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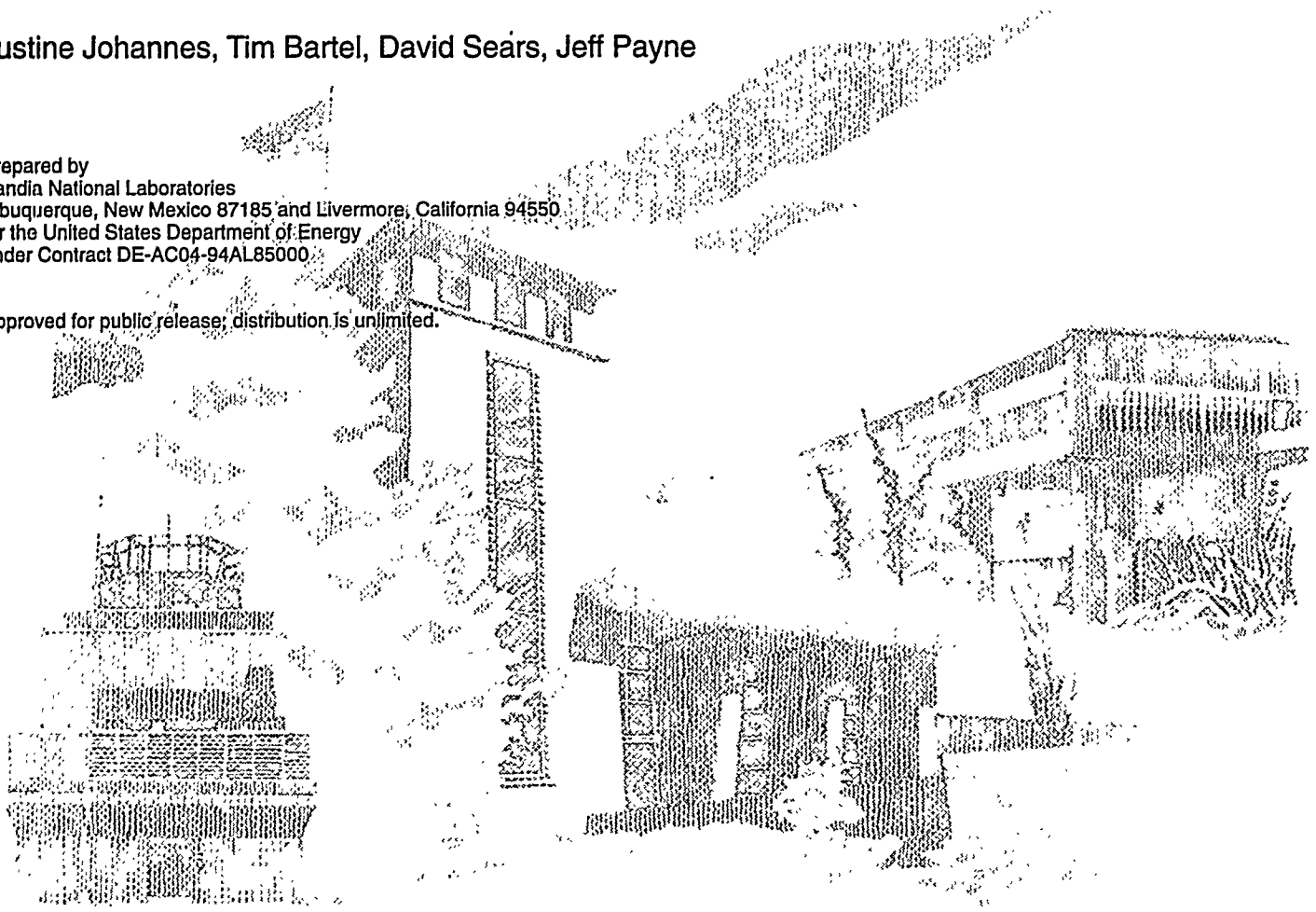
Gemini: A Hybrid Plasma Modelling Capability for Low Pressure Systems
User's Manual - V.1.7

Justine Johannes, Tim Bartel, David Sears, Jeff Payne

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550
for the United States Department of Energy
under Contract DE-AC04-94AL85000



SF2900Q(8-81)

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User's Manual - V.1.7

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ABSTRACT

Gemini is the coupling of Icarus, the Sandia National Laboratories (SNL) 2-D Direct Simulation Monte Carlo (DMSC) code, to MPRES, the University of Houston 2-D finite element plasma reactor code. Thus, Gemini is not a stand alone code. The primary application of Gemini is the simulation of inductively coupled plasma reactors that operate at low pressures (< 10mtorr) where continuum formulations of the transport equations begin to break down. Plasma parameters (electron density (ne), electron temperature (Te) and electrostatic fields (Er and Ez)) are computed in MPRES and interpolated onto the DSMC grid. This allows transport of the neutrals and ions to be performed using the DSMC method while including electron impact reactions and field transport effects. A sample calculation including appropriate input files is given.

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Overview

Gemini is an extension of Icarus, the Sandia National Laboratories (SNL) 2-D DSMC code, to include 2-D plasma effects, (i.e., electron density (n_e), electron temperature (T_e) and electrostatic fields (E_r and E_z)) cylinderical. The primary application of Gemini is the simulation of inductively coupled plasma reactors that operate at low pressures (< 10mtorr) where continuum formulations of the transport equations begin to break down. An alternative to continuum formulations for predicting transport is the direct simulation monte carlo (DSMC) method which has been validated for flows ranging from free molecular to several atmospheres. However, the disparate time scales of heavy particle (ions and neutral) transport and electron transport make it computationally intractable to solve the entire plasma reactor problem using DSMC. The way around this has been to solve electron properties and electrostatic fields using a continuum code (University of Houston MPRES code) and solve for heavy particle transport using DSMC (Icarus). MPRES solves for n_e, T_e, E_r and E_z which are mapped into Icarus to include electron impact reactions and field transport effects in the DSMC solution. **As such, Gemini is not a stand alone code but rather a coupling of MPRES and Icarus.**

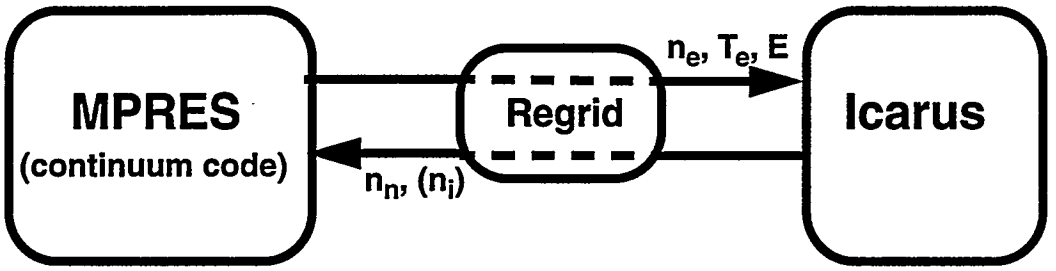
Gemini solutions contain the same simplifying assumptions used in MPRES to determine n_e, T_e, E_r and E_z. The reactor is divided two regions, bulk plasma and sheath. The bulk is solved assuming local charge neutrality and the sheath is described by a semi-analytical model developed by M. Riley (Sandia Report SAND95-0775). The positive and negative ion densities are solved using the corresponding mass balance equations and the electron density is calculated through the charge neutrality constraint. The electrons are assumed to be in Boltzmann equilibrium, implying that the electric field force almost balances the electron pressure force in the momentum balance equation.

The Icarus portion of a Gemini simulation requires little deviation from a standard neutral flow simulation. The electro-static fields are included to determine ion transport and the voltage drop across the sheath is used to determine angular and energy distributions of ions at the wafer. The spatially varying electron temperature and electron density are imposed on the DSMC grid to compute spatially varying electron impact reaction probabilities determined by $(n_e \bullet k(T_e) \bullet \Delta t)$.

Gemini results are contained in both MPRES and Icarus output files; n_e, T_e, E_r and E_z are contained in an MPRES output file (*FInput*) and heavy particle number densities, velocities and temperatures are found in a Icarus output file format (*cell.**).

