FUN3D v13.4 Training

Session 13: Time-Dependent Simulations

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Session Scope

- What this will cover
  - How to set up and run time-accurate simulations on static meshes
    - Subiteration convergence: what to strive for and why
    - Nondimensionalization
    - Choosing the time step
    - Input / Output
- What will not be covered
  - Moving-mesh, aeroelastics (covered in follow-on sessions)
- What should you already be familiar with
  - Basic steady-state solver operation and control
  - Basic flow visualization

Introduction

- Background
  - Many of problems of interest involve unsteady flows and may also involve moving geometries
  - Governing equations written in Arbitrary Lagrangian-Eulerian (ALE) form to account for grid speed
  - Nondimensionalization often more involved/confusing/critical
- Compatibility
  - Compressible/incompressible paths
  - Mixed elements; 2D/3D
  - Dynamic grids
  - Not compatible with generic gas model
- Status
  - Incompressible path exercised very infrequently for unsteady flows

Governing Equations

- Arbitrary Lagrangian-Eulerian (ALE) Formulation

$$\frac{\partial(\vec{Q}V)}{\partial t} = -\oint_{\partial V}\left(\overline{\overline{F}} - \vec{q}\vec{W}^T\right)\cdot\vec{n}dS - \oint_{\partial V}\overline{\overline{F}}_v\cdot\vec{n}dS = \vec{R} \qquad \vec{Q} = \frac{\oint_V \vec{q}\,dV}{V}$$

$\vec{W} =$ Arbitrary control surface velocity; Lagrangian if $\vec{W} = (u,v,w)^T$ (moves with fluid); Eulerian if $\vec{W} = 0$ (fixed in space)

- Discretize using N^th order backward differences in time, linearize $\vec{R}$ about time level n+1, and introduce a pseudo-time term:

$$\left[\left(\frac{V^{n+1}}{\Delta\tau} + \frac{V^{n+1}\phi_{n+1}}{\Delta t}\right)\overline{\overline{I}} - \frac{\partial\vec{R}^{n+1,m}}{\partial\vec{Q}}\right]\Delta\vec{Q}^{n+1,m} = \vec{R}^{n+1,m} - \frac{V^{n+1}\phi_{n+1}}{\Delta t}\left(\vec{Q}^{n+1,m} - \vec{Q}^n\right) - \ldots + \vec{R}^{n+1}_{GCL}$$

$$= \overline{\vec{R}^{n+1,m}} + O(\Delta t^N)$$

- Physical time-level t^n ; Pseudo-time level τ^m
- Want to drive ***subiteration residual*** $\overline{\vec{R}^{n+1,m}} \rightarrow 0$ using pseudo-time subiterations at each time step – more later – otherwise you have more error than the expected $O(\Delta t^N)$ truncation error

Time Advancement - Namelist Input

- The **`&nonlinear_solver_parameters`** namelist in the **`fun3d.nml`** file governs how the solution is advanced in time
- Relevant entries - *default values shown* - some definitely need changing:

```
&nonlinear_solver_parameters
  time_accuracy         = 'steady'   (i.e. not time accurate)
  time_step_nondim      = 0.0
  subiterations         = 0
  schedule_iteration    = 1      50
  schedule_cfl          = 200.0 200.0
  schedule_cflturb      = 50.0   50.0
  pseudo_time_stepping = "on"
  temporal_err_control = .false.
  temporal_err_floor    =  0.1
/
```

- Let's look at these in some detail (defer **`time_step_nondim`** to last)

Time Advancement - Order of Accuracy

- Currently have several types of backward difference formulae (BDF) that are controlled by the **`time_accuracy`** component:
  - In order of formal accuracy: BDF1 (**`1storder`**), BDF2 (**`2ndorder`**), $BDF2_{OPT}$ (**`2ndorderOPT`**), BDF3 (**`3rdorder`**), MEBDF4 (**`4thorderMEBDF4`**)
  - Can pretty much ignore all but $BDF2_{OPT}$ and BDF2
    - BDF1 is least accurate; little gain in CPU time / step over 2nd order; for moving grids can be helpful to start out with BDF1 (rare)
    - BDF3 not guaranteed to be stable; feeling lucky?
    - MEBDF4 only efficient if working to very high levels of accuracy - *including spatial accuracy* - generally ***not*** for practical problems
    - $BDF2_{OPT}$ *(recommended)* is a stable blend of BDF2 and BDF3 schemes; formally 2nd order accurate but error is ~1/2 that of BDF2; also allows for a more accurate estimate of the temporal error for the error controller (p.8)

