LeMANS User Guide

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Getting Started

LeMANS is a parallel CFD code developed for the simulation of high-enthalpy hypersonic atmospheric flows. Simulations should be run on the Flux parallel cluster at the University of Michigan Center for Advanced Computing (CAC). (Note that, with modifications to the *Makefile*, LeMANS may be run on any MPI capable parallel machine or single processor Linux computer. LeMANS can also be run as a DOS command line application in Windows, by compiling with Microsoft Visual C++.) As a first step before using LeMANS, you should apply for an account on Flux through the CAC website:
https://www.engin.umich.edu/form/cacaccountapplication
Accounts are available for all University of Michigan students, and for others with submission of an external access form.

Once you have an account, you will need an SSH client, such as PuTTY for Windows, to connect to Flux. You can access Flux by logging into `flux-login.engin.umich.edu` using your U-M Login ID and Kerberos Password. If you're logging in from off-campus, you'll either want to use the U-M VPN client (http://www.itcom.itd.umich.edu/vpn/) or SSH to a publicly available login node like `login.itd.umich.edu` or `login.engin.umich.edu`, and then from there login to flux-`login.engin.umich.edu`.

After logging in to your account, download the latest trunk version of LeMANS from the SVN repository to your local work directory. Next, at the Linux command prompt, type “cd sources” to enter the LeMANS source directory, then compile the LeMANS by typing “make”. If the code compiles properly, a new executable file *lemans* will be created. To compile a serial version of LeMANS, type “make serial”.

Obtaining a Copy of LeMANS

After logging in to your account, download the latest trunk version of LeMANS from the SVN repository to your local work directory by doing the following:

1) First, checkout a copy of the entire LeMANS package:

svn checkout svn+ssh://uniquename@login.itd.umich.edu/afs/umich.edu/group/acadaff/ngpd/svn-repos/svnlemans DirWhereFullWorkingCopyGoes

2) Next, make a copy of the trunk into the /branches directory, which will be your branch:

cd DirWhereFullWorkingCopyGoes
svn cp trunk branches/YourBranchName (this should be your initials or uniquename)

svn update
svn commit -m "Created $uniquename's branch"

3) Remove your local FullWorkingCopy (but you just committed it to the server so you can retrieve your branch in the next step):

cd ../
rm -r DirWhereFullWorkingCopyGoes

4) Now, checkout just your branch so no accidental updating of the trunk occurs:

svn checkout svn+ssh://uniquename@login.itd.umich.edu/afs/umich.edu/group/acadaff/ngpd/svn-repos/svnlemans/lemans/branches/YourBranchName DirWhereYourBranchWorkingCopyGoes

Now you have your branch checked out and can update it however you want. A quick reference sheet of subversion commands is found in /docs. There is exhaustive documentation on SVN at http://svnbook.red-bean.com/.

Mesh Generation

LeMANS uses Fluent format mesh files, which may be generated using the commercial codes Pointwise/Gridgen and Gambit. These programs are installed on all CAEN computers in North Campus computing labs. When creating a mesh in Pointwise, ANSYS FLUENT must be specified as the solver, and only the following boundary conditions should be used: wall, symmetry, pressure_farfield (for inflow boundaries), and pressure_outlet (for outflow boundaries). No more than one boundary of each type may be specified for each surface. If the grid is generated in Pointwise, make sure that the grid orientation aligns with the computational direction using the "Orient…" command under the "Edit" menu in Pointwise. A mesh file should be generated with the extension ".cas" for Pointwise/Gridgen and ".msh" for Gambit.

To install Pointwise on your personal computer located on the University of Michigan campus, go to the download page at www.pointwise.com, and follow the installation instructions. Once Pointwise is installed, specify the license server by setting the environment variable

PWID_LICENSE_FILE = 27026@license-pointwise.engin.umich.edu

It is typical for viscous meshes to stretch the cells near the wall to capture the sharp gradients in the boundary layer. A general rule of thumb is to set the height of the first cell near the wall such that the first cell Reynolds number is between 0.1 and 1.0. The first cell Reynolds number is defined as,

$$Re_w = \frac{\rho_w a_w \Delta y}{\mu_w}$$

where ρ_w is the density at the wall, a_w is the speed of sound at the wall, μ_w is the viscosity at the wall, and Δy is the height of the first cell away from the wall.

