STATDOSE for 3D dose distributions

H.C.E. McGowan, B.A. Faddegon and C-M Ma
Ionizing Radiation Standards
National Research Council of Canada, Ottawa

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Source tex file is: `$OMEGA_HOME/doc/statdose/statdose.tex`

Abstract

`STATDOSE` is an interactive program for analyzing 3-dimensional dose distributions generated by DOSXYZ. This report describes the structure and functions of STATDOSE, how to compile and run STATDOSE, and the input and output requirements for plotting 1-dimensional dose distributions using the *Grace* plotting package (`xmgrace` command).

Contents

1 Introduction

STATDOSE is an interactive computer program for 3-dimensional dose analysis and plotting 1-dimensional dose distributions using the *Grace* plotting package. 3D dose data such as that generated using the EGS4 user-code DOSXYZ [1], developed at NRCC for the OMEGA project, are examples of typical dose data. STATDOSE functions include normalization, re-binning, plotting and analysis of the dose distributions. Distributions can also be compared both statistically and graphically. Graphs to aid in statistical analysis of the distributions, as well as both cross-plots and depth-doses, are provided by STATDOSE.

STATDOSE was originally written by H.C.E. McGowan and B.A. Faddegon for analyzing dose results generated by DOSXYZ and plotting dose distributions through PLOT_XVGR, a subroutine written by M. Barfels and D.W.O. Rogers. Both programs were modified and new scripts were written in order to compile and run STATDOSE on both SUN and Silicon Graphics machines. This report is a shortened version of the original program report and revised to reflect changes and additions. The following sections contain an overview of STATDOSE and a user's manual. Programming documentation is not included, as the source code, *statdose.mortran*, has extensive in-line documentation.

In order to run STADOSE one should first install *Grace* plotting package (providing the xmgrace command).

2 Description of STATDOSE

2.1 Files Related to STATDOSE

STATDOSE was written in MORTRAN3, a FORTRAN preprocessor, on a UNIX system. The executable code must be run on a UNIX system with the *Grace* graphics package and facility for running C shell scripts. Files which are essential to the operation of STATDOSE are as follows:

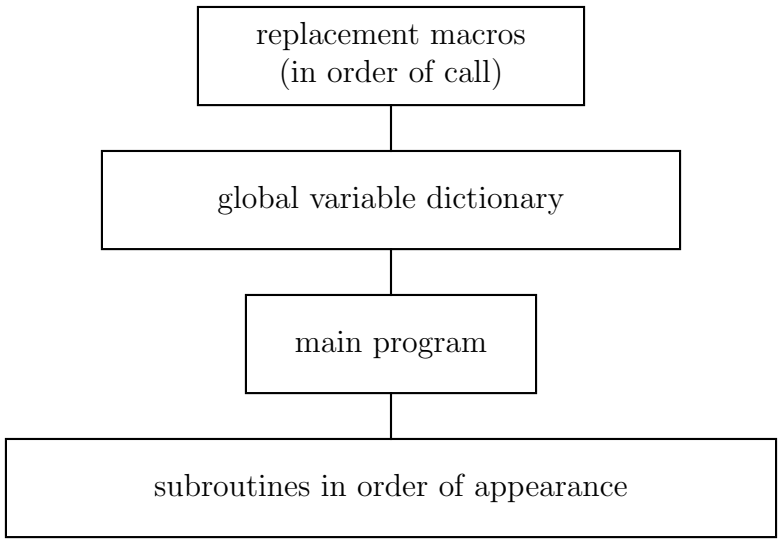
- *statdose.mortran* (MORTRAN program)
- STATDOSE (C-shell script, used to run STATDOSE)
- *compile_statdose* (C-shell script, used to compile STATDOSE)
- *plot_xvgr.f* (FORTRAN program, used to invoke xmgrace with preset options)
- *filename.3ddose* (files containing 3D dose-data generated by DOSXYZ)
- *plot_xvgr.par* (sample parameter file required by *plot_xvgr.f*)
- *plot_xvgr.bat* (sample data file required by *plot_xvgr.f*)