Time Advancement - Subiterations (1/4)

- Can think of each time step as a mini steady-state problem
- Subiterations (**`subiterations`** > 0) are essential
  - Subiteration control in *each time step* operates exactly like iteration control in a steady state case:
    - CFL ramping is available for mean flow and turbulence model – however, be aware that ramping schedule should be < **`subiterations`** or the specified final CFL won't be obtained
      - *We almost never ramp CFL for time-accurate cases*
      - If used, CFL ramping starts over each time step
    - Caution: the *spatial* accuracy flag, **`first_order_iterations`**, starts over each time step, so make sure you don't have this on
- Pseudo-time term helpful for large time steps
  - We *always* use it in our applications
  - **`pseudo_time_stepping = "on"`** `(default)`

Time Advancement - Subiterations (2/4)

- How many subiterations?
  - In theory, should drive subiteration residual "to zero" each time step – but you cannot afford to do that
  - Otherwise have additional errors other than $O(\Delta t^2)$ (if 2nd order time)
- In a perfect world, the answer is to use the ***temporal error controller***
  - **`temporal_err_control = .true.`**
  - **`temporal_err_floor = 0.1`** => iterate until the subiteration residual is 1 order lower than the (estimated) temporal error (0.01 => 2)
  - Subiterations kick out when this level of convergence is reached OR subiteration counter > **`subiterations`**
  - (empirically) 1 order is about the minimum; 2 orders is better, BUT…
  - Often, either the turbulence residual converges slowly or the mean flow does, and the max subiterations you specify will be reached
  - When it kicks in, the temporal error controller is the best approach, and the most efficient; even if it doesn't kick in, it can be informative

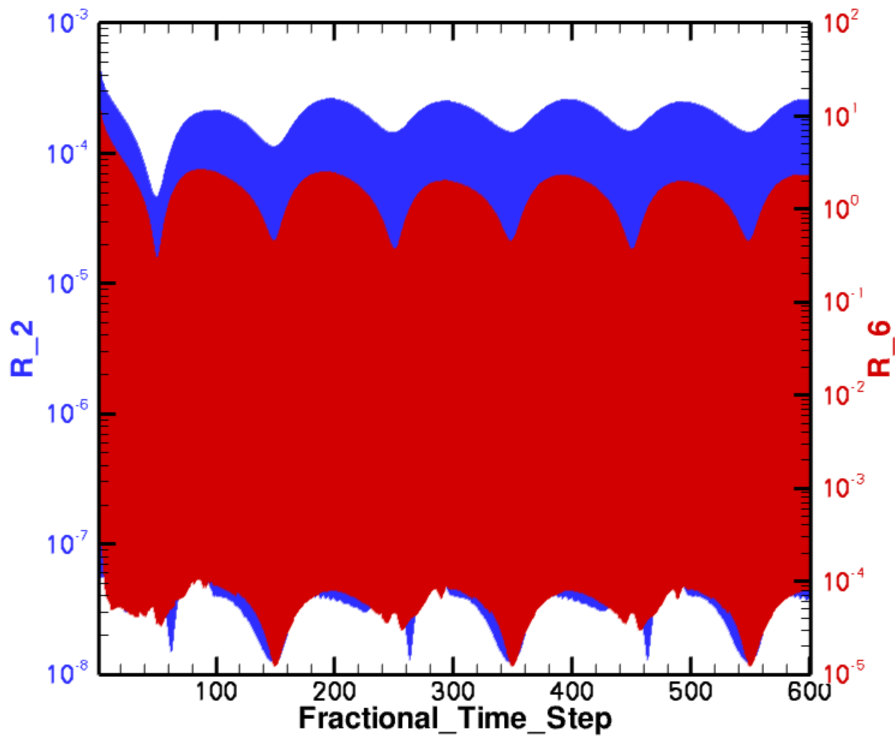
Time Advancement - Subiterations (3/4)

