DAFoam Workshop 2021

v2.2.5

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Objectives

After this workshop, you should be able to

- Get familiar with the high-fidelity design optimization framework MACH-Aero.
- Describe the details in the OpenFOAM and DAFoam configuration files (e.g., controlDict, fvSchemes, runScript.py).
- Run aerodynamic optimization with DAFoam.
- Adjust the configuration files for a new case

A few notes

- We assume you are familiar with basic concepts of **CFD**, e.g., finite volume method, initial and boundary conditions, and discretization, and basic **Linux commands**, e.g., create, copy, modify, and save files.
- This workshop focuses on how to **use** DAFoam.
- This workshop has **hands-on** examples.
- **Stop** me at any time if you have questions.
- The online meeting will be **recorded**.
- All the materials are available at `https://github.com/dafoam/workshops`.

Outline

1 DAFoam Introduction

2 MACH-Aero Framework

3 Airfoil aerodynamic optimization

4 Wing aerodynamic optimization

DAFoam Introduction

What is DAFoam ?

DAFoam : **D**iscrete **A**djoint with Open**FOAM**

DAFoam can be used to :

- Compute derivatives for a large number of design variables
- Couple with gradient-based algorithms for optimizations
- Run OpenFOAM primal solvers to generate CFD samples
- Easily access the residuals, indexing, and file IO operations, etc.

What is OpenFOAM ?

- OpenFOAM : **Open**-source **F**ield **O**peration **A**nd **M**anipulation
- OpenFOAM is written in C++ and contains libraries to facilitate numerical operation of field variables (e.g., solving linear equations, computing partial derivatives in a PDE)
- Building on these libraries, OpenFOAM includes more than 80 solvers (binary executives) that solve a wide range of PDEs.
- OpenFOAM also contains a wide range of utilities for pre- and post-processing (e.g., generate unstructured meshes, check mesh quality)

DAFoam supports only the ESI OpenCFD branch of OpenFOAM v1812

There are three main branches for OpenFOAM :

- **ESI OpenCFD**. Latest version : OpenFOAM-v2012
- The OpenFOAM Foundation. Latest version : OpenFOAM-v8
- Extend project. Latest version : foam-extend-4.0

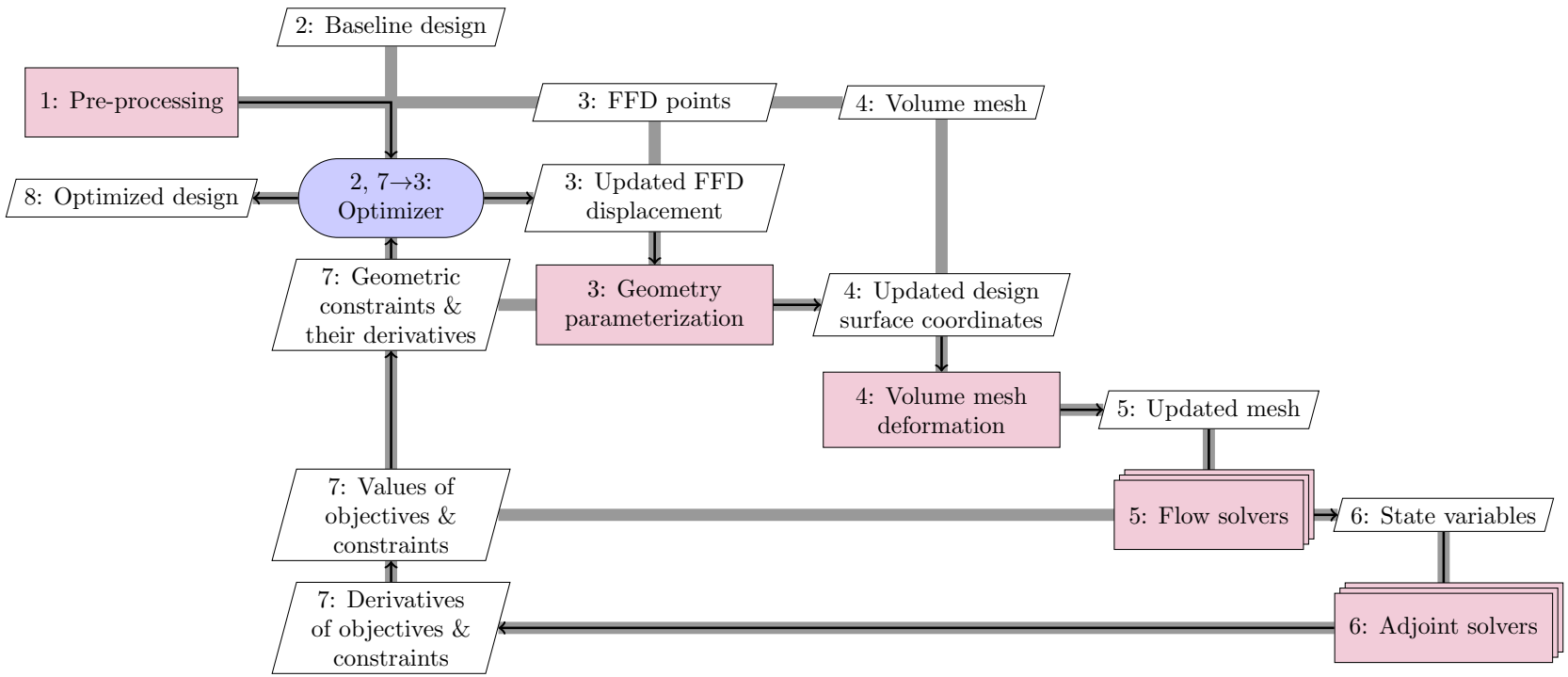
DAFoam development timeline

- 2014-04 Project started in the MDOLab, University of Michigan
- 2018-05 First DAFoam paper published in Computers & Fluids
- 2019-06 Code became open source
- 2020-01 Extended for multiple solvers
- 2020-07 DAFoam upgraded to version 2
- 2020-12 Added Jacobian-free adjoint with AD

MACH-Aero Framework

MACH-Aero framework

MACH-Aero is a high-fidelity design optimization framework developed by the MDOLab at University of Michigan. MACH-Aero is open source at : `https://github.com/mdolab/MACH-Aero`



XDSM diagram for the MACH-Aero framework. The diagonal blocks are the modules (libraries) used in an optimization. The off-diagonal blocks are date transfer. All the modules are wrapped with Python.

Pre-processing module

Goal : Generate mesh and free-form deformation (FFD) control points

Mesh needs to be in OpenFOAM format. Possible tools :

- blockMesh and snappyHexMesh utilities from OpenFOAM.
- pyHyp (`https://github.com/mdolab/pyhyp`) from MACH-Aero.
- Commercial software such as ICEM-CFD, Pointwise.

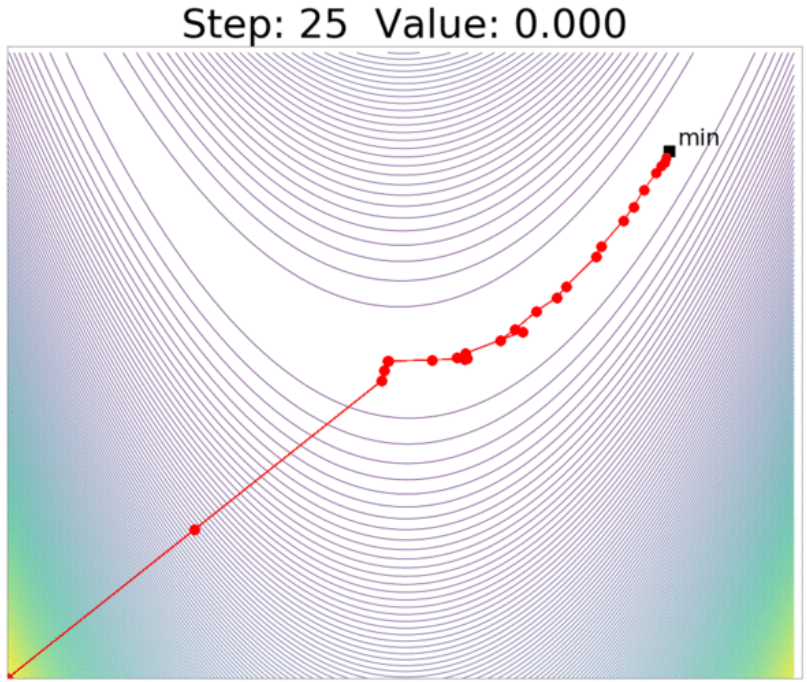
FFD file needs to be in the **plot3D** format. Possible tools :

- Python scripts such as genFFD.py.
- Commercial software that can generate structured meshes in the plot3D format, e.g., ICEM-CFD

Optimizer module

Goal : Receive function values and derivatives and update the design variables

MACH-Aero uses pyOptSparse to set up optimization problems `https://github.com/mdolab/pyoptsparse` (Design variables, objective and constraint functions, and optimizers : SNOPT, SLSQP, IPOPT, etc.)

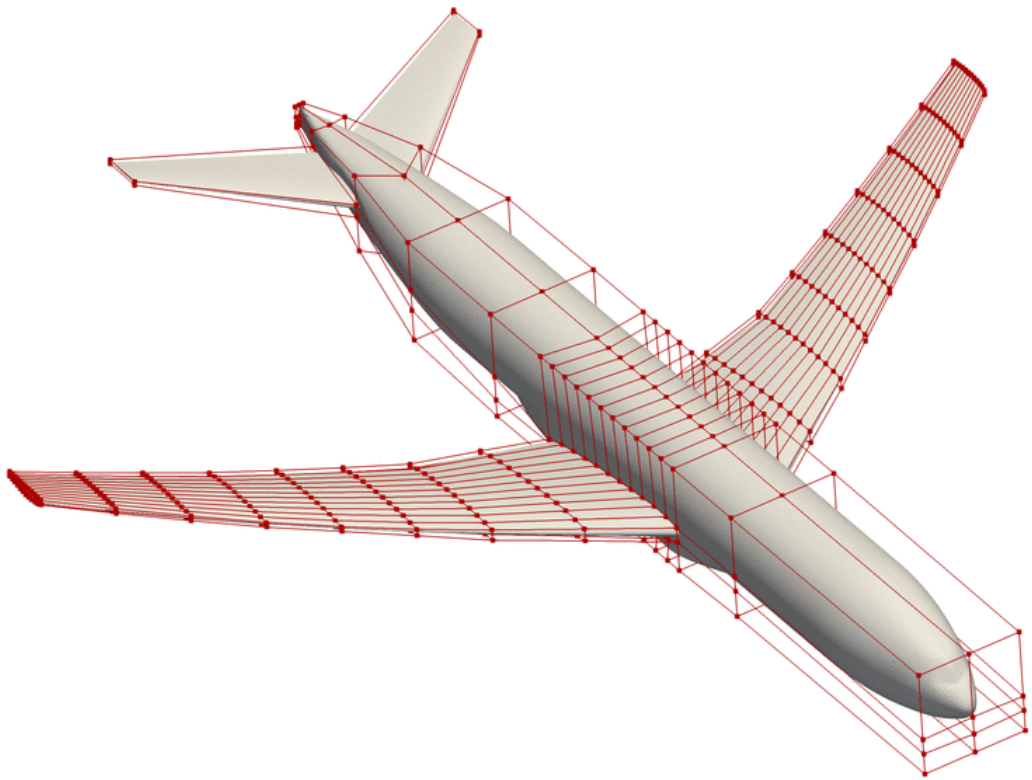


Optimization of the Rosenbrock function using gradient-based algorithms

Geometry parameterization module

Goal : Receive the updated design variables and change the design surface geometry or mesh.

We use the pyGeo module to parameterize the geometry through the free-form deformation (FFD) approach
(`https://github.com/mdolab/pygeo`)

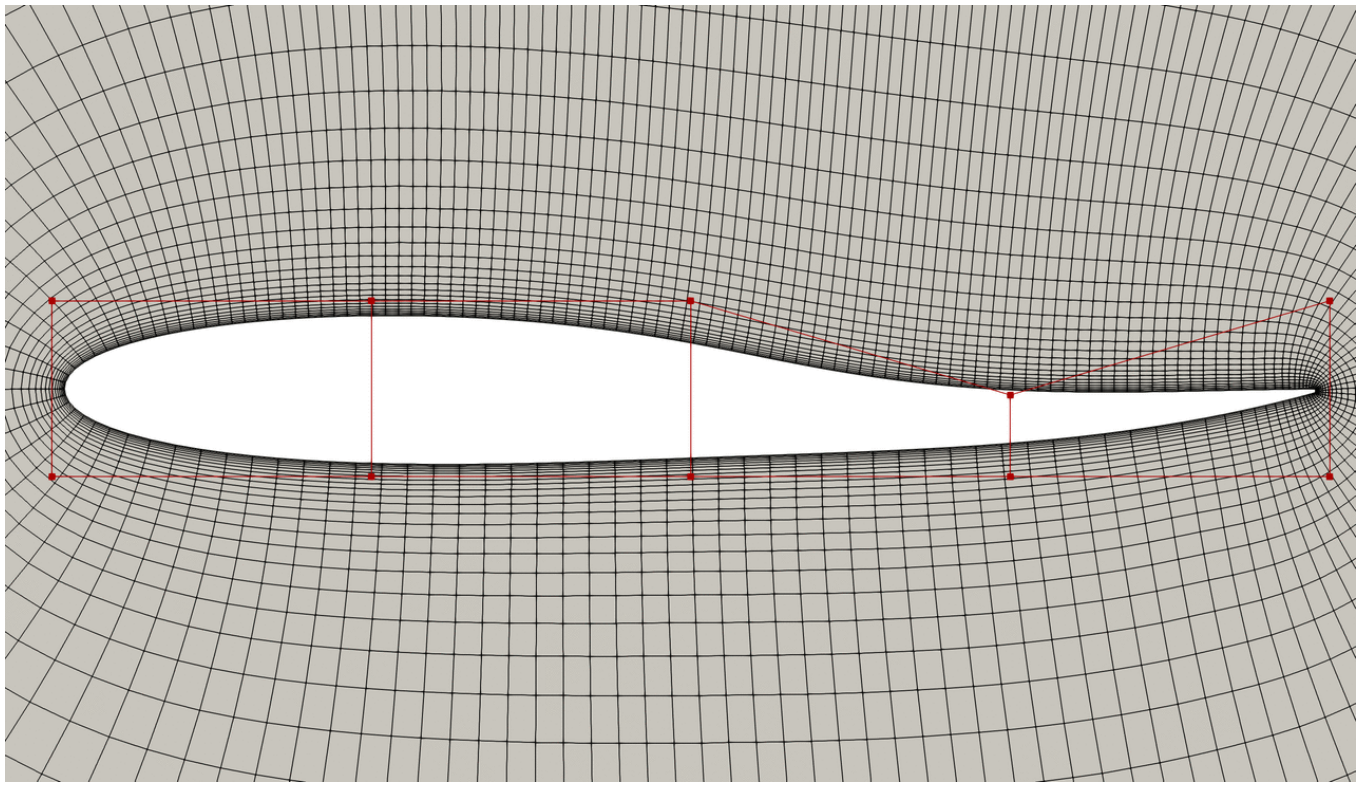


FFD control points (red) for an aircraft configuration

Volume mesh deformation module

Goal : Receive the design surface mesh and update the volume mesh coordinates

We use the IDWarp module to deform the volume mesh through an inverse distance weighting approach. It works for both structured and unstructured meshes. (`https://github.com/mdolab/idwarp`).

