD documentation)
- When using MASSOUD with FUN3D, you must always use the design variable linking option, even if simply set to the identity matrix

Maximize L/D for Transonic Flow Over a Wing

Files Required in `description.1` Directory

`design.usd.1`

```
# this is input sd file for MASSOUD
# number of row == number dvs within MASSOUD
# number of col == final number  dvs
#(row) (col) (#of nonzero rows)
10 11 10
    d   1d   2d   3d   4d   5d   6d   7d   8d   9d  10d  11d
    1    1    0    0    0    0    0    0    0    0    0    0
    2    0    1    0    0    0    0    0    0    0    0    0
    3    0    0    1    0    0    0    0    0    0    0    0
    4    0    0    0    1    0    0    0    0    0    0    0
    5    0    0    0    0    1    0    0    0    0    0    0
    6    0    0    0    0    0    1    0    0    0    0    0
    7    0    0    0    0    0    0    1    0    0    0    1
    8    0    0    0    0    0    0    0    1    0    0    1
    9    0    0    0    0    0    0    0    0    1    0    1
   10    0    0    0    0    0    0    0    0    0    1    1
```

- Our demo problem uses 166 variables; this sample file only shows 10 raw variables plus 1 linked variable for clarity
- Linked variable is equal combination of raw DV's 7-10

Maximize L/D for Transonic Flow Over a Wing

Files Required in `description.1` Directory

`massoud.1`

```
#MASSOUD INPUT FILE
# runOption (0 analysis), (> 0 sd using user's dvs ) (-1, sd using massoud's dvs)
166
# core (0 incore solution)(1 out of core solution)
0
# input parameterized file
design.gp.1
# design variable input file
design.1
# input sensitivity file (used for runOption > 0
design.usd.1
# output file grid file
new1.plt
# output tecplot file for viewing
model.tec.1
# file containing the design variables group
designVariableGroups.1
# user design variable file
customDV.1
```

- This file tells MASSOUD the names of its input/output files for the 1st body
- The first value specifies the number of linked MASSOUD design variables
  - If linking matrix is identity, this is just the number of raw MASSOUD design variables
- The remainder of the inputs are filenames; they should remain as is, but with the integer value in each name set to the index of the current body

Maximize L/D for Transonic Flow Over a Wing

Files Required in `description.1` Directory

`fun3d.nml`

- This is the nominal solver input deck for your case
- The adjoint solver also uses this input
  - If the adjoint requires different values (e.g., stopping tolerance), you can override these values with CLOs given in `command_line.options`
- It should contain the necessary inputs to run the baseline case
- The optimization will override values as needed using CLOs (e.g., angle of attack, etc.)

`[project].fgrid, [project].mapbc`

- This is the nominal mesh for your baseline case in whatever grid format is convenient

Maximize L/D for Transonic Flow Over a Wing

Files Required in `description.1` Directory

`rubber.data`

- This is the main design control file used to define the design variables and their bounds, objective functions, and constraints for the current design point
- It also stores current values of functions and sensitivities
- A copy of this file is placed in the `model.1` directory at the beginning of an optimization and is continuously updated with the current values of the design variables, objective/constraint functions, and all gradient information
  - If you want to know the latest info during a design, it's probably in here

Maximize L/D for Transonic Flow Over a Wing

Files Required in `description.1` Directory

`rubber.data`: Design Variable Block

- In general, for each design variable, you must set several fields
  - Active (0=no, 1=yes), baseline value, upper and lower bounds (if active)
- First subsection lays out global design variable information including Mach number, angle-of-attack, yaw, noninertial rates
- This is followed by an input stating the number of bodies to be designed
- Then for each body:
  - Fixed number of rigid motion variables – leave these alone (used for unsteady flows)
  - Number of shape variables and their inputs – these correspond directly to the MASSOUD variables previously discussed
    - When setting bounds for shape variables, it pays to be conservative – the optimizer will exploit every radical shape it can dream up
    - You can quickly get into unsolve-able or invalid/crossed-up geometries
    - You can always loosen up the bounds and restart the design if needed