- Be wary reaching conclusions about the effect of time-step refinement unless the subiterations are "sufficiently" converged for each size step
- How to monitor and assess the subiteration convergence:
  - Printed to the screen, so you can "eyeball" it
  - With temporal error controller, if the requested tolerance is not met, message(s) will be output to the screen:
    - **`WARNING: mean flow subiterations failed to converge to specified temporal_err_floor level`**
    - **`WARNING: turb flow subiterations failed to converge to specified temporal_err_floor level`**
    - Note: when starting unsteady mode, first timestep ***never*** achieves target error (no error estimate first step, so target is 0)
    - Note: x-momentum residual (**`R_2`**) is the mean-flow residual targeted by the error controller
  - Plot it (usually best)

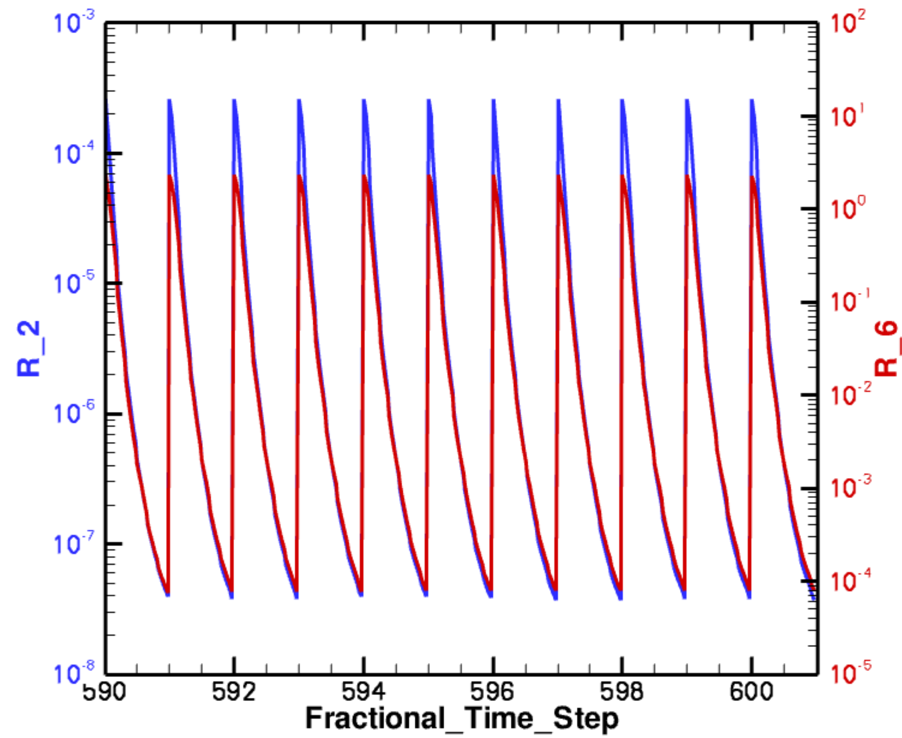
Time Advancement - Subiterations (4/4)

- Tecplot file (ASCII) with subiteration convergence history is output to a file: **`[project]_subhist.dat`**
  - Plot (on log scale) **`R_2`** (etc) vs **`Fractional_Time_Step`**
  - Also contains Cl, Cd, Cm to assess force convergence in a time step

All Time Steps



Final Few Time Steps



Nondimensionalization of Time

- Notation: * indicates a dimensional variable, otherwise nondimensional; the reference flow state is usually free stream (“ ∞ “), but need not be
- Define:
  - L^*_{ref} = reference length of the physical problem (e.g.,chord in ft)
  - L_{ref} = corresponding length in your grid (considered *nondimensional*)
  - a^*_{ref} = reference speed of sound (e.g., ft/sec) (compressible)
  - U^*_{ref} = reference velocity (e.g., ft/sec; compressible: U^*_{ref} = Mach a^*_{ref})
  - t^* = time (e.g., sec)
- Then nondimensional time in FUN3D is related to physical time by:
  - $t = t^* \, a^*_{ref} \, (L_{ref}/L^*_{ref})$ (compressible)
  - $t = t^* \, U^*_{ref} \, (L_{ref}/L^*_{ref})$ (incompressible)
  - *Usually* have $L_{ref}/L^*_{ref} = 1^*$, but need not - e.g., typical 2D airfoil grid
  - L_{ref}/L^*_{ref} appears because Re in FUN3D is input *per unit grid length*

