

FUN3D v13.4 Training

Session 9:

Thermochemical Nonequilibrium Simulations

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Aerothermodynamics Branch



Learning Goals

What we will cover:

- Description of data files, namelist options, and functionality unique to the generic gas path
 - Thermodynamics, Transport Properties, Chemical Kinetics, Radiation, Ablation
 - LAURA functionality
 - Grid adaptation and alignment for prismatic grids (Line adaptation).
 - Eigenvalue limiting control
- Troubleshooting

What we will *not* cover:

- Specific guidance on how the suite of namelist parameters are defined to provide converged solutions for sample applications – consult “A Tutorial for the Generic Gas Path in FUN3D”, NASA-TM-2014-218658

Additional Reference Material

U.S. persons who have been approved to receive the high-energy-physics options in FUN3D may also obtain NASA/TM-2014-218658 for detailed examples.

NASA/TM-2014-218658



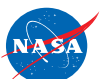
A Tutorial for the Generic Gas Path in Fun3D

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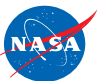
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Release

- 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)

Presence of Files in Working Directory

Red = must have in working directory.

Blue = will use copy in working directory if present; else will use copy in [install-prefix]/share/physics_modules.*

Green = required in working directory if special options are requested.*

*If you receive an error message that a file is not found, then it is likely that the installation is flawed. You can copy the file from Physics_Modules into the working directory.

Thermodynamics Data

- **species_thermo_data** (Section B.8 of manual)
- The majority of simulations do not require changes to this file – exceptions include:
 - Add pseudo species to describe combustion products in an approximate way to save resources.
 - Provide parametric variation to thermal relaxation models.
 - Value of $C_p(T)$ frozen at curve fit extrema is not an acceptable option.

```
N
&species_properties
elec_impct_ion = 4.196 ! 14.53 ! 4.196 from excited state
siga = 5.e-20, 0., 0.
mol_wt = 14.
/
3
0.00000000E+00 0.00000000E+00 0.25000000E+01 0.00000000E+00
0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00
0.56104638E+05 0.41939093E+01 200.000 1000.000
0.88765014E+05 -0.10712315E+03 0.23621883E+01 0.29167201E-03
-0.17295151E-06 0.40126579E-10 -0.26772276E-14 0.00000000E+00
0.56973513E+05 0.48652358E+01 1000.000 6000.000
0.54751811E+09 -0.31075750E+06 0.69167827E+02 -0.68479881E-02
0.38275724E-06 -0.10983677E-10 0.12779860E-15 0.00000000E+00
0.25505856E+07 -0.58487697E+03 6000.000 20000.000
```

Collision Cross Section Data - 1

- **species_transp_data** (Section B.10 of manual)
- Original LAURA log-linear fit between 2000K and 4000K
 - $\log_{10}(\pi\Omega^{(1,1)})$ and $\log_{10}(\pi\Omega^{(2,2)})$ in m^2
- Supplanted by high-order fit data if available (next slide)
- The majority of simulations do not require changes to this file – exceptions include:
 - Need quick look at new species transport property model.

Ar Ar

-14.6017 -14.6502 -14.5501 -14.6028 ! trr132+kestin et al

Ar CH4

-14.5827 -14.6319 -14.5328 -14.5806 ! kestin et al

Collision Cross Section Data - 2

- **species_transp_data_0** (Section B.11 of manual)
- Sources
 - Wright, M.: Recommended Collision Integrals for Transport Property Computations Part 1: Air Species. AIAA J., vol. 43, no. 12, 2005, pp. 2558-2564.
 - Wright, M.: Recommended Collision Integrals for Transport Property Computations Part 2: Mars and Venus Entries. AIAA J., vol. 45, no. 1, 2005, pp. 281-288.
- Supersedes log-linear fit data if available (previous slide)
- The majority of simulations do not require changes to this file.
- The data file contains all original sources and details of the curve fits.

