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Laura Users Manual: 5.1-41601

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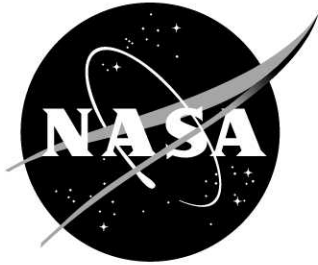
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Abstract

This users manual provides in-depth information concerning installation and execution of LAURA, version 5. LAURA is a structured, multi-block, computational aerothermodynamic simulation code. Version 5 represents a major refactoring of the original Fortran 77 LAURA code toward a modular structure afforded by Fortran 95. The refactoring improved usability and maintanability by eliminating the requirement for problem-dependent re-compilations, providing more intuitive distribution of functionality, and simplifying interfaces required for multiphysics coupling. As a result, LAURA now shares gas-physics modules, MPI modules, and other low-level modules with the FUN3D unstructured-grid code. In addition to internal refactoring, several new features and capabilities have been added, e.g., a GNU-standard installation process, parallel load balancing, automatic trajectory point sequencing, free-energy minimization, and coupled ablation and flowfield radiation.

Contents

1 Introduction

The users manual consists of seven sections. Section 2 gives an overview of new features, capabilities, and bug fixes. System requirements and installation are covered in Section 3, followed by code execution instructions in Section 4. Section 5 presents input files, their formats, and detailed information on their contents while Section 6 covers output files. Ancillary utilities are explained in Section 7, and the last section, Section 8, presents illustrative example cases.

2 New in This Version

LAURA v5.1 offers several new enhancements and bug fixes since the previous released version, v5.0:

- Major Enhancements

  - Surface recession
  - Multiple blocks per processor
  - Automatic load balancing

- Minor Enhancements

  - Updated kinetic, transport, and thermodynamic data
  - MPI efficiency improvements
  - Consistent `laura_blayer.dat` across block interfaces
  - GNU-standard installation `make check`
  - Simplified reaction diagnostic messages

- Bug Fixes

  - Occasional NaNs in `laura_blayer.dat` file
  - Memory leak in I/O section of the code
  - Error in one of 10 possible ranges in equilibrium-air formulation
  - Incorrect shear stress signs in output files
  - Deficiency in `super-catalytic` and `fully-catalytic` options
  - Error in algorithm for cases with inactive blocks
  - Evaluating boundary layer properties for inviscid flow
  - Error in Stefan-Maxwell diffusion model
  - Linf location initialization
  - Multiblock align shock

3 Installation

LAURA requires a Fortran 95 compiler, and if parallel processing is desired, a Message Passing Interface (MPI) implementation.[1] Some optional utilities require Ruby.[2] The installation and subsequent execution of LAURA assumes a Unix-like operating system or compatibility layer.[3] After the code is unpacked from the LAURA release tarball,

```
% tar zxf laura-5.1-Z.tar.gz  (unpack gzipped tarball)
% cd laura-5.1-Z
```

where Z is a revision track number. LAURA is installed via GNU build system,[4] which entails executing a sequence of four commands: `configure`, `make`, `make check`,[5] and `make install`.[6]

3.1 Sequential installation

To configure, compile, test, and install a sequential version of LAURA for use with a single processor, first make a subdirectory of `laura-5.1-Z` to store the configuration. For example,

```
% mkdir g95-seq
% cd g95-seq
```

if using the g95 Fortran compiler;[7] and then proceed with the typical GNU build sequence,

```
% ../configure FC=g95 --prefix=$PWD
% make
% make check
% make install
```

Note that `configure`'s `--prefix` option specifies the root directory for installing build artifacts—the default is `/usr/local`. In this example, it is set to the current working directory, `g95-seq` so executables will be installed in `g95-seq/bin` and data files will be copied to `g95-seq/share/laura` and `g95-seq/share/physics_modules` directories.

To use LAURA and associated utilities, set your search path to include `$PWD/bin`, e.g.,

```
setenv PATH ${PWD}/bin:$PATH  (for csh)
export PATH=${PWD}/bin:$PATH  (for sh)
```

---

[1]For example, OpenMPI or MPICH.

[2]See ruby-lang.org.

[3]For non-Unix-like systems, compatibility layers are available from mingw.org (minimal) and cygwin.com (maximal).

[4]See gnu.org/software/autoconf/.

[5]The `make check` command is optional. It will attempt to run small test cases.

[6]The `make install` command may require administrator privileges depending on your installation location.

[7]g95.org

3.2 MPI Installation

An MPI-enabled installation (to allow multiple processors) is similar to the sequential installation except the configuration command has the `--with-mpi` option instead of the `FC` Fortran compiler variable, e.g.,

```
% ../configure --prefix=$PWD \
               --with-mpi=/usr/local/pkgs/ompi_1.2.8-intel_11.0-028
```

Another difference is that an MPI-enable configuration will produce an executable named `laura_mpi` instead of `laura`.

In either case, `config.log` contains a record of the `configuration` command used, and `configure`'s `--help` option details all available configuration options.

4 Execution

The following steps outline a typical simulation cycle.[8]

Step 1. To start LAURA, a PLOT3D structured grid file is needed — see Section 5.2 on page 10 for more info. You may externally generate a grid using grid generation packages, such as Gridgen™, Grid*Pro*, and so forth, or use LAURA's interactive `self_start` utility to generate a single-block structured grid for simple families of 2D, axisymmetric and 3D blunt bodies—see Section 7.7 on page 49.

> **Step 1a.** Using `self_start`. To use `self_start` to generate a single-block grid, simply execute this interactive utility, e.g.,
>
> ```
> % self_start
> ```
>
> and answer all the questions. After a successful execution, this utility will have generated the following files:
>
> ```
> assign_tasks   laura_bound_data
> laura.g        laura_namelist_data   self_start.log
> ```
>
> Examine the grid, `laura.g`, and proceed to Step 2.

> **Step 1b.** External Grid Generation. Generate a single- or multi-block structured grid with the following rules:
>
> i. Right-handed grid coordinates
> ii. Longitudinal axis of the body aligned with the x-axis, oriented nose-to-tail

---

[8]See Section 8 on page 50 for complete worked examples and Appendix A on page 62 for how to restart cases run with versions of LAURA prior to version 5.

and write the grid coordinates into a PLOT3D file, `laura.g`. Run the interactive `bounds` utility (see Section 7.1 on page 47) and answer all the questions regarding the grid block topology:

```
% bounds
```

This utility will automatically generate `laura_bound_data`, the connectivity file.

Step 2. If you did not use `self_start`, create `assign_tasks` (see Section 7.6 on page 49 for more info) and a `laura_namelist_data` file or copy the sample file from the `[install_prefix]/share/laura` directory, where `[install_prefix]` is the installation prefix specified when LAURA was installed. Edit this file for your case—see Section 5.4 on page 13 for more detail.

Step 3. Create a `tdata` file (see Section 5.5 on page 30) to define the gas model condition for your specific simulation.[9]

Step 4. Run LAURA,

```
% laura
```

or

```
% mpirun -np [#] laura_mpi
```

where `#` is the number of available processors. By the end of this step, the following files will have been generated:

```
conv.out
laura_new.g          laura_new.rst
laura_surface.q      laura_flow.q
laura_surface.mcr    laura_flow.mcr
```

Examine these files before proceeding to the next step.[10]

Step 5. Change `irest` flag in the `laura_namelist_data` (see Section 5.4 on page 13) from 0 to 1, and copy the new generated grid and solution files to `laura.g` and `laura.rst` files; i.e.,

---

[9]A sample `tdata` is available in the `[install_prefix]/share/physics_modules` installation directory. The other datafiles that reside in this directory, e.g., `kinetics_data`, `species_thermo_data`, `species_transp_data`, and `species_transp_data_0`, may also be copied and tailored to suit a different thermodynamic model, curve-fit data, or thermochemical reactions are needed. See Section 5.5 on page 30 for more detail.

[10]See Section 6 on page 42 for complete description of laura output files.

```
% cp laura_new.g laura.g
% cp laura_new.rst laura.rst
```

Step 6. Repeat the previous two steps until iterative convergence.

5   Input Files

Nominally, LAURA requires five input files as shown in the upper section of Table 1. Depending on the simulation requirements, however, other files may also be necessary and are shown in the second section of Table 1. All files are plain ASCII text unless otherwise noted.

Table 1: LAURA input files.

Filename	Content
assign_tasks	Sweep and relaxation directions
laura.g*	PLOT3D grid
laura_bound_data	Grid block face boundary conditions
laura_namelist_data	Simulation configuration
tdata	Gas model
hara.in	Radiation mechanisms
kinetic_data	Specie reactants and products
laura.rst†	Flowfield solution for restart
laura.trn	Transition location and length
laura_trajectory_data	Trajectory points
laura_vis_data	Viscous term treatment
species_thermo_data	Specie thermodynamics
species_transp_data	Collision cross-sections
species_transp_data0	High-order collision cross-sections
surface_property_data	Thermochemical surface properties

* Fortran unformatted binary, 3-D whole, multiblock PLOT3D.
† Fortran unformatted binary.

The following subsections describe all input files in detail, beginning with the nominally required files and then proceeding alphabetically as shown in the table.

5.1   assign_tasks

This file defines sweep and relaxation directions for each grid block. Each line, corresponding to each grid block, has six integers that are separated by at

least one space. These integers correspond to `nbk`, `mbk`, `mbr`, `lstrt`, `lstop`, and `mapcpu` where

<u>nbk</u>

Block number.

<u>mbk</u>

Sweep direction. The assigned value can be either 1, 2, or 3, corresponding to i-, j-, or k-direction, respectively.

<u>mbr</u>

The line relaxation direction. Note: must be different than the sweep direction.

Options are:

0: Point-implicit, i.e., no line-relaxation

1: Line-implicit along i coordinate

2: Line-implicit along j coordinate

3: Line-implicit along k coordinate

<u>lstrt</u>

The starting grid index in the sweep direction. Typically 1 .

<u>lstop</u>

The ending grid index in the sweep direction. Typically 0, which is shorthand for the maximum index.

<u>mapcpu</u>

CPU number for block `nbk`. Must be greater than zero. To run with a single processor, set this value to 1 for all grid blocks.

When starting a new simulation where the k-coordinate runs from the vehicle surface to the freestream boundary, sweeping in the k-coordinate and solving point-implicitly is recommended, i.e. `mbk = 3` and `mbr = 0`. After the shock has stabilized, switch to streamwise sweeps and solve line-implicitly along the k-coordinate, i.e. `mbk = 1` and `mbr = 3`.

5.1.1 Example 1: Multiple Blocks per CPU or Vice-versa

Suppose the grid has 2 blocks, but the number of available processors is not the same as the number of grid blocks. The user does not need to change any of the input files and can simply specify the number of processors available, e.g.,

```
% mpirun -np [#] laura_mpi
```

where **#** is the number of available processors. LAURA automatically assigns processors to blocks such that each processor receives approximately same number of grid cells.

5.1.2 Example 2: Deactivating Grid Blocks

Suppose the grid has 50 blocks, but only blocks 20–25 need to be updated. In this case, `assign_tasks` would contain only the active blocks, e.g.,

```
20  3   0   1    0     1
21  3   0   1    0     2
22  3   0   1    0     3
23  3   0   1    0     4
24  3   0   1    0     5
25  3   0   1    0     6
nbk mbk mbr lstrt lstop mapcpu
```

5.2 `laura.g`

This file is a multi-block, 3D-whole PLOT3D file in Fortran unformatted binary format with double-precision reals. For convenience, here is a sample of the Fortran 95 code that LAURA uses to read this file:

```
open ( 25, file='laura.g', form='unformatted' )
read(25) nblocks
...allocate i,j,kblk(nb) and grid memory...
read(25) (iblk(nb),jblk(nb),kblk(nb),nb=1,nblocks)
do nb = 1, nblocks
  ix1 = iblk(nb) ; jx1 = jblk(nb) ; kx1 = kblk(nb)
  ...allocate grid(nb)%x,y,z memory...
  read(25) (((grid(nb)%x(i,j,k),i=1,ix1),j=1,jx1),k=1,kx1), &
           (((grid(nb)%y(i,j,k),i=1,ix1),j=1,jx1),k=1,kx1), &
           (((grid(nb)%z(i,j,k),i=1,ix1),j=1,jx1),k=1,kx1)
end do
```

A file of this format, but named `laura_new.g`,[11] is generated by LAURA at the end of a successful run. This file is required and must have a right-handed coordinate system. Figure 1 shows the default `laura` coordinate orientation. LAURA does not require a specific coordinate or grid orientation but the angle-of-attack definition is predefined — see Section 5.4.3 on page 18 for more info.

---

[11]When running a trajectory sequence, the file will be named `laura_####.g` where `####` is the trajectory point index.
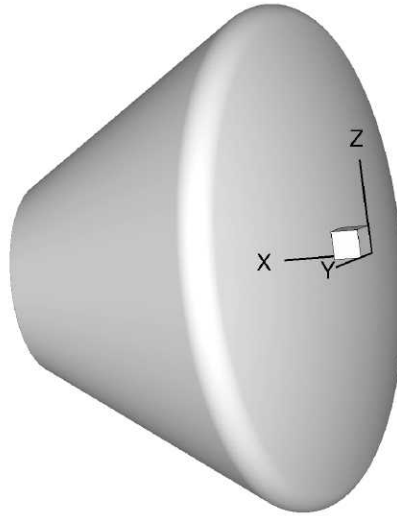
Figure 1: Default LAURA coordinate system orientation.

5.3 laura_bound_data

Grid block face boundary types are defined in laura_bound_data where each line corresponds to a grid block and contains six integers, one for each of the six faces: i_{min}, i_{max}, j_{min}, j_{max}, k_{min}, and k_{max}. Each integer specifies either a physical boundary condition or block-to-block interfaces. An illustrative example is analyzed toward the end of this section.

This file is required and is generated automatically for grids created by LAURA's self_start utility—see Section 7.7 on page 49. This file can also be created by using LAURA's interactive utility, bounds, by answering questions for each block.

Valid face types are as follows:

-9,...,0: Solid surface boundary. Up to ten different solid surface boundaries may be specified. Thermochemical properties of solid surfaces that are different than type 0, which are specified in laura_namelist_data, are defined in surface_property_data file—see Section 5.15 on page 41.

1: Outflow boundary (extrapolation).

2: Symmetry boundary across $y = $ constant.

3: Farfield/Freestream boundary.

4: Symmetry boundary across $x = $ constant or $z = $ constant.

5: Reflection boundary across $j = 1$ symmetry (valid for axi-symmetric and/or 2D grids).