Files which are left behind by the operation of STATDOSE are as follows:

- *plotname.xvparam* (`xmgrace` parameter file for a plot, written by *plot_xvgr.f*)
- *plotname.xvplt* (`xmgrace` data file for a plot, written by *plot_xvgr.f*)
- *xvgr_script* (Bourne-shell script, written by *plot_xvgr.f* and used to invoke `xmgrace`)

2.2 Structure and Functions of *statdose.mortran*

The *statdose.mortran* code is written in MORTRAN3 and consists of the main program, subroutines, and MORTRAN replacement macros. The code has the following structure:



Documentation occurs at the beginning of each subroutine. There is also extensive in-line commenting. Error checking of user input is minimal.

2.2.1 Subroutines

The `STATDOSE` subroutines coincide with the menus and sub-menus used for interactive parameter selection. Choosing an option during execution will cause a subroutine specific to that task to be called. Below is a list of the subroutines and corresponding menu options. All subroutine names are italicized:

- *mainmenu* –Display Main menu
  - *readdose* –Read in Dose Distributions
  - *statsmenu* –Display Statistical Analysis menu
    - *stats* –Calculate Statistics
  - *normmenu* –Display Normalization menu

    - *scale* –Rescale Distribution
    - *averagedose* –Normalize to Average Dose
    - *centralmax* –Normalize to Maximum Dose Along Central Axis
    - *specvoxel* –Normalize to Dose in a Specific Voxel
    - *denormalize* –Restore the Original Distribution Dose Array
  - *rebinning* –Rebin a Distribution
  - *plotmenu* –Plot curves from Distributions
    - *plotdose* –Plot Profiles of one Distribution
    - *compareplot* –Compare Plot Profiles from Multiple Distributions
  - *save* –Save Distributions

There are also subroutines which perform tasks within the menu option subroutines.

- *newlettercount* –Counts the Number of Letters in a Character String
- *plotfreq* –Plots Frequency Distribution Graphs

More details are given in the documentation at the beginning of the MORTRAN code for each subroutine.

2.3 Subroutine *Plot_xvgr.f*

Plot_xvgr.f is a FORTRAN subroutine for setting various `xmgrace` plot parameters, and then creating files which pass this information on to `xmgrace` . `xmgrace` produces a graph from the information in the files. Documentation of *plot_xvgr.f* is located at the beginning of the Fortran code. This subroutine is now included in *statdose.mortran*.

2.4 Scripts

2.4.1 *compile_statdose* script

compile_statdose' is a script to MORTRAN and Fortran compile *statdose.mortran*. Depending on what machine the program is running on the executable file is saved as *statdose.$my_machine.exe* (*e.g.*, on a SUN SPARC machine $my_machine = "sparc"). In order to run `STATDOSE` on any machines one should compile `STATDOSE` on those machines by issuing the following command:

```
compile_statdose
```

2.4.2 *statdose* script

The `STATDOSE` script executes *statdose.$my_machine.exe*, depending on what machine it is running on. Two data files, *plot_xvgr.par* and *plot_xvgr.bat*, required for plotting in `xmgrace` data format are linked to logical units 11 and 31, respectively. The following command may be issued to execute *statdose*:

statdose	to run the program

3 Format of DOSXYZ 3D Dose Data

3.1 *filename.3ddose format*

DOSXYZ is a general-purpose EGS4 user code, developed for the OMEGA project, to do Cartesian coordinate dose calculations (see "DOSXYZ User's Manual" by Ma *et.al.*(1995)). The 3D dose data generated by DOSXYZ is stored in a file with extension *.3ddose*. The simulation geometry and 3D dose results are stored the following format:

Row/Block 1 — number of voxels in x,y,z directions (e.g., n_x, n_y, n_z)

