Session 13: Thermochemical Nonequilibrium Simulations

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Session Overview

- Background
- Restrictions (ITAR)
- New Required Data Files
- Set-up fun3d.nml
- New Boundary Conditions
- Required Command Line Option
- Challenges to Stagnation Region Heating
    - Multi-dimensional Reconstruction
- Examples
- Future Plans

Code Background

- LAURA (1987 - present)
  - Langley Aerothermodynamic Upwind Relaxation Algorithm
  - Multi-block, structured grid, cell-centered, finite-volume
  - Thermochemical equilibrium and nonequilibrium (Earth, Mars) with Park's two-temperature model
  - Roe's scheme, Yee's STVD limiter, Harten's entropy fix, central difference viscous terms (the devil I know!)
  - Tuned for Cray vector architecture - extensive use of conditional compilation
- FUN3D (perfect gas, 1989 - present)
  - Unstructured grid, node-based, finite volume
  - perfect gas, incompressible to supersonic domains
  - Multiple upwind options including Roe's scheme, weighted least-squares gradients into Barth or Venkat limiter, Green-Gauss viscous terms
  - Adjoint equation solution for grid adaptation and optimization

Merged Code

FUN3D (Generic Gas Path, 2001 - present)

- Re-factor FUN3D to accommodate multiple species, energies, momenta, coupled 2eq turbulence models
- Create PHYSICS MODULES directory to bring thermodynamic, kinetic, transport, and turbulence models from LAURA and VULCAN into FUN3D
- Adopt Extreme Programming conventions with continuous, automated testing

LAURA V (2005 - present)

- Production capability in FUN3D slow to mature
  - Poor quality heating on tetrahedral grids
  - Columbia accident investigation and Return to Flight
- Re-factored LAURA using FUN3D data structures and modules
  - PHYSICS MODULES
  - Continuous, automated code testing
- Modular structure simplified addition of HARA radiation and ablation

Restrictions

- ITAR - International Traffic in Arms Regulations
  - US Government codes explicitly written for simulation of flows over vehicles traveling at hypersonic velocities are treated as ITAR restricted
  - Contents of the PHYSICS_MODULES directory contain the models required for high temperature gas dynamic simulations
    - Baseline FUN3D contains only perfect gas models and is not considered ITAR (though it is export controlled)
    - Contents of PHYSICS_MODULES are treated as ITAR - are not released unless specifically requested and approved
- A separate request for the generic gas path and a new usage agreement are required

Configuration

Follow instructions for baseline FUN3D but include one additional option:

../configure --enable-hefss …

(hefss: high energy flow solver synthesis)

PHYSICS_MODULES

- equilibrium_air.f90
- hara_radiation.f90
- shared_gas_variables.f90
- shared_hara_variables.f90
- catalysis.f90
- surface.f90
- chemical_kinetics.f90
- thermal_relaxation.f90
- thermodynamics.f90
- transport_property.f90
- turb_gen.f90

Data files - should not need modification

- kinetic_data
- species_thermo_data
- species_transp_data
- species_transp_data_0

Data file - modify to define thermochemical model

- tdata

Thermochemical nonequilibrium model: tdata

```
Two Temperature
N   6.217e-20
O   7.758e-09
N2   0.737795
O2   0.262205
NO   1.e-09
N+ 7.261e-35
O+ 1.179e-35
N2+ 1.495e-35
O2+ 3.785e-33
NO+ 4.567e-24
e- 8.352e-29
```

Thermal nonequilibrium

Species name followed by mass fraction in mixture

Air as Perfect Gas in tdata

perfect_gas

DEFAULTS for air are:

gamma = 1.4

mol_wt = 28.8

suther1 = 0.1458205E-05

suther2 = 110.333333

prand = 0.72

Generic Perfect Gas in tdata

perfect_gas

&species_properties

gamma =	Ratio of specific heats
mol_wt =	Molecular weight
suther1 =	Sutherland constant 1
suther2 =	Sutherland constant 2
prand =	Prandtl number

/

Sutherlands Constants in tdata

Note that the constants for Sutherland's law in the namelist species_properties define viscosity in SI units using the equation:

$$\mu = suther1 \frac{T^{3/2}}{T + suther2}$$

Constants for Sutherland's law often appear in other units and/or in the form

$$\mu = \mu_{ref} \left(\frac{T}{T_{ref}} \right)^{3/2} \frac{T_{ref} + suther2}{T + suther2}$$

$$suther1 = \mu_{ref} \frac{T_{ref} + suther2}{T_{ref}^{3/2}}$$

Equilibrium Gas in tdata

equilibrium_air_t	tannehill model
equilibrium_air_r	eq_air_coeffs.asc eq_air_lk_up.asc

Recommended Model for Return from LEO in tdata

N 0.

O 0.

N2 0.737795

O2 0.262205

NO 0.

Generic Gas Options in fun3d.nml

```
&governing_equations
  eqn_type = "generic"
  viscous_terms = "laminar"
  chemical_kinetics = "finite-rate"
  thermal_energy_model = "frozen"
/
```

eqn_type: cal_perf_compress, cal_perf_incompress, generic
viscous_terms: inviscid, laminar, turbulent
chemical_kinetics: frozen, finite-rate
(only engaged if tdata contains two or more species names)
thermal_energy_model: frozen, non-equilib
(only engaged if first line of tdata is “two temperature”)

Generic Gas Options in fun3d.nml

```
&reference_physical_properties
  gridlength_conversion =   .0254
  dim_input_type = "dimensional-SI"
  temperature_units = "Kelvin"
  velocity =    6920.0
  density =   5.750E-005
  temperature =    202.0
  temperature_walldefault =    800.0
  angle_of_attack =  -50.6
  angle_of_yaw =   0.0
/
```

The generic gas path does not accept Mach number and Reynolds number to define free stream conditions.

Generic Gas Options in fun3d.nml

```
&inviscid_flux_method
  flux_limiter = "minmod"
  first_order_iterations = 0
  flux_construction = "stvd"
  multi_dim_recon_flag  = 0   (0,1,2)
  re_cell_cutoff = 400.0000     (NA)
  re_cell_cutoff_expon = 8      (NA)
  re_cell_cutoff_dir =  2         (freq. update direction)
  rhs_u_eigenvalue_coef =   0.5
  lhs_u_eigenvalue_coef =   1.0
/
```

Generic Gas Options in fun3d.nml

```
&nonlinear_solver_parameters
  time_accuracy = "steady"                steady, 1storder
  time_step_nondim =    1.0
  pseudo_time_stepping = "on"
  subiterations =            2
  schedule_number =   2
  schedule_iteration = 1        200
  schedule_cfl =   5.e+06   5.e+06
  invis_relax_factor =   2.
  visc_relax_factor =    1.
/
```

Generic Gas Options in fun3d.nml

```
&linear_solver_parameters
  meanflow_sweeps = 2
  line_implicit = "off"
/
```

meanflow_sweeps: 1 or 2 to initialize, 20 to 30 final

Generic Gas Options in fun3d.nml

```
&code_run_control
  steps =     10000
  stopping_tolerance =   1.00E-100
  restart_write_freq =        500
  restart_read = "on"
  jacobian_eval_freq =  1
/
```

jacobian_eval_freq: keep small until shock sets up

convergence is judged by heating - expect residual to freeze

(Note that the command line option --no_smart_jupdate must be invoked in order that the jacobian _eval_freq is engaged.)