The Case Directory

As a next step in setting up a LeMANS simulation, you will need to create a new case directory. As an example, create a directory *lemans_testcase* by typing "mkdir lemans_testcase". Note that the command "mkdir" is listed with a number of other useful Linux commands in the document *nyxQuickSheet.pdf* included in the LeMANS release package.

Next, the following files should be copied to the newly created case directory:

- The executable file *lemans* from the directory sources/

  This file may be copied by typing "cp lemans_source_directory/lemans lemans" at the command prompt from the case directory. If the file *lemans* exists in the case directory but is not recognized as an executable (i.e. no "x" is found under file attributes when you type "ll" at the command prompt) then type "chmod +x lemans" to convert this file to an executable

- Input files required by LeMANS, as found in the inputs/ directory: *prob_setup.dat*, *chemistry.dat*, *diff.dat*, *electronic.dat*, *lerc.dat*, *mod_milikan.dat*, *vis.dat*, *rot_non_eq.dat*, *omega11.dat*, and *omega22.dat* (more information on each of these files is provided below)

- A Fluent format mesh file (.msh)

- Additional input files required by the Finite-Rate Surface Chemistry (FRSC) module: *frsc.inp* and *lewis.bulk*.

- A PBS batch submission script, such as *run_parallel* in the inputs/ directory

Information on PBS batch script files can be found at
http://cac.engin.umich.edu/resources/systems/nyx/pbs
The file *run_parallel* included in the inputs/ directory contains the following text, which should be altered as appropriate for the intended simulation:

```
#!/bin/sh
#PBS -S /bin/sh
#PBS -N CASE_NAME
#PBS -A iainboyd1_flux
#PBS -l qos=flux
#PBS -l nodes=2:ppn=8,walltime=2:00:00
#PBS -q flux
#PBS -m abe
#PBS -V
#
echo "I ran on:"
cat $PBS_NODEFILE
#
cd $PBS_O_WORKDIR
mpiexec ./lemans
```

Here `CASE_NAME` is the simulation name (any name may be used which does not begin with a number and does not include any spaces) and `nodes=2:ppn=8` specifies that two different nodes will be used with 8 processors per node, for a total of 16 processors. The designation

`walltime=2:00:00` means that the simulation will stop automatically after 2 hours. The option `-A iainboyd1_flux` means that you are requesting to use resources available to the iainboyd group (you must be authorized to use these resources), and `-q flux` means that the job will be submitted on the flux queue. Using the option `-m`, the user will receive an email when the simulation begins (`b`), ends (`e`), or aborts (`a`).

Input Files

For most LeMANS simulations, the only input files (excluding the mesh file) which should be altered from the files in the inputs/ directory are *prob_setup.dat*, *chemistry.dat*, and *frsc.inp* (when using the FRSC Module). All other input files can be copied from the inputs/ directory with no modifications. Note that, if possible, the input files *prob_setup.dat* and *chemistry.dat* should be modified using a Unix/Linux text editor such as vi. If these files are altered with a text editor in Windows, then the command dos2unix may have to be used to remove Windows end-of-line indicators which can interfere with file reading in LeMANS. (For example, type "dos2unix *dat" from the command line in the case directory.) Useful information for each required input file is provided below.

prob_setup.dat

This is the main "problem setup" file for a LeMANS simulation, and contains a number of different values for numerical parameters and boundary conditions. All dimensional values should be given in SI units (m/s, kg/m3, K, etc.) Each parameter in this file is described as follows:

`IS_AXIS`
This specifies whether an axisymmetric simulation will be run. It should be set to 1 for an axisymmetric simulation, or 0 for a two dimensional planar or three dimensional simulation.

`IS_VISCOUS`
This should be set to 0 for an inviscid flow simulation, or 1 for a viscous flow simulation.

`IS_ADIAB`
This should be set to 0 if an isothermal wall boundary condition is desired, or 1 for adiabatic walls. In most simulations `IS_ADIAB` should equal 0.