6: Venting boundary. (See Section 5.4.14 on page 30 for more details.)

7: Reflection boundary across i face singularity with periodic j boundary.

>1000000: This seven digit boundary number defines block-to-block face connectivity. The first digit is always 1. The next three digits identifies the block number that is shared with the current block. The 5th digit defines which i, j, or k face of the neighboring block is shared where 1 corresponds to i_{min}, 2 corresponds to i_{max}, and so forth. The last two digits identify the relation of the remaining two indices: The 6th digit can be either 1, 2, 3, or 4 where values of 1 or 3 mean the first index of the host face is in the same direction as the first or second index of the neighboring face, respectively, and values of 2 or 4 mean the adjoining indices are in the opposite direction. The last digit can be either a 1 or 2 and indicates whether the second indices of the host and neighboring faces are in the same direction or they are in the opposite direction, respectively.

For example, consider a block with the following `laura_bound_data` boundary condition numbers:

```
1006421  1002111     2    1005121     0        3
```

The first integer, 1006421, shows that i_{min} of this block is shared with j_{max} (fifth digit) of block 6 (the first three digits after 1). The first and second indices of the host face are j and k, respectively. Because the j index is connected to i, the first and second indices of the neighboring face are i and k, respectively, The 2 in the 6th digit shows that the j index of the host face is in opposite direction of the i index of the neighboring face. The last digit, 1, indicates that k indices of the host and and neighboring faces are along the same direction. This configuration is illustrated in Figure 2.
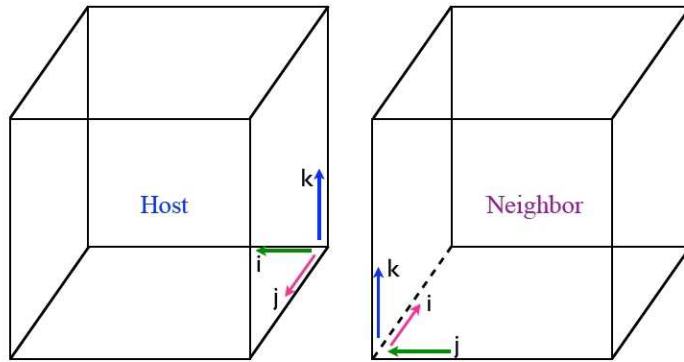
Figure 2: Illustration used for block connectivity example.

The second and fourth boundary-type integers can be explained similarly. The third boundary-type integer (corresponding to the j_{min} face) specifies a

y-constant symmetry plane; the fifth boundary-type integer (corresponding to the k_{min} face) specifies is a solid-wall boundary condition; and the last digit (corresponding to the k_{max} face) specifies a freestream boundary.

5.4 `laura_namelist_data`

Simulation configuration is specified through `laura_namelist_data` and is required. This file is read as a Fortran 95 namelist and has the form,

```
&laura_namelist
 velocity_ref = 5000.0 ! Free stream velocity, m/s
 density_ref  = 0.023  ! reference density, kg/s
 tref         = 250.0  ! Free stream temperature, K
 alpha        = 25.0   ! Angle-of-attack in xz plane, degrees
[ variable     = value  ! Optional comment ]
 /
```

where `variable` and their possible `values` are described in the following sections, which are grouped according to farfield/freestream and aerodynamic coefficient reference quantities; thermochemical nonequilibrium flags; molecular transport flags; turbulent transport models flags; numerical parameters; grid adaptation, alignment, and doubling parameters; radiation and ablation flags; grid-file description; venting boundary condition flags; and solid surface boundary condition flags. Note that for all but the parameters shown in the above example, reasonable defaults have been chosen and only those parameters that differ from the defaults need to be specified.

Detailed description of parameters and/or flags with their units and default values is presented under each of the above categories. The order of these parameters is arbitrary but is given here alphabetically for better readability.

5.4.1 Ablation Flags

`ablation_option`

An integer that specifies whether the pyrolysis ablation rate and wall temperature are computed in addition to the char ablation rate. This option only effects cases with `bprime_flag` equal to 0 or 1.

Options are:

0: The pyrolysis ablation rate and wall temperature are computed, in addition to the char ablation rate, assuming steady-state ablation.

1: The pyrolysis ablation rate and wall temperature are held constant (they are set to the values present in `ablation_from_laura.m`) while the char ablation rate is computed.

<u>ablation_verbose</u>

A logical flag to print out developer focused info on convergence of ablation. Default: `.false.`

<u>blowing_model_0</u>

Character indicator for ablation model specification. Default: '`none`'

Options are:

'`FIAT`'

This '`FIAT`'[12] option computes the blowing rate and surface temperature as a function of heating rate, pressure, and ablator elemental mass fractions. The user must specify the elemental mass fractions for char and pyrolysis gas or default of 100% carbon will be employed.

'`none`'

No ablation-flowfield coupling.

'`specified`'

This option specifies a blowing or suction rate as a function of pressure (see `mdot_pressure_0`). The user must specify the elemental mass fractions for pyrolysis gas or default of 100% carbon will be employed. Any specification for elemental mass fraction of char is ignored in this option.

'`equil_char_quasi_steady`'

This option solves the equilibrium surface ablation problem. The energy balance, elemental mass balance, and char equilibrium constraint are solved to obtain the char ablation rate, wall temperature, and elemental composition at the surface. Along with the pressure from the normal momentum equation, these values define the equilibrium species composition at the wall. The user must specify the surface temperature type to be `surface energy balance` — see Section 5.4.10 on page 25 for more info.

Presently, this model does not include an in-depth material response computation, which would provide the pyrolysis ablation rate and conductive heat flux into the solid material. These two values are required for solving the previously mentioned surface equations. To approximate these values, the steady-state ablation assumption is made, which specifies that the pyrolysis ablation rate is proportional to the char ablation rate and the in-depth conduction is proportional to the enthalpy at the surface.

---

[12]FIAT is a stand alone software and is needed if `blowing_model_0`='`FIAT`'. Request for access to FIAT can be made to NASA Ames Research Center.

In the present framework of steady-state ablation, the ablation material is completely defined by `CHONSi_frac_pyrolysis_0` (thus `CHONSi_frac_char_0` is ignored in this option). These are defined below. Note that the computed ablation rate is the sum of the pyrolysis and char components. (See Sections 8.3 on page 57 and 8.4 on page 58 for recommended procedure for an unspecified ablation computation.)

'`quasi_steady`'

This option specifies a quasi-steady ablation rate as a function of local pressure, heating rate, and temperature. The sublimation temperature and heat of ablation are specified by the user for a given ablator as a function of pressure. (See `t_sublimation_0` and `h_ablation_0`.) If the surface temperature is less than the sublimation temperature a zero blowing rate is defined. Otherwise the blowing rate is given by $\dot{m} = q/\Delta H_{abl}$ with appropriate non-dimensionalization employed before use. The user must specify the elemental mass fractions for pyrolysis gas or default of 100% carbon will be employed. Any specification for elemental mass fraction of char is ignored in this option. The user must specify the surface temperature type to be `surface energy balance` — see Section 5.4.10 on page 25 for more info.

`bprime_flag`

An integer defining if the b-prime approach is applied. Applicable only for `blowing_model_0` = '`equil_char_quasi_steady`'. See Section 5.4.1 on the preceding page for more details of its application. Default: `0`

Options are:

0: Do not use bprime approach, and instead use a rigorous diffusion model. This option is consistent with the "Fully-Coupled" approach defined in Ref. [1].

1: Use b-prime approach. This option is consistent with the "Partially-Coupled" approach defined in Ref. [1].

2: Hold the ablation rate and wall temperature constant from the restart file, while applying the rigorous diffusion model (thus, the surface energy balance and char equilibrium constraint are not satisfied). This option is sometimes useful when transitioning from a `bprime_flag = 1` computation to a `bprime_flag = 0` computation.

`char_density_0`

Density of the char, kg/m^3. Default: 256.29536

CHONSi_frac_char_0

This rank 1 vector of extent 5 sets elemental mass fraction of C, H, O, N, and Si species from char. Elemental mass fractions must be in this order and the sum of elemental mass fractions must equal 1.0 . Default: `CHONSi_frac_char_0 = 1.0, 0.0, 0.0, 0.0, 0.0`

CHONSi_frac_pyrolysis_0

This rank 1 vector of extent 5 sets the elemental mass fractions of pyrolysis gas species, which are C, H, O, N, and Si. Elemental mass fractions must be in this order and the sum of elemental mass fractions must be 1. Default is Graphite: `CHONSi_frac_pyrolysis_0 = 1.0, 0.0, 0.0, 0.0, 0.0`

compute_mdot_initial

An integer defining if the ablation rates are computed before the first flowfield iteration.

Options are:

0: Applies the ablation rates and wall temperatures present in the `ablation_from_laura.m` file.

1: Computes the ablation rates and wall temperatures before the first flowfield iteration.

freq_wall

For `bprime_flag = 1`, it is an integer defining frequency of update to ablation wall boundary conditions. For `bprime_flag = 0`, it is an integer defining frequency of update to the surface energy balance solution, which defines the wall temperature, while `nexch` defines the frequency of update to the remaining surface equations — see Section 5.4.8 on page 23 for more info on `nexch`. Default: 50

h_ablation_0

A rank 1 vector of extent 3 used to compute the heat of ablation in MJ/kg for `quasi_steady` blowing option as

$$
\begin{aligned}
\texttt{h\_ablation\_0(1)} \quad &+ \quad (\texttt{h\_ablation\_0(2)})\log p_w \\
&+ \quad (\texttt{h\_ablation\_0(3)})(\log p_w)^2
\end{aligned} \tag{1}
$$

where p_w is the local pressure, in atmospheres. Example $\Delta H_{abl} = 28.0 - 1.375 \log p_w + 27.2 (\log p_w)^2$. Default: 0.0

mdot_pressure_0

A rank 1 vector of extent 2 is used to set the blowing or suction distribution defined as

$$
\texttt{mdot\_pressure\_0(1)} + (\texttt{mdot\_pressure\_0(2)})\frac{p}{\rho_\infty V_\infty^2} \tag{2}
$$

where p is the local pressure, ρ_∞ is the reference density, and V_∞ is the reference velocity. Positive value produces blowing distribution, while negative value produces suction distribution. Default: 0.0

<u>t_sublimation_0</u>

A rank 1 vector of extent 3 used to compute the sublimation temperature in degrees Kelvin for `quasi_steady` blowing option as

$$
\begin{aligned}
\texttt{t\_sublimation\_0(1)} \quad + \quad & (\texttt{t\_sublimation\_0(2)}) \log p_w \\
+ \quad & (\texttt{t\_sublimation\_0(3)})(\log p_w)^2
\end{aligned}
\tag{3}
$$

where p_w is the local pressure, in atmospheres. Example $T_{sub} = 3797.0 + 342.0 \log p_w + 30.0(\log p_w)^2$. Default: 0.0

<u>uncoupled_ablation_flag</u>

An integer defining if an uncoupled ablation analysis is applied. The uncoupled ablation option is included to provide a baseline solution for the coupled ablation analysis. Default: 0

Options are:

0: Do not apply an uncoupled ablation analysis. It means that the coupled ablation analysis discussed in Section 8.3 on page 57 is applied.

1: Apply an uncoupled ablation analysis to a converged non-ablating flowfield. The procedure for applying the uncoupled ablation analysis is discussed in Section 8.4 on page 58.

<u>virgin_density_0</u>

Density of virgin material, kg/m^3. Default: 544.627742

5.4.2 Aerodynamic Coefficient Reference Quantities

<u>bref</u>

Yaw moment coefficient reference length, grid-units. Default: 1.0

<u>cref</u>

Pitching moment coefficient reference length, grid-units. Default: 1.0

<u>sref</u>

Reference area for aerodynamic coefficients, grid-units. Default: 1.0

<u>xmc</u>

x-coordinate of moment center, grid-units. Default: 0.0

ymc

y-coordinate of moment center, grid-units. Default: `0.0`

zmc

z-coordinate of moment center, grid-units. Default: `0.0`

5.4.3 Farfield/Freestream Reference Quantities

alpha

Angle-of-attack in xz plane, degrees, such that

$$u = cos(\alpha)cos(yaw); v = -sin(yaw); w = sin(\alpha)cos(yaw) \qquad (4)$$

where u, v, and w are velocities in x-, y-, and z-coordinate, respectively. Default: `0.0`

density_ref

Free stream density, kg/m^3. Default: `0.001`

rpm

Spin rate, RPM. This is applicable only to axisymmetric cases. Default: `0.0`

tref

Free stream temperature, K. Default: `200.0`

velocity_ref

Free stream velocity, m/s. Default: `5000.0`

yaw

Sideslip angle in xy plane, degrees. Default: `0.0`

trajectory_data_point

Pickup simulation from this line in the file `laura_trajectory_data`.

Default: `0` if `laura_trajectory_data` is not present.

Default: `1` if `laura_trajectory_data` is present.

Note that the reference quantities are defined consistently across the trajectory using the values supplied in namelist above. The reference quantities are NOT reset according to the time varying free stream conditions. Consequently, dimensionless values of density and velocity in free stream will not generally equal 1. Dimensionless values of total enthalpy in free stream will not equal 0.5 which may impact post-processing tools that are key on a specific number for total enthalpy to detect the boundary-layer edge.

The algorithm is most efficient if the restart solution is converged (or nearly converged so that line-implicit relaxation may be applied) at free stream conditions equal to the reference quantities in `laura_namelist_data`. If one wishes to pickup a computation for `trajectory_data_point` > 1 then it is best to start at the converged restart file for the previous trajectory point. Restart files and post processing files for each trajectory point have the trajectory point number included as part of the root name. Thus if one wants to pickup at trajectory point 12 one should copy `laura_0011.rst` to `laura.rst` and (if grid is being updated) `laura_0011.g` to `laura.g`. This advice is offered because restart solutions are converted according to the ratio of density and velocity between adjacent trajectory points to bring interior initial conditions closer to the new inflow boundary conditions.