Additional Surface Boundary Conditions

4001 - 4009: map from 1st to 9th occurrence of namelist &surface_properties in file surface_property_data

&surface_properties
surface_group_name = “RCG”
surface_temperature_type = “radiative equilibrium”
emiss_a = 0.89
catalysis_model = “Stewart-RCG”
/

Additional Surface Boundary Conditions

surface_group_name: your identifying name

surface_temperature_type: constant, adiabatic, radiative equilibrium, surface_energy_balance

$$\varepsilon = emiss\_a + T(emiss\_b + T(emiss\_c + T\, emiss\_d))$$

$$q = \varepsilon \sigma T^4$$

surface_temperature: specify value if constant different from default

catalysis_model: super-catalytic, non-catalytic, equilibrium-catalytic, Stewart-RCG, Zoby-RCG, Scott-RCG, fully-catalytic

Catalytic Boundary Conditions

Super-catalytic: Species mass fractions set to free stream conditions

Equilibrium-catalytic: Species mass fractions in equilibrium at wall temperature and pressure

Fully-catalytic: 100% of atoms diffusing to wall recombine to form homogeneous, neutral diatom. All other ions are neutralized.

Finite-catalytic: Fraction of atoms undergoing homogeneous recombination is function of wall temperature.

Non-catalytic: $J_i = 0$

Execution

For the near term the generic path requires use of command line option: --lmpi_io 0

nodet_mpi --lmpi_io 0

party --lmpi_io 0

This path carries additional data for restart and post-processing and the requisite updates for Version 11 io have not been completed.

Goals

Start with "reasonable grid" on CAD description of vehicle / system of arbitrary complexity

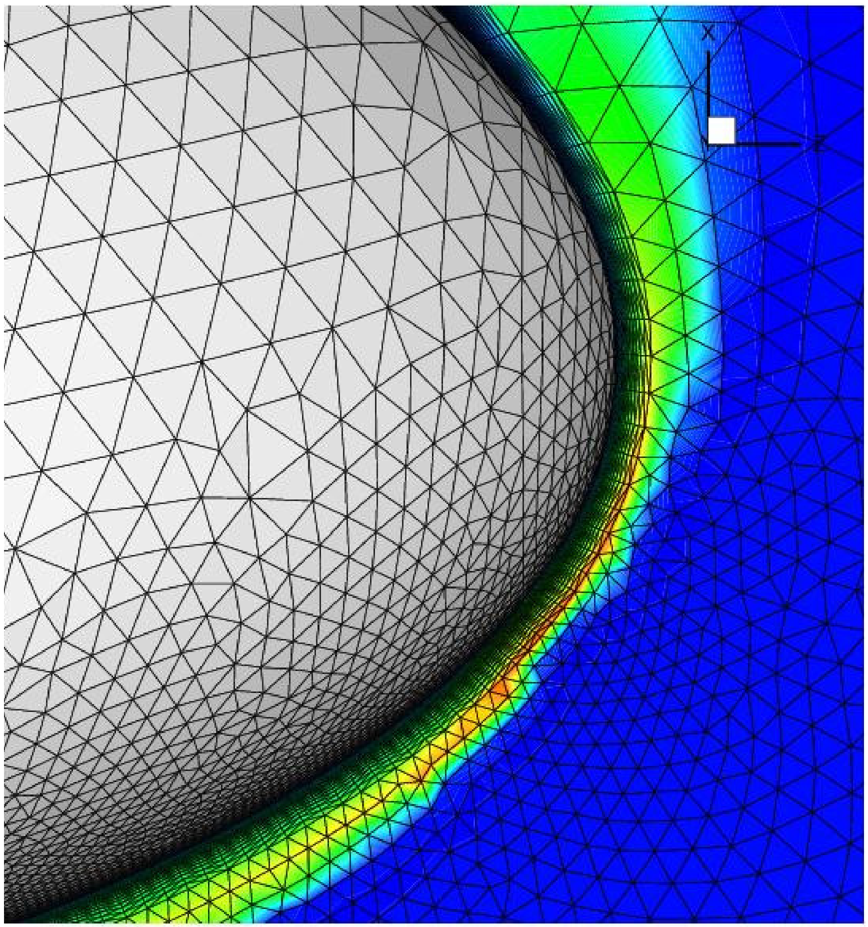
- "Reasonable" means sufficient resolution to initialize a CFD simulation.

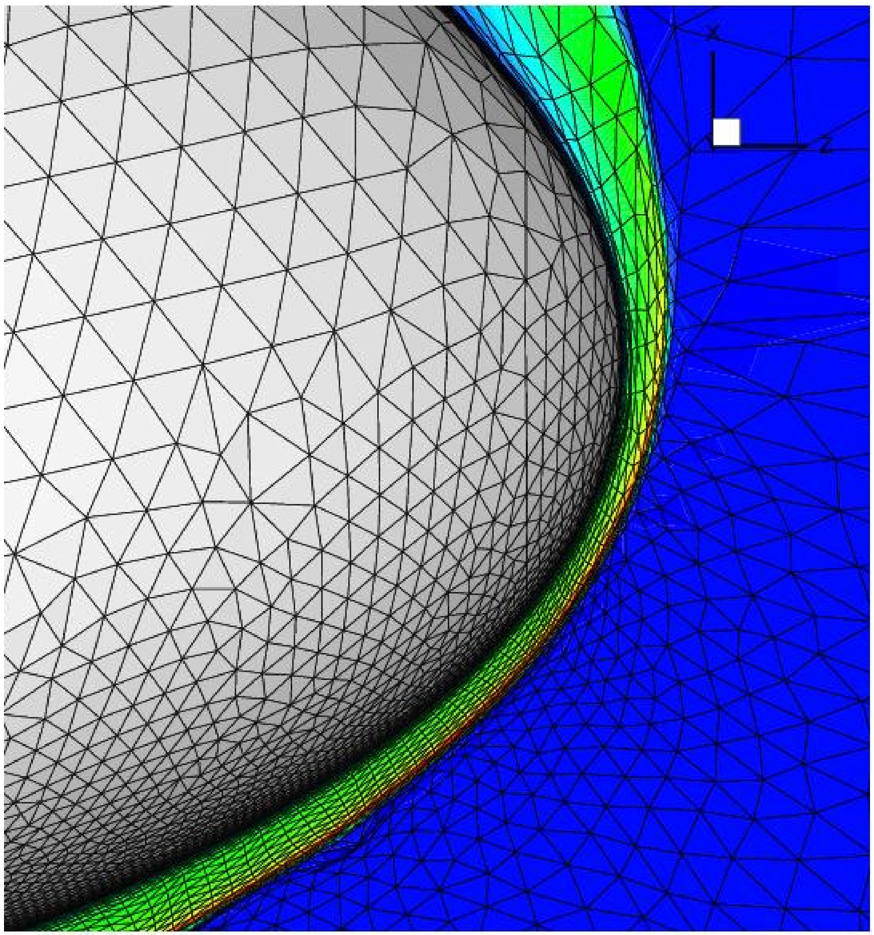
Finish with CFD simulation accurate to user specified convergence criteria with physics model uncertainties bounded by validation tests.