Coupling Strategies

Coupling MPRES and Icarus requires variables (n_e,T_e, E_r and E_z) to be mapped from a Finite Element Grid (MPRES) to a DSMC grid (Icarus). The offset between the two grids are specified in the MPRES.inp file, the center of the wafer is assumed to be the origin. Mapping is performed by Regrid, see Figure 1. Regrid is contained in the Icarus code package, and is described in the Icarus documentation (Sandia Report SAND96-0591).



Two different strategies that can be used to couple MPRES and Icarus; weak coupling, and strong coupling. The coupling strategy determines how much information is cycled between MPRES and Icarus during a Gemini simulation. Coupling strategies are defined below:

Weak Coupling. Only neutral profiles are cycled from Icarus to MPRES to compute updated electron properties. This approach is the most robust and requires the least amount of computational time. The disadvantage is that electron properties and electrostatic fields (from MPRES) are not required to be consistent with the final Icarus ion densities. Ion profiles predicted in MPRES are different from those computed in Icarus due to different boundary conditions and transport formulations.

Strong Coupling. Both neutral and ion profiles are cycled from Icarus to MPRES to compute updated electron properties. This method results in a self consistent solution. Unfortunately, it requires considerably more computation time and is less robust. If intermediate ion profiles computed in Icarus have large discontinuities MPRES will not converge to a solution.

File Transfers

Strong and Weak Coupling:

A shell script is used to automate the code coupling and the file transfer for a Gemini calculation, see Appendix A. The recommended protocol is to run MPRES in a stand-alone fashion to generate a good starting solution for Icarus, the output files from MPRES (*FInput* and *Sheath*) are run through Regrid to generate *dsmc.restart, dsmc.plasma* and *dsmc.em.* The *dsmc.in* Icarus file requires an additional command line argument, read efield, to recognize that a plasma calculation is being performed and that *dsmc.plasma* and *dsmc.em* are required to start Icarus. Once Icarus is running, the shell script (mpres.csh) is started to automate the remaining file transfers. The coupling strategy is controlled by specifications made in two different files; *MPRES.inp2* and *dsmc.map. MPRES.inp2* controls the MPRES modules that run during coupling, for weak cou-

pling neutral transport is not performed in MPRES so module 3 is turned off. Both ion and neutral transport modules (1 and 3) are turned off for strong coupling. The *dsmc.map* file is used to specify which variables are mapped into the MPRES restart file, both ion and neutral profiles are mapped back for strong coupling.

The coupling frequency is determined by the control variable "gemini flag" defined in the Icarus *inputfile* (for an explanation of this file refer to Icarus documentation). An example of the *inputfile* used for a weakly coupled calculation is given in the example problem (page 31).

Files:

Below is a list of the files required from the various codes to perform a Gemini Calculation

MPRES	Icarus	Regrid	Shell Script
MPRES.inp1*	dsmc.in (*inputfile*)	glow.map	DSMC.OUT
MPRES.inp2	dsmc.in2 (for MP)	dsmc.map	MPRES.COUNT
MPRESgrid.inp	dsmc.node (if restart)	FInput	
mmat.inp	dsmc.restart (if restarting)	Sheath	
	dsmc.em (from Regrid)	dsmc.in2	
	dsmc.plasma (from Regrid)		

* Files *MPRES.inp1* and *MPRES.inp2* are the same format as the input file *MPRES.inp* described in the MPRES documentation. *MPRES.inp1* has all of the modules operating to generate the initial solution to use for coupling. *MPRES.inp2* has module 3 (and possibly 1) turned off for coupling.

Example Problem: Chlorine Plasma in GEC Reference Cell

Problem Description:

Input Gases: Chlorine (Cl_2)

Reactor Conditions: 185 watts @ 13.56MHz deposited power (MPRES)
Stainless steel wafer (no etching), no wafer bias (MPRES)
20 mtorr reactor pressure (MPRES)
Inlet 15 sccm Cl_2

Chemical Species:

	Mwt	Mass	Variable Hard Sphere diameter
Cl	35.45 gm/gmole	0.59×10^{-25} kg	3.831×10^{-10} m
Cl^+	35.45 gm/gmole	0.59×10^{-25} kg	3.831×10^{-10} m
Cl^-	35.45 gm/gmole	0.59×10^{-25} kg	3.831×10^{-10} m
Cl_2	70.91 gm/gmole	1.18×10^{-25} kg	5.405×10^{-10} m
Cl_2^+	70.91 gm/gmole	1.18×10^{-25} kg	5.405×10^{-10} m
$SiCl_2$	98.99 gm/gmole	1.65×10^{-25} kg	8.000×10^{-10} m

use a mixture viscosity coefficient of 1.00 @ 300 K for DSMC calculation

Icarus Boundary conditions:

inlet: ring radius= 0.1252 m
15 sccm Cl_2 inlet distributed over outer ring radius
use an inlet temperature of 255.79 K and a velocity of 200 m/s

outlet: annular pump
pump speed maintained at 0.00829 m^3/sec.

Icarus Surface Boundary Conditions:

- 100% thermal accommodation
- 100% diffuse surface reaction
- Temperature of all surfaces = 300 K

- Surface Chemistry:

	Sticking Coefficient
$Cl \rightarrow {}^1/_2\ Cl_2$	0.1
$Cl^+ \rightarrow Cl$	1.0
$Cl^- \rightarrow Cl$	1.0
$Cl_2^+ \rightarrow Cl_2$	1.0
$Cl_2^- \rightarrow Cl_2$	1.0

- Gas Phase Chemistry:

$Cl^+ + Cl$	-->	$Cl + Cl^+$	Charge Exchange
$Cl_2^+ + Cl_2$	-->	$Cl_2 + Cl_2^+$	Charge Exchange
$Cl^+ + Cl^-$	-->	$Cl + Cl$	
$Cl_2^+ + Cl^-$	-->	$2Cl + Cl$	

Cl^-	detachment -->	Cl	(rx 5)
Cl_2	attachment -->	Cl	(rx 6)
Cl_2	dissociation -->	$2Cl$	(rx 1)
Cl_2	ionization -->	Cl_2^+	(rx 2)
Cl	ionization -->	Cl^+	(rx 3)
Cl_2^+	attachment -->	$2Cl$	(rx 4)

Example *MPRES.inp* file:

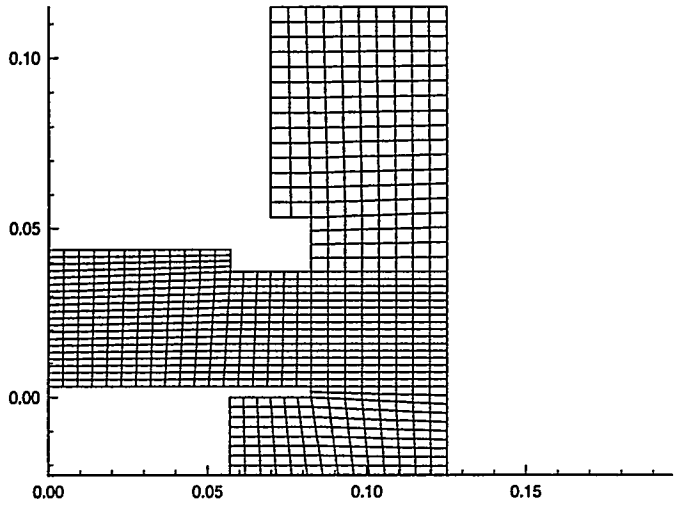
```
**************************************************************************
********
*       INPUT FILE
*        for the
*    MPRES v2.2d
* Copyright 1995, University of Houston
**************************************************************************
********
* RUN INFO
**************************************************************************
* The GD code is based on a modular approach. It consists of three separate
* modules that are coupled. Module (1)solves for the ion density profiles,
* (2)solves for the EM fields and electron temperature profiles and (3)solves
* for the neutral density profiles. The user should specify which modules are
* to be executed in a successive mode, by using the appropriate flag (1->RUN
* MODULE, 0->SKIP MODULE)
* Module-1  Module-2  Module-3
  1         1         1
* The user should also specify the time for which each module is run (in
* seconds) before switching to the next module.
* Module-1  Module-2  Module-3
  3.7e-7    370.e-9   2.e-4
*
* Enter 1 below to solve for bias potentials. The bias simulation
* is done as a postprocessing step, and can be time consuming.
* If capacitive coupling from the coils is to be included, it
* is necessary that module 2 also be run.
*
* Bias Circuit Simulation (1>Run Simulation, 0>Skip)
 0
*
* Convergence is reached once every quantity at every node (of the mesh) in
* every module changes by less than Tolerance over the integration run time
* of each module.
* Tolerance(relative)
  0.05
*
**************************************************************************
********
* Plasma Generation Info
* List here information for the ORMAX power deposition solver.
* ORMAX requires the lower left hand corner to be at 0,0 (ORMAX coordinates),
* enter the z offset relative to the GD grid here (normally > 0). r=0 is assumed
* to be a centerline.
*
* Grid (nr, nz)  Maximum r, z (m)        z offset(m)    number of coils
    40  46    0.1252  0.13795         0.02290          5
*
* Enter below parameters for the applied fields. Note that the
* complex lead current is used only as an initial condition when
```

```
* a target power greater than 0 is specified.
*
* Frequency(Hz) lead current (A)  Target Power (w)
  13.56d6  (-25.00d0, 0.d0)  185.0
*
* Enter below parameters for substrate biasing. These include the excitation
* frequency (Hz), the amplitude of the applied potential(V), and the size of the
* blocking capacitor (Farads). Also include the effective capacitance of the wafer
* subsurface and the wafer itself (also in Farads). All must be real numbers.
*
* Bias Frequency  Vbias  Cblocking  Csubsurface  Cwafer  CQuartz
  13.56d6        00.   3.0d-9   1.20d-10     3.2d-10  2.20d-10
*
* Collision Cross Section (electron - neutral) (m^-2)
 5.0d-19
*
* Mach Number for Ions Entering Sheath
 1.0
*
* Offset for DSMC Grid relative to GD grid
 0.0032
*
* GAS INFO
**********************************************************************
* Pressure (Pa)  Gas Temperature (K)  Ion Temperature (eV) Residence time(s)
   2.667           500.              0.12           6.5154e-2
* List the species to be considered in the simulation by: symbol, charge,
* molecular mass (a.m.u.), mobility coefficient (uN), diffusion coefficient (DN)
* The symbol used for the species should NOT start with a number as this will
* be used to specify the stoichiometry of the reaction process. Diffusion
* coefficients for charged species can be computed internally according to
* Einstein's relation (therefore there is no need for the user to calculate it).
* If the user wishes to specify it then the GD code will use the externally
* specified diffusion coefficient. Neutral species must have mobility equal to
* zero.
* Symbol Charge   a.m.u   Mobility(m-V-s)^-1  Diffusion (m-s)-1
  e     -1    5.4860e-4   6.4200d23           0.
  Cl2+    1   71.0        5.6151e21          0.
  Cl+     1   35.5        6.4838e21          0.
  Cl-    -1   35.5        6.4838e21          0.
  Cl      0   35.5        0.                 6.2133e20
  SiCl2   0   99.086      0.                 2.4984e20
  Cl2     0   71.0        0.                 4.5345e20
* Feed Gases
* List the symbols of the feed gases along with each species' feed ratio. The
* feed ratios must add up to 1.0 and must be separated from the symbols by
* spaces. Also, since the pressure is assumed constant the number degrees of
* freedom is equal to the number of species considered minus one. Therefore
* the first species listed will have its density inferred from the total gas
* density.
   Cl2   1.0
**********************************************************************
********
* Initial Conditions
```

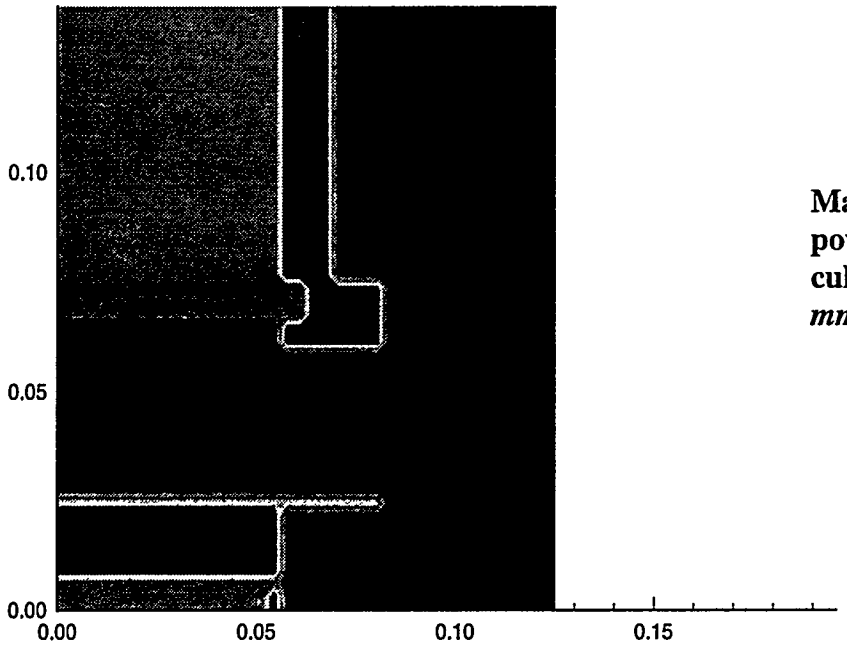
```
**********************************************************
* In this section of the input file the initial conditions of each of the
* variables has to be specified. In the event this is a restart run GD will
* discard the following data and use as initial conditions those specified by
* the user. The initial conditions for clarity and simplicity are uniform
* throughout the reactor. Densities should be given in m^-3 and temperature in
* eV. The electron density will be computed internally to satisfy
* electroneutrality. No need to follow the same order as above. The initial
* condition of the inferred feed species (the first species listed above)
* will be calculated and so should not be provided.
 Cl   1.0e20
 SiCl2 0.0e00
 Cl+  1.0e16
 Cl-  1.0e16
 Cl2+ 1.0e16
 Te   2.0
**************************************************************************
********
* CHEMISTRY
**************************************************************************
* Notes on Entries:
* Character line entries have two formatting requirements:
* 1. Only spaces can be used as separators, tabs are not supported.
* 2. Every species symbol (e.g. Ar) must be preceded and followed by one or more
* spaces. Thus, 2Cl should be written as 2 Cl, or 2Cl+ should be written as
* 2 Cl+.
*
*  GAS PHASE
* List all chemical reactions that GD should account for in the BULK. After ":"
* specify the energy loss that en electron will experience. In case the reaction
* does not involve electron impact the value after ":" should be 0.0. In the
* case where the collision process is an elastic electron impact collision
* process the word "momentum" should be written and the code will compute
* internally the energy exchange.
 Cl2 + e  -> 2 Cl       + e  : 3.12
 Cl2 + e  -> Cl2(B3P)*    + e  : 2.49
 Cl2 + e  -> Cl2(21P&21S)* + e  : 9.25
 Cl  + e  -> Cl(4s)*     + e  : 8.90
 Cl  + e  -> Cl(4p)*     + e  : 10.40
 Cl  + e  -> Cl(3d)*     + e  : 10.90
 Cl  + e  -> Cl(5p)*     + e  : 11.80
 Cl  + e  -> Cl(4d)*     + e  : 12.00
 Cl  + e  -> Cl(5d)*     + e  : 12.40
 Cl2 + e  -> Cl2*        + e  : 0.0689
 Cl2 + e  -> Cl2+        + 2 e : 11.47
 Cl  + e  -> Cl+         + 2 e : 12.99
 Cl2 + e  -> Cl-         + Cl  : 0.0
 Cl2+ + e  -> 2 Cl           : 0.0
 Cl- + e  -> Cl          + 2 e : 3.61
 Cl2+ + Cl- -> Cl2       + Cl  : 0.0
 Cl+ + Cl- -> 2 Cl           : 0.0
 3 Cl     -> Cl2         + Cl  : 0.0
 Cl  + e  -> Cl          + e  : momentum
 Cl2 + e  -> Cl2         + e  : momentum
```

```
*  SURFACE CHEMISTRY
* List all chemical reactions that GD should account for on boundaries. After
* ":" specify the reaction probability (for each reactant). The reactions may
* consist of only one type of gas phase reactant, however, there is no limit
* on the number or types of products. All reactions should have integer
* stoichiometry.
* Include the surface type in each reaction, as a catalyst or reactant.
* 4 surface types are currently supported:
* M1
* M2
* Si
* Q
* The interpretation of the above symbols is determined by the reaction list,
* given below. The symbols were chosen to be mnemonic for common materials.
 Cl+ + M1 -> Cl + M1        : 1.0
 Cl2+ + M1 -> Cl2 + M1      : 1.0
 2 Cl + M1 -> Cl2 + M1      : 0.1
 Cl+ + Si -> Cl + Si        : 1.0
 Cl2+ + Si -> Cl2 + Si      : 1.0
 2 Cl + Si -> Cl2 + Si      : 0.1
 Cl+ + Q  -> Cl + Q         : 1.0
 Cl2+ + Q  -> Cl2 + Q       : 1.0
 2 Cl + Q  -> Cl2 + Q       : 0.1
***----------------------------------------------------------------------------
* Below the rate cofficients for each of the above listed GAS PHASE reactions must be
* given as a function of the mean electron temperature (eV). In the case where
* the  reaction rate coefficient (m3/s) of a certain reaction process is not
* electron energy dependent the reaction rate constant is enough.
*----------------------------------------------------------------------------
*  Cl2  + e  -> 2Cl        + e
0.10000  1.7649e-33
0.37273  2.4546e-19
etc....,
```