Maximize L/D for Transonic Flow Over a Wing

Files Required in `description.1` Directory

```
################################################################################
######################## Design Variable Information ###########################
################################################################################
Global design variables (Mach number / angle of attack)
Index Active          Value                Lower Bound             Upper Bound
 Mach     0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
  AOA     0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
  Yaw     0   0.0000000000000000E+00  0.0000000000000000E+00 0.0000000000000000E+00
xrate     0   0.0000000000000000E+00  0.0000000000000000E+00 0.0000000000000000E+00
yrate     0   0.0000000000000000E+00  0.0000000000000000E+00 0.0000000000000000E+00
zrate     0   0.0000000000000000E+00  0.0000000000000000E+00 0.0000000000000000E+00
Number of bodies
    1
Rigid motion design variables for body 1 (name of body 1, less than 80 cols)
  Var Active          Value                Lower Bound             Upper Bound
RotRate   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
RotFreq   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
RotAmpl   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
RotOrgx   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
RotOrgy   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
RotOrgz   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
RotVecx   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
RotVecy   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
RotVecz   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
TrnRate   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
TrnFreq   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
TrnAmpl   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
TrnVecx   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
TrnVecy   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
TrnVecz   0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
Parameterization Scheme (Massoud=1 Bandaids=2 Sculptor=4)
1
Number of shape variables for body 1 (name of body 1, less than 80 cols)
  166
Index Active          Value                Lower Bound             Upper Bound
    1     0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
    2     0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
    3     0   0.0000000000000000E+00  0.0000000000000000E+00 0.5000000000000000E+01
.
.
```


Maximize L/D for Transonic Flow Over a Wing

Files Required in `description.1` Directory

`rubber.data`: Function Block

- These sections lay out the objective/constraint function definitions
- First input is the total number of composite functions being specified (sum of objectives + constraints)
- Then, for each function:
  - Is it an objective function (1) or a constraint (2)
  - If it is a constraint, what are the upper and lower bounds (otherwise dummies)
  - How many component functions are used to build up the composite function
  - Time step interval defining the function (leave as dummies – for unsteady design)
  - Composite function weight/target/power: for further generality, described in manual
  - Then the list of component functions:
    - Boundary index it applies to (0 means all boundaries)
    - Keyword identifying the function type (see manual)
    - Value (dummy – this is an output during the optimization)
    - Weight/target/power to be applied to current component function
    - The remainder of the function block is devoted to sensitivity outputs – you can place dummies here, *but there must be a line corresponding to every design variable*

Maximize L/D for Transonic Flow Over a Wing

Files Required in `description.1` Directory

```
################################################################################
############################ Function Information ##############################
################################################################################
Number of composite functions for design problem statement
    1
################################################################################
Cost function (1) or constraint (2)
    1
If constraint, lower and upper bounds
    0.0 0.0
Number of components for function   1
    1
Physical timestep interval where function is defined
    1 1
Composite function weight, target, and power
1.0 0.0 1.0
Components of function   1: boundary id (0=all)/name/value/weight/target/power
    0 clcd          0.000000000000000           1.000   20.00000 2.000
Current value of function   1
            0.000000000000000
Current derivatives of function wrt global design variables
            0.000000000000000
            0.000000000000000
.
.
.
Current derivatives of function wrt rigid motion design variables of body   1
            0.000000000000000
            0.000000000000000
.
.
.
Current derivatives of function wrt design variables of body   1
            0.000000000000000
            0.000000000000000
.
.
.
```

