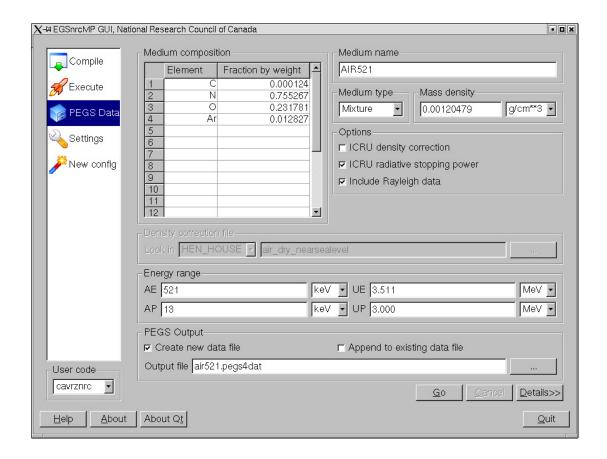
EGSnrcMP: the multi-platform environment for **EGSnrc**

I. Kawrakow, E. Mainegra-Hing and D. W. O. Rogers
Ionizing Radiation Standards
National Research Council of Canada
Ottawa, K1A OR6

September 2006

NRCC Report PIRS-877



 $A vailable \ on-line \ via: \\ http://irs.inms.nrc.ca/software/egsnrc/documentation.html$

EGSnrc Code System Licence

The EGSnrc code system (i.e. all pieces of code saying they are subject to the EGSnrc Licence, including routines related to the 1999 and later versions of EGSnrc and EGS_Windows, all associated source code, the NRC databases related to multiple scattering and spin correction, as well as the NRC user codes DOSRZnrc, FLURZnrc, CAVRZnrc, CAVSPHnrc, EDKnrc and SPRRZnrc, all scripts and all associated documentation) are copyrighted material owned by the National Research Council of Canada, all rights reserved. Those portions of the system for which the copyright is owned jointly or wholly by the Stanford Linear Accelerator Center, are distributed under a formal NRC/SLAC agreement.

- 1) The NRC grants the user a non-transferable, non-exclusive licence to use this system free of charge only for non-commercial research or educational purposes. All proprietary interest, right, title and copyright in the EGSnrc code system remains with NRC.
- 2) The express, written consent of NRC is required if the EGSnrc code system or any part or derivative thereof or data generated by the code is used by an individual or an organization for developing a commercial product or service.
- 3) The express, written consent of NRC is required if this code system or any part thereof is to be used in a fee for service application, either clinically or by consultants.
- 4) The express, written consent of NRC is required if the NRC spin correction or multiple scattering data bases are to be used directly or indirectly in any other application, either commercial or non-commercial.
- 5) The code system must be obtained from NRC. Users may not copy nor distribute the code system or parts thereof.
- 6) NRC disclaims any warranties, expressed, implied or statutory, of any kind or nature with respect to the software, including without limitation any warranty of merchantability or fitness for a particular purpose. NRC shall not be liable in any event for any damages, whether direct or indirect, special or general, consequential or incidental, arising from the use of the software.
- 7) This licence supercedes all prior communications and agreements, written or oral, concerning the EGSnrc code system. No amendment or waiver of terms is effective unless in writing, signed by both parties and specifically states the intention to affect this licence.
- 8) This licence is governed by the laws of Ontario and Canada applicable therein. The user consents to the jurisdiction of the federal court and the courts of Ontario.

-End of	Licence——-
---------	------------

The intent of the above may best be given by example. If you are at a not-for profit institution, and are not working under a contract or grant from a commercial organization, you have a free licence to use EGSnrc. If you work for a commercial organization (except a hospital), then you may only use EGSnrc if your organization has a licence agreement with NRC. If you work at a hospital but are using the code solely for internal or personal research purposes, you have a free licence to use EGSnrc. If you work for any type of organization, and your work is sponsored by a commercial organization for any purpose related to commercial use, then you need a licence agreement with NRC.

The scripts and GUIs are distributed under the GNU GPL which is with the system.

Abstract

This manual describes the NRC EGSnrcMP multi-platform environment for running the EGSnrc Monte Carlo code system for simulating the transport of photons and electrons. In previous distributions of EGSnrc, the system was run in the csh scripts and structure that had been developed to work in a Unix environment with EGS4. The EGSnrc code itself and the scripts in particular meant the system would not run on Windows platforms, and the scripts had become very hard to maintain since they had grown to handle many more situations than originally designed for. The EGSnrcMP environment is a ground-up reworking of the way EGSnrc is maintained and run. The code itself has been reworked slightly to allow the same code to work on all operating systems (with some very minor exceptions which are handled by alternate coding of some macros), and the scripts reworked to be far more flexible and powerful. In addition, graphical user interfaces to run the codes and installation have been developed based on the Qt GUI toolkit library.

Contents

	No	tation		5
1	Intr	Introduction		7
	1.1	Intent	of this report	7
	1.2	Overv	iew of the changes	7
	1.3	Brief o	description and comparison to the previous system	8
2	Inst	alling	EGSnrc	10
	2.1	Unix/	Linux platforms	10
		2.1.1	Libraries or compilers to be separately obtained	10
		2.1.2	Traditional Linux/Unix Installation	10
		2.1.3	Other installation alternatives for Linux	12
			$2.1.3.i$ egs_install GUI	12
			2.1.3.ii egs_install_self GUI	12
		2.1.4	The test_egsnrcmp_distribution script	12
	2.2	Windo	ows platforms	13
		2.2.1	Libraries or compilers to be separately obtained	13
		2.2.2	Downloading the necessary files	13
		2.2.3	Installation	14
	2.3	Install	lation on Mac OSX	14
	2.4	A wor	d about the Qt library	15
3	Нох	w to de	efine the environment	17

4	Hov	v to create an executable user-code	18
	4.1	Compilation using Makefiles	18
		4.1.1 Default use of make	18
		4.1.1.i user-code.make	18
		4.1.2 Other targets with make	19
		4.1.3 Running make for different configurations	19
	4.2	Compilation using egs_gui	20
	4.3	Compilation using mf user-code (Unix/Linux specific)	21
	4.4	Location of executables	21
5	Run	ning a standard EGSnrc user-code interactively	22
	5.1	Executing a user-code using egs_gui and egs_inprz	22
	5.2	Executing an NRC user-code using command-line arguments	23
	5.3	Executing a user-code using the scripts (Unix/Linux specific)	24
6	Running a standard EGSnrc user-code in batch mode		
	6.1	Informing EGSnrcMP about your batch queuing system	25
	6.2	Using exb or run_user_code_batch	25
	6.3	Using batch mode with the GUIs	26
	6.4	NRC user-code command-line arguments for batch mode	26
7	Hov	v to create a new data set using PEGS4	27
	7.1	Using egs_gui	27
	7.2	Using pegs4.exe	28
8	The	file structure	29
	8.1	\$HEN_HOUSE	29
	8.2	\$EGS_HOME	31
9	Hov	v the EGSnrcMP environment works	32
	9.1	\$HEN_HOUSE/specs: Config files	32
		9.1.1 What is a config file?	32
	9.2	Pre-compiled components for Windows	33
10	egs_	init and $\operatorname{\sf egs_finish}$	33
	10.1	user-code.io file format	36
11	A C	interface for EGSnrc	37

	Inde	ex	60
17	Refe	erences	5 9
		B.3 \$HEN_HOUSE/makefiles/standard_makefile	56
		B.2 An example user-code .make file: ranmar_test.make	55
		B.1 Makefile (tutor1)	53
	App	pendix B: Examples of a Makefile	53
		A.4 windows.spec	52
		A.3 unix.spec	51
		A.2 all_common.spec	48
		A.1 pgf77.conf	47
		pendix A: An example config file	47
16	Kno	own restrictions	45
	15.2	Creating a Distribution	45
	15.1	Using CVS	44
15	Usir	ng the system at NRC	43
14	How	v to upgrade your old EGS user-code	43
	13.3	Random number generators	42
		Fortran compilers	42
		Static vs non-static	42
13		ciency considerations	42
	12.2	Parallel job submission	41
		egs_c_utils	41
12		allel runs	40
		11.1.5 Known limitations of C interface	40
		11.1.4 The tutor4c user-code	39
		11.1.3 What is needed for a C-written EGSnrc user-code	38
		11.1.2 Main interface header files: $egs_interface1.h$ and $egs_config1.h$.	37
		11.1.1 Macros for the C interface: egs_c_interface1.macros	37
	11.1	\$HEN_HOUSE/interface: Interface for C-written user-codes	37

List of Figures

1	Screen shot of the egs_gui after compiling tutor1	20
2	Screen shot of the ${\tt egs_gui}$ after running a DOSRZnrc job in batch mode	23
3	Screen shot of the egs_gui set to calculate a data set for air using the ICRU Report 37 density effect	27
4	Structure of the \$HEN_HOUSE area. Note that several sub-subdirectories in the gui subdirectories have been suppressed	30
5	The user's area \$FGS HOME in the EGSnrcMP environment	31

Nomenclature

The nomenclature with the EGSnrcMP environment is somewhat confusing to start, and hence a brief set of definitions is provided. The \$ identifies an environment variable and the forward slashes, /, are separators on Unix/Linux. Although on Windows the notation is different (%var% and \), for simplicity throughout the text we will use the first notation.

- \$HEN_HOUSE is the directory on which the EGSnrc system is maintained. It can be anywhere on the file system except that no spaces are permitted in the path (and so, Windows users can not install the system on e.g. C:\Documents and Settings\user\HEN_HOUSE). On Unix/Linux systems the HEN_HOUSE variable is set for the user in the egsnrc_cshrc_additions or egsnrc_bashrc_additions files. On Windows systems it must be defined in the user's environment (this can be done by the installation wizard).
- \$EGS_HOME is the main directory for an individual user's user-codes. The environment variable EGS_HOME must be defined to point to this directory. On Windows systems this can be automatically done by the installation program. On Unix and Linux systems, users must define this variable in their shell initialization file (typically .cshrc for C-shell and derivatives or .bashrc or .profile for Bourne shell and derivatives).
- \$EGS_CONFIG is the absolute path to the file describing the config which is to be used. It must be defined by the environment. On Windows systems it can be automatically defined by the installation program, On Linux and Unix system users must define it in their shell initialization file.

- Config is a set of variable definitions for various EGSnrc directories, compiler name and compilation options, etc. These definitions are stored in a config file pointed to by the environment variable EGS_CONFIG, which is created during the installation/configuration process. The config file is included by all make files when building an EGSnrcMP user-code and is also used by some of the Unix shell scripts.
- \$my_machine is the name used to refer to a config. It is used to distinguish different Fortran files and executables related to different configs and also the different bin and lib areas which contain files specific to a given config on both \$HEN_HOUSE and \$EGS_HOME. This variable is defined in the \$EGS_CONFIG file and selected by the user during installation/configuration. This variable, i.e., \$my_machine, is also called CONFIG_NAME at various places in the documentation.
- egs_gui is a GUI for compiling and executing a user-code, for running the PEGS4 code and for adjusting settings and creating a new config. For Linux and Unix users the alias egsgui is defined, which executes egs_gui in the background and discards all diagnostic messages printed to standard output.
- egs_inprz is a GUI for working with input files for the RZ user-codes, compiling and executing an RZ user-code and for adjusting settings and creating a new config. For Linux and Unix users the alias egsinprz is defined, which executes egs_inprz in the background and discards all diagnostic messages printed to standard output.
- egs_install is a GUI for installing/configuring the EGSnrcMP system. A reduced version of this GUI is used by egs_gui and egs_inprz for adjusting settings and creating a new config.
- \$PATH is the environment variable which tells the system where to find executable codes and
 it must include the \$my_machine subdirectory of
 \$HEN_HOUSE/bin and \$EGS_HOME/bin.

1 Introduction

1.1 Intent of this report

This report describes a major revision of the EGSnrc system's structure, but not any changes in the physics of the system. The underlying rationale was to develop a system that could work on the Microsoft and Mac OSX platforms as well as Unix/Linux platforms while minimizing the differences in the source code required. At the same time we needed to rework the Unix scripts to be more flexible. The previous system was based on assumptions about compilers that were native to most systems, whereas today there are a variety of compilers available for many systems. To accomplish these goals required some minor changes in the coding of the EGSnrc system itself and a minor modification of the initialization calls required in user-codes. These changes are documented here, as are the new GUIs and installation scripts.

1.2 Overview of the changes

There have been several improvements in the EGSnrc system, which make the installation, maintenance and use of the system much simpler and, at the same time, portable to other operating systems:

- EGSnrc data file units and user-defined I/O units are opened explicitly through a call to subroutine egs_init, which must be step 0 in every EGSnrc user-code. Symbolic links are not needed anymore and the previously used .environment file is replaced by the .io file.
- The EGSnrc system and the user-codes are now built using make, a standard tool on Linux and Unix systems. Windows users can use the GNU version of make.
- Config files (*.conf) are used to describe a combination of operating system and Fortran compiler. This implies that one can use the same EGSnrc installation from different operating systems and/or use different compilers by just switching the current config.
- Command-line arguments can be passed to a user-code to specify things like the input file, the .pegs4dat file, the name for output files, the \$HEN_HOUSE and \$EGS_HOME directories, flags for a batch run, etc.. One can list all available options by using the -h or -help command line option.
- Utilities are available for managing I/O units
- For Unix/Linux systems, a more efficient and general parallel job submission and processing approach has been implemented.
- An interface for accessing EGSnrc data structures and calling EGSnrc subroutines from a C program is now available, *i.e.*, user-codes can be written in C or C++.

- Besides the gz, bz2 and tar archives, new archives are created using the zlib library for compressing files using an in-house format (*.egszip files). This way, archives can be uncompressed by the EGSnrcMP installation program on any operating system without relying on external uncompressing utilities that might not be available.
- Three graphical user interfaces are available for working with the EGSnrcMP environment: egs_install, egs_inprz and egs_gui. The first one is a graphical installation utility that can be used for creating or updating the EGSnrcMP environment and further configs (operating system-compiler combinations). The second one is for working with the NRC RZ user-codes suite (see Reports PIRS-702[1] and PIRS-801[2]). The third one can be used to work (compile, run) with any EGSnrc user-code and produce PEGS4 data sets. The two latter GUI's can also invoke a reduced version of egs_install, called egs_configure for creating new configs.
- The spin data base is now in binary format, *i.e.*, it is 5 times smaller than the text version and can be read much faster. ICRU density effect correction files for calculating electron stopping powers for elements and compounds are distributed in single files and split during installation.
- On Windows, GNU make is included in the installation in case it is not available on the user's system. If no Fortran compiler is available, users are asked by the installation GUI whether it should install the GNU C, C++ and Fortran compilers from the EGSnrc distribution site.
- All NRC user-codes distributed with the system have been cleaned up to use system independent wrapper functions and subroutines for date and time, hostname, etc.
- The main system and the NRC user-codes distributed with the system have been adapted so that no global static compilation switch is required.

