FUN3D v13.4 Training

Session 12: Feature- and Adjoint-Based Error Estimation and Mesh Adaptation

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Learning Goals

- Background on adaptation
- Manual step-by-step output adaptation cycle
- Describe the scripts that automate this process

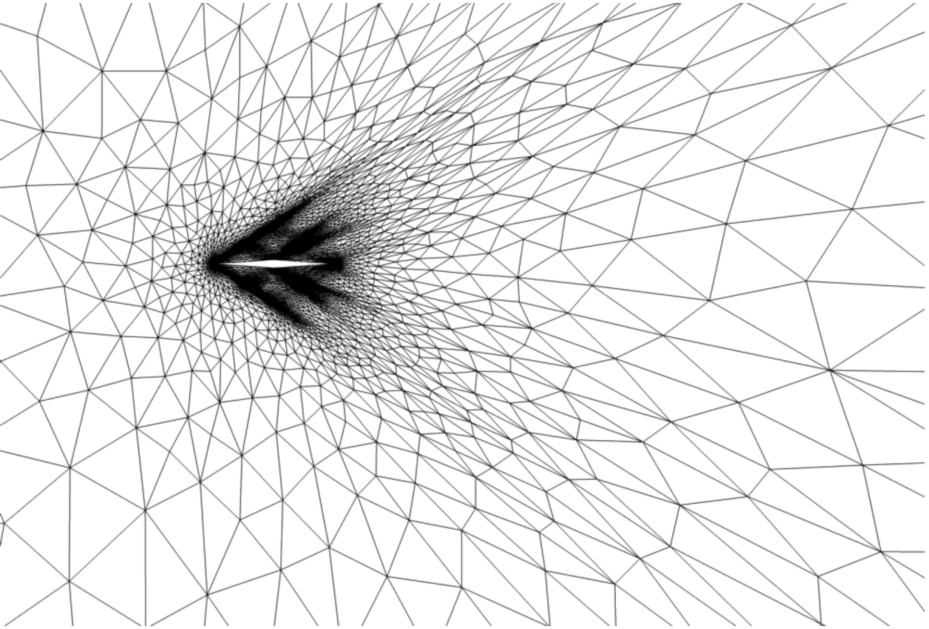
Available Adaptation Modes

- Split into error-estimation/metric construction and adaptive mechanics
- Output-based adaptation for capabilities with an adjoint
- Feature-based adaptation for other flow solver capabilities
- Anisotropic metric-based triangular and tetrahedral grid adaptation with a frozen mixed element boundary layer that can be subdivided
- Experimental grid adaptation for time accurate simulations
- Controlled with the `&adapt_mechanics` and `&adapt_metric_construction` namelists
- See FUN3D user manual grid adaptation overview section and complete namelist description

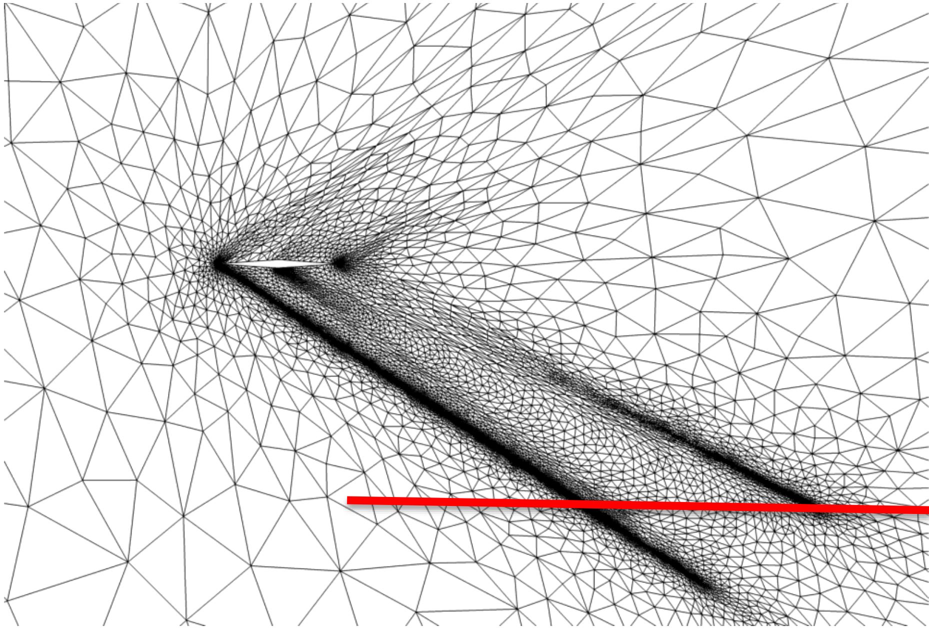
Output-Based Adaptation

- Mathematically rigorous approach involving the adjoint solution that reduces estimated error in an engineering output
- Uniformly reducing discretization error is not ideal from an engineering standpoint - some errors are more important to outputs

Adapted for Drag



Adapted for Shock Propagation



Local Error and Output Adaptation

Feature based

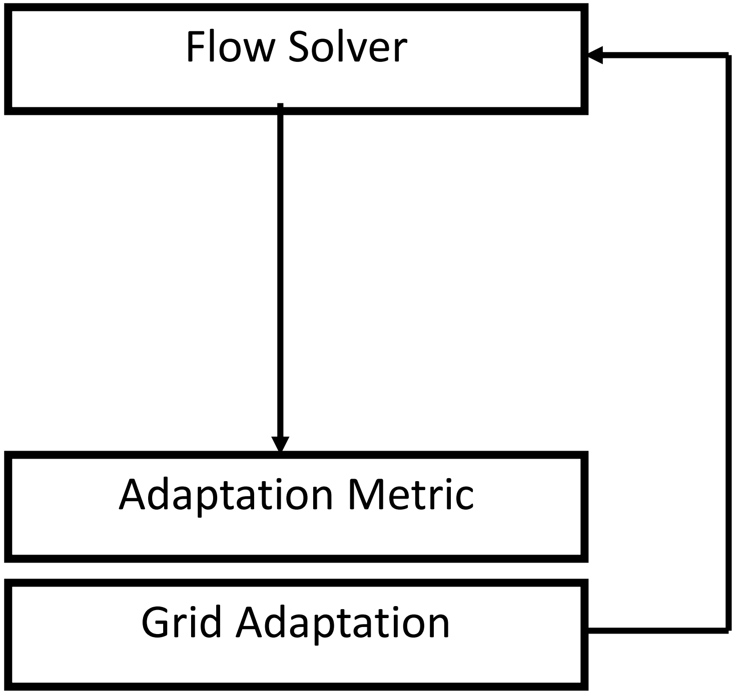
- Flow solver/physics agnostic
- Not as robust
- Requires more manual interaction