5.4.4 Grid Adaptation, Alignment, and Doubling Parameters

`beta_grd`

This parameter controls grid points normal to the body (k-grid points) are controlled by the following grid stretching function:

$$k_i^* = 1 - \beta \frac{\frac{\beta-1}{\beta+1}^{\frac{k_{max}-k_i}{k_{max}}} - 1}{\frac{\beta-1}{\beta+1}^{\frac{k_{max}-k_i}{k_{max}}} + 1} \tag{5}$$

where k_i^* are new grid points. The `beta_grd` parameter defines the β coefficient in equation 5. No stretching will be performed if $\beta < 1$. Recommended value is 1.15, if used. Default: `0.0`

`ep0_grd`

Grid clustering around the shock is designed using the following function:

$$\overline{k^{**}}_i = \epsilon_0 \overline{k_i^*}^2 (1 - \overline{k_i^*})(\overline{k_i^*} + \mathtt{fsh}) + \overline{k_i^*} \tag{6}$$

where $\overline{k_i}$ refers to normalized value and k_i^* is defined by equation 5. `ep0_grd` assigns the ϵ_0 coefficient in equation 6. Maximum recommended value is 25/4, if used. Default: `0.0`

`kmax_final`

The target number of grid cells in the k-direction. Triggered by the global L2 error norm set by `kmax_error`, cells along the k direction are increased by a factor of `kmax_factor` until reaching `kmax_final`. Any value less than the number of k grid cells in `laura.g` file will be ignored, i.e., no coarsening. This option requires all blocks to be active. Default: `0.0`

kmax_error

When the global L2 error norm reaches this value, the number of grid cells in the k direction increases by a factor of `kmax_factor` until the maximum allowable grid cells, `kmax_final`, is reached. This option requires all blocks to be active. Default: 0.01

fctrjmp

This parameter is used to detect bow shocks. Bow shock is first detected when the sensing parameter defined by `jumpflag` exceeds by this value, while searching from inflow boundary. Default: 1.05

frac_line_implicit

This positive parameter, which must be less than or equal 1, sets a fraction of the line-implicit direction that is assigned in `assign_tasks` (see Section 5.1 on page 8). This parameter, which supersedes the given assignments in `assign_tasks`, will be applied to all the active blocks. This parameter is recommended where there might be an instability issue such as across strong shocks. Default: 0.7

fsh

Fraction of arc length distance between body and inflow boundary where bow shock is captured. Default: 0.8

fstr

This parameter approximately defines fraction of k-cells in boundary layer region. Default: 0.75

jumpflag

An integer flag to select the sensing parameter to be used in detecting position of captured shock for grid adaption. Default: 2

Options are:

0: Redistributes grid points in k-direction for the target cell Reynolds number defined by `re_cell` parameter, without changing the domain boundary.

1: Selects pressure as the sensing parameter.

2: Selects density as the sensing parameter.

3: Selects temperature as the sensing parameter.

4: Scales the grid distance in the k-direction up by the value defined by `fctrjmp` parameter.

maxmoves

An integer number to assign maximum number of times that grid adaption is performed. The value of zero, however, can be used for unlimited number of times. Default: `0`

max_distance

This real number defines maximum distance from the body surface that grid outer boundary can be moved away by any one of the flags. This is often useful especially when adapting shock into wake, where the adapting grid may become skewed due to presence of sharp gradients. This value defines the maximum length of the wake. Default: `1.0E+6`

movegrd

An integer number for number of cycles between each grid alignment. A zero value disables any grid alignment. Default: `0`

re_cell

This value defines the target cell Reynolds number at the wall after a grid movement. Default: `2.0`

The cell Reynolds number is defined as

$$Re_{cell} = \rho c \Delta n / \mu \tag{7}$$

Here ρ is the flow density, c is the sound speed, Δn is the cell height, and μ is the flow viscosity.

5.4.5 Grid File Description

dimensionality

A string flag to select the dimensions of the problem. Default: '3D'. Available options are:

'axisymmetric'

This option selects axisymmetric flow solution. This requires a domain with single-cell width in the j-direction.

'2D'

This selects two-dimensional problem, which requires a domain with single-cell width in the j-direction.

'3D'

This option solves three-dimensional problems.

grid_conversion_factor

This parameter scales the grid to meter. One grid unit equals `grid_conversion_factor` meters. Default: `1`

single_precision_grid

Logical flag: .true. if grid points in the laura.g file are stored as single precision values, otherwise double precision is assumed. Default: .false.

5.4.6 Initialization

init_vel_fctr

A real number between 0 and 1 to reduce the initial velocities u, v, w within the domain to avoid creating a vacuum for wake flow problems, which may lead to an invalid solutions. The initial near zero velocity has also shown to ease up the formation of bow shock. Default: 0.01

5.4.7 Molecular Transport Flags

ivisc

An integer flag to engage viscous terms (inviscid=0/viscous=2). Default: 2

mass_driven_diff

A logical flag to engage binary diffusion driven by mass fraction gradient. Default: .false.

multi_component_diff

A logical flag to engage multi-component diffusion by Stefan-Maxwell equation sub-iterations. Default: .false.

mole_driven_diff

A logical flag to engage binary diffusion driven by mole fraction gradient. Default: .true.

navier_stokes

A logical flag to select equation set for Thin-Layer Navier Stokes or Full Navier Stokes. The navier_stokes = .false. may be used to select Thin-Layer Navier Stokes. Default: .false.

pressure_diffusion

A logical flag to engage pressure diffusion term on Stefan-Maxwell approximation. Default: .false.

schmidt_number

A constant Schmidt number may be specified to calculate diffusivities. If the value is negative, diffusivities are computed directly from collision cross sections. Default: -1.0

prandtl_number

A constant Prandtl number may be specified to calculate conductivities. If the value is negative, conductivities are computed directly from collision cross sections. Default: `-1.0`

5.4.8   Numerical Parameters

cfl1

Initial value of CFL number. Default: `5.0`

cfl2

Final value of CFL number. Default: `5.0`

epsa

Eigenvalue limiting factor. Default: `0.3`

hrs

The maximum total CPU time for simulation, hours. Default: `10`

iramp

Number of cycles to ramp from `cfl1` to `cfl2`. Default: `200`

irest

An integer flag to start the simulation either using freestream values (`irest = 0`), or using the existing solution from `laura.rst` file (`irest = 1`). Default `0`

iterwrt

Number of cycles between saves of all output files—see Section 6 on page 42. Default: `200`

jupdate

Number of cycles between jacobian updates. Default: `10`

ncyc

Number of global iterations. Default: `1000`

nexch

Number of cycles between exchange of data between processors and updating boundary conditions. Default: `2`

nitfo

Number of cycles using 1st-order spatial accuracy. Default: `0`

<u>nordbc</u>

Boundary condition calculation using 1st-order (`nordbc = 1`) or 2nd-order (`nordbc = 2`) accuracy. Default: `1`

<u>ntran</u>

Number of cycles between transport properties update. Default `1`

<u>rf_inv</u>

Inviscid relaxation factor. Default: `3.0`

<u>rf_vis</u>

Viscous relaxation factor. Default: `1.0`

<u>rf_chem</u>

Chemical source term reduction factor sometimes useful to "ease in" simulations very close to equilibrium. This factor, which must be greater than 1.0 when it is used, changes the answers and must ultimately equal 1.0 in the final simulation. Default: `1.0`

<u>rmstol</u>

A real number to stop the iterations after L2 norm residual reaches this value. Default: `1.0E-10`

<u>sub_iterations</u>

An integer number to control multiple passes through the linear solver, which has been found to increase robustness for some high energy applications. Default: `1`

5.4.9 Radiation Flags

<u>radiation</u>

A logical flag to enable coupling between radiation equation(s) and flow equations. See Section 8.2 on page 56 for coupled radiation procedure. Default: `.false.`

<u>radiation_input_only</u>

A logical flag to enable creation of input file `hara_out.m` to compute radiation outside of LAURA when `radiation` is `.false.`. Default: `.false.`

<u>maxrad</u>

An integer number to assign maximum number of calls to radiation interface. The value of zero can be used for unlimited number of times. Default: `0`

<u>nrad</u>

Number of iterations between calls to HARA. Default: `500`

iinc_rad, jinc_rad

Increment between i and j lines, respectively at which radiation profile is computed. Interim lines are interpolated. Default: 1 (Compute every line.)

frac_rad_new

Relaxation factor on radiation. $\nabla(q_{rad}) = frac\_rad\_new\nabla(q_{rad})^n + (1 - frac\_rad\_new)\nabla(q_{rad})^{n-1}$. Default: 1.0

absorptivity

Fraction of incident radiative energy absorbed by the wall. Affects surface energy balance and computation of radiative equilibrium wall temperature. Default: 1.0

tw_rad_flag

An integer flag to engage Tauber-Wakefield approximation for radiation cooling on surface-energy balance (on=1/off=0). Default: 0

5.4.10 Solid Surface Boundary Condition Flags

catalysis_model_0

A character identifier for selecting catalysis model for surface type 0 (see Section 5.3 on page 11). This flag is good only for multi-species reacting gases and will be ignored for single-specie gas models. The catalysis model name must be surrounded by quotation marks, e.g., ' '. Default: 'super-catalytic'

Available catalysis models are:

'CCAT-ACC'

This option uses the following surface catalytic coefficients [2] for catalyzing atomic oxygen and nitrogen to molecular oxygen and nitrogen, respectively.

$$\gamma_O = \begin{cases} 13.5e^{-8350/T_w^*} & T_w^* \le 1359.0 \ K \\ 5.0 \times 10^{-8}e^{18023/T_w^*} & T_w^* > 1359.0 \ K \end{cases} \tag{8}$$

$$\gamma_N = \begin{cases} 4.0e^{-7625/T_w^*} & T_w^* \le 1475.0 \ K \\ 6.2 \times 10^{-6}e^{12100/T_w^*} & T_w^* > 1475.0 \ K \end{cases} \tag{9}$$

where T_w^* is calculated as

$$T_w^* = \begin{cases} \min(\ \max(1255.0, T_w),\ 1659.0) & \text{for } \gamma_O \\ \min(\ \max(1255.0, T_w),\ 1900.0) & \text{for } \gamma_N \end{cases} \tag{10}$$

'CSiC'

This option uses the following surface catalytic coefficients [2] for catalyzing atomic oxygen and nitrogen to molecular oxygen and nitrogen, respectively.

$$\gamma_O = 6.415 \times 10^{-4} e^{3498.4/T_w^*} \tag{11}$$

$$\gamma_N = 3.993 \times 10^{-4} e^{4402/T_w^*} \tag{12}$$

where T_w^* is given as

$$T_w^* = \min(\ \max(1100.0, T_w),\ 1920.0) \tag{13}$$

'CSiC-SNECMA'

This option uses the following surface catalytic coefficients [2] for catalyzing atomic oxygen and nitrogen to molecular oxygen and nitrogen, respectively.

$$\gamma_O = \gamma_N = 9.593 \times 10^{-5} e^{7002.9/T_w^*} \tag{14}$$

where T_w^* is given as

$$T_w^* = \min(\ \max(1350.0, T_w),\ 1920.0) \tag{15}$$

'equilibrium-catalytic'

This option sets species concentrations to equilibrium values at wall pressure and temperature based on elemental mass fractions in the cell above the solid surface boundary.

'fully-catalytic'

This option assumes that all the atomic and ionized oxygen, nitrogen, carbon, and so forth catalyzes to molecular oxygen, nitrogen, carbon, and so on, respectively; i.e.,

$$\gamma_O = \gamma_N = \gamma_C = ... = 1 \tag{16}$$

'non-catalytic'

This option assumes that no atomic or ionized oxygen, nitrogen, carbon, and so forth catalyzes to molecular oxygen, nitrogen, carbon, and so on, respectively; i.e.,

$$\gamma_O = \gamma_N = \gamma_C = ... = 0 \tag{17}$$

'RCC-LVP'

This option uses the following surface catalytic coefficients [2] for catalyzing atomic oxygen and nitrogen to molecular oxygen and nitrogen, respectively.

$$\gamma_O = \begin{cases} 7.5 e^{-8283/T_w^*} & T_w^* \leq 1499.0\ K \\ 2.5 \times 10^{-7} e^{17533/T_w^*} & T_w^* > 1499.0\ K \end{cases} \tag{18}$$

$$\gamma_N = \begin{cases} 6.0 \times 10^{-2}e^{-2605/T_w^*} & T_w^* \le 1529.0 \ K \\ 1.5 \times 10^{-5}e^{10080/T_w^*} & T_w^* > 1529.0 \ K \end{cases} \tag{19}$$

where T_w^* is calculated as

$$T_w^* = \begin{cases} \min(\ \max(1255.0, T_w),\ 1799.0) & \text{for } \gamma_O \\ \min(\ \max(1255.0, T_w),\ 1954.0) & \text{for } \gamma_N \end{cases} \tag{20}$$

'Scott-RCG'

This option uses the following surface catalytic coefficients [3] for catalyzing atomic oxygen and nitrogen to molecular oxygen and nitrogen, respectively.

$$\gamma_O = 16.0e^{-10271/T_w} \quad 1400 \le T_w \le 1650 \tag{21}$$

$$\gamma_N = 7.14 \times 10^{-2}e^{-2219.0/T_w} \quad 1090 \le T_w \le 1670 \tag{22}$$

The same equations will be used even if the wall temperature, T_w, is out of the specified range, in which case a warning will be issued to the `stdout`.

'Stewart-RCG'

This option uses the following surface catalytic coefficients [2] for catalyzing atomic oxygen and nitrogen to molecular oxygen and nitrogen, respectively.

$$\gamma_O = \begin{cases} 5.0 \times 10^{-3}e^{-400/T_w} & T_w \le 502 \\ 1.6 \times 10^{-4}e^{1326/T_w} & 502 < T_w \le 978 \\ 5.2e^{-8835/T_w} & 978 < T_w \le 1617 \\ 39 \times 10^{-9}e^{21410/T_w} & 1617 < T_w \end{cases} \tag{23}$$

$$\gamma_N = \begin{cases} 5.0 \times 10^{-4} & T_w \le 465 \\ 2.0 \times 10^{-5}e^{1500/T_w} & 465 < T_w \le 905 \\ 10.0e^{-10360/T_w} & 905 < T_w \le 1575 \\ 6.2 \times 10^{-6}e^{12100/T_w} & 1575 < T_w \end{cases} \tag{24}$$

'super-catalytic'

This option sets the species mass fractions to free stream values as defined in `tdata`—see Section 5.5 on page 30.