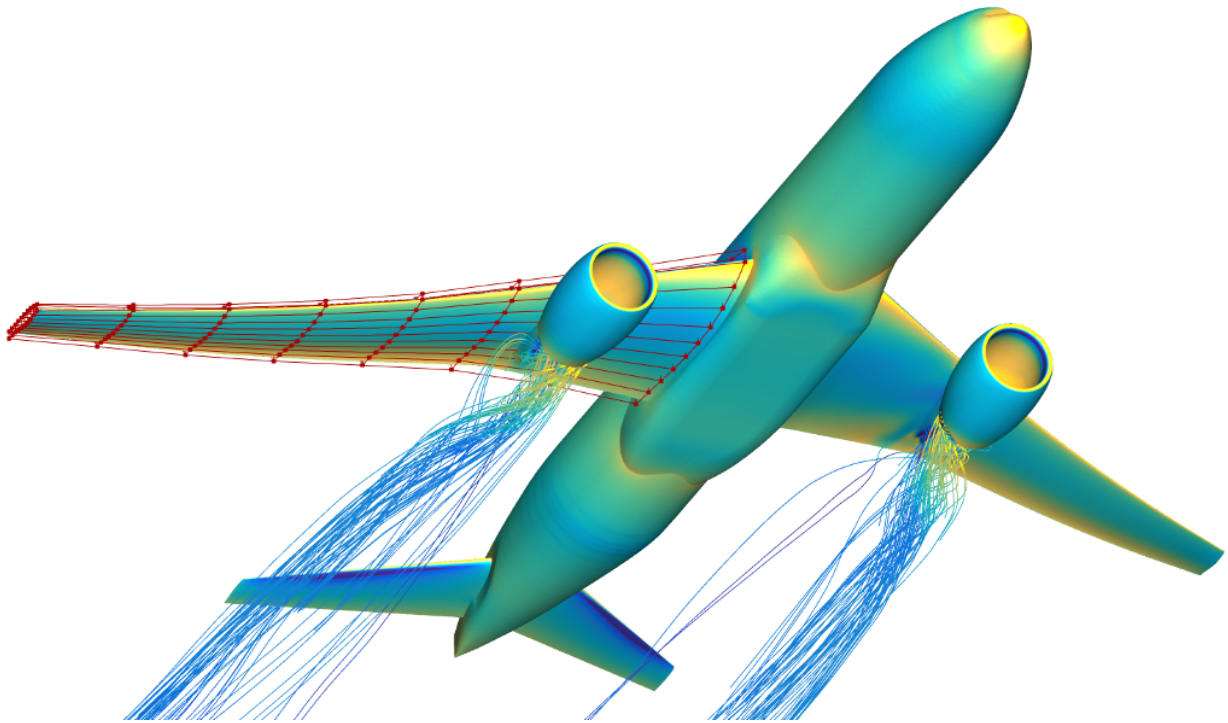


Example of deformed mesh

Primal solution module

Goal : Receive the update volume mesh and compute the objective and constraint functions, as well as state variables (e.g., velocity and pressure). For fluid mechanics, it is also called flow simulation.

We use Cython to compile OpenFOAM's solvers, e.g., simpleFoam, into C++ libraries and call them from Python. We do **NOT** use the OpenFOAM's built in binary solvers in optimization.

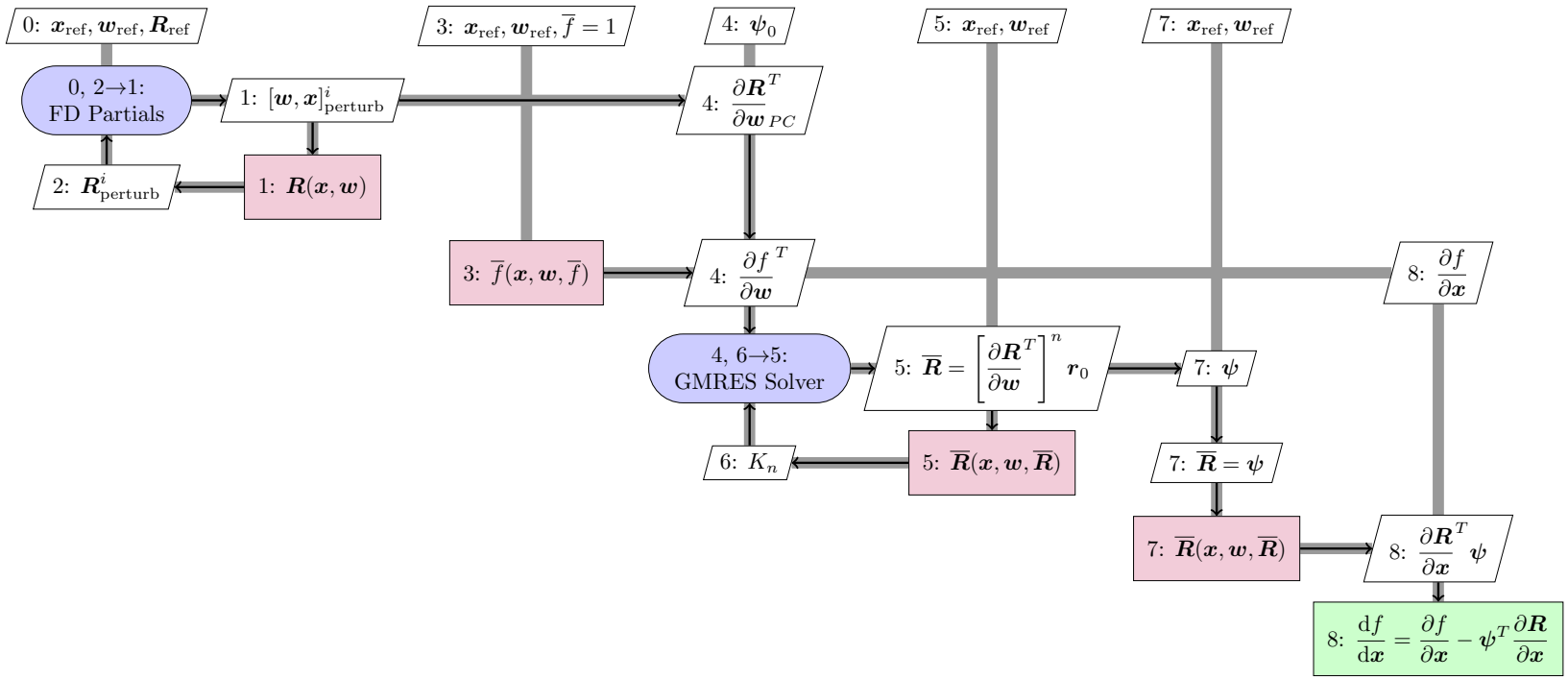


Aircraft aerodynamic analysis with OpenFOAM

Adjoint solution module

Goal : Receive the state variables and compute the total derivatives of objective functions with respect to all design variables

We implemented efficient derivative computation in DAFoam using the Jacobian-free adjoint approach. The derivative is machine-precision accurate.



Jacobian-free adjoint diagram in DAFoam.

Airfoil aerodynamic optimization

Outline

- How to use the DAFoam docker image
- How to run an optimization
- How to visualize the result
- How to read the optimization log file
- Details of configuration files
- How to change the configuration files for a new case

How to use the DAFoam docker image

Download DAFoam Docker image and examples

The easiest way to run DAFoam optimizations is to use the DAFoam Docker image

First, install Docker following this website :

`https://dafoam.github.io/mydoc_get_started_download_docker.html`

Once done, verify the installation by running :

```
docker --version
```

Then run this command to download the DAFoam Docker image :

```
docker pull dafoam/opt-packages:v2.2.5
```

Finally, download the workshop examples at :

`https://github.com/dafoam/workshops`

How to start a Docker container

If you use Linux or MacOS, open a terminal and use the `cd` command to go this folder on your local computer. If you put the workshops folder in the $HOME directory, the command may look like :

```
cd $HOME/workshops/2021_Summer/examples/naca0012/incompressible
```

Then, run this command to start a Docker container :

```
docker run -it --rm -u dafoamuser --mount \
"type=bind,src=$(pwd),target=/home/dafoamuser/mount" \
-w /home/dafoamuser/mount dafoam/opt-packages:v2.2.5 bash
```

If you use Windows, open the Prompt Command terminal, use the `cd` command to go to the above folder, and run this command :

```
docker run -it --rm -u dafoamuser --mount \
"type=bind,src=%cd%,target=/home/dafoamuser/mount" \
-w /home/dafoamuser/mount dafoam/opt-packages:v2.2.5 bash
```

Once in a Docker container, you should see something like :

```
dafoamuser@cddb89839078:~/mount$
```

More information about the Docker container

What does the above command do ?

- Start a Docker container (a light-weight virtual machine)
- Mount (link) your computer's current directory to the container's /home/dafoamuser/mount directory
- Login the container as dafoamuser and go to the mounted dir
- Set the relevant DAFoam environmental variables.

A few notes :

- Treat the Docker container as disposable, i.e., start one container for one optimization run. If the optimization is running and you want to kill it, press `ctrl+c` or `ctrl+\` to kill the job, then run `exit` to quit the container
- Do not store simulation results in the container because they will be deleted after you exit. Run simulations on the mounted space `/home/dafoamuser/mount` instead
- dafoamuser has the sudo privilege and its password is : dafoamuser

How to run an optimization

How to run an optimization (1/3)

Summary of the naca0012/incompressible case.

Optimizer	IPOPT
Flow and adjoint solvers	DASimpleFoam
Geometry	NACA0012
Mesh	4 032 cells
Objective function	C_d
Design variables	20 FFDs and α
Constraint	$C_l = 0.5$, thickness, volume, TE/LE
U_∞	10 m/s
Re	6.7$\times 10^5$
Turbulence Model	Spalart–Allmaras

How to run an optimization (2/3)

Once in a Docker container, you should see something like :

```
dafoamuser@cddb89839078:~/mount$
```

Run this command to double check if you are in the correct directory :

```
ls
```

After running the above command, you should see something like :

```
0.orig Allclean.sh FFD constant genAirFoilMesh.py paraview.foam
preProcessing.sh profiles runScript.py system
```

How to run an optimization (2/3)

Once in a Docker container, you should see something like :

```
dafoamuser@cddb89839078:~/mount$
```

Run this command to double check if you are in the correct directory :

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```

After running the above command, you should see something like :

```
0.orig Allclean.sh FFD constant genAirFoilMesh.py paraview.foam
preProcessing.sh profiles runScript.py system
```

How to run an optimization (3/3)

Now you should be in the right directory. There are two main steps to run a case.

First, run this command for pre-processing (mesh generation) :

```
./preProcessing.sh
```

Then, use this command to run the flow simulation :

```
python runScript.py | tee 2>&1 logOpt.txt
```

The optimization log will be printed to the screen and saved to `logOpt.txt`. In addition, the optimizer will write a separate log to the disk. For the IPOPT optimizer we use in this tutorial, it is `opt_IPOPT.txt`.

The optimization converged in 17 steps and took about 10 minutes.

How to visualize the results

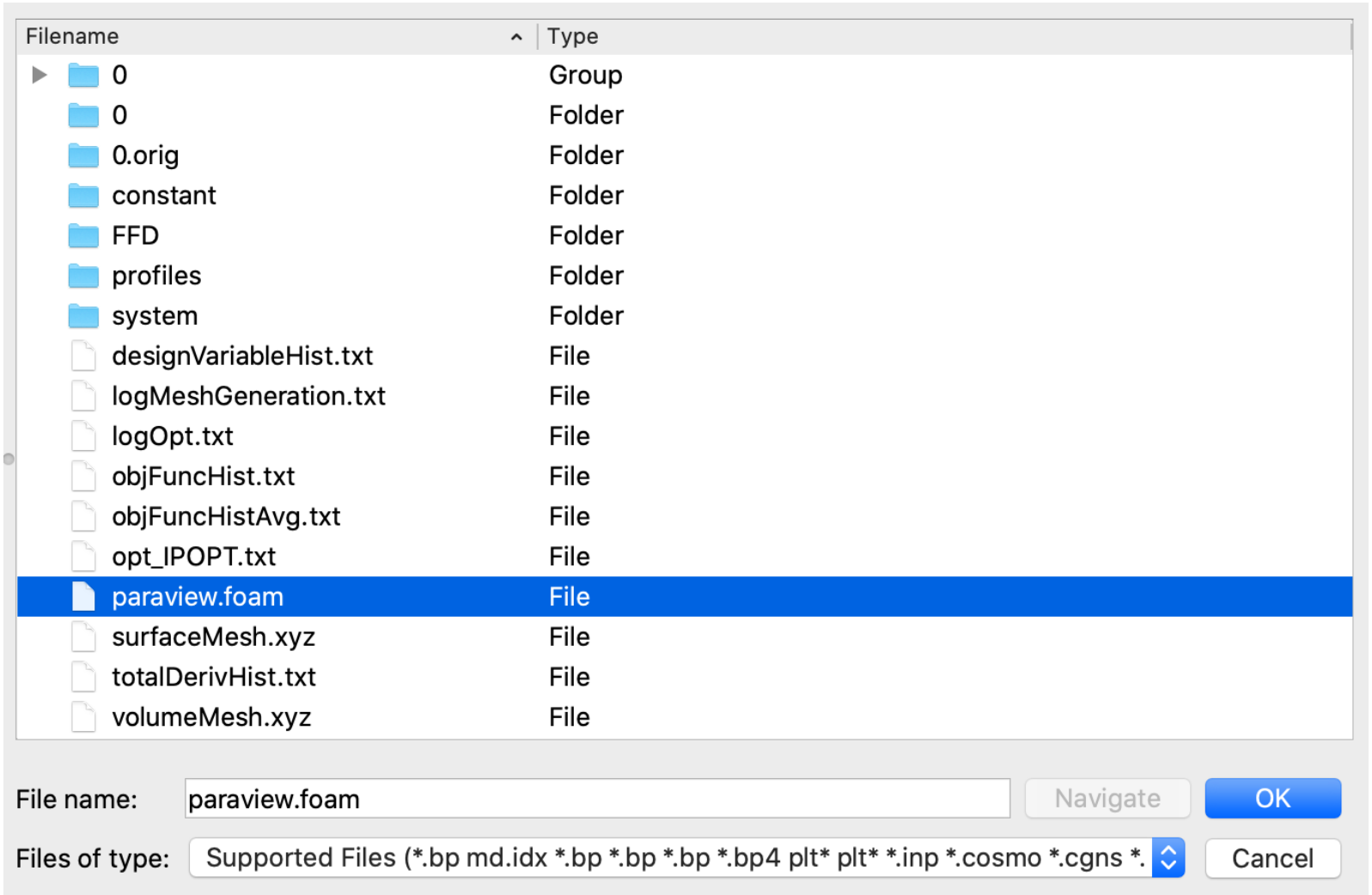
How to visualize the results (1/7)

We use Paraview ; an open-source post-processing tool to visualize the optimization results.