Output (adjoint) based

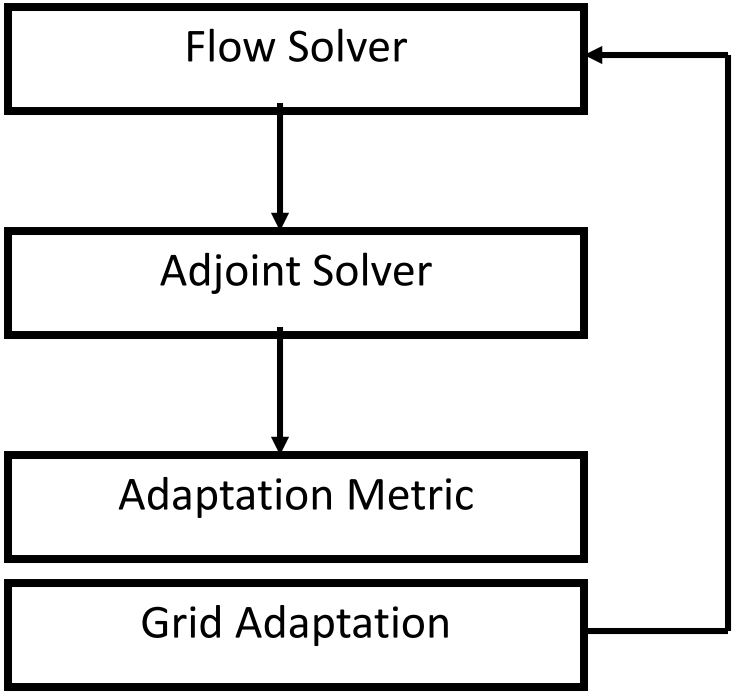
- Requires adjoint solution
- More robust
- Transport of errors
- Fewer user controlled parameters

Adaptation Process

Local error based

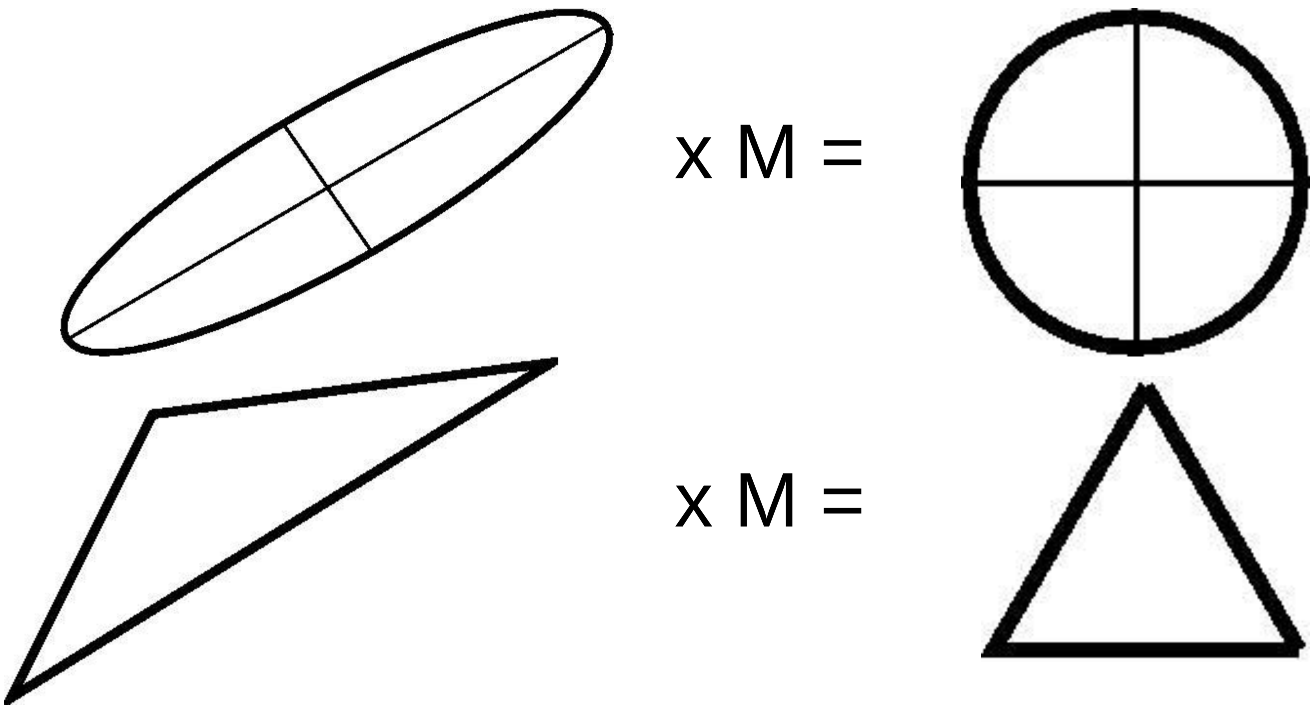


Output (adjoint) based



Metric Adaptation Mechanics

- Parallel node insertion, node movement, element collapse, and element swap to iteratively drive mesh to satisfy an anisotropic metric M



Metric

- Many methods are available in literature to construct the metric
- Most commonly used methods in FUN3D are based on a reconstructed Hessian (`adapt_hessian_method`) of a scalar (`adapt_hessian_key`), i.e. Mach number

Metric Adaptation Mechanics

- Selectable with `adapt_library` in `&adapt_mechanics` or driven with scripts
- FUN3D is distributed with
  - refine/one (mature, development stopped)
  - refine/two (under development, 2D, mixed elements)
- FUN3D can interact with external tools
  - BAMG (Bidimensional Anisotropic Mesh Generator)
  - In-house proprietary tools
- refine is also available https://github.com/NASA/refine

Venditti Adaptation Metric

- Output-based size specification scales the stretching and orientation of the Mach Hessian grid metric (Venditti and Darmofal)
- This error is typically evaluated on an embedded grid (with a large memory requirement) with an interpolated solution `adapt_error_estimation='embed'`
- `adapt_error_estimation='single'` is an single grid heuristic

$$e_\kappa = \frac{|(\hat{\lambda} - \bar{\lambda})R(\hat{u})| + |(\hat{u} - \bar{u})R_\lambda(\hat{\lambda})|}{2}$$

$$\frac{h_{\text{request}}}{h_{\text{current}}} = \left(\frac{e_{\text{tol}}}{\sum e_\kappa} \frac{e_{\text{tol}}}{N e_\kappa} \right)^\omega$$

