Technical Report RAL-TR-96-099

# A User Guide for the Laser-Plasma Simulation Code: MED103 

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December 1996

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ISSN 1358-6254

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# A user guide <br> for the laser-plasma simulation code: MED103 

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#### Abstract

Many features have been added to the laser plasma simulation code Medusa [1] over the last few years. This was renamed Med101 [2] in 1989 and now Med103. The new features in the latest version include: the coupling of the energies involved in the atomic processes of excitation. ionization, etc... (in the non-LTE time-dependent average atom model) to the free electron energy balance equation, which allows realistic simulations of rapidly heated plasmas found in short-pulse high-intensity laser-produced plasmas. The new version also includes a high-field corrections to inverse bremsstrahlung absorption, tunnel ionization, a non-local electron heat conduction subroutine as well as a package for the modelling of collisional in addition to recombination x -ray lasers. Complete details for running this code are given including: an explanation of the input parameters. instructions for running on the Rutherford Appleton Laboratory DEC ALPHA (AXPRL2), UNIX farm (OSFSERV) and the superscalar computer (COLUMBUS). The code is capable of simulating a wide range of laser-produced plasma experiments in 1 D planar, cylindrical or spherical geometry with a choice of ionization and equation of state models.


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## 1 Introduction

This document outlines recent modifications to the laser fusion code MED101 [1, 2] (now renamed MED103). Like MED101, MED103 is a one dimensional Lagrangian hydrodynamic code which is capable of modelling a wider range of experiments. Improvements to the physics in the program include

1) Coupling of the energies involved in excitation and ionization, when using the time-dependent average atom model, to the free electron energy balance equation[3]. This allows realistic simulations of, for example, high-Z targets where a large fraction of the absorbed laser energy is consumed in the processes of excitation and ionization of the plasma.
2) Calculation of Ne-like collisional X-ray laser gain [3] in addition to H -like, Li-like and Na -like recombination schemes. Atomic data [4] is available in the code for 27 levels of 4 Ne -like ion configurations ( $2 s^{2} 2 p^{6}, 2 s^{2} 2 p^{5} 3 s, 2 s^{2} 2 p^{5} 3 p, 2 s^{2} 2 p^{5} 3 d$ ) and for the following elements: $\mathrm{Si}(\mathrm{Z}=14), \operatorname{Ar}(\mathrm{Z}=18)$, $\mathrm{Ti}(\mathrm{Z}=22), \mathrm{Fe}(\mathrm{Z}=26), \mathrm{Ge}(\mathrm{Z}=32)$ and $\mathrm{Kr}(\mathrm{Z}=36)$.
3) A high field correction to inverse bremsstrahlung, a non-local heat conduction subroutine [5] as well as the option to switch on tunnel ionization (This is useful for the simulation of short pulse high intensity laser interaction with gas targets).
4) More control over the initial conditions of the beam/target and over the simulation. For example it is now possible to specify the maximum time step DTMAX used by the code (useful for the simulation of very short pulses). It is also possible to restart the code from where it left off in a previous run with the possibility of changing irradiation conditions (laser wavelength for example). 5) When dealing with multiple Gaussian pulse irradiation with largely different pulse lengths (ie. a femtosecond pulse following a nanosecond ASE prepulse), it is no longer necessary to use a small value of DTMAX to perform the simulation. The code 'looks ahead' for short pulses and adjusts the time step so as to sample the short pulse adequately.
The source code for MED103 has also been 'cleaned-up' and some errors corrected. MED103 now compiles and runs on COLUMBUS, the UNIX farm (OSFSERV), and DEC ALPHA (AXPRL2) without any modifications.
There are four different NAG/GKS graphics programs to post-process MED103 output:
5) FLIP3 - this is the most useful and it plots the hydrodynamic variables (velocity, mass density, electron density, pressure, electron and ion temperatures, and average ionization) vs. distance for different times, and also the hydrodynamic variables (cell coordinates plus velocity etc.) vs. time for each cell
6) ION3 - this plots the ground state number density of the different ionization stages vs. distance at different times during the interaction. ION3 also displays the zoning of the run. This can be useful to ensure that there are enough cells in the regions of interest
7) XRLREC3 - this plots the recombination X-ray laser gain vs. distance at different times, and also the space-integrated gain for different lines (i. e. alpha, beta etc.) vs. time as would as measured by experiment.
4)XRLCOL3 this plots the Ne-like collisional X-ray laser gain vs. distance at different times.

Each graph has a panel at the top containing details of the input data used for that particular run. The graphics packages were written initially to run on the old IBM and use NAG GKS routines. They produce postscript files which can be viewed on any X-windows display using ghostview and either printed at Rutherford or transferred to the user's local site and printed on a local postscript printer.

## 2 Getting started

If you don't already have an account on the Unix farm (OSFSERV) or the DEC ALPHA (AXPRL2) contact the Theory and Computation group at the Central Laser Facility (telephone: 01235 445481/446344). Information and documentation on the available computing services can be found on the word wide web (http://www.cis.rl.ac.uk/services.html)
In the following sections commands that exist in batch or script files or commands that can be typed in by the user will be printed

## IN THIS TYPEFACE or this typeface

### 2.1 A note to users of MED101

When implementing any modification to the code, I have tried to do it in a way which leaves the code upward compatible (i.e it can run old data sets without any changes). This philosophy has been adhered to, except for the use of the variable SAHA. In MED101, when the X-ray laser calculation is switched on (ICXRL=1) the code automatically uses the time dependent non-LTE ionization ( $\mathrm{Z}^{*}$ ) from the solution to the non-LTE average atom model rate equations. In MED103 it is necessary to set (SAHA=2.0) for the code to calculate the ionization from the nonLTE average atom rate equations independently of the value of ICXRL. The ionization energy is also calculated and included in the solution to the free electron energy balance equation. With SAHA=2, either the perfect gas (NLPFE=T) or the degenerate gas (NLPFE=F, STATE=0) equations of state may be used.
If the user mixes the non-LTE model (SAHA=2) with the LTE Thomas Fermi equation of state ( $\mathrm{NLPFE}=\mathrm{F}$ and $\mathrm{STATE}=1,2$ or 3 ) either inadvertently or purposefully the code will calculate the ionization energy from the non-LTE model while the pressure is calculated from the TF model. This choice is arbitrary and is thermodynamically inconsistent. Therefore this is not advised. Typical settings of SAHA, NLPFE, STATE, ICXRL are given in the examples in this manual. An example input data file (FPAP2.DAT) for the modelling of the $x$-ray laser experiment is shown next. A similar example was also given in the med 101 manual[2].

```
FLUDRINE FIBRE (med103 version: saha=2.0)
0.53 microns, 3.5e12 W/m/rad, 70 ps FWHM,
8 micron diameter, perfect gas EOS
```

```
****************************************************
```

\$NEWRUN
XAMDA1 $=0.53 \mathrm{E}-6$, GAUSS $=1.0, \quad$ ANPULS $=1.0, \quad$ TOFF $=1.0$,
PLENTH=4.2E-11, $\operatorname{PMAX}=3.50 \mathrm{E} 12, \mathrm{PMULT}=2.381$,
$\mathrm{NGEOM}=2, \quad \operatorname{PIQ}(55)=0.0, \operatorname{TEINI}=300.0, \operatorname{TIINI}=300.0$,
MESH=50, RINI=4.E-06, RHDGAS $=2635.0$, RF1 $=0.9000$,
$X Z=9.0, \quad X M A S S=19.0, \quad \quad F N E=1.0$,
ZGLAS $=0.0$, DRGLAS $=0.0 \mathrm{E}-06$, ROGLAS $=0.0, \quad \mathrm{RF} 2=0.9999$,
$X Z 2=0.0, \quad$ XMASS2 $=0.0, \quad$ FNE2 $=1.0$,
ZPLAS $=0.0$, $\operatorname{DRPLAS}=0.00 \mathrm{E}-0$, ROPLAS $=0.0, \quad \mathrm{RF} 3=0.9999$,
$X Z 1=0.0, \quad$ XMASS1 $=0.0, \quad H Y D R O G=0.0$,
NPRNT $=-100, \mathrm{TSTOP}=1 . \mathrm{E}-09, \quad \mathrm{NRUN}=999999$,
NP3=1, $\quad$ NLEMP $=F$,
NLBRMS $=T$, FLIMIT $=10.0$,
ANABS $=0.2, \quad \mathrm{FHOT}=0.0, \quad$ FTHOT $=-1.0, \quad$ RHOT $=1.0$,
STATE=0.0, NLPFE=t, saha=2.0,
ICXRL=1, IFRSTA=1, ILOSTA=0, IHISTA=3,
ISTAGE=1, IDFLG=0, ROPMUL=1.0, ITBFLG=1, ISTFLG=0,

```
IPUFLG=0, TPON=2.15E-10, TPOFF=2.85E-10,
NLP=1, NUP=3, RMPD=0.002, DLAMDA=81.0E-08,
NLMAX=2, FLSHORT=0.0001, FLLONG=0.55,
    nlres=f,
$END
```