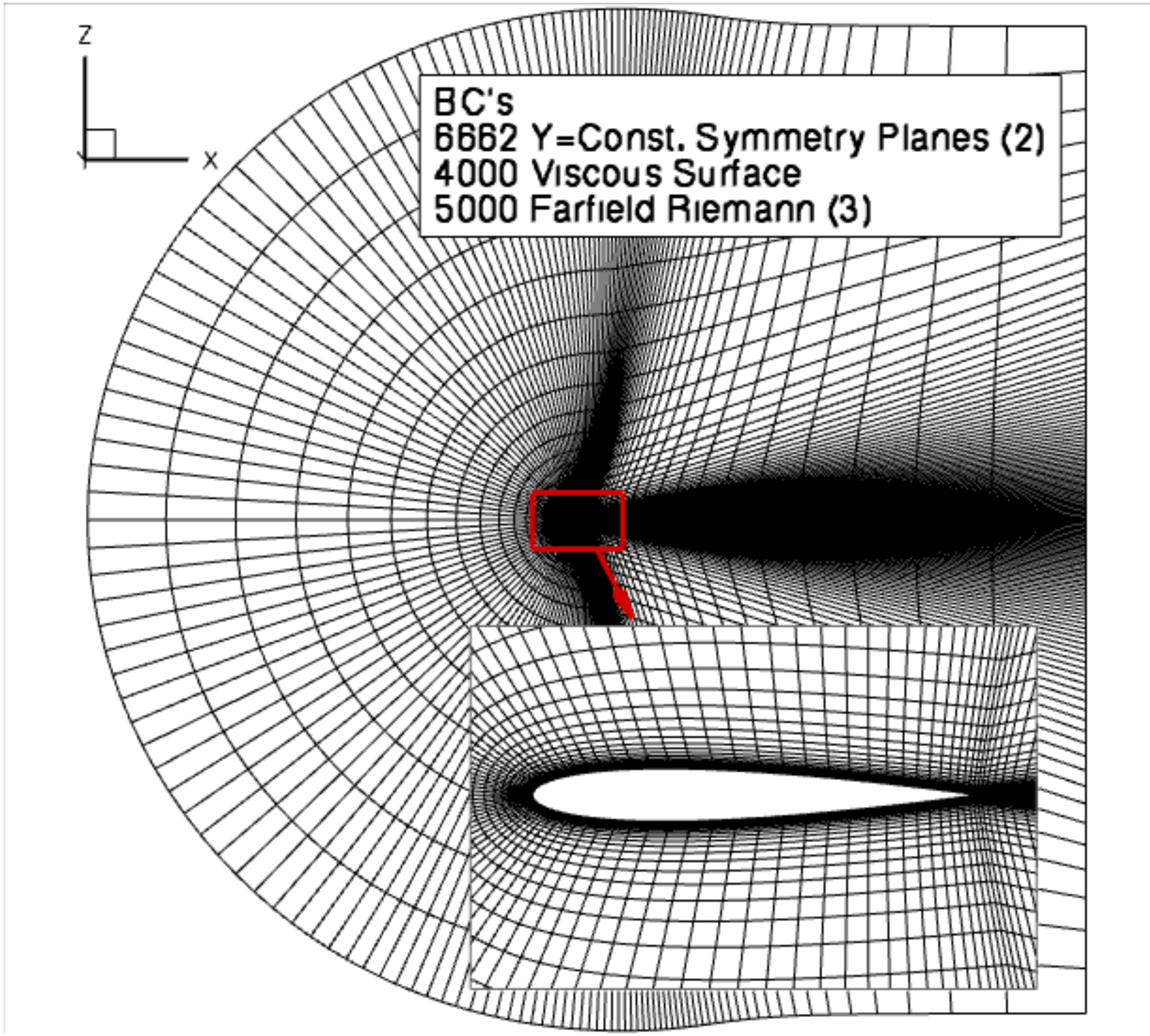
Determining the Time Step

- Identify a ***characteristic time*** t^*_{chr} that you need to resolve with some level of accuracy in your simulation; perhaps:
  - Some important shedding frequency f^*_{shed} (Hz) is known or estimated $t^*_{chr} \sim 1 / f^*_{shed}$
  - Periodic motion of the body $t^*_{chr} \sim 1 / f^*_{motion}$
  - A range of frequencies in a DES-type simulation $t^*_{chr} \sim 1 / f^*_{highest}$
  - If none of the above, you can estimate the time it takes for a fluid particle to cross the characteristic length of the body, $t^*_{chr} \sim L^*_{ref} / U^*_{ref}$
  - $t_{chr} = t^*_{chr}\, a^*_{ref}\, (L_{ref}/L^*_{ref})$ (comp) $t_{chr} = t^*_{chr}\, U^*_{ref}\, (L_{ref}/L^*_{ref})$ (incomp)
- Say you want N time steps within the characteristic time:
  - $\Delta t = t_{chr} / N$ = **`time_step_nondim`**
- Figure an absolute *minimum* of N = 100 for reasonable resolution of t_{chr} with a 2nd-order scheme - really problem dependent (*frequencies > f* may be important*); but don't over resolve time if space is not well resolved too

Tutorial Case: Unsteady Flow, High AoA (1/7)

- Test case located in: tutorials/flow_unsteady_airfoil_high_AoA
  - **`run_tutorial.sh`** script starts with a 2000 time step restart file, runs an additional 100 steps, and makes plots that follow
- Consider flow past a (2D) NACA 0012 airfoil at 45^o angle of attack - the flow separates and is unsteady