- Download Paraview at `https://www.paraview.org/download/`.
- For MacOS, download `ParaView-5.8.1-MPI-OSX10.12-Python2.7-64bit.dmg` and install the .dmg package
- For Ubuntu, download `ParaView-5.8.1-MPI-Linux-Python2.7-64bit.tar.gz`, extract the tarball, and run the paraview executive in the ParaView-5.8.1-MPI-Linux-Python2.7-64bit/bin folder
- For Windows, download `ParaView-5.8.1-Windows-Python3.7-msvc2015-64bit.zip`, extract the zip and run the paraview executive in the ParaView-5.8.1-Windows-Python3.7-msvc2015-64bit/bin folder

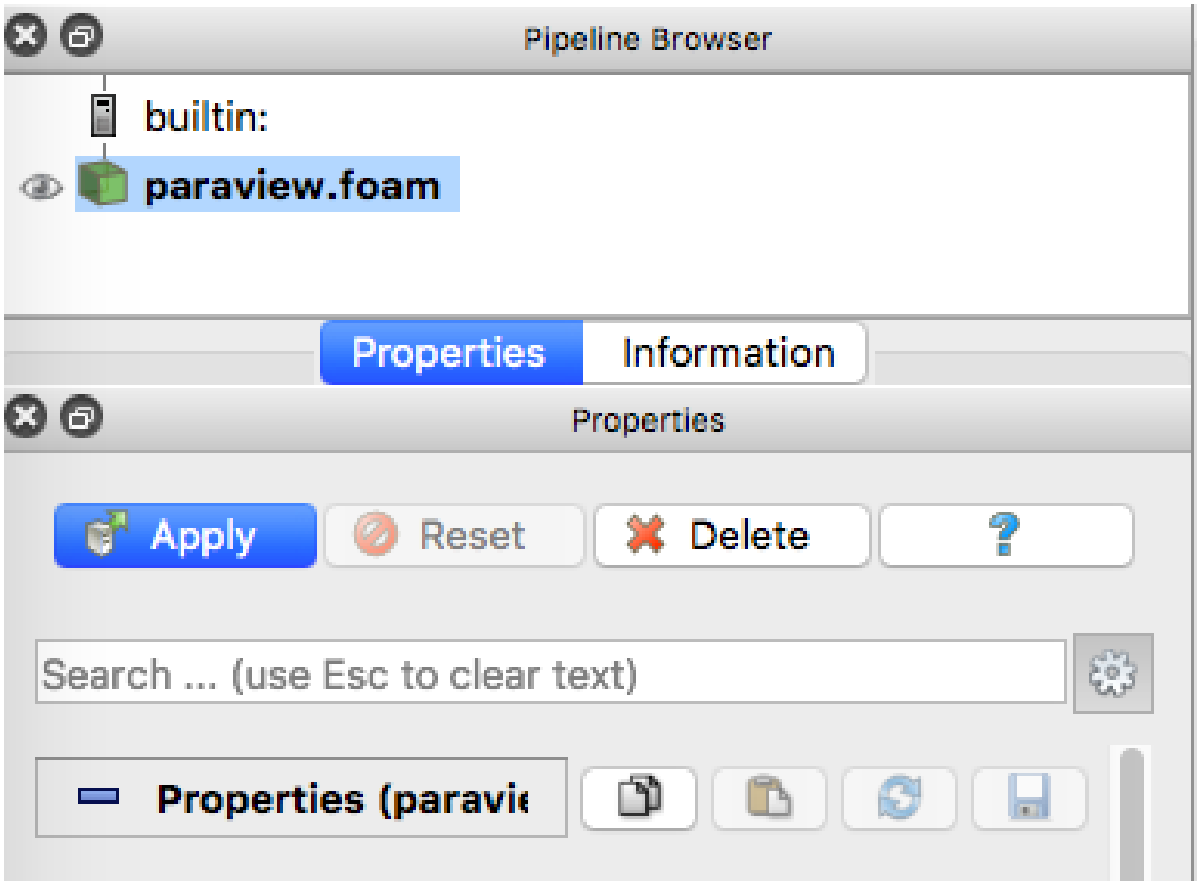
How to visualize the results (2/7)

In Paraview, click `File->Open`. In the pop up window, select `paraview.foam` in the `naca0012/incompressible` folder, and click `OK`.



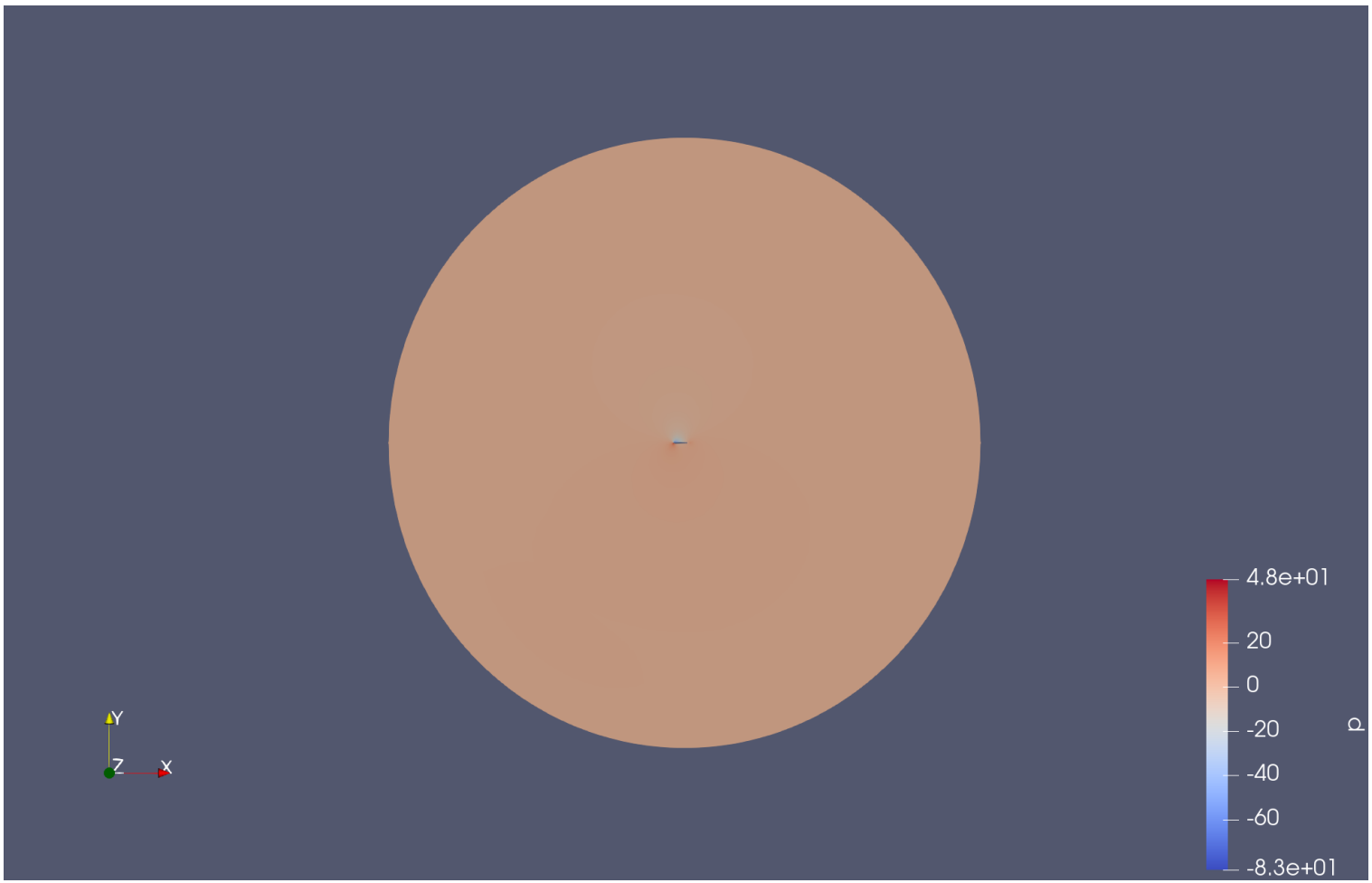
How to visualize the results (3/7)

Then, on the left properties window, hit `Apply`.



How to visualize the results (4/7)

Finally, you can see the simulation results for the NACA0012 airfoil on the right layout window

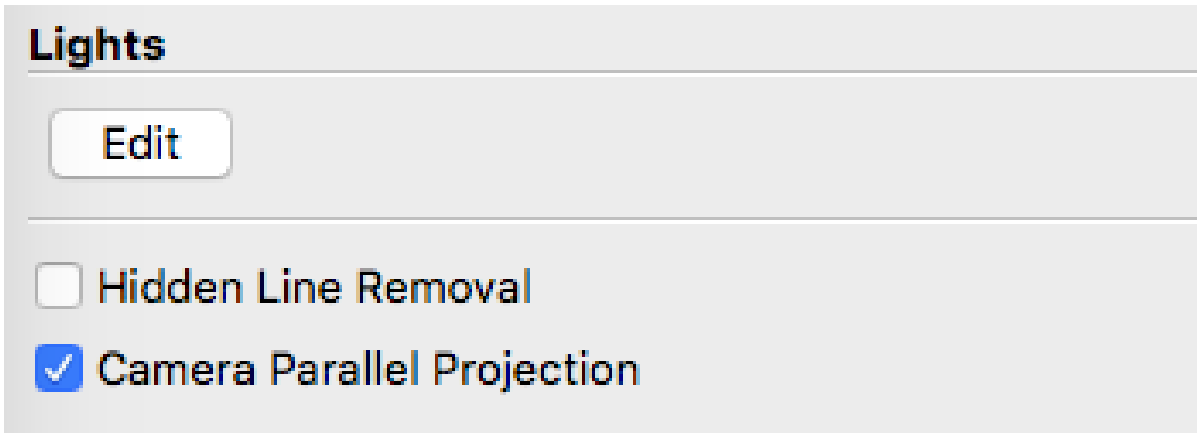


How to visualize the results (5/7)

You can scroll your mouse wheel to zoom-in and zoom-out, and hold your middle wheel, you can pan the view.

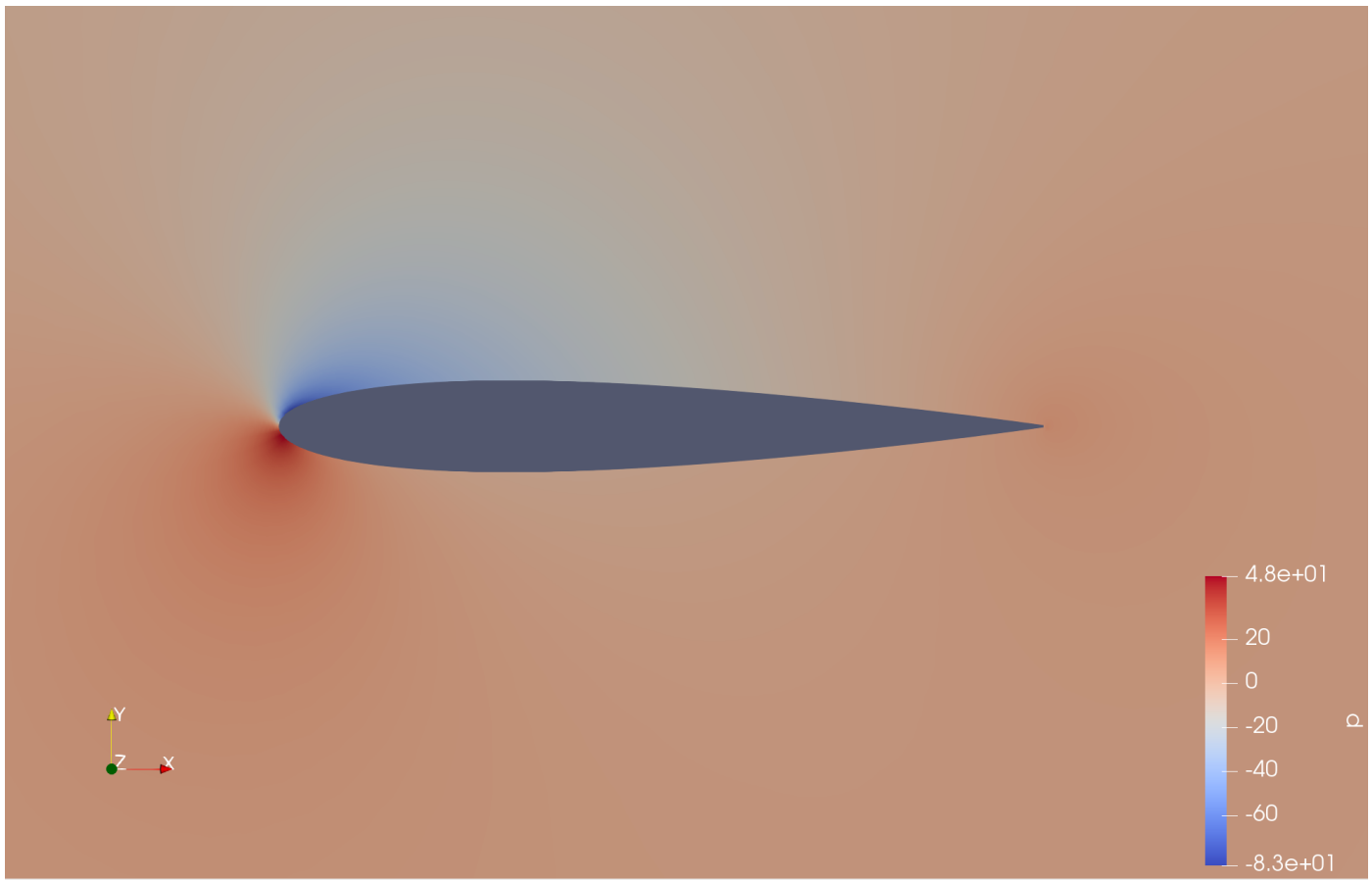
We also recommend enable the `Camera Parallel Projection` option by first clicking this icon on the left properties bar

Then, scroll down and check `Camera Parallel Projection`



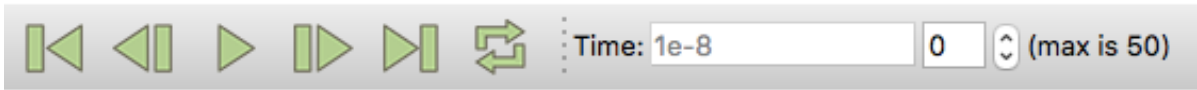
How to visualize the results (6/7)

Now, you can zoom-in to view the detailed pressure field around the airfoil (scroll your mouse wheel).



How to visualize the results (7/7)

Now you can hit the `play` button on the top bar to visualize the evolution of pressure and shape during the optimization.



Play

If you want to look at another variable, change the range of the variable, or change the surface representation (e.g., visualize the mesh), check the top bar as shown below.

Set data range

Variable to load

Surface representation

How to read optimization log files

How to read `opt_IPOPT.txt`

`opt_IPOPT.txt` is the very first file we need to check during or after the optimization. We want to look at the objective, feasibility (inf_pr) and optimality (inf_du).