Row/Block 2 — voxel boundaries (cm) in x direction(n_x +1 values)

Row/Block 3 — voxel boundaries (cm) in y direction (n_y +1 values)

Row/Block 4 — voxel boundaries (cm) in z direction (n_z +1 values)

Row/Block 5 — dose values array ($n_x n_y n_z$ values)

Row/Block 6 — error values array (relative errors, $n_x n_y n_z$ values)

General Rules of reading the dose and statistical uncertainty (error) results:

- read one by one (across columns) to get dose (error) readings in x direction
- read every (n_x)-th value to get readings in y direction
- read every ($n_x n_y$)-th value to get readings in z direction

It should be noted that `STATDOSE` is capable of analyzing dose results of format described above, not confined to the dose results generated by DOSXYZ only. This means that `STATDOSE` can be used to analyze 1D, 2D, and 3D dose results generated by other programs so long as the dose data files have the same format as described above. For 1D dose results along x-axis, for instance, one can ouput the geometry and dose data in the following format:

Row/Block 1 — number of voxels in x,y,z directions ($n_x, 1, 1$)

Row/Block 2 — voxel boundaries (cm) in x direction (n_x +1 values)

Row/Block 3 — voxel boundaries (cm) in y direction (2 values)

Row/Block 4 — voxel boundaries (cm) in z direction (2 values)

Row/Block 5 — dose values (n_x values)

Row/Block 6 — error values (n_x values)

3.2 A Sample *filename.3ddose* File

The following Table shows a sample 3D dose data and the file format. The doses are scored for a cubic geometry consisting of 4 x 4 x 4 voxels. Each voxel has a volume of 8 x 8 x 8 cm^3. The center of voxel (2,1,3) has coordinates (-4,-12,4). The dose in the voxel is 6.0, and is shown in bold face in the above table.

Row(block) Number		Column Number				
		1	2	3	4	5
1	(1)	4	4	4		
2	(2)	-16.0000	-8.0000	0.0000	8.0000	16.0000
3	(3)	-16.0000	-8.0000	0.0000	8.0000	16.0000
4	(4)	-16.0000	-8.0000	0.0000	8.0000	16.0000
5	(5)	1.0000	2.0000	2.0000	1.0000	2.0000
6		8.0000	8.0000	2.0000	2.0000	8.0000
7		8.0000	2.0000	1.0000	2.0000	2.0000
8		1.0000	2.0000	4.0000	4.0000	2.0000
9		4.0000	16.000	16.000	4.0000	4.0000
10		16.000	16.000	4.0000	2.0000	4.0000
11		4.0000	2.0000	3.0000	6.0000	6.0000
12		3.0000	6.0000	24.000	24.000	6.0000
13		6.0000	24.000	24.000	6.0000	3.0000
14		6.0000	6.0000	3.0000	4.0000	8.0000
15		8.0000	4.0000	8.0000	32.000	32.000
16		8.0000	8.0000	32.000	32.000	8.0000
17		4.0000	8.0000	8.0000	4.0000	
18	(6)	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01
19		1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01
20		1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01
21		1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01
22		1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01
23		1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01
24		1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01
25		1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01
26		1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01
27		1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01
28		1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01
29		1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01
36		1.0000 E-01	1.0000 E-01	1.0000 E-01	1.0000 E-01	

4 Running Statdose

4.1 Introduction

STATDOSE can be invoked using the script *statdose*. It is imperative that at least one dose distribution be read in before attempting any type of analysis. After a distribution is loaded, it can be normalized, rebinned, plotted and written to disk. Statistical comparisons can be performed if only two or more dose distributions have been read in, and the voxel geometries (bin boundaries) are identical.

The following section outlines the STATDOSE options and explains what each STATDOSE option will do and what input it requires. Most options have default values which are listed in brackets beside the prompt. In most cases, this default value is 0, which is synonymous with a carriage return. Entering a default value will usually bounce the program back to the previous menu. In the case where the required user input is a character string, the default value listed beside the prompt will be set by hitting carriage return.