Shuttle Forebody Grids

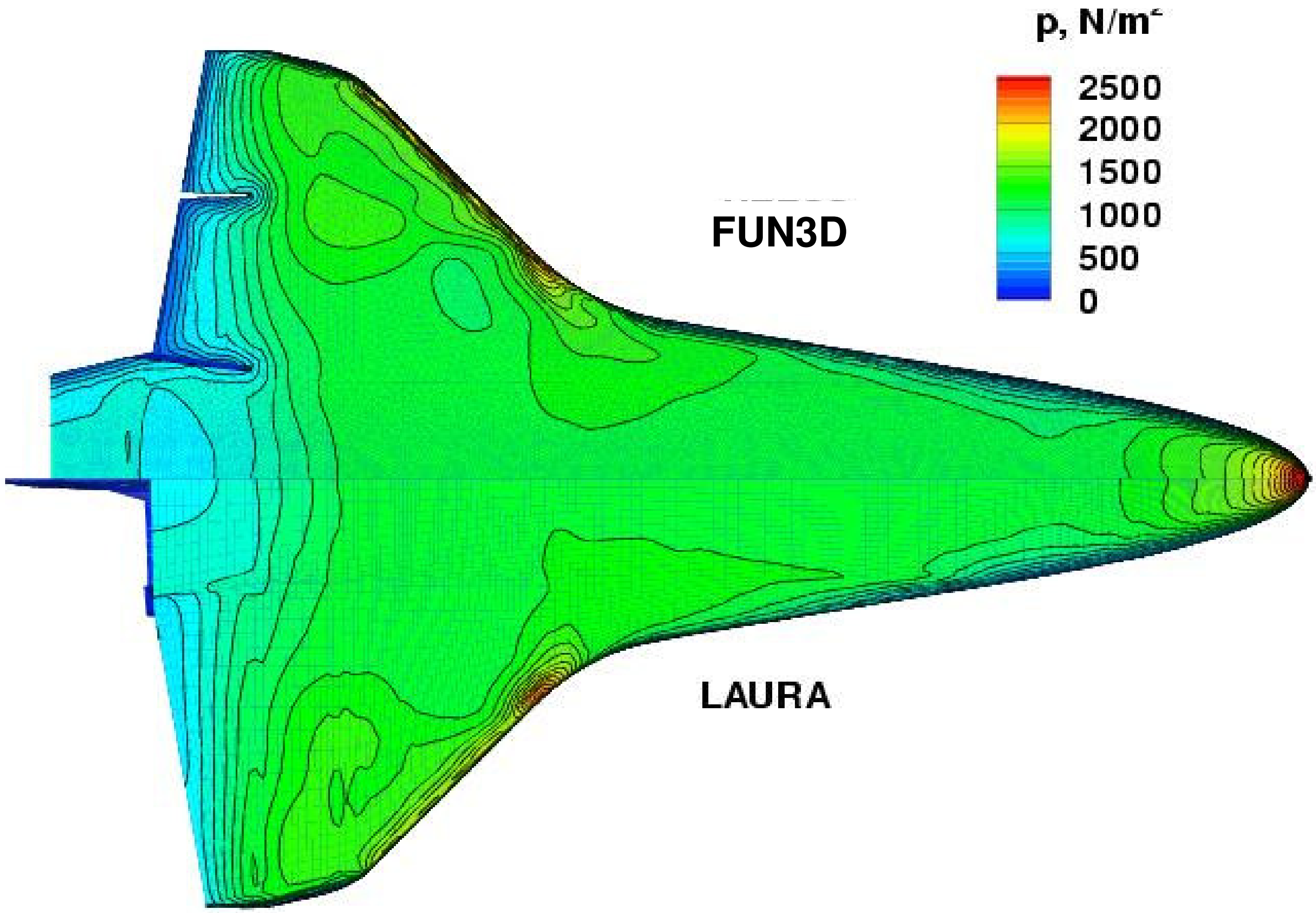
STS–2 72.4 km

$V_\infty = 6920$ m/s $\rho_\infty = 5.75\ 10^{-5}$ kg/m^3 $\alpha = 39.4$ deg

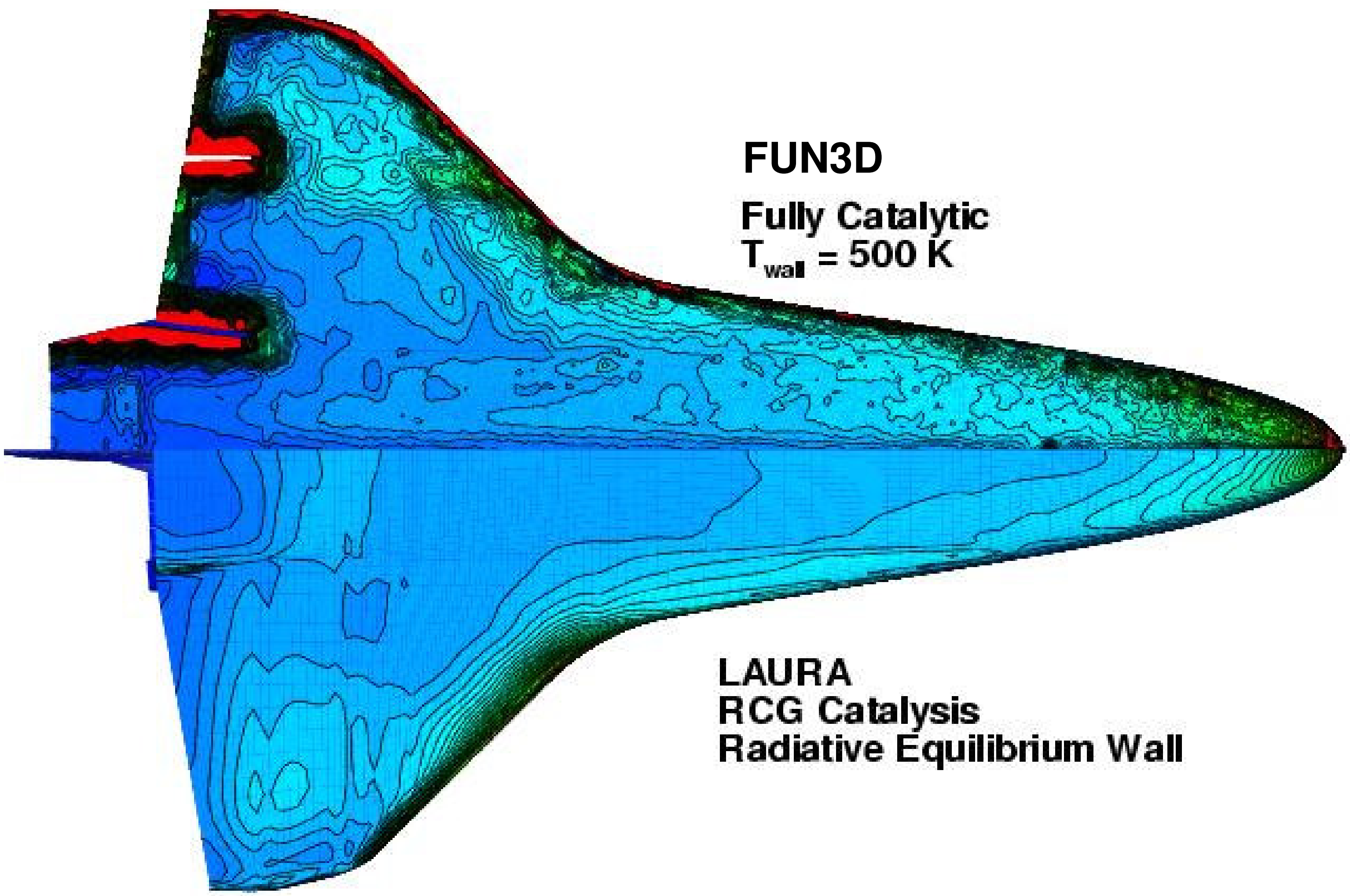




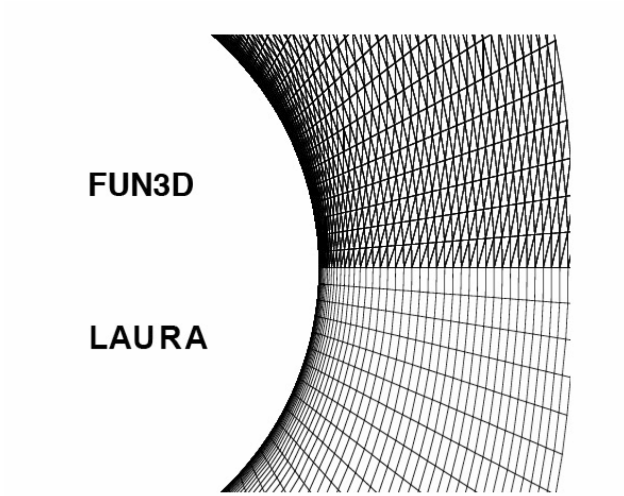
Windside Pressure Contours

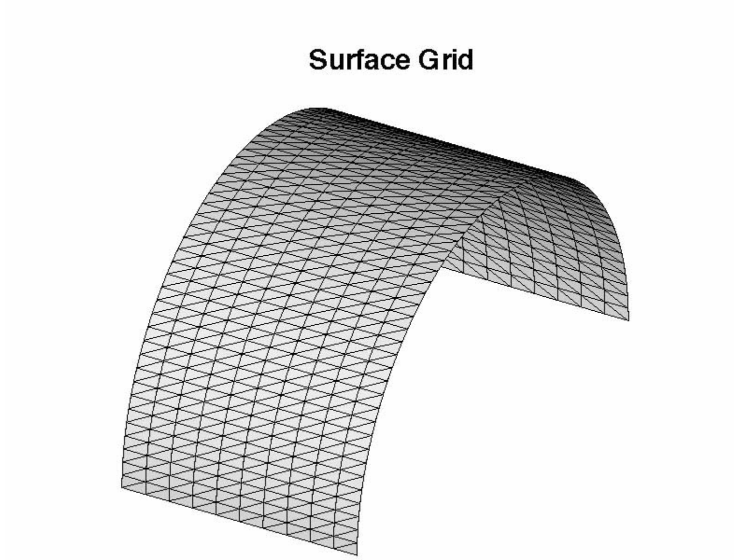


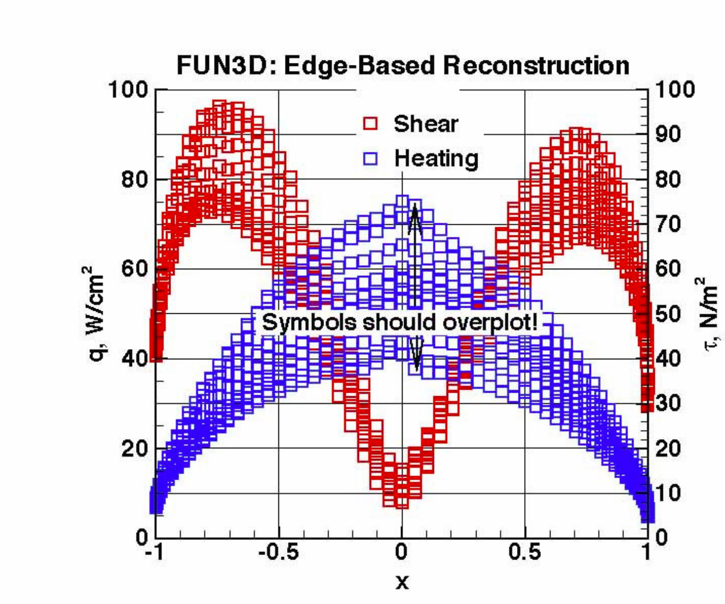
Windside Heating Contours

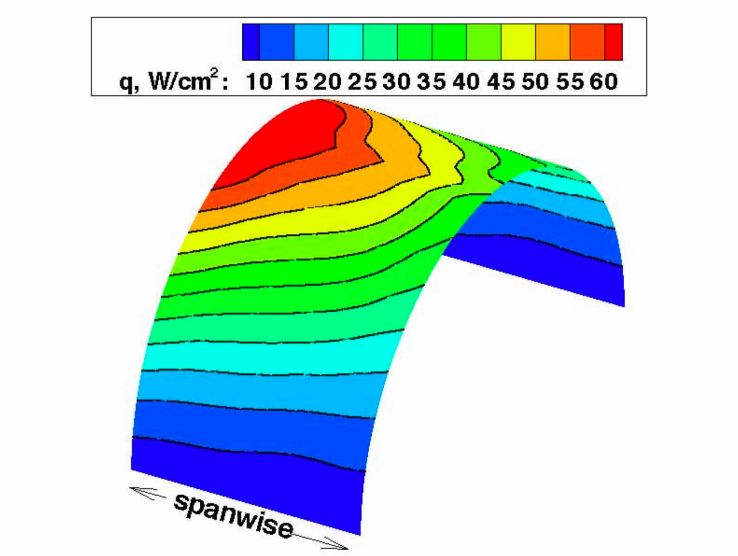


The Challenge Problem - Mach 17 Flow Over Cylinder