Our objective function:

$$f = (L/D - 20)^2$$

Maximize L/D for Transonic Flow Over a Wing

`ammo/design.nml`

- We are now finished setting things up in the `description.1` directory
- There is one more file that needs to be set up in the `../ammo` directory
- The `design.nml` file controls the actual optimization procedure
- Everything in this namelist file is pretty self-explanatory, but a few reminders:
  - '`opt_algorithm`': DOT/BIGDOT=1, KSOPT=3, PORT=4, NPSOL=5, SNOPT=6
  - '`what_to_do`': analysis=1, sensitivity analysis=2, optimization=3
  - Note you can specify the mpirun executable name
    - Useful if executable is called '`mpiexec`', '`aprun`', or otherwise on your system
  - Otherwise, see extensive documentation for this namelist in the manual

```
&design
  base_directory = 'path/to/your/design/case'
  what_to_do     = 1
  mpirun_prefix  = 'mpiexec'
/
```

Maximize L/D for Transonic Flow Over a Wing

Running a Function Evaluation

- Things are now ready for execution
- The first thing I typically do is just run a function evaluation to see that the parameterization and all of the inputs are set correctly
- To do this, edit `design.nml` and set `what_to_do` to `1`
- From the `ammo` directory, the command line that is used to run this case is

```
./opt_driver --sleep_delay 5
```

  - The `'--sleep_delay 5'` instructs the design driver to wait 5 seconds in between operations – allows NFS caching to keep up
  - Different systems may require more time (or none)

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Running a Function Evaluation

- The first thing that you will see is MASSOUD evaluating the parameterization for each body, defining the surface grid coordinates at the baseline position
- The flow solver will then start up, but prior to the solve, you will see an auxiliary solution take place that represents the interior mesh movement based on the elasticity equations
  - For this first step at the baseline position, you should see very small numbers for the `"Natural Error Est"` (close to machine zero): this indicates the current surface mesh is very close to the requested surface mesh
- After the actual flow solution takes place, the solver will evaluate each of the objective and constraint functions you posed:

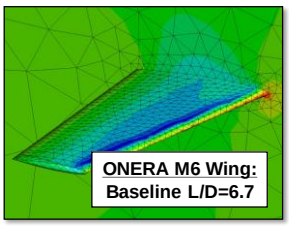
```
Current value of function     1      178.087727962997
```

- This marks the end of a successful function evaluation
- Always wise to plot the flow solver convergence – you want to run enough iterations to get a "reasonable" answer (outputs resolved beyond what you are expecting from design changes), but you don't necessarily need to drive it into the ground

Maximize L/D for Transonic Flow Over a Wing

Running a Function Evaluation

```
[MASSOUD Screen Output]

 Sleeping to allow file system time to catch up...

 Executing: mpiexec nodet_mpi --animation_freq -1 --design_run --irest 0 --write_mesh inviscid

FUN3D 12.7-74063 Flow started 05/20/2015 at 14:38:54 with 24 processes
  [Echo of fun3d.nml]
  [Usual preprocessing info]
 Using linear elasticity to reposition grid...

 reading ../rubber.data ...
 reading:../Rubberize/model.tec.1.sd1
 Iter      Natural Err Est          Error Estimate      Restarts
    0   0.648914658284637E-16   0.000000000000000E+00         0

 Iter           density_RMS  density_MAX   X-location   Y-location   Z-location
    1  0.725550147064997E-04  0.46595E-03  0.34893E-01  0.60683E-01  0.00000E+00
       Lift  0.657554528793843E-01         Drag  0.319926994134964E-01
...
   74  0.207836490870309E-09  0.82846E-08  0.22500E+01  0.45000E+01  0.65000E+01
       Lift  0.881383268442809E-01         Drag  0.132438291863532E-01

 Writing boundary output: inviscid_tec_boundary.dat
  Time step: 74, ntt: 74, Prior iterations: 0

 Writing inviscid.flow (version 11.8) lmpi_io 2
  inserting current history iterations 74
 Time for write: .0 s
 Current value of function            1   178.087727962997
 writing ../rubber.data ...
 global element counts below i4 limit, write as 'stream'
 wrote inviscid.b8.ugrid in     0.0000
 Done.
 Analysis complete.
```