`WALL_CAT` (previously called `IS_SUPER_CAT`)
Set this to 0 for no species recombination at wall boundaries (non-catalytic wall), 1 for complete species recombination at any wall boundaries (super-catalytic wall), 2 for recombination of charged species at the wall (list their neutral counterparts in *chemistry.dat*), or 3 for the FRSC module. Note that this value is not used if `IS_CHEM_REAC` equals 0.

`IS_RAD_WALL`
Set to 1 for a radiative wall boundary condition for non-catalytic wall, 2 for radiative wall boundary condition with the FRSC module, or 3 for the steady-state energy balance. Note that options 2 and 3 are only used if `WALL_CAT` equals 3. The radiative wall boundary condition models a wall as a non-conducting blackbody surface, where the local wall temperature is automatically set so that convective heat transfer from the gas is balanced by radiative heat transfer from the surface. For options 1 and 2, the surface temperature is calculated by solving:

$$q_{conv} + q_{diff} = \sigma \epsilon T_w^4$$

where ϵ is the surface emissivity (user specified). For option 3, the surface temperature is calculated by solving the steady-state energy balance:

$$q_{conv} + q_{diff} = \sigma \epsilon T_w^4 + (h_w - h_a)\frac{\dot{m}}{C_y}$$

where h_w is the gas-phase enthalpy at the wall, h_a is the enthalpy of the virgin material (user specified), $\dot{m}$ is the mass blowing rate due to ablation, and C_y is the char yield which is defined as the ratio of the char density to the density of the virgin ablator (user specified).

`IS_CHEM_REAC`
This should be set to 1 to simulate a gas flow with chemical reactions. Otherwise set this to 0.

`IS_VIB_NON_EQ`
Set to 1 to allow for vibrational nonequilibrium. If set to 0, then vibrational excitation is neglected.

`IS_ROT_NON_EQ`
Set to 1 to allow for rotational nonequilibrium. If set to 0, then the rotational mode is assumed to be fully excited.

`NS`
This gives the number of species, and must be an integer greater than 1. The number used here must equal the number of species specified in the input file *chemistry.dat* (discussed below).

`RHO_INF_0` through `RHO_INF_10`
This gives the inflow mass density (in kg/m3) for each species. If, for example, 5 species are used in the simulation, then `RHO_INF_0` through `RHO_INF_4` may have nonzero values, while `RHO_INF_5` through `RHO_INF_10` must equal 0.

`V_INF_0`, `V_INF_1`, `V_INF_2`
These give the inflow bulk velocity in m/s in the x-direction, y-direction and z-direction, respectively.

`TT_INF`
This gives the inflow translational temperature (if `IS_ROT_NON_EQ = 1`) or translational-rotational temperature (if `IS_ROT_NON_EQ = 0`) in Kelvin.

`TR_INF`
This gives the inflow rotational temperature (if `IS_ROT_NON_EQ = 1`) in Kelvin.

`TV_INF`
This gives the inflow vibrational temperature (if `IS_VIB_NON_EQ = 1`) in Kelvin.

`TT_WALL`
This gives the isothermal wall translational temperature (if `IS_ROT_NON_EQ = 1`) or translational-rotational temperature (if `IS_ROT_NON_EQ = 0`) in Kelvin.

TR_WALL
This gives the isothermal wall rotational temperature (if IS_ROT_NON_EQ = 1) in Kelvin.

TV_WALL
This gives the isothermal wall vibrational temperature (if IS_VIB_NON_EQ = 1) in Kelvin.

MOD_MILLIKAN
This is only used if IS_VIB_NON_EQ is set to 1. If MOD_MILLIKAN equals 1, than a modified version of the Millikan and White correlation for vibrational relaxation is used. If this equals 0, than the standard Millikan and White correlation is employed.

IS_GUPTA
This should usually be set to 0 if the inflow velocity is less than 10,000 m/s; otherwise a value of 1 should be used. The Gupta mixing rule for viscosity and thermal conductivity in a mixture is used when IS_GUPTA equals 1, and the Wilke mixing rule is used when IS_GUPTA equals 0.

IS_CLN
This specifies whether a constant Lewis number, given as equal to the below value Le, will be used. If IS_CLN equals 0 then a separate Lewis number is calculated for each species from kinetic theory expressions. This is only used if IS_GUPTA is set to 1.

