FUN3D v12.7 Training

Session 7: Supersonic and Hypersonic Perfect Gas Simulation

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Session Overview

- How to use FUN3D to compute **perfect gas** supersonic and hypersonic flows (`eqn_type="compressible"`)
  - What are the challenges and strategies
  - Inviscid flux types and inviscid flux gradient limiters options that work the best for supersonic and hypersonic flows
  - Required practice for running adjoint with gradient limiters for design and grid adaptation
- Methods to initialize supersonic and hypersonic flows
- Example of a hypersonic flow application
- What to do when things go wrong
- The focus is on high-speed flows, but the strategies discussed can be used in other flow regimes

Perfect and Generic Gas Simulation

- The input parameters described in this talk are only valid for (`eqn_type="compressible"`)
- Generic gas input parameters are different, but the philosophy is similar
- Work is underway to merge the options where possible, but consult generic gas specific documentation for details

What Are the Challenges?

- The inviscid terms can be discontinuous, i.e., when there are shocks
  - Entropy problem: strong shocks can cause difficulties in inviscid flux schemes especially near points in the flow where the dissipation vanishes
  - Monotonicity problem: shocks cause discontinuities that make robust implementation of higher order schemes difficult
- The inviscid terms can be a problem when there is strong expansion
  - Positivity problem: strong expansions can cause difficulties such that the local conditions approach a vacuum
  - Sonic rarifaction or “expansion shock” problem: strong expansions near the sonic point where dissipation due to the u-a eigenvalues vanishes can cause difficulties
- Turbulence modeling challenges compound these issues but are not the focus of this talk

Inviscid Flux Types

- Inviscid flux schemes fall into several categories:
  - Contact preserving, i.e., good for viscous flows
    - Flux difference splitting scheme of `flux_construction = "roe"`
      - Non positivity near vacuum conditions
      - The sonic rarefaction problem
      - The "carbuncle" problem
      - Non preservation of the total enthalpy in shocks
      - Entropy fixes (Eigenvalue smoothing) exist for some but not all of these problems
    - Flux splitting schemes such as `flux_construction = "hllc"` and `"ldfss"` may display some limited unphysical behavior at very strong normal shocks
  - Non-contact preserving, i.e. not usually good for viscous flows
    - Flux vector split scheme, `flux_construction ="vanleer"`, has desirable qualities
      - Positivity near vacuum conditions
      - Preservation of the total enthalpy in shocks

Inviscid Flux Types

- Inviscid flux schemes fall into several categories:
  - Hybrid or “blended” schemes
    - The `flux_construction = “dldfss”` scheme is a blend of two schemes
      - The `vanleer` scheme at shocks via a shock detector
      - The `ldfss` scheme near walls via a shock and boundary layer detector

Inviscid Flux Gradient Limiter Types

- Gradient limiters are available in two types:
  - Edge based : limiting is done on an edge by edge basis, `flux_limiter = "minmod"`, `"vanleer"`, `"vanalbada"` and `"smooth"`
    - They are less dissipative and they work pretty well on hex grids but they are not as robust on mixed element or tetrahedral grids.
    - They are not "freezable" and may cause convergence to get hung up by limiter cycling. They also can not be used when using the adjoint solvers
  - Stencil based : limiting is done based on the max and min reconstructed higher order edge gradients that exist over the entire control volume "stencil", `flux_limiter = "barth"`, `"hvanleer"`, `"hvanalbada"`, `"hsmooth"`, and `"venkat"`
    - They are more robust but more dissipative and work on all grid types
    - They are "freezable", i.e. they can be frozen after a suitable number of iterations which sometimes will allow the solution to converge further
    - They must be frozen when solving adjoint equations
    - Limiters with the "h" prefix include a heuristic stencil based pressure limiter to increase robustness

Realizability

- Nonphysical (negative density or pressure) reconstructions are set to cell averages (first order) accompanied with a “realizability” warning
- Nonlinear density and pressure updates are floored to a ratio of freestream with the `f_allow_minimum_m` namelist variable
  - The default floor may need to be lowered if the simulation requires it