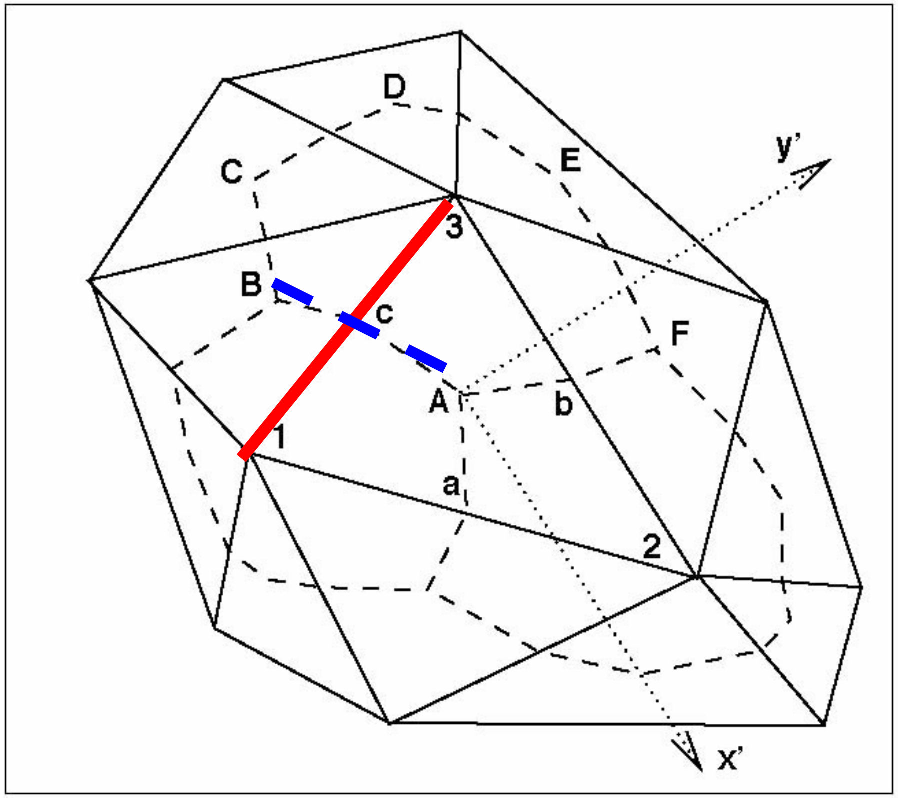








One Dimensional, Edge Based Reconstruction

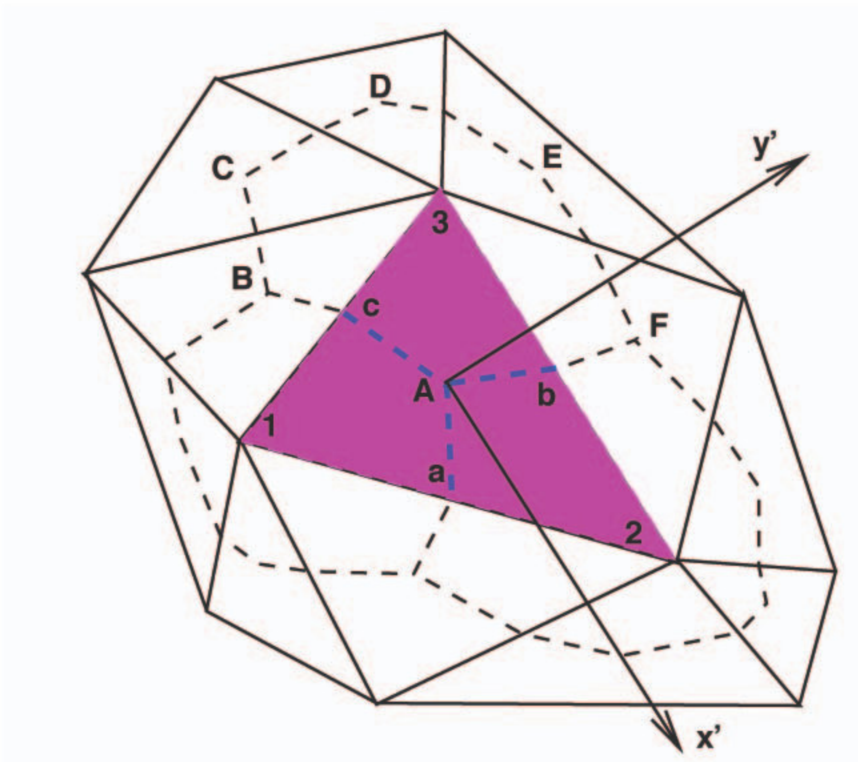


Loop over edges (red)

Compute flux f_c across single face separating two nodes (blue)

$$f_c(q_1, q_3, \nabla q_1, \nabla q_3)$$

Three-Dimensional, Element Based Reconstruction



The metrics used here are identical to those already used in the viscous flux formulation.

Loop over elements (magenta)