Example MPRES grid - Uses input files *MPRESgrid.inp* and *mmat.inp*



Finite Element grid for MPRES specified in *MPRESgrid.inp*



Material mesh for power deposition calculation in MPRES - *mmat.inp*

Example Regrid *glow.map* file - convert FInput to dsmc.em, dsmc.plasma & dsmc.restart:

```
* this is the glow mapping file
* The star in the first line is a comment statement
* the mapping given below are the same as defaults
* defined in the code
*
* the glow index is the order the var. appears in the
* output file.
*
* z/r are converted to meters and the direction is
* reversed on z. The DSMC VAR. 1 defines z and
* 2 defines R
*
* the first 10 spaces are defined for char. use only...
* var. name     dsmc var    glow    default/mult
z              1          2      -1.0
r              2          1      1.0
*
* the DSMC VAR 51 through 100 define the species number
* density. The order is give by adding the species number
* to 50. i.e. species 1 is indexed as 51 , 2 as 52 , etc.
*
* var. name     dsmc var    glow    default/mult
n_cl           51          7      1.
n_cl+          52          5      1.
n_cl-          53          6      1.
n_cl2          54          9      1.
n_cl2+         55          4      1.
n_Sicl2        56          8      1.
*
* the DSMC VAR 100 through 200 defines the species V x/z
* velocity. The order is give by adding the dsmc species number
* to 100. The glow output provides no velocity data
* so a value of -1 in the glow col., tells the mapping code
* to apply the constant value in col. 4 over the entire domain.
*
* var. name     dsmc var    glow    default/mult
Vz_cl          101         -1      0.0
Vz_cl+         102         -1      0.0
Vz_cl-         103         -1      0.0
Vz_cl2         104         -1      0.0
Vz_cl2+        105         -1      0.0
Vz_Sicl2       106         -1      0.0
*
* the DSMC VAR 200 through 300 defines the species V y/r
* velocity. The order is give by adding the dsmc species number
* to 200. The glow output provides no velocity data
* so a value of -1 in the glow col., tells the mapping code
* to apply the constant value in col. 4 over the entire domain.
*
* var. name     dsmc var    glow    default/mult
Vr_cl          201         -1      0.0
```

```
Vr_cl+          202      -1       0.0
Vr_cl-          203      -1       0.0
Vr_cl2          204      -1       0.0
Vr_cl2+         205      -1       0.0
Vr_Sicl2        206      -1       0.0
*
* the DSMC VAR 300 through 400 defines the species trans. temp.
*  The order is give by adding the dsmc species number
* to 300. The glow output provides no temp. data
* so a value of -1 in the glow col., tells the mapping code
* to apply the constant value in col. 4 over the entire domain.
*
* var. name     dsmc var     glow    default/mult
tt_cl           301      -1       500.0
tt_cl+          302      -1       500.0
tt_cl-          303      -1       500.0
tt_cl2          304      -1       500.0
tt_cl2+         305      -1       500.0
tt_Sicl2        305      -1       500.0
*
* the DSMC VAR 400 through 500 defines the species rot. temp.
*  The order is give by adding the dsmc species number
* to 400. The glow output provides no temp. data
* so a value of -1 in the glow col., tells the mapping code
* to apply the constant value in col. 4 over the entire domain.
*
* var. name     dsmc var     glow    default/mult
tr_cl           401      -1       500.0
tr_cl+          402      -1       500.0
tr_cl-          403      -1       500.0
tr_cl2          404      -1       500.0
tr_cl2+         405      -1       500.0
tr_Sicl2        406      -1       500.0
*
* the DSMC VAR 500 through 600 defines the species vib. temp.
*  The order is give by adding the dsmc species number
* to 500. The glow output provides no temp. data
* so a value of -1 in the glow col., tells the mapping code
* to apply the constant value in col. 4 over the entire domain.
*
* var. name     dsmc var     glow    default/mult
tv_cl           501      -1       500.0
tv_cl+          502      -1       500.0
tv_cl-          503      -1       500.0
tv_cl2          504      -1       500.0
tv_cl2+         505      -1       500.0
tv_Sicl2        506      -1       500.0
*
* the DSMC VAR 600 through 700 defines the species weights cxy
* The order is give by adding the dsmc species number
* to 600. The glow output provides no weight. data
* so a value of -1 in the glow col., tells the mapping code
* to apply the constant value in col. 4 over the entire domain.
* NOTE: as the code is set up the cxy are over-written by the
```

```
* values in the dsmc.in2 file.
*
* var. name      dsmc var     glow    default/mult
cxy_cl           601       -1       1.0
cxy_cl+          602       -1       1.0
cxy_cl-          603       -1       1.0
cxy_cl2          604       -1       1.0
cxy_cl2+         605       -1       1.0
cxy_Sicl2        606       -1       1.0
*
* the DSMC VAR 1000 through 2000 defines the species rates
* The order is give by adding the dsmc species number.
* THE VALUE IN COL. 4 IS THE INDEX OF THE ELECTRON NUMBER
* DENSITY WHICH IS MULT. BY THE GLOW RATE.....
*
* var. name      dsmc var     glow    default/mult.
Te               1001       10       1.0
ne               1002       3        1.0
*
* the DSMC VAR 2000 through 3000 defines the em mapping
* Ex/z is defined as 2001 and Ey/r is defined as 2002
*
* var. name      dsmc var     glow    default/mult
Ez               2001       13      -1.00
Er               2002       12       1.00
*
* If a mapping is not provided in the file the constant
* default values defined in the code are used...
```