Calorically Perfect Supersonic Flow

- Maximum Mach number in computational domain < 3.0 such that:
  - Shocks are relatively weak
  - Expansion fans are relatively weak
- Inviscid flux options suitable for these applications:
  - When Euler: `viscous_terms = "inviscid"`
    - `flux_construction = "vanleer", "ldfss", "hllc" or "roe"`
  - When Navier-Stokes: `viscous_terms = "laminar" or "turbulent"`
    - `flux_construction = "ldfss", "hllc", or "roe"`
- Inviscid flux gradient limiter options most suitable for these applications:
  - `flux_limiter = "vanleer", "vanalbada", "hvanleer", or "hvanalbada"`
- For applications that require solving the adjoint:
  - `flux_construction = "vanleer" or "roe"`
  - `flux_limiter = "hvanleer" or "hvanalbada"`

Calorically Perfect Hypersonic Flow

- Maximum Mach number in computational domain > 3.0 such that:
  - Shocks may be strong, especially when there are normal shocks
  - Expansion fans may be strong
- Inviscid flux options suitable for these applications:
  - When Euler: `viscous_terms = "inviscid"`
    - `flux_construction = "vanleer" or "dldfss"`
  - When Navier-Stokes: `viscous_terms = "laminar" or "turbulent"`
    - `flux_construction = "dldfss"`
- Inviscid flux gradient limiter options most suitable for these applications:
  - `flux_limiter = "hvanleer" or "hvanalbada"`
- For applications that require solving the adjoint:
  - `flux_construction = "vanleer" or "roe"`
  - `flux_limiter = "hvanleer" or "hvanalbada"`

Nonlinear Equations

- When solving nonlinear equations (e.g., Euler, Navier-Stokes), the initial guess is critical!
- Transients can be much more challenging than the steady solution
  - Solution under and over shoots can be aggravated
  - Nonphysical states may be transited
  - Boundary conditions are less robust with large gradients nearby
  - Linear system solution scheme and nonlinear defect correction solution schemes can become unstable

Strategy

- Perform the simulation in phases
  - Initialization
  - Target solution scheme
  - Optional end game that freezes limiter for better iterative convergence.
- Initialization is the primary challenge to success for high speed, internal, and propulsion flows

Initialization Strategies

- The default initialization fills the domain with freestream flow and applies strong boundary conditions
  - Creates high gradients adjacent to the boundary
  - Sets up an unphysical expansion on backward facing surfaces
- The goal of initialization is to improve this default flow field with one that establishes the physical mechanisms of the simulations (e.g., boundary layers, shear layers, recirculation zones)
  - Moves large gradient regions away from the boundaries and into the interior of the domain
- You have the freedom to use methods that are inaccurate as long as you later restart the solution with an appropriate method for your simulation
  - Includes changing boundary conditions, freestream conditions, etc.

Initialization Strategies

- Use `first_order_iterations` to create a spatially first-order solution
  - This helps the nonlinear update because there are less approximations in defect correction
- Use a more dissipative flux scheme
  - Roe with excessive Eigenvalue smoothing
    - `rhs_u_eigenvalue_coef, lhs_u_eigenvalue_coef, rhs_a_eigenvalue_coef, lhs_a_eigenvalue_coef`
  - “`vanleer`” for Navier-Stokes
- Restart from a lower Mach number or angle of attack solution
- Slow down (lower CFL number or physical time step)
  - This aids the stability of the linear solve and nonlinear updates
- Combinations of these strategies

Initialization Strategies

- Explicitly initialize with the `&flow_initialization` namelist
  - Fill plenums with subsonic high density and pressure gas
  - Place a subsonic wake behind an aft facing step
  - Surround the entire vehicle with a sphere of post shock flow conditions (subsonic high density and pressure gas)
  - May reduce the execution time by allowing the use of larger CFL numbers