4.2 Read Dose Distributions

The major features of the 'Read Dose Distributions' option are:

- the names of the *.3ddose* files (up to 40) in the current directory will be listed for the user
- the routine will loop, prompting first for the number of the file to read in, and then number under which to store it
- up to 5 files can be read in
- files can be read in at any time during a STATDOSE run
- previously loaded files can be overwritten
- numbering of file need not be consecutive

4.3 Statistical Analysis

In order to perform any of the statistical analysis routines, at least two distributions must be loaded. The two distributions selected for comparison must have the same structure (ie. the same number of bins and the same bin boundary values). If either of these two conditions is not met, the program will display a message and prompt the user for more input. Statistical analysis includes calculation of the chi-squared/degree of freedom and RMS deviations, the maximum absolute or percent difference in dose and the maximum dose along the central axis for the two distributions being compared. In addition, STATDOSE produces plots of the dose difference or percent dose difference distribution and of the chi-squared distribution.

First, the user specifies whether he/she wishes to deal with a dose difference distribution or a percent dose difference distribution. `STATDOSE` has 3 possible definitions for percent dose difference. Thus, the user has a total of 4 options:

Option 1 – Plot frequency vs D1-D2

Option 2 – Plot frequency vs (D1-D2)/[(D1+D2)/2)] * 100

Option 3 – Plot frequency vs (D1-D2)/[max avg central axis dose] * 100

Option 4 – Plot frequency vs (D1-D2)/SQRT(ERR1**2+ERR2**2)

Where D1 and D2 are the doses in the same voxel from the 2 distributions, and ERR1 and ERR2 are the errors in D1 and D2 respectively. Options 2 and 3 comprise the 3 different definitions of percent dose difference. In Option 2, the percentage difference is calculated with respect to the average of D1 and D2. Option 3 calculates the average with respect to the maximum average (ie average between the 2 distributions) central axis (Z-axis) dose. In Option 4, the difference of Option 1 is scaled by the square root of the sum of the errors in the two doses. Note that if there are no systematic differences between the two distributions, then we expect that Option 4 will produce a distribution with a peak at $\sim$1.

After selecting the type of distribution, the user selects one of 3 possible methods for scaling the plot. The equations used by `STATDOSE` to determine the binning structure for each scaling option are listed below:

Option 1 – Limit Frequency Distribution to Maximum Dose Difference or Maximum Percent Dose Difference

$$W_{bin} = \delta_{max}/INT(n/2-1) \tag{1}$$

Option 2 – Limit Frequency Distribution to Maximum Dose along the Central Axis

$$W_{bin} = D_{max}/INT(n/2-1) * 10. \tag{2}$$

Option 3 – Custom Bin Width

$$W_{bin} = user\ entered\ bin\ width \tag{3}$$

W_{bin} is the calculated width of the bins (bin width can be a real number), n is the number of bins desired (selected by the user), δ_{max} is the maximum dose difference, and D_{MAX} is the maximum dose along the central axis. INT is the FORTRAN type cast to an integer. Note that Option 2 above, in which the plot is limited to the maximum dose along the central axis, only makes sense if the user is plotting a dose difference distribution and, thus, cannot be chosen if the the user has selected one of the percent dose distributions.

The 2 sets of options described above apply only to the dose difference distribution, not the chi-squared distribution. The latter is always calculated the same way, regardless of whether

the user chooses a dose difference or percent dose difference distribution, and is always plotted on a scale from 0-10.

For each of the program options, the user will be asked to select the number of a file or files on which to perform the appropriate action.

4.4 Normalization

This option asks the user to select the number of the data set to normalize. The normalized dose distribution replaces the original dose distribution and the product of the normalization factors applied to a given distribution is stored. The original distribution is retrieved with the 'denormalize' option, which divides the normalized distribution by the stored factor. If the distribution has been rebinned, the result of denormalization will be the original distribution, with all rebinning left intact.