### 2.2 What is needed to run the code

To run MED103 you will need an input data file. An example for the simulation of a recombination x -ray laser experiment was given above. Another example (AL100FS.DAT) is given below. This specifies an Al target which is irradiated by a $100 \mathrm{fs}, 10^{17} \mathrm{~W} / \mathrm{cm}^{2}$ pulse which is preceeded by an ASE prepulse of 1 ns duration and $10^{11} \mathrm{~W} / \mathrm{cm}^{2}$ peak intensity. Both pulses peak at 1 ns (simulation time). The meaning of all the input parameters is explained in 'Explanation of the input parameters' section. A third example for the simulation of a Ne-like x-ray laser experiment is also given in 'Changing the input data' section .
alioofs: al target planar geom 0.268 um
2 PULSES: $100 \mathrm{FS}, 1 . E 17 \mathrm{~W} / \mathrm{CM}^{\wedge} 2$ ON TOP OF 1NS $1 . E 11 \mathrm{~W} / \mathrm{CM} 2$ ASE DEGENERATE GAS, E BALANCE, ANABS $=0.25$

```
$NEWRUN
XAMDA1=0.268E-6, TON=0., TOFF=1.,
GAUSS=1.0, ANPULS=2.0,
PMAX=1.E15, PLENTH=0.6E-09, PMULT=1.6666666667,
XASER1 (38)=1.E21, XASER1 (42)=60E-15, XASER1 (46)=16666.66667,
    NGEOM=1, PIQ(55)=2.0,
        MESH=65, RINI=4.5E-6, RHOGAS=2700., RF1=0.9999,
        XZ=13., XMASS=27., FNE=1.0,
            ZGLAS= 20., DRGLAS=.5000E-06, ROGLAS=2700., RF2=0.8711,
            XZ2=13.0, XMASS2=27.00, FNE2=1.0,
                ZPLAS=00., DRPLAS=0.00E-06, ROPLAS=2700., RF3=0.9999,
                XZ1=13., XMASS1=27., HYDROG=0.0,
        TEINI=11604.5000, PIQ(86)=11604.50, PIQ(89)=11604.50,
        TIINI=11604.500, PIQ(87)=11604.50, PIQ(90)=11604.50,
        PIQ(92)=1., PIQ(93)=1., PIQ(94)=1.,
        PIQ(85)=1., PIQ(88)=1., PIQ(91)=1.,
    NLHF=T, NLTNL=T, NLOMT3(10)=T, FLIMIT=10.,
    NLBRMS=T,
    NLCRI1=T, ANABS=0.25, FHOT=0.0, FTHOT=-1.0, RHOT=1.0,
    NLPFE=F, STATE=0.0, SAHA=2.0,
        ICXRL=0, ISTAGE=1,
        IFRSTA=1, ILOSTA=0, IHISTA=3,
        IDRFLG=0, DRMUL=1.0,
    NLRES=F,
    NPRNT=100., TSTOP=1.1E-9, NRUN=999999, DTMAX=1.E-11,
    NP3=1, NLEMP=F,
    $END
```

You will also need a command (DCL) file to run on the DEC ALPHA or a script file to run on the UNIX farm or COLUMBUS. Examples of these files are given in the following sections. Copies of all the files listed in this manual can be obtained from directory DISK_USER3:[AD1.PUBLIC] on machine AXPRL2.RL.AC.UK.

### 2.3 Running on the DEC ALPHA

The TCP/IP address for DEC ALPHA is AXPRL2.RL.AC.UK (or 130.246.12.10). In addition to the input data file, a DCL command file is needed to run med103 on the DEC ALPHA. An example is listed below.

```
! COMMAND FILE MED103.COM TO RUN MED103 ON AXPRL2
$SET DEFAULT DISK_USER3:[AD1.MED103]
$FORTRAN/REAL_SIZE=64/ALIGN=ALL MED103
$LINK/EXECUTABLE=MED103 MED103
$ASSIGN AL100FS.DAT FORO05
$CREATE/DIRECTORY WEEK_DISK:[PUBLIC.HEEK.AD1]
$ASSIGN WEEK_DISK:[PUBLIC.WEEK.AD1]DAL100FS.OUT FOR006
$ASSIGN WEEK_DISK:[PUBLIC.WEEK.AD1]XAL100FS.OUT FORO11
$ASSIGN WEEK_DISK:[PUBLIC.WEEK.AD1]IAL100FS.OUT FORO12
$ASSIGN WEEK_DISK:[PUBLIC.WEEK.AD1]FAL100FS.OUT FORO13
$ASSIGN WEEK_DISK:[PUBLIC.WEEK.AD1]RAL100FS.OUT FORO15
$DELETE *.LIS;*
$DELETE *.OBJ;*
$DELETE *.MAP;*
$RUN MED103
$DELETE MED103.exe;*
$DEASSIGN FOROO5
$DEASSIGN FOR006
$DEASSIGN FORO11
$DEASSIGN FORO12
$DEASSIGN FORO13
$DEASSIGN FORO15
$EXIT
```

The first line is a comment line. The next line sets the default working directory to the directory where MED103.FOR and the input data are kept on the DEC ALPHA. You will have to change this to point to the directory where you keep your files. The next two lines compile and link the code. the executable file is given the name MED103. The next line assigns an input data file to fortran stream 5 so it can be read by the code. MED103 reads its input from stream 5. In this case the input file is AL100FS.DAT.
The next line creates a subdirectory on WEEK_DISK for writing the output. In this version of the command file all the output from the code is written in the temporary directory WEEK_DISK. Files in this directory are inspected at midnight each night and are deleted if they are more than 7 days old. If you want to keep any of the files in the WEEK directory you should copy them to your own disk space. The next 6 lines assign the streams to various output file names. MED103 produces a number of output files depending on the input. Data is always output on stream 6 (OAL100FS.OUT in this case), stream 13 (FAL100FS.OUT) and stream 15 (RAL100FS.OUT). OAL100FS.OUT will contain details of the input data and defaults set by the program plus all the output data in an easy-to-read form (see section 3 for some sample output). FAL100FS.OUT contains the hydrodynamic variables in a form suitable for the graphics package FLIP3. Stream 12 (IAL100FS.OUT) contains the ionization data in a form suitable for ION3. Stream 11 (XAL100FS.OUT) contains the X-ray laser output in a form suitable for the graphic package XRLREC3 or XRLCOL3. Streams 15 is used for the restart feature. The code dumps all variables specifying the target on stream 15 (RAL100FS.OUT) (every time it produces an output on stream 6). When restarting a previous run the code reads the necessary variables from stream 15.

The next 3 lines clear some disk space by deleting files which were created during the compilation and link stage and are no longer needed. The next line runs the programme. The following line deletes the executable file MED103. If you do not want to recompile the code every time you run it, you can keep the executable file MED103 by putting a comment (!) in front of it. The next 7 lines deassign all the fortran streams and finally the jobs terminates.
Batch jobs are submited to the DEC ALPHA using the standard DCL command SUBMIT. To run this DCL command file as a batch job you will have to enter something like

SUBMIT/QUEUE=LONGQ/NOTIFY MED103
Almost immediately you will be sent a message.

```
JOB MED103 (QUEUE LONGQ, ENTRY 205) PENDING
    pending statuS CauSEd by queue stopped STate
```

20.5 is the job number. If for some reason you decide to cancel this job type

DELETE/ENTRY=205 LONGQ
If the job is already executing you should specify LONGQ_EXEC instead of LONGQ as in

## DELETE/ENTRY=205 LONGQ_EXEC

When the job starts running a LOG file MED103.LOG is created in your top directory. Any error messages (total amount of CPU time used when the job finishes) are written to this file.
You can find out about the status of your batch job by typing

## SHOW QUEUE/BATCH

The queue LONGQ has a maximum time limit of 6 hours. To allow for batch jobs requiring different resources, a number of different queues are available. You can find out the names, limits etc ... of the other queues by typing

## SHOW QUEUE/BATCH/FULL

this will list all the queues and also give you the maximum amount of CPU time allowed on any one queue.
When the job has finished you will be sent a message such as
JOB MED103 (QUEUE LONGQ_EXEC, ENTRY 250) COMPLETED
Any output files will be sent to the files specified in the ASSIGN statements above. More help on the different commands can be obtained interactively using HELP. for example
heLP SUBMIT
There are also a number of online documents including a user's guide for the Alpha. To find out the list of available documents type

DIR RALCCD_DOCUMENTATION
Both text and postscript versions of the files are available. The file names for the user guide are RALCCD_DOCUMENTATION:ALPHA_VMS.TXT and
RALCCD_DOCUMENTATION:ALPHA_VMS.PS. These can be printed on one of the printers at RAL or transferred to the users home and printed locally.

### 2.4 Running on OSFSERV Unix farm

The TCP/IP address for OSFSERV is osfserv.rl.ac.uk (or 130.246.104.2). Jobs are run on the OSFSERV Unix farm using a script file. Note that the Unix operating system is case sensitive (unlike VMS on the DEC ALPHA). A script file for ruming med103 (med 103.scr) is shown next

```
# medi03.scr:
# QSUB -mb -me
# 0$ -eo
# O$ -q long
# @$ -lt 360:00
# 0$
#
cd /home/osfserv/ad1/med103
ln -f -s -/med103/xal100fs.out fort.11
ln -f -s -/med103/ial100fs.out fort.12
ln -f -s -/med103/fal100fs.out fort.13
ln -f -s -/med103/ral100fs.out fort.15
f77 -o med103 -r8 -align dcommons med103.for
med103 < "/med103/al100fs.dat > "/med103/oal100fs.out
```

The first line is a comment line. The next line sends a mail at beginning and end of request execution. This can then be checked using the command elm for example. The next line directs all error messages that are normally appended to the standard error file (stderr) to the standard output file (stdout). The next lines queues the request in the long queue. Other currently available queues are short, medium and large queues. The next lines set a limit of 360 minutes and the following two lines are comments.
The line beginning with ed changes directory to where the med103 files are kept. You should change this to point to the directory where you keep your files. The next line links the file xal100fs.out to fortran stream 11 and the linking to files is repeated for stream 12, 13 and 15. Stream 11 (xal100fs.out) contains the X-ray laser output in a form suitable for the graphic package xrlrec3 or xrlcol3. Stream 12 (ial100fs.out) contains the ionization data in a form suitable for the ion3 package. Stream 13 (fal100fs.out) contains the hydrodynamic variables in a form suitable for the graphics package flip3. Streams 15 is used for the restart feature. The code dumps all variables specifying the target on stream 15 (ral100fs.out) (every time it produces an output on stream 6). When restarting a previous run the code reads the necessary variables from stream 15.
Under Unix if a file already exists and a new file is created with the same name, the new file will override the old one. The old data is therefore lost. This is unlike VMS where the new file is given a different version number from the old, thus keeping the old data.
The line beginning with $\mathbf{f 7 7}$ compiles and links the file med103.for in double precision and creates the executable file med103. If you do not want to recompile the code every time you run it, you can keep the executable file med 103 by putting a comment (\#) in front of $\mathbf{f 7 7}$. The final line runs med103 and reads the standard fortran input (stream 5) from al100fs.dat and writes the standard output (stream 6) in file oallo0fs.out.
Batch jobs are submited to the Network Queuing System (NQS) using the standard command qsub. To run the above script file as a batch job just type
qsub med103.scr
Almost immediately you will be sent a message.
Request 18821.osf01.cc.rl.ac.uk submitted to queue: long.
18821.osf01 is the request-id.