'Zoby-RCG'

This option uses the following surface catalytic coefficients [4] for catalyzing atomic oxygen and nitrogen to molecular oxygen and nitrogen, respectively.

$$\gamma_O = 9.41 \times 10^{-3}e^{-658.9/T_w} \quad 900 \le T_w \le 1500 \tag{25}$$

$$\gamma_N = 7.14 \times 10^{-2} e^{-2219.0/T_w} \quad 1090 \leq T_w \leq 1670 \tag{26}$$

The same equations will be used even if the wall temperature, T_w, is out of the specified range, in which case a warning will be issued to the screen.

emiss_a_0, emiss_b_0, emiss_c_0, emiss_d_0

Real number values to calculate emissivity, ϵ, for solid surface boundary type (see Section 5.3 on page 11) from the following equation:

$$\epsilon = \epsilon_a + \epsilon_b T_w + \epsilon_c T_w^2 + \epsilon_d T_w^3 \tag{27}$$

where T_w is the surface temperature. Values for ϵ_a, ϵ_b, ϵ_c, and ϵ_d are defined by emiss_a_0, emiss_b_0, emiss_c_0, and emiss_d_0, respectively. Default: emiss_a_0=0.89, emiss_b_0=0.0, emiss_c_0=0.0, emiss_d_0=0.0

ept

Under-relaxation parameter for radiative equilibrium wall temperature:

$$q_{i,j}^{n+1} = (1 - \mathtt{ept} q_{i,j}^n) + \mathtt{ept} q_{i,j}^{n+1} \tag{28}$$

where n denotes iteration level, $q_{i,j}^{n+1}$ is the most recent value of convective heat flux, $q_{i,j}$, $q_{i,j}^n$ is the value of convective heat flux from the previous iteration as adjusted by previous application of this formula, and $q_{i,j}^{n+1}$ is the newly adjusted value for convective heat flux at the $n+1$ iteration level. Default: 0.01

surface_temperature_type_0

Character identifier for surface temperature model selection. Default: 'constant'

Options are:

'adiabatic'

Surface temperature will be such that there is no heat transfer between the surface and the gas adjacent to the surface.

'constant'

The surface temperature stays constant as given by twall_bc value.

'radiative equilibrium'

The surface temperature is calculated so that the heat flux to the wall, q_w, is in equilibrium with radiation heat flux:

$$q_w = \epsilon \sigma T_w^4 \tag{29}$$

where σ is the Stefan-Boltzmann constant, and ϵ is the surface emissivity defined by emiss_a_0, emiss_b_0, emiss_c_0, emiss_d_0 values.

'surface energy balance'

> This option is required for ablating surfaces to compute surface temperature as a function of the surface energy balance and the relevant surface chemistry kinetics.

surface_group_name_0

Character descriptor for surfaces with solid surface boundary types (see Section 5.3 on page 11). Any character can be specified to group solid surface boundaries. Default: 'default surface 0'

twall_bc

Initial wall temperature for solid surface boundaries, K. (See Section 5.3 on page 11.) The wall temperature stays constant as specified by this parameter if surface_temperature_type_0 = 'constant'. Default: 500.0

5.4.11 Thermochemical Nonequilibrium Flags

chem_flag

An integer flag to engage chemical source term for non-equilibrium flow (on=1/off=0). Default: 0

therm_flag

An integer flag to engage thermal source term for non-equilibrium flow (on=1/off=0). Default: 0

5.4.12 Time Accurate Flags

itime

An integer flag to engage (itime = 1) or disable (itime = 0) time accurate simulation. Default: 0

subiters

An integer number to specify number of iterations between each time step for time-accurate simulations. Default: 10

5.4.13 Turbulent Transport Models

prandtl_turb

Turbulent Prandtl number. Default: 0.9

schmidt_turb

Turbulent Schmidt number. Default: 0.9

<u>turb_int_inf</u>

Farfield turbulent intensity non-dimensionalized by square of the reference velocity. Default: `0.001`

<u>turb_model_type</u>

An integer flag to select turbulence modeling. Default: `0`

Options are:

`-1`: Baldwin-Lomax algebraic turbulence model. [5]

`-2`: Cebeci-Smith algebraic turbulence model. [5]

`0`: Laminar flow, i.e., no turbulence model.

<u>turb_vis_ratio_inf</u>

Farfield ratio of turbulent to laminar viscosity. Default: `0.01`

<u>xtr</u>

Transition location along x-axis in grid units. Default: `0.0`

5.4.14 Venting Boundary Condition Flags

<u>vacuum_pressure_coefficient</u>

This parameter, which is in N/m^2 sets the pressure coefficient behind type 6 boundaries (see Section 5.3 on page 11), which forces flow out of the domain. This coefficient is defined as

$$\texttt{vacuum\_pressure\_coefficient} = \frac{p_0 - p_\infty}{2}. \tag{30}$$

where p_0 is back pressure where the gas is venting out, and p_∞ is farfield pressure. Default: `0.0`

<u>vacuum_pressure_factor</u>

Factor on pressure across type 6 boundary to force flow out of domain.

$$\texttt{vacuum\_pressure\_factor} = \frac{p_0}{p_1}, \tag{31}$$

where p_1 is the pressure just before the gas vents out. Default: `0.01`

5.5 `tdata`

The gas model is defined in this file. It contains a list of key words, sometimes followed by numeric values, which identify components of the gas model. One or more spaces must be present between keyword and values when appearing on the same line. Spaces may appear to the left or right of any key word. The first line of the file must not be blank, however.

The following subsections describe available gas model options.

5.5.1 Perfect Gas

The perfect-gas option is engaged with either of the following keywords: `perfect_gas`, `PERFECT_GAS`, `Perfect_Gas`, or `Perfect_gas`.

If no further data is provided in this file, this single line `tdata` file will assume the following parameter values in SI units:

```
gamma   =   1.4
mol_wt  =  28.8
suther1 =   0.1458205E-05
suther2 = 110.333333
prand   =   0.72
```

Here, `gamma` is the gas specific heat ratio, `mol_wt` is the gas molecular weight, `prand` is the gas Prandtl number, and `suther1` and `suther2` are the first and second Sutherland's viscosity coefficients, s_1 and s_2, respectively, defined as

$$\mu = s_1 \frac{T^{3/2}}{T + s_2} \tag{32}$$

These values can be modified and explicitly defined in the `tdata` by the keyword `&species_properties` in the second line followed by the gas parameters and `/` at the last line of the file. For example,

```
perfect_gas
&species_properties
gamma = 1.4
mol_wt = 28.0
suther1 = 0.1E-05
suther2 = 110.3
prand   = 0.7
/
```

5.5.2 Equilibrium Gas

To engage the Tannehill curve fits for thermodynamic and transport properties of equilibrium air [6], the following keyword should be used in the first line of the `tdata` file: `equilibrium_air_t`. No additional inputs or files are required to engage the Tannehill option for equilibrium air.

To use a table look-up capability for equilibrium gases [7], the following keyword should be placed in the `tdata` file, instead: `equilibrium_air_r`. Note that this option still uses the Tannehill transport properties.

5.5.3 Mixture of Thermally Perfect Gases

If the gas is a mixture of thermally perfect gases and multi-species transport solution is desired the species names followed by their mass fractions must be

provided in the `tdata` file. Thermal state of the gas may be defined as the first entry by either of the following flags:

one

> This flag assumes that all the species are thermally in equilibrium state. That is translational temperature, T, and vibrational temperature, T_v are equal. This is known as *one-temperature*, 1-T, model.

two

> This flag assumes that energy distribution in the translational and rotational modes of heavy particles (not electrons) are equilibrated at translational temperature, T, and all other energy modes (vibrational, electronic, electron translational) are equilibrated at vibrational temperature, T_v. This is known as *two-temperature*, 2-T, model.

FEM

> This option, called Free-Energy Minimization, causes the species continuity equations to be replaced with elemental continuity equations and equilibrium relations for remaining species.

One temperature model is assumed if thermal state of the gas is not provided in the first line of the `tdata` file. In this case, the first line must contain species information. Note, the first line must not be blank.

Subsequent file entries include species names and their mass fractions at freestream/farfield boundary. Only one specie per line is allowed. The species mass fraction at the boundary is defined in the same line as the species name separated by one or more spaces. If no value appears to the right of the species name then that species is assumed not to be present at the boundary but may be produced through chemical reactions elsewhere in the flowfield.

Example 1: 1-T, 5-species air model: In this example, only molecular oxygen and nitrogen are present on freestream/farfield boundary, but atomic nitrogen and oxygen and nitric oxide may be produced elsewhere in the flow field due to chemical reactions.

```
one
N2   .767
N
O2   .233
O
NO
```

Example 2: 2-T, 11-species air model: In this example, the gas is assumed to be a mixture of 11 thermally perfect gases. A solution to a thermal non-equilibrium state of the gas is also desired (2-T model).

```
two
N2   .767
N
O2   .233
O
NO
O2+
O+
NO+
e-
```

5.6 `hara.in`

This file is required for coupled radiation simulations and controls the radiation models used by the HARA radiation module [8, 9]. No lines may be added or deleted from this file, only the numbers for each option may be altered.

The first section of the file specifies whether a particular radiation mechanism is treated. For atomic species, these consist of lines, photoionization edges, and the negative ion continuum. For molecular species, this consists of molecular band systems. If the user is unaware of the dominant mechanisms, then all those associated with species present in the flowfield should be treated.

The part of this file starting with

```
1 .... specify the N atomic line model
```

allows the user to choose the atomic line model for each atom. A value of 1 applies the recommended model, which consists of the individual treatment of strong individual atomic lines and groups of weak multiplets. A value of 2 applies a more approximate model consisting of grouped multiplet lines.

The part of this file starting with

```
2 .... specify the model for the N electronic states
```

allows the user to choose the electronic state model applied for each atom. A value of 1 applies the Boltzmann assumption, while a value of 2 applies a collisional-radiative non-Boltzmann model, which is recommended for most applications. The same options apply to

```
2 .... specify the model for the molecular electronic states
```

for all molecular band systems.

The line

```
1 .... use triangles to for optically thin atomic lines?
```

specifies whether optically-thin atomic lines are modeled as triangles to reduce computational time. This option has shown to result in a negligible loss of accuracy while greatly reducing the computational time, and is therefore recommended.

The final line specifies whether a photoionization edge shift is applied. For most applications this this option may be set to `0`.

5.7 `kinetic_data`

This file defines possible chemical reactions and is optional. By default, `kinetic_data` is read from `[install-prefix]/share/physics_modules`, but if present in the local run directory, LAURA will read reactions from the local file instead.[13]

Reactants and products can be any species defined in the `species_thermo_data` file—see Section 5.12 on page 37. A sample entry looks like this,

```
O2 + M     <=>    2O + M                                    1
2.000e+21   -1.50   5.936e+04                               2
teff1 = 2                                                   3
exp1 = 0.7                                                  4
t_eff_min = 1000.                                           5
t_eff_max = 50000.                                          6
C = 5.0                                                     7
O = 5.0                                                     8
N = 5.0                                                     9
H = 5.0                                                    10
Si = 5.0                                                   11
e- = 0.                                                    12
```

The first line specifies the reaction while line 2 provides three coefficients of an Arrhenius-like equation,

$$K_f = c_f T_{eff}^\eta e^{-\epsilon_0/kT_{eff}} \tag{33}$$

where c_f is the pre-exponential factor, η is the power of temperature dependence on the pre-exponential factor, ϵ_0 is the Arrhenius activation energy, and k is the Boltzmann constant. The arrowheads in line 1 signify the allowed directionality of the reaction. The symbol $=>$ denotes forward reaction only while $<=>$ denotes forward and backward rates are computed. The coefficients in line 2 correspond to c_f, η, and ϵ_0/k, respectively. For reactions with a generic collision partner, `M`, such as this one, these coefficients correspond to Argon; and other collision partners and their efficiencies (multipliers of c_f)

---

[13]The precise installation location is given by LAURA during startup. It can also be found on Unix-like systems from the executable itself by issuing the command `strings laura | grep share`.

are specified on lines following line 5 and 6, which give the valid temperature range for the reaction. The effective temperature, T_{eff}, is defined according to a given integer number in line 3; Default: 2

teff1,teff2

Flag defining formula to compute the effective temperature T_{eff} for the forward rate and backward rate, respectively. It is engaged for the case of thermal nonequilibrium. Options for teff are:

1: $T_{eff} = T_{tr}$

2: $T_{eff} = T_{tr}^{exp1} T_v^{1-exp1}$

3: $T_{eff} = T_v$

where T_{tr} and T_v are translational and vibrational temperatures, respectively. Default: 1

exp1

The exponent used to define the effective temperature when teff1 = 2 (forward rate) or teff2 = 2 (backward rate). See previous equations for teff options. Default: 0.7

t_eff_min

The minimum temperature for T_{eff} to compute reaction rates to circumvent stiff source terms. Default: 1000.

t_eff_max

The maximum temperature for T_{eff} to compute reaction rates to circumvent stiff source terms. Default: 50000.

5.8 laura.rst

This Fortran-unformatted binary file has the flowfield solution for every grid cell, boundary surface values, and grid cell derivatives for each block face. The number of variables in this file varies depending on number of conservation equations that LAURA needs to solve as specified through the tdata and laura_namelist_data files. A file of this format, but named laura_new.rst,[14] is generated by LAURA at the end of a successful run. The laura.rst file is required only if restarting from a prior run, i.e., irest = 1 in laura_namelist_data as described in Section 5.4.8 on page 23.

---

[14]When running a trajectory sequence, the file will be named laura_####.g where #### is the trajectory point index.

5.9 `laura.trn`

Turbulent transition location and transition length are specified in `laura.trn`.[15] One line of data consisting of four integers followed by at least one space with the following entries per block is required: `block_number`, `turbulent_flag`, `transition_location`, and `transition_length_factor` where

`turbulent_flag`

One of `-1`, `0`, or `1`, which correspond to laminar, transition location in block, or fully turbulent flow, respectively.

`transition_location`

Specified as an x coordinate. This value used only if `turbulent_flag` is `0`.

`transition_length_factor`

Defined as (transition length)$/L$, where L is the distance from the nose to the transition location. Use `0` for instantaneous transition.

5.10 `laura_trajectory_data`

This file is used to sequentially simulate points along a trajectory. Each line of the file defines a single trajectory point. The trajectory point data is entered in free format with time, velocity, density, temperature, alpha, and yaw in MKS units (6 entries per line). The simulation will start at trajectory point 1 by default unless another line number is specified in the `laura_namelist_data` using the namelist variable trajectory_data_point.

The restart solution files and post processing files for each trajectory point are saved with a four digit number added to the usual root name of these files corresponding to the trajectory point number.

5.11 `laura_vis_data`

This file contains the data set that overrides the default viscous terms in the i-, j-, and k-directions. There are four integers consisting of block number and toggles for each viscous term per line in this file: `blk_num`, `ivis`, `jvis`, and `kvis` where `ivis`, `jvis`, and `kvis` are viscous terms in the i-, j-, and k-directions, respectively. The viscous-term flag options are:

0: Viscous terms are not engaged in the respective direction; i.e. inviscid flow.

---

[15]LAURA transition files from versions prior to 5 can also be used.

1: Viscous terms and a reduced eigenvalue limiter are engaged in the respective direction. The reduced eigenvalue limiter is to prevent distortion of computed heating.