1.3 Brief description and comparison to the previous system

In the previous system, the user used a series of scripts to perform various tasks. The scripts egs_compile and egs_run were used to compile and run user-codes. At the compilation stage, the user_code.configuration file was used to specify all the different source code modules to be used to create the user_code, e.g., dosrznrc.mortran, srcrz.mortran, ranlux.macros, ranlux.mortran etc.. At run time, the file user_code.environment was used to associate various Fortran I/O units to explicit file names.

While the previous system was flexible in many ways, there were several serious draw-backs. Firstly, the egs_compile and egs_run scripts hardwired various assumptions about compilers and operating systems which meant, e.g., that if you were using the GNU g77 FORTRAN compiler on a Solaris system, the scripts didn't work and had to be changed. These scripts didn't work at all under Microsoft Windows and the method used to associate I/O units with specific files was not portable to the Windows environment.

To avoid the above problems, the EGSnrcMP environment has been developed. The increased flexibility has come at the cost of increased complexity in the implementation, but

the vast majority of this is hidden from the user and the new system should be easy to use once a few new concepts are understood.

An important concept is that of the \$EGS_CONFIG environment variable. This variable points to a file with all the relevant information about the environment being used such as the operating system being run under, the compiler to be used and its switches. The user is able to set up several environments within one installation (e.g., using different compilers or different hardware or different operating systems) and then alternate between them by resetting the \$EGS_CONFIG variable. The \$HEN_HOUSE/bin and \$HEN_HOUSE/lib areas (see figure 4, page 30) then have separate subdirectories corresponding to each \$EGS_CONFIG environment. This is discussed in more detail in the next section.

To overcome the problems of defining I/O units, two new subroutines have been added to the EGSnrc system, egs_init and egs_finish which handle the I/O units. This involves two new features. One is the ability of the user-codes to read command line inputs (e.g., -p tutor_data specifies that the pegs4 dataset tutor_data.pegs4dat is to be used) and also the use of the file user_code.io which allows arbitrary Fortran I/O units to be associated with arbitrary files (analogous to the old .environment files). The new routine means that the EGSnrc system now explicitly opens and closes files using their specific names, thereby making the code portable to the Windows system. The use of these new capabilities are described below in section 10, page 33.

The final major component on the new environment is the use of make files in the compilation process rather than scripts. There is a version of GNU make available for the Windows OS so that this makes the EGSnrcMP environment portable across different operating systems. In a similar vein, the reworking of the I/O routines means that one can run most user-codes directly without using an egs_run script.

2 How to install EGSnrc using the EGSnrcMP environment

2.1 Unix/Linux platforms

2.1.1 Libraries or compilers to be separately obtained

It is essential to have a working Fortran compiler for installing and using the EGSnrc system. If no Fortran compiler is available, the installation process aborts. The GNU suite of compilers is available for free and can be downloaded at http://www.gnu.org

A working make utility is needed for building the different system components and the user-codes. Make utilities from different Unix flavours tend to differ. The main system has been tested and found to work with make on AIX, OSF1, IRIX, SunOS, HP-UX and Linux. The Makefiles for the C interface will only work with the GNU version of make.

The new EGSnrc system uses the Qt library version 3.1 or higher for the graphical user interfaces. Most Linux distributions include the Qt library these days, since the popular Desktop Environment KDE is based on this library. However, if the Qt library is not available in the user's system, one can download it for free at http://www.trolltech.com. For more information about installing Qt, see section 2.4, page 15.

To take advantage of the new EGSnrc C interface, a working C or C++ compiler is required. Again, the GNU suite of compilers can be installed.

2.1.2 Traditional Linux/Unix Installation

The traditional method for installing EGSnrc is to run an installation script after obtaining several tar files, either from the web site (http://irs.inms.nrc.ca/software/egsnrc/download.html) or from a CD (only handed out to those taking a course).

This is still a viable method. The files that must be downloaded are:

```
V4_EGSnrc.tar[ |.gz|.bz2]
V4_EGSgui.tar[ |.gz|.bz2]
V4_manuals.tar[ |.gz|.bz2]
V4_user_codes.tar[ |.gz|.bz2]
V4_spinms.tar[ |.gz|.bz2]
```

where [|.gz|.bz2] indicates that you need one of the file formats, the shortest one for which you have the code installed for uncompressing the format (*i.e.*, gunzip for .gz and bunzip2 for .bz2). If you have none of them, just get the uncompressed tar files.

The only absolutely essential file is V4_EGSnrc.tar. The file V4_spinms.tar has changed format from previous versions (binary file is much shorter and is read much faster but the physics is unchanged), so it needs to be downloaded even if you have the previous version. The other three tar files are also highly recommended.

All of these files need to be placed on a single subdirectory since the install script assumes

this. But the location of the EGSnrc system is independent of where the tar files are kept.

In addition to the above files, one needs the script install_egs. It is easiest if it is copied to the same area as the above files, but, in principle, it can be stored anywhere that the user has write permission (and in particular it must be copied from the course CD).

Prior to starting the installation, one must ensure that the environment variable QTDIR is defined to point to the Qt library installation directory if you want to install the GUIs (see section 2.1.1).

The traditional installation process is followed by issuing the command ./install_egs (after ensuring that the file is executable). Note that one MUST NOT redirect the output from the install script since this script is interactive, unlike in past releases. On the other hand, the script does create several output files. The files install.status and install.log are both on the directory from which install_egs is run and they inform the user what has happened in install_egs.

By far the most complex part of the installation is handled by the script configure which is called from within install_egs. The configure script establishes the parameters for a given config file related to the compiler used and the options chosen (see section 9.1). This script leaves the file config.log on \$HEN_HOUSE/scripts (which is where the script configure resides). Note that the user can run this script separately to create another config file and then alternate between configs by changing the environment variable EGS_CONFIG. This allows, e.g., easy switching between compilers.

Another component of the installation is handled by another script, which may be called from within install_egs, viz., finalize_egs_foruser. This script leaves behind a log file called finalize_\$USER.log on \$HEN_HOUSE/scripts where this script is also found. The purpose of this script, which can be run independently, is to set up an individual user's area. For a single user, this area is usually set up on the same account as the HEN_HOUSE. However, for an installation with many users, the HEN_HOUSE may be on one account and each user's area on their independent accounts, in which case finalize_egs_foruser needs to be run for each user's account (but must be run by someone with write permission on the users account and the \$HEN_HOUSE)..

The final component of the installation that may be called from within the install_egs script is the generation of the GUIs. This can also be done independently by going to the GUI area \$HEN_HOUSE/gui and executing a make command after the environment variable \$EGS_CONFIG has been defined.

The installation scripts require many inputs, usually with good defaults suggested. In most cases, if the response is unclear, typing help will generate a message with further information.

Once the install_egs script has been run, there are three statements that must be added to your .cshrc, .bashrc or .profile file (depending on which shell you run in interactively). These are near the end of the output from install_egs and involve setenv EGS_HOME (or export EGS_HOME for .bashrc), setenv EGS_CONFIG and source (appropriate_directory)_egsnrc_cshrc_additions or source (appropriate_directory)_egsnrc_bashrc_additions.

Once these additions have been made to your .cshrc or .bashrc file, you must source the

file to bring these definitions into effect. Note that you may want to redefine EGS_CONFIG if you want to use an alternative compiler or another configuration of some sort.

The egsnrc_cshrc(bashrc)_additions file also sources the file \$HOME/.egsnrc_cshrc_additions or \$HOME/.egsnrc_bashrc_additions. This file allows the user to tailor their personal environment although this could be done directly in your .cshrc or equivalent file directly.

The final component of the installation is setting up the information needed for doing runs in batch mode on the user's system. This is discussed below in section 6, page 25.

2.1.3 Other installation alternatives for Linux

2.1.3.i egs_install GUI

An alternative way of installing the system on a Linux system is to use the graphical user interface called egs_install (vs the script install_egs described above). This GUI uses the Qt library and the binary on the distribution site (size ~ 9Mb) has been created with the GNU C++ compiler version 2.95.3 statically linked to the Qt 3.2.1 library on a SuSE 7.3 Linux system. We have successfully tested this binary of the installation GUI on the following Linux systems: SuSE 8.2, Red Hat 9.0 and Mandrake 9.1. There is no guarantee that this binary will run properly on older systems (and it is guaranteed that it will not run on systems that are so old that they use the a.out format for executables.).

This GUI works on the same set of tar files as described above in section 2.1.2 except that it uses the *.egszip format of all the files (this format is like a .gz file, but the GUI has built-in routines for reading it). The GUI looks for these files on the local area and if they are not found, on the user's request the GUI will download them from the EGSnrc distribution site. The user can select the specific system components that should be downloaded/uncompressed. This allows the flexibility of partial future updates.

The installation GUI is based on the Qt system but is statically linked so the user does not need to install the Qt libraries to use the install GUI. However, as part of the installation process, the user is asked to make the GUIs for running the codes egs_gui and egs_inprz and to do this, one needs the Qt libraries installed (see section 2.4).

2.1.3.ii egs_install_self GUI

This GUI is identical to the previous one except that the file includes all the necessary files, *i.e.*, it is a self-extracting binary. As a consequence the file is much larger (~ 23 Mb).

2.1.4 The test_egsnrcmp_distribution script

The script test_egsnrcmp_distribution is found on \$HEN_HOUSE/scripts. It exercises the distribution and can be used to create a file with the output from various test runs by issuing:

test_egsnrcmp_distribution >& test_distribution_machine.out &

These can be compared to the output from the same script run on various machines and found on the area \$HEN_HOUSE/scripts/test_distribution_outputs.

2.2 Windows platforms

2.2.1 Libraries or compilers to be separately obtained

It is essential to have a working Fortran compiler for installing and using the EGSnrc system. On the EGSnrc distribution site, the archive V4_MinGW.egszip contains a Windows version of the GNU suite of compilers (C, C++ and Fortran) and other related tools. For more information on the GNU suite of compilers for Windows the user is referred to http://www.mingw.org

During installation, if no Fortran compiler is found, the user is asked whether the GNU compiler should be installed by the setup program. If no Fortran compiler is available, the installation process must be cancelled by the user since it will not be possible to build the EGSnrc system and the user-codes.

Another key element in the new EGSnrc system is the GNU make utility. Since it might not be available on a Windows system, we have also included a free distribution of GNU make, which is copied to the system's binary directory.

The new EGSnrc system uses the Qt library for the graphical user interfaces. With the Windows installation, version 3.2 of this library is included and copied to the EGSnrc binary directory of the current config. Since the GUI's are distributed in executable form, there is no need for compiling them at installation time. All the sources for the GUI's are distributed under the GPL with EGSnrc and can therefore be modified to meet a user's needs. However, the user must possess a licensed copy of the Qt library for Windows and a C++ compiler (MS, Borland and recently GNU) in order to be able to re-compile.

2.2.2 Downloading the necessary files

To install the EGSnrc system, the different components (system files, user-codes, spin data base, documentation, etc.) and the installation GUI (egs_install.exe) can be directly downloaded from the EGSnrc distribution site. The distribution files have the *.egszip extension and are created using the zlib data-compression library (see

http://www.gzip.org/zlib/). They can be placed together anywhere as the installation program will prompt for their location in case they are not on the same location (default).

There are two alternatives to the installation method outlined above: the self-extracting executable file egs_install_self.exe with all system components included (size ~ 30 Mb) or the smaller executable file egs_install.exe (size ~ 4Mb). The latter approach will have the installation program check on its current location for system components (*.egszip files) and if none is found, it will ask whether it should download them from the EGSnrc distribution site (http://irs.inms.nrc.ca/software/egsnrc/download.html) or else it will inquire for the location of the distribution files.

If no compiler is found, the user is prompted whether the installation GUI should install the GNU Fortran, C and C++ compilers and the GNU make utility on \$HEN_HOUSE\gnu. Once the GNU compilers are installed, the PATH environment variable for the current user is updated with the binary directory for the GNU tools \$HEN_HOUSE\gnu\bin.

2.2.3 Installation

The installation wizard guides the user through the whole process requiring information related to files location, compilers to use, what kind of installation the user wants, etc. Firstly, on the environment page, the installation utility asks the user for the location of the EGSnrc system (environment variable HEN_HOUSE) and the user area (environment variable EGS_HOME, where the user keeps his/her user codes). On the next screen, the system configuration page, the user is required to enter among other things, a name for the configuration file if there was no previous configuration or else, a combo box displays the current configuration file together with a list of available configurations. The environment variable EGS_CONFIG points to the current configuration file, which is the control centre of the system and contains many specifications of the particular compiler-operating system combination.

These environment variables need to be set prior to using the EGSnrc system. This can be done by the user after finishing the installation or the installation program can take care of it if the user selects this option on the GUI (set HEN_HOUSE, set EGS_HOME and set EGS_CONFIG check boxes).

Once all the information has been entered, one can start the installation process, which first uncompresses the files into the selected system location (HEN_HOUSE) and then performs a series of tests for the selected Fortran and C compilers. The results of these tests are used to create the system/compiler dependent files machine.mortran and machine.macros. The installation utility then starts the actual building of the EGSnrc system, by creating the Mortran3 string processor mortran3.exe and the PEGS4 data pre-processing tool pegs4.exe. After the EGSnrc system is installed, if the user requested it, a user area is created with all the NRC user codes and a user pegs4 data directory. Finally, user codes previously selected by the user on the wizard, are compiled and the path to the location of the executable files on the system and user areas is added to the environment PATH variable, if it was not already appended.

2.3 Installation on Mac OSX

Most of the installation instructions about Linux/Unix systems (see section 2.1) apply to Mac OSX. Both, the script and graphical installation wizard, worked on our test systems (fairly old hardware running Mac OSX 10.2 and Mac OSX 10.3). There are few restrictions and differences:

- The self-extracting installation method does not work on Mac OSX.
- If you want to use the command line interface and your default shell is bash, you have to put the environment variable initializations in the file .profile in your home directory instead of .bashrc.
- When starting the GUIs from a shell, you have to use open egs_gui or open egs_inprz. Because of this difference, some of the aliases defined in the egsnrc_*_additions files will not work for Mac OSX.

• If you want to be able to start the GUIs directly (*i.e.* not from a shell), you have to define the EGS_CONFIG, EGS_HOME and HEN_HOUSE environment variables in a file named environment.plist in the directory \$HOME/.MacOS. This is a XML file that may or may not already exist. If the file does not exist, create it and put the following in it:

Note that the directory definitions (EGS_HOME and HEN_HOUSE) MUST end with a slash. If the file already exists, just insert somewhere the 3 definitions.