You can find out about the status of your batch job by typing

## qjob

This also tell tells you on which host your request is running (osf01, osf02, osf03, osf04 or osf05). If for some reason you decide to cancel your request and assuming your request is queued on osf03.cc.rl.ac.uk type
qdel -h osf03 18821.osf01
If the job is already executing you should also specify $-k$

```
qde1 -k -h osf03 18821.osf01
```

The queue long has a maximum time limit of 24 hours. To allow for batch jobs requiring different. resources, a number of different queues are available. You can find out the names, limits etc ... of the other queues by typing

```
more /usr/local/doc/osfserv/nqs_limits.txt
```

this will list all the queues and also give you the maximum amount of CPU time allowed on any one queue. When the job has finished you will be sent a mail which you can view using elm for example. The file med103.scr. 018821 which contains any error messages is also created. More help on the different commands can be obtained interactively using the command man. for example

## man qsub

There are also a number of online documents including a user's guide for OSFSERV. To find out the list of available documents type

## Is /usr/local/doc/osfserv

Bot text and/or postscript versions of the files are available. The file names for the user guide are/usr/local/doc/osfserv/osflgd.txt and /usr/local/doc/osfserv/osf1gd.ps. These can be printed on one of the printers at RAL or transferred to the users home and printed locally.

### 2.5 Running on COLUMBUS

The TCP/IP address for COLUMBUS is columbus.rl.ac.uk (or 130.246.12.27). A script file for running med 103 on columbus (med103.scr) is shown next

```
# med103.scr:
# @$
cd /home/columbus5/ad1/med103
ln -f -s /home/columbus5/ad1/med103/xal100fs.out fort.11
ln -f -s /home/columbus5/ad1/med103/ial100fs.out fort.12
ln -f -s /home/columbus5/ad1/med103/fal100fs.out fort.13
ln -f -s /home/columbus5/ad1/med103/ral100fs.out fort.15
f77 -o med103 -r8 -fast -align dcommons med103.for
med103 < /home/columbus5/ad1/med103/al100fs.dat > oal100fs.out
```

This is similar to the script file used in osfserv (see section 2.3 for an explanation). Batch jobs are submited to the Network Queuing System (NQS) using the standard command qsub. To run the above script file as a batch job just type
qsub -q e2 med103.scr

Notice the queue name (e2) is now given in the command line instead of the script file. Almost immediately you will be sent a message.

Request 16104 is submitted to queue e2.
16104 is the request-id.
You can find out about the status of your batch job by typing
qstat
If for some reason you decide to cancel your request type
qdel 16104
If the job is already executing you should also specify $-k$
qdel -k 16104
The queue $\mathbf{e} 2$ has a maximum time limit of 6 hours. To allow for batch jobs requiring different resources, a number of different queues are available. You can find out the names, limits etc ... of the other queues by typing
more /usr/local/doc/columbus/batch_queues.txt
this will list all the queues and also give you the maximum amount of CPU time allowed on any one queue. When the job finishes, any error messages are written to the file med103.scr.e. More help on the different commands can be obtained interactively using the man command. for example man qsub

There are also a number of online documents. To find out the list of available documents type
Is /usr/local/doc/columbus

## 3 Changing the Input Data File

This is the most important part of the process by which you may edit the input data file in order to create the conditions you desire. MED103 reads in data using NAMELIST. The NAMELIST is a non-standard FORTRAN extension that works on COLUMBUS, OSFSERV, the DEC ALPHA and other machines (although the control character may change from a dollar to something else). A typical data file may look like this (GE1C.DAT)

```
GE TARGET (NE-LIKE SCHEME) MODELLED IN planar GEOMETRY
100 mic wide ( }99.5\mathrm{ micron , 0.5 micron Ge) anabs=0.20
I=2.0e13W/cm2 gaussian ,1.06 micron,Ideal Gas
************************************************************************
    $NEWRUN
    XAMDA1=1.06E-6, GAUSS=1.0, PMAX=2.0E17, ANPULS=1.0,
    PLENTH=0.36E-09, pmult=1.389, toff=1.0e-06,
        MESH=40, RINI=99.5E-6, RHDGAS=5323., RF1=0.4232,
        XZ=32.0, XMASS=72.61, FNE=1.0,
            ZGLAS=10., DRGLAS=0.250E-06, ROGLAS=5323., RF2=0.9999,
            XZ2=32., XMASS2=72.61, FNE2=1.0,
                ZPLAS=20., DRPLAS=0.250E-06, ROPLAS=5323., RF3=0.9181,
            XZ1=32., XMASS1=72.61, HYDROG=0.0,
    NGEOM=1, PIQ(55)=0.0, TEINI=300.,TIINI=300.,
    NLRES=f, NPRNT=-100,TSTOP=1.00e-09, NRUN=999999,
    NP3=1, NLEMP=F,
    NLBRMS=T, FLIMIT=10.0,
    NLCRI1=T, ANABS=0.20, FHOT=0.0, FTHOT=-1.0, RHOT=1.0,
    NLPFE=f, state=0.0, saha=2.0,
        ICXRL=1, ISTAGE=4,
        IFRSTA=1, ILOSTA=09, IHISTA=11,
        IDFLG=0, ROPMUL=1.0, ITBFLG=0, ISTFLG=0,
        idrflg=1, drmul=1.0, IPUFLG=0,
            NLMAX=2, FL(1)=0.10e00,fI(2)=0.30,
        ak1=1., ak2=1., ak3=1., ak4=1., ak8=1., ak9=1.,
    $END
```

There is a space in the first column of this file before the $\$$, this is necessary so don't remove it. The four lines written before the $\$$ have no effect and are thus like a comment space. These lines do, however, get printed out by the code so they may be used to identify any particular run (assuming you change them). These lines are necessary as the code expects four lines of something before it starts to read the NAMELIST file. The first of these four lines is also included in the titles given to the graphics output packages so if each run is sensibly labelled it should be easier to reconcile all the MED103 output you will inevitably generate. Going through this NAMELIST file will provide a user with just about all they need to know about controlling MED103. The order in which the data appears in the NAMELIST is not significant. Also if a constant is not declared in the NAMELIST then it should default to some reasonably sensible value. This is why most input data files do not have all the control variables shown in the following list.
Note: When editing this file make sure all lines (except the last) have a comma at the end.
Below the letters C,I,R and L refer to character, integer, real and logical constants respectively. D denotes the default value. The default value may stop the code from falling over but it will not necessarily give sensible results for your problem.

### 3.1 Explanation of the input parameters

### 3.1.1 Geometry

- NGEOM (I) $\mathbf{D}=3$ This variable sets the geometry of the problem; 1 is planar, 2 is cylindrical and 3 is spherical. Note: the X-ray laser calculations will at present only work in cylindrical and planar geometries.


### 3.1.2 Laser

- XAMDA1 (R) D=10.0E-6 laser wavelength (m).
- GAUSS (R) $\mathrm{D}=\mathbf{0 . 0}$ This sets the laser pulse shape.

GAUSS $=1.0$ gives a gaussian pulse shape. A single Gaussian pulse is given by

$$
P(t)=P M A X \times \exp \left(-((t-P M U L T * P L E N T H) / P L E N T H)^{2}\right)
$$

GAUSS $=-1.0$ gives a triangular pulse given by

$$
P(t)=P M A X \times t / P L E N T H(\text { for } 0 \leq t \leq P L E N T H)
$$

and

$$
P(t)=P M A X \times(T O F F-t) /(T O F F-P L E N T H)(\text { forPLENTH } \leq t \leq T O F F)
$$

GAUSS $=-2.0$ gives a triangular pulse with a flat top (For a pecification see Fig. 1 Appendix C).

GAUSS $=0.0$ gives an isentropic pulse. For a specification of the isentropic pulse see [1] or look in subroutine laser.

- TON (R) $\mathrm{D}=0.0$ This defines the turn-on time of the laser (in s). This is normally set to 0.0 .
- TOFF (R) $\mathbf{D = 0 . 0}$ This defines the turn-off time of the laser (in s). This is normally set to a large value such as 1.0. This does not mean that you will run for a simulation time of 1 second as other control factors will stop the run well before this.
- PMAX (R) $\mathrm{D}=0.0$ This is the peak power of the laser in units of $\mathrm{W} \mathrm{m}^{-2}$ for planar targets, $W \mathrm{~m}^{-1} \mathrm{rad}^{-1}$ for cylindrical targets and $W$ ster ${ }^{-1}$ for spherical targets. Note: The summary print-out also includes a factor called PEQUIV which shows the equivalent surface irradiance in $\mathrm{W} \mathrm{cm}^{-2}$ for any of the three geometries. In this way one can check that, for example, a planar experiment modelled in cylindrical geometry has the right surface irradiance.
- PLENTH (R) $\mathbf{D}=\mathbf{0 . 0}$ In the case of one Gaussian pulse, this is the time from the peak of the laser pulse to the value at which the laser is only $e^{-1}$ of its maximum value (in s). This may be approximated to PLENTH $=0.6 \times$ FWHM.
- PMULT (R) $\mathbf{D}=0.0$ In the case of one Gaussian pulse, this is the number of PLENTH times at which the run starts before the peak of the pulse. The larger the number the slower the turn-on of the laser, this helps avoid shocks at the beginning. However, the larger the number, the longer the code will have to run and the more CPU time it will use.
- ANPULS (R) $\mathbf{D}=\mathbf{0 . 0}$ When using Gaussian pulses (GAUSS=1.), this sets the number of Gaussian pulses. Set this to $1.0,2.0,3.0,4.0$ or 5.0 . Each of the additional 4 pulses is determined by specifying the peak power, width and time of peak, in a way similar to specifying (PMAX, PLENTH and PMULT) for the first pulse. The variable which are used for this purpose are shown in Table 1, Appendix C, and an example input data file which uses two pulses can be seen in AL100FS.DAT in this manual.
ANPULS is also used to specify 2 pulses when GAUSS=-2., The variables needed to specify' the second pulse in thi case, are given in italic in Fig 1 of Appendix C.