Feature based Metric

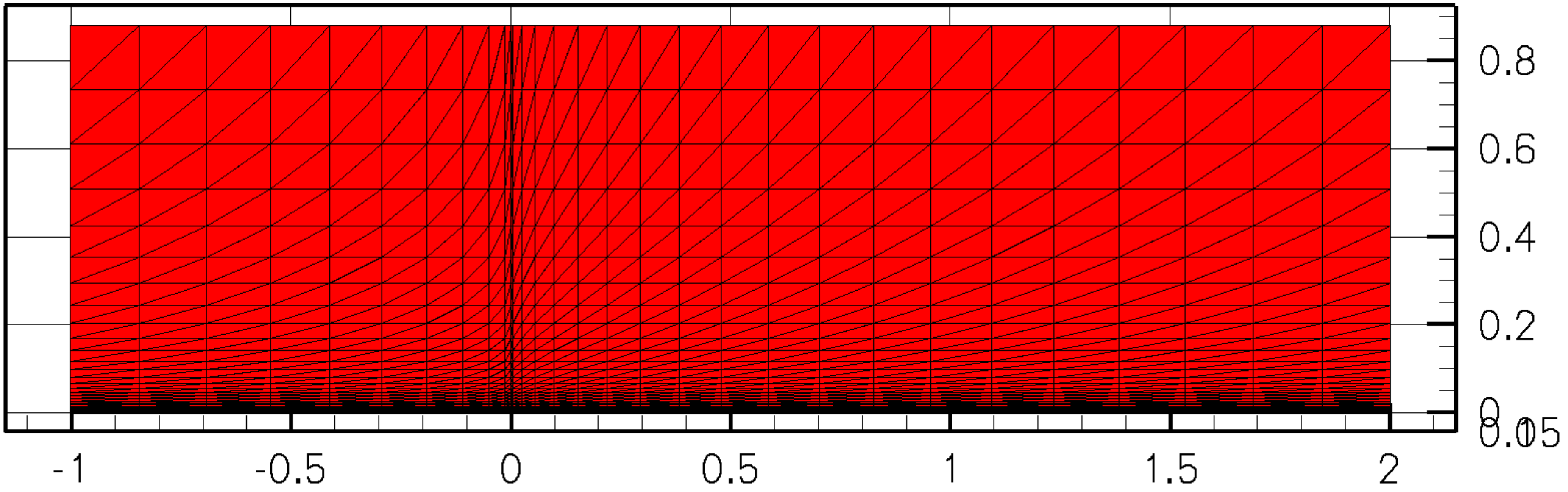
- Implemented in the Venditti framework where the nodal error estimate is replaced with a function of a solution scalar
  - `adapt_feature_scalar_key`
  - `adapt_feature_scalar_form`
- See Bibb, et al. AIAA-2006-3679 for details and Shenoy, Smith, Park AIAAJA 2014 DOI:10.2514/1.C032195 for a recent application

Cases

- Single output-based cycle performed manually on a supersonic flat plate
- Fully scripted diamond airfoil drag adaptation in supersonic flow

Supersonic Flat Plate

- Mach 2, 1,000,000 Reynolds number, Spalart-Allmaras turbulence model



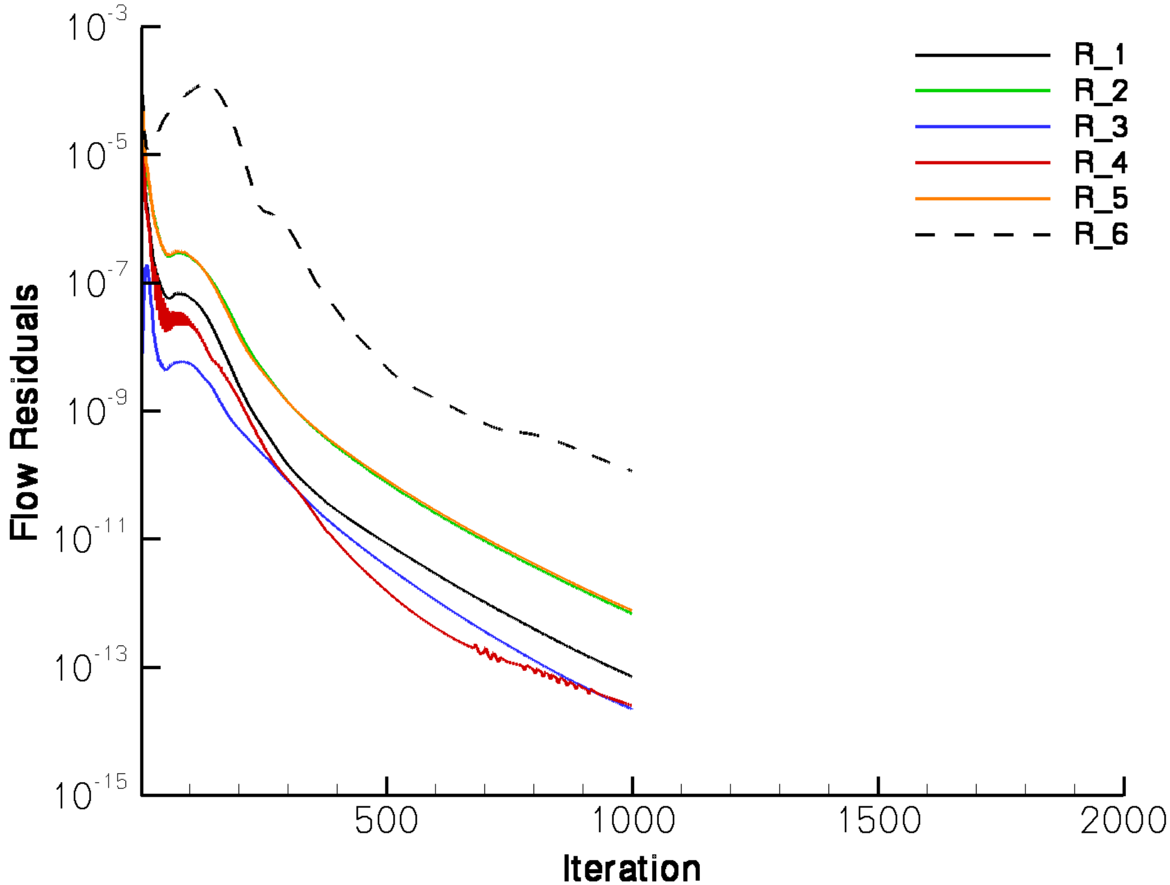
Initial Flow Solution

- Follow the design directory layout convention
- Grid and `fun3d.nml` should be in a directory named `Flow`

```
$ cd Flow
$ mpirun -np 8 nodet_mpi
```