• It appears that Mac OSX executables are not backward compatible (the installation wizard compiled on the 10.3 system did not run on the 10.2 system). On the web we are providing the installation wizard compiled on 10.2. It runs on 10.2 and 10.3 but there is no guarantee that it will work on earlier Mac OSX versions.

Please note that we typically do not have access to a Mac OSX system and therefore can not provide support for this platform.

2.4 A word about the Qt library

The GUIs were developed using Qt, a multi-platform, C++ Graphical User Interfaces toolkit that enables building efficient, portable and maintainable GUI applications. Qt is a fully object-oriented, easily extensible C++ application framework that enables rapid building of state-of-the-art GUI applications. For more information please see http://www.trolltech.com.

We started developing the GUIs with Qt version 3.0. Considering the new developments and improvements in the Qt library since then, we strongly recommend that the user installs the latest available version of this library to avoid possible conflicts with older versions.

On Linux we have built and run the EGSnrc GUIs successfully for version 3.1.1 and up for SuSE 7.3 and 8.2, Red Hat 9.1 and Mandrake 9.0. Since KDE, the most widespread Graphical Desktop Environment for Linux, uses the Qt C++ cross platform GUI toolkit for KDE development, the Qt library is shipped in most Linux distributions. When installing

a different Qt library to the one that comes with the Linux distribution on the user's machine, one should **never** perform the installation on top of the existing Qt library, *i.e.*, one should select a different location. This is to avoid rendering the KDE Desktop environment unusable since it has been compiled with the older Qt library.

To install the Qt library for Unix/Linux and Mac OSX:

Download the compressed archive qt-x11-free-3.2.x.tar.gz (Unix/Linux) or qt-mac-free-3.x.x.sit from the Trolltech Web site http://www.trolltech.com by going to the Downloads section and clicking on the Qt/X11 Free or the Qt/Mac Free link.

Uncompress the archive and copy the Qt directory to a desired location.

Read the INSTALL ASCII file in the Qt directory for environment settings and after setting the necessary environment variables, and from the Qt directory run

./configure -thread -no-xft -fast

Note the ./ in front of configure to make sure the correct one is invoked. The switch -thread is needed since some of the GUIs use multi-threaded processes and the switch -fast is optional to speed up the Qt building process by not building the numerous examples and tutorials. The switch -no-xft is needed on some systems to prevent problems related to fonts not used by the GUI anyway.

Once configure has finished, run make, again from the Qt directory, to build the library. Note that this can take a few hours on GHz range machines.

On Windows, we provide the Qt library in the form of a dynamic link library (dll), which is used by the graphical user interfaces egs_gui.exe and egs_inprz.exe which are distributed in binary form. If for some reason the user intends to re-compile these GUIs, he/she will have to obtain a licensed version of the Qt library.

3 How to define the environment

In the above we have already mentioned what needs to be done to define the EGSnrcMP environment but here we will summarize.

On the Windows systems, the installation GUI handles all the definitions needed (\$EGS_HOME, \$EGS_CONFIG etc).

On Linux/Unix systems one must include some definitions in the shell initialization files .cshrc, .bashrc or .profile depending on which shell you use for interactive runs.

```
.cshrc
```

setenv EGS_HOME path_to_directory_holding_users_codes setenv EGS_CONFIG path_to_file_holding_conf_file source path_to_hen_house/scripts/egsnrc_cshrc_additions Note that EGS_HOME is typically \$HOME/egsnrc/ and EGS_CONFIG is typically path_to_hen_house/specs/name.conf.

This latter file defines \$PATH to include \$HEN_HOUSE/bin/\$my_machine and \$EGS_HOME/bin/\$my_machine.

.bashrc

export EGS_HOME=path_to_directory_holding_users_codes
export EGS_CONFIG=path_to_file_holding_conf_file
. path_to_hen_house/scripts/egsnrc_bashrc_additions

This latter file defines \$PATH to include \$HEN_HOUSE/bin/\$my_machine and \$EGS_HOME/bin/\$my_machine.

Note that the definition of EGS_HOME requires the slash at the end.

One must also set up the information needed for doing runs in batch mode on the user's system. This is discussed below in section 6, page 25.

4 How to create an executable user-code

In the original EGSnrc environment and the EGS4 Unix environment, compilation of user-codes, both the Mortran and Fortran steps, was handled by C-shell scripts and made use of user-code.configuration files which told the scripts what source code files to include in a given user code.

In the EGSnrc system, this approach has been replaced by the Makefile approach which can be used on both Unix/Linux systems and on Windows systems (by way of the GNU make utility). This approach is much more flexible and means one system can be maintained for the two major operating environments. At the same time, some scripts have been written which allow the old compilation commands and syntax to be used, just to make the transition easier.

As discussed above (section 2.1.2, page 10 and section 2.2.3, page 14) an important part of the process is to have various environment variables set (viz., EGS_HOME, EGS_CONFIG and HEN_HOUSE) and on Unix/Linux systems to include a variety of other variables by sourcing either the egsnrc_cshrc_additions or egsnrc_bashrc_additions files from .cshrc or .bashrc files (depending on which shell you work in interactively).

In the following we start by describing the use of Makefiles to compile EGSnrc user-codes and then describe the use of the GUIs and the scripts.

4.1 Compilation using Makefiles

Makefiles are a system for compilation whereby dependencies are formally defined and when a compilation is asked for, the Makefile only does the compilation for those components which have changed. In this context, compiling includes the Mortran pre-processor step, the Fortran compilation step and the linking step. These steps combine to create an executable file from Mortran source files.

4.1.1 Default use of make

To compile a user-code, go to the directory containing the user-code.mortran source (usually \$EGS_HOME/user-code) and issue the command make. This default use of make will create the user-code executable with optimization turned on.

When one issues the command make on the area \$EGS_HOME/user-code, this first uses the file \$EGS_HOME/user-code/Makefile (see appendix B, page 53) which in turn includes the files \$EGS_CONFIG, user-code.make and \$HEN_HOUSE/makefiles/standard_makefile. Note that \$EGS_CONFIG also includes the files \$HEN_HOUSE/specs/all_common.spec and \$HEN_HOUSE/specs/unix.spec or \$HEN_HOUSE/specs/windows.spec. Fortunately the user does not need to touch any of these files except user-code.make.

4.1.1.i user-code.make

The file user-code.make is where the user tells the system what pieces of source code to

include in the user-code. An example is given in Appendix B.2 (see page 55). By default the user-code includes nine files, as defined by the following statement in \$HEN_HOUSE/specs/all_common.spec:

```
SOURCES =
          $(EGS_SOURCEDIR)egsnrc.macros \
           $(MACHINE_MACROS) \
           $(RANDOM).macros \
           $(USER_CODE).mortran \
           $(RANDOM).mortran \
           $(EGS_UTILS)nrcaux.mortran \
           $(MACHINE_MORTRAN) \
           $(EGS_SOURCEDIR)egs_utilities.mortran \
           $(EGS_SOURCEDIR)egsnrc.mortran
```

Note that each of the continuation lines above begins with a tab. These defaults can be overridden by including a modified version of the above statement in user-code.make, but otherwise this statement is not needed in user-code.make. This .make file can often be very simple.

4.1.2 Other targets with make

Makefiles define 'targets' to be made and these can include a variety of options. The following targets are defined in the EGSnrc Makefiles file:

make opt	Build the user-code executable with optimization turned on.
make noopt	Build the user-code executable with optimization turned off.
make debug	Build a user-code executable for debugging
make fortran	Mortran step only.
make clean	Remove the fortran file, mortjob file, mortlst file and the various executables.

4.1.3 Running make for different configurations

As mentioned before (section 2), EGSnrc config files define important system specifications and the environment variable EGS_CONFIG points to the current config file. If a user wants to build a user-code for a config other than the current one, all he/she has to do is invoke make and pass a new value for the EGS_CONFIG environment variable to it, i.e.

```
make EGS_CONFIG=new_config_file
```

replacing temporarily the value of EGS_CONFIG. This way any variable values used in the

Makefiles can be replaced. For more information on EGSnrc configs and config files the user is referred to section 9.

The general command for running make is:

make [opt|nooopt|debug|fortran|clean] [EGS_CONFIG=new_config_file]

4.2 Compilation using egs_gui

egs_gui is a graphical user interface (GUI) for doing various tasks related to EGSnrc. When using egs_gui, one does not need to go to the user-code directory since one is given an explicit choice between all of the user-codes that are available. On Unix/Linux the alias egsgui runs the GUI in the background and filters out the diagnostic messages whereas direct use of egs_gui runs in the foreground and prints a variety of diagnostic messages to the terminal.

If you want to change the config file prior to doing the compilation, click on the settings icon in the GUI and select one of the available config files.

Alternatively, if you have write permission on the \$HEN_HOUSE, you can use the 'New config' screen in the GUI to create a new config file.

For the specific case of the RZ user-codes, the user can also build these codes using the egs_inprz GUI in a similar fashion as with egs_gui. On Unix/Linux the alias egsinprz runs the GUI in the background.

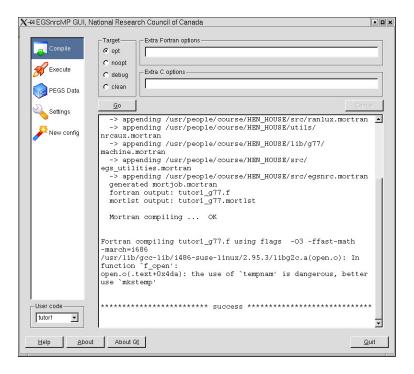


Figure 1: Screen shot of the egs_gui after compiling tutor1.

4.3 Compilation using mf user-code (Unix/Linux specific)

For compatibility with the old usage, the script \$HEN_HOUSE/scripts/compile_user_code has been written. It has several possible arguments.

```
compile_user_code [mf|m] user_code [a] [opt|noopt|debug] [config=XXX]
```

The script compiles user_code. All other options are optional and in fact the parameter 'a' is not used (present for compatibility)

mf => Mortran and Fortran compile and then linkm => Mortran compile and create the Fortran file

debug => create executable ready for a debug run

config=XXX => use the config file specified as a full pathname instead of the default which
is \$EGS_CONFIG.

4.4 Location of executables

After creation of the executable file, it is placed on the area specified by \$HEN_HOUSE/bin/\$my_machine if it is a system wide file such as mortran3 or pegs4 or on \$EGS_HOME/bin/\$my_machine if it is an individual's user-code.

5 Running a standard EGSnrc user-code interactively

Once a standard user-code has been built, one can execute it using command line options or through one of the two available GUI's, viz., egs_gui or egs_inprz. The egs_inprz GUI creates/modifies input files, compiles and runs the NRC RZ user-code suite. In contrast the egs_gui GUI compiles and executes any EGSnrc user-code and creates PEGS4 data files but does not create input files. On Unix/Linux systems one can also use the scripts run_user_code and run_user_code_batch to execute the user-code interactively and to submit EGSnrc jobs to a queuing system respectively (see section 6 page 25).

5.1 Executing a user-code using egs_gui and egs_inprz

The egs_gui can be used under Windows or Unix/Linux to execute an already compiled user-code. The use is mostly self-explanatory but a few points are worth noting.

- The user can select where to look for the PEGS4 data set. By default the GUI looks on either the user's PEGS4 area (\$EGS_HOME/pegs4/data) or the system PEGS4 area (\$HEN_HOUSE/pegs4/data). If data files are obtained from other locations, these are remembered by the GUI
- In the lower left corner the user selects which user-code to execute. The available list consists of all subdirectory names in the \$EGS_HOME area.
- The input file name does not need the extension (which must be .egsinp).
- On Windows the batch option is currently not available

As mentioned above, if the user wants to run the RZ user-codes with the ability of modifying/creating input files, egs_inprz can be used instead of egs_gui. Pressing on the execute button of the GUI brings up a dialog with the execution options which are identical to those in egs_gui. For more information on how to work with egs_inprz, the user can start the GUI and press on the Help button to display its manual in html format.

On Unix/Linux systems the following aliases are defined in the shell addition files \$HEN_HOUSE/scripts/egsnrc_[bash|csh]rc_additions:

egsgui is aliased to \$HEN_HOUSE/bin/\$my_machine/egs_gui and runs it in background and ignores the usually unnecessary diagnotic messages from the script.

egsinprz is aliased to \$HEN_HOUSE/bin/\$my_machine/egs_inprz

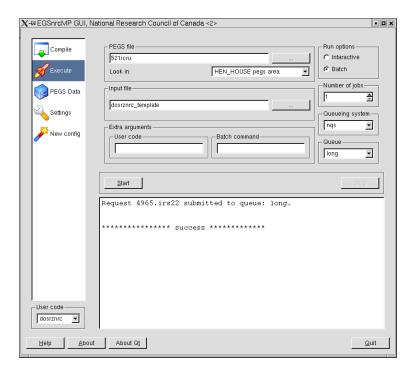


Figure 2: Screen shot of the egs_gui after running a DOSRZnrc job in batch mode.

5.2 Executing an NRC user-code using command-line arguments

User codes can be executed directly on the command line in a Unix or DOS shell using

user_code -p pegs_file [-i ifile] [other args]

where user_code is the name of the user code (e.g. tutor1, cavrznrc, etc) and pegs_file is the name of the PEGS4 data file. The -i ifile argument specifies that input comes from the file named ifile.egsinp on the user code area, this argument is only necessary if the user code requires an input file. other args are other optional arguments (see below). For instance, to execute the tutor1 tutorial code, which needs the PEGS data file tutor_data.pegs4dat and no input, use

tutor1 -p tutor_data

To execute the cavrznrc user code using the cavrznrc_template.egsinp file distributed on the cavrznrc area, use

cavrznrc -p 521icru -i cavrznrc_template

Here is a list of all standard arguments understood by EGSnrc user codes that employ the egs_init subroutine (see section 6.4 on page 26 concerning the input for batch runs):

-i orinput ifile	Specifies that the input file is ifile.egsinp
-o oroutput ofile	Output data will be written to ofile.egslog, ofile.egslst, etc., instead of ifile.egslog, ifile.egslst, etc.
-p orpegs-file file_name	Use the pegs4 data file file_name.pegs4dat. The system will look for it in the HEN_HOUSE and the users pegs4 data areas
-H orhen-house dir	Change the HEN_HOUSE to be dir instead of the directory specified in the machine.macros file.
-e oregs-home dir	Change EGS_HOME to be dir instead of the directory specified by the EGS_HOME environment variable
-b orbatch	Specify this is a batch run. See next section.
-P orparallel nparallel	Run nparallel jobs simultaneously
-j orjob njob	This is job # njob
-h orhelp	Print this help message and exit

Note that arguments can be given in arbitrary order.