Chemical Kinetic Data

- **kinetic_data** (Section B.9 of manual)
- Advantageous to keep local copy for parametric studies involving thermochemical nonequilibrium.

O2 + M <=> 2O + M
2.000e+21 -1.50 5.936e+04
teff1 = 2
exp1 = 0.7
t_eff_min = 1000.
t_eff_max = 50000.
C = 5.0
O = 5.0
N = 5.0
H = 5.0
Si = 5.0
e- = 0.

! JTHT Vol 15 No 1 pp76-90 2001 (Ref 1)

N + e- <=> N+ + e- + e-
2.500e+34 -3.82 1.682e+05
teff1 = 3
teff2 = 3

! Ref 1



Radiation Data

- **hara_data, hara_namelist_data** (Section B.12 of manual)
- Define *gas_radiation* and *rad_use_impl_lines* in **fun3d.nml**.
- Coupled radiation requires implicit lines spanning entire domain.

```
&governing_equations  
  eqn_type      = 'generic'  
  viscous_terms = 'laminar'  
  gas_radiation = 'coupled'  
  rad_use_impl_lines = .true.  
/
```

Thermochemical Model

- **tdata** (Section B.7 of manual)

| | | | |
|-------------------------|---------|---------|---------|
| perfect_gas | one | two | FEM |
| &species_properties | N2 .767 | N2 .767 | N2 .767 |
| gamma = 1.4 | N | N | N |
| mol_wt = 28.8 | O2 .233 | O2 .233 | O2 .233 |
| suther1 = 0.1458205E-05 | O | O | O |
| suther2 = 110.333333 | NO | NO | NO |
| prand = 0.72 | | O2+ | O2+ |
| / | | O+ | O+ |
| | | NO+ | NO+ |
| | | e- | e- |

Multiple Inflow Boundaries

tdata

one temperature

model

N2 1.0

O2

H2

O

H

OH

H2O

N2 0.7686

O2 0.2314

H2 1.0000

O 0.0000

H 0.0000

OH 0.0000

H2O 0.0000

fun3d.nml

&boundary_conditions

wall_temperature(1) = 1305.0

wall_temp_flag(1) = .true.

wall_catalysis_model(1) = 'non-catalytic'

plenum_id(2) = 3

plenum_t0(2) = 1000.0

plenum_p0(2) = 3800.0

.

.

plenum_id(6) = 3

plenum_t0(6) = 900.0

plenum_p0(6) = 16000.0

Governing Equations – fun3d.nml

- Detail in manual Sec. B.4.6

```
&governing_equations
  eqn_type = "generic"
  viscous_terms = "laminar"
  chemical_kinetics = "finite-rate" ! "frozen"
  thermal_energy_model = "non-equilb" ! "frozen"
  gas_radiation = "off" ! "on"
  rad_use_impl_lines = .false.
  multi_component_diff = .false.
/
```

Inviscid_flux_method – fun3d.nml

- Detail in manual Sec. B.4.9

```
&inviscid_flux_method  
  flux_construction = 'stvd' ! 'roe' ! 'multidm'  
  flux_limiter = 'minmod_gg' ! 'hvanalbada'  
  gen_turb_advectn_ho = .false.
```

```
multidm_option = 1  
fixed_direction = .true.
```



Some improvement
of heating on
tetrahedral grids.

```
adptv_entropy_fix = .true.  
rhs_u_eigenvalue_coef = 0.5  
lhs_u_eigenvalue_coef = 1.0  
rhs_a_eigenvalue_coef = 0.5  
lhs_a_eigenvalue_coef = 1.0  
re_min_vswch = 5.  
re_max_vswch = 50.
```



Eigenvalue limiting
controls to suppress
carbuncle but enable
accurate heating on
prismatic grids.

```
pole_gradient = .false.
```