Compute flux f_{cAa}, f_{cAb}, and f_{bAa} for the three faces (blue) separating the three nodes defining the element

$$f_{cAa} = f_{x'} n_{cAa,x'} + f_{y'} n_{cAa,y'}$$

$$f_{cAb} = f_{x'} n_{cAb,x'} + f_{y'} n_{cAb,y'}$$

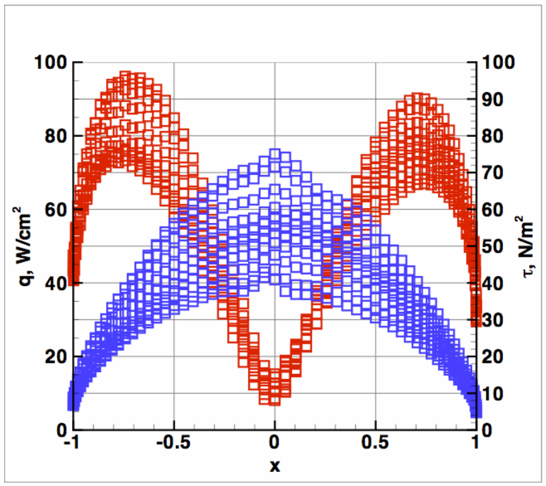
$$f_{bAa} = f_{x'} n_{bAa,x'} + f_{y'} n_{bAa,y'}$$

$$f_{x'}(q_{R,x'}, q_{L,x'}, \nabla q_{R,x'}, \nabla q_{L,x'})$$

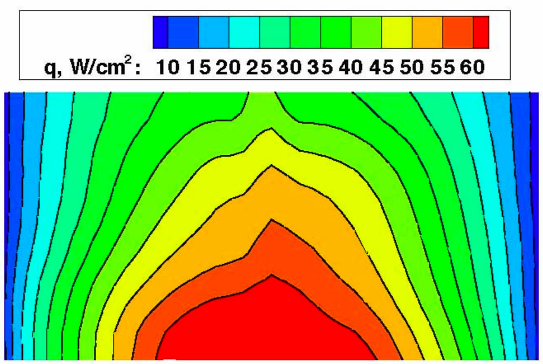
$$f_{y'}(q_{R,y'}, q_{L,y'}, \nabla q_{R,y'}, \nabla q_{L,y'})$$