5.3 Executing a user-code using the scripts (Unix/Linux specific)

For compatibility with the old usage, the script \$HEN_HOUSE/scripts/run_user_code has been written and the command ex has been aliased to this script. See the next section for the corresponding exb command. The general command for running ex is

```
ex user_code input_file pegs_file [noopt]
```

the first three parameters **must** be entered in that order to mantain backward compatibility with the old system. The input file and the PEGS4 data file can be entered with or without extension.

noopt is optional and tells the script to use the executable compiled with no optimizations.

6 Running a standard EGSnrc user-code in batch mode

6.1 Informing EGSnrcMP about your batch queuing system

Before running an EGSnrc user-code in batch mode, you must inform the EGSnrcMP environment about what queuing system you are using. At present batch operations are not available for Windows.

The default batch submission system assumed is the standard Unix job submission tool at. In the directory \$HEN_HOUSE/scripts, three files are provided which contain specific definitions for the at, NQS and PBS batch submission systems. These files are named:

batch_options.batch_system

where batch_system stands for at, nqs or pbs, the three systems that happen to be available at NRC. If the user wants to make NQS, PBS or any other system the default job submission system, he/she can define the environment variable EGS_BATCH_SYSTEM to be nqs, pbs or the name of the other queuing system for which they have created a batch_options.batch_system file modelled on the exisiting files.

```
batch_options.at
batch_options.nqs
batch_options.pbs
```

To use the names of the queues at your local installation, you must edit the names found near the bottom of the appropriate batch_options.batch_system file on \$HEN_HOUSE/scripts.

6.2 Using exb or run_user_code_batch

The script \$HEN_HOUSE/scripts/run_user_code_batch (alias: exb) is for submitting EGSnrc jobs to a queuing system taking advantage of the new implementation for parallel processing in EGSnrc (see section 12, page 40). The general command for using exb is

```
exb user_code input_file pegs_file [noopt] [queue_type] [options]
```

The first three parameters **must** be entered in that order to maintain backward compatibility with the previous EGSnrc/EGS4 systems. The input file and the PEGS4 data file can be entered with or without extension. The rest of the parameters can be in an arbitrary order. The [options] can be any combination of the following

noopt (optional) tells the script to use the executable compiled with no optimizations. queue_type gives the name of the batch queues used at your local installation. By default, queue_type is set to long. This is discussed further in section 6.1 above.

6.3 Using batch mode with the GUIs

On Unix/Linux if the batch mode is selected in the GUIs, then the queuing system and queue inputs become active. The default values are those in use at NRC. The GUI recognizes which queuing systems are available by looking on \$HEN_HOUSE/scripts for files in the form batch_options.batch_system where batch_system is the name of the remote job submission system.

6.4 NRC user-code command-line arguments for batch mode

In section 5.2 on page 23, the command-line inputs to the standard NRC user-codes are described. There is one further parameter available for jobs which are being run in batch, viz.:

-b or --batch

Specify this is a batch run. The difference between a batch run and an interactive run is that in batch mode unit 6 is connected to a file, whereas in interactive mode unit 6 output goes to the standard output. The file name in a batch run is determined as follows:

- * it is set to ofile.egslog, if ofile was specified with the -o option,
- * it is set to ifile.egslog, if there was no -o option used but an input file was specified with -i
- * it is set to test.egslog, if neither -i nor -o was used

Note that the user does not use this feature directly since the GUIs and the exb script take care of using it properly.

7 How to create a new data set using PEGS4

7.1 Using egs_gui

By far the easiest way to create a new pegs data set is using the egs_gui GUI which allows you to input the standard variables needed and to search the density effect corrections easily. Figure 3 presents a screen shot of the GUI.

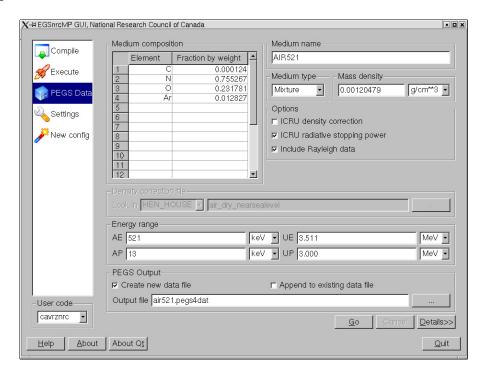


Figure 3: Screen shot of the egs_gui set to calculate a data set for air using the ICRU Report 37 density effect.

The GUI does not keep the input file but executes the code directly. There is also no output listing but the traditional output information is available by hitting the 'Details' button on the GUI after execution.

The PEGS4 data set created is put on \$EGS_HOME/pegs4/data using the filename specified by the user, with an extension .pegs4dat and thus it is necessary that \$EGS_HOME/pegs4/data and especially \$EGS_HOME are defined. If one wants to create a dataset on the \$HEN_HOUSE/pegs4/data area, this can be done by going to the Settings screen and entering the absolute path for \$HEN_HOUSE as the value for \$EGS_HOME, assuming of course that the user has write permission on \$HEN_HOUSE. Note that the user is given the option of creating a stand-alone data file or of appending the new data to an already existing data set. The code also appends information about each data set created to the file \$EGS_HOME/pegs4/data/pegs4.log. Here is an example of the pegs4.log file after 2 data sets have been created.

```
>more pegs4.log
medium = ARGON512
data generated on: Thu Nov 13 14:46:22 2003
type=ELEM rho= 1.7800E-03 ne= 1 iunrst=0 epstfl=0 iaprim=1
Rayleigh data not included
cross section data from: /usr/people/course/HEN_HOUSE/pegs4/pgs4pepr.dat
form factor data from: /usr/people/course/HEN_HOUSE/pegs4/pgs4form.dat
     5.12000E-01 ap=
                        1.00000E-03 ue=
                                          6.00000E-01 up=
data written to: /usr/people/group1/egsnrc/pegs4/data/argon.pegs4dat
medium = air 521
data generated on: Thu Nov 13 15:04:37 2003
type=MIXT rho= 1.2048E-03 ne= 4 iunrst=0 epstfl=1 iaprim=1
Rayleigh data included
density correction file: /home/course/HEN_HOUSE/pegs4/density_corrections/
                                   compounds/air_dry_nearsealevel.density
cross section data from: /home/course/HEN_HOUSE/pegs4/pgs4pepr.dat
form factor data from: /home/course/HEN_HOUSE/pegs4/pgs4form.dat
                                          3.51100E+00 up=
      5.21000E-01 ap=
                        1.00000E-03 ue=
                                                            3.00000E+00
data written to: /home/group1/egsnrc/pegs4/data/air521icru.pegs4dat
```

7.2 Using pegs4.exe

The egs_gui GUI can handle most PEGS4 jobs perfectly well, but there are some options which are not available via the GUI (e.g., the GUI assumes IUNRST=0 always, and the GUI cannot handle some of the PLOT and testing functions which are described in Report PIRS-701[3], nor can it use the GASP feature for scaling the density of gases in atmospheres). In these cases one needs to use pegs4.exe directly.

The usage is somewhat different from the previous EGSnrc or EGS4 environments since all parameters are now passed on the command line instead of as parameters to a script. To run the code it is best to go to the directory where the input file is stored (ifile.pegs4inp has the same format as defined in the EGSnrc manual) and issue the command:

```
pegs4.exe -i ifile [-o ofile] [-a] [-d density] [-x CrossSectData] \
                                                      [-e HEN_HOUSE]
                    => ifile.pegs4inp is the input file
 -i ifile
                    => if present output file is $EGS_HOME/pegs4/data/ofile.pegs4dat
 -o ofile
                       \& if not present output is $EGS_HOME/pegs4/data/ifile.pegs4dat
                    => if present that output is appended to [i|o]file.pegs4dat
 -a
 -d density
                    => if present density effect is in density.density
 -x CrossSectData => if present use $HEN_HOUSE/pegs4/CrossSectData for
                       photoelectric cross sections
 -e HEN_HOUSE
                    => if present store data on $HEN_HOUSE/pegs4/data
                       rather than $EGS_HOME/pegs4/data
 -h or --help
                    => print this help screen
```

The density effect files are only used if both the -d input is present and the flag EPSTFL=1 is part of the input file. This option is normally used to introduce an ICRU Report 37 density effect correction[4, 5], but can be used for any density effect in principle.

The -x option is there to allow use of the enhanced low-energy photo-electric cross section data set which basically uses the XCOM photo-electric and pair production cross sections[6] instead of the original EGS4 data set. The original data are in

\$HEN_HOUSE/pegs4/pgs4pepr.dat and the new data are in

\$HEN_HOUSE/pegs4/pgs4pepr_xcom_full.dat. For a description of the upgraded data set, see ref [7]. We want to thank Jan Seuntjens, Fadi Hobeila and Wamied Abdel-Rahman of McGill University for making this data set available in the correct format. If this option is not present, the standard \$HEN_HOUSE/pegs4/pgs4pepr.dat data set is used.

8 The file structure of the EGSnrcMP environment

As in the original EGS4 and EGSnrc environment, the EGSnrcMP environment uses two areas, one for keeping the system files (\$HEN_HOUSE or %HEN_HOUSE% on Windows) and another for the user files (\$EGS_HOME or %EGS_HOME% on Windows). System files on \$HEN_HOUSE can be common to several users or each user could have his/her own \$HEN_HOUSE if desired. The rationale behind having two different locations for the system and the user(s) is maintenance. While a user could be working on a specific user-code, updates and corrections can be introduced in the system without interference.

8.1 \$HEN_HOUSE

The directory structure of EGSnrc has changed, now files are regrouped according to their function within the system. See figure 4 for a summary of the \$HEN_HOUSE. While subdirectories doc, pegs4, mortran3, spectra (former ensrc_spectra) remain unchanged, the general system source files are placed together in \$HEN_HOUSE/src, more problem specific files (geometry dependent, user implementation dependent) can be found in \$HEN_HOUSE/utils and the cross section data files used by EGSnrc are placed in \$HEN_HOUSE/data. The tutor codes and the NRC user-codes are now located in \$HEN_HOUSE/user_codes.

The installation program can place \$HEN_HOUSE anywhere the person doing the installation has write permission, but it is most common to use \$HOME/HEN_HOUSE on Unix/Linux systems. On Windows systems, the \$HEN_HOUSE area *must not* contain spaces. This limitation is due to the use of the GNU make utility. One should therefore use *e.g.* C:\HEN_HOUSE and not use C:\Documents and Settings or C:\Program Files.

\$HEN_HOUSE in EGSnrcMP environment

```
'---- bin
                                       <=all executables
       '---- g77
                                       <=one subdirectory for each config
      '---- pgf77
'---- data
                                       <=cross section data for EGSnrc</pre>
'---- doc
                                       <=pdf versions of all manuals</pre>
      '---- pirs877
'---- gui
                                       <=GUI's for installation, running etc
       '---- egs_configure
       '---- egs_gui
      '---- egs_inprz
       '---- egs_install
'---- interface
                                       <=source re C interface to EGSnrc</pre>
'---- lib
                                       <=source re machine/OS dependencies</pre>
      '---- g77
                                       <=one subdirectory for each config
      '---- pgf77
'---- makefiles
                                       <=standard makefiles for all user-codes
'---- mortran3
                                       <=preprocessor source and makefiles</pre>
'---- pegs4
                                       <=data preparation package
      '---- data
                                       <=some prepared data sets</pre>
       '---- density_corrections
                                       <=ICRU 37 density effect corrections
               '---- compounds
               '---- elements
'---- pieces
                                       <=misc source
'---- previewRZ
                                       <=Tcl/Tk code to display RZ geometries
'---- specs
                                       <=config dependent spec files
'---- spectra
                                       <=useful spectra for user-codes to use
'---- src
                                       <=major sources for EGSnrc</pre>
'---- user_codes
                                       <=source & related files: NRC user-codes</pre>
       '---- cavsphnrc
                                         <=cavity calculations spheres
       '---- dosrznrc
                                         <=dose calculations RZ geometry</pre>
       '---- examin
                                         <=examine PEGS4 data sets</pre>
       '---- flurznrc
                                         <=fluence calculations RZ geometry
       '---- edknrc
                                         <=spherical energy deposition kernels</pre>
                                         <=stopping-power ratios RZ geometry</pre>
        '---- sprrznrc
       '---- tutor1
                                         <= tutorial codes
        '---- tutor1c
                                         <= C version of the tutorial code
     '---- tutor7
'---- utils
                                       <=geometry,source,plotting,timing etc</pre>
```

Figure 4: Structure of the \$HEN_HOUSE area. Note that several sub-subdirectories in the gui subdirectories have been suppressed.

8.2 \$EGS_HOME

In the original EGSnrc distributions, the user's EGSnrc area was assumed to be in \$HOME/egsnrc. This is still a logical choice for Linux/Unix users but for generality, this area is now consistently referred to as \$EGS_HOME so the user may place it anywhere and possibly switch between multiple versions. The same restriction on the path name as for \$HEN_HOUSE applies to \$EGS_HOME, i.e. Windows users should not select e.g. C:\Documents and Settings\some_user\egsnrc as their EGS_HOME directory. Otherwise the structure of the user's area is very similar to the past (see Figure 8.2) although the files associated with each user-code have changed somewhat. Note in particular that the previously hidden concatenation of all source code (.mortjob.mortran) is no longer a hidden file.

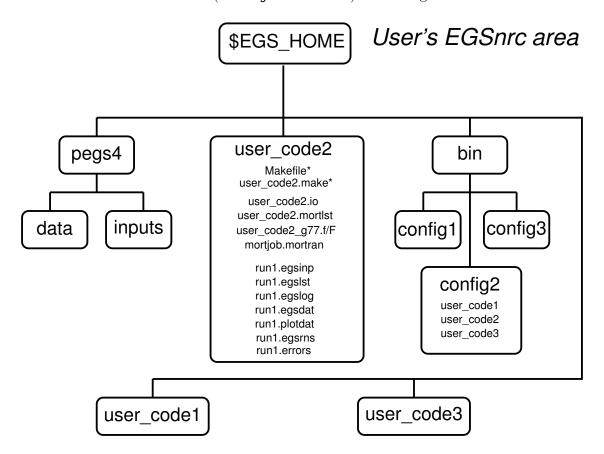


Figure 5: The user's area, \$EGS_HOME in the EGSnrcMP environment.

9 How the EGSnrcMP environment works

9.1 \$HEN_HOUSE/specs: Config files

9.1.1 What is a config file?

If a system is to work on a multi-platform environment, it needs to differentiate among combinations of operating systems and compilers for it to work properly. As described below, user-codes are compiled using Makefiles (see section 4.1) and the config file is an input for the Makefiles and the config name is used as part of a variety of file names. Therefore, when installing the system, the user should choose a meaningful config name that would for instance represent the settings selected by the user (compiler name, operating system, type of CPU, etc.). A suggestion is made to the user for the config name by the installing program, based on the operating system and CPU architecture (canonical name). The user can accept the suggested name, but any other name can be used and in particular, shorter ones may be preferable.