Boundary Conditions – fun3d.nml

- Detail in manual Sec. B.4.18

```
wall_temperature(:) = 1.  
wall_temp_flag(:) = .false.  
wall_radeq_flag(:) = .false.  
wall_emissivity(:) = 0.8  
wall_emissivity_b(:) = 0.  
wall_emissivity_c(:) = 0.  
wall_emissivity_d(:) = 0.  
wall_temp_relax(:) = 0.001  
wall_catalysis_model(:) = 'super-catalytic'  
catalytic_efficiency_o(:) = 0.  
catalytic_efficiency_n(:) = 0.  
plenum_t0(:) = 1000.  
plenum_p0(:) = 1000.  
plenum_id(:) = 0  
fixed_in_id(:) = 0  
fixed_in_rho(:) = 0.  
fixed_in_uvw(:,1:3) = 0.  
fixed_in_t(:) = 0.  
fixed_in_tv(:) = 0.  
fixed_in_turb(:,1:7) = 0.
```

Turbulent Diffusion Model – fun3d.nml

- Detail in manual Sec. B.4.10
- Algebraic models available if implicit lines span domain.
 - *baldwin-lomax*
 - *cebeci-smith*
- Models tested in the generic gas path
 - *sa-catris*
 - *kw-sst*
 - *kw-sst2003*
 - *wilcox-kw98*
 - *wilcox-kw06*

Boundary Output Variables– fun3d.nml

- Detail in manual Sec. B.4.27
- The units of convective heating (*heating*) and radiative heating (*q_rad*) are W/cm².
- The units of shear in the x, y, and z directions (*shear_x*, *shear_y*, and *shear_z*, respectively) are in N/m².
- The units of temperature (*tt*, *tv*) are in K.
- All other variables are non-dimensionalized by reference density, velocity, and length - consistent with units used to demonstrate the Mach number independence principle.

| Variable | Non-dimensionalization |
|----------|--------------------------------|
| ρ | ρ_{ref} |
| u | V_{ref} |
| v | V_{ref} |
| w | V_{ref} |
| a | V_{ref} |
| p | $(\rho_{ref} V_{ref}^2)$ |
| e | V_{ref}^2 |
| h | V_{ref}^2 |
| μ | $(\rho_{ref} V_{ref} L_{ref})$ |

Grid Adaptation – fun3d.nml

- Detail in manual Sec. B.4.34
- Line adaptation available if implicit lines span domain.

&adapt_mechanics

ladapt_fsh = 0.8

ladapt_fstr = 0.75

ladapt_fctrjmp = 1.05

ladapt_re_cell = 1.

ladapt_beta_grd = 0.

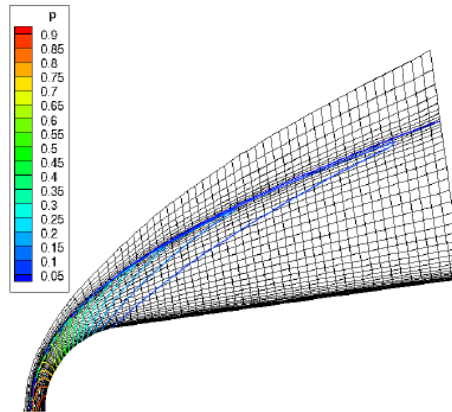
ladapt_ep0_grd = 0.

ladapt_jumpflag = 2

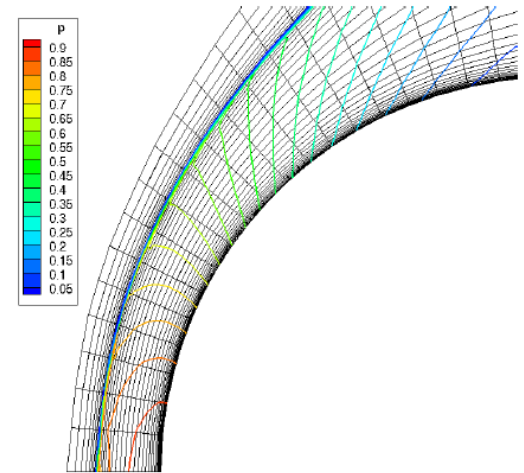
ladapt_freq = 200

ladapt_max = 1000

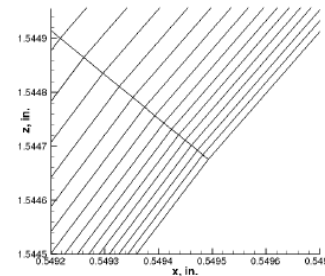
/



(a) Global view.