2: Viscous terms are engaged but an unmodified eigenvalue limiter is retained to maintain stability.

The following defaults will be applied if this file is not present in the working directory:

If `ivisc = 0` in `laura_namelist_data` (see Section 5.4 on page 13) then inviscid flow is specified and `ivis`, `jvis`, and `kvis` are set to zero for all blocks by default.

If `ivisc = 2` and `navier_stokes = .false.` in the `laura_namelist_data` file then the default is a function of the wall boundary condition. If the wall boundary on the i_{min} or i_{max} face of block n is a solid surface (see Section 5.3 on page 11) then `ivis(n) = 2`, otherwise `ivis(n) = 0`. In like manner, if the wall boundary on the j_{min} or j_{max} face of block n is a solid surface then `jvis(n) = 2`, otherwise `jvis(n) = 0`. The default specification for `kvis(n)` is set to 1 if k_{min} or k_{max} of block n is a solid surface, otherwise `kvis(n) = 0`. This default recognizes that the standard orientation is for the solid wall on the k_{min} surface and the reduced eigenvalue limiter is required in this case.

If `ivisc = 2` and `navier_stokes = .true.` in `laura_namelist_data` then the default is `ivis = 2`, `jvis = 2`, and `kvis = 1` for all the blocks.

There may be circumstances where the user wishes to override these defaults. If a block is away from the stagnation streamline crossing the shock into the boundary layer then a more accurate heating on side walls (i and/or j) will be returned using `ivis` and/or `jvis` set to 1 without sacrificing stability. In the case of cavities, a block may sit over a cavity and not have any solid boundaries itself but has a well defined boundary layer streaming into it from an adjacent block. In this case, even though the block has no solid boundaries itself, it should engage viscous terms to capture the entering shear layer.

Example: To override the default values and to reset viscous terms in block number 3 to `ivis = 1`, `jvis = 0`, and `kvis = 1`, and in block number 5 to `ivis =0`, `jvis =1`, and `kvis =1` the `laura_vis_data` would look like:

```
3 1 0 1
5 0 1 1
```

5.12 `species_thermo_data`

The `species_thermo_data` file is the master file for species thermodynamic data.[16] Each species record consists of the species name, a species properties namelist - `&species_properties`, the number of thermodynamic property curve fit ranges, and the curve fit coefficients for each range [10]. No blank line is allowed in this file.

---

[16]The `species_thermo_data` file should only be changed by developers.

Elements of the `&species_properties` namelist are:

molecule

A logical flag to determine whether the species is molecule (composed of more than one atom); If the species is molecule then `molecule = .true.`, otherwise `molecule = .false.`

ion

A logical flag to identify the charged particle. `ion = .true.` for charged particles except for neutrals and electrons. This flag initializes electron-neutral energy exchange cross section and sum of the charges.

charge

An integer number to determine number of positive charges in particle. If `ion = .false.` then `charge = 0`.

elec_impct_ion

This real number to set the energy for neutrals (i.e. `ion=.false.`) in electron volts (eV) that is required to liberate an electron when the neutral impacts with free electron.

mol_wt

A real number to set the molecular weight of the particle. This parameter is always required.

siga

An array of three real numbers, which correspond to curve fit coefficients for electron-neutron energy exchange cross section defined as

$$\sigma_{en} = a + bT + cT^2 \tag{34}$$

where σ_{en} is the electron-neutron energy exchange collision cross section in m^2, a, b, and c are the curve fit coefficients, and T is the gas temperature [11,12]. The format to define these coefficients is `siga=a, b, c`. For example, `siga=7.5e-20, 0, 0`.

disoc_ener

A real number to set dissociation energy of molecule in electron volts (eV).

alantel

A real number to set Landau-Teller constant to compute vibrational relaxation time for molecule. These are defined in Ref. [13]. This variable is required if `molecule=.true.`.

cprt0

A non-dimensional real number that defines translational-rotational heat capacity that is normalized by gas constant. This is equal to

$$cprt() = \frac{f+2}{2} \tag{35}$$

where f is the number of degrees of freedom in translation and rotation. The defaults for atoms and diatomic molecules are 2.5 and 3.5, respectively.

Example: A portion of the `species_thermo_data` that provides thermodynamic properties of carbon is shown below.

```
C                                                                   1
&species_properties                                                 2
molecule = .false.                                                  3
ion = .false.                                                       4
charge = 0                                                          5
elec_impct_ion = 11.264                                             6
siga = 7.5e-20, 5.5e-24, -1.e-28                                    7
mol_wt = 12.01070                                                   8
/                                                                   9
3                                                                   10
  0.64950315E+03 -0.96490109E+00  0.25046755E+01 -0.12814480E-04    11
  0.19801337E-07 -0.16061440E-10  0.53144834E-14  0.00000000E+00    12
  0.85457631E+05  0.47479243E+01  200.000  1000.000                 13
 -0.12891365E+06  0.17195286E+03  0.26460444E+01 -0.33530690E-03    14
  0.17420927E-06 -0.29028178E-10  0.16421824E-14  0.00000000E+00    15
  0.84105978E+05  0.41300474E+01  1000.000  6000.000                16
  0.44325280E+09 -0.28860184E+06  0.77371083E+02 -0.97152819E-02    17
  0.66495953E-06 -0.22300788E-10  0.28993887E-15  0.00000000E+00    18
  0.23552734E+07 -0.64051232E+03  6000.000 20000.000                19
```

The species name is defined in line 1. Between lines 2 and 9 species properties are defined. These parameters and/or flags state that the carbon molecular weight is 12.0107, and the species is neither a molecule nor a charged particle, but it can liberate an electron when its energy reaches 11.264 eV after it is impacted with a free electron.

Line 10 shows that there are three thermodynamic property curve fits for temperature ranges of 200 K $< T <$ 1,000 K, 1,000 K $< T <$ 6,000 K, and 6,000 K $< T <$ 20,000 K. Each data range consists of 12 real numbers with a restriction of 4 real numbers per line. The first 10 real numbers are the thermodynamic curve fit coefficients, and the last two real numbers identify the temperature range for the given curve fit coefficients. These coefficients are used to calculate the following thermodynamic properties

$$c_p(T)/R = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \quad (36)$$

$$h(T)/RT = -a_1 T^{-2} + a_2 T^{-1} ln\ T + a_3 + a_4 \frac{T}{2} + a_5 \frac{T^2}{3} + a_6 \frac{T^3}{4} + a_7 \frac{T^4}{5} + \frac{a_9}{T} \quad (37)$$

$$s(T)/R = -a_1 \frac{T^{-2}}{2} - a_2 T^{-1} + a_3 ln\ T + a_4 T + a_5 \frac{T^2}{2} + a_6 \frac{T^3}{3} + a_7 \frac{T^4}{4} + a_{10} \quad (38)$$

where T is the gas temperature, R is the universal gas constant, c_p, h and s are the species specific heat, enthalpy and entropy, respectively, and a_i are the provided curve fit coefficients in `species_thermo_data`.

The following corrections will be applied if the gas temperature is out of the given range for the given curve fit coefficients:

$$c_p(T) = c_p(T^*) \tag{39}$$

$$h(T) = h(T^*) + (T - T^*)c_p(T^*) \tag{40}$$

$$s(T) = s(T^*) + ln \frac{T}{T^*} c_p(T^*) \tag{41}$$

where

$$T^* = \begin{cases} T_{lower} & \text{for } T < T_{lower} \\ T_{upper} & \text{for } T > T_{upper} \end{cases} \tag{42}$$

5.13 `species_transp_data`

This file[17] contains log-linear curve fit coefficients for species collision cross section that are defined based on temperature range of 2,000–4,000 K [14]. This temperature range spans boundary-layer temperatures for typical hypersonic entry. The curve fit for the given coefficients is poor, however, at temperatures below 1,000 K. A higher order curve fit data is available in `species_transp_data_0`, which supersedes that of `species_transp_data`—see Section 5.14.

```
  Ar Ar                                                        1
 -14.6017 -14.6502 -14.5501 -14.6028 ! trr132+kestin et al    2
  Ar+ Ar+                                                      3
 -11.48 -12.08 -11.50 -12.10                                   4
  Ar N2                                                        5
 -14.5995 -14.6475 -14.5480 -14.5981 ! kestin et al           6
  Ar CO                                                        7
 -14.5975 -14.6455 -14.5459 -14.5964 ! kestin et al           8
```

5.14 `species_transp_data_0`

This file[18] provides collision cross section coefficients for a higher order curve fit data [15, 16] than those are in the `species_transp_data` file—see Section 5.13. The data in `species_transp_data_0` supersedes the data in `species_transp_data` if the file is placed in the working directory hosting the simulation.

```
  O2 N     1 1 1      (c)
           -1.1453028E-03  1.2654140E-02 -2.2435218E-01  7.7201588E+01
           -1.0608832E-03  1.1782595E-02 -2.1246301E-01  8.4561598E+01
            1.4943783E-04 -2.0389247E-03  1.8536165E-02  1.0476552E+00

  NO N     1 1 1      (c)
           -1.5770918E-03  1.9578381E-02 -2.7873624E-01  9.9547944E+01
```

---

[17]The `species_transp_data` file should only be changed by developers.

[18]The `species_transp_data_0` file should only be changed by developers.

```
           -1.4719259E-03   1.8446968E-02  -2.6460411E-01   1.0911124E+02
            2.1014557E-04  -3.0420763E-03   2.5736958E-02   1.0359598E+00

  NO O      1 1 1      (c)
           -1.0885815E-03   1.1883688E-02  -2.1844909E-01   7.5512560E+01
           -1.0066279E-03   1.1029264E-02  -2.0671266E-01   8.2644384E+01
            1.4145458E-04  -1.9249271E-03   1.7785767E-02   1.0482162E+00

  END END   1 1 0
              0. 0. 0. 0.
              0. 0. 0. 0.
```

5.15 surface_property_data

This file is required if there are more than 1 solid surface boundary types (see Section 5.3 on page 11) and the surface conditions of these solid surfaces differ from those specified in `laura_namelist_data` (see Section 5.4 on page 13).

Surface boundary properties of each solid surfaces must be bounded by:

```
&surface_properties

/
```

The first instance of the parameters defines properties for surfaces of type `-1` (note that properties of type `0` are defined in `laura_namelist_data`), the second instance defines properties for surfaces of type `-2`, and so on (see Section 5.3 on page 11 for different solid surface types.)

The parameters that can be defined for each solid surface boundary are:

blowing_model

See Section 5.4.1 on page 13 for more details and a complete list of options. Default: 'none'

catalysis_model

See Section 5.4.10 on page 25 for more details and a complete list of options. Default: 'super-catalytic'

char_density

Density of the char, kg/m^3. Default: 256.29536

CHONSi_frac_char

See Section 5.4.1 on page 13 for more details and a complete list of options. Default: CHONSi_frac_char = 1.0, 0.0, 0.0, 0.0, 0.0

CHONSi_frac_pyrolysis

See Section 5.4.1 on page 13 for more details and a complete list of options. Default: CHONSi_frac_pyrolysis = 1.0, 0.0, 0.0, 0.0, 0.0

`emiss_a, emiss_b, emiss_c, emiss_d`

Real numbers to assume emissivity constant coefficients for solid surface boundary type (see Section 5.3 on page 11) surface emissivity, ϵ, which is calculated as

$$\epsilon = \epsilon_a + \epsilon_b T_w + \epsilon_c T_w^2 + \epsilon_d T_w^3 \tag{43}$$

where T_w is the surface temperature. Values for ϵ_a, ϵ_b, ϵ_c, and ϵ_d are defined by `emiss_a`, `emiss_b`, `emiss_c`, and `emiss_d`, respectively. Default: `emiss_a=` 0.89, `emiss_b=0`, `emiss_c=0`, and `emiss_d=0`

`h_ablation`

See Section 5.4.1 on page 13 for more details and a complete list of options. Default: 0.0

`mdot_pressure`

See Section 5.4.1 on page 13 for more details and a complete list of options. Default: 0.0

`surface_group_name`

Character descriptor for surfaces with solid surface boundary types—see Section 5.3 on page 11. Any character can be specified to group solid surface boundaries. Default: '`undefined surface`'

`surface_temperature`

Initial wall temperature in K for the solid surface boundary. This variable is similar to `twall_bc` in Section 5.4.10 on page 25. The wall temperature stays constant as specified by this parameter if `surface_temperature_type` = '`constant`'. Default: value of `twall_bc`.

`surface_temperature_type`

A character identifier for surface temperature model. See Section 5.4.10 on page 25 for options and their descriptions. Default: '`constant`'

`t_ablation`

See Section 5.4.1 on page 13 for more details and a complete list of options. Default: 0.0

`virgin_density`

Density of virgin material, kg/m^3. Default: 544.627742

6 Output Files

LAURA generates the files listed in Table 2 on the facing page regardless of inputs specified. A description of each output file is presented after a brief discussion of `stdout` output.

Table 2: Laura output files.

Filename	Content	Format
`laura.mcr`	Variables names in `laura.q`	Tecplot™
`laura.q`	Flowfield solution	Plot3D
`laura_blayer.dat`	Boundary layer edge data	Tecplot™
`laura_conv.out`	Time step, CPU time, and residuals	ASCII
`laura_new.g`	Volume grid	Plot3D
`laura_new.rst`	Flowfield solution for restart	Binary
`laura_surface.mcr`	Variables names in `laura_surface.q`	Tecplot™
`laura_surface.g`	Surface grid	Plot3D
`laura_surface.q`	Surface solution	Plot3D

In addition to files, Laura writes some information on the screen. After initial configuration information such as grid block sizes, `laura_namelist_data` specifications, and `tdata` gas physics, the screen output is divided to five distinctive categories: block number, task number, L_∞ including location and equation, and L_2 of mixture continuity, xyz-momenta, and energy equations.

The L_2 norm is defined as

$$L_2 = \sum_{i=1}^{N} \left(\frac{|R_i|}{\rho_i} \right)^2 \tag{44}$$

where N is the total number of grid cells times the number of conservation equations, R is the residual, and ρ is the mixture density.