The config name is used by the EGSnrc system to create the binary and library directory for a given config, *i.e.*, executable and machine dependent files created for config CONFIG_NAME are stored in \$HEN_HOUSE/bin/CONFIG_NAME and \$HEN_HOUSE/lib/CONFIG_NAME respectively. All these settings are stored in a config file (*.conf) in \$HEN_HOUSE/specs and the environment variable EGS_CONFIG must point to the current (desired) config file. On Linux/Unix systems this must be set in the user's .cshrc or .bashrc file (*e.g.*, in .cshrc one needs the statement setenv EGS_CONFIG /home/course/HEN_HOUSE/specs/pgf77.conf). Although we commonly use the config name for the config file name, *i.e.*, CONFIG_NAME.conf, this is not required and as with the config name, the config file name can be freely chosen by the user.

Depending on the installation procedure chosen, a config file is created by the \$HEN_HOUSE/scripts/configure script or by the installation GUI. At any time, the user who owns the \$HEN_HOUSE area may create additional config files using the \$HEN_HOUSE/scripts/configure script (Unix/Linux only) or one of the 3 GUIs (egs_install, egs_gui or egs_inprz). The later method works for Windows and Linux. When running the configure script it is important that \$HEN_HOUSE NOT be set from a previous (non MP) EGSnrc or EGS4 installation.

The process of creating a config file involves the following steps:

- Determine compiler name and compilation options to be used
- Check for the availability of various Fortran intrinsics (e.g data_and_time, etime, hostnm, etc.,) data types (e.g. integer*8), record length for binary I/O, etc.
- Based on the results of the previous step, create the files machine.macros and machine.mortran in \$HEN_HOUSE/lib/\$my_machine and the config file in \$HEN_HOUSE/specs
- Compile the Mortran3 preprocessor and create the hex data file using these compiler settings and place them in \$HEN_HOUSE/bin/\$my_machine.

• Compile the PEGS4 program using the newly created Mortran3 executable and the new Fortran compiler settings

Appendix A presents examples of a config file created on a Linux system which has a pgf77 compiler (Portland Group). Also presented there are three files which are included in config files. \$HEN_HOUSE/specs/all_common.spec, which is common to all config files and \$HEN_HOUSE/specs/unix.spec and \$HEN_HOUSE/specs/windows.spec which are common to config files on Unix/Linux and windows installations respectively.

The syntax of these config files is fairly simple and self-explanatory. Users are encouraged to take a look at them for a better understanding of their functions. Note that while config files can have any name, we are reserving the extension *.spec for specification files from the EGSnrc system and the *.conf for user-created config files. This convention can of course be replaced by any other.

It is worth noting that after creating a new config the user may want to compile the various GUIs for the new config. After switching to the new config, this is most easily accomplished by going to the \$HEN_HOUSE/gui directory and typing make.

9.2 Pre-compiled components for Windows

On Windows (NT/2000/XP) many object and executable files are created at NRC and included in the distribution, e.g., the graphical user interfaces, egs_c_utils.obj, etc.. These files can be found in \$HEN_HOUSE/pieces/windows together with a copy of the Qt library dll and the executable for GNU make. At installation time they are just copied to their corresponding location.

10 Using external files: egs_init and egs_finish

Any EGSnrc simulation requires that the user-code have access to a variety of I/O files (e.g., data files, listing files, standard output, standard input, etc.). These can be divided into two broad classes, those that are "routine" and used by all codes, and those specified by the user. In the original EGSnrc environment and the EGS4 Unix environment, the association between Fortran I/O unit numbers and external files was handled by the run scripts and the .environment files by linking the standard Fortran names for these files (fort.n) to the specific files of interest. In the EGSnrcMP environment this is done by explicitly opening and closing the files by their proper names from within the code. The advantage of doing this is that it works on Unix/Linux systems and on Windows systems.

To handle this the user must call two additional routines at the start and end of the user-code, viz., egs_init and egs_finish and the user must create a .io file for each user-code to associate particular units with specific file name extensions. All one has to do is include a call to subroutine egs_init before any other executable statement in the user-code. This is called step 0 in the user-code (but really has to be the first executable step in the code and is often found in Step 2 since step 1 has no executable statements usually). Similarly, egs_finish

should be the last executable statement when the user-code is run (including after error conditions). Both of these subroutines are found in \$HEN_HOUSE/src/egs_utilities.mortran and this source file is automatically included in all EGSnrc compilations.

The subroutine egs_init does many things.

• egs_init initializes arrays and default values (this replaces BLOCK DATA in EGSnrc since, for large arrays, the GNU compiler was very slow initializing block data)

• egs_init processes command-line arguments, including:

```
- -p pegs_file
- -i ifile
- -o ofile
- -b
- [-e| --egs-home] new_egs_home_location
- [-H| --hen-house] new_hen_house_location
```

- egs_init opens default EGSnrc data file units
- opens specific I/O units defined in the .io file found in the user-code area (user-code.io). See section 10.1 below for the format.
- moves files associated with this particular job to a temporary working directory which is a subdirectory of the user-code directory.
- prints a summary of the configuration and other system info to standard output (*i.e.*, the terminal).

The following comments apply to the above points.

The PEGS4 data file specified by -p pegs_file, is used if it is passed as a full pathname and found. Otherwise, the subroutine looks in turn for:

```
$EGS_HOME/pegs4/data/pegs_file,
$EGS_HOME/pegs4/data/pegs_file.pegs4dat
$HEN_HOUSE/pegs4/data/pegs_file
$HEN_HOUSE/pegs4/data/pegs_file.pegs4dat
```

If a -i ifile option was given as an argument, ifile.egsinp is opened as Fortran unit 5. The input file MUST be in the user-code directory, *i.e.*, on \$EGS_HOME

If the run is a batch run (*i.e.*, the -b option was present on the command line), Fortran unit 6 is connected to an output file with a .egslog extension instead of going to standard output. The algorithm for determining the .egslog file name is the following: If the -o ofile option was present, the output to unit 6 will go to ofile.egslog If there was no -o option, but there is an input file specified with -i ifile, output to unit 6 will go to ifile.egslog If neither of the above is true, the output will go to test.egslog.

During run time, all output from the program (the .egslog file and all other files specified in the .io file (see section 10.1) are kept in the temporary working directory. After successful completion, egs_finish moves all output back to the user-code area and removes the temporary working directory. This implies that if, for whatever reason, the job terminates prematurely, the temporary working directory, with all the outputs, will be left behind.

The name of the temporary working directory is created using egsrun_getpid_ifile_hostname, if there was an input file, or egsrun_getpid_noinput_hostname, if there was no input file specified. Here, getpid is the process id returned by the getpid() intrinsic and hostname is the host name as determined by egs_get_hostnm().

EGS_HOME is normally taken from the environment variable EGS_HOME. However, one can overwrite the environment variable by giving the -e | --egs-home new_egs_home_location command line parameter. EGS_HOME must be set, either via the environment or via the command line, otherwise the job will abort.

HEN_HOUSE is set to the value defined in machine.macros, which is created by the configure script or the configuration wizard in the GUI. This value can be overwritten by giving the -H | --hen-house new_hen_house_location option on the command line. HEN_HOUSE is NOT taken from the environment.

Subroutine egs_finish does three things.

- closes all the currently open I/O files
- moves any files on the subdirectory for this run back to the user-code directory
- prints a summary of the CPU time used on the standard output

10.1 user-code.io file format

The user-code.io file is specific to each user-code and is found in \$EGS_HOME/user-code along with user-code.mortran etc.. This file is used to associate specific file names with Fortran unit numbers used within the user-code and subroutine egs_init then opens these files. The file format is an integer followed by a filename extension. The integer is the Fortran unit to be associated with the file in the user-code. The file extension is appended to the file name to be used for output. This will either be the name specified by the user for output (e.g., by the -o ofile command line specification, see section 10 or, if that is not specified, then by default the input file base name (i.e., ifile from ifile.egsinp). For cases in which neither ifile nor ofile are specified, the value of test is used. For example:

- 4 .egsdat
- 15 .egserr
- 1 .egslst

will result in connecting unit 4 to the file ifile.egsdat (or ofile.egsdat or test.egsdat, see above) to unit 4, [i|o]file.egserr to unit 15, etc.. Lines starting with a pound sign (#) are ignored. Note that file name extensions can not exceed 10 characters.

11 A C interface for EGSnrc

11.1 \$HEN_HOUSE/interface: Interface for C-written user-codes

The EGSnrcMP system provides a C interface so that user-codes can be written in C (or C++). The necessary files are on \$HEN_HOUSE/interface. The files are egs_c_interface1.macros, egs_interface1.h and egs_interface1.c. The standard Makefile to be included by makefiles for C user-codes is c_makefile in the makefiles subdirectory of \$HEN_HOUSE. Examples of user-codes implemented in C are tutor1c, tutor2c and tutor4c.

11.1.1 Macros for the C interface: egs_c_interface1.macros

The purpose of the file egs_c_interface1.macros is:

- To slightly re-organize EGSnrc common blocks so that a relatively small number of common blocks needs to be exported as C structures. In particular, all variables that define a certain aspect of a cross section or the modelling of some process (e.g. ibrdst, which defines the bremsstrahlung cross section to be used, spin_effects, which defines whether spin effects should be modelled in electron elastic scattering, etc) are removed from the respective EGSnrc common block in which they are normally defined and combined into a single common block called xsection_options and are accessible from the_xoptions, which is a pointer to a struct EGS_XOptions.
- To re-define most of the arrays that have the dimension of the number of geometrical regions to be scalar variables (e.g. ecut, pcut, smaxir, etc.). The rationale behind this is that (i) the core EGSnrc system should be as much independent of the geometry as possible (ii) if the user needs a region-by-region variation of these quantities, memory can be dynamically allocated in the C written user-code depending on the actual number of regions instead of being statically allocated in the EGSnrc Fortran routines. There is a process defined that the user writing a code in C must follow to implement region-by-region variation of the various quantities.
- To re-define various EGSnrc macros that have been introduced into the EGSnrc system specifically for the purpose of providing non-Fortran interfaces to EGSnrc. One example of such a macro is \$start_new_particle; which is defined as dummy in egsnrc.macros but is replaced with a call to a function that the user needs to implement in egs_c_interface1.macros.

11.1.2 Main interface header files: egs_interface1.h and egs_config1.h

The header file egs_interface1.h provides the main interface to EGSnrc. Its purpose is to define C structures corresponding to the exported EGSnrc common blocks, the EGSnrc functions visible to the user and the functions that the user must implement in order to have a functional EGSnrc user-code. egs_interface1.h includes the header files egs_config1.h

and array_sizes.h. The latter must be present in the user-code directory and must define the C-preprocessor macros MXMED to be the maximum number of different media and MXSTACK to be the maximum number of particles that the EGSnrc stack can hold. The former is created during the EGSnrc installation/configuration, defines the name mangling scheme of the Fortran compiler used to compile the EGSnrc Fortran routines via the C-preprocessor macros F77_OBJECT and F77_OBJECT_, and can be found in the lib/\$my_machine subdirectory of \$HEN_HOUSE. Different Fortran compilers generate different internal names for Fortran subroutines and functions (name mangling). For instance, given the Fortran subroutine test, one of the following C function names will be necessary to call this subroutine from C: test, test_, TEST or TEST_. It is even worse for a subroutine or function named some_test: some_test, some_test_, some_test__, SOME_TEST, SOME_TEST_ and SOME_TEST_ are all possible results. Because of this, one has to use F77_OBJECT(test, TEST) or F77_OBJECT_(some_test, SOME_TEST) to refer to Fortran subroutines, functions and common blocks. Because this is quite tedious, egs_interface1.h defines C-preprocessor macros for referring to important EGSnrc objects, e.g. egsHatch() can be used to call the HATCH subroutine, egsInit() can be used to call the initialization routine, etc. In addition, egs_interface1.h defines pointers to C-structures corresponding to the exported EGSnrc common blocks, e.g. one can use the_stack->E to access the array containing the energies of particles on the stack, instead of using the cumbersome F77_OBJ(stack, STACK).E.

11.1.3 What is needed for a C-written EGSnrc user-code

A user-code written in C must provide the following components:

- Implementation of the void egsHowfar() function. This function must calculate the distance t to the next geometry boundary along the direction of motion of the top particle on the stack. The position and direction of the top stack particle are in the_stack->x[i], the_stack->y[i], the_stack->z[i] (position) and the_stack->u[i], the_stack->v[i], the_stack->w[i] (direction). Here, i = the_stack->np 1. This function must then compare this distance to the intended step length (in the_epcont->ustep) and
 - If you wish to discard the particle immediately, set the_useful->idisc to a positive value and return. If the particle is to be discarded after the step is complete, then set the_useful->idisc to a negative value and return.

Otherwise,

- just return, if t > the_epcont->ustep
- set the_epcont->ustep to t, set the_epcont->irnew to the new region number and set the_useful->medium_new to the medium in the new region, if t < the_epcont->ustep
- If there is a region change and you wish to implement region-by-region variation of cut-off energies, maximum step size or non default mass density, then: set the_epcont->ecut_new to the desired value to have a non-default electron cut-off energy, the_epcont->pcut_new to the desired value to have a non-default photon

cut-off energy, set the_etcontrol->smax_new to have a maximum geometrical electron step-size restriction in the new region and set the_useful->rhor_new to have a non-default mass density in the new region.

- Implementation of the void egsHownear(float *tperp) function. This function must set tperp to the perpendicular distance to the closest boundary. If this is impossible (because e.g. the geometry is too complex), tperp must be set to 0 but this means that the entire calculation will be done in single scattering mode and take much longer.
- Implementation of the void egsAusgab(const int *iarg) function. This is where the actual scoring is being done, see section 3.7 of the EGSnrc manual for details[3].
- Implementation of the void egsStartParticle() function. This function is called just before the transport of a "new" particle starts (either directly from the source or a new particle from the particle stack). This function must set the_useful->medium to the medium index of the region the particle is in. If a region-by-region variation of threshold energies is to be obtained, the_bounds->ecut or the_bounds->pcut must be set to the desired value (depending on the particle charge).
- Provide a main function. The main function must
 - Call egsInit(int argc, char **argv) (where argv are the command-line arguments and argc their number) before accessing any EGSnrc data
 - Identify to the EGSnrc system all media that make up the geometry using the int egsAddMedium(const char *medname, int len) function. The return value of this function is the index of the medium in the internally maintained list of media (and so, if one calls this function with a medium name that was previously added, this function will return the index of the previously added medium).
 - Initialize cross section data needed at run time via a call to egsHatch().
 - Simulate a given number of particles by placing one or more particles on the stack (the_stack) and calling egsShower().
 - Close all Fortran I/O units and remove temporary files by calling egsFinish().