Initial Flow Solution

- Flow solver (primal) convergence history



Initial Adjoint Solution

- Adjoint function is defined in `rubber.data`
  - Only need to set the cost function, the other design inputs no used
- This is a integral of pressure along a line
  - Target off-body pressures required for sonic boom prediction

```
...
Components of func 1: boundary id (0=all)/name/value/weight/target/power
    0 boom_targ   0.000000000000000    1.0    0.00000 1.000
...
```

Initial Adjoint Solution

- The `boom_targ` function requires an additional namelist in `fun3d.nml`

```
&sonic_boom
 x_lower_bound =  0.0
 x_upper_bound =  1.0
 nsignals = 1
 y_ray(1) =  0.05
 z_ray(1) =  0.1
/
```

Initial Adjoint Solution

- Initial `fun3d.nml` adjoint solver parameters

```
&code_run_control
  steps             = 200
  stopping_tolerance = 1.0e-13
  restart_read      = "off"
/
```

Typically run less adjoint iterations

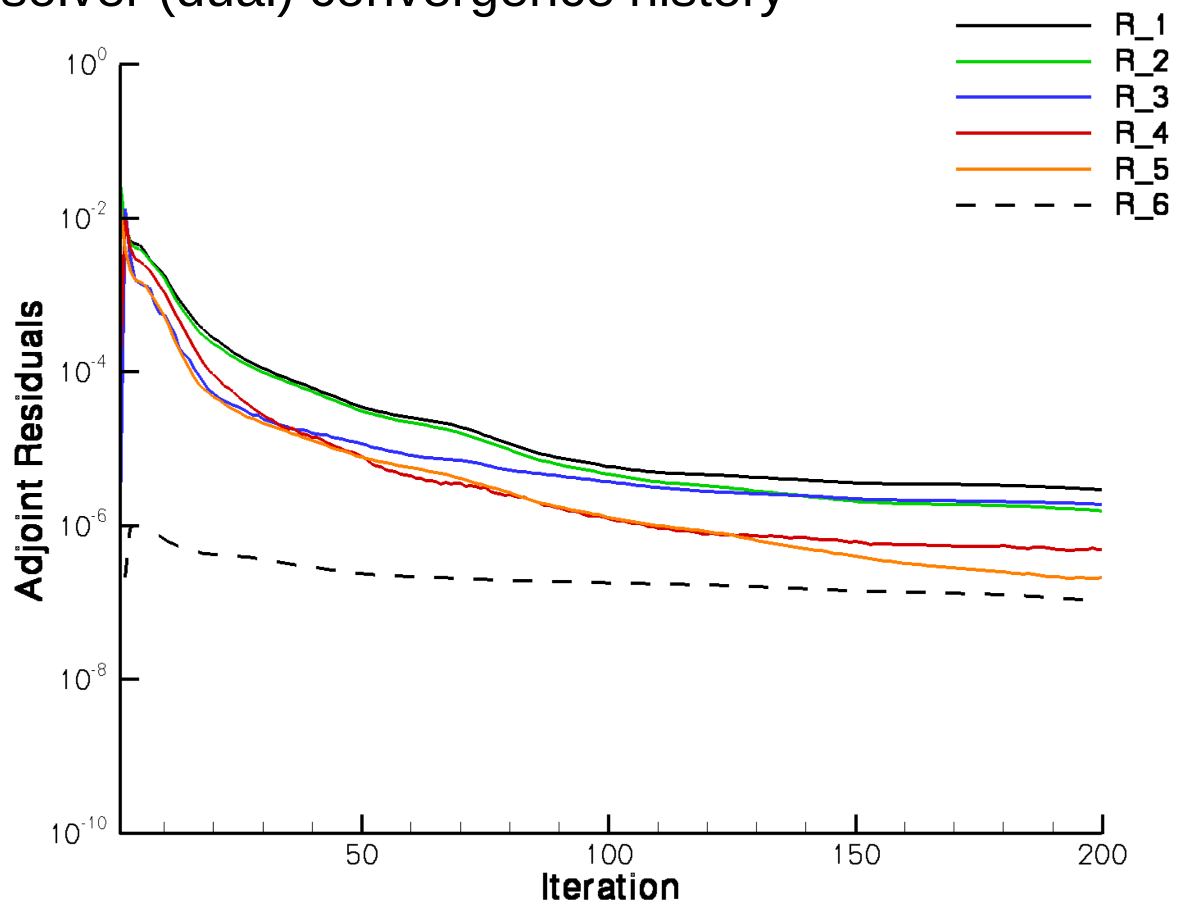
Initial Adjoint Solution

- Follow the design directory layout convention
- Grid and `fun3d.nml` should be in a directory named `Flow`
- The file `rubber.data` should be in the directory above
- Adjoint solver should be run in a directory named `Adjoint`

```
$ cd Adjoint
$ mpirun -np 8 dual_mpi --outer_loop_krylov
```