The location of the maximum L_∞ residual is shown by four integer numbers after the norm itself. The first three integer numbers correspond to i-, j-, and k-indices of the corresponding block, and the last number is the equation number, `n_eqn`. The total number of equations, `n_eqn_max`, is defined as

$$\texttt{n\_eqn\_max} = \texttt{n\_species} + 3 + \texttt{n\_energy} \tag{45}$$

where `n_species` and `n_energy` are number of species and energy equations, respectively. The equation number corresponding to species is based on the species order defined in `tdata` followed by the x-, y-, and z-momentum equation numbers. For example, consider block 11 for the following sample screen output,

```
Reading block sizes from laura.g
  block =   10 task =  10  Linf: 0.63E+02  23  24  86  1  L2eq: 0.31E+00 0.11E-01 0.12E-01 0.12E-01 0.32E-01 0.27E-02
> block =   11 task =  11  Linf: 0.12E+04  21   2  86 14  L2eq: 0.42E+01 0.10E+01 0.17E+00 0.95E+00 0.88E+00 0.28E-01 <
  block =   12 task =  12  Linf: 0.31E+03  11   7  87  5  L2eq: 0.20E+01 0.38E+00 0.22E+00 0.28E+00 0.35E+00 0.11E-01
  block =    6 task =   6  Linf: 0.68E+02   6  24  87  1  L2eq: 0.39E+00 0.17E-01 0.80E-02 0.28E-01 0.37E-01 0.32E-02
  block =    2 task =   2  Linf: 0.66E+02   3  24  87  1  L2eq: 0.49E+00 0.27E-01 0.88E-02 0.53E-01 0.53E-01 0.38E-02
  block =    4 task =   4  Linf: 0.17E+03  24   1  87 14  L2eq: 0.89E+00 0.12E+00 0.47E-01 0.14E+00 0.12E+00 0.75E-02
  block =    9 task =   9  Linf: 0.65E+02  21  24  86  1  L2eq: 0.43E+00 0.26E-01 0.36E-01 0.47E-01 0.48E-01 0.32E-02
  block =   14 task =  14  Linf: 0.78E+02   2  24  86  1  L2eq: 0.66E+00 0.63E-01 0.27E-01 0.22E-01 0.67E-01 0.36E-02
  block =    7 task =   7  Linf: 0.71E+03  14   2  87 14  L2eq: 0.27E+01 0.51E+00 0.11E+00 0.69E+00 0.55E+00 0.22E-01
  block =    1 task =   1  Linf: 0.22E+03  24   4  87 14  L2eq: 0.11E+01 0.13E+00 0.29E-01 0.14E+00 0.13E+00 0.90E-02
  block =    8 task =   8  Linf: 0.26E+03   6   1  87 14  L2eq: 0.10E+01 0.14E+00 0.97E-01 0.19E+00 0.16E+00 0.82E-02
  block =    5 task =   5  Linf: 0.78E+02   1  24  87  1  L2eq: 0.47E+00 0.22E-01 0.23E-01 0.52E-01 0.50E-01 0.35E-02
  block =    3 task =   3  Linf: 0.45E+03  24  16  87 14  L2eq: 0.21E+01 0.35E+00 0.80E-01 0.41E+00 0.34E+00 0.18E-01
  block =   13 task =  13  Linf: 0.15E+03  17   2  87  5  L2eq: 0.98E+00 0.73E-01 0.63E-01 0.65E-01 0.88E-01 0.39E-02
  step =   10  time =    57.20 sum(abs(task error)) =  0.28E+02 L2 norm =   0.17E-02
```

which is for 14-block, 11-species, two-temperature case. The maximum change is shown to be from z-momentum equation `n_eqn=14` located on i=21, j=2, and k=86 of block 11.

See Section 7.5 on page 49 for a description of the `laura_stdout_to_tec` utility, which can convert this output into a Tecplot™-compatible format.

6.1 `laura.mcr`

Tecplot™ macro used to label variables contained in `laura.q` file.

6.2 `laura.q`

PLOT3D function file for post-processing volume solution. Most of the variables in this file are non-dimensionalized according to Table 3. The actual number of variables in this file depends on the condition specified in the input files.

Table 3: laura.q variables

Variables	Definition	Normalized by
$c_{N,N2,...}$	Species mass fraction	-
u, v, w	Velocity components	U_∞
E	Total energy per unit mass	U_∞^2
e_j	Energy mode j per unit mass	U_∞^2
T	Translational temperature	-
T_v	Vibrational temperature	-
ρ	Density	ρ_∞
M_w	Molecular weight	-
p	Pressure	$\rho_\infty U_\infty^2$
c	Sonic velocity	U_∞
e	Static energy per unit mass	U_∞^2
e_v	Vibrational energy per unit mass	U_∞^2

6.3 `laura_blayer.dat`

Boundary layer edge, and wall surface properties and shock stand off distance are written in this ASCII and Tecplot™ readable file. Below is an example showing the header of the file with their orders. Note that the species mass fraction will be written in the exact same order as provided by user in `tdata` file—see Section 5.5. Also, the vibrational temperature will only be written if two temperature is selected in `tdata`.

In addition to these properties, angle-of-attack, Mach and Reynolds-number-per-grid-unit will be provided in this file as auxiliary parameters.

```
TITLE ="BL EDGE PROPERTIES"
VARIABLES = "xw (m)"
"yw (m)"
"zw (m)"
"rhow (kg/m^3)"
"pw (Pa)"
"Tw (K)"
"Tvw (K)"
"Hw (J/kg)"
"muw (Pa.s)"
"c<sub>N2</sub>w"
"c<sub>O2</sub>w"
"c<sub>N</sub>w"
"c<sub>O</sub>w"
"c<sub>NO</sub>w"
"qw (W/m^2)"
"tauwx (Pa)"
"tauwy (Pa)"
"tauwz (Pa)"
"rhoe(kg/m^3)"
"pe (Pa)"
"Te (K)"
"Tve (K)"
"He (J/kg)"
"ue (m/s)"
"ve (m/s)"
"we (m/s)"
"Me"
"mue (Pa.s)"
"c<sub>N2</sub>e"
"c<sub>O2</sub>e"
"c<sub>N</sub>e"
"c<sub>O</sub>e"
"c<sub>NO</sub>e"
"delta (m)"
```

```
"deltastar (m)"
"theta (m)"
"Re-ue (1/m)"
"CH (kg/m^2.s)"
"Stand-off (m)"
DATASETAUXDATA Common.AngleOfAttack="-70.000"
DATASETAUXDATA Common.ReferenceMachNumber=" 7.130"
DATASETAUXDATA Common.ReynoldsNumber="  4037.    "
ZONE T="laura_blayer: Block  1"
..
..
```

6.4 `laura_conv.out`

Time steps and residuals history are written in this file. Some of the flow conditions, such as angle-of-attack, free stream conditions, Mach number, Reynolds-number-per-grid-unit, etc. are also repeated at the beginning of the file. As shown in the following sample, step number, clock time, sum of all the residuals in all active tasks, and the overall L_2 norm of the residuals are written in this file. The overall L_2 norm is defined as:[19]

$$L_2 = \frac{\sum_i (|rhs_i|/\rho_i)^2}{CFL^2} \tag{46}$$

where rhs is the residual and ρ is the density.

```
Step      0 time=      4.53
step  =  10  time =     10.87 sum(abs(task error)) =  0.27E-03 L2 norm =   0.92E-12
step  =  20  time =     17.13 sum(abs(task error)) =  0.26E-03 L2 norm =   0.88E-12
step  =  30  time =     23.40 sum(abs(task error)) =  0.25E-03 L2 norm =   0.84E-12
step  =  40  time =     29.65 sum(abs(task error)) =  0.25E-03 L2 norm =   0.81E-12
    .
    .
```

See Section 7.4 on page 49 for a description of the `laura_conv_to_tec` utility, which can convert this file into a Tecplot™-compatible format.

6.5 `laura_new.g`

The PLOT3D grid file includes any changes associated with grid adaptation or grid doubling during the run. The name must be changed to `laura.g` if user wants to restart with this new grid on the next run—see Section 5.2 on page 10 for more information on the file format.

6.6 `laura_new.rst`

The restart file contains volume and surface data required for restart from end of current run. The name must be changed to `laura.rst` if user wants to restart from this new solution file.

---

[19]The overall L_2 norm definition is different than the L_2 norm defined for each equation by Equation 44.

6.7 `laura_surface.mcr`

Tecplot™ macro used to label variables contained in `laura_surface.q`.

6.8 `laura_surface.g`

PLOT3D 3d whole multiblock surface grid file. See Section 5.2 on page 10 for more information on the file format.

6.9 `laura_surface.q`

PLOT3D function file for post-processing surface solution. The number of variables in this file depends on the conditions specified in the `laura_namelist_data`. Some of the surface variables are presented in Table 4.

Table 4: laura_surface.q variables.

Variables	Definition	Unit
T	Surface temperature	K
p	Surface pressure	N/m^2
τ_x, τ_y, τ_z	Wall shear stresses	N/m^2
q_{conv}	Convective heat flux	W/cm^2
q_{rad}	Radiative heat flux	W/cm^2
ϵ	Surface emissivity	-
$mdot$	Blowing or Suction rate	kg/m^2-s

7 Laura Utilities

LAURA has several interactive utilities that automatically generate some of the required input files or otherwise aid running and post-processing LAURA simulations. These utilities are explained here:

7.1 `bounds`

This interactive utility creates `laura_bound_data` that contains block connectivity data. This utility reads the volume grid data from a PLOT3D structured grid, `laura.g`. See Section 5.2 on page 10 for more detail on the file format. Here is a sample of an interactive session with `bounds`:

```
 Enter precision of laura.g : 1 = single, 2 = double
2
 Do you want all type 9 bounds to default to type 8?
 Enter 1 for yes or 0 for no: (0)
0
```

```
       .
       .
BLOCK  =    1 k =  1 BOUNDARY

Area  =    0.26821087E+03
(Xcntr,Ycntr,Zcntr) = (-0.63020306E+02, 0.91387367E+02,-0.63128987E+03)

Enter ITYPE: (0)
0
       .
       .
```

The first question is about the precision of `laura.g`. Note that any grid file created by LAURA or one of its utilities is created in double-precision.

The second question is about type 8 and type 9 boundary data. These boundary types are given for the block faces that are shared between two blocks. A type 9 requires an identical orientation of indices across the shared boundary (increasing i to increasing i, increasing j to increasing j, and increasing k to increasing k). A type 8 accommodates more general connectivity.

7.2   convert_bound_data

The utility converts old (pre LAURA.5) `STRTfiles/bound_data.strt` files to the new `laura_bound_data` format. Usage: `convert_bound_data bound_data.strt`.

7.3   convert_laura

This interactive utility converts cases run with prior versions of LAURA.5—see Appendix A on page 62. This utility generates `laura.g`, from `old.rst`, and a new restart, `laura_new.rst`.

The following file are either required or optional prior to the execution of this utility:

old.2eq

   This file, which may have a different root name, has two-equation turbulent model information. This file is optional.

old.ep+

   This file, which may have a different root name, has algebraic turbulent model information. This file is optional.

old.qtw

   This file, which may have a different root name, has surface temperature information. This file is optional. If this file is provided, free stream density and velocity are also needed. LAURA uses this information to approximately calculate the related parameters needed to be in `laura_new.rst`.

old.rst

This file, which may have a different root name, is the old restart file that contains volume and surface data. The utility will ask for the precision of the data and the numbers of grid-blocks that are in this file. This file is required.

laura_bound_data

Use the convert_bound_data utility, or see Appendix A on page 62 to convert this file from old format. This file is required.

7.4 laura_conv_to_tec

This utility translates the LAURA convergence history file, laura_conv.out, described in Section 6.4 on page 46 into a form usable by Tecplot™.
Usage: laura_conv_to_tec [options].

7.5 laura_stdout_to_tec

To allow task-specific convergence history plotting, this utility translates the LAURA standard output stream described in Section 6 on page 42 into a convergence history file for each task suitable for Tecplot™.
Usage: laura_stdout_to_tec [options] [file].

7.6 make_assign_tasks

Given the number and blocks and processes, the make_assign_tasks utility will generate a default assign_tasks (point relaxation with k-sweeps).
Usage: make_assign_tasks n_blocks n_processes.

7.7 self_start

This interactive utility generates a single-block structured grid, laura.g, for families of 2D, axisymmetric and 3D blunt bodies. This utility will also generate laura_bound_data. Schematics of several blunt body families are shown in Figure 3 on the next page. Note that for axisymmetric geometries, the symmetry boundaries must be on the y-axis. Parameters for defining a probe shape are shown in Figure 4 on page 51.

7.8 shuffle_laura

This interactive utility modifies (shuffles) variables in the LAURA restart, laura.rst, to enable continuation of simulation if the gas model variables or parameters including number of species, thermal nonequilibrium, radiation, ablation, and turbulence model are modified. The users will be prompted to provide necessary information.
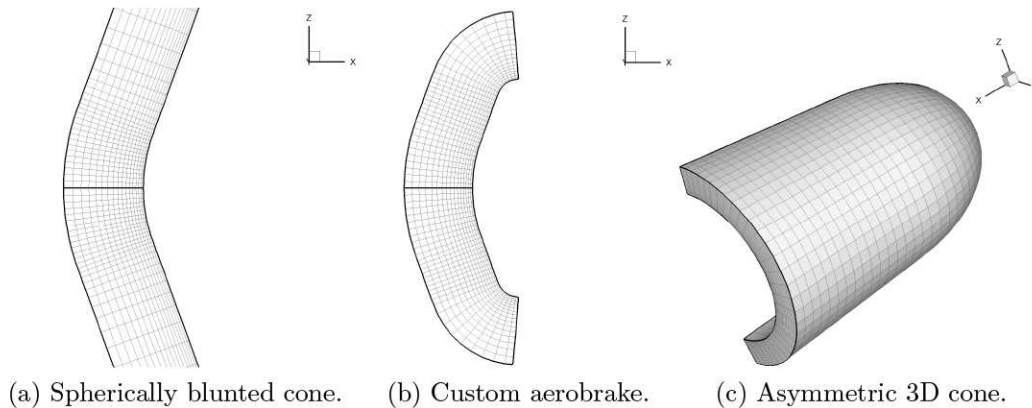
(a) Spherically blunted cone. (b) Custom aerobrake. (c) Asymmetric 3D cone.

Figure 3: Sample geometries generated by `self_start` utility.