The main.c files in the tutor1c and tutor2c directories of \$HEN_HOUSE/user_codes use the EGSnrc C interface to implement the functionality of the traditional tutor1 and tutor2 user-codes. They can be taken as a starting point for developing your own user-code in C or C++.

11.1.4 The tutor4c user-code

The C interface as described above requires an additional file called user_code.macros (where user_code is the name of the user-code) to be placed in the user-code directory. This file defines the maximum number of media (\$MXMED) and the maximum number of particles on the stack (\$MXSTACK) used during the Mortran and Fortran compilation steps of the EGSnrc system. One must therefore make sure that these array sizes are the same as the

array sizes defined in the array_sizes.h header file. The tutor4c user-code provides a C implementation of tutor4 where array sizes in the C part and in the Mortran/Fortran part are determined by a single file array_sizes.h. This alternative implementation requires that the EGSnrc Fortran sources are pre-processed by the C-preprocessor. On many systems (all Linux and Unix systems that we have tried and on Windows using the GNU compiler), this is automatically accomplished by having a .F extension for Fortran source files. Unfortunately, some Fortran compilers for Windows do not automatically pre-process a .F file or require weird options to do so. We have therefore deemed the tutor4c implementation not portable enough to designate it as the main EGSnrc C-interface implementation. But if the tutor4c implementation works for your operating system/compiler combination it is preferable to the main C interface.

11.1.5 Known limitations of C interface

- The Makefiles will only work with GNU make.
- On a Windows system, we can successfully compile and link the distributed user codes written in C using the GNU Fortran compiler and the Microsoft Visual Studio C++ compiler, but running the so created executables produces obviously wrong results. We are currently investigating the reasons for this behaviour.

12 Parallel runs

Running jobs in parallel requires special coding of the user-code. What is described in this section applies to the general purpose codes distributed with the EGSnrc system (DOSRZnrc etc).

In the original EGSnrc implementation of parallel runs for the NRC user-codes, the scripts asked each node to do (1/n)th of the calculation, where n was the number of nodes or computers used. This was inefficient when nodes had different CPU speeds and in practice meant that the calculation took as long as the slowest computer. In addition, parallel processing required a special script that had to "know" the syntax of input files for all parallelized user-codes so that it could modify the number of histories and the initial random number seed(s) when creating input files for the separate jobs. To overcome this drawback, the new system includes a parallel processing option for the NRC user-codes in which parallel processing is controlled via a "job control file" (JCF) placed in the user-code directory (the file name is ofile.lock where ofile is the name of the output file(s) that will be created by the job). This implies that \$EGS_HOME must be the same for all nodes participating in the parallel execution. This can be accomplished, e.g. by placing the \$EGS_HOME directory on an NFS file system for Unix/Linux installations or on a network share that is mapped to the same drive for Windows installation. The JCF is created by the first job, which reads from the input file the number of histories to be simulated, takes a small portion of them, writes the remainder to the JCF and starts simulating its portion of histories. Subsequent parallel jobs read the number of histories to be run and the number of jobs currently running (set to 1 by the first job) from the JCF, take a small portion of them and increment the

number of running jobs. When any job finishes execution of the small portion of histories it was simulating, it reads the JCF, takes some fraction of the remaining histories and writes the updated number of histories remaining to be done to the JCF. If no histories are left, the job performs statistical analysis, writes its data to ofile.egsdat, and decrements the number of running jobs in the JCF. If this number is greater than one, the jobs simply exits. If the remaining number of running jobs is zero (i.e. this is the only job still running), the job reads the data output by all other parallel jobs to .egsdat files, combines them, writes the combined results, removes the JCF and exits.

The advantage of this system is that, in the worst case, one waits for the slowest machine to execute the last group of histories, and if the groups of histories are small enough, this is a short period of time. In addition, no separate script is required that "knows" about the syntax of input files. Finally, no separate run that combines the results is required, as it was the case with the previous parallel processing implementation. The disadvantage is that each user-code must be coded to perform the above tasks.

12.1 egs_c_utils

To make the approach just described feasible, it is necessary to lock the JCF while a particular job is accessing it so that it becomes impossible for two jobs to modify the JCF at the same time. The JCF must be unlocked by the job when done with reading/writing to the file. Since it is impossible to lock/unlock a file using Fortran, tools for locking and unlocking a file were written in C. The corresponding C files are the source file egs_c_utils.c and the header files egs_c_utils.h and egs_config1.h. During installation, egs_c_utils.c is compiled and the resultant object file is copied together with the source and header files to \$HEN_HOUSE/lib/\$my_machine.

To see how these routines are used, please check the source for the DOSRZnrc or CAVRZnrc codes.

12.2 Parallel job submission

If the user-code is set up to handle them, parallel jobs can be submitted on Unix/Linux systems using one of the GUIs or the exb command. For both GUIs (egs_gui or egs_inprz), the only difference between submitting a single batch job (see section 5.1) and a parallel job is that the number of jobs must be set to greater than one in the relevant input box. In a similar way, when using the exb command, the only difference between submitting a single batch job (see section 6.2) and a parallel job is that one has to pass an additional argument of the form p=njob to the exb script, e.g.:

exb cavrznrc my_input my_pegs_data batch=pbs p=10

will initiate a cavrznrc run with 10 parallel jobs using my_input.egsinp as input file, my_pegs_data as a PEGS4 data set and PBS as the queuing system. It is important to note that there should not be any spaces for arguments of the from xxx=yyy passed to the exb script.

13 Efficiency considerations

For some of the standard NRC EGSnrc user-codes, we have obtained efficiency improvements, of the order of 30 to 40% on a given machine, through a variety of steps.

13.1 Static vs non-static

In the past, the EGSnrc system required 'static' switches on the Fortran compilers because EGS was written in the times when all variables in subroutines were saved from one call to the next. This is not standard Fortran and the compiler switches used to ensure the variables are all saved caused some inefficiency (of the order of 10%). We have ensured that these switches are no longer needed in the EGSnrc system itself and have done the same for the user-codes distributed with the system (CAVRZnrc etc). However, users with their own user-codes must ensure that this is the case for their user-codes before using the default switches which we now employ.

13.2 Fortran compilers

We have also found that Fortran compilers can vary a great deal in the speed of the code they produce on a given machine. When using the GNU g77 compilers, we have found that using version 3.3 of the gcc compiler can increase the execution speed of the calculation by more than 20% compared to using version 2.95.3. Using the Portland Groups pgf77 compiler can further increase the efficiency by another 5% compared to using gcc 3.3.

13.3 Random number generators

In table 7 of the EGSnrc Manual[8] there is a comparison of the timing of a particular calculation using different 'luxury levels' for the RANLUX random number generator.

We have found that by recoding the RANMAR random number generator to include a function subroutine to calculate a group of random numbers whenever the current supply has run out, we (a) avoid the frequent use of the subroutine call and (b) reduce the size of the Fortran source considerably because the random number generator is used so often that when the entire generator is coded in-line, the total length of the code increases substantially. The result is that for one of our major production codes (CAVRZnrc) there was a significant improvement in computation time, just because the executable is considerably smaller and fits into the fast memory.

With this change in place, we have found that using the RANMAR random number generator is about 10% faster than using the RANLUX generator with a luxury level of 1.

14 How to upgrade your old EGS user-code

If you have written an EGSnrc user-code, the major change required to use the EGSnrcMP environment is to insert the subroutine calls call egs_init as step 0 in the code and call egs_finish as the last statement in the code (see section 10, page 33). In addition you need to create a user-code.io file on \$EGS_HOME/user-code (see section 10.1, page 36) and a user-code.make file on the same area (see section 4.1.1.i, page 18). The final step is then to copy a generic Makefile to the user-code area (see appendix B.2, page 53 for a Makefile example) and follow the directions in the header of the Makefile.

If your user code makes the assumption that local variables are automatically saved, you have to either find the appropriate switch for your compiler (e.g. -fno-automatic for the GNU compiler, -static for many Unix compilers, etc.) or you have to determine which variables really need to be static and save them using save statements in the appropriate subroutines.

If you want to adapt your user code to the new parallel processing implementation, use as a starting example the implementation in cavrznrc.mortran by searching for pieces of code enclosed between #ifdef HAVE_C_COMPILER and #endif. You will of course need a working C compiler that is capable of compiling egs_c_utils.c.

If you are starting from an EGS4 user code you must first convert it to using EGSnrc. This is described in detail of Section 5 of the EGSnrc Manual, Report PIRS-701[3].

15 Using the system at NRC

This section is just for people who are working at NRC.

At NRC the system is maintained under CVS control with the repository on the area /home/cvsroot/HEN_HOUSE.

To get the HEN_HOUSE and all the associated files onto your own area, execute: /home/cvsroot/CVSROOT/update_egs.

This builds the system on \$HOME/HEN_HOUSE, creating the subdirectory if not there and only updating changed files if you already have the system. This script also compiles various codes if needed because of changes (mortran3, pegs4). Note that the compilations are done for 3 compilers and need the following statement in your .login or .cshrc file:

setenv LD_LIBRARY_PATH /home/iwan/gcc33/lib:\$LD_LIBRARY_PATH to pick up the libraries for gcc3.3.

To have access to the standard files, you need to have: setenv HEN_HOUSE and setenv EGS_CONFIG \$HEN_HOUSE/specs/\$your config file in your .cshrc and/or .profile.

15.1 Using CVS

To change a file on your local area:

blank means check in/commit all files in this directory or below which have been changed.

filename means just this file

directory means just contents of that directory and below.

All options leave just readonly versions of each file affected. Note that if the ci fails, use cvs update which will merge your changed version with that in the repository and then allow you to ci (possibly after manually resolving problems with the merge).

To print a record of log messages:

cvs log filename: prints a record of the log messages for this file.

To get the changes that others have made to the system, and merge the changes into a file you are working on (but don't be editing it when you do this): cvs update [filename|directory|blank]

blank means update all files in this directory or below which have been changed.

filename means update just this file

directory means update contents of that directory and below.

All of the above will try to merge changes with any files that you have editable and leave them editable.

The above command will **not** pick up any new directories in the repository unless you add -d right after the command update.

The preferred alternative is to execute /home/cvsroot/CVSROOT/update_egs which updates everything on \$HOME/HEN_HOUSE and also rebuilds any files which are dependent on changes that have been made.

To add a directory or file:

First create the file or directory. Then:

cvs add [directory|filename] where both are full pathnames

and then for the files only, you must:

cvs ci filename

To compare file to what is in repository:

cvs diff filename does a diff against repository.

15.2 Creating a Distribution

On the NRC system, go to \$HOME/HEN_HOUSE/tools/distribution. Make sure that you have environment variable QTDIR set. For some reason the default of /usr/lib/qt3 does not work but /home/course/qt_current does work. Then issue the command make linux_distribution which leads to the Unix/Linux distribution being created on this area. You can create the entire distribution (including Windows specific files) by using just make. Note, however, that the various Windows executables and object files must have been created in advance on the Windows 2000 server by going to \$HEN_HOUSE/pieces/windows and executing make there. This will only succeed if you have set up your environment (path including Visual Studio binary directory, GNU compiler binary directory and make binary directory, environment variable QTDIR set to point to the latest Qt Windows installation and path including \$(QTDIR)/bin.

Note that the list of files included in the distribution is defined in $$HOME/HEN_HOUSE/admin/egsnrc_list$ and near the top of this file the version identifier pre-pended to all tar files (e.g., V4_) is defined.$

The actual distribution is created by the program make_distribution.cpp which is on \$HOME/HEN_HOUSE/tools/distribution.

A complete distribution also requires the install script, either \$HOME/HEN_HOUSE/tools/install_egs or the gui equivalent.

16 Known restrictions

- Red Hat 9.0: Some of the graphical user interfaces, egs_install and egs_inprz, developed using the Qt library, hang and freeze the whole OS system when using the GNOME desktop environment and the Qt library version 3.1 that come with Red Hat 9.0. For reasons beyond our comprehension, the freeze does not occur with Red Hat 9.0, Qt 3.1 when using the KDE desktop environment
- SUSE 9.0: The GNU compiler distributed with SUSE 9.0 (a pre-release of version 3.3) is broken and fails to compile the egs_inprz GUI. If you are running SUSE 9.0 you should install the GNU compiler from source (see http://gcc.gnu.org/) or look for an updated rpm package from SUSE.
- Windows: Makefiles for the EGSnrcMP system will only work with GNU make.exe
- Windows: When writing user codes in C and using the Microsoft C/C++ compiler in combination with the GNU Fortran compiler, it is not possible to use single precision versions of the math library functions such as acosf, atanf, cosf, logf, etc. (use of these functions results in random crashes and/or wrong numerical results). Solution: Use the double precision math library functions instead.
- Windows: When running an EGSnrc user code compiled with the GNU fortran compiler from a drive that has its access permissions restricted and in addition there is a virus scanner monitoring each I/O operation running, execution fails with an error

coming from the GNU I/O library (endfile: truncation failed in endfile...) Solution: Don't restrict access permissions or run from a drive where you have full permissions.

- Windows: The Lahey Fortran 95 compiler version 5.7 or earlier does not invoke automatically the C pre-processor on Windows. But on Linux it does! This means that compiling the NRC RZ user-codes will fail.
 - **Solution**: If the EGSnrcMP system is being used **only** on Windows, remove/commentout all code between the #ifdef #endif constructs, including them, throughout the NRC RZ user-codes and any other user-code using this construct.
- C interface: The Makefiles for the user codes written in C only work with the GNU version of make.
- Mac OSX with GNU compilers: The building of the tutor1c user code fails because of an undefined reference to the acosf function. Solution: Replace the call to acosf in egsAusgab() with a call to acos with a double precision argument.

Appendix A: An example config file

Note that for all the files shown in the appendices, one should check that current versions of the files on the system for changes since these will not always be the current versions.