(b) Detailed view.



(c) Near wall view.

Line Extraction Utility

- From the utils directory of your configuration use
 - `plot3d_to_aflr3` to convert from plot3d, multiblock, structured grid to aflr3 unstructured grid
 - `aflr3_line_extraction` to extract lines from surface to the inflow boundary

abcfcd% `aflr3_line_extraction`

...

Input 0 for 3D, any other integer for 2D:

`0`

...

Input 1 or 2 to change inputs, any other integer to proceed:

`1`

Project rootname: `coupled_radiation`

...

Current, two-dimensional flag = F

Type 1 to change, any other number to keep as is: `0`

twod= F

...

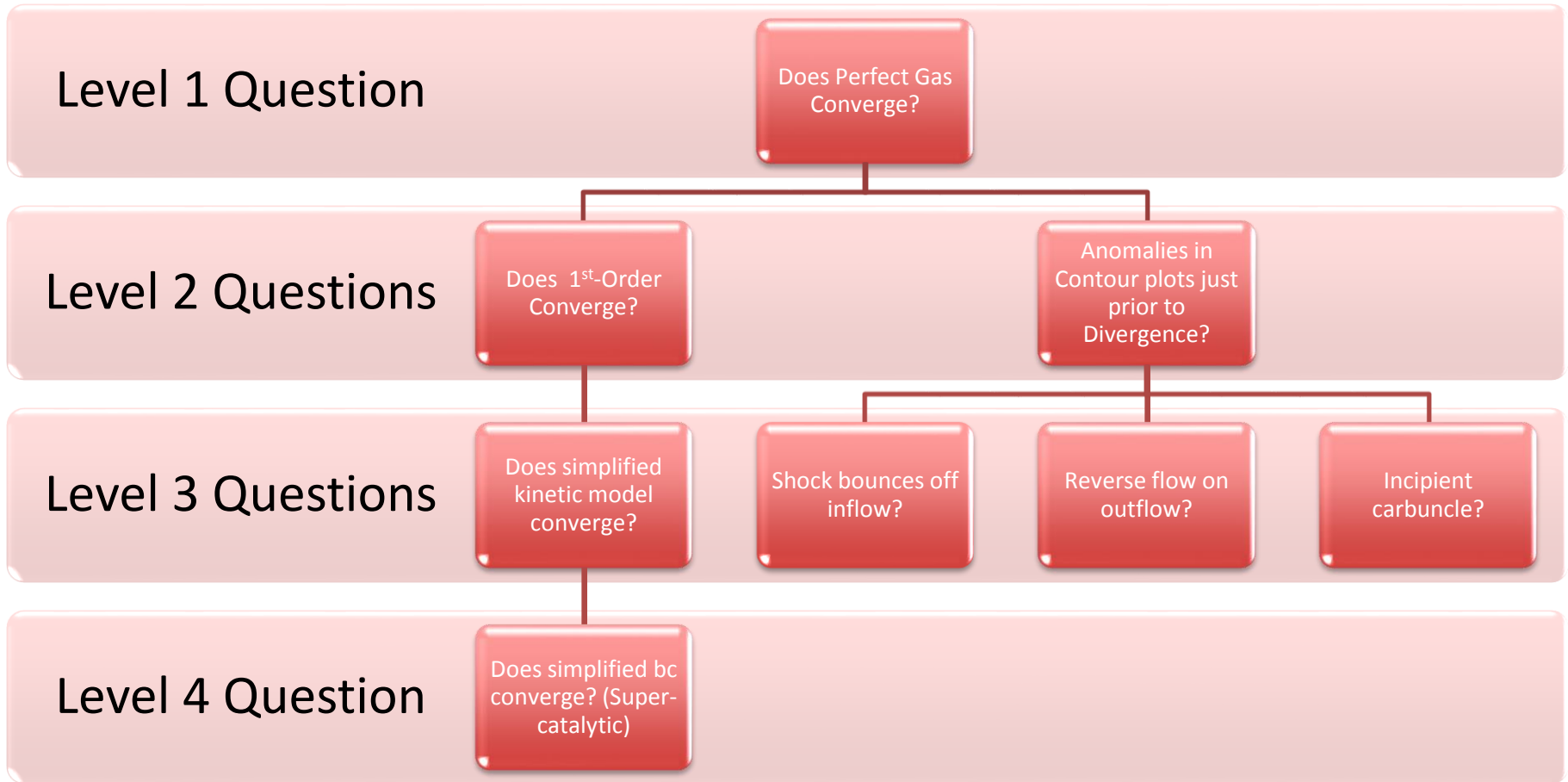
Extracted formatted lines file : `coupled_radiation.lines_fmt`