Initial Adjoint Solution

- Adjoint solver (dual) convergence history



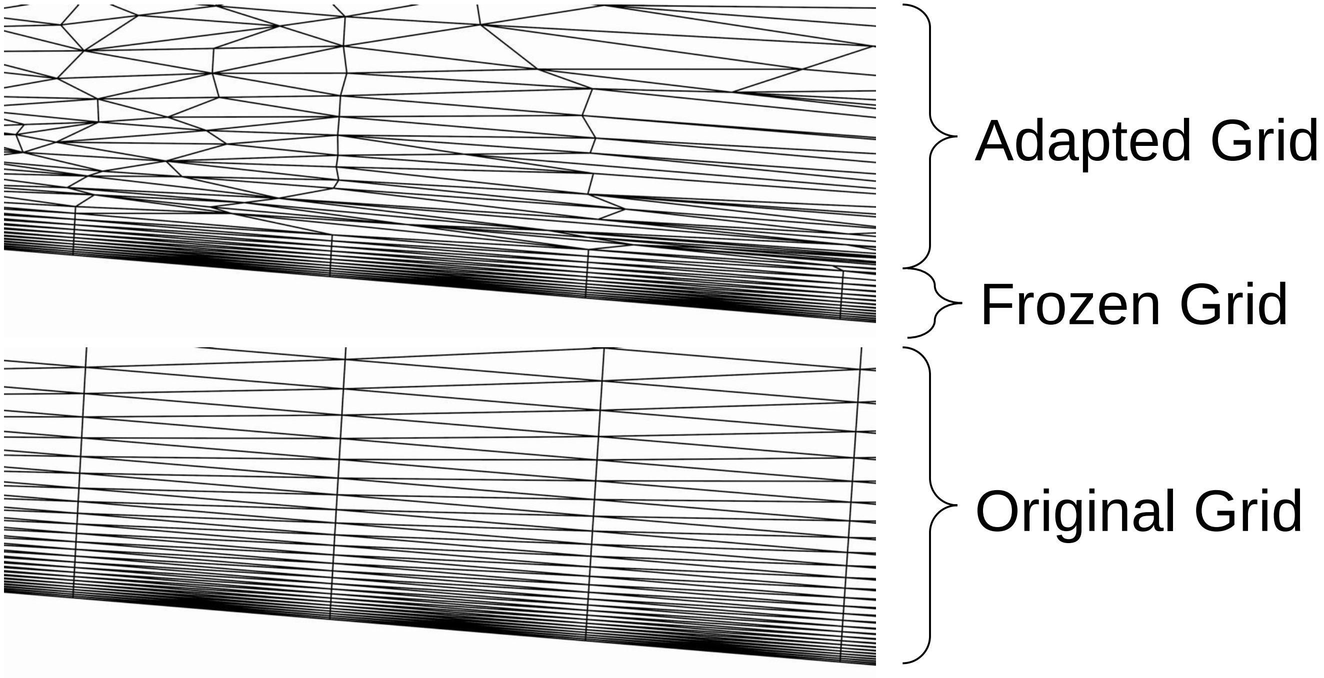
Output-Based Adaptation

- Output-based adaptation `fun3d.nml` parameters

```
&adapt_mechanics
  adapt_project   = 'box02'
  adapt_freezebl = 0.001
/
```

New project name

Frozen boundary layer



Output-Based Adaptation

- Planar geometry is specified to `refine/one` with `faux_geom`
- Place in the same directory that the adaptation is executed (`Adjoint`)

```
7
1 xplane          -1.000000000000000
2 xplane           2.000000000000000
3 yplane           0.000000000000000
4 yplane           0.100000000000000
5 zplane           0.000000000000000
6 zplane           0.000000000000000
7 zplane           0.881362940781450
```

Number of planes

Each plane with normal and position

Initial Adjoint Solution

- Follow the design directory layout convention
- Grid and `fun3d.nml` should be in a directory named `Flow`
- The file `rubber.data` should be in the directory above
- Adjoint grid adaptation should be run in a directory named `Adjoint`

```
$ cd Adjoint
$ mpirun -np 8 dual_mpi --rad --adapt
```

`--rad` = Residual Adjoint Dot-product

`--adapt` = Activates grid adaptation

Adapted Flow Solution

- Initial `fun3d.nml` grid and flow conditions

```
&project
  project_rootname = "box02"
/
&raw_grid
  grid_format = "aflr3"
  data_format = 'stream'
/
&code_run_control
  steps                = 1000
  stopping_tolerance = 1.0e-13
  restart_read         = "on"
/
```

New project name

New grids are always AFLR3 (ugrid) stream format

The solution is interpolated

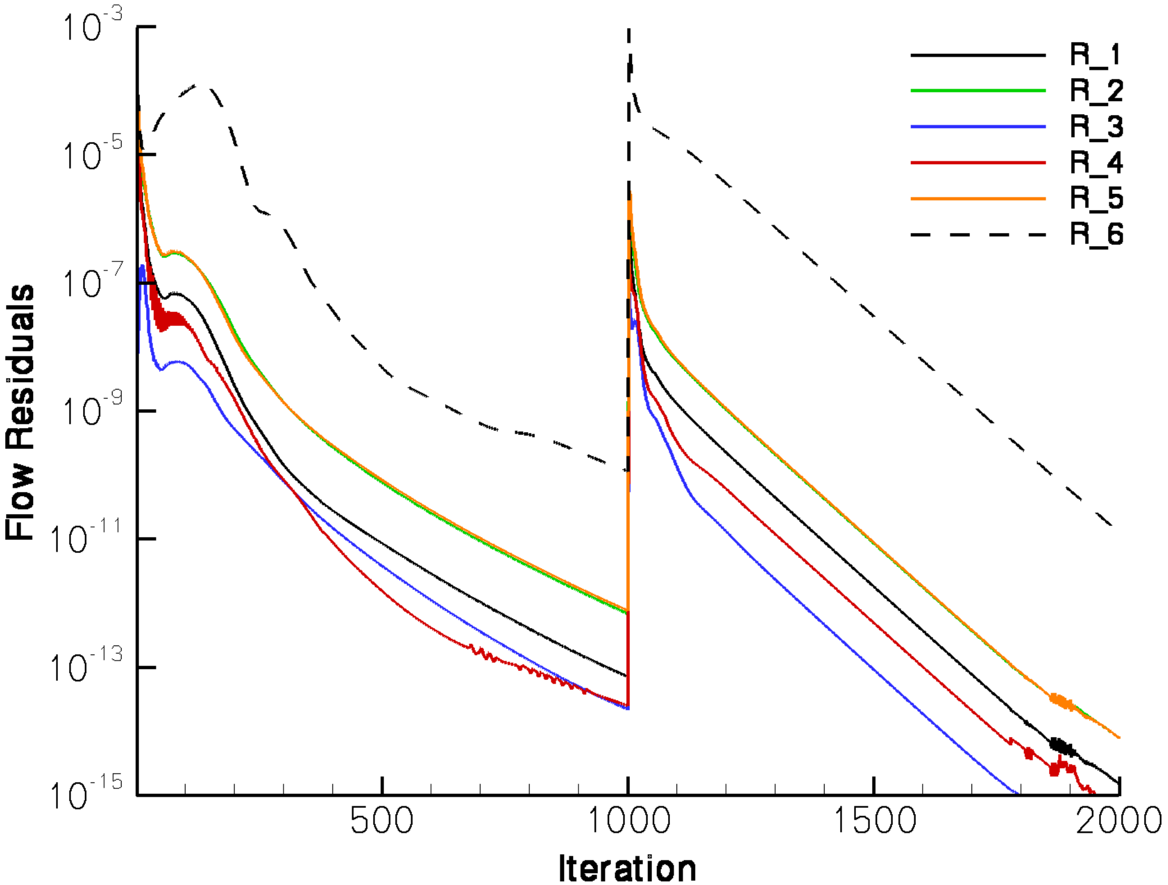
Adapted Flow Solution

- Follow the design directory layout convention
- Grid and `fun3d.nml` should be in a directory named `Flow`