8   Sample Cases

8.1   Sphere: 5-species Air, Thermo-chemical Nonequilibrium

A working directory is created in which all requisite files are assembled. The utility `self_start` is used to generate a grid and the initial template for some required input files within this working directory. A verbatim transcript of an interactive session using `self_start` follows.

```
% self_start
 Select dimensionality:
 1 = Axisymmetric
 2 = Two-dimensional
 3 = Three-dimensional
1
 Select geometry:
 1 = Conic (cone/wedge, paraboloid, etc.).
 2 = Aerobrake (includes AFE without axis singularity).
2
 Select aerobrake type:
 0 = AFE
 1 = hemisphere
 2 = customized aerobrake
1
Enter radius (m) {      1.000000}:
1.
 Select number of cells along symmetry plane.
30
 Enter number of cells in k direction, prior to any doubling
16
```
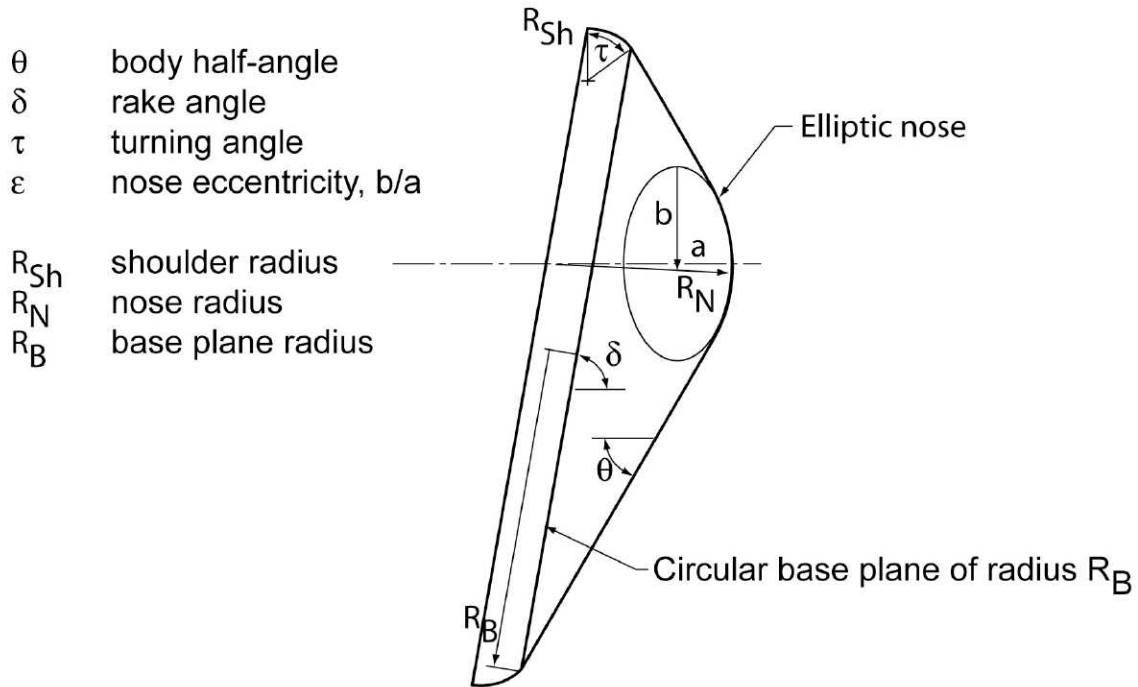
θ   body half-angle
δ   rake angle
τ   turning angle
ε   nose eccentricity, b/a

R_{Sh} shoulder radius
R_N nose radius
R_B base plane radius

Figure 4: Definition of probe shape parameters used by self_start.

At this point the grid file laura.g, the boundary data file laura_bound_data, the task assignment file assign_tasks, and the namelist file laura_namelist_data are created. The boundary data file does not require any further modification. The task assignment file is set for point-implicit relaxation - the standard practice for starting any simulation. The namelist file requires editing to define free stream conditions and possibly alter default settings. The edited file used for the first run of the test case follows.

```
&laura_namelist
velocity_ref = 5000. ! reference velocity, m/s
density_ref  = 0.001 ! reference density, kg/m^3
tref         = 200.0 ! reference temperature, K
alpha        = 0.000 ! pitch angle, degrees
twall_bc     = 500.0 ! initial wall temperature, K
chem_flag = 1  ! 0 chemically frozen, 1 chemical source on
therm_flag = 1  ! 0 thermally frozen,  1 thermal source on
irest    = 0    ! 0 for fresh start, 1 for restart
ncyc     = 2000 ! global steps
jupdate  = 4    ! steps between update of jacobian
ntran    = 4    ! steps between update of transport properties
nitfo    = 1500 ! number of 1st-order relaxation steps
iterwrt  = 200  ! steps between saves of intermediate solution
rf_inv   = 3.0  ! inviscid relaxation parameter
rf_vis   = 1.0  ! viscous relaxation parameter
```

```
movegrd  = 100   ! number of steps between calls to align_shock
maxmoves = 0     ! maximum number of calls to align_shock
re_cell  = 0.1   ! target cell Reynolds number at wall
fsh      = 0.6   ! target bow shock position arc length fraction
kmax_error = 0.005 ! error norm for doubling grid in k-dir.
kmax_final = 64 ! max number cells in k dir after all doubling
nexch    = 2     ! steps between exchange of info in mpi
frac_line_implicit = 0.7 ! fraction of line by block tri-dia
surface_temperature_type_0 = `radiative equilibrium'
catalysis_model_0 = `super-catalytic'
emiss_a_0 = 0.89
ept = 0.010      ! relaxation factor on read eq wall bc
axi_symmetric = .true.
two_dimensional = .false.
xmc =    0.0000
ymc =    0.0000
zmc =    0.0000
grid_conversion_factor =    1.0000
sref =  0.43633E-01
cref =   2.0000
/
```

The first 5 variables of the namelist in this particular template (other variable orderings are acceptable) deal with free stream conditions. The user must set these values, otherwise the user will get the default values assuming laminar flow of a perfect gas at 5 km/s and 0.001 kg/m^3. In this case both the chem_flag and therm_flag are reset to 1 to turn on the chemical and thermal source terms. Other template values are defined to provide a reasonable compromise between solution robustness and convergence rate for a fresh start solution (irest = 0). The template calls for 2,000 relaxation steps (ncyc) in the initial run with jacobian updates (jupdate) and transport property updates (ntran) requested every four relaxation steps. The first 1,500 iterations are executed using first-order spatial accuracy (nitfo)—second-order accuracy does not contribute significantly to the solution evolution in the initial relaxation period. The inviscid and viscous relaxation factors (rf_inv = 3 and rf_vis = 1) multiply the respective contributions to the Jacobian matrices and provide damping of the update. Larger values sometimes improve robustness for more energetic flows but are not required in this case.

Template values for grid movement are movegrd = 100, maxmoves = 0 (unlimited number of moves), re_cell = 0.1, and fsh = 0.6. These values are approximately tuned for optimal response in the opening relaxation process from a fresh start where the body materializes in a supersonic flow. Allowing the grid to move every 100 steps provides frequent opportunity to follow the evolution of the shock front as it initially is collapsed on the surface and then reflects off the surface into the oncoming flow. Setting re_cell to 0.1 provides very tight stretching near the wall. If there is a large difference between the wall temperature and the temperature of the first cell center off the wall then the upwind algorithm may fail to sense the wall

- the boundary condition using the Roe's averaged interface may admit a supersonic flow directed toward the wall at the interface. This condition subverts the ability of the inviscid, no-slip boundary to properly engage. The tighter near wall resolution enables the upwind scheme to sense the wall under all wall temperature conditions tested to date. Setting $\mathtt{fsh} = 0.6$ targets the captured bow shock location at 60% of the distance between the wall and the inflow boundary, providing adequate margin for the shock to reflect outward without striking the inflow boundary prior to the next grid update.

Automated grid doubling in the k direction is controlled by the triggering error norm magnitude ($\mathtt{kmax\_error} = 0.005$) and the maximum number of cells in the k direction ($\mathtt{kmax\_final} = 64$). Recall that the grid was initialized with only 16 cells in the k direction with the $\mathtt{self\_start}$ utility. The grid will double to 32 cells in the k direction (normal to the wall) when the L2 norm first drops below 0.005. It will double again when the error norm next falls below this trigger point. The selection of a trigger point for more complex problems (three-dimensional, highly energetic) may require user experimentation: trigger too high and the grid doubles too early causing a lot of extra work; trigger too low and the solution may ring (limit cycle) on a coarse grid and never engage a finer grid.

The template setting therefore updates the boundary condition after completion of a forward and backward sweep through the domain. Other template values are not discussed here. They are consistent with default values as described in Section 5.4 and are included for the users convenience.

Gas property data files must now be copied (or linked) from the $\mathtt{share/physics\_modules}$ installation directory into the working directory prior to executing laura. The files include $\mathtt{species\_thermo\_data}$ (thermodynamic curve fit data), $\mathtt{species\_transp\_data}$ and $\mathtt{species\_transp\_data\_0}$ (collision cross section data for computing transport properties), $\mathtt{kinetic\_data}$ (chemical kinetic source term data) and $\mathtt{tdata}$ (the gas model specific to the current simulation). The $\mathtt{tdata}$ file is generally the only file that requires editing by the user. For the case of 5 species air in thermochemical nonequilibrium the file $\mathtt{tdata}$ is defined as follows.

```
Two Temperature
N   6.217e-20
O   7.758e-09
N2  0.737795
O2  0.262205
NO  1.e-09
```

The fresh start run for this example case is now ready to be executed. It is assumed that the executable file laura is available in the working directory. This case is small enough to be run in interactive mode. For the purposes of discussion, it is convenient to capture the output in a file called $\mathtt{out\_01}$.

```
% laura >& out_01        (for csh)
% laura > out_01 2>&1    (for sh)
```

The user should note several types of information in $\mathtt{out\_01}$. The beginning of this file contains diagnostic information regarding presence of optional files, free

stream conditions, and kinetic model diagnostics including warnings regarding absence of some allowed third body collision partners. Lines beginning with "step =" keep track of the relaxation step number, elapsed wall time, sum of the L1 norms over all conservation equations, and the L2 norm. Lines beginning with "block =" keep track of the L1 norm for mixture continuity, x-momentum, y-momentum, z-momentum, total energy, and vibrational-electronic energy residuals. The statement `Calling align_shock...` appears after every 100 steps (`movegrd` = 100). The statement `Saving restart and plot files.` followed by intermediate values of aerodynamic coefficients appear after every 200 steps (`iterwrt` = 200). The grid doubles automatically after step 472 from 16 to 32 cells in the k direction when the error norm first drops below 0.005.

```
block =     1  task =    1 err:  0.17E+01  0.30E+00  0.61E-15  0.44E+00  0.38E+00  0.53E-01
step  = 472  time =     24.65 sum(abs(task error)) =  0.29E+01 L2 norm =    0.50E-02

Increased kmax to  32
block =     1  task =    1 err:  0.69E+05  0.54E+02  0.31E-14  0.51E+02  0.14E+04  0.40E+03
step  = 476  time =     25.09 sum(abs(task error)) =  0.70E+05 L2 norm =    0.97E+08
```

In general, there is a large jump in the error norm following a grid move or grid doubling which rapidly diminishes to pre-adjustment levels. A second doubling from 32 to 64 cells occurs after step 1348.

```
block =     1  task =    1 err:  0.15E+01  0.47E+00  0.13E-14  0.34E+00  0.45E+00  0.47E-01
step  = 1348  time =    113.30 sum(abs(task error)) =  0.28E+01 L2 norm =    0.49E-02

Increased kmax to  64
block =     1  task =    1 err:  0.47E+05  0.46E+02  0.39E-14  0.41E+02  0.82E+03  0.23E+03
step  = 1352  time =    114.19 sum(abs(task error)) =  0.49E+05 L2 norm =    0.46E+08
```

The interim solution for pressure contours after the first 2,000 steps is shown in Figure 5a on the next page. The corresponding surface pressure and heating distributions are shown in Figure 5b. The deep blue zone in front of the sphere represents undisturbed free stream conditions. The deep red indicated the high pressure stagnation region. The captured shock is approximately located at 60% of the distance between the spherical surface and the inflow boundary. The surface pressures and shock shape will be shown to be nearly converged at this point but the heating rates are still far from converged. Converging the boundary layer profile is the focus of the remaining relaxation steps.

Line relaxation is engaged at this point by editing `assign_tasks`, sweeping around the sphere in the i direction and applying line relaxation across the boundary layer in the k direction.

```
 1    1    3    1    0    1
```
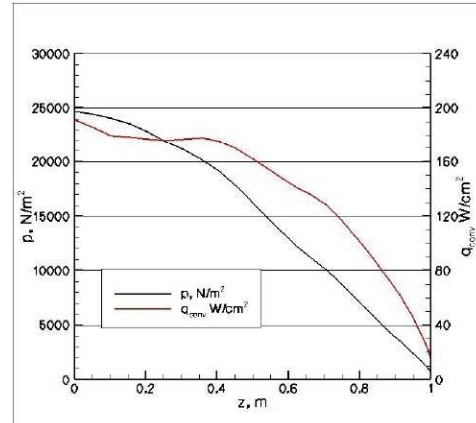
The adapted grid and restart files are renamed to start the second run.

```
% cp laura_new.g laura.g
% cp laura_new.rst laura.rst
```
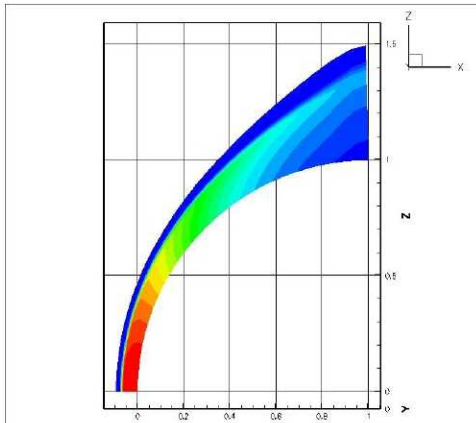
Changes or additions to the file `laura_namelist_data` are indicated below.
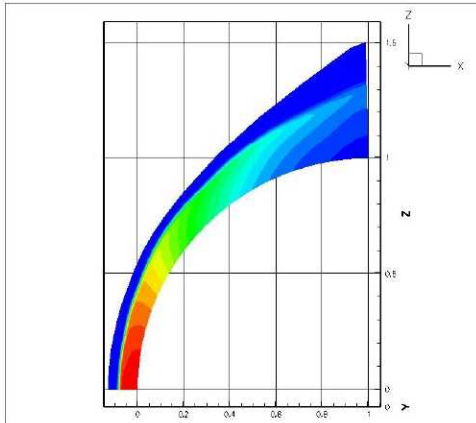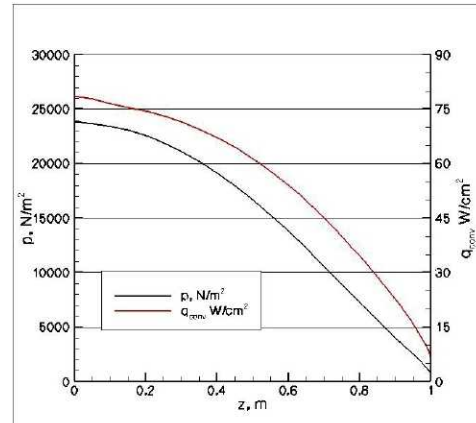
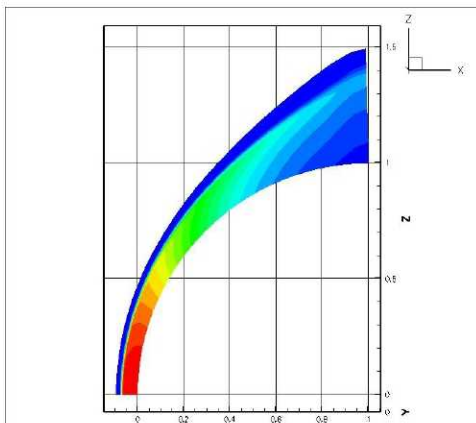(a) Pressure contours - interim solution after 2000 steps

(b) Surface pressure and heating - interim solution after 2000 steps

(c) Pressure contours - converged solution after 4000 steps.