A.1: pgf77.conf

The following config file was created by the script \$HEN_HOUSE/scripts/configure to use the pgf77compiler on a linux system. Note that this file includes the two files, all_common.spec and unix.spec.

```
#************************
# EGSnrc config file
# Created by configure version 1.0 on Wed Nov 12 12:11:10 EST 2003
# Attention: all changes you make to this file may be lost next time
# you run configure.
DSEP = /
my_machine = pgf77
canonical_system = i686-pc-linux-gnu
make_prog = make
HEN_HOUSE = /usr/people/course/HEN_HOUSE/
SPEC_DIR = $(HEN_HOUSE)/specs/
# Include the standard Unix spec file
include $(SPEC_DIR)unix.spec
# Include definitions common for all systems.
# These are mainly directory names, executable names, etc.,
# which are constructed from the previous definitions.
include $(SPEC_DIR)all_common.spec
# Fortran compiler name and options
F77 = pgf77
FCFLAGS =
FOPT = -fast
FDEBUG = -g -C
FLIBS =
FOUT = -0
# C compiler name and options
CC = gcc
C_FLAGS = -02
```

```
# You can use the following make varibale for
# including additional object files in the link
# process
USER_EXTRA_OBJECTS =
# We have a C compiler that successfully compiled egs_c_utils.c
# For simplicity in the Makefiles, we always include egs_c_utils.o
# in the link step, even if the functions are not used. This is not
# too wasteful as egs_c_utils.o is quite small.
EGS_EXTRA_OBJECTS = $(HEN_HOUSE)/lib/$(my_machine)/egs_c_utils.o
# FC_FLAGS gets used for compiling the EGSnrc fortran routines and for
# linking for EGSnrc user-codes written in C. We set FC_FLAGS by
# default to be given by $(FCFLAGS) $(FOPT). This is OK for most
# compilers. Unfortunately, some Fortran compilers insert a default
# main function and then complain about multiply defined main
# (theirs and the main of the user-code written in C), unless a special
# flag is passed. For instance, the PGI compiler needs -Mnomain.
# As I don't know how to test for this feature, it is left up to you
# to read the documentation of your compiler and adjust FC_FLAGS in
# case it does not work.
FC_FLAGS = $(FOPT) $(FCFLAGS) -Mnomain
```

A.2: all_common.spec

The following file (\$HEN_HOUSE/specs/all_common.spec) is included in the config file and thereby into all standard Makefiles. Note in particular that this piece of code is where the list of "standard" SOURCE codes are defined. These can be overridden for a specific user-code in the user-code.make file found on \$EGS_HOME/user-code (see Appendix B.2, page 55).

```
# it under the terms of the GNU General Public License as published by
# the Free Software Foundation; either version 2 of the License, or
# (at your option) any later version.
# The standard Makefile
EGS_MAKEFILE = $(HEN_HOUSE)makefiles$(DSEP)standard_makefile
# The standard Makefile for user codes written in C.
EGS_C_MAKEFILE = $(HEN_HOUSE)makefiles$(DSEP)c_makefile
# Relative directories for executables and libraries
BIN_SUBDIR = bin$(DSEP)$(my_machine)$(DSEP)
LIB_SUBDIR = lib$(DSEP)$(my_machine)$(DSEP)
# Main installation executables and libraries
EGS_BINDIR = $(HEN_HOUSE)$(BIN_SUBDIR)
EGS_LIBDIR = $(HEN_HOUSE)$(LIB_SUBDIR)
#
# User executables and libraries
USER_BINDIR = $(EGS_HOME)$(BIN_SUBDIR)
USER_LIBDIR = $(EGS_HOME)$(LIB_SUBDIR)
#
# EGSnrc sources
EGS_SOURCEDIR = $(HEN_HOUSE)src$(DSEP)
# Utilities coming with EGSnrc
EGS_UTILS = $(HEN_HOUSE)utils$(DSEP)
# The default random number generator
# You can overwrite either on the command line or in your
# Makefile
RANDOM = $(EGS_SOURCEDIR)ranlux
# User code directory
EGS_USERCODES = $(HEN_HOUSE)user_codes$(DSEP)
# The main area user code directory
MAIN_UCODE_DIR = $(EGS_USERCODES)$(USER_CODE)$(DSEP)
# The fortran file (without extension) to be created by the Mortran compiler
FORTRAN_FILE = $(USER_CODE)_$(my_machine)
# The executable
EXECUTABLE = $(USER_BINDIR)$(USER_CODE)$(WHAT)$(EXE)
```

```
# What about OMEGA stuff? I'm puting it in here for now, so
# that I can play around with the local makefiles.
OMEGA = $(HEN_HOUSE)omega$(DSEP)
# Mortran stuff
MACHINE_MORTRAN = $(EGS_LIBDIR)machine.mortran
MACHINE_MACROS = $(EGS_LIBDIR)machine.macros
MORTRAN_EXE = $(EGS_BINDIR)mortran3.exe
MORTRAN_DATA = $(EGS_BINDIR)mortran3.dat
# The standard set of files
SOURCES = $(EGS_SOURCEDIR)egsnrc.macros \
  $(MACHINE_MACROS) $(RANDOM).macros \
  $(USER_CODE).mortran \
  $(RANDOM).mortran $(EGS_UTILS)nrcaux.mortran $(MACHINE_MORTRAN) \
  $(EGS_SOURCEDIR)egs_utilities.mortran $(EGS_SOURCEDIR)egsnrc.mortran
#
# PEGS4 stuff
PEGS4_EXE = $(EGS_BINDIR)pegs4.exe
# Replacement for various scripts
# Do we need this ?
EGS_COMPILE = $(EGS_BINDIR)egs_compile$(EXE)
# The fortran file extension
FEXT = f
# The following set of definitions is for interfacing EGSnrc to C/C++
# C/C++ interafece file directory
C_INTERFACE = $(HEN_HOUSE)interface$(DSEP)
# Include directories for the C/C++ compiler
C_INCLUDES = -I$(HEN_HOUSE)lib$(DSEP)$(my_machine) -I$(HEN_HOUSE)interface -I.
# The set of mortran files needed for the C/C++ interface
            $(EGS_SOURCEDIR)egsnrc.macros \
C_SOURCES =
$(MACHINE_MACROS) $(C_INTERFACE)egs_c_interface1.macros \
$(RANDOM).macros\
$(USER_CODE).macros \
$(RANDOM).mortran \
$(MACHINE_MORTRAN) \
$(EGS_SOURCEDIR)egs_utilities.mortran \
$(EGS_SOURCEDIR)egsnrc.mortran
```

A.3: unix.spec

The following file, \$HEN_HOUSE/specs/unix.spec, is used on Unix/Linux systems and contains those aspects of the Makefile which are different on Unix and Windows systems.

```
# $Id unix.spec, v 1.4 2003/11/14 01:12:02 iwan Exp $
#
# This file gets used by Make on Unix systems.
# Copyright Iwan Kawrakow and the National Research Council of Canada
# Initial version: Iwan Kawrakow, March 2003
# The suffix of an executable
EXE =
SHELL = /bin/sh
# Sometimes I want to just leave a line blank in the output.
# When I just say echo, stupid Windows prints ECHO is off.
# => I'm using echo $(empty) and defining $(empty) to be really empty on Unix
empty =
# Check if a file exists and if not, copy it from the second argument.
# If the file exists, check if it is more recent than the other
GET_FILE = if test -f $0; then \
         echo $(MAIN_UCODE_DIR)$@ is more recent than local version; \
         cp $(MAIN_UCODE_DIR)$@ $@; \
         echo Copied $(MAIN_UCODE_DIR)$@ to local area; \
       fi
CHECK_USER_CODE = \
       if test -f $(USER_CODE).mortran; then \
         if test -f $(MAIN_UCODE_DIR)$(USER_CODE).mortran; then \
           $(MAKE) -s $(USER_CODE).mortran \
            depend=$(MAIN_UCODE_DIR)$(USER_CODE).mortran \
             check_message="$(the_message)"; \
         else \
           echo "$(USER_CODE).mortran does not exist on HEN_HOUSE"; \
         fi \
       else \
         if test -f $(MAIN_UCODE_DIR)$(USER_CODE).mortran; then \
           cp $(MAIN_UCODE_DIR)$(USER_CODE).mortran $(USER_CODE).mortran; \
           echo "Copied $(USER_CODE).mortran from HEN_HOUSE area"; \
         fi \
       fi
# Some system dependent commands
REMOVE = rm - f
CHECK_DIR = test -d $0 ||
MKDIR = ( echo Creating directory $0 && mkdir $0 )
```

A.4: windows.spec

```
# $Id windows.spec, v 1.5 2003/11/14 01:12:02 iwan Exp $
# This file gets used by Make on Windows systems.
# Initial version: Iwan Kawrakow, March 2003
# Copyright Iwan Kawrakow and the National Research Council of Canada
# iwan@irs.phy.nrc.ca
# The file extension of executables
EXE = .exe
# Sometimes I want to just leave a line blank in the output.
# When I just say echo, stupid Windows prints ECHO is off.
# => I'm using echo $(empty) and defining $(empty) to be realy empty on Unix
    but to be a . on Windows
empty = .
# Check if a file exists and if not, copy it from the second argument.
# If the file exists, check if it is more recent than the other
FILE_TEST = if not exist $1 ( copy $2 $1 & \
              echo "Copied $1 from $(dir $2) to local area" ) \
              else ( echo "$1 on $(dir $2) is more recent than local $1")
# Use the above in a make rule for a file
GET_FILE = $(call FILE_TEST,$0,$<)</pre>
CHECK_USER_CODE = \
       if exist $(USER_CODE).mortran ( \
         if exist $(MAIN_UCODE_DIR)$(USER_CODE).mortran ( \
           $(MAKE) -s $(USER_CODE).mortran \
             depend=$(MAIN_UCODE_DIR)$(USER_CODE).mortran \
             check_message="$(the_message)" \
       ) \
       else ( echo $(USER_CODE).mortran does not exist on HEN_HOUSE ) \
       ) \
       else (\
         if exist $(MAIN_UCODE_DIR)$(USER_CODE).mortran ( \
           copy $(MAIN_UCODE_DIR)$(USER_CODE).mortran $(USER_CODE).mortran \
           echo Copied $(USER_CODE).mortran from HEN_HOUSE area \
       ) \
# Some system dependent commands
REMOVE = del /Q /F /S
CHECK_DIR = if not exist $0
MKDIR = echo Creating directory $0 && mkdir $0
```

Appendix B: Examples of a Makefile

The use of Makefiles is discussed in section 4.1, page 18.

B.1: Makefile (tutor1)

The Makefile is found on the same area as the user-code which is to be compiled. It is usually a very simple piece of code. All it really does is define the specific USER_CODE for the rest of the Makefile and then includes several other files which are part of the Makefile, viz.:

- the current config file (*i.e.*, \$EGS_CONFIG see an example config file above in Appendix A.1, page 47 and a general discussion of config files in section 9.1.1, page 32);
- USER_CODE.make from the same area as the user-code;
- the standard_make file (which does the bulk of the work). This is \$HEN_HOUSE/makefiles/standard_makefile which is defined as EGS_MAKEFILE in \$HEN_HOUSE/specs/all_common.spec (see appendix A.2 above) which is included as part of the config file.

```
#
  $Id Makefile,v 1.2 2003/11/03 19:45:37 iwan Exp $
#
#
  A generic Makefile for a EGSnrc user code that uses mortran source
  files only.
#
#
  To use it, copy it to your usercode directory and
#
    - set the name of your user code in the line USER_CODE = ...
#
    - create a file named xxx.make where xxx is the name of your user code
#
      In the simplest possible case this file is empty.
#
      You can use it to specify an alternative set of sources,
#
      select the random number generator (ranlux vs ranmar), etc.
#
      See the .make files in tutor1-tutor7 and the NRC RZ codes
#
      for examples.
#
#
  Initial version: Iwan Kawrakow, March 2003
# First include the active EGSnrc configuration.
# EGS_CONFIG is a environment variable that must be
# set to point to the EGSnrc config file.
# This file defines the compiler name, compiler options, various
# directories, the standard set of Mortran sources needed to
# build a user code, etc. The configuration file is created
# during the EGSnrc installations and can be found in
```

```
# $HEN_HOUSE/specs.
include $(EGS_CONFIG)
# Then define the user code name
USER_CODE = tutor1
# User code specific definitions for Make
include $(USER_CODE).make
# That's all we need. Now we can use the standard EGSnrc Makefile to
# build the code with optimization, no optimization, debug and to also
# clean up. We have the following targets defined:
#
# make
                         Build the user code executable with optimization
# make opt
                         turned on.
# make noopt
                         Build the user code executable with optimization with
#
                         optimization turned off.
#
                         Build a user code executable for debugging
# make debug
#
# make fortran
                         Mortran step only.
                         Remove the fortran file, mortjob file, mortlst file
# make clean
#
                         and the various executables.
include $(EGS_MAKEFILE)
```

B.2: An example user-code make file: ranmar_test.make

The following is an example of a user-code's individual .make file. It is chosen as an example because it changes the random number generator from the default ranlux generator to the optional ranmar generator and it redefines the pieces of SOURCE code which make up the user-code (in this case adding \$EGS_UTILS/timing.macros and removing \$EGS_SOURCEDIR/egsnrc.mortran). These default SOURCES are defined in \$HEN_HOUSE/specs/all_common.spec (see section 16, page 48).

```
#
# $Id ranmar_test.make, v 1.2 2003/12/08 04:28:56 dave Exp $
# Make definitions for ranmar_test
# Initial version: Iwan Kawrakow, March 2003
#
# The RNG
#
RANDOM = $(EGS_SOURCEDIR)ranmar
# We don't use parallel preprocessing => don't link egs_c_utils.o
EGS_EXTRA_OBJECTS =
# The mortran sources
# Note: order is important!
# Note: don't forget the leading tabs on continuation lines!
SOURCES = \
      $(EGS_SOURCEDIR)egsnrc.macros \
      $(EGS_UTILS)timing.macros\
      $(MACHINE_MACROS) \
      $(RANDOM).macros\
      $(USER_CODE).mortran \
      $(RANDOM).mortran \
      $(MACHINE_MORTRAN) \
      $(EGS_SOURCEDIR)egs_utilities.mortran
```