Maximize L/D for Transonic Flow Over a Wing

Running a Gradient Evaluation

- Now lets test a sensitivity analysis
- Edit `design.nml` and set `what_to_do` to `2`
- Submit the job just as before
- The first thing that will take place is a function evaluation, just as before
- After the function evaluation takes place, MASSOUD will fire up again to evaluate the linearizations of the surface mesh coordinates with respect to the design variables
- FUN3D's adjoint solver will then start up:
  - You will see a solution taking place; this is the flowfield adjoint
  - Afterwards, you will see another solution occurring; this is the elasticity adjoint for the mesh
  - The final step is to update the `model.1/rubber.data` file with the sensitivity information
- This marks the end of a successful sensitivity analysis
- Again, it is wise to plot the convergence of the flowfield adjoint system
  - This convergence history is in the `model.1/Adjoint/[project]_hist.dat` file
  - In general, you want 2-3 orders of magnitude convergence; this is usually sufficient for reasonable sensitivity information

Maximize L/D for Transonic Flow Over a Wing

Running a Gradient Evaluation

```
[Function Evaluation]

[MASSOUD Screen Output]

Sleeping to allow file system time to catch up...

Executing: mpiexec dual_mpi --rmstol 1.e-3 --getgrad --irest 0 --force_stream_file
FUN3D 12.7-74063 Adjoint started 05/20/2015 at 14:44:00 with 24 processes
 [Echo of fun3d.nml]
 [Usual preprocessing info]

 Iter            adjoint RMS  adjoint MAX   X location   Y location   Z location
    1  0.707037901636711E+00  0.30235E+01  0.57720E+00  0.95000E+00  0.13288E-01
    2  0.221413741319278E+02  0.77671E+03  0.22500E+01  0.45000E+01  0.65000E+01
    3  0.252132505507981E+02  0.85665E+03  0.22500E+01  0.45000E+01  0.65000E+01
…
   79  0.108404219416308E-02  0.48685E-01  0.20671E+00  0.43560E+01  0.19196E+01
   80  0.961305851711102E-03  0.43086E-01  0.20671E+00  0.43560E+01  0.19196E+01

 Performing linear elasticity adjoint...

 reading ../rubber.data ...
  Using defaults for move_relaxation.schedule.
 Boundary 1 allowed to deform with y=constant constraint
 Iter      Natural Err Est         Error Estimate      Restarts
    0   0.540562915758561E+04   0.100000000000000E+01         0
    1   0.351062487957891E+02   0.649438719756149E-02         0
   11   0.426070657988252E-02   0.788198090485649E-06         0
 writing ../rubber.data ...
 Done.
 Sensitivity analysis complete.
```


Maximize L/D for Transonic Flow Over a Wing

Running the Optimization

- If you got this far, things are looking pretty good – we've checked that everything is set up to run functions and gradients correctly, which is all the optimizer depends on
- Now we're ready to try an actual optimization
  - Edit `design.nml` and set `what_to_do` to `3`; submit the job like usual
- Now you will see a lot of function and gradient evaluations going by, as the optimizer starts to change design variables and search for an optimum solution
- One easy way to monitor progress is to grep your screen output:
  - **`'grep "Current value" screen.output':`**

```
Current value of function           1   178.087727962997
Current value of function           1   137.781363854615
Current value of function           1   109.428434387371
Current value of function           1   95.6295324769749
Current value of function           1   98.1556907116245
Current value of function           1   90.6778940684516
Current value of function           1   90.5396512437177
Current value of function           1   87.6654699895390
Current value of function           1   87.6871503037963
Current value of function           1   87.1318763195701
Current value of function           1   86.8957999910668
Current value of function           1   87.3525539085617
Current value of function           1   86.5144811775675
Current value of function           1   86.8116026938974
Current value of function           1   86.2791203108911
Current value of function           1   86.2399423689607
Current value of function           1   86.2399415584093
```