### 3.1.3 Numerical and Target Design

MED103 was previously designed to model three layer ICF targets comprising the inner gas fill, the middle glass shell and an outer plastic shell. The code was modified to allow the user to control the contents of the inner gas fill (referenced as neon). In practise this meant that one could decide that the proportion of 'neon' was, say, $100 \%$ and that the 'neon' should have an atomic charge number of, for example, 79.0 (i. e. gold). This meant that the inner fill was solid gold. The code has now been modified to allow the user to alter not only the inner gas fill but to overwrite the 'glass' and 'plastic' constituents of the second and third shell. In this way MED103 now allows the user complete control over a three layer target. Some of the names given to the desired quantities will seem odd. This is because the modifications to MED103 have been made with the intent of making the code upwardly compatible with older versions (i. e. MED103 should run with an old data file with no modifications and produce the same results, except perhaps where a correction or modification to the physics has been made. Note however that the wavelength is now called XAMDA1, not LAMDA1).

- MESH (I) $\mathrm{D}=40$ This controls the total number of cells used in ALL THREE layers. This number should not exceed 200, but this can easily be changed in the code if necessary. The larger this number is, the more accurately the layer will be modelled but the longer the code will take to run. A typical value for MESH is 60.
- ZGLAS (R) $\mathrm{D}=0.0$ This controls the number of cells in the second layer or 'glass' layer. Note: this number is a real. If no second layer is desired then set ZGLAS $=0.0$
- ZPLAS (R) $\mathrm{D}=0.0$ This controls the number of cells in the third layer or 'plastic' layer. Note: this number is a real. If no third layer is desired then set ZPLAS $=0.0$
- RINI (R) $\mathrm{D}=4.8 \mathrm{E}-4$ This sets the thickness of the inner layer or 'gas' fill(m). Each cell will then be RINI/(MESH-ZGLAS-ZPLAS) thick, e. g. if $\mathrm{RINI}=10.0 \mathrm{E}-6$ and $\mathrm{MESH}=60$, ZGLAS $=20.0$ and ZPLAS $=20.0$ then the cell thickness in the inner layer will be $0.5 \mathrm{E}-6$ meters. The setting of this value becomes more complicated with the use of the arithmetic gridding factors (see later parameters and appendix A).
- DRGLAS (R) $\mathrm{D}=0.0$ This sets the thickness of the second layer $(\mathrm{m})$. The thickness of the individual zones is then DRGLAS/ZGLAS. If no second layer is desired then specify DRGLAS $=0.0$. (Note: if ZGLAS $=0.0$ then DRGLAS is set to 0.0 )
- DRPLAS (R) $\mathbf{D = 0 . 0}$ This sets the thickness of the third layer $(m)$. The thickness of the individual zones is then DRPLAS/ZPLAS. If no third layer is desired then specify DRPLAS $=0.0$. (Note: if ZPLAS $=0.0$ then DRPLAS is set to 0.0 )
- RHOGAS (R) D=124.0 This is the density of the inner layer or 'gas fill'. Units are $\mathrm{kgm}^{-3}$.
- ROGLAS (R) D=0.0 This is the density of the middle layer or 'glass shell'. Units are $\mathrm{kgm}^{-3}$.
- ROPLAS (R) D=0.0 This is the density of the outer layer or 'plastic shell'. Units are $\mathrm{kgm}^{-3}$.
- XZ (R) $\mathrm{D}=1.0$ This is the atomic number of the inner layer or 'gas fill' material.
- XZ2 (R) $\mathrm{D}=14.0$ This is the atomic number of the middle layer or 'glass shell' material.
- XZ1 (R) $\mathrm{D}=6.0$ This is the atomic number of the outer layer or 'plastic shell' material.
- XMASS (R) $\mathrm{D}=1$. This is the atomic mass number of the inner layer or 'gas fill' material.
- XMASS2 (R) $\mathbf{D}=\mathbf{2 8 . 0 8 5 5}$ This is the atomic mass number of the middle layer or 'glass shell' material.
- XMASS1 (R) $\mathrm{D}=12.011$ This is the atomic mass number of the outer layer or 'plastic shell' material.
- FNE (R) $\mathbf{D = 0 . 0}$ This is the fraction of the material specified by XZ, XMASS and RHOGAS that is used in the inner layer. The remaining fraction is divided equally between deuterium and tritium. This is really only useful for modelling ICF targets, to fill the inner layer entirely with a specified material set $\mathrm{FNE}=1.0$.
- FNE2 (R) $\mathrm{D}=0.0$ This is the fraction of the material specified by XZ2, XMASS2 and ROGLAS that is used in the middle layer. The remaining fraction is set to be silicon. Again, this is left-over from modelling ICF targets. To get control specify FNE2=1.0.
- HYDROG (R) $\mathbf{D}=\mathbf{0 . 0}$ This controls the fraction of hydrogen in the plastic or outer shell. If HYDROG $=0.0$ then the outer layer is composed entirely of the material specified by XZ1, XMASS1 and ROPLAS. Anything greater than 0.0 will result in a plastic of some form. For example, to obtain $\mathrm{CH}_{2}$ use $\mathrm{HYDROG}=0.67$.
As stated earlier MED103 has been altered to allow the user control over the constituent materials in all three layers. If a mixed layer is desired then the atomic numbers and mass numbers should be averaged. From the point of view of modelling the hydrodynamics, averaging the atomic and mass numbers is acceptable, providing the real density is used for the material. For example, to have a plastic layer as the inner target layer corresponding to CH then the charge number would be 3.5 and the mass number would be 6.5 with a density of $1000 \mathrm{kgm}^{-3}$. Note: this does not make sense for X-ray laser calculations (see below).
- RF1 (R) D=0.99999 This controls the arithmetic gridding in the 'gas fill' or inner layer.
- RF2 (R) $\mathrm{D}=0.99999$ This controls the arithmetic gridding in the 'glass' or middle layer.
- RF3 (R) $\mathrm{D}=0.99999$ This controls the arithmetic gridding in the 'plastic' or outer layer.

For a definition of RF1, RF2 and RF3 see appendix A. A simple fortran programme which calculates the RF value given the total thickness, the thickness of the first cell and the number of meshes is given in appendix B.
When using planar geometries it is possible to specify whether the left and right boundaries of the mesh are fixed or free. This is controlled by the variable PIQ(55). Bear in mind that MED103 treats the laser as travelling from right to left (from a high cell number towards cell number 1).

- PIQ(55) (R) $\mathrm{D}=0.0$ PIQ(55) is set to 0.0 by default and if NGEOM $\neq 1$ then the left boundary is fixed with $\mathrm{PIQ}(55)$ controlling the right boundary. A thin foil, for example, would be best modelled with $\operatorname{PIQ}(55)=2.0$. The various combinations are:
* 0.0 Left boundary fixed. Right boundary free.
* 1.0 Left boundary fixed. Right boundary fixed.
* 2.0 Left boundary free. Right boundary free.
* 3.0 Left boundary free. Right boundary fixed.


### 3.1.4 Physics

- TEINI (R) $D=1.0 E 3$ This is the initial temperature of the electrons, normally set to a value of, typically, 300 K . It is now possible to specify a different initial electron temperatures for each layer if desired (see table 2 in Appendix C).
- TIINI (R) $\mathrm{D}=1.0 \mathrm{E} 3$ This is the initial temperature of the ions, normally set to the same value as TEINI, typically, 300K. It is now possible to specify a different initial ion temperatures in each layer if desired (see table 2 in Appendix C).
- ANABS (R) D=0.0 This is the amount of laser energy that having reached critical density (i. e. having been to some extent depleted by inverse bremsstrahlung absorption) is deposited in the plasma by resonance absorption. Typically $10 \%-20 \%$ (e. g. ANABS $=0.2$ ). Note: this only works if NLCRI1=.TRUE.
- FHOT (R) $\mathbf{D}=0.0$ This is the fraction of laser energy absorbed by resonance absorption that gets converted to hot electrons, typically 0.1 . This is not the same as setting the amount of laser energy deposited by resonance absorption.
- FTHOT (R) D=0.0 This determines the way in which the code calculates the hot electron temperature $T_{H}$.
If FHOT $>0.0$ then $T_{H}=$ FTHOT $\times T_{e c}$ where $T_{e c}$ is the electron temperature at critical density. If FHOT $<0.0$ then $T_{H}=-$ FTHOT $\times f\left(I \lambda^{2}\right)$ where $f\left(I \lambda^{2}\right)$ is the LASL compilations of $T_{H}$ versus $I \lambda^{2}$.
The transport of energy of hot electrons is handled by splitting the Maxwellian distribution into 10 groups and performing a $\mathrm{dE} / \mathrm{dx}$ calculation for each group. see subroutine ABSORB for details.
- RHOT (R) D=0.0 This controls the transport of hot electron energy after the electrons have made a single pass through the target. If RHOT $=1.0$ the energy remaining at this time is deposited throughout the target uniformly. If $\mathrm{RHOT}=0.0$ then the remaining energy is lost. Typical value of RHOT is 1.0 .
- FLIMIT (R) $\mathrm{D}=\mathbf{0 . 0}$ This is the control of the flux limiter where

$$
F L I M I T=\frac{\text { classical free streaming limit }}{\text { desired flux limit }}
$$

A typical value of FLIMIT is 10.0 (i. e. the desired flux limit is 0.1 )

- PIQ(27) (R) $\mathrm{D}=0.0$ It is possible to vary the thermal conductivity of the electrons, $K_{e}$, using

$$
K_{e}=K(\text { Spitzer }) \times(1.0+P I Q(27))
$$

As all elements of the PIQ array default to zero the conductivity will be the Spitzer value by default.