  - Re_{c^*} = 4.8 million, M_{ref} = 0.6, *assume* a^*_{ref} = 340 m/s
  - chord = 0.1m, chord-in-grid = 1.0 so L_{ref}/L^*_{ref} = 1.0/0.1 = 10 (m^{-1})
  - Say we know from experiment that lift oscillations occur at ~450 Hz
  - $t^*_{chr} = 1 / f^*_{chr}$ = 1 / 450 Hz = 0.002222 s
  - $t_{chr} = t^*_{chr}\, a^*_{ref}\, (L_{ref}/L^*_{ref})$ = (0.002222)(340)(10) = 7.555
  - $\Delta t = t_{chr} / N$ so Δt = 0.07555 for 100 steps / lift cycle
  - By way of comparison, for M = 0.6, a^*_{ref} = 340 m/s, and L^*_{ref} = 0.1 m it takes a fluid particle ~ (0.1)/(204) = 0.00049 s to pass by the airfoil; this leads to smaller, more conservative estimate for the time step, by about a factor of 4

Tutorial Case: Unsteady Flow, High AoA (2/7)



Tutorial Case: Unsteady Flow, High AoA (3/7)

- Flow viz: output u-velocity and y-component of vorticity
- Relevant fun3d.nml namelist data (note: many defaults assumed)

```
&project
   project_rootname = "n0012_i153"
   case_title = "NACA 0012 airfoil, 2D Hex Mesh"
/
&global
   boundary_animation_freq = 5
/
&raw_grid
    grid_format = "aflr3"
    data_format = "ASCII"
    twod_mode   = .true.
/
&reference_physical_properties
   mach_number       = 0.60
   reynolds_number   = 4800000.00
   temperature       = 520.00
   temperature_units = 'Rankine'
   angle_of_attack   = 45.0
/
```

Tutorial Case: Unsteady Flow, High AoA (4/7)