A successful optimization should reduce the objective function values, and the feasibility and optimality should drop below the prescribed tolerance (1e-6 for this tutorial).

```
iter    objective   inf_pr  inf_du lg(mu) ||d|| lg(rg) alpha_du alpha_pr ls
0  2.0820238e-02 1.61e-07 1.43e-02 0.0 0.00e+00 -  0.00e+00 0.00e+00 0
1  2.0522813e-02 3.29e-04 6.87e-02 -5.9 7.45e-03 - 9.54e-01 1.00e+00h 1
2  1.9625311e-02 2.41e-03 2.67e-01 -7.3 2.14e-02 - 9.69e-01 1.00e+00h 1
3  1.9219882e-02 1.06e-03 4.45e-03 -4.4 3.51e-02 - 9.89e-01 1.00e+00h 1
4  1.9054431e-02 1.56e-04 2.14e-03 -4.9 9.26e-02 - 1.00e+00 1.00e+00h 1
5  1.8964830e-02 5.90e-05 1.25e-03 -5.8 5.98e-02 - 1.00e+00 1.00e+00h 1
.........
13  1.7376934e-02 2.93e-05 2.45e-04 -6.7 2.93e-02 - 1.00e+00 1.00e+00h 1
14  1.7376357e-02 6.27e-07 3.25e-06 -8.4 7.27e-03 - 1.00e+00 1.00e+00h 1
15  1.7376337e-02 1.09e-07 1.56e-06 -10.2 3.16e-03 - 1.00e+00 1.00e+00h 1
16  1.7376337e-02 6.04e-10 1.03e-06 -11.0 1.07e-04 - 1.00e+00 1.00e+00h 1
17  1.7376337e-02 2.50e-09 5.61e-07 -11.0 6.01e-04 - 1.00e+00 1.00e+00h 1
```

Flow and adjoint equations

In flow solution, the steady-state incompressible Navier-Stokes equations are solved using the finite-volume mesh with the SIMPLE algorithm :

$$\nabla \cdot \boldsymbol{U} = 0$$

$$(\boldsymbol{U} \cdot \nabla)\boldsymbol{U} + \nabla p - \nabla \cdot \nu_{eff}(\nabla \boldsymbol{U} + \nabla \boldsymbol{U}^T) = 0$$

In adjoint solution, the adjoint equation is solved using a Jacobian free method to get the adjoint vector ψ

$$[\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{W}}]^T \psi = \frac{\partial f}{\partial \boldsymbol{W}}$$

Then, the adjoint vector is used to compute the total derivative $\mathrm{d}f/\,\mathrm{d}\boldsymbol{x}$.

$$\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}} = \frac{\partial f}{\partial \boldsymbol{x}} - [\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{x}}]^T \psi$$

How to read `logOpt.txt` (1/8)

Basic information.

```
-------------------------------------------------------------------------------
|                                DAFoam v2.2.5                                |
-------------------------------------------------------------------------------
Selecting RAS turbulence model SpalartAllmaras // Turbulence model
...
Global Cells: 4032 // Mesh cells
DAFoam option dictionary: // All DAFoam options
{
  solverName     DASimpleFoam;
  primalMinResTol 1e-08;
  ...
}
+---------------------------------------+
|     All IDWarp Options:               |
+---------------------------------------+
 {'LdefFact': 1.0, // All IDWarp options
  'aExp': 3.0,
  'alpha': 0.25,
  ....
#-----------------------------#
Total Volume Nodes :   17640
#-----------------------------#
{'all': [3, 4], // Design surface information
 'allsurfaces': [0, 1, 2, 3, 4],
 'designsurfaces': [3, 4],
```

How to read `logOpt.txt` (2/8)

Before running the optimization, it automatically finds the angle of attack to match the target CL (0.5). This is also called solveCL.

```
+-------------------------------------------------------------------------+
|               Running SolveCL to find alpha that matches target CL      |
+-------------------------------------------------------------------------+
eps: 0.01 tol: 0.0001 maxit: 10 // eps: solveCL finite-difference step size
+-------------------------------------------------------------------------+
|                   Evaluating Objective Functions 000                    |
+-------------------------------------------------------------------------+
Design Variables:
{'alpha': array([5.+0.j]), ... }
...
Setting U = (9.961947 0.87155743 0) at inout // setting U field based on alpha
...
Time = 400
U Initial residual: (1.5179219e-08 1.1995847e-08 1.5597788e-08)
U   Final residual: (1.1435775e-09 9.1588646e-10 1.3379879e-09)
...
yPlus min: 14.568982 max: 100.52633 mean: 60.130968 // flow solution prints y+
CD-part1-force: 0.020495205 // CD and CL at Time = 400
CL-part1-force: 0.48750507
ExecutionTime = 8.69 s ClockTime = 10 s
Time = 425 // flow converged in 425 steps
Minimal residual 9.8369143e-09 satisfied the prescribed tolerance 1e-08
alpha: 5.000000, CL: 0.487505 // first solved alpha and CL
... // repeat the solveCL
alpha: 5.139185, CL: 0.500000 // final alpha and CL
Completed! alpha = 5.139185
```

How to read `logOpt.txt` (3/8)

Once solveCL is done, the optimization starts. It first prints the initial design variables, constraints, bounds, etc.

```
Optimization Problem -- opt
=============================================================================
Objective Function: aeroFuncs
Objectives
   Index  Name            Value         Optimum
       0  CD     0.E+00     0.E+00
Variables (c - continuous, i - integer, d - discrete) // design variables
   Index  Name        Type      Lower Bound          Value      Upper Bound    Status
       0  alpha_0       c      0.E+00     5.139185E+00    1.E+01
       1  shapey_0      c     -1.E-01     0.E+00     1.E-01
       2  shapey_1      c     -1.E-01     0.E+00     1.E-01
       3  shapey_2      c     -1.E-01     0.E+00     1.E-01
       ....
Constraints (i - inequality, e - equality) // constraints
Index  Name                          Type    Lower     Value    Upper   Status  Pi(N/A)
0  DVCon1_volume_constraint_0          i   1.E+00    0.E+00    3.E+00    L    9.E+100
1  DVCon1_thickness_constraints_0      i   8.E-01    0.E+00    3.E+00    L    9.E+100
2  DVCon1_thickness_constraints_0      i   8.E-01    0.E+00    3.E+00    L    9.E+100
3  DVCon1_thickness_constraints_0      i   8.E-01    0.E+00    3.E+00    L    9.E+100
    ....
```

How to read `logOpt.txt` (4/8)

Then, the coloring is computed. The coloring information will be used to compute the Jacobian matrices, e.g., dRdWTPC.

```
+-------------------------------------------------------------------------+
|                         Running Coloring Solver                         |
+-------------------------------------------------------------------------+
...
Calculating dRdW Coloring..
number of uncolored: 36223 1
ColorSweep: 100 8 s
number of uncolored: 23511 1
ColorSweep: 200 10 s
number of uncolored: 11178 1
ColorSweep: 300 12 s
number of uncolored: 544 1
ColorSweep: 324 13 s
...
Calculating dFdW CD-part1 Coloring...
...
```

How to read `logOpt.txt` (5/8)

It first solves the flow and computes the initial objective function.

```
+-------------------------------------------------------------------------+
|                    Evaluating Objective Functions 005                   |
+-------------------------------------------------------------------------+
Design Variables:
OrderedDict([('alpha', array([5.139184882352932])), ('shapey', array([0., ...
     0.]))]) // all design variable values for this flow solution.
...
// Check mesh quality before actually run the flow solution. If checkMesh fails,
      the flow solution will not run.
Checking mesh quality for time = 0
Overall domain bounding box (-17.36956 -18.580929 0) (18.72809 18.580929 0.1)
Mesh has 3 geometric (non-empty/wedge) directions 3{1}
Mesh has 3 solution (non-empty) directions 3{1}
Boundary openness (-4.6536375e-19 -3.9490374e-19 -5.6880426e-16) OK.
Max cell openness = 2.4445483e-16 OK.
Max aspect ratio = 97.871471 OK.
Minimum face area = 2.2541308e-06. Maximum face area = 4.2248202. Face area
     magnitudes OK.
Min volume = 2.2541308e-07. Max volume = 0.42248202. Total volume = 105.2804.
     Cell volumes OK.
Mesh non-orthogonality Max: 22.749125 average: 2.5479332
Non-orthogonality check OK.
Face pyramids OK.
Max skewness = 1.4324517 OK.
Coupled point location match (average 0) OK.
Mesh OK. // checkMesh passes
```

How to read `logOpt.txt` (6/8)

After the flow solution converges, it will print the objective and constraint function values.

```
Time = 200
U Initial residual: (8.0489602e-08 6.5681323e-08 1.9305741e-07) // U residual
U  Final residual: (6.1866068e-09 4.979837e-09 1.6009007e-08)
p Initial residual: 2.1616161e-07 // p residual
p  Final residual: 1.4795847e-08
Time step continuity errors : sum local = 3.8277947e-10
                              global = -1.6582597e-11
                           cumulative = 0.00015887025
nuTilda Initial residual: 2.2029223e-09 // turbulence variable residual
         Final residual: 2.1250661e-10
Bounding nuTilda>1e-16
yPlus min: 14.224415 max: 101.14689 mean: 59.937027 // y+
CD-part1-force: 0.020820085 // drag coefficient
CL-part1-force: 0.50000308 // lift coefficient
ExecutionTime = 51.83 s ClockTime = 58 s
Time = 286
Minimal residual 9.8182915e-09 satisfied the prescribed tolerance 1e-08
// Print the converged objective and constraint functions for this solution
Objective Functions:
{'DVCon1_volume_constraint_0': 1., 'DVCon1_thickness_constraints_0': array([1.,
     ... 1.]), 'CD': 0.020820238430313175, 'CL': 0.5000001610403806, 'fail':
     False}
Flow Runtime: 6.38911
```

How to read `logOpt.txt` (7/8)

Next, the adjoint is solved. Once done, the sensitivity will be printed.

```
+---------------------------------------------------------------------+
|              Evaluating Objective Function Sensitivities 000        |
+---------------------------------------------------------------------+
// Use coloring-FD method to compute preconditioner matrix dRdWTPC
Computing dRdWTPC 60 s
dRdWTPC: 0 of 325, ExecutionTime: 63 s
dRdWTPC: 100 of 325, ExecutionTime: 66 s
dRdWTPC: 200 of 325, ExecutionTime: 69 s
dRdWTPC: 300 of 325, ExecutionTime: 71 s
dRdWTPC: 324 of 325, ExecutionTime: 72 s
// Use reverse-mode AD to compute dFdW
Calculating dFdW using reverse-mode AD
// Solve dRdWT * psi = dFdW
Solving Linear Equation... 71 s
Main iteration 0 KSP Residual norm 3.216462234506e-02 72 s
Main iteration 100 KSP Residual norm 2.746557320396e-06 78 s
Main iteration 168 KSP Residual norm 3.080824419769e-10 82 s
// Compute dFdXv and dRdXV^T * psi using reverse mode AD
Calculating dFdXv using reverse-mode AD
Calculating [dRdXv]^T * Psi using reverse-mode AD
// print the sensitivity
Objective Function Sensitivity:
{'DVCon1_volume_constraint_0': {'alpha': array([[0.]]), 'shapey': array
     ([[-0.474621871902189 , -0.4746218719021887, 0.4746218719021891,
     ..., -0.2001199262333018, 0.2001199262333017,
      0.2001199262333014]])}, 'DVCon1_thickness_constraints_0': {'alpha': array
           ([[0.],
```

How to read `logOpt.txt` (8/8)

The above flow-adjoint solution will be repeated until the optimization converges. Then, the summary of optimization will be printed.

```
Optimization Problem -- opt
=============================================================================
    Objective Function: calcObjFuncValues
    Solution:
-----------------------------------------------------------------------------
Total Time:              708.2673 // total run time
User Objective Time :   192.3354
User Sensitivity Time : 514.5540
Calls to Objective Function : 26
Calls to Sens Function :     18
Objectives
    Index  Name           Value         Optimum
        0  CD       1.737634E-02    0.E+00 // optimized objective function
Variables (c-continuous, i-integer, d-discrete) // final design variables
    Index  Name       Type     Lower Bound          Value     Upper Bound    Status
        0  shapey_0      c    -1.E-01    1.157639E+00    1.E-01
        1  shapey_1      c    -1.E-01    1.481845E-02    1.E-01
....
Constraints (i - inequality, e - equality) // final constraint
  Index  Name                                Type         Lower          Value
       Upper    Status       Pi
  0  DVCon1_volume_constraint_0   i   1.E+00    1.E+00    3.E+00        l    9.E+100
  1  DVCon1_thickness_constraints_0 i 8.E-01   8.E-01    3.E+00        l    9.E+100
....
  33  CL                          e   5.E-01    5.E-01    5.E-01             9.E+100
```

The `designVariableHist.txt` file

History of design variables for each optimization iteration.

```
"Optimization_Iteration_000":
{
    "alpha": [ 5.139184882352932e+00 ],
    "shapey": [ 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00, 0.000000000000000e+00 ]
},

"Optimization_Iteration_001":
{
    "alpha": [ 5.138060485220683e+00 ],
    "shapey": [ -1.235388756207046e-05, -1.235388756207046e-05, 1.235388756207046e-05, 1.235388756207046e-05, 3.971763945166782e-03, 3.971763945166782e-03, 5.496896582781271e-03, 5.496896582781271e-03, 8.426675160166613e-05, 8.426675160166613e-05, 5.443509660246530e-04, 5.443509660246530e-04, -2.427500654732843e-03, -2.427500654732843e-03, -1.724052589118788e-03, -1.724052589118788e-03, 2.093032867706464e-05, 2.093032867706464e-05, -2.093032867706464e-05, -2.093032867706464e-05 ]
},
```