Le
This is the Lewis number, defined as the ratio of thermal diffusivity to mass diffusivity. A value around 1.4 should usually be used. Note that this value is not used in a simulation if IS_GUPTA equals 1 and IS_CLN is set to 0.

IS_SECOND_ORDER
A second order simulation will be run if a value of 1 is used here, and a first order simulation will be run if a value of 0 is used. A value of 1 is recommended, although the first order solver may work better if convergence is excessively slow using the second order solver. Note that (as described below) in an implicit simulation INV_RELAX must equal 1.5 if IS_SECOND_ORDER is 1; otherwise INV_RELAX must equal 1 for a first order implicit simulation.

IS_MSW
This should usually be set to 1, and is used to activate a modified form of Steger-Warming flux vector splitting for reduced diffusion in boundary layers. If IS_MSW equals 0 then the standard Steger-Warming scheme is employed.

DISS_BL_DIST
Default boundary layer distance (parameter d_0 in Eq. 3.11 in Scalabrin's Thesis). This value should be larger than the boundary layer thickness but smaller than the shock stand-off distance.

IMPLICIT
A value of either 0, 1 or 2 may be used here. An explicit simulation is run if IMPLICIT equals 0, a point-implicit simulation is run if IMPLICIT equals 1, and a line-implicit simulation is run if IMPLICIT equals 2. Line-implicit simulations will have the most rapid convergence, but the line-implicit solver may have stability problems for certain flowfield geometries.

MAX_TIME_STEP
This gives the maximum time step size (in s) in an implicit simulation, and is used only if IMPLICIT is *not* set to 0. The following values are recommended: 10^{-7} for a wind-tunnel model where the characteristic length scale is on the order of 1 cm; 10^{-6} for a flight model with a characteristic length scale on the order of 10 cm; and 10^{-5} for simulating the flow around a full scale Apollo-like object with a length scale on the order of 1 m. This value limits how aggressive the implicit scheme is; the more aggressive, the faster the simulation finishes, but the more likely that the solution becomes unstable and the code crashes.

MAX_CFL_NUMBER
This gives the maximum CFL number in an implicit simulation, and should general be between 10 and 10,000. LeMANS begins a simulation with a CFL of 0.01 and ramps up the CFL number based on the number of iterations until it reaches MAX_CFL_NUMBER. Note that the maximum time step is limited by this value as well as MAX_TIME_STEP.

CONV_CRITERION
This is the convergence criterion for residuals (usually 1.E-15).

MAX_N_ITER
This gives the maximum number of iterations before a simulation stops.

PRINT_ITER
This gives the frequency (in iterations) for printing output and restart files. A value between 100 and 1000 should be used in most simulations.

GRID_FACTOR
This gives a multiplicative factor to scale all coordinates in the mesh file. If coordinates entered in the grid generation program are in units of m, then a value of 1 should be used here. If coordinates are in mm, then a value of 1000.0 should be used.

MESH_FILENAME
The name of the computational grid.

Optional input parameters in prob_setup.dat

IS_OMEGA (DEFAULT 0)
Set to 1 to use updated collision cross-section data (obtained from DOI: 10.2514/1.16713) to compute the mixture transport properties.

PRESSURE_SWITCH_FACTOR (DEFAULT 6.0)
The value for the parameter used to switch from the modified to the original Steger-Warming scheme near shock waves.

IS_EL (DEFAULT 1)
Set this to 0 to neglect the electronic/electron energy and decouple it from the vibrational energy.

IS_PREF_ROT (DEFAULT 0)
Set to 1 in a reacting flow simulation for preferential dissociation at higher rotational energy levels. This should generally be set to 0.

IS_PREF_VIB (DEFAULT 0)
Set to 1 in a reacting flow simulation for preferential dissociation at higher vibrational energy levels. This should generally be set to 0.

EMISSIVITY (DEFAULT 1.0)
The surface emissivity used when IS_RAD_WALL is equal to 1, 2, or 3.

IS_LOMAX (DEFAULT 0)
Set to 1 to use the Baldwin-Lomax algebraic turbulence model.