Solution Scheme

- See the advantages and disadvantages of the available fluxes and limiters
- Adjust (ramp) the CFL number for the best convergence rate
- Expect the solution convergence to stall due to limiter buzz

End Game

- Optionally freeze the gradient limiter to overcome limiter buzz
  - Make sure the solution is sufficiently converged

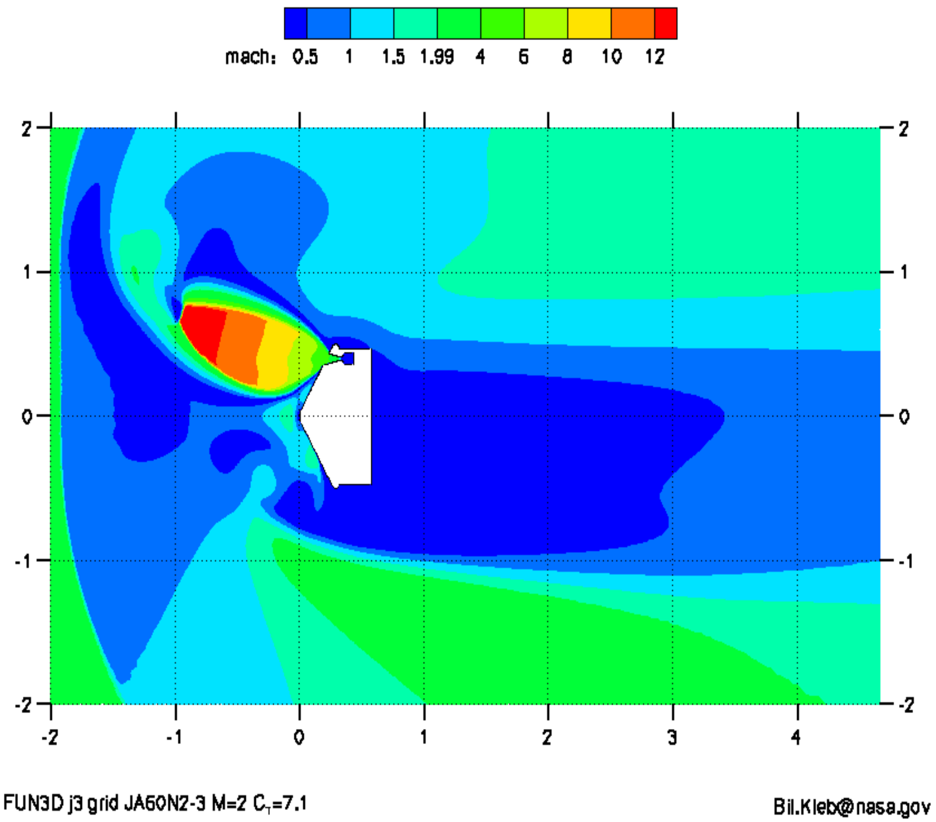
Multiple Step Approach

- Applications with shocks and expansions may need to be run in multiple steps
  - Step 1 : Run solution first order while scheduling the CFL number to evolve the solution to a quasi-steady state;
    - Initialize the flow appropriately
    - Set `first_order_iterations` to the same as the number of iterations specified by `steps`
    - Use `schedule_iteration`, `schedule_cfl`, and `schedule_cflturb` to slowly increase CFL number
  - Step 2 : Restart solution higher order while scheduling the CFL number to compute the final solution;
    - Read the restart file, i.e. `restart_read = "on"`
    - Set `first_order_iterations` = 0
    - The CFL ramping of `schedule_iteration`, `schedule_cfl`, and `schedule_cflturb` may need to be less aggressive