- NLOMT3(10) (L) $D=F$ This controls whether non local electron heat conduction is used instead of flux limited Spitzer formulation (above). For planar geometry the formulation by Luciani et al[7] is used. This is generalized to cylindrical and spherical geometry using an approximate (and less rigorous) method.
- STATE (R) $\mathrm{D}=0.0$ The ions always have a perfect gas equation of state regardless of the value of NLPFI (see next section). If NLPFE $=\mathrm{T}$ then the electrons also use the perfect gas equation of state. If $\mathrm{NLPFE}=\mathrm{F}$ then the equation of state is decided by the value given to STATE. Typically, STATE $=3.0$ is reasonable when using $\operatorname{SAHA}=1.0$. If NLPFE $=T$, this will save CPU time but the physics may not be strictly applicable to your specific situation. The values of STATE are


## * 0.0 Fermi Dirac

* 1.0 Thomas Fermi
* 2.0 Thomas Fermi with quantum corrections
* 3.0 Thomas Fermi with modified corrections to give correct solid density.
- SAHA (R) $\mathrm{D}=\mathbf{0} .0$ SAHA determines whether or not to calculate ionization equilibrium. If SAHA $=0.0$, the material is assumed to be fully ionized.
If $S A H A=1.0$ then the ionization is calculated from Saha's equation $(Z \leq 18)$ or the ThomasFermi model for higher $Z$ values.
If $S A H A=2.0$ then the ionization is calculated from the time-dependent solution of the average atom rate equations.
Note: If the X-ray laser calculations are turned on, then the ionization balance must be calculated using $\mathrm{SAHA}=2.0$.
- PONDF (R) $\mathbf{D}=\mathbf{0 . 0}$ This controls whether or not the ponderomotive force of the laser is included in the momentum equation. PONDF $=1.0$ includes the ponderomotive force. This uses a very crude prescription for the ponderomotive force and should be used with caution. The ponderomotive force is calculated in the WKB approximation only and the code calculations will be illustrative rather than quantitative (see subroutine FORMP).


### 3.1.5 Physics: Logical Switches

This section details the logical switches that control whether certain pieces of physics are to be included in the calculation. If switch=.TRUE. (or T) the part is included, if switch=.FALSE. (or F) it is not.

- NLTNL ( $L$ ) $D=F$ This controls whether tunnel ionization is included in the average atom rates.
- NLABS (L) $\mathbf{D = T}$ This controls whether the absorption of laser radiation by inverse bremsstrahlung is included in the calculation.
- NLHF (L) D=F This controls whether a high field correction is applied to the absorption of laser radiation by inverse bremsstrahlung.
- NLBRMS (L) $\mathbf{D = T}$ This controls whether radiation from bremsstrahlung in the plasma is included in the calculation.
- NLBURN (L) $\mathrm{D}=\mathrm{T}$ This controls whether burning of fusion fuel is included in the calculation.
- NLCRI1 (L) $\mathbf{D}=\mathbf{T}$ This controls whether any laser energy is dumped at critical density in the calculation.
- NLDEPO (L) D=T This controls whether any energy from fusion products is included in the calculation.
- NLECON (L) $D=T$ This controls whether electron heat conduction is included in the calculation.
- NLICON (L) D=T This controls whether ion heat conduction is included in the calculation.
- NLFUSE (L) D=T This controls whether fusion from D-D, D-T and D-He3 (if present) is included in the calculation.
- NLMOVE (L) D=T This controls whether fluid motion is included in the calculation.
- NLPFE (L) D=T This controls whether the equation of state for electrons is the perfect gas EOS.
- NLPFI (L) $\mathrm{D}=\mathrm{T}$ This controls whether the equation of state for ions is the perfect gas EOS.
- NLX (L) D=T This controls whether ion-electron collisional relaxation is included in the calculation.


### 3.1.6 Run Control

- NLRES (L) $\mathbf{D}=\mathbf{F}$ This switch specifies if the code should restart a previous run. If this switch is set to true ( T ), the code will read the previous simulation dump from fortran stream 15 and carry on from there.
- TSTOP (R) D=1.0E-6 This is the time in the simulation at which the calculation stops (units are seconds).
- NRUN (I) $D=100$ This is the maximum number of time steps that the code is allowed to run for. Set this to something large (e. g. 80000) so that the code will always terminate because of TSTOP rather than NRUN - this makes it easier to terminate the run exactly when you want.
- NPRNT (R) $\mathbf{D = 1 0 0 . 0}$ This is the number of time steps between printer (and restart and graphics files) dumps. If NPRNT is negative then this number becomes the number of picoseconds between successive printer (and restart and graphics files) output. For example, to produce a printout every 100 femtoseconds use NPRTNT=-0.1.
- NLEMP (L) D=T This controls whether you receive reams of diagnostic print-out when the code falls over. Probably best set to .FALSE.
- NP3 (I) $\mathrm{D}=(\mathrm{MESH} / 20)$ This how often the range of cells is sampled in order to provide output for the printer and graphics dumps, i. e. it is part of a construct

```
        DO 10 I=1,MESH,NP3
                        WRITE ...
10 CONTINUE
```

Set $N P 3=1$.

### 3.1.7 Code Control

This section lists some of the parameters available to the user for altering some of the numerical parameters in the code. Generally, these values should not be altered unless a specific problem is encountered, it is best to seek advice.

- DELTAT (R) $\mathbf{D}=1.0 \mathrm{E}-18$ This is the initial timestep, the code will automatically choose its own value for this after a few time steps. Something small, typically $10^{-18} \mathrm{~s}$ (the defanlt) is recommended.
- DTMAX ( R ) $\mathrm{D}=1 . \mathrm{E}-09$ This is the maximum time step that the code is allowed to use.
- AK0 (R) D=5.0 The is the maximum allowable ratio of successive time steps. Set AK0 to something large (e. g. 100.0) if message 'time centering is damaged' appears.
- AK1, AK2, AK3, AK4, AK5 (R) $\mathbf{D}=\mathbf{0 . 2 5 , 0 . 2 5 , 0 . 2 5 , 0 . 2 5 , 0 . 0}$ These numbers control the choice of timestep by the code. Refer to routine TIMSTP. AK1 controls the CFL condition: $\Delta t<\Delta r / c_{s}$. AK2-4 control the range of density, ion temperature and electron temperature respectively, AK5 is not used at present.
- AK8, AK9, (R) $\mathrm{D}=\mathbf{0 . 2 5 , 0 . 2 5}$ These numbers also control the choice of timestep by the code when usind the average atom model (SAHA=2.). Refer to routine TIMSTP. AK9 was introduced to control the change in average ionization state (useful when tunnel ionization is switched on). AK8 was introduced to control the change in energy input in a given computational cell (useful when simulating high peak power short pulses). Note: AK6 and AK7 are not used at present.
- NLITE ( $\mathbf{L}$ ) $\mathrm{D}=\mathrm{T}$ This is a logical switch that controls iterations on $T_{i}, T_{e}$ and $U$ (the internal energy). Since the thermal conductivity is non-linear it is best to iterate. Calculations which have electron thermal conduction switched off could set NLITE $=\mathrm{F}$.
- DUMAX, DTEMAX, DTIMAX (R) $\mathbf{D}=0.1,0.1,0.1$ The maximum fractional change in $U, T_{e}$ and $T_{i}$ which represent acceptable convergence.
- NITMAX (I) $D=5$ The maximum number of iterations before code stops due to the iterations failing to converge.


### 3.1.8 X-Ray Laser Calculations

One of the major new additions in MED103 and MED101 are subroutines for calculating X-ray laser gain in collisional [5] as well as recombining plasmas [6]. The recombining option is suitable for the three main single active electron atom/ion lasing schemes (i. e. H-like, Li-like and Na-like) and the collisional option is only implemented for the Ne-like scheme. An option for modelling photopumping is included. The x-ray laser subroutines are an integral part of MED103 but are switched off by default so that users only interested in modelling hydrodynamics may do so by setting (ICXRL=0).
When X-ray laser gain is calculated the non-LTE time dependent average atom model should be used to calculate the fractions of different ion stages within the plasma by setting SAHA=2. The Xray laser data output includes gain as a function of radius for every time frame dumped, refraction of the X-ray beam (based upon the width and length of the X-ray laser target which is supplied by the user) and a spatially integrated measure of gain that may be compared directly with the experimental results of X-ray laser experiments [6]. All of this data is printed out on the standard MED103 printout but is also written to data files for interpretation by the graphics packages. The X -ray laser code will run in cylindrical and planar geometries.

There is also an option to add a scaling factor to the opacity of the resonance lines when using the average atom model. This is by default set to zero (i. e. no absorption of the resonance line is included), if the scaling factor flag is set equal to 1 then a variable scaling factor may be used (this has been included to investigate the best agreement with recombination experimental results).
As a sub-set of the X-ray laser calculations the spatially dependent ion densities of selected ionic species may also be output. Only the ground state number densities are calculated (typically $90-99 \%$ of the ions are in their ground state). An option is supplied to calculate exactly what percentage of all of the ion states is in the ground state.
All of these options are controlled by various switches and variables now included in the NAMELIST file. For the Integer type switch set the variable equal to 1 for the particular calculation to be carried out.
Note: in X-ray laser calculations pure atomic numbers and atomic mass numbers (XZ and XMASS etc.) must be used. However the real densities of the target materials should be used. For example. to model the carbon in a plastic target in an X-ray laser calculation use a density of $1000 \mathrm{kgm}^{-3}$ (if it uses a plastic target) rather than using the higher density appropriate for pure carbon, but with a charge number of 6 and a mass number 12 .