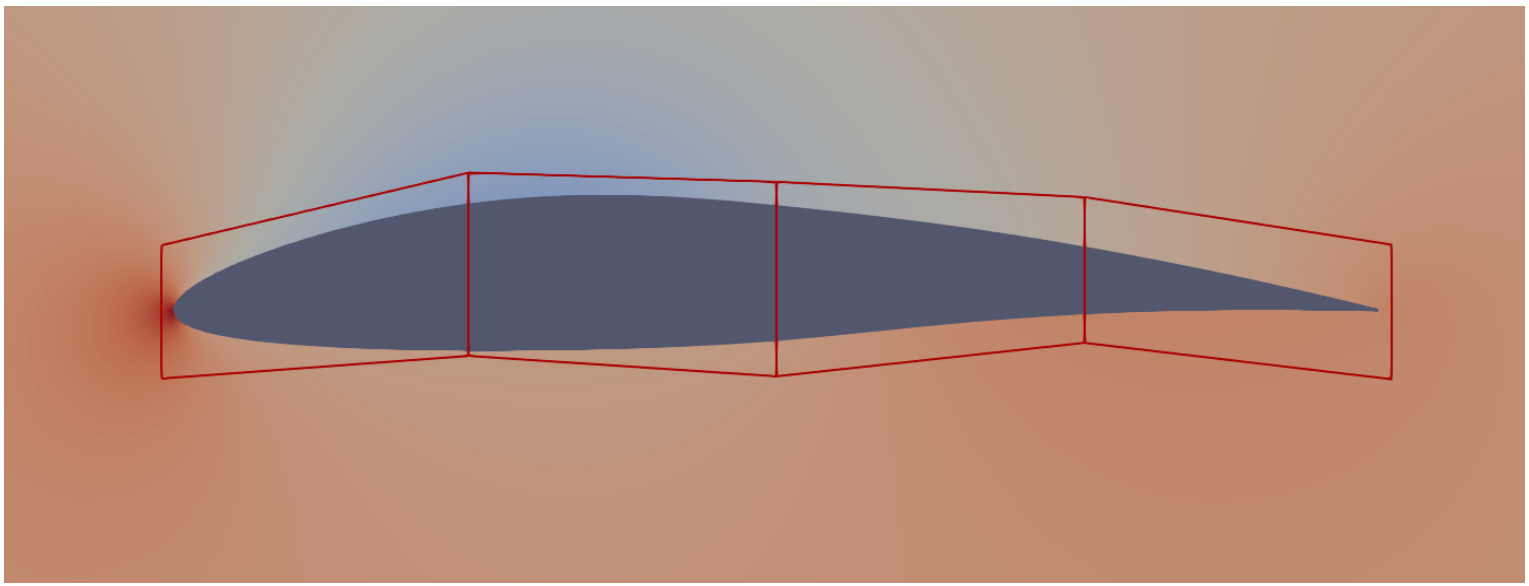
The `totalDerivHist.txt` file

History of total derivatives for each optimization iteration.

```
"Optimization_Iteration_000":
{
    "CD":
    {
        "alpha": [ 2.381623783762163e-03 ],
        "shapey": [ 3.511738965024154e-02, 3.492803545911542e-02, 3.200526828155191
             e-02, 3.180742702790106e-02, -5.892921319923614e-03,
             -5.902649387894162e-03, -1.144491483889070e-02, -1.146224282703606e
             -02, 3.177596591834314e-03, 3.187838214393225e-03, 5.929329231273673e
             -03, 5.924254135909747e-03, 1.890598489691082e-02, 1.890517540541186e
             -02, 2.059253838399523e-02, 2.058682490230581e-02, -4.818825079285534e
             -02, -4.825193433777377e-02, -4.993259758381555e-02,
             -4.999215109265394e-02 ]
    },
    "CL":
    {
        "alpha": [ 8.937240609804091e-02 ],
        "shapey": [ 2.077894737521315e-04, -1.527570234134256e-03,
             2.343608210441325e-01, 2.313962121945553e-01, 5.213755772675160e-01,
             5.206263437653107e-01, 7.036309452552799e-01, 7.024872477694163e-01,
             6.103749428633083e-01, 6.102302620088286e-01, 6.073417189281215e-01,
             6.070507720759699e-01, 1.583138188229053e+00, 1.583146820754854e+00,
             1.411095707919306e+00, 1.410944411517188e+00, -2.663221976842125e+00,
             -2.663605056859560e+00, -3.004362538425141e+00, -3.004690618705639e+00
              ]
    }
},
```

The `deformedFFD.dat` file

We can load the optimized airfoil geometry with the deformed FFD (deformedFFD_018.dat) in Paraview. The deformedFFD_018.dat is in Tecplot format.



Deformed FFD points and airfoil shape at the last optimization iteration.

Details of configuration files

Folders and files before the optimization

```
naca0012/incompressible
|-- 0.orig // initial fields and boundary conditions
|-- constant // flow and turbulence property definition
|-- FFD // folder that contains the FFD file
|-- profiles // naca0012 profile coordinate for mesh generation
|-- system // flow discretization, setup, time step, etc
|-- Allclean.sh // script to clean up the simulation results
|-- genAirFoilMesh.py // python script called by preProcessing.sh
|-- paraview.foam // dummy file for paraview post-processing
|-- preProcessing.sh // bash script to generate the mesh
|-- runScript.py // main run script for optimization
```

NOTE : The `0`, `constant`, and `system` folders are OpenFOAM essential, and the rests are for DAFoam optimization

Folders and files after the optimization

```
naca0012/incompressible
|-- 0 // initial fields and boundary conditions
|-- 0.00000001 // flow solution for the baseline design
|-- 0.00000002 // flow solution for the 1st opt iteration
|-- 0.00000018 // flow solution for the final opt iteration
|-- constant // flow and turbulence property definition
|-- FFD // folder that contains the FFD file
|-- profiles // naca0012 profile coordinate for mesh generation
|-- system // flow discretization, setup, time step, etc
|-- Allclean.sh // script to clean up the simulation results
|-- deformedFFD_018.dat // deformed FFD points for the final opt iter
|-- dRdWColoring_1.bin // computed coloring files
|-- DVConstraints.dat // visualization of constraints (Tecplot format)
|-- designVariableHist.txt // history of design variables during opt
|-- genAirFoilMesh.py // python script called by preProcessing.sh
|-- logMeshGeneration.txt // log file for mesh generation
|-- logOpt.txt // full log file for optimization
|-- objFuncHist.txt // objective history for ONE flow solution
|-- opt_IPOPT.txt // log file output by optimizer IPOPT
|-- paraview.foam // dummy file for paraview post-processing
|-- preProcessing.sh // bash script to generate the mesh
|-- runScript.py // main run script for optimization
|-- totalDerivHist.txt // history of total derivative during opt
|-- surfaceMesh.xyz // surface mesh generated by pyHyp
|-- volumeMesh.xyz // volume mesh generated by pyHyp
```

The `0` folder (1/2)

The `0` folder contains files for all the state variables, and their initial and boundary values are defined in these files

```
0
|-- nut         // turbulence viscosity
|-- nuTilda     // working variable in the SA turbulence model
|-- p           // pressure
|-- U           // velocity
|-- k           // k for SST turbulence model
|-- omega       // omega for SST turbulence model
|-- epsilon       // epsilon for kEpsilon turbulence model
```

The 0 folder (2/2)

Open 0/U and check the initial and boundary conditions for velocity. Similarly, we need to define the conditions for all other variables

```
// U magnitude 10 m/s. The internal and boundary field values defined in 0/U
     will be overwritten by DAFoam when running optimization. This is because we
      have define the boundary values in "primalBC"-"daOptions" of runScript.py
internalField uniform (10 0 0);
boundaryField
{
    "(wing.*)"          // boundary patch name for wing*
    {
        type            fixedValue;     // boundary type
        value           uniform (0 0 0); // boundary value
    }
    symmetry1           // symmetry plane
    {
        type            symmetry;
    }
    symmetry2
    {
        type            symmetry;
    }
    inout               // far field, usually no need to change
    {
        type            inletOutlet;
        inletValue      $internalField;
        value           $internalField;
    }
}
```

The `0.00000018` folder

Open 0.00000018/U.gz and check the final converged velocity field for the optimized design. NOTE : the `internalField` is no longer `uniform` as in the 0/U file.

```
internalField nonuniform List<vector> // nonuniform internal field
4032
(
(3.9243226 -1.290095 -0.0028988106)
(3.7305871 -0.99840567 -0.0027730653)
(3.554621 -1.3012481 -0.0028666955)
(3.8325503 -0.95915536 -0.003049858)
(3.947682 -0.94315159 -0.0028641267)
(4.2338067 -1.0326866 -0.0031121561)
(2.738578 -0.99318945 -0.0026861221)
(3.2447924 -0.87974595 -0.0029403715)
(4.3552657 -0.78274271 -0.0032382407)
(3.9498574 -0.91532577 -0.0028354695)
(4.5629592 -1.0266758 -0.0031897207)
(4.8687782 -0.9436423 -0.0033734098)
(3.6192063 -0.29059501 -0.0019943858)
.....
```

NOTE : The `0.00000018` folder also contains the optimized (deformed) mesh points in 0.00000018/constant/polyMesh/points.gz, which is different from the baseline mesh points in constant/polyMesh/points.gz (see next slide)

The `constant` folder (1/3)

The `constant` folder contains mesh, flow and turbulence property definitions.

```
constant
|-- polyMesh  // mesh points, faces, and boundary info
    |-- boundary     // mesh boundary patch names and types
    |-- faces.gz     // mesh faces
    |-- neighbour.gz // face neighbour info
    |-- owner.gz     // face owner info
    |-- points.gz    // baseline mesh point coordinates
|-- transportProperties // flow properties
|-- turbulenceProperties // turbulence model
```

The `constant` folder (2/3)

The `bounary` file defines the name and type of the boundary patches

```
5 // number of boundary patches
(
    symmetry1   // name of the mesh boundary patch, symmetry plane
    {
        type            symmetry; // type of the boundary patch
        nFaces          4032;     // number of faces in the patch
        startFace       7938;    // start face
    }
    wing   // wing surface
    {
        type            wall;
        nFaces          126;
        startFace       16002;
    }
    inout // far field
    {
        type            patch;
        nFaces          126;
        startFace       16128;
    }
    ...
)
```

The `constant` folder (3/3)

The `transportProperties` file defines flow properties

```
transportModel Newtonian;
nu 1.5e-5; // define the molecular viscosity
```

The `turbulenceProperties` file defines turbulence model

```
simulationType RAS; // RAS=RANS in OpenFOAM
RAS
{
    RASModel      SpalartAllmaras; // the SA turbulence model
    turbulence    on;
    printCoeffs   off;
}
```

The `system` folder (1/5)

The `system` folder contains

```
system
|-- controlDict  // defines system parameters such as time step
|-- createPatchDict // parameters used by the createPatch utility
|-- decomposeParDict // mesh decomposition parameters for parallel run
|-- fvSchemes // discretization schemes
|-- fvSolution // linear equation solution strategy
```

The `system` folder (2/5)

The `control` file contains flow setup such as step size

```
startFrom       startTime;  // simulation starts from startTime
startTime       0;          // if startFrom=startTime, define it here
stopAt          endTime;    // simulation ends at endTime
endTime         1000;       // define endTime here
deltaT          1;          // time step
writeControl    timeStep;   // how to write the results
writeInterval   1000;       // write flow field every 1000 steps
purgeWrite      0;          // whether to purge intermediate output
writeFormat     ascii;      // binary or ascii output format
writePrecision  8;          // Write precision for data output
writeCompression on;        // Compress the output files with .gz format
timeFormat      general;    // time format
timePrecision   8;          // time IO accuracy
runTimeModifiable true;     // Allow modification during runtime
// Do not print solver performance from OpenFOAM, the information
// printed to the screen will be completely controlled by DAFoam
DebugSwitches
{
  SolverPerformance 0;
}
```

The `system` folder (3/5)

The `decomposeParDict` contains parallel run setup. NOTE : there is no need to manually change this file, because it will be automatically generated by DAFoam when the optimization runs.

```
numberOfSubdomains   4;  // number of decomposed domain
method               scotch;
```

The `system` folder (4/5)

The `fvSchemes` file contains discretization definition for each variable

```
ddtSchemes
{
    default                                 steadyState;
}
gradSchemes
{
    default                                 Gauss linear;
}
divSchemes // NOTE: need to specify divergence discretization for each variable
{
    default                                 none;
    div(phi,U)                              bounded Gauss linearUpwindV grad(U);
    div(phi,nuTilda)                        bounded Gauss upwind;
    div((nuEff*dev2(T(grad(U)))))           Gauss linear;
    div((-devRhoReff.T()&U))                Gauss linear;
}
interpolationSchemes
{
    default                                 linear;
}
laplacianSchemes
{
    default                                 Gauss linear corrected;
}
```

The `system` folder (5/5)

The `fvSolution` file contains strategy for linear equation solution

```
SIMPLE
{
    consistent                      false; // don't use SIMPLEC
    nNonOrthogonalCorrectors        0;
}
solvers
{
    "(p|p_rgh|G)" // linear GaussSeideil solver for p equations
    {
        solver                      GAMG;
        smoother                    GaussSeidel;
        relTol                      0.1;
        tolerance                   0;
    }
}
relaxationFactors // NOTE: need to specify relaxation for each variable
{
    fields
    {
        "(p|p_rgh)"                 0.30;
    }
    equations
    {
        "(U|T|e|h|nuTilda|k|epsilon|omega)" 0.70;
    }
}
```

The `preProcessing.sh` script (1/4)

The `preProcessing.sh` script is used to generate mesh. We first run genAirFoilMesh.py to read the airfoil coordinates from the profiles folder and generate structured mesh using pyHyp and output the mesh as volumeMesh.xyz.

```
python genAirFoilMesh.py > log.meshGeneration
```

The `genAirFoilMesh.py` script reads :

```
########## user input ################
prefix = "./profiles/"
airfoilProfilePS = prefix + "NACA0012PS.profile"
airfoilProfileSS = prefix + "NACA0012SS.profile"
ZSpan = 0.1 # width in the z direction
nSpan = 2 # how many points in z
# PS parameters
dX1PS = 0.005 # first dx from the LE
Alpha1PS = 1.2 # clustering from the LE
dX2PS = 2e-3 # first dx from the TE
Alpha2PS = 1.2 # clustering from the TE
dXMaxPS = 0.02 # max dx for PS
...
# TE parameters
NpTE = 5 # number of points for blunt TE
# 3D
NpExtrude = 33 # how many points to extrude for the 3D volume mesh
yWall = 4e-3 # first layer mesh length
marchDist = 20.0 # march distance for extruding
```

The `preProcessing.sh` script (2/4)

Then, we use the plot3dToFoam utility to convert the plot3D mesh volumeMesh.xyz to OpenFOAM format and store the mesh in `constant/polyMesh`

```
plot3dToFoam -noBlank volumeMesh.xyz >> log.meshGeneration
```

After running the above command, the volumeMesh.xyz will be converted to the OpenFOAM mesh. However, in the boundary patch file `constant/polyMesh/boundary`, there is only one boundary patch, and reads :

```
1
(
    defaultFaces
    {
        type            wall;
        inGroups        1(wall);
        nFaces          9324;
        startFace       8946;
    }
)
```

The `preProcessing.sh` script (3/4)

Then, we run autoPatch to automatically split the boundary patches. Here the argument 60 means split the mesh based on 60 degree feature angle (lower this value will generate more patches). Essentially, this call will modify the `constant/polyMesh/boundary` file and generate new patches called auto0, auto1, auto2, etc.

```
autoPatch 60 -overwrite >> log.meshGeneration
```

Once done, `constant/polyMesh/boundary` reads :

```
6
(
    ...
    auto0
    {
        type            patch;
        nFaces          4536;
        startFace       8946;
    }
    ...
    auto4
    {
        type            patch;
        nFaces          4536;
        startFace       13482;
    }
)
```

The `preProcessing.sh` script (4/4)

The above generated boundary file has boundary names such as auto0, auto1, auto2, etc. Now group and rename the above generated patches to meaningful names, e.g. wing, symmetry, etc, see system/createPathDict

```
createPatch -overwrite >> log.meshGeneration
```

`system/createPathDict` reads :

```
patches
(
    ...
    {
        name wing; // Name of new patch
        patchInfo // Dictionary to construct new patch from
        {
            type wall;
        }
        // How to construct: either from 'patches' or 'set'
        constructFrom patches;
        // which patches to group and renamed as "wing"
        patches (auto2 auto3);
    }
    ...
);
```

The airfoil coordinates

When running the above `genAirFoilMesh.py` script, it will look for the airfoil coordinates in the `profiles` folder. NOTE : We need to define the upper profile (SS ; suction side) and lower profile (PS ; pressure side) separately. The range of x needs to be from 0 to 1. And we need to manually delete the last few points to make a blunt trailing edge. In other words, the last point should have x≈0.999, instead of 1.0

```
NACA0012SS.profile
0.0000000 0.0000000 # coordinate should start from 1
0.0005839 -.0042603
0.0023342 -.0084289
...
0.9947532 -.0019938
0.9976658 -.0015870
0.9994161 -.0013419 # end at about 0.999; we have deleted the last few points
```

```
NACA0012PS.profile
0.0000000 0.0000000 # coordinate should start from 1
0.0005839 0.0042603
0.0023342 0.0084289
...
0.9947532 0.0019938
0.9976658 0.0015870
0.9994161 0.0013419 # end at about 0.999; we have deleted the last few points
```

The FFD folder

We use the FFD/genFFD.py script to generate the FFD points and save it in the plot3D format (FFD/wingFFD.xyz).