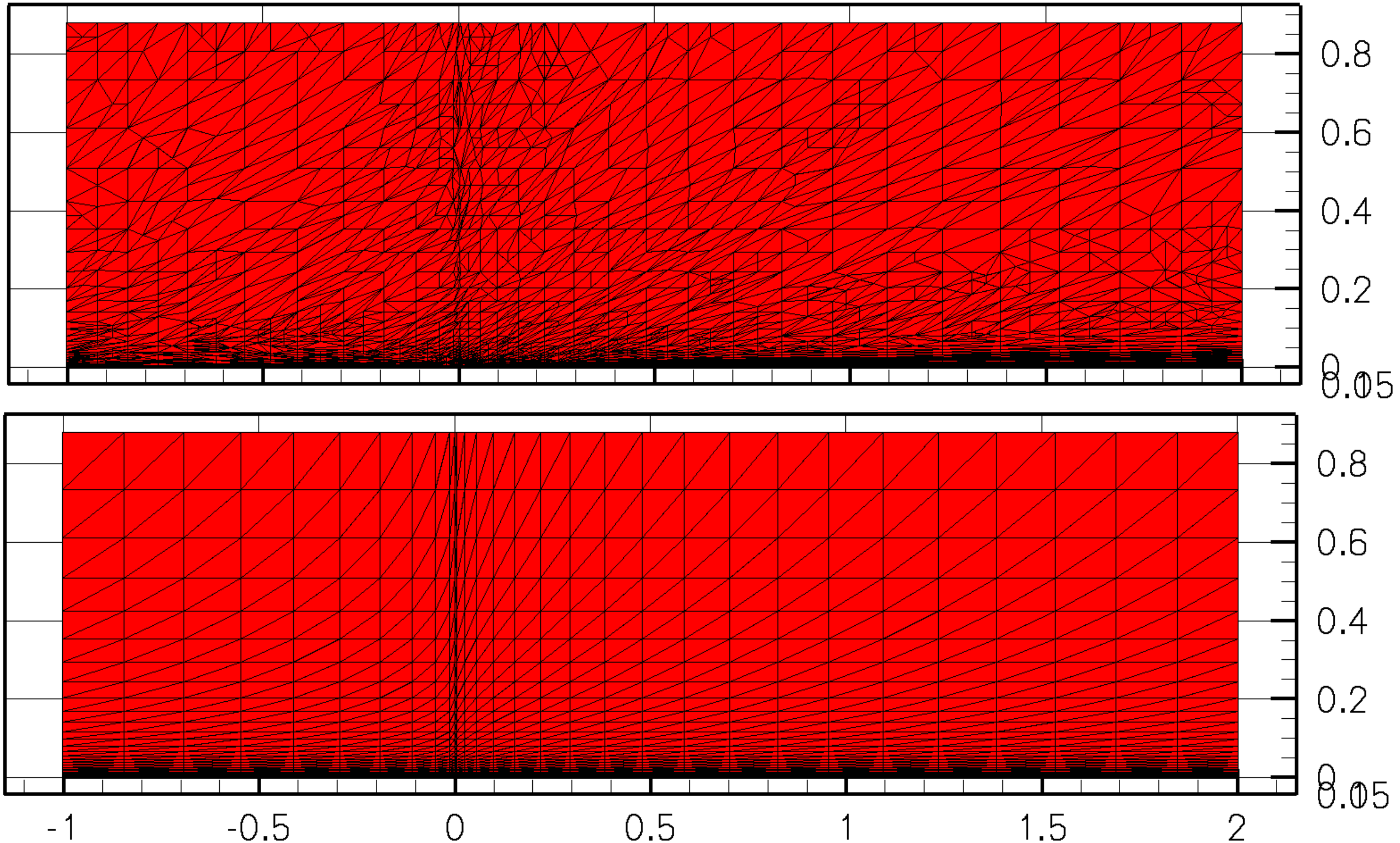
```
$ cd Flow
$ mpirun -np 8 nodet_mpi
```