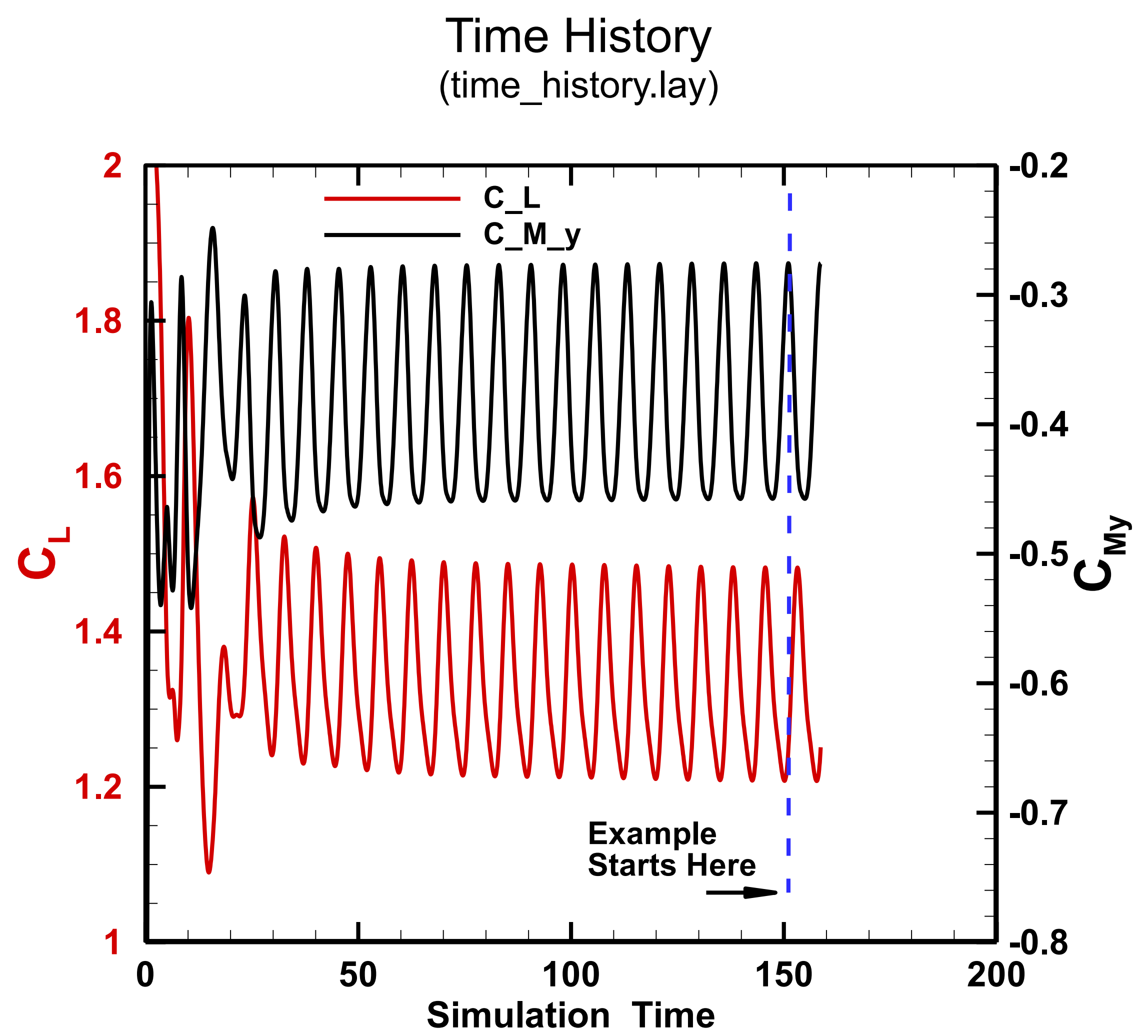
- Relevant fun3d.nml namelist data (cont)

```
&force_moment_integ_properties
    x_moment_center = 0.25
 /
&nonlinear_solver_parameters
    time_accuracy        = "2ndorderOPT" ! Our Workhorse Scheme
    time_step_nondim     = 0.07555       ! 100 steps/cycle @ 450 Hz
    temporal_err_control = .true.        ! Enable error-based kickout
    temporal_err_floor   = 0.1           ! Exit 1 order below error estimate
    subiterations        = 30            ! No more than 30
    schedule_cfl         = 50.00 50.00 ! constant cfl each step; no ramping
    schedule_cflturb     = 30.00 30.00
 /
&code_run_control
    steps        = 100  ! need ~2000 steps to be periodic from freestream

 /

 &boundary_output_variables
   primitive_variables = .false. ! turn off default
   y = .false.     ! So tecplot displays correct 2D orientation by default
   u = .true.
   vort_y = .true.
 /
```

