History, overview and recent improvements of EGS4

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> *"Halitosis is better than no breath at all."*
> W C Fields

1 History of the EGS Code System

A great deal of the content of the following historical sections of this report has been plagiarised unashamedly from the original EGS3 (**E**lectron **G**amma **S**hower Code Version **3**) document authored by Richard Ford and Ralph Nelson [1]. There are several reasons for this aside from laziness. This history predates one of the author's (AFB) involvement with EGS and he found it very difficult to improve upon the words penned by Ford and Nelson in that original document. Moreover, the EGS3 manual is now out-of-print and this history might have eventually been lost to the ever-burgeoning EGS-community now estimated to be at least 6000 strong. There had been one previous attempt to give a historical perspective of EGS [2]. However, this article was very brief and did not convey the large effort that went into the development of EGS. In this report the historical section on EGS4 as well as the summary of EGS3 to EGS4 conversion and the overview of EGS4 was taken directly from the EGS4 manual [3]. This is done for completeness only. The EGS4 manual gives much more detail and ought to be referred to for technical details. Finally, recent improvements to EGS4 are listed herein and represent the first time that this information is available in one place. The reader should consult the references cited in this report for more details regarding motivation and implementation.

1.1 Before EGS

The Monte Carlo method was originally suggested by Ulam and von Neumann [4], and was first used by Goldberger [5] in order to study nuclear disintegrations produced by high-energy particles. The first application of the Monte Carlo technique to study shower production was done by Wilson [6]. Wilson's approach was a simple graphical-mechanical that was described as follows:

> *"The procedure used was a simple graphical and mechanical one. The distance into the lead was broken into intervals of one-fifth of a radiation length (about 1 mm). The electrons or photons were followed through successive intervals and their fate in passing through a given interval was decided by spinning a wheel of chance; the fate being read from one of a family of curves drawn on a cylinder...*
>
> *A word about the wheel of chance; The cylinder, 4 in. outside diameter by 12 in. long is driven by a high speed motor geared down by a ratio 20 to 1. The motor armature is heavier than the cylinder and determines where the cylinder stops. The motor was observed to stop at random and, in so far as the cylinder is concerned, its randomness is multiplied by the gear ratio..."*
>
> from R. R. Wilson, *op. cit.*

Although apparently quite tedious, Wilson's method was still an improvement over the analytic methods of the time—particularly in studying the average behavior and fluctuations about the average [7].

The first use of an electronic digital computer in simulating high-energy cascades by Monte Carlo methods was reported by Butcher and Messel [8, 9], and independently by Varfolomeev and Svetlolobov [10]. These two groups collaborated in a much publicized work [11] that eventually led to an extensive set of tables describing the shower distribution functions [12]—the so-called "shower book".

For various reasons two completely different codes were written in the early-to-mid-1960's to simulate electromagnetic cascades. The first was written by Zerby and Moran [13, 14, 15] at the Oak Ridge National Laboratory and was motivated by the construction of the Stanford Linear Accelerator Center and the many physics and engineering problems that were anticipated as a result of high-energy electron beams showering in various devices and structures at that facility. This code had been used by Alsmiller and others [16, 17, 18, 19, 20, 21, 22] for a number of studies since its development[1].

The second code was developed by Nagel [24, 25, 26] and several adaptations had been reported [27, 28, 29]. The original Nagel version, which Ford and Nelson called SHOWER1, was a FORTRAN code written for high-energy electrons ($\leq$ 1000 MeV) incident upon lead in cylindrical geometry. Six significant electron and photon interactions (bremsstrahlung, electron-electron scattering, ionization-loss, pair-production, Compton scattering, and the photoelectric effect) plus multiple Coulomb scattering were accounted for. Except for annihilation, positrons and electrons were treated alike and were followed until they reached a cutoff energy of 1.5 MeV (total energy). Photons were followed down to 0.25 MeV. The cutoff energies were as low as or lower than those used by either Messel and Crawford or by Zerby and Moran.