(d) Surface pressure and heating - converged solution after 4000 steps.

(e) Pressure contours - 1.e-12 error norm solution after 5600 steps.
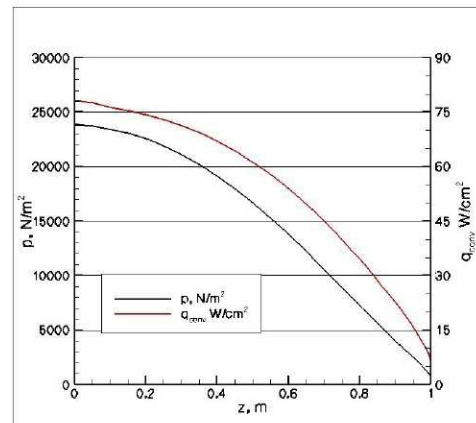
(f) Surface pressure and heating - 1.e-12 error norm solution after 5600 steps.

Figure 5: Solutions to the sphere test problem: $V_\infty = 5{,}000$ m/s, $\rho_\infty = 0.001$ kg/m^3, $T_\infty = 200$ K, 5-species air, thermochemical nonequilibrium, radiative equilibrium wall, $\epsilon = 0.89$, and super-catalytic wall boundary.

```
irest   = 1 ! 0 for fresh start, 1 for restart
jupdate = 20 ! steps between update of jacobian
ntran   = 20 ! steps between update of transport properties
nitfo = 0 ! number of 1st-order relaxation steps
rf_inv = 2.0 ! inviscid relaxation parameter
rf_vis = 2.0 ! viscous relaxation parameter
movegrd = 400 ! number of steps between calls to align_shock
maxmoves =  3 ! maximum number of calls to align_shock
frac_line_implicit = 0.7
```

At the conclusion of these next 2,000 steps (4,000) total the L2 norm has dropped to 0.74e-06 and the solution is converged. The solution for pressure contours after 4,000 steps is shown in Figure 5c. The corresponding surface pressure and heating distributions are shown in Figure 5d. Significant reduction in heating level and smoothing of the stagnation region profile has occurred using the line relaxation across the boundary layer during this second set of 2,000 relaxation steps.

Line relaxation across the entire shock layer (**frac_line_implicit** = 1.0) can be accommodated in this case if the relaxation factors (**rf_inv** and **rf_vis**) are increased to 5. The tolerance for convergence of the L2 norm (rmstol) is set to 1.e-12. Grid movement is switched off (movegrd = 0). The latest grid and restart files are renamed as before to start the third run. The third run reaches the convergence criteria in 1,600 additional relaxation steps, a drop of 6 orders of magnitude in the L2 norm. The solutions (Figure 5e and Figure 5f) are nearly identical to the corresponding figures at 4,000 steps.

```
block =    1  task =    1 err:  0.14E-04  0.50E-05  0.11E-14  0.36E-05  0.40E-05  0.53E-06
step  = 1580  time =   335.39 sum(abs(task error)) =  0.27E-04 L2 norm =   0.10E-11

block =    1  task =    1 err:  0.14E-04  0.48E-05  0.12E-14  0.35E-05  0.39E-05  0.51E-06
step  = 1600  time =   339.63 sum(abs(task error)) =  0.26E-04 L2 norm =   0.98E-12

Aerodynamic Coefficients
c_x = -0.8854
c_y = -0.0000
c_z =  0.6950
c_l = -0.0000
c_m =  0.3514
c_n =  0.0000
```

8.2 Coupled radiation procedure

Starting with the converged non-radiating LAURA solution, the **shuffle_laura** routine must be applied to the **laura.rst** file, and the option to convert from uncoupled to coupled radiation must be chosen—see Section 5.4.9 on page 24 for more info on radiation flags. The new .rst file created by **shuffle_laura** must then be renamed to **laura.rst**. The radiation input file, **hara.in**, which is also created by **shuffle_laura** must be revised according to Section 5.6 on page 33. Furthermore, the following lines must be added to the **laura_namelist_data** file:

```
radiation = .true.
nrad = 5000
```

```
frac_rad_new = 0.8
iinc_rad = 3
jinc_rad = 3
```

The first of these, `radiation`, must be set to true. The parameter `nrad` specifies the number of flowfield iterations between calls to HARA, `frac_rad_new` specifies the fraction of the most recent HARA calculation applied to the LAURA solution, and `iinc_rad` and `jinc_rad`, respectively, specify the increment in the treated points along the surface and in the spanwise direction. For `axisymmetric` cases, `jinc_rad` must be 1. For relatively weakly coupled radiation, such as Earth lunar-return conditions [17], `nrad` may be set to 1,500 for the first two calls to HARA, and 3,000–5,000 for the subsequent calls. For strongly coupled flows, such as Mars-return entry to Earth [18], `nrad` should be set to 500 for the first two calls to HARA, and 1,000 for the rest.

8.3   Unspecified ablation procedure - Coupled

The recommended procedure for an unspecified ablation computation, meaning the ablation rate and wall temperature is computed as part of the flowfield solution (instead of being specified by the user), is as follows:

1: Obtain a non-ablating solution assuming an equilibrium catalytic and radiative equilibrium wall. Include only species required for a non-ablating solution.

2: Apply the `shuffle_laura` utility to the converged non-ablating solution. Choose the ablation option and increase the number of species to the amount required to accommodate ablation species. Add the ablation species to `tdata`.

3: Modify `laura_namelist_data` to include the following—see Section 5.4.1 on page 13 for more info on ablation parameters:

```
surface_temperature_type_0 = 'surface energy balance'
blowing_model_0 = "equil_char_quasi_steady"
CHONSi_frac_pyrolysis_0 = 0.547, 0.093, 0.341, 0.019, 0.000
CHONSi_frac_char_0 =      0.488, 0.000, 0.273, 0.000, 0.239
ept = 0.01
nexch    = 2
freq_wall = 50
bprime_flag = 1
compute_mdot_initial = 1
ablation_option = 0
rmstol = 1.0e-12
hrs = 100.0
ablation_verbose = .true.
```

where `CHONSi_frac_pyrolysis_0` and `CHONSi_char_pyrolysis_0` should be changed to represent the material of interest. Setting `bprime_flag = 1` specifies that an approximate film coefficient diffusion model is applied in the

surface elemental mass balance. This model is robust enough to apply to a converged non-ablating flowfield. For this option, `freq_wall` specifies how often the cells at the wall are updated (instead of `nexch`). A value of 50 seems to work for both weakly and strongly ablating cases. In addition, `ept` represents the fraction of the new ablation solution, which includes the ablation rate, wall temperature, and wall species. The `rmstol` and `hrs` values are included to prevent premature termination of the computation.

4: Run LAURA for roughly 24,000 iterations. During each ablation computation, data is printed out for each point on the body, indicated by `l`. The level of convergence is indicated with `mdot residual` at the end of ablation computation:

$$\texttt{mdot residual} = \sum_l (\Delta \dot{m})^2 \tag{47}$$

Usually, `mdot residual = 1.E-2` or lower indicates that ablation computation is adequately converged within 1%.

5: If the user considers the b-prime approach of sufficient accuracy, then the computation is finished. If the user wishes to apply a rigorous diffusion model at the surface, consistent with that applied throughout the flowfield, then the following modifications should be made to `laura_namelist_data`:

```
freq_wall = 500
bprime_flag = 0
```

Setting `bprime_flag = 0` specifies the rigorous diffusion model at the surface [1]. This model is significantly less robust than the b-prime approach, which is why it requires the solution of the b-prime approach as an initial condition. With `bprime_flag = 0`, the energy equation is solved separately from the elemental mass balance and char equilibrium constraints. The number of flowfield iterations between solutions of the energy equation is governed by `freq_wall`, while the other equations are governed by `nexch`. In general, `freq_wall` should be much greater than `nexch`. The energy equation requires the convective heating, which must be allowed to converge to a meaningful value after the wall properties are perturbed. Note that with `bprime_flag = 0`, the ablation calls are significantly quicker than for `bprime_flag = 1`, and nothing is printed to the screen.

6: Run LAURA until the ablation rate, wall temperature, and convective heating reach steady values within one percent. After each solution of the energy equation, an increase in the residual will be seen. Unlike the b-prime approach, this value can be reduced within a reasonable number of iterations to `1e-7`, or lower.

8.4 Unspecified ablation procedure - Uncoupled

The uncoupled ablation analysis (defined in detail in Ref. [1]) differs from the coupled analysis in that the influence of ablation on convective heating is treated approxi-

mately using the blowing correction. In this uncoupled analysis, ablation is never introduced into the flowfield, and it consists of simply a post-processing step to the non-ablating flowfield. The recommended procedure for an uncoupled ablation analysis involves the same first two steps listed in Section 8.3 on page 57 for a coupled analysis. After those steps, modify `laura_namelist_data` to include the following:

```
surface_temperature_type_0 = 'surface energy balance'
blowing_model_0 = "equil_char_quasi_steady"
CHONSi_frac_pyrolysis_0 =   0.8822, 0.0283., 0.0866, 0.0029, 0.0
ept = 1.0
bprime_flag = 1
uncoupled_ablation_flag = 1
ncyc  = 0 ! global steps
```

where `CHONSi_frac_pyrolysis_0` and `CHONSi_char_pyrolysis_0`, should be changed to represent the ablator material of interest. Note that `ncyc = 0` is required. The final step is to run LAURA. This will first call the ablation model. Then it will print out an updated `laura_surface.q` file with the computed ablation rate, wall temperature, and altered convective heating (from the blowing correction) values. LAURA will then terminate without executing any flowfield iterations.

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Appendix A

Migrating Cases from Prior Versions

Follow the following steps to start LAURA simulations run with LAURA prior to version 5.

Step 1. Create a new working directory and change to it

```
% mkdir [Working Directory]
```

Step 2. Copy following required files from the old directory:

```
% cp /old/root.rst old.rst
% cp /old/root.tsk assign_tasks
% cp /old/STRTfiles/bound_data.strt laura_bound_data
```

and, depending on the case, these files:

```
% cp /old/root.qtw old.qtw
% cp /old/root.2eq old.2eq
```

Step 3. Use the LAURA convert_bound_data utility, or edit laura_bound_data so that there are only integer numbers in this file and there is 6 integers separated by at least one space per line per computational block. For example, the original file may look something like:

```
C:CDATADATADATADATADATADATADATADATADATADATADATADATADATADATADATA

C::::::  $Name:   $

      data ( itype(i,   1), i=1,6 )
     &          /      1, 1002111,       2,       1,       0,       3 /
      data ( itype(i,   2), i=1,6 )
     &          / 1001211,       1,       2,       1,       0,       3 /

C::CDATADATADATADATADATADATADATADATADATADATADATADATADATADATADATADATA
```

Edit the file to look like this:

```
      1   1002111        2       1       0       3
1001211         1        2       1       0       3
```

Step 4. Run the interactive convert_laura utility and answer all the questions. This utility creates laura.rst and laura.g files. You will have an option either to keep the prior-to-version-5 coordinate system orientation or to rotate the grid to the version 5 coordinate system orientation. As of version 5, LAURA uses $+x$-axis as the body normal direction while prior to

(a) Prior to Version 5. (b) Version 5.

Figure A6: LAURA coordinate system orientations.

version 5 LAURA used the $+z$-axis as the body-normal direction. The two orientations are show in Figure A6.

To run LAURA with LAURA grid orientation prior to version 5, use the following formula to get a new angle-of-attack, α:

$$\alpha_{new} = \alpha_{old} - 90 \qquad (A48)$$

Step 5. Copy the example `laura_namelist_data` file to your working directory from the `[installs_prefix]/share/laura` directory, where `install_prefix` is the installation prefix specified when LAURA was installed.

```
% cp [install_prefix]/share/laura/laura_namelist_data .
```

Use this file as a template to define the simulation parameters. Refer to Section 5.4 on page 13 for complete list of options. You must change `irest = 0` to `irest = 1`, otherwise the solution will be initialized to free stream conditions.

Step 6. Edit `assign_tasks` so that there are only integer numbers in this file. For example, the original file may look something like this:

```
CASE:
C:::::: $Name: $

  1  3  0  1   0    1
  2  3  0  1   0    2
blk swp rlx strt stop task
```

Edit the file to read like this:

```
1   3   0   1   0   1
2   3   0   1   0   2
```

Note: you can also use the LAURA utility `make_assign_tasks` to generate a new `assign_tasks`.

Step 7. If necessary, create the file `laura_vis_data` (see Section 5.11 on page 36 for more detail.)

Step 8. Modify `tdata` file (see Section 5.5 on page 30) to define the gas model condition for your specific simulation. The species order in this file must match the species order used in the prior version of LAURA. The other data files should not be changed.[A20]

Step 9. Run LAURA as usual—see Section 4 on page 6.

[A20]These files may be changed if different thermodynamic model, curve-fit data, or thermo-chemical reaction is needed—see Section 5.5 on page 30 for more detail.

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14. ABSTRACT
This users manual provides in-depth information concerning installation and execution of LAURA, version 5. LAURA is a structured, multi-block, computational aerothermodynamic simulation code. Version 5 represents a major refactoring of the original Fortran 77 LAURA code toward a modular structure afforded by Fortran 95. The refactoring improved usability and maintanability by eliminating the requirement for problem-dependent re-compilations, providing more intuitive distribution of functionality, and simplifying interfaces required for multiphysics coupling. As a result, LAURA now shares gas-physics modules, MPI modules, and other low-level modules with the FUN3D unstructured-grid code. In addition to internal refactoring, several new features and capabilities have been added, e.g., a GNU-standard installation process, parallel load balancing, automatic trajectory point sequencing, free-energy minimization, and coupled ablation and flowfield radiation.

15. SUBJECT TERMS
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