- ICXRL (I) $\mathrm{D}=0$ This is a switch that controls whether the X -ray laser calculations are to be included.
- ISTAGE (I) $\mathbf{D}=1$ This controls the scheme used in the calculation:

1 H-like
2 Li-like
3 Na-like
4 Ne -like

- DLAMDA (R) $\mathrm{D}=81.0 \mathrm{E}-8$ If ISTAGE $\leq 3$, DLAMDA is the wavelength of the main X-ray lasing transition (units are cm ).
- IFRSTA (I) $\mathbf{D}=\mathbf{0}$ This is a switch that controls whether the spatially dependent ion densities are included in the calculation. This can only be carried out at present when SAHA $=2$.
- IDFLG (I) $\mathrm{D}=\mathbf{0}$ This is a switch that controls whether trapping of the resonance line is included in the calculation of the average atom level populations.
- ROPMUL (R) $\mathbf{D}=0.0$ This is the scaling factor that alters the escape factor of the resonance line in the calculation. Set equal to 0.0 if no trapping is desired (or set IDFLG=0), set $=1.0$ if full trapping is to be included. Any other value chosen for this variable is up to you.
- ITBFLG (I) $\mathrm{D}=10$ No thermal band. 1 Forces the population of the highest level to be in LTE.
- ISTFLG (I) $\mathbf{D}=0$ This controls whether motional Stark broadening is to be included in the calculation (NB: Only data for carbon is at present included). 0 Motional Stark broadening is not included. 1 Motional Stark broadening is included on the Balmer alpha line.
- IPUFLG (I) $\mathrm{D}=0$ This controls whether photopumping is to be included in the calculation.
- TPON (R) D=0.0 This is the time at which the photopumping is switched on (units are seconds).
- TPOFF (R) $\mathbf{D = 0 . 0}$ This is the time at which the photopumping is switched off (units are in seconds).
- NLP (I) $\mathrm{D}=0$ This is the lower level (corresponding to the principal quantum number of the state in question) with which a coincidence photopumping line is to be included.
- NUP (I) $\mathbf{D}=\mathbf{0}$ This is the upper level (corresponding to the principal quantum number of the state in question) with which a coincidence photopumping line is to be included.
- RMPD (R) $\mathbf{D}=\mathbf{0 . 0}$ This is the modal photon density of the pumping radiation.
- FLSHORT (R) $\mathbf{D}=0.1$ This is the short length of the X-ray laser gain medium (i. e. the width of the gain region), units are in cm . (This is the same as FL(1))
- FLLONG (R) $D=1.0$ This is the long length of the X-ray laser gain medium, units are in cm . (This is the same as FL(2))
The sub-set of the X-ray laser calculations that allows the spatially dependent ion densities of selected ion species in ground state to be calculated are controlled by ILOSTA and IHISTA. These specify the range of ionization stages that the calculation will use.
- ILOSTA (I) $\mathbf{D}=1$ This is the number of electrons in the most ionized ion to be considered (the ion with the least bound electrons). For example, if ILOSTA $=0$ then the code will supply data on completely stripped ion densities, if ILOSTA $=1$, H -like ions, and so on.
- IHISTA (I) $D=2$ This is the number of electrons in the least ionized ion to be considered (the ion with the most bound electrons). For example, if ILOSTA $=1$ and IHISTA=3 then the code will supply the spatially dependent ion densities of H -like, He-like and Li-like ions.
- IGSTAT (I) $\mathrm{D}=0$ This is a switch that controls whether the total number of ions in all ionization stages in the ground state, is calculated. This can be used to check whether the data supplied by the routines controlled by ILOSTA and IHISTA is reasonably valid. A high percentage of ions in the ground state means that this data is good. Note: Because this call calculates all of the possible ground state ions, it tends to eat up CPU time, so allow extra. time if you include this.


## 4 General Hints

The following section outlines briefly the steps that a user should go through in order to set up data for a run.

- Specify laser wavelength, power (check units and geometry), pulse shape and duration. For Gaussian pulses set ANPULS to the number used ( $\leq 5$ )
- Specify the target material/s. Build the target from the inner layer outwards, i. e. if only one layer is desired then use the inner or 'gas' fill layer. Check MESH is greater than (ZPLAS+ZGLAS). Check values of arithmetic gridding factor, if used. Check adjacent layers do not have a difference of more than a factor of 2 in mass (this applies when different target materials are used in different layers). For example, if layer 1 has a material with a density of $x \mathrm{kgm}^{-3}$ then if layer 2 has a material with density $2 x \mathrm{kgm}^{-3}$ then the cell size of layer 2 should be half that of layer 1 .
In specifying the physics the following applies to most normal situations:
- Always set RHOT=1.0 and $\mathrm{FTHOT}=-1.0$
- If you know the absorption in a particular experiment that you are simulating, set NLABS $=\mathrm{F}$ and $\mathrm{ANABS}=$ actual absorption. If you have no information on the amount of hot electrons generated, set $\mathrm{FHOT}=0.5$.
- The most useful way to get output over your run is to set it to print out data between $10-20$ times over the duration of the run. This is most accurately controlled by using NPRNT with a negative value so that it prints at specific times rather than using a positive value that prints out after a specific number of timesteps (the difference between print-outs then varies), i. e. $\operatorname{NPRNT}=\left[\mathrm{NT}\left[\left(\mathrm{TSTOP}^{*} 10^{12}\right) / 10.0\right.\right.$.]
- Give TIINI and TEINI identical values.
- When modelling recombination X-ray lasers, generally speaking, use cylindrical geometry. If the aim is to model a planar experiment then the code may be used provided the radius of the target is made large enough to model the plasma expansion as approximately planar. A general rule of thumb is to have the radius the same size as the width of the planar target to be modelled. This may, however, produce a plasma that cools too quickly and incorrectly model the resulting gain. If a larger radius is used the expansion will be more similar to a planar expansion. If in doubt, set at least one run to use real planar expansion and use this as the lower limit of the observed gain.


### 4.1 Common Error Messages

There are two fairly common error messages:

- TIME CENTERING DAMAGED means that the ratio of successive time steps is less than Ali $0^{-1}$. The remedy for this is to make AK0 larger, for example, set $\mathrm{AK} 0=100.0$. There is no penalty in run time and only a small likelihood of a serious numerical error.
- ITERATIONS FAIL TO CONVERGE VARIABLE $n$ IN CELL $l$. This is self-explanatory, the variable $n$ corresponds to the quantities: $1=$ velocity, $2=$ density (specific volume), $3=T_{i}$ and $4=T_{e}$. The approach should be to reduce the value of $\mathrm{AK} n$ (e. g. AK4 if $T_{e}$ fails to converge) to a smaller value. There will be an increase in run time as the values of AK $n$ are reduced but the exact amount is unpredictable.
- POPULATIONS FAILED TO CONVERGE IN CELL $n$. This will only be seen in the time dependent ionization part of the code. This normally happens only at low temperatures whenever a cell starts to heat up at the very beginning of a code run. At the start of the run the system will try to ionize very rapidly; if the timestep is too large (the timestep is determined by the hydrodynamics) then the calculation determining the ionization will fail to converge. If this only occurs at the start of the code (within 100 ps ) then ignore it - the system will settle down after a short time. If the message occurs late in the run then there may be something wrong with the way the run has been set up.
- There are messages DENSITIES/TEMPERATURES TOO LOW. These will only normally be seen if the code has been allowed to run for extremely long times (e. g. greater than $10^{-5}$ ).


## 5 Dealing with the output

When the job has finished on AXPRL2, OSFSERV or COLUMBUS (or has failed due to lack of time or space, or because of an error) all the output files will be sent to the files specified in the COMMAND or SCRIPT file. You can either view them on screen using and editor (EDIT on AXPRL2 and emacs on OSFSERV and COLUMBUS for example) or print them. you can use the LPEM command to run a preprocessor on the output files. The output can be formatted in portrait or landscape mode with either one, two or four pages to a sheet of paper. The number of lines per page and characters per line can also be altered.
The following pages which show some typical MED103 output on stream 6, obtained using the input data file below (AL100FS.DAT) where formatted using

Ipem -u2 -ol -f oal100fs.out oal100fs.pem
before being printing using
lpr oal100fs.pem
Table 1.1: title page, input data as read from stream 5 and a summary of the data. The remainder of the output comprises frames for the initial and later times (determined by the value of NPRNT) similar to tables 1.2 to 1.6
Table 1.2: Hydrodynamic conditions of target at specified times. All quantities are calculated at the cell centre except the velocity which is calculated at the cell edge. For mixtures $Z$ is the average atomic number.
Table 1.3: Laser-related variables across target at specified time. (Intensity, absorption coefficient. etc...)
Table 1.4 and 1.5: non-LTE populations from the average atom model and corresponding LTE populations for the same density and temperature. This is only printed if SAHA=2.
Table 1.6: Ground state ion fractions and densities for some ion stages specified by ILOSTA and IHISTA. This is only printed if $S A H A=2$ and IFRSTA $=1$.

## 21 ratary planar orom $0.26 \mathrm{~m}_{\mathrm{u}}$


degenarate Get, 5 belance, anabs=0.25

evmary of the input dace
veraion 103 supporting xrl H-, ki-, 8a-1ike racembination

:I mplawantatlon, Aug 1991-Dea 1996::


Table 1.1: title page, input data as read from stream 5 and a summary of the data.


Table 1.2: Ilydrodyamic conditions of target at specified time.


Table 1.3: laser-rolated variables across targel at specified time.


Table 1.1: non-LTE populations from the average atom model in each cell.


Table 1.5: ITE populations from the average atom model in each cell.


Table 1.f: Ground state ion fractions and deusities for different ion stages

### 5.1 Using the Graphics Packages

The packages FLIP3, ION3, XRLREC3 and XRLCOL3 are all available for interpretation of the files output by MED103 on streams 11, 12 and 13.

1) FLIP3 - this plots the hydrodynamic variables (velocity, density, pressure, electron and ion temperatures, and average ionization) vs. distance for different times, and also the hydrodynamic variables (cell edge and centre plus velocity etc.) vs. time for each cell
2) ION3 - this plots the ground state number density of the different ionization stages vs. distance at different times during the interaction. ION3 also displays the zoning of the run. This can be useful to ensure that there are enough cells in the regions of interest.
3) XRLREC3 - this plots the recombination X-ray laser gain vs. distance at different times, and also the space-integrated gain for different lines (i. e. alpha, beta etc.) vs. time as would as measured by experiment.
4) XRLCOL3 - this plots the Ne-like collisional X-ray laser gain vs. distance at different times, and also the space-integrated gain for different lines (i. e. alpha, beta etc.) vs. time as would as measured by experiment.
The use of the above packages on AXPRL2 is described next. The fortran files for these programmes can be obtained from DISK_USER3:[AD1.PUBLIC] on machine AXPRL2.RL.AC.UK. These packages can also be run on OSFSERV and COLUMBUS using appropriate script files.
All the graphs produced include six lines of data, (including a run name) compiled from the input data file recording, detailing most of the parameters used in that MED103 run.