The availability of Nagel's dissertation [25] and a copy of his original shower program provided the incentive for Nicoli [28] to extend the dynamic energy range and flexibility of the code in order for it to be made available as a practical tool for the experimental physicist. Nicoli's modifications of SHOWER1 fell into three categories:

1. High-energy extensions to the least-squares fits for total interaction probabilities and branching ratios.
2. Provisions for including boundary-condition interrogation in the transport cycle, allowing for particle marking and/or discarding and the use of generalized energy cutoffs for electrons and photons.
3. The handling of input/output requirements.

In August, 1966 the Nicoli version (SHOWER2) was brought to SLAC by Nagel, who had been working at MIT and had consulted with Nicoli on the above changes and extensions. The SLAC Computation Group undertook the task of getting the code running on the IBM-360 system and generalizing the program to run in elemental media other than just lead. The latter was facilitated by a set of hand-written notes—brought to SLAC in 1966 by Nagel [30]—on the best way to accomplish this task and V. Whitis was assigned the job. Whitis left SLAC in the summer of 1967 and his work, which consisted mainly of a series of fitting programs written in the ALGOL language, was passed on to one of us (WRN)[2]. Under Nelson's direction, a programmer (J. Ryder) constructed SHOWER3 in modular form and wrote a pre-processing code called PREPRO that computed fit-coefficients for the cross-section and branching-ratio data needed by SHOWER3. The values of these constants depended on the material in which the shower

[1] According to Alsmiller[23], the Zerby and Moran source code vanished from ORNL and they were forced to work with an octal version.

[2] Nagel's computer programme was recovered from a trash receptacle at SLAC by WRN. Although no printout of the code could be found, the punch cards had been sequenced in columns 73-80 and they were easily sorted by machine.

was to be simulated. During the summer of 1972 the Ryder version of SHOWER3/PREPRO was successfully tested for several different elements by B. Talwar under the direction of Nelson, thus bringing SHOWER3/PREPRO into an operational status.

Meanwhile, interest in a computer code capable of simulating electromagnetic cascade showers had been developing for several years at the High Energy Physics Laboratory (HEPL) at Stanford University where a group led by R. Hofstadter and E. B. Hughes was continuing their development of large NaI(Tl) Total Absorption Shower Counters (TASC's) [31]. A method of accurately predicting shower behavior in these counters was needed. A version of Nagel's code (SHOWER2) was obtained from Nelson in the fall of 1970; however, efforts to scale from lead to NaI were uncertain and led to a growing conviction that a generalized code was necessary. Thus it was that Richard Ford undertook the task of generalizing SHOWER2 to run is any element, mixture, or compound in September, 1971—an effort similar to the one already underway by Ryder, Talwar, and Nelson that resulted in the final version of SHOWER3/PREPRO.

Ford obtained a copy of a Ryder version of SHOWER3/PREPRO and Nagel's notes from Nelson. In addition to the references mentioned in Nagel's notes, the Messel and Crawford "shower book" [12], as well as the review by Scott [32] on multiple scattering, were found to be very useful sources of information. The essential physics was formulated and the coding was completed by February, 1972. At that time the HEPL version was called SHOWER (now referred to as SHOWER4) and the corresponding preprocessor was completely new and was called SHINP (for **SH**ower **INP**ut). Both codes were in FORTRAN and were made operational on the IBM-7700 machine at HEPL—a second generation experimental data-acquisition computer. A number of interesting studies were subsequently performed, including calculations of detector resolutions and expected self-vetoes in gamma detectors due to backscattered photons from shower detectors downstream.

In January, 1974 it appeared likely that HEPL's computer would be sold. In addition, the Hofstadter group was involved in an experiment at SLAC that required shower simulations and the SHOWER4/SHINP codes were therefore made operational on the considerably faster and more efficient IBM-360/91 at SLAC. During the calculations that had been performed at HEPL, a couple of errors were found in the sampling routines that would have been detected earlier if it had been possible to test this in a more systematic way. Therefore, it was decided to incorporate into the new version being brought to SLAC test facilities to insure the correctness of these sampling routines. In order to facilitate comparison between the sampled secondary spectra and the theoretical distributions, the preprocessing code was split up and modularized into subprograms.