Challenge Problem Revisited

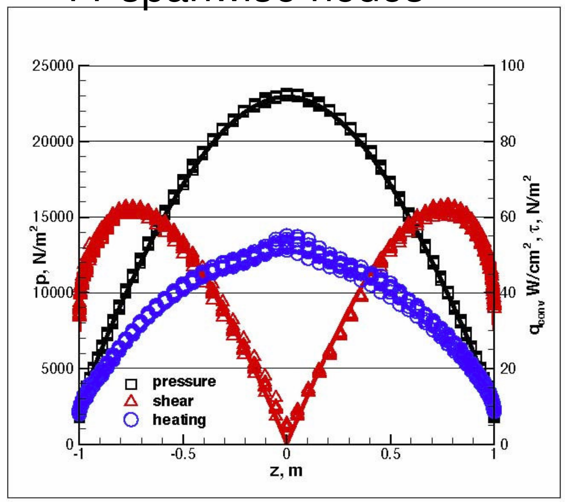
Original



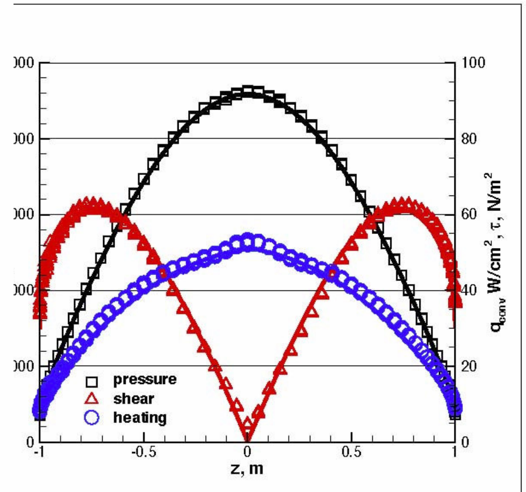
heating



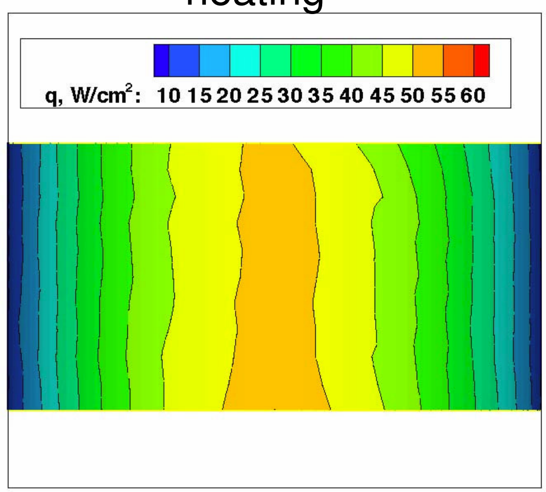
11 spanwise nodes



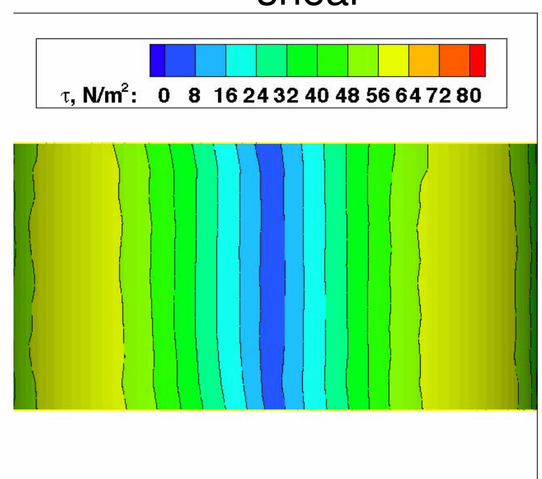
7 interior nodes



heating

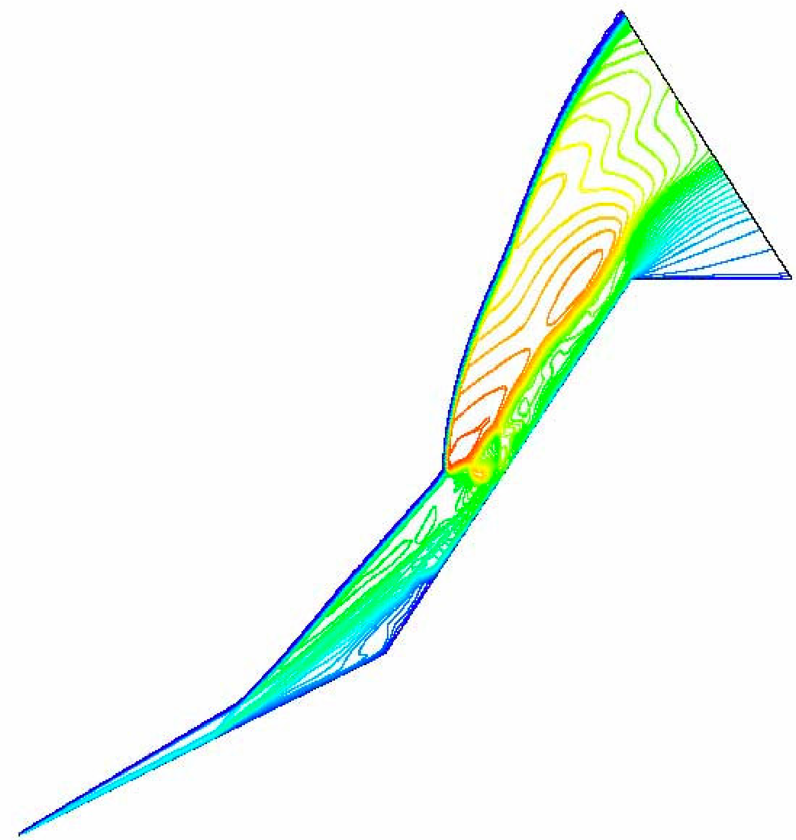


shear



Sharp Double-Cone

Temperature

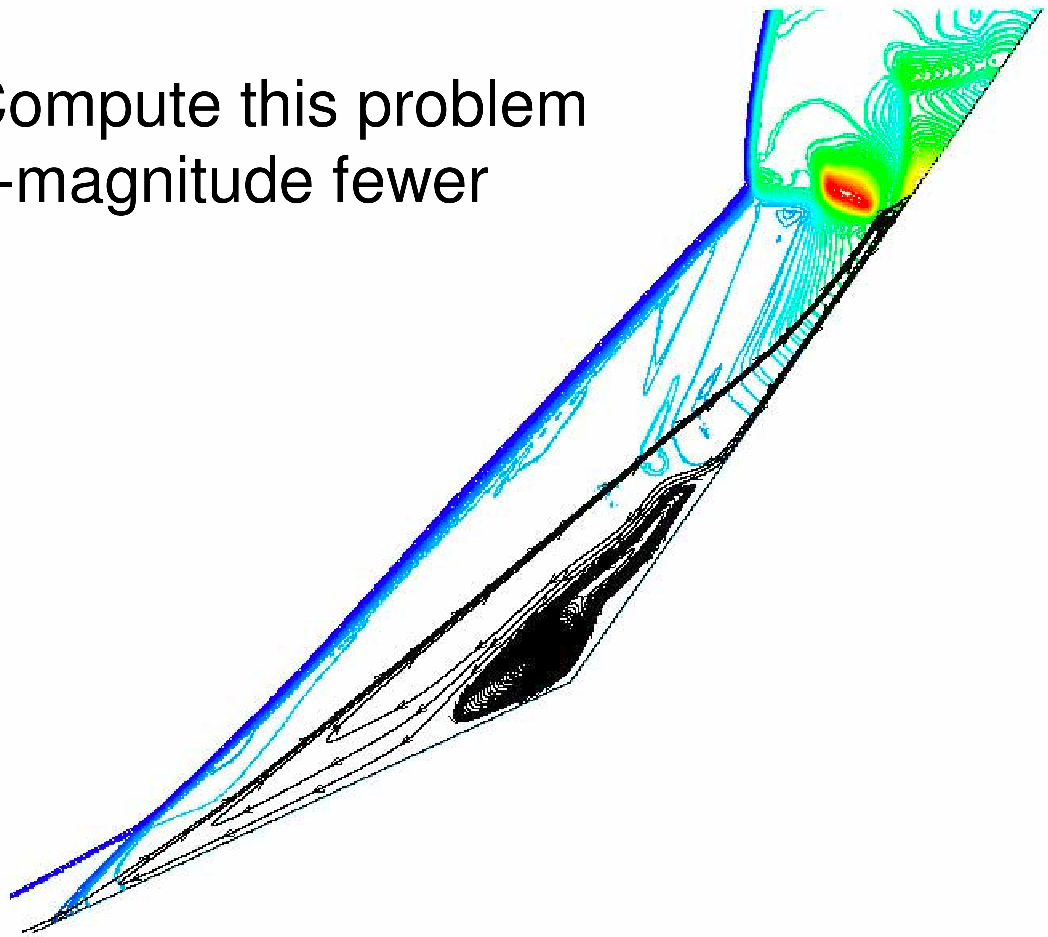


Run 28 (Holden et. al)
Mach 9.6
Re = 144000 m^{-1}
perfect gas (N_2)