...

Done!

Check that nodes
span the entire
domain!

Troubleshooting



Possible Remedies

- Level 0
 - Consult NASA-TM-2014-218658 for a test case most like your case for guidance in selecting namelist parameters.
- Level 1
 - If perfect gas fails to converge, then there is likely a problem with grid quality or boundary conditions. Capturing surface contour plots, contour plots in the symmetry plane, or contour plots in cut planes through “challenging” topological features will often reveal problems with the grid or boundary conditions. Plot streamlines to confirm consistency with boundary conditions.
- Level 2
 - If first-order fails to converge and Level 1 checks pass, then the problem is likely one or more of the following conditions: overaggressive cfl ramping, inadequate eigenvalue limiting, temperature transient causes instability in the kinetic model.
- Level 3
 - If simplified kinetic model works where more complete model fails then additional limiting on max / min temperatures may be required for offending reactions. Proceed with caution that real physics isn’t compromised!
- Level 4
 - If simple (Dirichlet) bc converges, then a more conservative (smaller) relaxation factor may be required for the radiative equilibrium wall boundary (wall_temp_relax(:)).

Warnings

64 0.226705883950811E-05 0.80561E-05 0.2348E-01 0.5379E-02 0.1232E+00 3
Lift -0.189740078163752E-02 Drag 0.679775300136714E-02
INFO: Temperature below 1.0000 4 times. Reset. Min: 0.50000
INFO: Temperature below 1.0000 6 times. Reset. Min: 0.50000
INFO: Temperature below 1.0000 9 times. Reset. Min: 0.50000

- Such warnings (and related involving density) are not necessarily a problem.
- Usually, they are indicative of an undershoot or overshoot across a captured shock as its position evolves.
- Often, they disappear as the solution converges.
- Occasionally, they persist indicating a shortcoming of the limiter.
- If the number of occurrences keeps growing, the solution is diverging.

Summary

- Generic gas path simulations require additional data files available in the PHYSICS_MODULES directory.
- Recommended flux reconstruction and limiting options are documented in the tutorial.
- Not all options for the compressible gas path are available for the generic gas path.
 - Not all of the turbulence models are engaged in the generic gas path.
 - Not all of the boundary conditions are engaged in the generic gas path.
 - Not all of the flux reconstruction option are engaged in the generic gas path.
 - Usually, engagement will only require accommodation of correct equation of state or speed of sound.
- Prismatic grids orthogonal to the boundary layer, free shear layers, and captured shocks are HIGHLY recommended if accurate simulation of surface heating and shear is required.
 - The *multidm* option can be engaged for an all-tetrahedral grid to improve simulation quality, but this option is not as effective as a good grid.
 - The utility *aflr3_make_tets* will convert a mixed-element grid into tetrahedra.