Example Regrid *dsmc.map* file - convert cell.* to new FInput file for coupling:

```
* this is the dsmc mapping file
* The star in the first line is a comment statement
* the mapping given below are the same as defaults
* defined in the code
*
* the glow index is the order the var. appears in the
* output file.
*
* z/r are converted to meters and the direction is
* reversed on z. The DSMC VAR. 1 defines z and
* 2 defines R
*
* the first 10 spaces are defined for char. use only...
* var. name      dsmc var    glow    default/mult
z              1          2      -1.0
r              2          1      1.0
*
* the DSMC VAR 51 through 100 define the species number
* density. The order is give by adding the species number
* to 50. i.e. species 1 is indexed as 51 , 2 as 52 , etc.
* The number density is converted from (#/cm^3) to (#/m^3)
*
* var. name      dsmc var    glow    default/mult
n_cl           51          19      1.0
n_cl+          52          -1      1.0
n_cl-          53          -1      1.0
n_cl2          54          22      1.0
n_cl2+         55          -1      1.0
n_Sicl2        56          21      1.0
*
* the DSMC VAR 100 through 200 defines the species V x/z
* velocity. The order is give by adding the dsmc species number
* to 100. The value of -1 in the glow col., tells the mapping code
* not to interpolate the dsmc varible into the new glow.inp file.
*
* var. name      dsmc var    glow    default/mult
Vz_cl          101         -1      0.0
Vz_cl+         102         -1      0.0
Vz_cl-         103         -1      0.0
Vz_cl2         104         -1      0.0
Vz_cl2+        105         -1      0.0
Vz_Sicl2       106         -1      0.0
*
* the DSMC VAR 200 through 300 defines the species V y/r
* velocity. The order is give by adding the dsmc species number
* to 200. The value of -1 in the glow col., tells the mapping code
* not to interpolate the dsmc varible into the new glow.inp file.
*
* var. name      dsmc var    glow    default/mult
Vr_cl          201         -1      0.0
Vr_cl+         202         -1      0.0
Vr_cl-         203         -1      0.0
```

```
Vr_cl2          204      -1       0.0
Vr_cl2+         205      -1       0.0
Vr_Sicl2        206      -1       0.0
*
* the DSMC VAR 300 through 400 defines the species trans. temp.
*  The order is give by adding the dsmc species number
* to 300.
*
* var. name     dsmc var     glow    default/mult
tt_cl           301      29       1.0
tt_cl+          302      -1       1.0
tt_cl-          303      -1       1.0
tt_cl2          304      32       1.0
tt_cl2+         305      -1       1.0
tt_Sicl2        306      34       1.0
*
* the DSMC VAR 400 through 500 defines the species rot. temp.
*  The order is give by adding the dsmc species number
* to 400. The glow output provides no temp. data
* so a value of -1 in the glow col., tells the mapping code
* not to interpolate the dsmc varible into the new glow.inp file.
*
* var. name     dsmc var     glow    default/mult
tr_cl           401      -1       500.0
tr_cl+          402      -1       500.0
tr_cl-          403      -1       500.0
tr_cl2          404      -1       500.0
tr_cl2+         405      -1       500.0
tr_Sicl2        406      -1       500.0
*
* the DSMC VAR 500 through 600 defines the species vib. temp.
*  The order is give by adding the dsmc species number
* to 500. The glow output provides no temp. data
* so a value of -1 in the glow col., tells the mapping code
* not to interpolate the dsmc varible into the new glow.inp file.
*
* var. name     dsmc var     glow    default/mult
tv_cl           501      -1       500.0
tv_cl+          502      -1       500.0
tv_cl-          503      -1       500.0
tv_cl2          504      -1       500.0
tv_cl2+         505      -1       500.0
tv_Sicl2        506      -1       500.0
*
* the DSMC VAR 600 through 700 defines the species weights cxy
* The order is give by adding the dsmc species number
* to 600. The glow output provides no weight. data
* so a value of -1 in the glow col., tells the mapping code
* not to interpolate the dsmc varible into the new glow.inp file.
* NOTE: as the code is set up the cxy are over-written by the
* values in the dsmc.in2 file.
*
* var. name     dsmc var     glow    default/mult
cxy_cl          601      -1       1.0
```

cxy_cl+	602	-1	1.0
cxy_cl-	603	-1	1.0
cxy_cl2	604	-1	1.0
cxy_cl2+	605	-1	1.0
cxy_Sicl2	606	-1	1.0