IS_WALL_VALUE (DEFAULT 0)
Set this value to 1 to use the original Baldwin-Lomax turbulence model, which does not account for flows with pressure gradients. Note that this is only used is IS_LOMAX is equal to 1.

C_MUTM
This option sets the location of transition to turbulence. Note that this is only used is IS_LOMAX is equal to 1.

IS_SLIP (DEFAULT 0)
Velocity slip and temperature jump at the wall. Set this value to 1 to use a simple Maxwell-type slip boundary condition, 2 to use the Gökçen slip boundary condition, and 3 to use the Lockerby slip boundary condition.

ACCOM (DEFAULT 1.0)
Momentum and thermal accommodation coefficient. Note that this is only used if IS_SLIP is not set to 0.

SLIP_ITER
Iteration at which to start using the slip boundary conditions. Note that this is only used if IS_SLIP is not set to 0.

IS_VHS (DEFAULT 0)
Set this to 1 to use the variable hard sphere (VHS) viscosity model in place of the Blottner model. This allows for a different temperature dependence for the dynamic viscosity, and is recommended if LeMANS is used for comparison with DSMC simulation results. If the VHS model is employed, then the Blottner model constants A, B and C in *chemistry.dat* are replaced by the reference collision diameter, reference temperature, and temperature exponent in *rot_non_eq.dat*.

RHO_AMB_0 through RHO_AMB_10, V_AMB_0, V_AMB_1, V_AMB_2, TT_AMB, TR_AMB, TV_AMB
These parameters give ambient gas properties at simulation startup, and are analogous to the inflow properties discussed above. If these are not included, then by default ambient properties will equal the inflow properties.

RHO_AMB2_0 through RHO_AMB2_10, V_AMB2_0, V_AMB2_1, V_AMB2_2, TT_AMB2, TR_AMB2, TV_AMB2
These parameters give gas properties at simulation startup in an optional second ambient region, for which x-coordinates are greater than the value given by X_MIN_AMB2. This second region is useful to avoid instabilities or unphysical results in supersonic regions of a nozzle flow or wake regions of a hypersonic blunt body flow. In both cases, the density in ambient region 2 should be between one and two orders of magnitude lower than the density in ambient region 1.

X_MIN_AMB2 (DEFAULT 1.0E9)
This parameter is required when a second ambient region is used (see above), and gives the minimum x-value for ambient region 2. This value defines a plane normal to the x-axis which separates the two ambient regions.

MULTI_FILES (DEFAULT 1)
Set this to 0 to deactivate output file concatenation, so that separate output and wall data files are generated for each processor in a parallel simulation.

IS_GMV (DEFAULT 0)
Set this to 1 to allow output file creation in the General Mesh Viewer format. This may be useful if cell-based - rather than node-based - field data files are desired. (For information about General Mesh Viewer, see http://www-xdiv.lanl.gov/XCM/gmv/GMVHome.html).

LIMITER (DEFAULT 0)
Select the flux limiter used in a 2nd order simulation. The options are minmod (LIMITER=0), harmonic (LIMITER=1), and van Albada (LIMITER=2).

MINMOD_CUTOFF (DEFAULT 0.0)
The value used to detect a change in the slope when the minmod limiter is used.

GRAD_TYPE_CALC (DEFAULT 2)
This specifies the method used for calculating gradients, and should not usually be changed from the default value of 2.

IS_DEBUG (DEFAULT 0)
Set this to 1 to have LeMANS print out additional information during the main iteration loop. Note, however, that IS_DEBUG equal to 1 can result in relatively large stdout files if the simulation runs for many iterations.

IS_DP_RESTART (DEFAULT 0)
Set this to 1 to write the conserved variables in *restart.dat* in double precision. Note that a value of 1 results in larger *restart.dat* files.

IS_EL_ACTIV (DEFAULT 1)
Set this to 0 to deactivate the electronic/electron energy.

IS_PARTITION (DEFAULT 0)
Set this to 1 to have LeMANS read the partition files written by Pre-LeMANS. This option can significantly reduce the memory requirement, especially for large 3D simulations.

STAG_Y (DEFAULT 0.0)
The height (length) of the first face along the surface away from the axis of symmetry (Y = 0.0). This is used to output convergence data near the stagnation point when WALL_CAT is equal to 3 (FRSC module). The data includes convergence history of surface properties written to convergence_surf.dat and species production rate data written to convergence_rates.dat.