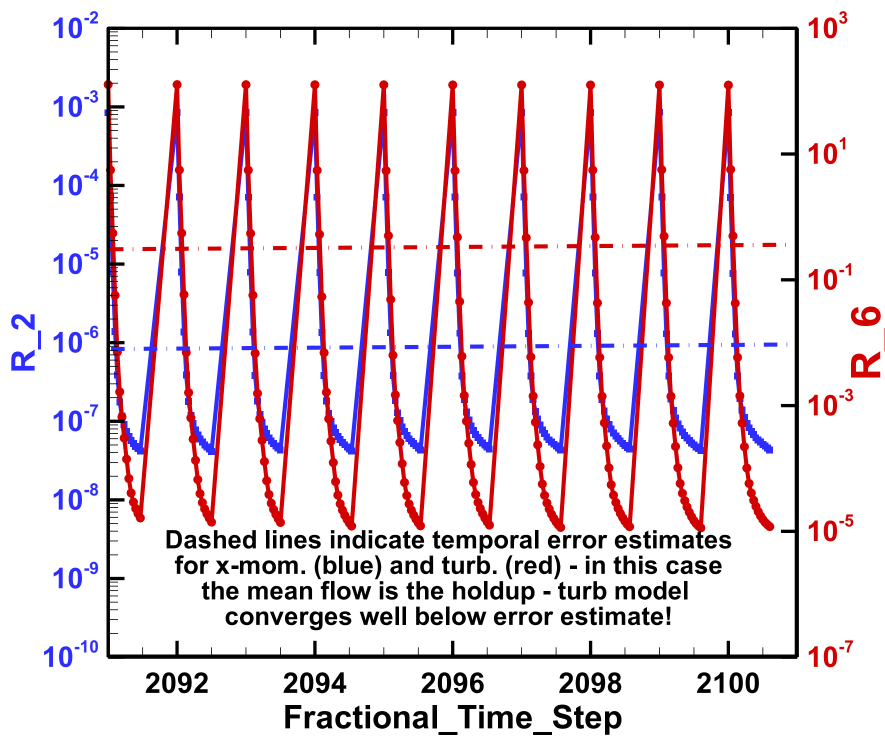
Tutorial Case: Unsteady Flow, High AoA (5/7)



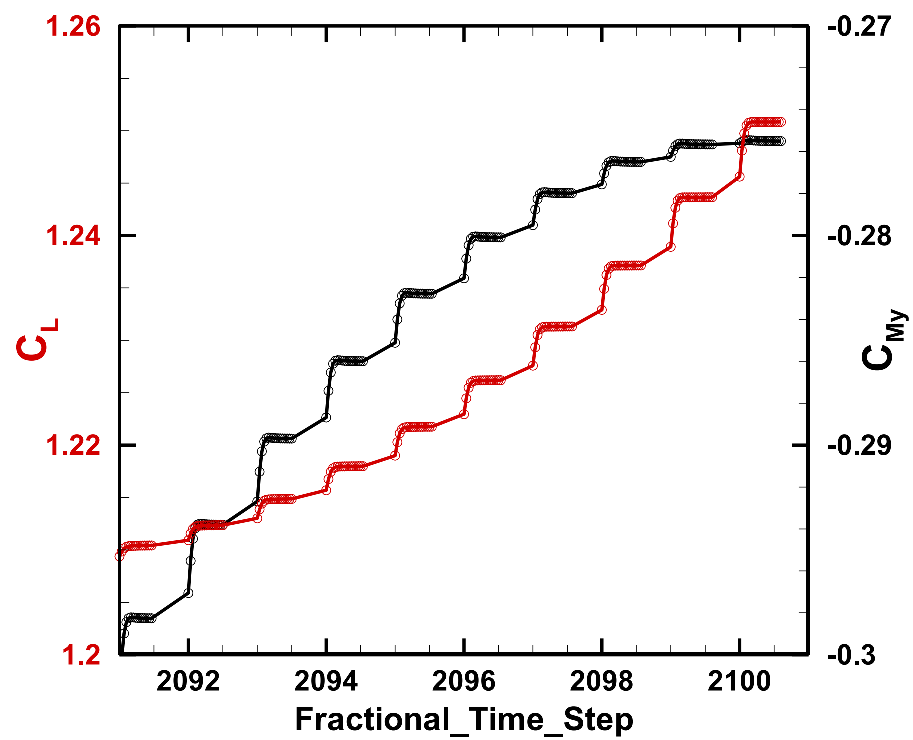
Tutorial Case: Unsteady Flow, High AoA (6/7)