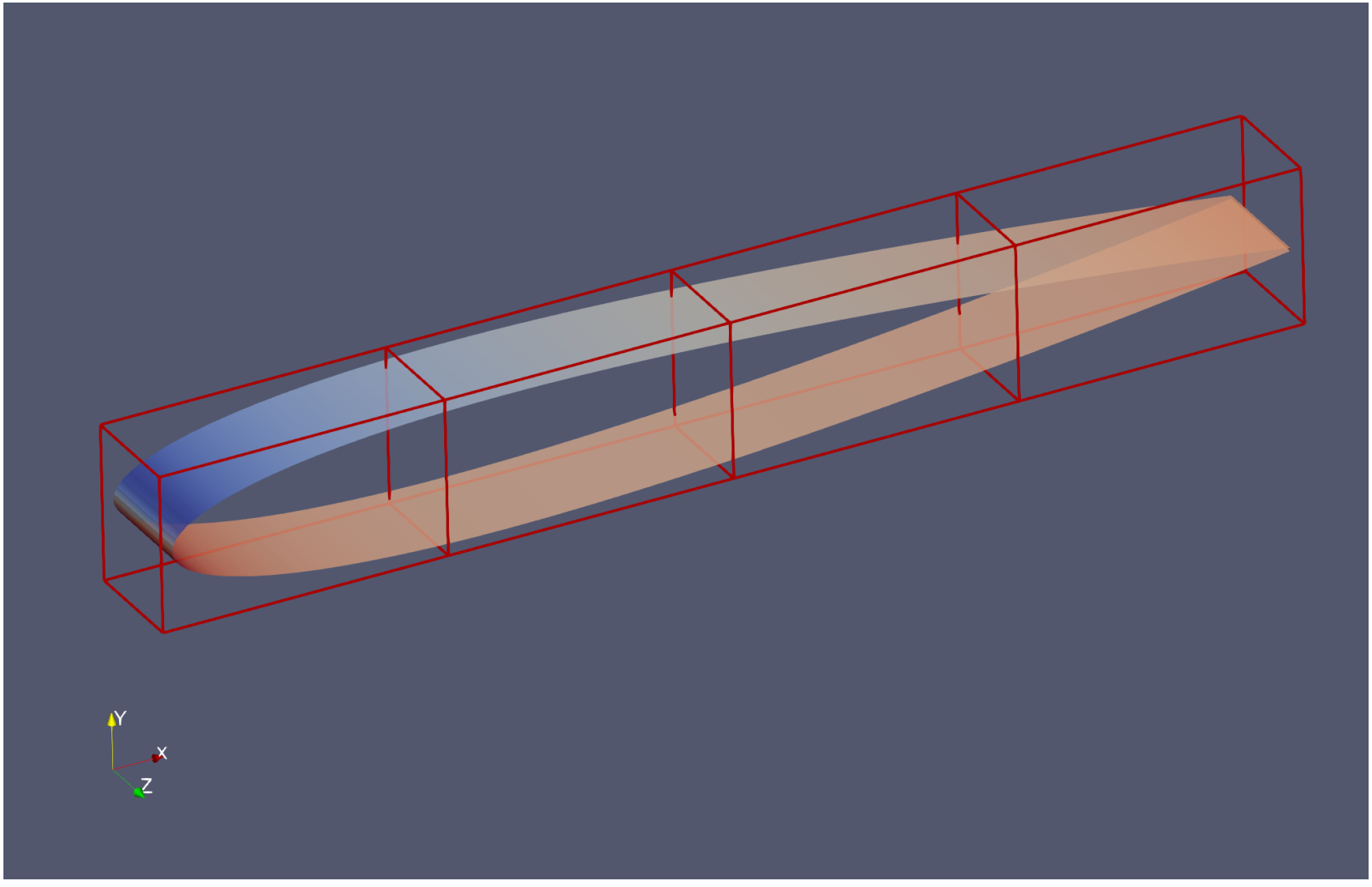
```
nBlocks = 1 # we only have one FFD block
nx = [5] # number of FFD points in the x direction
ny = [2]
nz = [2]
# we need to define the coordinates for the 8 corner points and the
# rest of points will be automatically generated by this script.
corners[0,0,:] = [-0.010,-.0700,0.0]
corners[0,1,:] = [-0.010,-0.0700,0.1]
corners[0,2,:] = [-0.010,0.0700,0.0]
corners[0,3,:] = [-0.010,0.0700,0.1]
corners[0,4,:] = [ 1.01,-.07,0.0]
corners[0,5,:] = [ 1.01,-.07,0.10]
corners[0,6,:] = [ 1.01,0.07,0.0]
corners[0,7,:] = [ 1.01,0.07,0.1]
```

Paraview has problems loading small plot3D files, so we can convert it to Tecplot format by running this command. Then we can load wingFFD.dat in Paraview.

```
dafoam_plot3d2tecplot.py wingFFD.xyz wingFFD.dat
```

Visualize the FFD points (wingFFD.dat) in Paraview

The FFD points have to completely contain the design surface ! !



The `runScript.py` script (1/11)

```
# ================
# Input Parameters
# ================
parser = argparse.ArgumentParser()
# we support slsqp, ipopt, and snopt
parser.add_argument("--opt", help="optimizer to use", type=str, default="ipopt")
# the default task is optimization (opt), we can also do runPrimal, runAjoint,
    verifySens, etc.
parser.add_argument("--task", help="type of run to do", type=str, default="opt")
args = parser.parse_args()
gcomm = MPI.COMM_WORLD

# Define the global parameters here
U0 = 10.0 # far field velocity
p0 = 0.0 # far field pressure (relative to the ref value)
nuTilda0 = 4.5e-5 # far field turbulence variables
k0 = 0.015
epsilon0 = 0.14
omega0 = 100.0
CL_target = 0.5 # target lift coefficient for optimization
alpha0 = 5.0  # guess of angle of attack for CL_target
A0 = 0.1 # reference area for normalizing lift and drag
```

The `runScript.py` script (2/11)

```
daOptions = {
    "designSurfaces": ["wing"], # design surface names
    "solverName": "DASimpleFoam", # solver name
    "adjJacobianOption": "JacobianFree", # Use Jacobian-free adjoint with AD
    "primalMinResTol": 1.0e-8, # flow solution residual tolerance
    "primalBC": { # set boundary condition here and overwrite 0/U, 0/p, etc.
        "U0": {"variable": "U", "patches": ["inout"], "value": [U0, 0.0, 0.0]},
        "p0": {"variable": "p", "patches": ["inout"], "value": [p0]},
        ...
        "useWallFunction": True, # use wall functions for turbulence variables
    },
    "objFunc": { # define objective function here
        "CD": { # first objective name is CD
            "part1": {
                "type": "force", # it is of "force" type
                "source": "patchToFace", # force is computed from selected patches
                "patches": ["wing"], # patch names for force computation
                "directionMode": "parallelToFlow", # force dir is parallel to flow
                "alphaName": "alpha", # provide angle of attack name for force dir
                "scale": 1.0 / (0.5 * U0 * U0 * A0), # scale to normalize force
                "addToAdjoint": True, # whether to compute adjoint for this objFunc
            }
        },
        "CL": { # second objective name is CL
                ...
                "directionMode": "normalToFlow", # force dir is normal to flow
                ...
        },
    },
```

The `runScript.py` script (3/11)

```
daOptions = {
    ...
    "adjEqnOption": { # adjoint solution options
        "gmresRelTol": 1.0e-8, # adjoint solutioin residual tolerance
        "pcFillLevel": 1, # preconditioner fill-in level
        "jacMatReOrdering": "rcm" # preconditioner re-ordering
    },
    "normalizeStates": { # state variable normalization values for adjoint
        "U": U0, # far field velocity to normalize U
        "p": U0 * U0 / 2.0, # dynamic pressure to normalize p (incompressible)
        "nuTilda": nuTilda0 * 10.0,
        "k": k0 * 10.0,
        "epsilon": epsilon0,
        "omega": omega0,
        "phi": 1.0, # always use 1.0 to normalize ph
    },
    # finite-difference step size for computing preconditioner
    "adjPartDerivFDStep": {"State": 1e-7, "FFD": 1e-3},
    # how frequent to recompute the preconditioner dRdWTPC
    "adjPCLag": 100,
    # provide an empty key for place holder (values to be assigned later)
    "designVar": {},
    # write the deformed FFD files during optimization
    "writeDeformedFFDs": True
}
```

NOTE : A complete list of daOptions are at :

`https://dafoam.github.io/doxygen/html/classdafoam_1_1pyDAFoam_1_1DAOPTION.html`

The `runScript.py` script (4/11)

```
# mesh warping parameters, users need to manually specify the symmetry plane and
      their normals
meshOptions = {
    "gridFile": os.getcwd(),
    "fileType": "openfoam",
    # point and normal for the symmetry plane
    "symmetryPlanes": [[[0.0, 0.0, 0.0], [0.0, 0.0, 1.0]], [[0.0, 0.0, 0.1], [0.0,
         0.0, 1.0]]],
}

# options for optimizers
if args.opt == "snopt":
    optOptions = {
        ...
    }
elif args.opt == "ipopt":
    optOptions = {
        "tol": 1.0e-6, # optimality
        "constr_viol_tol": 1.0e-6, # feasibility tolerance
        "max_iter": 50, # max number of optimization iterations
        "print_level": 5,
        "output_file": "opt_IPOPT.txt",
        "mu_strategy": "adaptive",
        "limited_memory_max_history": 10,
        "nlp_scaling_method": "none",
        "alpha_for_y": "full",
        "recalc_y": "yes",
    }
...
}
```

The `runScript.py` script (5/11)

```
# ========================
# Design variable setup
# ========================
def alpha(val, geo): # define the angle of attack function to update primalBC
    aoa = val[0] * np.pi / 180.0 # val[0] is the aoa in degree
    inletU = [float(U0 * np.cos(aoa)), float(U0 * np.sin(aoa)), 0] # U components
    DASolver.setOption("primalBC", {"U0": {"variable": "U", "patches": ["inout"],
        "value": inletU}}) # update U in primalBC based on aoa
    DASolver.updateDAOption() # update the value in the C++ layer
DVGeo = DVGeometry("./FFD/wingFFD.xyz") # read the FFD point
DVGeo.addRefAxis("bodyAxis", xFraction=0.25, alignIndex="k") # add ref axis
# select points
iVol = 0 # we only have one FFD block, so it is the 0th index
pts = DVGeo.getLocalIndex(iVol) # get all the FFD points
indexList = pts[:, :, :].flatten() # select all the FFD points [:,:,:]
PS = geo_utils.PointSelect("list", indexList)
# shape variables that move in the y direction within [-1.0:1.0]
DVGeo.addGeoDVLocal("shapey", lower=-1.0, upper=1.0, axis="y", scale=1.0,
     pointSelect=PS) # assign the PS to pointSelect
# update daOptions, the type of shape design variable is "FFD"
daOptions["designVar"]["shapey"] = {"designVarType": "FFD"}
# angle of attack variable defined by the alpha(val, geo) function above
DVGeo.addGeoDVGlobal("alpha", value=[alpha0], func=alpha, lower=0.0, upper=10.0,
     scale=1.0) # initial aoa is [alpha0] and the bounds are [0:10]
# update daOptions, the type of aoa design variable is "AOA", we also need to
# give patch names, flowAxis, and normalAxis to determine the force direction
daOptions["designVar"]["alpha"] = {"designVarType": "AOA", "patches": ["inout"],
    "flowAxis": "x", "normalAxis": "y"}
```

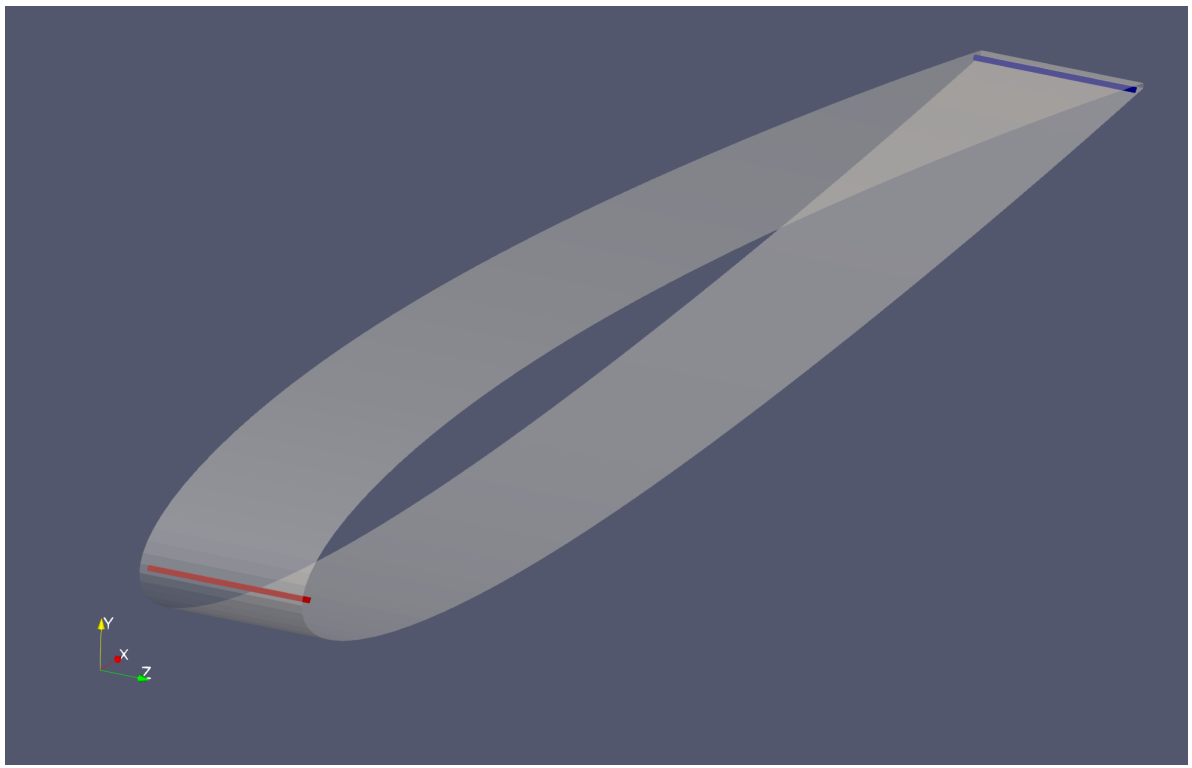
The `runScript.py` script (6/11)

No need to change this part

```
# ======================
# DAFoam initialization
# ======================
DASolver = PYDAFOAM(options=daOptions, comm=gcomm)
DASolver.setDVGeo(DVGeo)
mesh = USMesh(options=meshOptions, comm=gcomm)
DASolver.addFamilyGroup(DASolver.getOption("designSurfaceFamily"), DASolver.
    getOption("designSurfaces"))
DASolver.printFamilyList()
DASolver.setMesh(mesh)
evalFuncs = []
DASolver.setEvalFuncs(evalFuncs)
```