H_VIRGIN
Enthalpy of the virgin (unaffected) material used in the steady-state energy balance when WALL_CAT is equal to 3.

C_YIELD
Char yield used in the steady-state energy balance when WALL_CAT is equal to 3.

chemistry.dat

Gas species parameters and information for chemical reaction modeling are specified in this input file. For atmospheric flow simulations without ionization effects, the five species model given in the *chemistry.5sp.dat* file in the inputs/ directory can be used by renaming it *chemistry.dat*. For atmospheric simulations involving ionization, the included file *chemistry.11sp.dat* should be copied to the case directory and renamed *chemistry.dat*. Note that a value of 11 should be given for the number of species in *prob_setup.dat* if the 11 species model with ionization is employed.

The file is divided into three different sections, each of which ends with a line containing the word "END". The first section, which begins with the word "MODEL", contains either "00" or "90" and designates the chemistry model containing curve fits for equilibrium constants. For example, a value of 90 gives the Park 1990 model. Here 90 should be used unless ionization effects are being modeled, in which case 00 should be used.

The second section, which specifies individual species properties, begins with the word "SPECIES". This is followed by up to 11 lines containing information for each species in the simulation. Each line contains 12 different values, as follows:

1. Species name (e.g. N2)
2. Molecular weight, in kg/kmol
3. Enthalpy of formation, in SI units
4. Constant A for calculating species viscosity using the Blottner model
5. Constant B for calculating species viscosity using the Blottner model
6. Constant C for calculating species viscosity using the Blottner model
7. Translational specific heat at constant volume, equal to 1.5*Ru/MW where Ru is the universal gas constant and MW is the species molecular weight
8. Rotational specific heat at constant volume, equal to Ru/MW for a diatomic species or 0 for a monatomic species
9. Characteristic temperature of vibration
10. Dissociation energy (in J/kg) for use with a preferential dissociation model
11. Charge (Set to 0 for neutral species, 1 for ions and -1 for electrons.)
12. Species name OR neutral counterparts for charged species that recombine at the wall if WALL_CAT is set to 2 (list anything but 'e' for electrons)

The third section, which begins with the word "REACTIONS" gives information for all individual chemical reactions which are considered in a simulation. Values in this section should not generally be altered. For each reaction, the chemical equation showing reactants and products is first specified. The next line contains eight different values related to the corresponding reaction rates:

1. A temperature coefficient C_f in the forward reaction rate

2. A temperature exponent N_f in the forward reaction rate
3. A value E_f used in the forward reaction rate
4. A translational/rotational temperature exponent A for the forward reaction temperature T_f
5. A vibrational temperature exponent B for the forward reaction temperature
6. A rotational temperature exponent C for the forward reaction temperature if `IS_ROT_NON_EQ` is equal to 1
7. A translational/rotational temperature exponent A' for the backward reaction temperature T_b
8. A vibrational temperature exponent B' for the backward reaction temperature
9. A rotational temperature exponent C' for the backward reaction temperature if `IS_ROT_NON_EQ` is equal to 1
10. The minimum temperature T_{min} used for calculating forward and backward reaction temperatures

The forward reaction rate k_f is calculated as $k_f(T_f) = C_f T_f^{Nf} \exp(-E_f/T_f)$ where $T_f = \max\{T_{tr}^A T_v^B, T_{min}\}$ if `IS_ROT_NON_EQ` is 0 and $T_f = \max\{T_t^A T_v^B T_r^C, T_{min}\}$ if `IS_ROT_NON_EQ` is 1. Here T_{tr} is the translational/rotational temperature, T_t is the translational temperature, T_r is the rotational temperature, and T_v is the vibrational temperature. Likewise, the backward reaction is calculated as $k_b = k_f(T_b)/K_c(T_b)$, where K_c is the equilibrium constant and $T_b = \max\{T_{tr}^{A'} T_v^{B'}, T_{min}\}$ if `IS_ROT_NON_EQ` is 0 and $T_b = \max\{T_t^{A'} T_v^{B'} T_r^{C'}, T_{min}\}$ if `IS_ROT_NON_EQ` is 1. Note that both A+B (A+B+C) and A'+B' (A'+B'+C') must equal to 1.