- You can also observe (but don't change!) the file `model.1/rubber.data`

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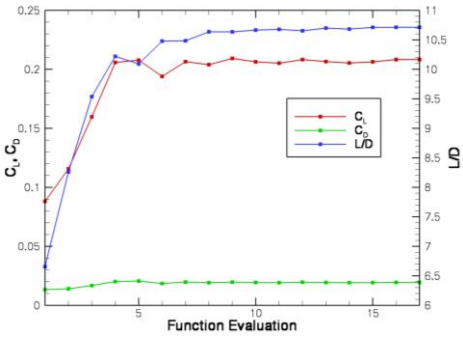
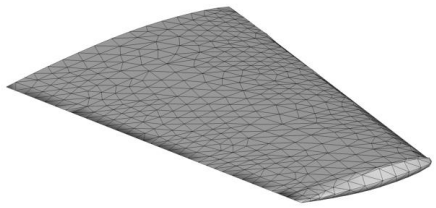
Post Mortem

- After the job finishes, PORT will summarize its performance in the file `model.1/port.output`
- Since each solution is a warm start, you can plot the entire flow solution history contained in `model.1/Flow/[project]_hist.dat`
- A history of the surface geometry is stored in `model.1/Rubberize/surface_history/model.tec.1.sd1.iteration.*`

Redesigned Wing:
L/D=10.7





What Could Possibly Go Wrong?

- The procedure can terminate due to CFD-related problems:
  - Running into negative volumes during a mesh movement (you can plot the history of the surface(s) using the files in `model.1/Rubberize/surface_history`)
    - Watch for invalid surfaces or unusually large changes
    - Be conservative in your lower/upper bounds!
  - The flowfield or the adjoint solution is unstable
    - Problem-dependent; get in touch for advice
- The procedure can also terminate due to hardware/environment problems
  - You run out of allocated time, a node dies, etc.
- Finally, the procedure can terminate if the optimizer has given up:
  - No more progress can be made due to constraints
  - The optimizer has hit the max number of functions/gradients you allowed
  - An optimal solution has been found

List of Key Input/Output Files

Input

- In `description.i` directory:
  - All files necessary to run solutions for `i`th design point (grid files, `fun3d.nml`, etc)
  - All parameterization files for i^{th} parameterized body
  - `command_line.options`
  - `rubber.data`
- `ammo/design.nml`

Output

- All files normally associated with running the solver
- `rubber.data`
- `port.output`
- Design history in `model.1/Rubberize/surface_history`

Summary of Design Optimization for Steady Flows

- That's more or less the basic pieces involved with running an optimization
- Lots of options we did not cover here; see manual or get in touch for help
  - How the wrappers work (`LibF90/analysis.f90`, `LibF90/sensitivity.f90`)
  - Parameterizations other than MASSOUD
  - Multipoint/multiobjective (tutorial on website)
  - Constrained problems (tutorial on website)
  - Running with other optimization packages (tutorial on website)
  - Body grouping, spatial transforms
  - Archiving files during optimization
  - Overset grids
  - Forward-mode sensitivity analysis using complex variables
  - Unsteady design (later session)

General Advice

- Become very comfortable with the flow solver
- Work the tutorials
- Learn how to set up parameterizations using MASSOUD and/or bandaids
- Try plugging in your own grids/parameterizations in the tutorials
- Ask questions – it's actually not that bad once you get up the learning curve

What We Learned

- General approach used by FUN3D for design optimization
- What is an adjoint
- What does a function/gradient evaluation consist of in terms of CFD
- Design variables in FUN3D
- Functions/constraints in FUN3D
- What is required of a geometry parameterization tool
- How to set up the inputs required for design optimization
- How to run function, gradient evaluations
- How to perform a basic design optimization
- What to watch out for and how to interpret results