The `runScript.py` script (7/11)

```
# ==================
# Constraint setup
# ==================
DVCon = DVConstraints()
DVCon.setDVGeo(DVGeo)
DVCon.setSurface(DASolver.getTriangulatedMeshSurface(groupName=DASolver.getOption(
      "designSurfaceFamily")))
# leading and trailing edge lines for volume and thickness constraints
leList = [[1e-4, 0.0, 1e-4], [1e-4, 0.0, 0.1 - 1e-4]] # RED line
teList = [[0.998 - 1e-4, 0.0, 1e-4], [0.998 - 1e-4, 0.0, 0.1 - 1e-4]] # BLUE line
```



The `runScript.py` script (8/11)

```
# volume constraint, we use the leList and teList as outer boundary and
# create 2x10 sample points defined by nSpan and nChord. Then, we project
# and these samle points to the airfoil surface to form trapezoid volumes
# the sum of these volumes is an approximated volume for the airfoil.
# We constrain the relative upper and lower bounds [1.0:3.0]
# based on the initial volume
DVCon.addVolumeConstraint(leList, teList, nSpan=2, nChord=10, lower=1.0, upper=3,
     scaled=True)

# thickness constraint, we use the leList and teList as outer boundary and
# create 2x10 sample points defined by nSpan and nChord. Then, we project
# and these samle points to the airfoil surface. The lengths of the projection
# lines are the local thickness of the airfoil. We constrain the relative
# upper and lower bounds [0.8:3.0] based on the initial local thickness
DVCon.addThicknessConstraints2D(leList, teList, nSpan=2, nChord=10, lower=0.8,
     upper=3.0, scaled=True)
```

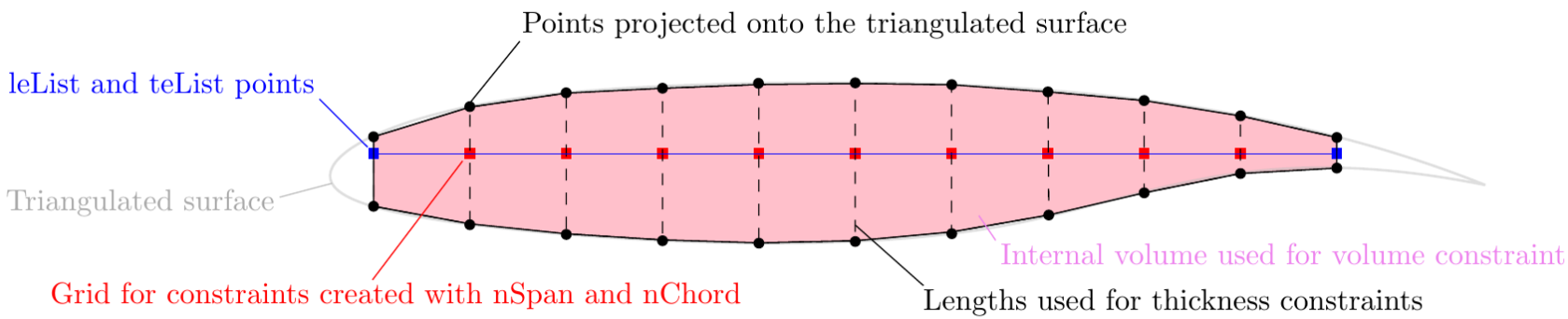
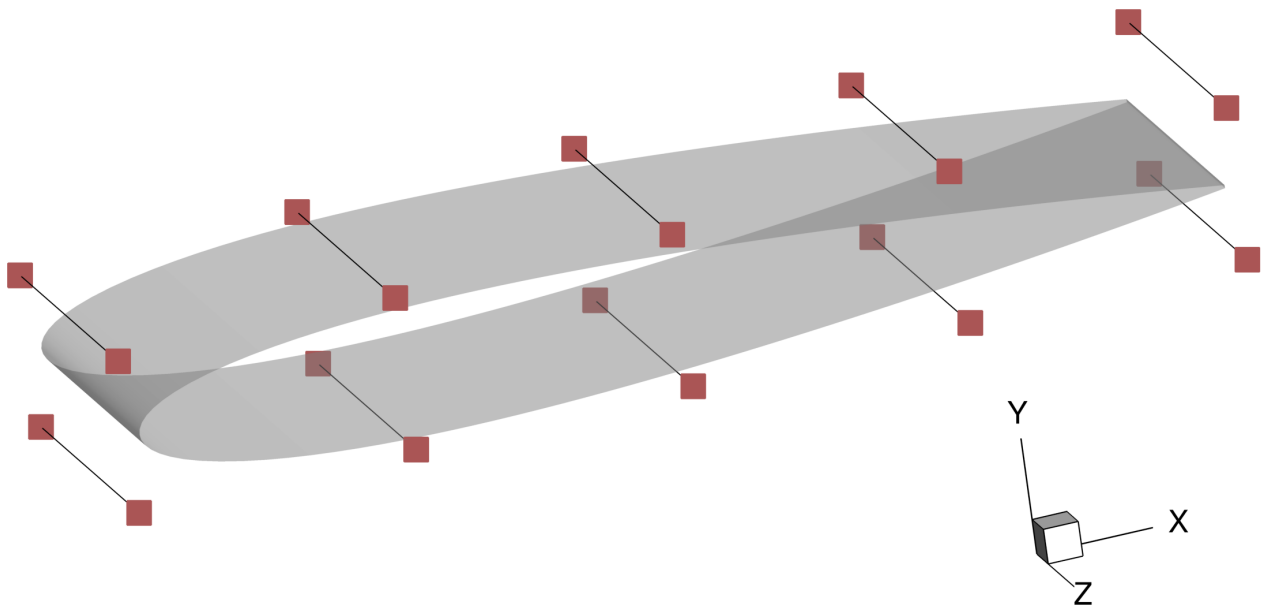


Diagram for volume and thickness constraints.

The `runScript.py` script (9/11)

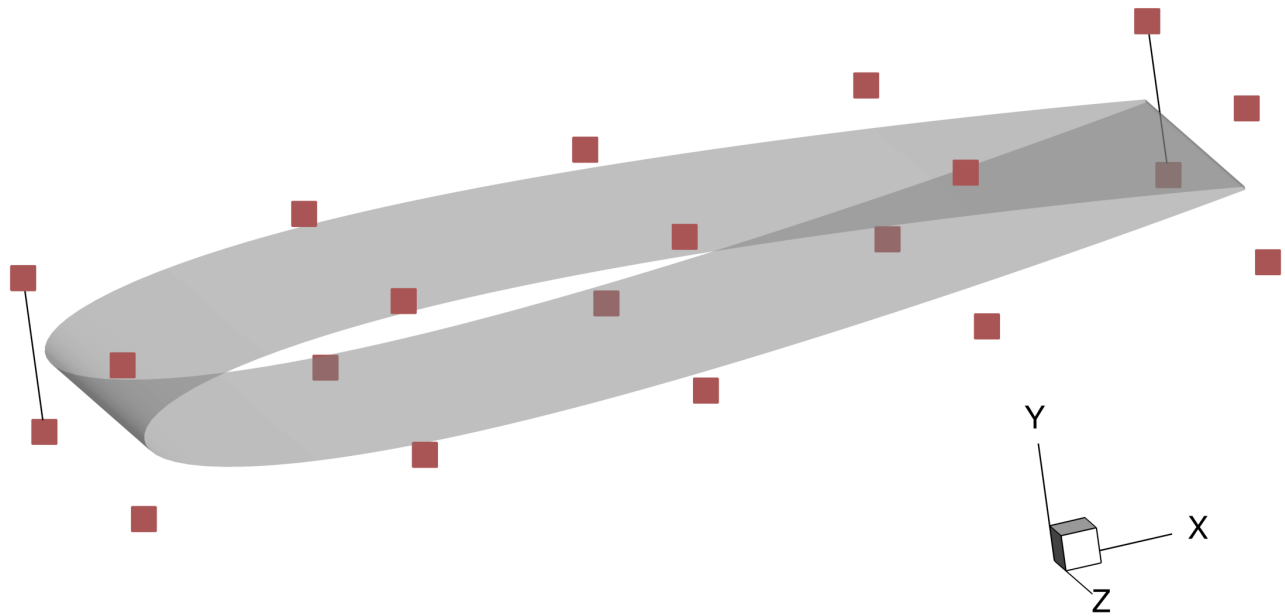
```
# Create linear constraints to link the shape change between k=0 and k=1
nFFDs_x = pts.shape[0] # the x size of pts array
indSetA = []
indSetB = []
for i in range(nFFDs_x):
    for j in [0, 1]:
        indSetA.append(pts[i, j, 1]) # linking k=0 and k=1
        indSetB.append(pts[i, j, 0])
DVCon.addLinearConstraintsShape(indSetA, indSetB, factorA=1.0, factorB=-1.0, lower
     =0.0, upper=0.0)
```



Black lines linking the FFD points movement between k=0 and k=1.

The `runScript.py` script (10/11)

```
# Create a linear constraint to fix the leading and trailing point.
indSetA = []
indSetB = []
for i in [0, nFFDs_x - 1]:
    # do not constrain k=1; it has been linked in the above symmetry constraint
    for k in [0]:
        indSetA.append(pts[i, 0, k])
        indSetB.append(pts[i, 1, k])
DVCon.addLinearConstraintsShape(indSetA, indSetB, factorA=1.0, factorB=1.0, lower
    =0.0, upper=0.0)
# write constraint visualization to a Tecplot file
DVCon.writeTecplot("DVConstraints.dat")
```



Black lines forcing the FFD points oppsitite movement at the LE and TE.

The `runScript.py` script (11/11)

```
# ====================================
# Initialize optFuncs for optimization
# ====================================
optFuncs.DASolver = DASolver # optFuncs.py has functions to run primal and adjoint
optFuncs.DVGeo = DVGeo
... # users usually don't need to change this part
# =======
# Task
# =======
if args.task == "opt":
    # run solveCL before opt. Need to specify which variables are AOA and lift
    alpha4CLTarget = optFuncs.solveCL(CL_target, "alpha", "CL")
    alpha([alpha4CLTarget], None) # once solveCL is done, set the correct alpha
    # create an pyOptSparse opt problem and set objFun function to run primal
    optProb = Optimization("opt", objFun=optFuncs.calcObjFuncValues, comm=gcomm)
    DVGeo.addVariablesPyOpt(optProb)
    DVCon.addConstraintsPyOpt(optProb)
    optProb.addObj("CD", scale=1) # set the objective function
    optProb.addCon("CL", lower=CL_target, upper=CL_target, scale=1) # CL constraint
    if gcomm.rank == 0:
        print(optProb)
    # run graph coloring before optimization
    DASolver.runColoring()
    # set sens function to run adjoint and solve the optimization problem
    opt = OPT(args.opt, options=optOptions)
    histFile = "./%s_hist.hst" % args.opt
    sol = opt(optProb, sens=optFuncs.calcObjFuncSens, storeHistory=histFile)
    if gcomm.rank == 0:
        print(sol)
```

The dafoam/dafoam/optFuncs.py script (1/2)

```
def calcObjFuncValues(xDV):
    """Update the design surface and run the primal solver to get objective
        function values.
    """
    Info("\n")
    Info("+--------------------------------------+")
    Info("|   Evaluating Objective Functions %03d |" % DASolver.nSolvePrimals)
    Info("+--------------------------------------+")
    Info("Design Variables: ")
    Info(xDV)
    a = time.time()
    # Setup an empty dictionary for the evaluated function values
    funcs = {}
    # Set the current design variables in the DV object
    DVGeo.setDesignVars(xDV)
    DASolver.setDesignVars(xDV)
    # Evaluate the geometric constraints and add them to the funcs dictionary
    DVCon.evalFunctions(funcs)
    # Solve the CFD problem
    DASolver()
    # Populate the required values from the CFD problem
    DASolver.evalFunctions(funcs, evalFuncs=evalFuncs)
    b = time.time()
    # Print the current solution to the screen
    Info("Objective Functions: ")
    Info(funcs)
    Info("Flow Runtime: %g" % (b - a))
    fail = funcs["fail"]
    return funcs, fail
```

The dafoam/dafoam/optFuncs.py script (2/2)

```
def calcObjFuncSens(xDV, funcs):
    """Run the adjoint solver and get objective function sensitivities.
    """
    Info("+---------------------------------+")
    Info("|Evaluating␣Objective␣Function␣Sensitivities␣%03d|"%DASolver..)
    Info("+---------------------------------+")
    a = time.time()
    # write the design variable values to file
    DASolver.writeDesignVariable("designVariableHist.txt", xDV)
    # write the deform FFDs
    DASolver.writeDeformedFFDs()
    # Setup an empty dictionary for the evaluated derivative values
    funcsSens = {}
    # Evaluate the geometric constraint derivatives
    DVCon.evalFunctionsSens(funcsSens)
    # Solve the adjoint
    DASolver.solveAdjoint()
    # Evaluate the CFD derivatives
    DASolver.evalFunctionsSens(funcsSens, evalFuncs=evalFuncs)
    b = time.time()
    # Print the current solution to the screen
    with np.printoptions(precision=16, threshold=5, suppress=True):
        Info("Objective␣Function␣Sensitivity:␣")
        Info(funcsSens)
        Info("Adjoint␣Runtime:␣%g␣s" % (b - a))
    # write the sensitivity values to file
    DASolver.writeTotalDeriv("totalDerivHist.txt", funcsSens, evalFuncs)
    fail = funcsSens["fail"]
    return funcsSens, fail
```

How to change the configuration files for a new case

How to change flow conditions ?

Change these in `runScript.py`

```
U0 = 10.0
p0 = 0.0
nuTilda0 = 4.5e-5
k0 = 0.015
epsilon0 = 0.14
omega0 = 100.0
```

How to use more mesh cells ?

Change the input parameters in `genAirFoilMesh.py`, e.g., reduce dX1PS, dX2PS, dXMaxPS, etc, and increase NpTE, NpExtrude.

```
########## user input ################
prefix = "./profiles/"
airfoilProfilePS = prefix + "NACA0012PS.profile"
airfoilProfileSS = prefix + "NACA0012SS.profile"
ZSpan = 0.1 # width in the z direction
nSpan = 2 # how many points in z
# PS parameters
dX1PS = 0.005 # first dx from the LE
Alpha1PS = 1.2 # clustering from the LE
dX2PS = 2e-3 # first dx from the TE
Alpha2PS = 1.2 # clustering from the TE
dXMaxPS = 0.02 # max dx for PS
...
# TE parameters
NpTE = 5 # number of points for blunt TE
# 3D
NpExtrude = 33 # how many points to extrude for the 3D volume mesh
yWall = 4e-3 # first layer mesh length
marchDist = 20.0 # march distance for extruding
```

How to use a different turbulence model ?

To use the kOmegaSST model, in the `constant/turbulenceProperties` file, change

```
simulationType RAS;
RAS
{
    RASModel      SpalartAllmaras;
    turbulence    on;
    printCoeffs   off;
}
```

to :

```
simulationType RAS;
RAS
{
    RASModel      kOmegaSST;
    turbulence    on;
    printCoeffs   off;
}
```

How to use more FFD points ?

To use 40 FFD points, in the `FFD/genFFD.py` file, change

```
nx = [5]
ny = [2]
nz = [2]
```

to :

```
nx = [10]
ny = [2]
nz = [2]
```

NOTE : Always use 2 points in the vertical direction, so ny=2. In addition, because in the z direction (spanwise), the airfoil is symmetry, so nz=2. For 3D wing cases, nz should be greater than 2.