### 5.1.1 FLIP3

FLIP3 reads data from stream 13 and writes to stream 16. For example, in order to display the hydrodynamic data from the example data file (AL100FS.DAT) you need a command file such the following.

```
!flip3.com
$set default disk_user3:[ad1.med103]
$fortran flip3.for
$link/executable=flip3 flip3,nag$libj06/lib,nagg$gks/lib,nag$library/lib,gks_opt/opt
$assign week_disk:[public.week.ad1]fal100fs.out for013
$assign week_disk:[public.week.ad1]fal100fs.ps for016
```

first execute the file using

## @FLIP3

then run the executable using

## RUN FLIP3

First you will be asked
DO YDU WANT TO READ DATA FOR ALL 65 POINTS? Y/N ?
Most times you should enter Y unless you want to read/plot data for a few cells only. Then you will be asked

```
DO YOU WANT TO
```

S Plot quantities vs SPACE
T Plot quantities vs TIME
X EXIT

Enter $S$ to plot quantities vs. space and $T$ to plot quantities vs. time. When plotting vs. space you will be asked
what do you want to plot

1. HYDRODYNAMIC VELOCITIES
2. DENSITY
3. PRESSURE
4. ELECTRON TEMPERATURE
5. ION TEMPERATURE
6. AVERAGE IONIZATION
7. ELECTRON DENSITY
8. RETURN TO SPACE-TIME-EXIT OPTION
```
Enter choice (0 - 7)
```

?
if you enter $1,2,3,4,5,6$ or 7 you will be asked

```
dO yOU WANT TO PLOT alL TIME FRAMES? y/N
```

If you answer Y you will be asked

```
DD YOU WANT LOGS ON THE Y-AXIS WHERE POSSIBLE? Y/N
```


## do you want the overall maxima for every time frame? y/N

Plotting the frames with the overall maxima allows comparisons to be made between the different time frames. If you answer N to this prompt each time frame will have local X and Y maxima (which will be different for every frame).
If you had entered N to the PLOT ALL TIME FRAME question you would be asked
DO YOU WANT TO SPECIFY FIRST AND LAST TIME(S) TD PLDT? Y/N
If you had entered N you will asked several questions about each time frame. These prompts are self-explanatory, if somewhat tiresome especially when there are many time frames. It is therefore advisable to specify the first and last time you want to plot.
If you had opted to plot against time by entering $T$ (instead of $S$ above) you will be prompted

```
DO YOU WANT to write data(time) in a file? Y/N
```

This is useful if you want to export the data file to another package for plotting (for example the radius as a function of time of all cells of an ICF target can be generated this way). Then you will be asked

```
WHAT DO YDU WANT TO PLOT?
```

1. CELL EDGES
2. HYDRODYNAMIC VELOCITIES
3. CELL CENTRES
4. DENSITY
5. PRESSURE
6. ELECTRON TEMPERATURE
7. ION TEMPERATURE
8. aVERAGE IONIZATION
9. ELECTRON DENSITY
O. RETURN TO SPACE-TIME-EXIT OPTION
```
ENTER CHOICE (0 - 9)
```

?

You are then given the option of only plotting part of the range on the X (time) or Y axis. You are then asked

```
dO yOU WANT TO PLOT ALL CELLS? Y/N
```

Any of the following types of responses are valid

## ALL

1 to 10
1,3,12 to 25,45
Except for the cell edges, velocities and cell centres it is not advisable to plot all the cells as the results are usually totally confusing.
Some example output from FLIP3 (and FAL100FS.OUT) are shown in Figs 1 and 2. Figure 1 a plot obtained by opting to plot log electron temperature vs. distance for all times not using the overall maxima for every time frame. Figure 2 shows the position of all cell centres plotted is. time.

### 5.1.2 ION3

ION3 reads data from stream 12 and writes to stream 15 . Therefore if your input data is in IAL100FS.OUT (as it would be if you used the COMMAND file in section 'RUNNING ON THE DEC ALPHA') and you want to call your output graphics file IAL100FS.PS, you need a command file such the following.

```
!ion3.com
$set default disk_user3:[ad1.med103]
$fortran ion3.for
$link/executable=ion3 ion3,nag$libj06/lib,nagg$gks/lib,nag$1ibrary/lib,gks_opt/opt
$assign week_disk:[public.week.ad1]ial100fs.out for012
$assign week_disk:[public.week.ad1]ial100fs.ps for015
```

first execute the file using
QION3
then run the executable using
RUN ION3
First you will be asked

```
DD YOU WANT TO PLOT ALL 65 POINTS? Y/N
```

Most times you should enter y unless you want to read/plot data for a few cells only. Then you will be asked

```
RAL GKS 1.38 ALPHA/VMS version
Enter minimum value of Y::(Default=1.40000E+01):
```

All prompts in ION3 have have sensible defaults and if you hit the ENTER key after each query you should obtain useful output.
Figure 3 shows one of the plots of ion density vs. distance (for 4 ion stages). The position of the cell edges are shown below the X -axis, allowing the zoning of the run to be monitered.

### 5.1.3 XRLREC3

XRLREC:3 plots the x-ray laser gain data for the recombination case (ISTAGE=1, 2 or 3 ). It reads data from stream 11 and writes to stream 14. Therefore if your input data is in XFPAP2.OUT and you want to call your output graphics file XFPAP2.PS, you need a command file such the following.

```
!xrlrec3.com
$set default disk_user3:[ad1.med103]
$fortran/nooptimize xrlrec3.for
$link/executable=xrlrec3 xrlrec3,nag$libj06/lib,nagg$gks/lib,nag$library/lib,gks_opt/opt
$assign week_disk:[public.week.ad1]xfpap2.out for011
$assign week_disk:[public.week.ad1]xfpap2.ps for014
first execute the file using
```


## QXRLREC3

then run the executable using

```
RUN XRLREC3
```

First you will be asked

```
DO YOU WANT TO USE ABSOLUTE TIME OR TIME RELATIVE
TO THE PEAK OF THE LASER PULSE? A/R
```

Enter A or R. You will then be asked $\mathrm{Y} / \mathrm{N}$ questions.

```
ncell 50 ngain 3
```

RAL GKS 1.38 ALPHA/VMS version
DO YOU WANT TO PLOT GAIN VS RADIUS? Y/N
You will also be given the option of plotting the alpha, beta etc. gain vs.time on separate plots and then of plotting all the gains on one plot.
Figure 4 shows some of the graphs obtained by plotting x-ray laser gain versus distance. Figure 5 shows the efective gains (spatially integrated) for Alpha, Beta and Gamma lines vs. time.

### 5.1.4 XRLCOL3

XRLCOL3 plots the x-ray laser gain data for the Ne-like collisional case (ISTAGE=4). It reads data from stream 11 and writes to stream 14. Therefore if your input data is in XGE1C.OUT and you want to call your output graphics file XGE1C.PS, you need a command file such the following.

```
!xrlrec3.com
$set default disk_user3:[ad1.medi03]
$fortran/nooptimize xrlcol3.for
$link/executable=xrlcol3 xrlcol3,nag$libj06/lib,nagg$gks/lib,nag$library/lib,gks_opt/opt
$assign week_disk:[public.week.ad1]xge1c.out for011
$assign week_disk:[public.week.ad1]xge1c.ps for014
```

first execute the file using

## @XRLCOL3

then run the executable using
RUN XRLCOL3

First you will be asked
do you want to use absolute time or time relative
TO THE PEAK OF THE LASER PULSE? A/R
Enter A or R . You will then be asked $\mathrm{Y} / \mathrm{N}$ questions.
RAL GKS 1.38 ALPHA/VMS version
dO YOU WANT TO PLOT GAIN VS RADIUS? Y/N
You will also be given the option of plotting the gain vs. time. on separate plots and then of plotting
Figure 6 shows some of the graphs obtained by plotting x-ray laser gain versus distance for the 196 Angstrom line, while Fig. 5 shows the efective gains (spatially integrated) for some lines (including the 196 Angstrom) vs. time.

AI TARGET planar GEOM 0.268um ngeom 1 prax: 1.000E+15 xandal: 2. 680E-07 plenth: 6.000E-10 pmult: 1.667E +00 fhot: $0.000 E+00 \times z: 13$. xmoss: 27. rini: 4.500E-06 xz2: 13. xmoss2: 27. fne2: 1. drglas: 5.000E-07 xz 1: 13. xmass1: 27. drplas: 0 . 000Et00 mesh: $65 \mathrm{zglas:} \mathrm{20}. \mathrm{zplas:} 0$. rf 1: 9.999E-01 rf2: 8.711E-01 rf3: 9.999E-01 xrl of $f$ dlanda: $0.000 E$ +OOAngstroms pequiv: $1.000 E+15 \mathrm{w} / \mathrm{m*} * 2$ opocity corrections of $f$


Figure 1: FILP3 output - Log electron temperature vs. distance.
Al TARGET planar GEOM 0.268 um ngeom 1 prrax: 1.000E+15
xamda1: 2.680E -07 plenth: $6.000 \mathrm{E}-10 \mathrm{pmul} \mathrm{t}: 1.667 \mathrm{E}+00$ fhot: $0.000 \mathrm{E}+00 \mathrm{xz}: 13$.
xrass: 27. rini: 4.500E-06 xz2: 13. xnass2: 27. fne2: 1. drgl as: 5. 000E-07
xz1: 13. xmass1: 27. drplas: $0.000 \mathrm{t}+00$ mesh: $65 \mathrm{zglas:} \mathrm{20}. \mathrm{zplas:} 0$.
rf 1: 9.999E-01 rf 2: 8.711E-01 rf3: 9.999E-01 xrl of f dlama: 0.000E + OOAngstroms pequiv: $1.000 \mathrm{E}+15 \mathrm{w} / \mathrm{m} * * 2$ opocity corrections of $f$


Figure 2: FILP3 output - position of all cell centres plotted vs. time.