Adapted Flow Solution

- Flow solver (primal) convergence history



Adapted and Original Flat Plate Grid

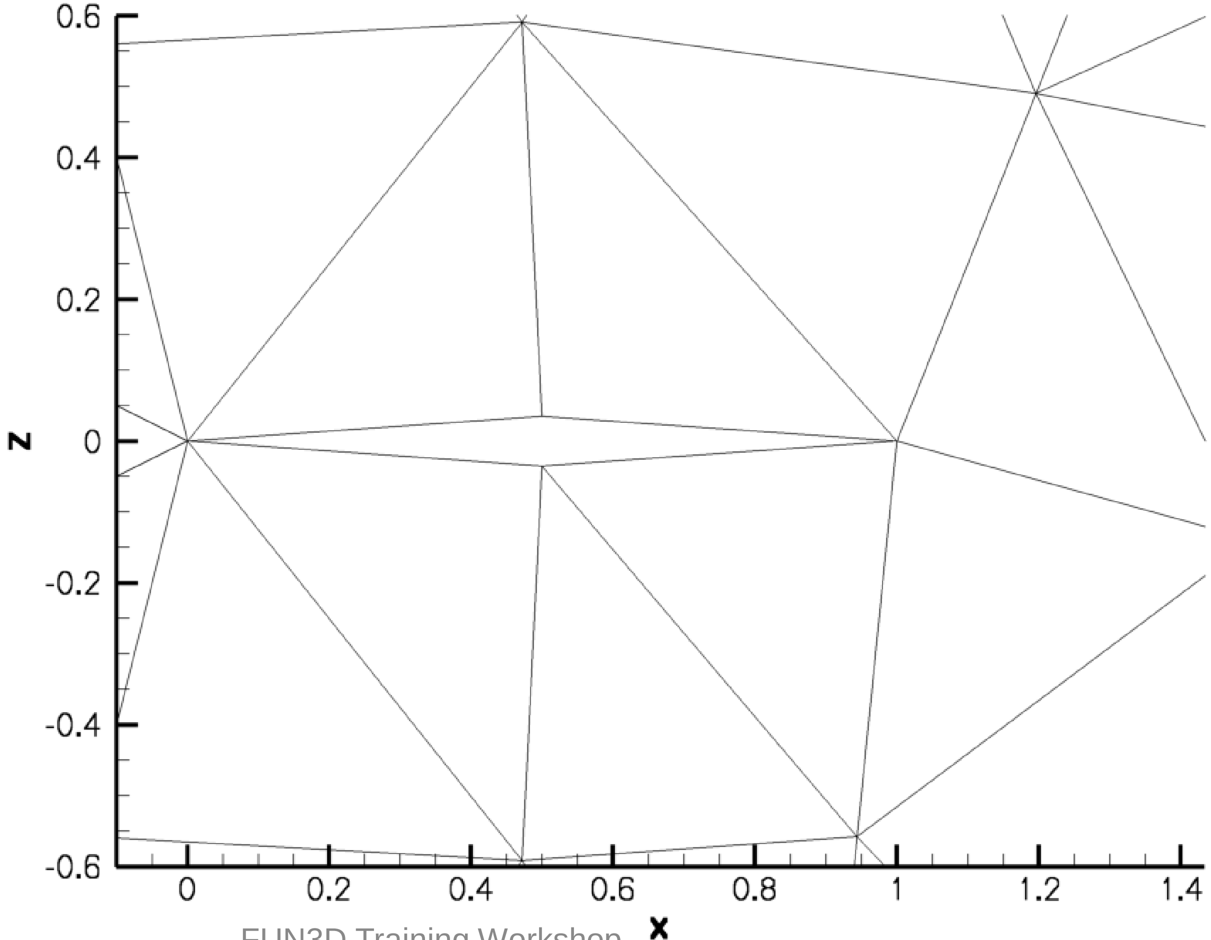


`F3D` script

- Domain specific language written in Ruby
- Simple syntax for driving adaptation with the power of a scripting language if needed
- Input file `case_specifics` is scanned for updates during adaptation allowing for computational steering
- All input files are expected to be in the current directory and are also scanned for updates
  - Files are copied to `Flow` and `Adjoint` as needed
- Can generate `rubber.data` with `$ f3d function cd`
- Subcommands to start, stop, and examine adaptation in progress
- Discussed in Grid Adaptation section of the user manual

Drag-Adapted Diamond Airfoil

- Mach 2.0, inviscid flow, extremely coarse initial BAMG grid



`F3D` input `case_specifics` example

- Keyword value pairs to add command line options, adjust namelist settings, and specify outer adaptation cycle iterations

```
root_project 'diamond'

number_of_processors 8

adj_cl " --outer_loop_krylov "

rad_nl["adapt_complexity"] = 200*(1.5**iteration)

all_nl['data_format']="'stream'" if (iteration>1)

first_iteration 1
last_iteration 10
```

Namelist Setup

- Initial `fun3d.nml` grid and flow conditions

```
&adapt_mechanics
 adapt_library = 'refine/two'
 adapt_project = 'diamond02'
/
&adapt_metric_construction
  adapt_hessian_method = 'grad'
  adapt_hessian_average_on_bound = .true.
  adapt_twod = .true.
  adapt_statistics = 'average'
  adapt_max_anisotropy = 10.0
  adapt_complexity = 1000
  adapt_gradation  = 1.5
  adapt_current_h_method = 'implied'
/
```

refine version 2 mechanics

`F3D` script

- Run with no subcommands for help

```
$ f3d
usage: f3d <command>

 <command>         description
 ---------         -----------
 start             Start adaptation
 view              Echo a single snapshot of stdout
 watch             Watch the result of view
 shutdown          Kill all running fun3d and ruby processes
 clean             Remove output and sub directories
 function [name]   write rubber.data with cost function [name]
```

`F3D` script

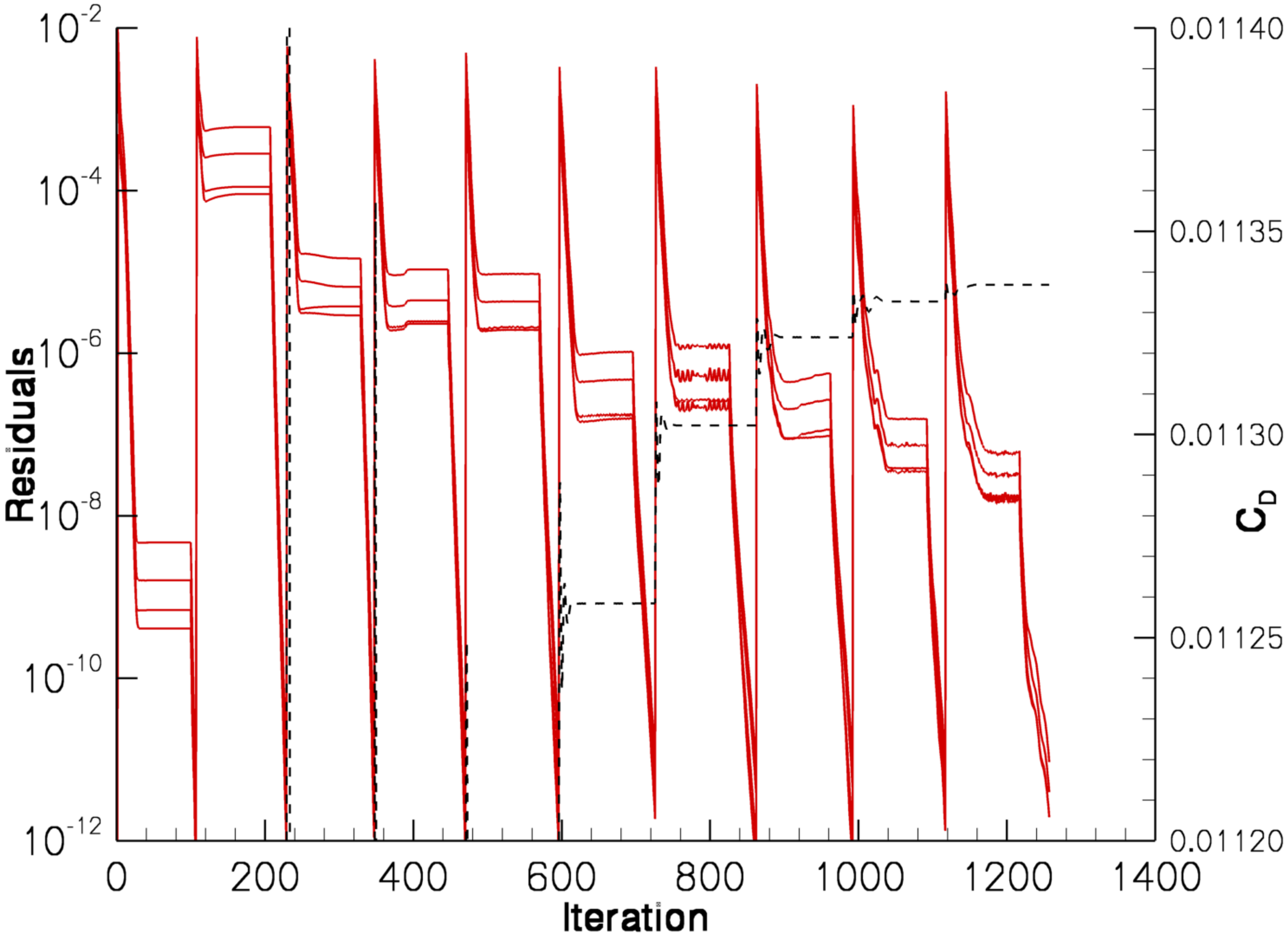
- To begin and watch progress

```
$ f3d start
$ f3d watch
```