How to optimize a different airfoil ?

- Generate the separated upper and lower airfoil coordinates and save them to the `profiles` folder (e.g., RAE2822PS.profile and RAE2822SS.profile). Remember to delete the last few points to get blunt TE.
- Modify `airfoilProfilePS` and `airfoilProfileSS` in `genAirFoilMesh` to let it link to the correct airfoil coordinate files.
- Modify the FFD corners coordinates, i.e., `corners[0,0,:]`, `corners[0,1,:]`, etc. in the `FFD/genFFD.py` file to make sure the FFD points fully contain the new airfoil surface.
- Run `./Allclean.sh` to clean up the previous runs
- Start a Docker container and run : `./preProcessing.sh && python runScript.py`

How to use a different solver (1/2) ?

Refer to `examples/naca0012/subsonic`, differences in runScript.py :

- There are new variables (e.g., T) in the global parameters. Also, we use absolute pressure p0=101325, instead of relative one
- "solverName" changed to "DARhoSimpleFoam"
- A new key "primalVarBounds" that sets the bounds for robust flow simulation
- In "normalizeStates", "p" is normalized by p0, insteady of dynamic pressure.

In addition, in the "0" folder, we have more variables, i.e., alphat and T. In the "constant" folder, the fluid properties are defined in "thermophysicalProperties" instead of "transportProperties". Also, in the "system" folder, "fvSchemes" and "fvSolution" have different setup that are specially designed for compressible flow solver DARhoSimpleFoam.

How to use a different solver (2/2) ?

Refer to `examples/naca0012/transonic`, it is similar to `examples/naca0012/subosnic`, except that :

- U0 is set to be at transonic speed
- "solverName" changed to "DARhoSimpleCFoam". Here C means SIMPLEC algorithm (consistent). This is needed for transonic conditions.
- "transonicPCOption" in "daOptions" is set to 1. This uses the transonic preconditioner to speed up the adjoint convergence
- In the "system" folder, "fvSchemes" and "fvSolution" have different setup that are specially designed for transonic flow conditions for DARhoSimpleCFoam.

How to use more CPU cores ?

If you want to run an DAFoam optimization using 4 CPU core, use this command :

```
mpirun -np 4 python runScript.py | tee 2>&1 logOpt.txt
```

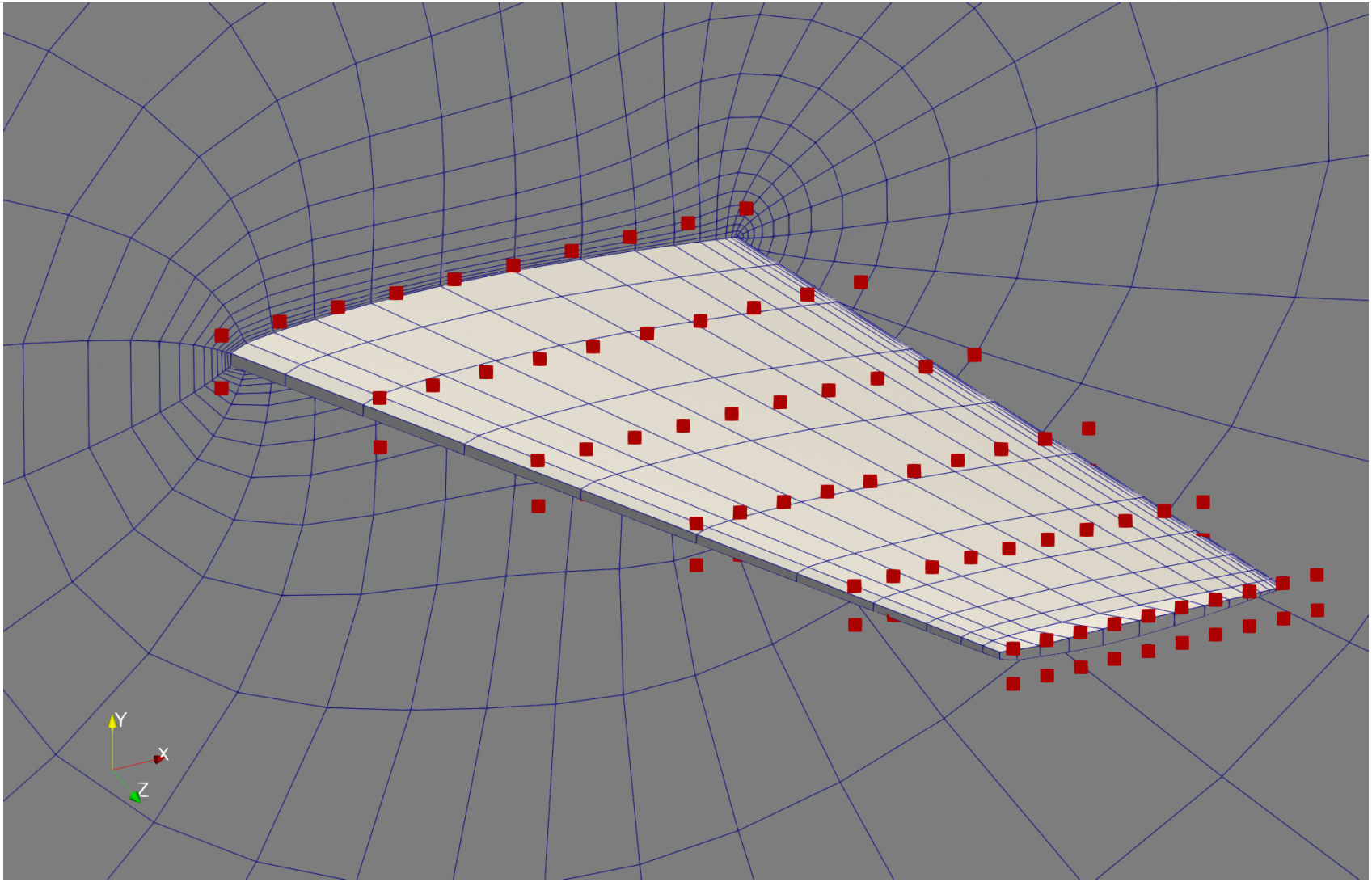
NOTE : Always run `./Allclean.sh` before running a new job !

Wing aerodynamic optimization

Optimization summary

Optimizer	IPOPT
Flow and adjoint solvers	DARhoSimpleFoam
Geometry	Onera_M6
Mesh	7 800 cells
Objective function	C_d
Design variables	120 FFDs and α
Constraint	$C_l = 0.25$, thickness, volume, TE/LE
U_∞	100 m/s
Re	5×10^6
Turbulence Model	Spalart–Allmaras

Mesh and FFD



How to run a wing optimization

Running a 3D wing optimization is similar to running an airfoil optimization. Open a new Docker container, and run this command for pre-processing (mesh generation) :

```
./preProcessing.sh
```

Then, use this command to run the flow simulation :

```
python runScript.py | tee 2>&1 logOpt.txt
```

The optimization log will be printed to the screen and saved to `logOpt.txt`. In addition, the optimizer will write a separate log to the disk. For the IPOPT optimizer we use in this tutorial, it is `opt_IPOPT.txt`.

The `preProcessing.sh` script

The overall mesh generation process is similar to the airfoil case. The main differene is that :

- We need to provide a surface mesh in the cgns or plot3D format (e.g., surfaceMesh.cgns). The surface mesh is usually generated by using commercial software such as ICEM-CFD and Pointwise. Refer to the MACH-Aero documentation for more details.
  `https://mdolab-mach-aero.readthedocs-hosted.com/en/latest/machAeroTutorials/overset_surface_mesh.html`
- We coarsen the surface mesh four times to create a very coarse volume mesh for demonstration. If you want to increase the mesh density, comment out one or more these lines :
  `cgns_utils coarsen surfaceMesh.cgns`
- The genWingMesh.py is used to extrude the surface mesh to volume mesh using pyHyp

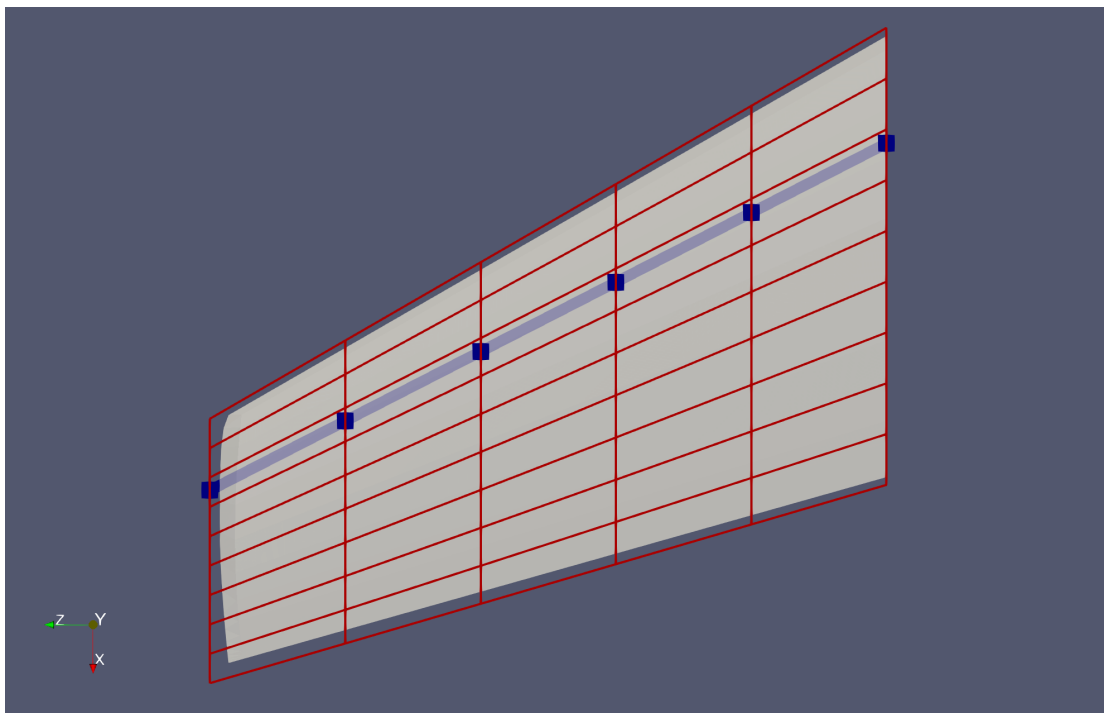
NOTE : We can run `preProcessing_snappyHexMesh.sh` to generate unstructured mesh instead. Refer to this link for more details :
`https://cfd.direct/openfoam/user-guide/v6-snappyhexmesh/`

The `runScript.py` script (1/4)

The `runScript.py` script is similar to the airfoil (subsonic) case. The main differene is that :

1. In the design variable setup, we create a reference axis (blue line) aligned with z and located at 25% chordwise (xFraction=0.25). Here nTwists=6 is the number of FFD layers in z. This ref axis will be used to twist the wing at these 6 spanwise locations

```
nTwists = DVGeo.addRefAxis("bodyAxis", xFraction=0.25, alignIndex="k")
```



The `runScript.py` script (2/4)

2. Similar to the alpha(val,geo) function, we define a twist(val, geo) function to twist the wing. Here we loop over all the spanwise locations except for the root and assign the design variable values from `val` to `geo.rot_z["bodyAxis"].coef[i]`. Then the `geo` object will actually twist the wing during optimization. Note that the first element in `val`, i.e., `val[0]` is the 2nd twist to the root, but `geo.rot_z["bodyAxis"].coef[0]` is the root twist, that is why we use `val[i-1]`.

```
def twist(val, geo):
    for i in range(1, nTwists):
        geo.rot_z["bodyAxis"].coef[i] = val[i - 1]
```

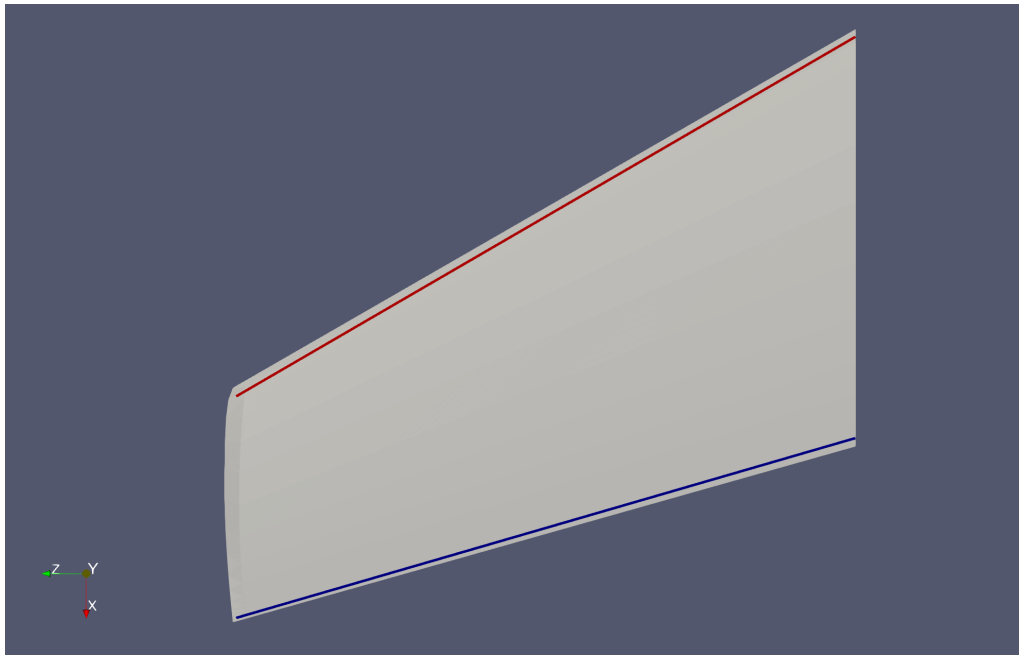
After that, we add the twist as the design variable. Again, we have only nTwists-1 twist variables, and their initial values are all zeros : `np.zeros(nTwists-1)`.

```
# twist
DVGeo.addGeoDVGlobal("twist", np.zeros(nTwists - 1), twist, lower
    =-10.0, upper=10.0, scale=1.0)
daOptions["designVar"]["twist"] = {"designVarType": "FFD"}
```

The `runScript.py` script (3/4)

3. Similar to the airfoil case, we need to define LE (red) and TE (blue) lines for the thickness and volume constraints

```
leList = [[0.01, 0.0, 1e-3], [0.7, 0.0, 1.19]]
teList = [[0.79, 0.0, 1e-3], [1.135, 0.0, 1.19]]
```



We do not impose symmetry constraints because it is a 3D case. Also, the LE and TE constrainst can be easily added by calling :

```
DVCon.addLeTeConstraints(0, "iLow")
DVCon.addLeTeConstraints(0, "iHigh")
```

The `runScript.py` script (4/4)

4. There are other minor changes, e.g., we add a "checkMeshThreshold" parameter in "daOptions" to relax the mesh quality tolerance, in "meshOptions", we have only one symmetry plane, as opposed to two symmetry planes in the airfoil case.

Useful links

- OpenFOAM user guide :
  `https://www.openfoam.com/documentation/user-guide`
- DAFoam documentation :
  `https://dafoam.github.io`
- MACH-Aero documentation :
  `https://mdolab-mach-aero.readthedocs-hosted.com`

Thank you !