A TARCET plat GeM 0.208 m ngeon 1 prox: 1.00E+15
xandal: 2 EBCE- 07 pl entr $6.00 E-10$ pral t: 1. $6 \pi+\infty$ fhot: Q.OOE +0 xZ 13.
xnass: 27. rini: $4500 \mathrm{E}-60 \times 22$ 13. xmassz 27. frez 1. drg as $500 \mathrm{E}-07$

rf1: 9.99E-01 rf2 8.711E-01 rfz 9.99E-01 xrl of $d$ and $0.00 E+00 A n g s t r o n s$
peqi v. 1. OCE $+15 \mathrm{w} / \mathrm{m} * 2$ poci ty corecti ons off


Figure 3: ION3 output - ion density vs. distance (for 4 ion stages)

## 





peqiv. 8 万 $5 \mathbb{E}+17 \mathrm{w} / \mathrm{m} * 2$ qaci ty corections off


Figure 4: XRLREC3 output - x-ray laser gain versus distance

FLUR NE FIERE (nod103 versi ar scha=20) ngean 2 prax: $3.50 \mathrm{E}+12$

xnuss: 19 rini: $4000-66$ x2: 0 xnuss2 0 fne2 1. dg as $000 E+\infty$

rf1: 9.00E-01 rf2 9. $99 E-01 \mathrm{rf} 39.99 E-01 \mathrm{xrl}$ an d andr \& 100E+OIAngstrans
peqi v. 8 万 $5 E+17 \mathrm{w} / \mathrm{m} * 2$ qai ty corections off

MED103 + XRLREC3 GAI N ON ALL LI NES VERSUS TI ME(PS)


Figure 5: XRLREC3 output - efective gains (spatially integrated) for Alpha, Beta and Camma lines vs. time.

CE TARCET (NEHIKE SOEME) NOCELED IN p anar CEngeorn 1 prox: 2 ONE 17
xardal: 1. OSE- 06 plentr $3.60 E-10$ pral t: $1.38 E+\infty$ f hat: $0.00 E+\infty 0 \times 2$



peqi v. $200 E+17 \mathrm{w} / \mathrm{n} * 2$ pacity corections off


Figure 6: XRLCOL3 output - X-ray laser gain versus distance

CE TARCET (NE LIKE SOEME) MODELD IN p anor CEngean 1 prox: $200 E+17$

xnuss: 73 rini: 9950 -65 xe2 32 xussiz 73. frez 1. of as $250 \mathrm{E}-07$
x21: 32 xrosst 73 drpl os $250 \mathrm{E}-07$ nast: 40 zglos 10. यp as: 20.
rff: 4.232-0irfz 9.99EE-01 rf3 9.181E-01 xrl an glos. 10. zplas 20.
peqiv. $200 E+17 \mathrm{w} / \mathrm{mm*2}$ qoi ty corections off


Figure 7: XRLCOL3 output - efective gains (spatially integrated) for some lines vs. time

## 6 Summary

It is hoped that this guide will provide enough detail for any user to run MED103. If you have any problems contact The Theory Group. The users are also advised to keep an unmodified version of the code and to include all personal additions/modification in a new version. When encoutering problems they should run the original version of the code and if the problem re-occurs, then contact the Theory Group with a copy of the input data file.
If people are actively engaged in writing some piece of code that changes the physics, this may be of interest to other users and we would like to hear about it. If some important piece of physics is lacking then of course, it would be our aim to include this in future versions of MEDUSA.

## References

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[6] GJ Pert and SJ Rose, Appl. Plys. B, 50, 307, (1990)
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## APPENDICIES

## A Arithmetic gridding

A further modification made in MED103 is the option of arithmetic gridding (this is where the thicknesses of the cells gradually increases or decreases within a layer rather than remaining identical). Each of the 3 layers may be altered independently. The gridding is based upon the formula:

$$
\begin{gathered}
w_{i}=\left(\frac{r_{j}^{i}-1}{r_{j}^{n}-1}\right) \times S \\
\Delta_{i}=w_{i}-w_{i-1} \\
\Delta_{1}=w_{1}
\end{gathered}
$$

where $w_{i}$ represents the co-ordinate relative to zero of the $i$ th cell boundary, $\Delta_{i}$ is the width of the $i$ th cell, $n$ is the number of cells in the layer, $i$ varies from 1 to $n$ and $S$ is the thickness of the layer (i. e. RINI, DRGLAS or DRPLAS). The factor in brackets varies between 0 and 1 depending on $i$ and the difference in cell thickness from one cell to the next is controlled by $r_{f}$ (i. e. RF1, RF2 or RF3).
If $r_{f}$ is almost but not quite equal to 1.0 (e. g. 0.99999 ) then the gridding will be linear as in the old versions of MEDUSA.
If $r_{f}=1.0$ the denominator is zero so the code resets any input from 1.0 to 0.99999 . This is also the default so to obtain a linear mesh either $r_{f}=1.0$ or $r_{f}=0.99999$ can be used.
It is only possible to fix any three of the four quantities $r_{f}, n, S$ and $\Delta_{1}$ (or any $\Delta_{i}$ ). Suppose, for example, we require a layer containing 10 cells to have its first cell 10 times larger than its 10 th cell. Using the formula

$$
r_{f}=\left(\frac{\Delta_{n}}{\Delta_{1}}\right)^{\frac{1}{n-1}}
$$

we find $r_{f}=0.7743$. Given $r_{f}$ and $n$ the thickness of the layer may be specified. If we to specify the thickness of the beginning and end cell we lose control over the total thickness of the layer. To calculate the total thickness of the layer (i. e. one of RINI, DRGLAS and DRPLAS) use

$$
S=\left(\frac{r_{f}^{n}-1}{r_{f}-1}\right) \times w_{1}
$$

If, for example, we set $\Delta_{1}=10 \mu \mathrm{~m}$ and $\Delta_{10}=1 \mu \mathrm{~m}$ then the total thickness of the layer MUST be $40.87 \mu \mathrm{~m}$. Alternatively if we set $S=100 \mu \mathrm{~m}$ (with $n=20$ and $r_{f}=0.8361$ ) then $w_{1}=24.47 \mu \mathrm{~m}$ and $w_{10}=2.447 \mu \mathrm{~m}$.
It is not possible to control the number of cells, the ratio, the total thickness and the individual thicknesses simultaneously.
This facility is very useful for a number of things. It can be used to ensure that the zoning is at its finest at the edge of a target where most detail is needed, without having to set up a large number of different layers. It can be used to interface between layers of differing cell width. This helps avoid jumps in the mass between consecutive cells that may cause problems.

## B A fortran program for calculating RF1, RF2 and RF3

```
c Program to calculate rf value when thickness of first zone,
c total thickness of shell and number of zones are specified
    PROGRAM MAIN
    IMPLICIT DOUBLE PRECISION (a-h, m-z)
    CHARACTER answer*1
c Inputting the data
    WRITE (6,1000)
1000 format(/1x,' Given the thickness of the first cell and the ',
        & 'total thickness, this code calculates the RF value',/1x)
    1 WRITE (6,*) 'Please enter Delta1(in any units): '
            READ (5,*) delta1
            WRITE (6,*) 'Please enter total thickness(same units as delta1):'
            READ (5,*) thickness
            WRITE (6,*) 'Please enter number of meshes:'
            READ (5,*) meshes
c Is the data correct????
            WRITE (6,*) , ,
    3 WRITE (6,*) 'Is the above information correct (y/n)?'
            READ (5,FMT='(A)') answer
            IF (answer .EQ. 'y' .OR. answer .EQ. 'Y') GOTO 5
            IF (answer .EQ. 'n' .OR. answer .EQ. 'N') GOTO 1
            GOTO 3
c Creating blank space
    5 DO i = 1, 1
        WRITE (6,*),'
            END DO
c Doing the calculation
    rdm = 1.0e30
    DO 10 i = 10000, 990000
            rf = float(i)*1.e-05
            IF(rf .EQ. 1.000) GOTO 10
            rd = (ABS (delta1-thickness*(rf-1)/(rf**meshes -1))/delta1)
            IF (rd .LT. rdm) THEN
                rf2 = rf
                    rdm = rd
            END IF
    10 CONTINUE
    rf = rf2
    rd = rdm
    del1=thickness*(rf-1.)/(rf**meshes-1.)
    deln=del1*rf**(meshes-1)
    delnm1 = del1*rf**(meshes-2)
    delnm2 = del1*rf**(meshes-3)
c Displaying the results
    WRITE (6,*) , RESULTS'
    WRITE (6,*) , -------'
    WRITE (6,*) Delta1 = ', delta1
    WRITE (6,*) , Total thickness =', thickness
```

```
    WRITE (6,*) ' Number of meshes = ', meshes
    WRITE (6,*) , ,
    WRITE (6,4000)rf,del1,deln,deln/delnm1
4000 format(' rf ',1pe14.7,' Delta1 = ',e14.7,' Deltan = ',e14.7,
    &' delta n/delat n-1 = ', e14.7)
    WRITE (6,5000)1/rf,deln,del1,delnm1/deln
5000 format(' rf ',1pe14.7,' Delta1 = ',e14.7,' Deltan = ',e14.7,
    &' delta n/delat n-1 = ', e14.7)
    WRITE (6,*) ' '
    WRITE (6,2000)
2000
    format(' Use rf .LT. 1 for meshes decreasing towards ',
    &'the laser beam (left to right)')
    WRITE (6,3000)
3000
    format( ' Use rf .GT. 1 for meshes increasing towards ',
    &'the laser beam ')
    WRITE (6,*) , ,
c Re-run the program???
    WRITE (6,*) ',
    20 WRITE (6,*) 'Do you want to calculate another value (y/n)? '
    READ (5, FMT='(A)') answer
    WRITE (6,*),'
    IF (answer .EQ. 'y' .OR. answer .EQ. 'Y') THEN
                GOTO 1
    ELSEIF (answer .EQ. 'n' .OR. answer .EQ. 'N') THEN
            GOTO 30
            ELSE
            GOTO 20
            ENDIF
30 STOP
    END
```


## C Special features



Figure 1: How to specify a triangular pulse with flat top (GAUSS $=-2$ ). Variables in italic are for a second pulse (ANPULS=2.).

Table 1: How to specify up to 5 Gaussian Pulses.

|  | Peak Power (Wm <br> Wm $^{-1}$ rad |
| :--- | :--- | :--- | :--- |
| 1st or Wster |  |

Table 2: How to set different initial temperatures and ionization states in the three layers.

|  | First (Inner) Layer | Second Layer | Third Layer |
| :--- | :--- | :--- | :--- |
| Initial Electron Temperature | TENI | PIQ(86) | PIQ(89) |
| Initial Ion Temperature | TIINI | PIQ(87) | PIQ(90) |
| Initial Value of Z* <br> (Averave Atom model only) | PIQ(92) | PIQ(93) | PIQ(94) |
| Minimum allowed value of $Z^{*}$ <br> (Averave Atom model only) | PIQ(85) | PIQ(88) | PIQ(91) |