- Subiterations converge? `grep "WARNING" screen_output | wc`
  - In this case, all steps converge to the specified tolerance

Subiteration Residuals, Final 10 Steps



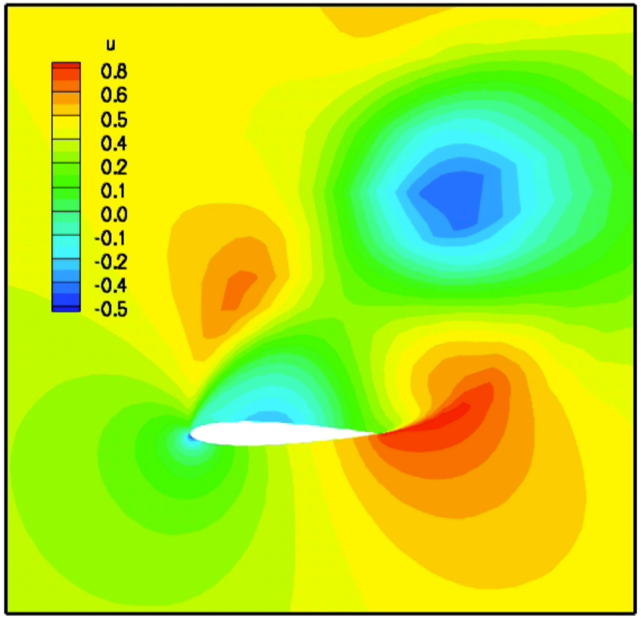
Subiteration Lift & PM, Final 10 Steps

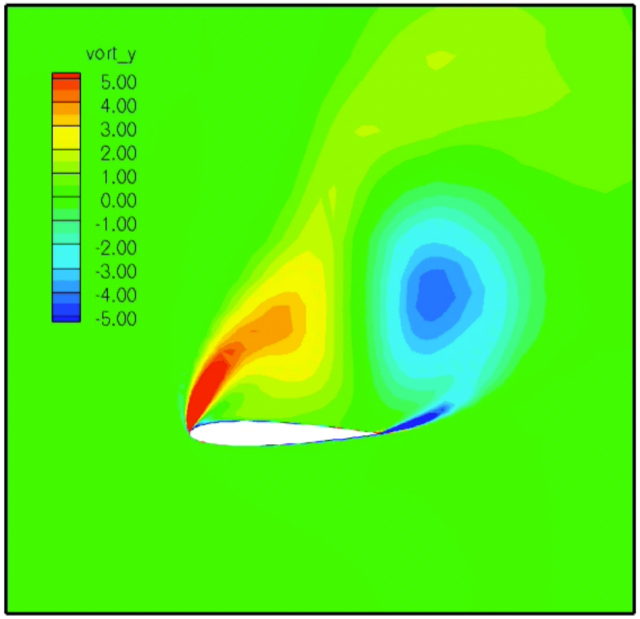


Tutorial Case: Unsteady Flow, High AoA (7/7)

- Animation of Results

X-Component of Velocity





Y-Component of Vorticity

List of Key Input/Output Files

- Beyond basics like **`fun3d.nml`**, etc.:
- Input
  - none
- Output
  - **`[project]_subhist.dat`**
  - Use to check subiteration residual and force/moment convergence