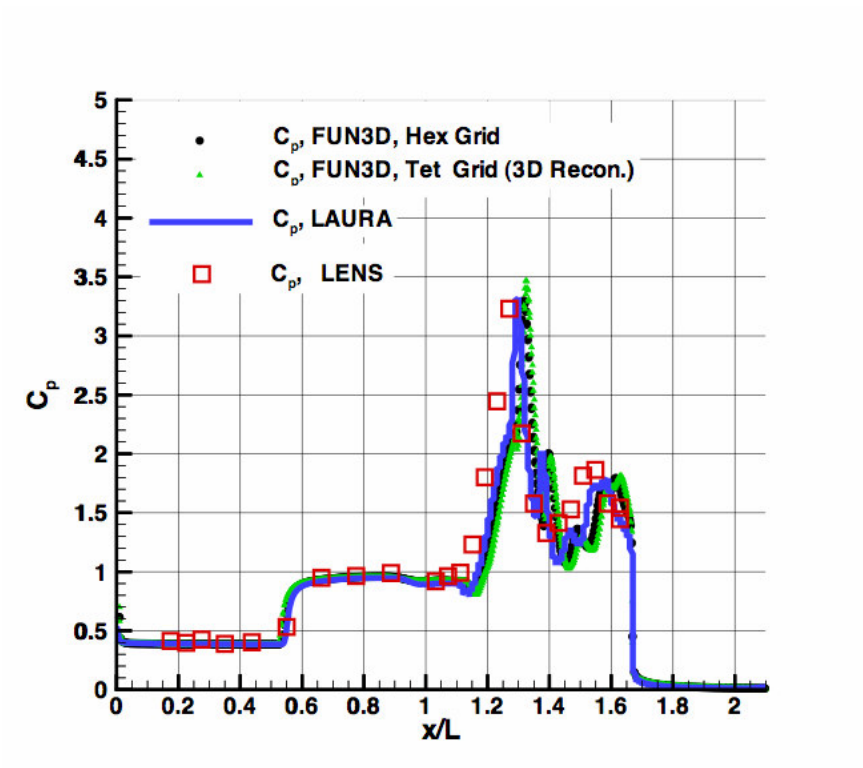
Sharp Double-Cone -- Separation Zones

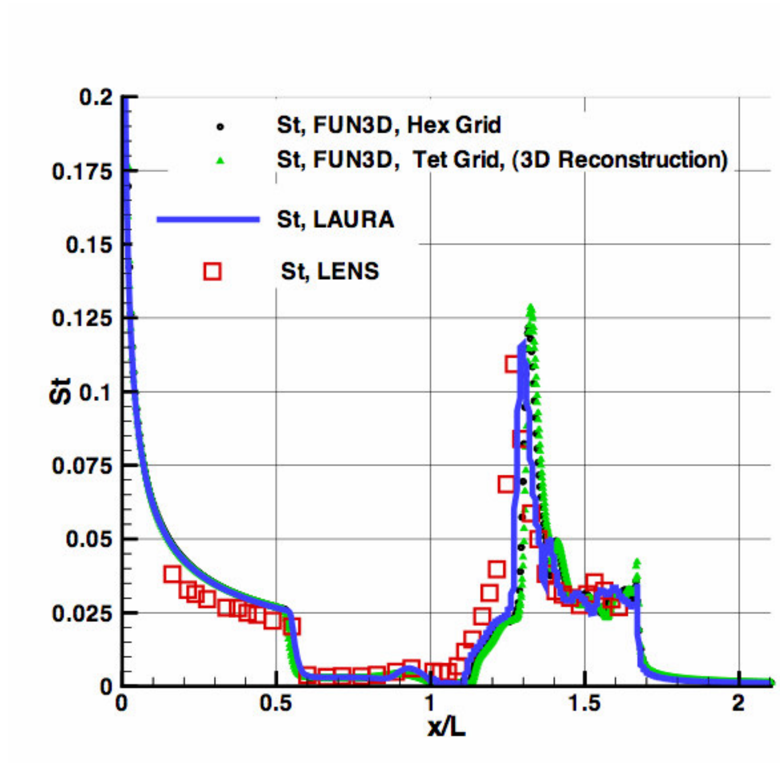
Pressure

Challenge: Compute this problem with order-of-magnitude fewer mesh points.



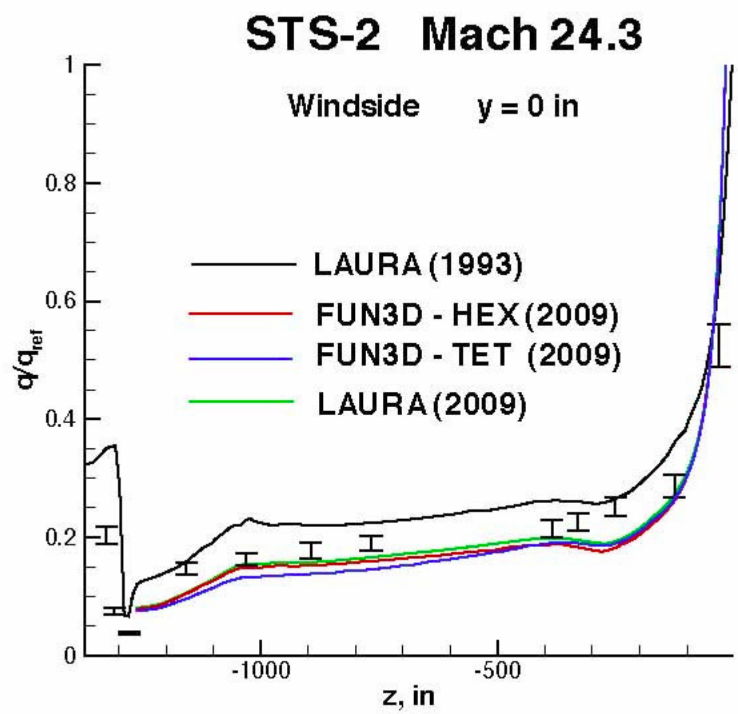
Sharp Double-Cone - Surface Pressure and Heating

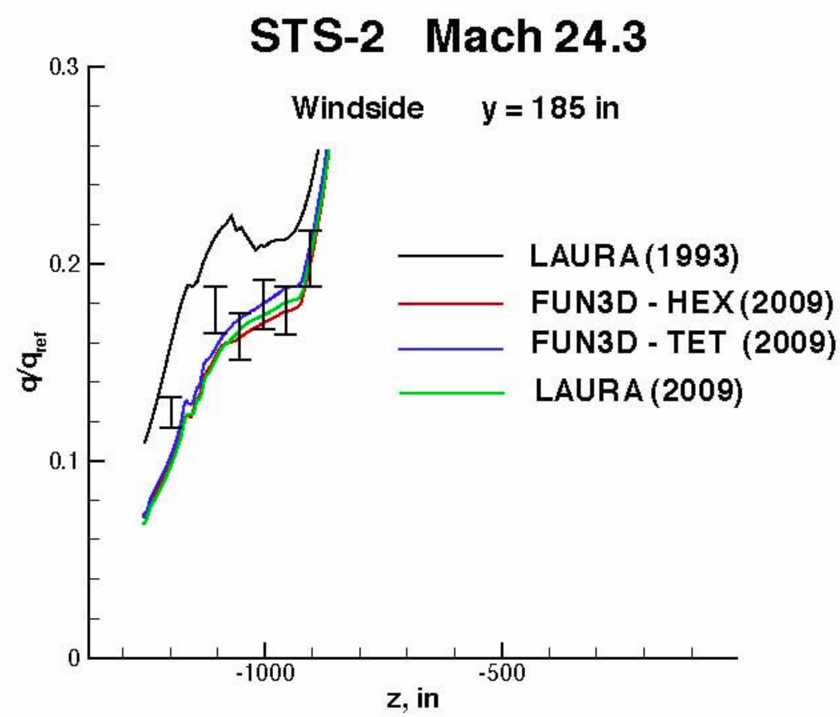


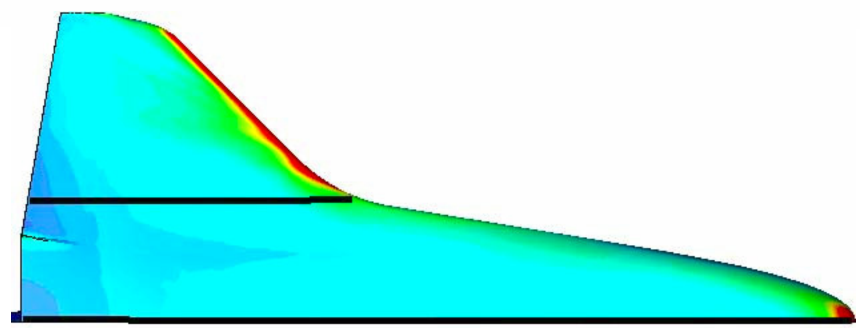


- Good agreement between codes and grid types.
- FUN3D multi-dimensional reconstruction had to be run time accurate.

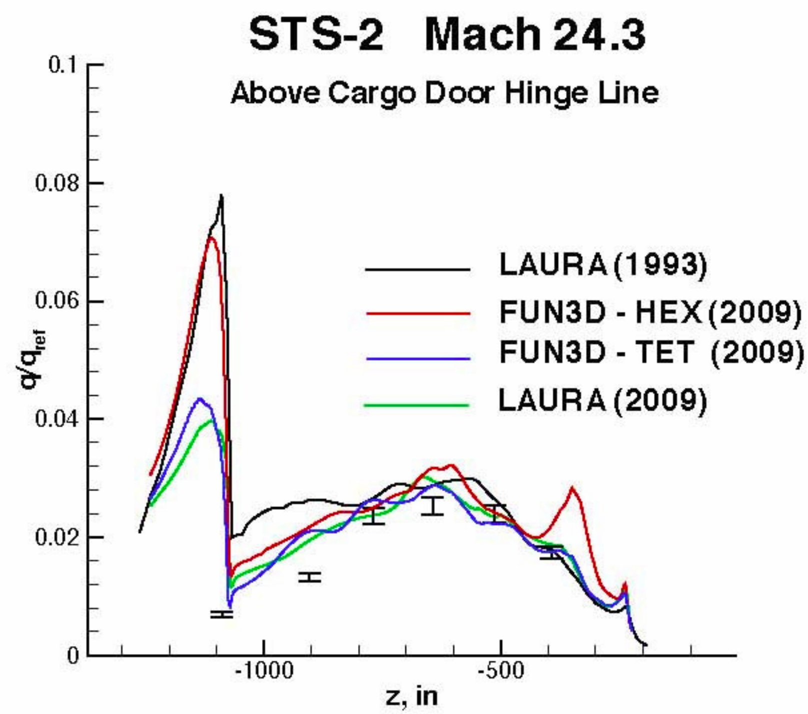
STS-2 Mach 24 -- Windside Surface Heating