Supersonic/Hypersonic Retro-propulsion Flow Example

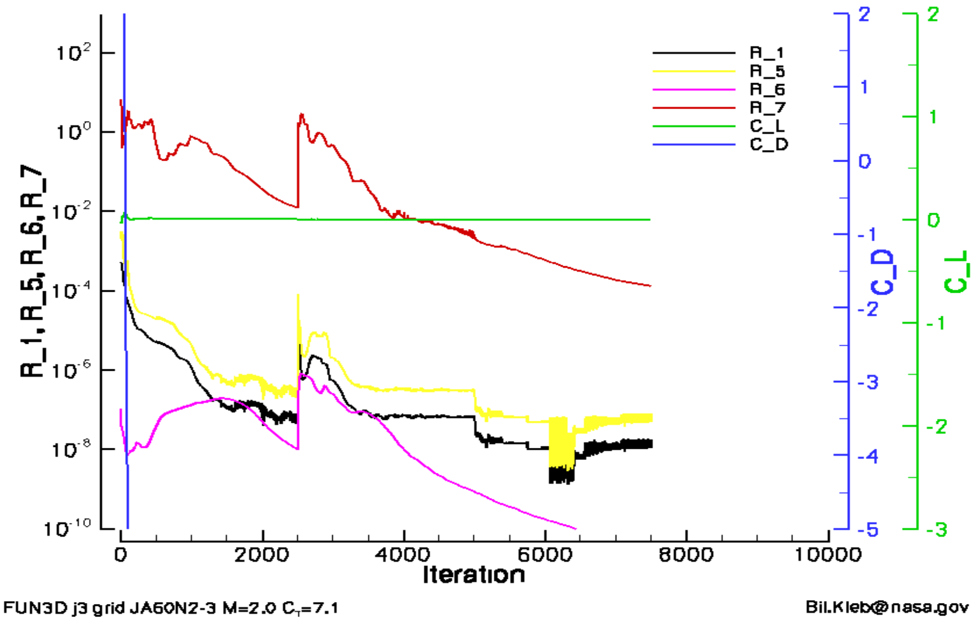
- Turbulent retro-propulsion re-entry plume flow in one run that includes the three phases
- Relevant namelist settings

```
&code_run_control
  steps                  = 7500
  restart_read    = 'off'
 /
 &inviscid_flux_method
  first_order_iterations = 2500
  freeze_limiter_interation = 5000
  flux_limiter = 'hvanalbada'
  flux_construction = 'dldfss'
 /
 &nonlinear_solver_parameters
  schedule_iteration =  1    100
  schedule_cfl       =  0.1   10.
  schedule_cflturb   =  0.01   1.
 /
```



Supersonic/Hypersonic Retro-propulsion Flow Example

- Switch from 1st order to 2nd order scheme occurs at 2500 iterations
- The `hvanalbada` limiter was frozen at 5000 iterations
- Continuity and energy equation residuals converged ~ 4 orders
  - Jet unsteadiness probably preventing further convergence
- Lift has converged, i.e. is no longer changing



Supersonic/Hypersonic Retro-propulsion Flow Example Some Observations

- Turbulent flow has made this case easier to run because of the added dissipation caused by the eddy viscosity in the retro-propulsion jet
- If this case were laminar, it would probably be more difficult to run
  - You would need to be careful that the `dldfss` flux scheme does not add too much dissipation by refining the grid
  - You may need to resort to a multiple step running approach or explicit initialization of the flow field

Diagnosis When Things Go Wrong

- Restart the solution and visualize just before an increase in the residual
- Create movies near the largest residual location
- Try to isolate the problem location
- Check your grid resolution near the maximum residual location
  - Under-resolved expansions can cause a lot of trouble
  - Really large grid aspect ratios near expansions can cause trouble
- Check to make sure your boundary conditions are well posed
  - This is especially true for internal flows

Diagnosis When Things Go Wrong

- Isolate the problem to linear system or nonlinear update
  - Invoke the `--monitor_linear` command line option
  - Set `linear_projection = .true.` or change the number of linear sweeps
  - Lowering CFL number can aid linear and nonlinear stability
  - Try a different initialization strategy

What We Learned

- Recommended use cases and descriptions of flux schemes
- Recommended use cases for gradient limiters and how to freeze them
- Initialization strategies
- What the convergence behavior may look like
- What to do when things go wrong