B.3: \$HEN_HOUSE/makefiles/standard_makefile

```
# $Id standard_makefile,v 1.8 2003/11/14 01:15:03 iwan Exp $
The main portion of a Makefile for the EGSnrc system.
  This file is included from all user code makefiles.
#
  Initial version: Iwan Kawrakow, March 2003
#
#
#
   Copyright Iwan Kawrakow and the National Research Council of Canada
#
   iwan@irs.phy.nrc.ca
#
#
   This file is free software; you can redistribute it and/or modify
   it under the terms of the GNU General Public License as published by
#
#
   the Free Software Foundation; either version 2 of the License, or
#
   (at your option) any later version.
#
# We want to be able to build 3 different targets:
#
    executable with optimization turned on (default)
#
    executable without optimization
#
    executable with debug symbols included
# The following is for distinguishing between the 3
   $(WHAT) gets appended to the user code name. It is empty for a default
#
           build (optimization turned on), is = _noopt for no optimization
#
           and _debug for debug symbols included.
#
   $(OPTLEVEL_F) is the optimization or debug flags passed to the
                fortran compiler. Depending on the target (opt, noopt or
#
#
                 debug), it gets replaced with the appropriate compiler
#
                flags.
#
   $(OPTLEVEL_C) is not used right now
# FOPT and COPT are defined in the config file EGS_CONFIG
#
WHAT =
OPTLEVEL_F = \$(FOPT)
OPTLEVEL_C = \$(COPT)
depend =
the_message = $(USER_CODE) on HEN_HOUSE area is more recent than local version
check_message = $(empty)
EXE_DIR = $(EGS_HOME)bin$(DSEP)$(my_machine)
# The following is the rule for building the executable
#
   The first line says that the executable is dependent on the
   fortran file. Because of this dependence, make will rebuild the
   executable whenever the prerequisite (the fortran file) is more
#
   recent than the executable using the rule on the second line
   (note the leading tab!!! without it it will not work)
```

```
# F77 and FLFLAGS are defined in the configuration file.
# OPTLEVEL_F is set depending on whether we build optimized, noopt or
# debug executable.
# $@ is an automatic make variable and gets replaced with the name
# of the target that initiated the invocation of this rule
# ( $(EXECUTABLE) in this case, which expands to something like
# $HOME/egsnrc/bin/Linux/cavrznrc)
# So, the actual command passed by make to the sehll will look
# something like
   g77 -03 -o /usr/people/iwan/egsnrc/bin/Linux/dosrznrc dosrznrc_Linux.F
$(EXECUTABLE): $(FORTRAN_FILE).$(FEXT) $(EGS_EXTRA_OBJECTS) $(EGS_USER_OBJECTS) $(EXE_DI
        @echo $(empty)
        @echo $(empty)
        @echo Fortran compiling $(FORTRAN_FILE).$(FEXT) using flags '$(FCFLAGS) $(OPTLEV
        @$(F77) $(FCFLAGS) $(OPTLEVEL_F) $(FOUT)$@ $(FORTRAN_FILE).$(FEXT) $(EGS_EXTRA_C
# The following 2 rules are to make sure that the user executable directory
# exists.
$(EXE_DIR): $(EGS_HOME)bin
        @$(CHECK_DIR) $(MKDIR)
$(EGS_HOME)bin:
        @$(CHECK_DIR) $(MKDIR)
# In order to determine whether the executable needs to be re-built,
# make will examine its pre-requisits ($(FORTRAN_FILE).$(FEXT) in this case).
# The following says that $(FORTRAN_FILE).$(FEXT) is dependent on the
# files listed in $(SOURCES). If the fortran file does not exist, or
# any of its pre-requisits listed in $(SOURCES) is more recent,
# it will get re-made using the rule on the second line.
# MORTRAN_EXE is the name of the mortran compiler defined in EGS_CONFIG
# MORTRAN_DATA is the name of the mortran hex data file defined in EGS_CONFIG
# The -d option tells the mortran compiler to use the next argument as the
# name of the hex data file
# The -f option tells the mortran compiler to use all subsequent arguments
# until another -x option as names of files that need to be concatenated
# in the given order to make the mortjob.
# The -o7 option tells the mortran compiler to write the resulting fortran
# output to the file name given by the next argument (7 us the unit mortran
# uses for that \Rightarrow -o7)
# The -o8 option tells the mortran compiler to write the resulting listing
# output to the file name given by the next argument.
$(FORTRAN_FILE).$(FEXT): $(SOURCES)
        @echo Mortran compilation for $@
        @$(MORTRAN_EXE) -d $(MORTRAN_DATA) -f $(SOURCES) -o7 $@ \
        -08 $(FORTRAN_FILE).mortlst
```

```
# The following rule is there just for convinience so that you can say
# make fortran
# to perform the mortran step only (corresponds to m user_code)
fortran: $(SOURCES)
        @echo Mortran compilation of $(USER_CODE)
        @$(MORTRAN_EXE) -d $(MORTRAN_DATA) -f $(SOURCES) \
        -o7 $(FORTRAN_FILE).$(FEXT) -o8 $(FORTRAN_FILE).mortlst
# The following rule tells make that $(USER_CODE).mortran is dependent on
# a file with the same name on the $HEN_HOUSE/$USER_CODE/ area.
# (DSEP is defined in EGS_CONFIG and is / for Unix and \ for Windows)
# GET_FILE is a system dependent shell script defined in EGS_CONFIG that
# - copies the mortran file from the main area to the user area,
     if the mortran file is not on the user area
# - prints a warning if the mortran file is on the user area but the
    main area file is more recent
$(USER_CODE).mortran: $(depend)
        @echo $(check_message)
check:
        @$(CHECK_USER_CODE)
# Build a optimized user code
opt:
        @$(MAKE) -s $(EXECUTABLE)
# Build a user code without optimization
noopt:
        @$(MAKE) -s WHAT=_noopt OPTLEVEL_F= OPTLEVEL_C=
# Build a user code for debugging
debug:
        @$(MAKE) -s WHAT=_debug OPTLEVEL_F="$(FDEBUG)" OPTLEVEL_C="$(CDEBUG)"
# Clean-up the user code directory.
clean:
        @echo $(REMOVE) mortjob.mortran $(FORTRAN_FILE).$(FEXT) $(FORTRAN_FILE).mortlst
        @$(REMOVE) mortjob.mortran $(FORTRAN_FILE).$(FEXT) $(FORTRAN_FILE).mortlst
        @$(MAKE) -s WHAT=_debug execlean
        @$(MAKE) -s WHAT=_noopt execlean
        @$(MAKE) -s WHAT= execlean
# Remove the executable.
execlean:
        @echo $(REMOVE) $(EXECUTABLE)
               $(REMOVE) $(EXECUTABLE)
# A 'phony' target always gets remade. As opt, noopt, debug, clean and
# execlean have no list of prerequisits so that make can determine whether
# they need to be remade, we declare them as phony.
.PHONY: opt noopt debug clean execlean
```

17 References

[1] D. W. O. Rogers, I. Kawrakow, J. P. Seuntjens, B. R. B. Walters, and E. Mainegra-Hing, NRC User Codes for EGSnrc, Technical Report PIRS-702(RevB), National Research Council of Canada, Ottawa, Canada, 2003.

- [2] E. Mainegra-Hing, User Manual for inputRZ, a GUI for the NRC RZ user-codes, Technical Report PIRS-801, National Research Council of Canada, Ottawa, Canada, 2002.
- [3] I. Kawrakow and D. W. O. Rogers, The EGSnrc Code System: Monte Carlo simulation of electron and photon transport, Technical Report PIRS-701, National Research Council of Canada, Ottawa, Canada, 2000.
- [4] ICRU, Stopping powers for electrons and positrons, ICRU Report 37, ICRU, Washington D.C., 1984.
- [5] S. Duane, A. F. Bielajew, and D. W. O. Rogers, Use of ICRU-37/NBS collision stopping powers in the EGS4 system, NRCC Report PIRS-0173, Ottawa, March (1989).
- [6] M. J. Berger and J. H. Hubbell, XCOM: Photon Cross Sections on a Personal Computer, Report NBSIR87–3597, NIST, Gaithersburg, MD20899, 1987.
- [7] J. P. Seuntjens, I. Kawrakow, J. Borg, F. Hobeila, and D. W. O. Rogers, Calculated and measured air-kerma response of ionization chambers in low and medium energy photon beams, in *Recent developments in accurate radiation dosimetry, Proc. of an Int'l Workshop*, edited by J. P. Seuntjens and P. Mobit, pages 69 84, Medical Physics Publishing, Madison WI, 2002.
- [8] I. Kawrakow and D. W. O. Rogers, The EGSnrc Code System: Monte Carlo simulation of electron and photon transport, Technical Report PIRS-701 (4th printing), National Research Council of Canada, Ottawa, Canada, 2003.

\mathbf{Index}

.bashrc, 17	example, 47
.conf files, 7, 33	config files, 19
.configuration, 18	config.log, 11
.cshrc, 17	CONFIG_NAME, 6, 32, 33
.egsdat, 23, 41	configure, 11
.egsinp, 22, 23, 35	CVS, 44
.egslog, 23, 26, 35	
.egslst, 23	dataset, 27
.egszip, 12, 13	defining the environment, 17
.environment, 33	efficiency, 42
environment file, 7	compilers, 42
ifile, 23	ranlux vs ranmar, 42
io file, 7, 9, 35, 36	static vs non static, 42
.make, 18, 19	EGS4, 43
ofile, 23	EGS-BATCH_SYSTEM, 25
.pegs4dat, 23, 27	egs_c_interface1.macros, 37
spec files, 33	egs_c_utils.c, 41
Topics interpretation	egs_c_utils.h, 41
Abdel-Rahman, 29	egs_compile, 8
all_common.spec, 18, 48	EGS_CONFIG, 5, 9, 11, 12, 17–21, 53
array_sizes.h, 39	egs_config1.h, 41
1 . 1 . 00 . 05	egs_configure, 8
batch, 23, 25	
batch runs, 25	egs_finish, 9, 33, 36
batch_options, 25	egs_gui, 6, 12, 20, 22 screen shot
BLOCK DATA replaced, 35	
C interface	compile, 20
known limitations, 40	execute, 22 egs_gui.exe, 16
C/C++ interface to EGSnrc, 37	EGS_HOME, 5, 12, 17, 18, 35
command-line arguments, 23	bin, 6, 17
batch, 26	bin/\$my_machine, 21
compile_user_code, 21	lib, 6
compilers, 8	must be set for PEGS4, 27
Fortran, 42	pegs4/data, 27
g77, 42	pegs4.log, 28
GNU	user-code, 43
Unix/Linux, 10	egs_init, 9, 23, 33
pgf77, 33, 42	command-line arguments, 23
Portland Group, 33	egs_inprz, 6, 12, 22
compiling	egs_inprz.exe, 16
GUI, 11	egs_install, 12
config, 25	egs_install.exe, 13
config file, 20, 32, 53	egs_install_self, 12
definition, 32	egs_install_self.exe, 13
dominuon, 02	050-11100011-0011.CAC, 10

egs_interface1.c, 37	pegs4, 29, 30
egs_interface1.h, 37	pgs4pepr.dat, 29
EGS_MAKEFILE, 53, 54	pgs4pepr_xcom_full.dat, 29
egs_run, 8	pieces, 30
EGS_SOURCEDIR, 55	previewRZ, 30
egs_utilities.mortran, 19	scripts, 11, 25
egsFinish(), 39	compile_user_code, 21
egsgui, 6, 20, 22	test_distribution_outputs, 12
egsinprz, 6, 22	specs, 18, 30, 32, 33
EGSnrc	\$my_machine, 32
binary directory, 33	all_common.spec, 18, 19, 48, 53, 55
installation, 10	unix.spec, 18
Unix/Linux, 10	windows.spec, 18
Windows, 13	spectra, 29, 30
egsnrc.macros, 19, 37	src, 29, 30
egsnrc.mortran, 19	egs_utilities.mortran, 34
egsnrc_bashrc_additions, 5, 12, 17, 18	user-codes, 30
egsnrc_cshrc_additions, 5, 12, 17, 18	user_codes, 29, 30
egsShower(), 39	tutor1c, 39
eh, 25	tutor2c, 39
ex, 24	tutor4c, 39
exb, 25, 41	utils, 29, 30
	hh, 25
finalize_\$USER.log, 11	Hobeila, 29
finalize_egs_foruser, 11	http://irs.inms.nrc.ca/software/egsnrc/, 10, 13
Fortran	http://www.gnu.org, 10
compilers, 42	http://www.gzip.org/zlib, 13
CACD 20	http://www.mingw.org, 13
GASP, 28	http://www.trolltech.com, 10, 15, 16
GNU compilers	1 //
Unix/Linux, 10	ifile, 26, 35
Windows, 13	ifile.egslog, 35
GUI	install.log, 11
compiling, 11	install.status, 11
installation, 12	install_egs, 11
HEN_HOUSE, 5, 18, 23, 28, 29	installation
bin, 6, 9, 17, 32, 33	egs_install, 12
bin/\$my_machine, 21	egs_install_self, 12
data, 29, 30	IUNRST, 28
doc, 29, 30	707 40 44
gui, 11, 30	JCF, 40, 41
interface, 30, 37	job control file, 40
lib, 6, 9, 30, 32	local batch quaves 25
\$my_machine, 32, 41	local batch queues, 25 local queue names, 25
makefiles, 18, 37	lock file, 41
standard_makefile, 18, 53, 54, 56	IOCA IIIC, TI
mortran3, 29, 30	Mac OSX, 14, 46
, ,	•

machine.macros, 32	RANDOM, 19
machine.mortran, 32	RANLUX, 42, 55
machine_macros, 19	RANMAR, 42
main.c, 39	Red Hat, 45
make, 7, 8, 18, 20	run_user_code, 24
targets, 19	run_user_code_batch, 25
Makefile, 18	, , ,
example, 53, 54	screen shot
standard, 48	$ m egs_gui$
MinGW.egszip, 13	compile, 20
my_machine, 6, 21	execute, 22
,, 0, 21	PEGS4, 27
noopt, 25	Seuntjens, 29
nqs, 25	SOURCES, 19
nrcaux.mortran, 19	speed, 42
,	compilers, 42
ofile, 26	ranlux vs ranmar, 42
ofile.egsdat, 41	static vs non static, 42
ofile.lock, 40	spinms, 8
	standard Makefile, 48
parallel runs, 24, 40	standard_make file, 53
PATH, 6, 13, 17	standard_makefile, 18
where set, 17	start_new_particle, 37
pbs, 25	SUSE, 45
PEGS4, 22, 27	,
command line inputs, 28	temporary working directory, 35
creating a new data set, 27	test.egslog, 35
data	test_egsnrcmp_distribution, 12
search path, 22, 35	the_stack, 39
pegs4.exe, 28	tutor1c, 37, 39
pegs4.log, 28	tutor2c, 37, 39
pgs4pepr.dat, 29	tutor4c, 37, 39
pgs4pepr_xcom_full.dat, 29	
screen shot	unix.spec, 18, 51
egs_gui, 27	user-code.configuration, 18
pgf77.conf, 47	user-code.io, 9, 35
pgs4pepr.dat, 29	user-code.make, 18, 19, 43
pgs4pepr_xcom_full.dat, 29	user_code.macros, 39
PIRS-701, 28, 43	USER_CODE.make, 53
PIRS-702, 8	WA DOO 11 10
Portland Group compiler, 42	V4_EGSgui.tar, 10
O+ 10 19	V4_EGSnrc.tar, 10
Qt, 10, 12	V4_manuals.tar, 10
installation, 16	V4_spinms.tar, 10
Qt library, 15	$V4_{user_codes.tar}$, 10
QTDIR, 11	Windows
queue_type, 25	Windows
queuing system, 25	downloading, 13

filename restrictions, 29
machine.macros, 14
machine.mortran, 14
make, 13
mortran3.exe, 14
pegs4.exe, 14
Qt, 13
Qt dll, 16
Restrictions, 46
windows.spec, 18, 52
working directory, 35
zlib library, 8, 13