`F3D` script

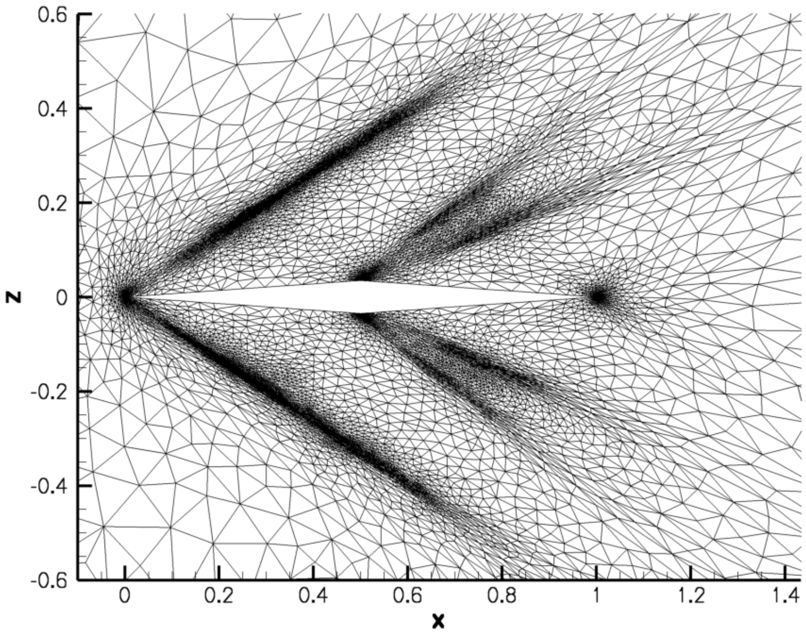
- Copies `fun3d.nml` into Flow directory and modifies it to set `project_rootname`, `restart_read`, and other options with the `nl_flo`, `nl_adj`, `nl_rad` hashes
- Backup copies of `fun3d.nml` are saved as `[project]_flow_fun3d.nml`, `[project]_dual_fun3d.nml`, and `[project]_rad_fun3d.nml`
- Backup copies of standard screen output are are saved as `[project]_flow_out`, `[project]_dual_out`, and `[project]_rad_out`

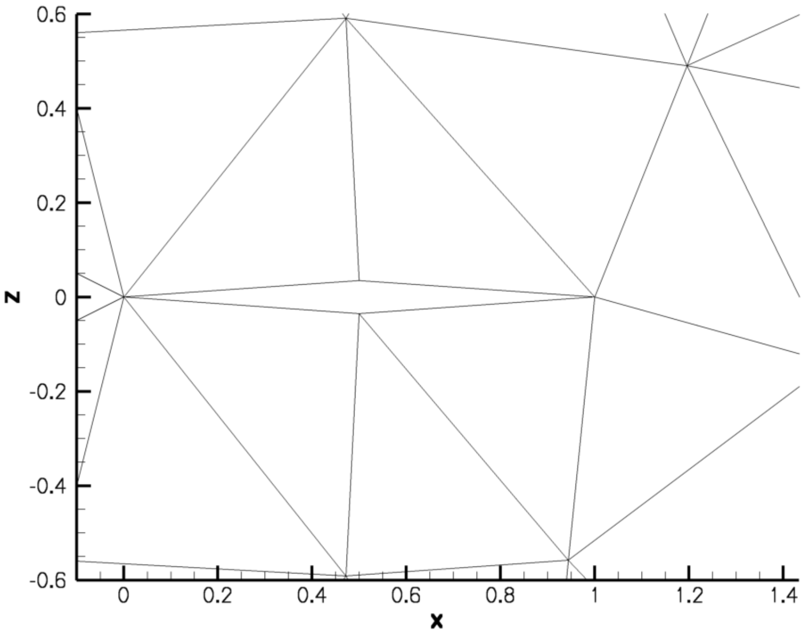
Drag-Adapted Diamond Airfoil



Drag-Adapted Diamond Airfoil

- Mach 2.0, inviscid flow





What Can Go Wrong?

- Flow solver did not produce a project.forces file on completion
  - Indicate a setup problem (first iteration)
  - Previous grid adaptation failed (error estimation, grid mechanics)
  - Flow solver crashed or diverged
- Examine `flow_out` for more details

```
/u/mpark/fun3d/opt/bin/f3d:149:in `readlines': No such file or
directory - Flow/diamond07.forces (Errno::ENOENT)
   from /u/mpark/fun3d/opt/bin/f3d:149:in `read_forces'
   from /u/mpark/fun3d/opt/bin/f3d:121:in `flo'
   from /u/mpark/fun3d/opt/bin/f3d:224:in `iteration_steps'
   from /u/mpark/fun3d/opt/bin/f3d:233:in `iterate'
   from /u/mpark/fun3d/opt/bin/f3d:310
```

What Can Go Wrong?

- Adjoint solver setup (particularly `rubber.data`)

Evolving Process

- Lightning talk
- Continuing development of refine grid mechanics (for CAD models)
- Implementation of error estimation techniques