Example Icarus *geometry.inp* file:

```
*-----------------------------------------------------------------------
*  astrick in column 1 indicates comment card
*-----------------------------------------------------------------------
*
 GEC/ICP -- 6 species chemb  grid4 p2.1b
*
*   point injection model for inlet
*
*-----------------------------------------------------------------------
*
   1    control:     -1 -- plot grid only;
*                     1 -- initialization & plot file
   1              0/1 for X-Y or Z-R flow
*-----------------------------------------------------------------------
*                  Initial Conditions
*-----------------------------------------------------------------------
   1              0/1 for vacuum/freestream
   0.            x-component of velocity, m/sec (ft/sec x 0.3048)
   0.            y-component of velocity, m/sec
   4.8e20         number density, molecules/m**3 (mol./ft**3 x 35.315)
   300.00          temperature, deg K (deg R/1.8)
*-----------------------------------------------------------------------
*                  Specie Information
*-----------------------------------------------------------------------
   6              Number of molecular species
*-----------------------------------------------------------------------
*   Cl   Cl+    Cl-    Cl2    Cl2+    SiCl2
    0.9  0.0    0.0    0.1    0.0      0.0
*-----------------------------------------------------------------------
*-----------------------------------------------------------------------
   3              internal structure of most complex molecule:
*                   3-monatomic, 4-rotation, 5-rotat. + vibrat.
   11             # of chem. rx. (from file chem)
*-----------------------------------------------------------------------
*                  Weighting Information (particles and time step)
*-----------------------------------------------------------------------
   2.0e10          base # of real mols. per simulation one
   1.E-06          base time step, sec
   4              cell weighting option
*-----------------------------------------------------------------------
*                  Collision Model Input
*-----------------------------------------------------------------------
   300.0          ref. temp. for VHS model, deg K
   1.0           temperature exponent of viscosity coeffs.
*-----------------------------------------------------------------------
*                . Surface Modelling Information
*-----------------------------------------------------------------------
   1.000          thacc: thermal accomodation coefficient
*-----------------------------------------------------------------------
*                  Misc input Section
*-----------------------------------------------------------------------
```

```
   7          vacuum pump region #
   0          ic region distribution
   1          wafer material type
   24          pressure iteration control pt.
   0
  0.0000        min radial expansion radius
   1.          ne mult
   0.          extra input 8
   0.          extra input 9
   1.0         use external cross-sections
*-------------------------------------------------------------------------
*                 Region Definition
*-------------------------------------------------------------------------
   8          number of regions (must be .le. 30)
   24          number of global points (must be .le.120)
*-----------------------------------
*    Global corner pt. coordinates
* Pt.       z (m)         r (m)
*-----------------------------------
  1        -0.0000          0.0
  2        -0.0341          0.0
  3        -0.0405          0.0
  4        -0.0405          0.05715
  5        -0.0341          0.05715
  6        -0.0341          0.08255
  7        -0.0500          0.08255
  8        -0.0500          0.06985
  9        -0.1118          0.06985
  10       -0.1118          0.08255
  11          -0.1118          0.1252
  12       -0.0341          0.1252
  13       -0.0000          0.1252
  14       -0.0000          0.08255
  15       0.0032          0.08255
  16       0.0032          0.0570
  17       0.0262          0.0570
  18       0.0262          0.08255
  19       0.0262          0.1252
  20       0.0362          0.08255
  21       0.0362          0.1252
  22       -0.0118          0.010
  23       0.00           0.05715
  24       -0.0163          0.1135
*-------------------------------------------------------------------------
*          Individual Region Definitions Follow
*          --REGION NUMBERS MUST BE SEQUENTIAL--
*-------------------------------------------------------------------------
*=========================================================================
   1 <------ Inputs specific to this region follow
*=========================================================================
   1.0          fnum multiplier
   1.0          dtm multiplier
   3           global points
   4
```

```
  23
  1
  40          number of cells along sides 1 and 3
  40          number of cells along sides 2 and 4
  0           sides 1 and 3 curvature: 0/1 for line/circular arc
  0           sides 1 and 3 cell spacing:
  0           sides 2 and 4 cell spacing:
  1           boundary type code for sides 1 - 4, resp.
  5
  9
  5
  3
*-------------------------------------------------------------------
*  Side Cell1 Cell2    Spec. refl.  Temp. K   Material#   Value
*-------------------------------------------------------------------
   2   1   100        0.000      373.00      2          0.
   3   1   100        0.000      373.00      3          1.
   4   1   100        0.000      373.00      1          0.
*-------------------------------------------------------------------
*              Region interface/matching
*     |-----> Only need if IVN > 0; then supply IVN pairs of (IVR,IVS)
*           Number adj.
*  Reg. side  reg. sides      Adj. sidel Adj. reg.
*             (IVN)          no. (IVS)l no. (IVR)
*-------------------------------------------------------------------
     1         0
     2         0
     3         2  1 -1  1  8
     4         0
*===================================================================
  2 <------ Inputs specific to this region follow
*===================================================================
  1.0         fnum multiplier
  1.0          dtm multiplier
  6           global points
  12
  13
  14
  20          number of cells along sides 1 and 3
  20          number of cells along sides 2 and 4
  0           sides 1 and 3 curvature: 0/1 for line/circular arc
  0           sides 1 and 3 cell spacing:
  0           sides 2 and 4 cell spacing:
  7           boundary type code for sides 1 - 4, resp.
  7
  52
  7
  1
*-------------------------------------------------------------------
*  Side Cell1 Cell2    Spec. refl.  Temp. K   Material#   Value
*-------------------------------------------------------------------
*    1   1    60        0.000      350.       8          1.
*    2   1    60        0.000      350.       6          1.
     3   1    60        0.000      350.       3          0.
```

```
*   4   1    60       0.000     350.       7        1.
*-----------------------------------------------------------------------
*              Region interface/matching
*      |-----> Only need if IVN > 0; then supply IVN pairs of (IVR,IVS)
*            Number adj.
*   Reg. side   reg. sides      Adj. sidel Adj. reg.
*              (IVN)         no. (IVS)l no. (IVR)
*-----------------------------------------------------------------------
      1         1    3 8
      2         1    4 3
      3         0
      4         1    2 5
*=======================================================================
   3 <------ Inputs specific to this region follow
*=======================================================================
   1.0          fnum multiplier
   1.0          dtm multiplier
  10            global points
  11
  12
   6
  25            number of cells along sides 1 and 3
  25            number of cells along sides 2 and 4
   0            sides 1 and 3 curvature: 0/1 for line/circular arc
   0            sides 1 and 3 cell spacing:
   0            sides 2 and 4 cell spacing:
   9            boundary type code for sides 1 - 4, resp.
   5
   5
   7
   3
*-----------------------------------------------------------------------
*  Side  Cell1  Cell2    Spec. refl.   Temp. K   Material#    Value
*-----------------------------------------------------------------------
    1    1     50        0.000        350.      3         1.
    2    1     50        0.000        350.      3         0.
    3    1     50        0.000        350.      3         0.
*-----------------------------------------------------------------------
*              Region interface/matching
*      |-----> Only need if IVN > 0; then supply IVN pairs of (IVR,IVS)
*            Number adj.
*   Reg. side   reg. sides      Adj. sidel Adj. reg.
*              (IVN)         no. (IVS)l no. (IVR)
*-----------------------------------------------------------------------
      1         2   3 -1 3 4
      2         0
      3         0
      4         1   2  2
*=======================================================================
   4 <------ Inputs specific to this region follow
*=======================================================================
   1.0          fnum multiplier
   1.0          dtm multiplier
   9            global points
```

```
 10
 7
 8
 20          number of cells along sides 1 and 3
 8           number of cells along sides 2 and 4
 0           sides 1 and 3 curvature: 0/1 for line/circular arc
 0           sides 1 and 3 cell spacing:
 0           sides 2 and 4 cell spacing:
 5           boundary type code for sides 1 - 4, resp.
 5
 7
 5
 3
*-------------------------------------------------------------------
*  Side Cell1 Cell2    Spec. refl.  Temp. K   Material#   Value
*-------------------------------------------------------------------
   1    1    50       0.000        350.      3           0.
   2    1    50       0.000        350.      3           0.
   4    1    50       0.000        350.      3           0.
*-------------------------------------------------------------------
*              Region interface/matching
*      |-----> Only need if IVN > 0; then supply IVN pairs of (IVR,IVS)
*           Number adj.
*   Reg. side  reg. sides      Adj. sidel Adj. reg.
*              (IVN)           no. (IVS)| no. (IVR)
*-------------------------------------------------------------------
      1        0
      2        0
      3        1       1  3
      4        0
*===================================================================================
  5 <------ Inputs specific to this region follow
*===================================================================================
  1.0         fnum multiplier
  1.0         dtm multiplier
 14           global points
 13
 19
 18
 15          number of cells along sides 1 and 3
 15          number of cells along sides 2 and 4
 0           sides 1 and 3 curvature: 0/1 for line/circular arc
 0           sides 1 and 3 cell spacing:
 0           sides 2 and 4 cell spacing:
 9           boundary type code for sides 1 - 4, resp.
 7
 5
 7
 2
*-------------------------------------------------------------------
*  Side Cell1 Cell2    Spec. refl.  Temp. K   Material#   Value
*-------------------------------------------------------------------
   1    1    20       0.000        350.00    3           1.
   3    1    20       0.000        350.00    2           0.
```

```
*-------------------------------------------------------------------
*              Region interface/matching
*     |-----> Only need if IVN > 0; then supply IVN pairs of (IVR,IVS)
*           Number adj.
*  Reg. side  reg. sides      Adj. sidel Adj. reg.
*             (IVN)         no. (IVS)| no. (IVR)
*-------------------------------------------------------------------
     1        2    3  6 3 -1
     2        1    4  2
     3        0
     4        1    2  7
*-------------------------------------------------------------------
*===================================================================
  6 <------ Inputs specific to this region follow
*===================================================================
  1.0         fnum multiplier
  1.0         dtm multiplier
 16           global points
 15
 18
 17
 10           number of cells along sides 1 and 3
 10           number of cells along sides 2 and 4
  0           sides 1 and 3 curvature: 0/1 for line/circular arc
  0           sides 1 and 3 cell spacing:
  0           sides 2 and 4 cell spacing:
  5           boundary type code for sides 1 - 4, resp.
  5
  7
  5
  3
*-------------------------------------------------------------------
*  Side Cell1 Cell2    Spec. refl.  Temp. K   Material#   Value
*-------------------------------------------------------------------
   1   1    40        0.000       350.00      3         0.
   2   1    40        0.000       350.00      3         0.
   4   1    40        0.000       350.00      3         0.
*-------------------------------------------------------------------
*              Region interface/matching
*     |-----> Only need if IVN > 0; then supply IVN pairs of (IVR,IVS)
*           Number adj.
*  Reg. side  reg. sides      Adj. sidel Adj. reg.
*             (IVN)         no. (IVS)| no. (IVR)
*-------------------------------------------------------------------
     1        0
     2        0
     3        1   1  5
     4        0
*-------------------------------------------------------------------
*===================================================================
  7 <------ Inputs specific to this region follow
*===================================================================
  1.0         fnum multiplier
  1.0         dtm multiplier
```

```
 18          global points
 19
 21
 20
 5          number of cells along sides 1 and 3
 10          number of cells along sides 2 and 4
 0          sides 1 and 3 curvature: 0/1 for line/circular arc
 0          sides 1 and 3 cell spacing:
 0          sides 2 and 4 cell spacing:
 5          boundary type code for sides 1 - 4, resp.
 7
 5
 5
 3
*-------------------------------------------------------------------
*  Side  Cell1  Cell2    Spec. refl.  Temp. K   Material#   Value
*-------------------------------------------------------------------
   1    1     40        0.000       350.00      4         0.
   3    1     40        0.000       350.00      4         0.
   4    1     40        0.000       350.00      4         0.
*-------------------------------------------------------------------
*              Region interface/matching
*     |-----> Only need if IVN > 0; then supply IVN pairs of (IVR,IVS)
*           Number adj.
*  Reg. side  reg. sides      Adj. sidel Adj. reg.
*             (IVN)         no. (IVS)| no. (IVR)
*-------------------------------------------------------------------
     1        0
     2        1  4  5
     3        0
     4        0
*===================================================================
  8 <------ Inputs specific to this region follow
*===================================================================
  1.0         fnum multiplier
  1.0          dtm multiplier
  5          global points
  6
  14
  23
  30          number of cells along sides 1 and 3
  15          number of cells along sides 2 and 4
  0          sides 1 and 3 curvature: 0/1 for line/circular arc
  0          sides 1 and 3 cell spacing:
  0          sides 2 and 4 cell spacing:
  7          boundary type code for sides 1 - 4, resp.
  5
  7
  5
  2
*-------------------------------------------------------------------
*  Side  Cell1  Cell2    Spec. refl.  Temp. K   Material#   Value
*-------------------------------------------------------------------
   2    1     60        0.000       373.        3         0.
```