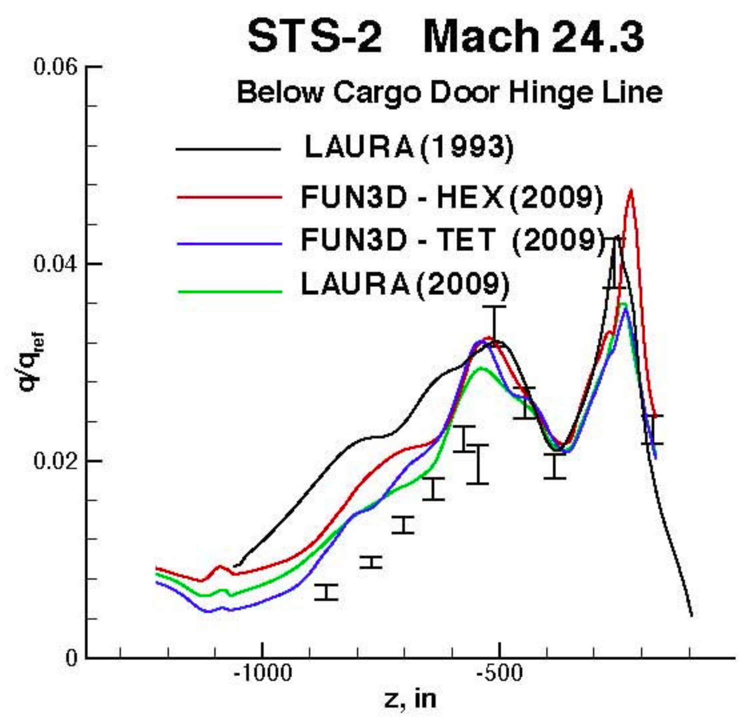


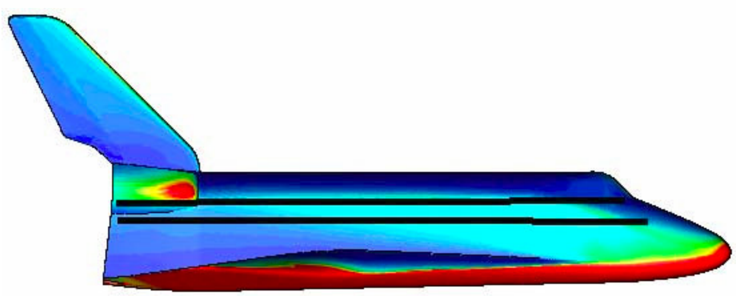




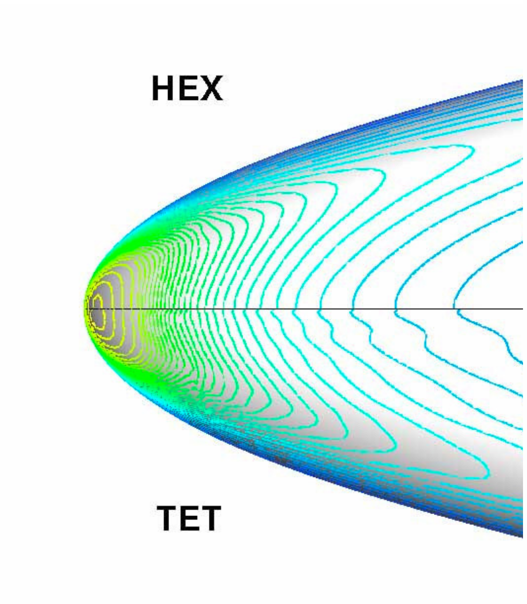
STS-2 Mach 24 -- Fuselage Surface Heating

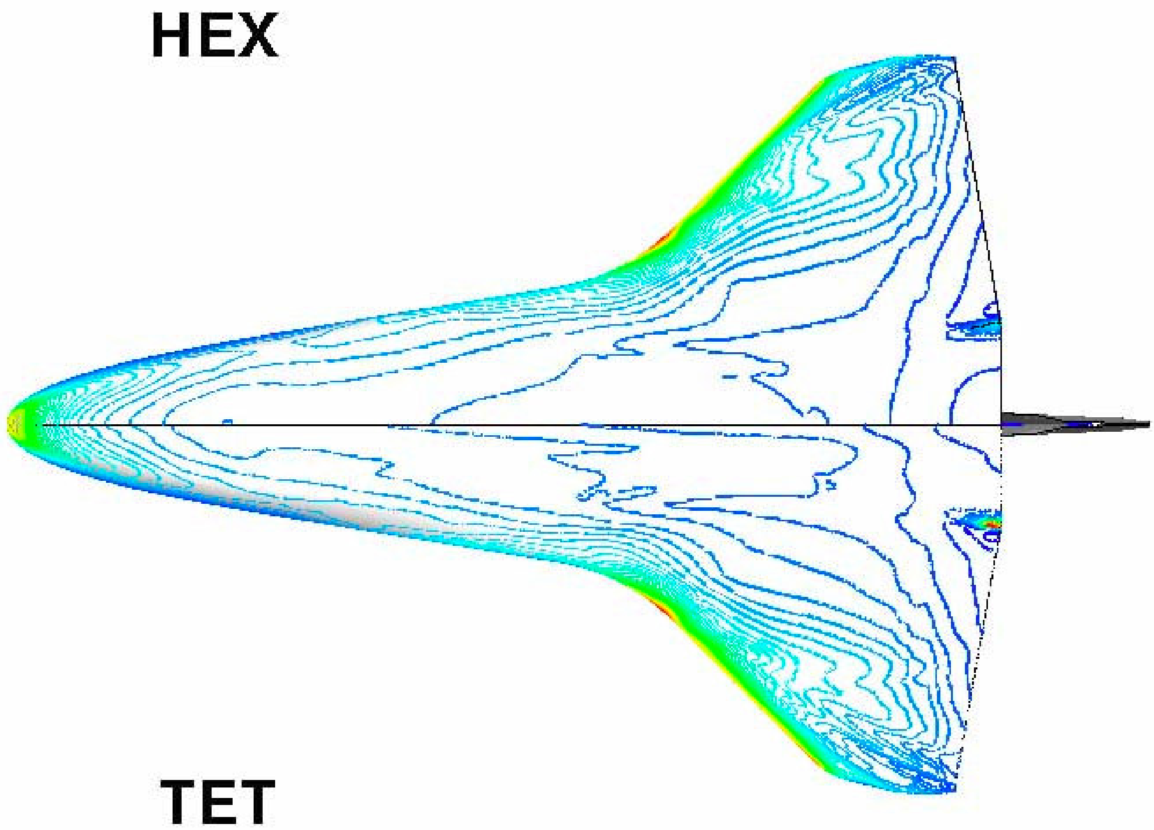






STS-2 Mach 24 -- Surface Heating Contours





Future Plans

- Update io consistent with version 11
- Resolve / understand symmetry plane issues
- Resurrect turbulence models
- Engage the adjoint for grid adaptation
- Engage PHYSICS_MODULES currently in LAURA for
  - Free-energy minimization
  - Coupled radiation using HARA
  - Coupled ablation