1. Apply Scaling Factor
    - prompts user for a scaling factor
    - multiplies all the dose values in the distribution by this factor
2. Normalize to Average Dose
    - finds the average dose for the distribution and the voxel where it occurs
    - each element of the dose array is divided by the average dose
3. Normalize to Maximum Dose Along Central Axis
    - finds the maximum dose along the central axis of a distribution, and the voxel where it occurs
    - each element of the dose array is divided by the maximum dose
4. Normalize to Dose in Specific Voxel
    - prompts the user for the coordinates of a voxel (enter 3 integers, separated by commas)
    - each element of the dose array will be divided by the dose in this voxel
5. Denormalize
    - reverses all normalizations performed on a dose distribution by dividing it by the stored cumulative normalization factor
    - denormalization will leave the binning structure intact

4.5 Rebinning

This option allows the user to choose the number of the dose distribution file to rebin, as well as the number and name of the rebinned file for plotting with `xmgrace` . Rebinning modifies the size of the bins in a dose distribution by a factor provided by the user. The rebinning factor must be an integer. For instance, a rebinning factor of 4 condenses the contents of 4 bins in the selected dose array into a single bin in a new dose array. Dose values in the 4 bins will be added together and averaged in order to calculate the new dose. Dose in any leftover bins will be added and averaged (where appropriate) and placed in the last bin of the new dose array. Currently, the routine only handles positive integral rebinning factors, since it cannot perform any sort of data interpolation. This means that the number of bins may only decrease (bins may only increase in size).

4.6 Plot

The routine has two plot options, 'Plot Profiles' and 'Comparison Plot'. Comparison Plot may be selected if there are two or more distributions loaded. Both plot options allow several cross-plots or depth dose curves to be plotted on a single graph. Curves which are parallel to the X and Y axes are referred to as cross-plots, and those parallel to the Z axis are depth-doses. Cross-plots and depth doses in which the curves are all parallel to a single axis of voxel geometry are allowed, but combinations of X,Y and Z axis plots **cannot** be mixed on a single graph. Dose values are plotted in the voxels which lie parallel to the axis selected and pass through the selected coordinates.

1. Plot Profiles
    - profiles all come from the same distribution
    - axis of profile must be an integer from 1-3, corresponding to X, Y and Z axes, respectively
    - graph title and output filename are arbitrary
    - number of curves must be an integer
    - prompts user for coordinates of each curve (enter 2 real numbers, separated by a comma)
2. Comparison Plot
    - profiles come from different distributions
    - axis of profile must be an integer from 1-3, corresponding to X, Y and Z axes, respectively
    - prompts user for coordinates of the curve (enter 2 real numbers, separated by a comma)
    - graph title and output filename are arbitrary
    - if selected, automatic offset will slightly offset the location coordinate of the curves plotted, the dose values are unchange (default is no offset)

Stored *plotname.xvparam* and *plotname.xvplt* files can be plotted by `xmgrace` directly, without using STATDOSE. The appropriate command to issue in order to retrieve the graph corresponding to these files is:

xvgr -autoscale xy -type xydy -device 1 plotname.xvplt -p plotname.xvparam

4.7 Save

Any dose distributions stored by the program can be saved. This means that normalized and rebinned distributions can be written to disk in a format that can be re-read by STATDOSE. The routine will display the names of all loaded files and prompt the user for the number(s) and name(s) of the file(s) to be stored. The current filename will be the default name under which the distribution will be stored, so be careful that you do not wipe out files that you meant to keep. This could happen if you attempt to save a normalized distribution and get carried away when hitting carriage returns!

5 References

[1] Ma C.-M., Reckwerd P, Holmes M., Rogers D.W.O. and Geiser B., "DOSXYZ User's Manual", *NRCC Internal Rep.* **PIRS-0509 (B)** (1995)