Example Icarus *spec* File:

```
**************************************
*     species data file          *
**************************************
*  number of species to input taken from problem description
*  input --- they MUST be the same
*-----------------------------------------------------------------------------------------
* ID
* Mwt    Mol. mass   Diam.   #Rot.Deg.   Rot.Rel.   Vib. Rel.  Vib.Temp.  specie wt.  charge
*          (kg)       (m)     Freedom     Coll. #    Coll. #     (K)
*-----------------------------------------------------------------------------------------
Cl
 35.45   0.59e-25  3.831e-10     0.0       0.0        0.0        0.0      1.0        0.0
Cl+
 35.45   0.59e-25  3.831e-10     0.0       0.0        0.0        0.0      0.0001     1.0
Cl-
 35.45   0.59e-25  3.831e-10     0.0       0.0        0.0        0.0      0.0001     -1.0
Cl2
 70.91   1.18e-25  5.405e-10     2.        5.         00.        0000.    1.00       0.0
Cl2+
 70.91   1.18e-25  5.405e-10     2.        5.         00.        0000.    0.0001     1.0
SiCl2
 98.99   1.647e-25 8.000e-10     2.        5.         0.0        0.0      1.0        0.0
*
*   some of these are based on Chemkin data provided by Ellen Meeks - SNLL
*
```

Example Icarus *chem* File:

```
*
* NOTE:  line 1 MUST have 8 integers
*      line 2 for type 0, -1, & -2 MUST have 5 real numbers
*      line 2 for type -3 MUST have 2 integers and 1 real number
*      line 3 for type -3 MUST have 6 real numbers
*
*
*
*       first number on line 1 defines reaction type:
*
*            0 -- standard Arrhenius collisional chemistry k = A T^B exp(-Ea/kT)
*                 second line variables:
*                 1 -- number of internal degrees of freedom
*                 2 -- Ea
*                 3 -- A
*                 4 -- B
*                 5 -- heat of rx (+ for exothermic) - joules
*
*           -1 -- Charge Exchange reaction with fixed rate
*                 second line variables:
*                 1 -- probability
*                 2 -- sigma CE (m^2)
*
*           -2 -- Charge Exchange reaction using model from Rapp & Frances(1962)
*                       sigma = ( k1 - k2*alog(vr) )**2
*                 second line variables:
*                 1 -- k1 for elastic collision
*                 2 -- k2 for elastic collision
*                 3 -- k1 for charge exchange
*                 4 -- k2 for change exchange
*
*           -3 -- Electron Impact reactions
*                 second line variables:
*                 1 -- equation type (if <0, T in K instead of eV)
*                 2 -- number of products (1 or 2)
*                 3 -- heat of formation (Frank-Candom)- joules
*                 third line variables:
*                 1 - 6 are fit coefficients
*
*
*  Chlorine chemistry example -- 11 reaction set
*
*     Cl, Cl+, Cl-, Cl2, Cl2+, SiCl2
*     1  2   3   4   5   6
*
*
Cl+ + Cl -> Cl + Cl+ (charge exchange)
-1     2    1     1   1   1  0  2
       0.75      120.e-20       0.  0.  0.
*
Cl2+ + Cl2 -> Cl2 + Cl2+ (charge exchange)
```

```
-1     5   4    1   1   4  0  5
       0.75     120.e-20      0.  0.  0.
*
Cl- + Cl -> Cl  + Cl- (charge exchange)
-1     3   1    1   1   1  0  3
       0.90     240.e-20      0. 0.   0.
*
*
Cl+ + Cl- -> Cl + Cl   (recombination)
0      2   3    1   1    1 0  1
       0.0   0.0      5.e-14     0.0     1.5e-18
*
Cl2+ + Cl- -> 2Cl + Cl   (recombination)
0      5   3   2  1    1   1   1
       0.0   0.0      5.e-14     0.0     1.26e-18
*
*
 Cl2 attachment to Cl + Cl-  (electron impact)
-3     4   4   1  1    1   0   3
       2   2   5.78e-19
       2.21e-16 0.485 -0.174 0.0 0.0 0.0
*
 Cl- detachment to Cl   (electron impact)
-3     3   3   1  0    1   0   0
       1   1  0.0
       2.94e-14 0.680 3.7994 0.0 0.0 0.0
*
  Cl2 dissociation to 2Cl  (electron impact)
-3     4   4   1  1    1   0   1
       1   2   0.96e-19
       3.99e-14 0.115 4.43 0.0 0.0 0.0
*
 Cl2 ionization to Cl2+  (electron impact)
-3     4   4   1  0    5   0   0
       1   1   0.0
       2.13e-14 0.771 11.7 0.0 0.0 0.0
*
 Cl ionization to Cl+   (electron impact)
-3     1   1   1  0    2   0   0
.      1  1    0.0
       2.96e-14 0.554 13.1 0.0 0.0 0.0
*
   Cl2+ attachment to 2Cl  (electron impact)
-3     5   5   1  1    1   0   1
       3   2  0.0
       9.0e-13 0.0258526 0.61 0.0 0.0 0.0
*
*
*   third body probabilities now follow
*
```

Example Icarus *surf_chem* file:

```
*
* this file contain surface chemistry information for the
* UH - GEOM1 Problem  Cl2 chemistry
*      Cl, Cl+, Cl-, Cl2, Cl2+, SiCl2
*      1  2  3  4  5  6
*
* variable order for each reaction:
* (Species-i) (Species-r) (degree of specular reflect) (Rx prob) (create prob)
*
4    number of material table types
*
* material 1 (wafer), wafer
1 4
1.  4.  0.   0.1    0.5
2.  1.  0.   1.0    1.0
3.  1.  0.   1.0    1.0
5.  4.  0.   1.0    1.0
*
* material 2, upper head
2  4
1.  4.  0.   0.1    0.5
2.  1.  0.   1.0    1.0
3.  1.  0.   1.0    1.0
5.  4.  0.   1.0    1.0
*
* material 3, chamber walls
3  4
1.  4.  0.   0.1    0.5
2.  1.  0.   1.0    1.0
3.  1.  0.   1.0    1.0
5.  4.  0.   1.0    1.0
* material 4, increase surface area recomb.rate
4  4
1.  4.  0.   0.1    0.5
2.  1.  0.   1.0    1.0
3.  1.  0.   1.0    1.0
5.  4.  0.   1.0    1.0
```

Example Icarus *inlet* file:

```
*
* new version of inlet file
*
2 number of tables
*
1 1 1   -- 15sccm -- point source -- new grid2
*       #/s
 0.038  6.717899e+18  0.00  -199.725   255.79  255.79  255.79  0.0 0. 0. 1.0  0. 0.
*
*     base case calc.
*
2  2 2    -- 10sccm distributed over the outer-ring radius
*        #/m2                    Tt                          Cl2
 -0.033     1.967e20   0.0    0.0     300.    300.     300.   0.0 0.0 0.0 1.0 0.0 0.0
 -0.004     1.967e20   0.0    0.0     300.    300.     300.   0.0 0.0 0.0 1.0 0.0 0.0
```

Example Icarus *cross_section* file:

```
*   cross section input file - overwrite the VHS based values
*
*   file for charged particles and neutral
*
9
2  1
30.e-20
2  4
30.e-20
2  6
30.e-20
3  1
30.e-20
3  4
30.e-20
3  6
30.e-20
5  1
30.e-20
5  4
30.e-20
5  6
30.e-20
```