The following six lines for each reaction give a mixture number density followed by various temperature coefficients corresponding to this number density in Park's chemistry models.

diff.dat

This file includes coefficients used in collision integrals for diffusion calculations. (See NASA technical report TP2867 for details.) This file should not be altered.

electronic.dat

This gives electronic levels (characteristic temperatures for electronic excitation) and electron degeneracies for each species. This file should not be altered.

lerc.dat

This file contains coefficients used in curve fits based on data from NASA Lewis Research Center (now NASA Glenn). This file should not be altered. Note that lerc.dat is only read during a LeMANS simulation if the chemical reaction model in *chemistry.dat* is set to "00", as in the 11 species file *chemistry.11sp.dat*. See the above section on *chemistry.dat* for details.

mod_milikan.dat

This gives coefficients used in the modified Millikan correlation for vibrational relaxation. This file should not be altered.

vis.dat

This gives coefficients used in collision integrals to calculate transport properties, based on the Gupta mixing rule. This file should not be altered.

omega11.dat and omega22.dat

These files contain diffusion ($\Omega^{1,1}$) and viscosity ($\Omega^{2,2}$) collision integrals in $Å^2$ as functions of temperature in Kelvin (obtained from DOI: 10.2514/1.16713) to compute mixture transport properties and are only used if `IS_OMEGA` is set to 1. This file should not be altered.

rot_non_eq.dat

This file contains species constants used to compute the rotational energy source terms. Some these parameters are also used in the VHS model if `IS_VHS` is set to 1. Detailed information can be found in Timothy Holman's PhD thesis. Each line contains 6 different parameters:

1. Species name
2. The constant Z_{rs}^{∞} used to calculate the rotational collision number
3. The constant T^* used to calculate the rotational collision number
4. Reference temperature T_{ref} (also used in the VHS model)
5. Temperature exponent ω (also used in the VHS model)
6. Reference collision diameter d_{ref} (also used in the VHS model)

lewis.bulk (required for FRSC module)

This file contains thermodynamic property data for condensed species. The data has been compiled by Gordon and McBride (NASA/TP-2002-211556) and is presented in the form of nine coefficients used to calculate thermodynamic properties as functions of temperature.

frsc.inp (required for FRSC module)

This file contains information regarding the chemistry model used by the FRSC module. The file is divided into three different sections: the phase and active site section, the species section, and the surface reaction(s) section.

Running a LeMANS simulation

From within the case directory, type "qsub run_parallel" to submit your job to the queue. You can view your job, as well as other jobs recently submitted on flux, by typing "qstat –a". Type "qstat –u username" to view only jobs you have submitted. To view jobs currently using iainboyd resources, type "showq -w acct=iainboyd1_flux". To cancel a job before completion, type "qdel" followed by the job number. Your job number appears before ".nyx.engin" on the line corresponding to your job when you type "qstat –a" or "qstat –u username". More details on NYX commands can be found at http://cac.engin.umich.edu/resources/systems/nyx/pbs.

Once a simulation starts running, a number of different files will be created. These files include a convergence file *convergence.plt*, a restart file *restart.dat*, as well as wall data and field data output files *wall_data.dat* and *output.dat*. Field data output files are periodically updated according to the `PRINT_ITER` interval specified in *prob_setup.dat*, and are given in Tecplot format.

To view field data in Tecplot, copy the file *output.dat* from the case directory onto your desktop. Next, open Tecplot, choose “Load data files” under the “File” menu, “Tecplot Data Loader, and select *output.dat*. Wall data may be viewed in Tecplot through a similar procedure.

The simulation convergence history may be viewed in realtime by typing “tail –f convergence.plt” at the command prompt. Alternatively, you can instead type "qpeek –f" followed by the job number to view the command line output generated by LeMANS if `IS_DEBUG` is set to 1. Variables displayed are the iteration number, maximum residual, cell number that corresponds to the maximum residual, L2 residual, time step size and CFL number. Press Ctrl+Shift+C to return to the command prompt. The convergence history can be also plotted in Tecplot using the procedure described above.