Example of *dsmc.in* file used for GEC weak coupling

```
# Test file for GEC/ICP Chlorine Plasma-test
log file                dsmc.log
output screen           100
zero flag               100
chemistry flag          1
efield flag             2
efield subcycle         1 1
subcycle                5
pump speed              0.001
pump control            100 2.67 .00001 .01 dsmc.pump
gemini flag             1000
read definition         1.0  dsmc.in2
load particles          1.8
read efield             dsmc.em dsmc.plasma
adapt flag              400 0.25
time factor             2.0
run                     4000 0
adapt flag              1000 0.25
output cells            3000
output surface          3000
output wafer            3000
time factor             2.0
run                     80000 1
#   coupled step #2
output cells            0
output surface          0
output wafer            0
run                     2000 0
output cells            2000
output surface          2000
output wafer            2000
run                     40000 1
#coupled step #3
output cells            0
output surface          0
output wafer            0
run                     2000 0
output cells            5000
output surface          5000
output wafer            5000
run                     50000 1
#coupled step #4
output cells            0
output surface          0
output wafer            0
run                     2000 0
output cells            3000
output surface          3000
output wafer            3000
run                     40000 1
```

Appendix A. Gemini Shell Script - Weak and Strong Coupling

```
#!/bin/csh -bf

#10-Jan-1995 Version 1.6
# mpres.csh
#
#Usage:
#       mpres.csh [1]
#

# Debugging
##set echo
##set verbose

#  Intialize variables
set ERROR=0
set MYNAME=`basename $0`
set MPRES_DATA="FInput"
set MPRES_COUNT="MPRES.COUNT"
set DSMC_FILE="DSMC.OUT"
set MPRES_OUTPUT="mpres.screen"
set MPRES_FLAG="MPRES.FLAG"
set ME=`basename $0`
set HOST=`uname -n`             # Hostname, e.g., bear
set SYS=`uname -s`              # OS Name, e.g., SunOS, IRIX
set VER=`uname -r`              # OS Release, e.g., 4.1.3, 5.3, 4.0F
set SYSTEM=${SYS}${VER}         # OS, e.g., SunOS4.1.3, SunOS5.3, IRIX4.0F

@ knt=1

# Determine OS and setup executables
switch  ("$SYSTEM")
  case "SunOS4*":
#    echo "  "${ME}: \"SunOS4 Block\" @ `date`
+   set MPRESEXE="/home/u/tjbarte/bin/mpres_sun"
+   set REGRID="/home/u/tjbarte/bin/regrid_sun"
      breaksw
  case "SunOS5*":                   # Solaris
#    echo "  "${ME}: \"SunOS5 Block\" @ `date`
     set MPRESEXE="/home/u/tjbarte/bin/mpres_sun"
     set REGRID="/home/u/tjbarte/bin/regrid_sun"
     breaksw
  case "IRIX*":             # SGI
#    echo "  "${ME}: \"IRIX Block\" @ `date`
     set MPRESEXE="/home/u/tjbarte/bin/mpres_sgi"
     set REGRID="/home/u/tjbarte/bin/regrid_sgi"
     breaksw
  case "HP*":               # HP
#    echo "  "${ME}: \"HP Block\" @ `date`
     set MPRESEXE="/home/u/tjbarte/bin/mpres_hp"
     set REGRID="/home/u/tjbarte/bin/regrid_hp"
     breaksw
  default:
```

```
    echo "  "${ME}: Unknown system, SYSTEM=$SYSTEM
    exit 1
  endsw

  # Verify Executables Exist
  if ( ! -e ${MPRESEXE} ) then
   echo "${MYNAME}:  ERROR - Executable ${MPRESEXE} does NOT exist"
   set ERROR=1
  endif
  if ( ! -e ${REGRID} ) then
   echo "${MYNAME}:  ERROR - Executable ${REGRID} does NOT exist"
   set ERROR=1
  endif

  # Check for errors so far
  if ( ${ERROR} ) then
   echo "${MYNAME}:  Exiting 1..."
   exit (1)
  endif


  # Process command line args:
  if ( "$1" != "" ) then
   if ( "$1" != "1" ) then
    echo "${MYNAME}: ERROR - Usage:  ${MYNAME} [1]"
    set ERROR=1
   else
    #  Process the existing data file
    if ( ! -e MPRES.inp ) then
     if ( ! -e MPRES.inp1 ) then
      echo "{$MYNAME}:  ERROR - File MPRES.inp1 AND MPRES.inp do NOT exist - Exiting
  10..."
      set ERROR=1
      exit (1)
     else
      cp MPRES.inp1 MPRES.inp
     endif  # if ( ! -e MPRES.inp1 ) then
    endif  # if ( ! -e MPRES.inp ) then
    $MPRESEXE
    sleep 5

    $REGRID $MPRES_DATA
    rm -f $MPRES_COUNT
    echo "1" > $MPRES_COUNT

    if ( ! -e "${MPRES_DATA}" ) then
     echo "${MYNAME}:  ERROR - File ${MPRES_DATA} does NOT exist"
     set ERROR=1
    else
     mv $MPRES_DATA $MPRES_DATA.$knt
    endif

   endif  # if ( "$1" != "1" ) then
  endif  # if ( "$1" != "" ) then
```

```
# MPRESEXE data file exist?
rm -f MPRES.inp
if ( ! -e MPRES.inp2 ) then
   echo "{$MYNAME}:  ERROR - File MPRES.inp2 does NOT exist"
   echo "{$MYNAME}:  ERROR - File MPRES.inp2 does NOT exist" >> $MPRES_OUTPUT
   set ERROR=1
  else
   cp MPRES.inp2 MPRES.inp
endif  # if ( ! -e MPRES.inp2 ) then

# Check for errors
if ( ${ERROR} ) then
  echo "${MYNAME}:  Exiting 2..."
  exit (1)
endif

touch $DSMC_FILE
chmod 644 $DSMC_FILE
rm -f $MPRES_OUTPUT
touch $MPRES_OUTPUT

# Loop - wait for DSMC data files
while ( 1 )

#  sleep 300
  sleep 100

  if ( -z "${DSMC_FILE}" ) then
    continue
  endif

  # Restartd2g
  rm -f glow.restart
  set INP_FILE=`cat ${DSMC_FILE}`
  chmod 644 $INP_FILE
  $REGRID $MPRES_DATA.$knt $INP_FILE
  sleep 5

  if ( ! -e glow.restart ) then
    echo "${MYNAME}:  ERROR - file glow.restart does NOT exist"
    echo "${MYNAME}:  ERROR - file glow.restart does NOT exist" >> $MPRES_OUTPUT
    set ERROR=1
    break
  endif

  mv -f FInput FInput_old
  mv glow.restart FInput

  # Increment counter
  @ knt++

  # gd
  rm -f $MPRES_OUTPUT
```

```
  rm -f $MPRES_FLAG
  $MPRESEXE > $MPRES_OUTPUT
  sleep 5

  if ( ! -e "${MPRES_FLAG}" ) then
    echo "${MYNAME}:  ERROR: MPRES did not converge - script aborted"
    echo "${MYNAME}:  ERROR: MPRES did not converge - script aborted" >> $MPRES_OUTPUT
    set ERROR=1
    break
  endif

  mv -f dsmc.restart dsmc.restart_last
  mv -f dsmc.plasma dsmc.plasma_last
  mv -f dsmc.em dsmc.em_last

  $RESG2D $MPRES_DATA

  if ( ! -e "${MPRES_DATA}" ) then
    echo "${MYNAME}:  ERROR - file ${MPRES_DATA} does NOT exist"
    echo "${MYNAME}:  ERROR - file ${MPRES_DATA} does NOT exist" >> $GD_OUTPUT
    set ERROR=1
    break
  endif
  mv $MPRES_DATA $MPRES_DATA.$knt

  rm -f $DSMC_FILE
  touch $DSMC_FILE
  chmod 644 $DSMC_FILE

  rm -f $MPRES_COUNT
  echo "${knt}" > $MPRES_COUNT

end  #  while ( 1 )

if ( ${ERROR} ) then
  echo "Exiting 3..."
  exit (1)
endif

# All done - all is well!!!
exit (0)

#
#       EOF:  mpres.csh
```

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