1.2 EGS1

About this time Nelson became interested in being able to use Ford's version of the code and offered to help support its further development. One of Ford's objectives was to make the preprocessor code produce data for the shower code in a form that was directly usable by the shower code with a minimum of input required by the user. In SHOWER3/PREPRO and in SHOWER4/SHINP, whenever it was desired to create showers in a new medium, it was necessary to look-up the photon cross sections in the literature and keypunch them for the preprocessing code to use. Subsequent to this it was necessary to select from several fits produced by the preprocessing code and to include this new information, consisting of many data cards, with other data used by the shower program. Ford rewrote the preprocessor to automatically produce all of the data needed by the shower code in a readily acceptable form and, with the assistance of Nelson, obtained photon cross sections for elements 1 to 100 from

Storm and Israel [33] on magnetic tape. Ford also separated the shower code's material-input from its control-input. For flexibility and ease of use, the `NAMELIST` read facility of FORTRAN-IV was utilized for reading-in control data in both the preprocessor and the shower codes. The resultant shower code was re-named EGS (**E**lectron-**G**amma-**S**hower) and its companion code was called PEGS (**P**reprocessor for **EGS**). This version, written completely in the FORTRAN-IV language, is referred to as Version 1 of the EGS Code System (or more simply EGS1 and PEGS1).

The sampling routines were tested using the internal test-procedure facility of EGS1 and, with the exception of the bremsstrahlung process, were found to be operating very nicely. In the bremsstrahlung case a ripple, amounting to only 5% but still noticeable, was observed when the sampled data were compared with the theoretical secondary distribution. This effect went away upon selection of another random number generator, and it was concluded that correlations in the original number generator were the cause. EGS1 was then tested against various experiments in the literature and with other Monte Carlo results that were then available and the authors found reasonable good agreement in all cases.

1.3 EGS2

By the fall of 1974 the Hofstadter group had obtained some hexagonal modular NaI detectors and the discovery of the J/ψ particle [34, 35] in November, 1974 opened up an exciting area of high-energy gamma-ray spectroscopy for which the modularized NaI detectors were ideally suited. EGS1, however, could not be readily used to simulate showers in complex geometries such as those presented by modular stacks of NaI. A good example of this was the Crystal Ball detector for which EGS1, under the direction of E. Bloom at SLAC, was modified to handle the particular geometry in question. Furthermore, Nelson had received a large number of requests from the growing list of EGS users, both at SLAC and elsewhere in the high-energy physics community, to improve further EGS1 so that complex geometries could be realized in the near future. Thus it was decided that EGS1, which was a one-region, one-medium code, should be generalized in order to handle many-region, many-media, complex, three-dimensional geometries.

It soon became clear that, in the time available at least, it would not be possible to construct a self-contained code that would have all of the control, scoring, and output options that might ever be wanted, as well as a geometry package that would automatically handle arbitrary complex geometries. Therefore, Ford decided to put in only the necessary multi-region structures, to replace all scoring and output code in EGS1 with a user interface, and to dispense with the EGS1 main control program completely. Thus EGS1 became a subprogram in itself with two user-callable subroutines (`HATCH` and `SHOWER`) that require two user-written subroutines (`HOWFAR` and `AUSGAB`) in order to define the geometry and do the scoring, respectively.

For added flexibility and portability, EGS1 and PEGS1 were rewritten in an extended FORTRAN language called MORTRAN2, which was translated by a (MORTRAN2) Macro Processor into standard FORTRAN. The part of EGS1 that was used to test the sampling routines was reconfigured into a separate main program called the TESTSR code, also written in MORTRAN2. These revisions were completed by the end of 1975 and the new versions of EGS, PEGS, and TESTSR comprise what is called Version 2 of the EGS Code System, or more simply EGS2, PEGS2, and TESTSR2.

1.4 EGS3

One part of EGS2 which seemed aesthetically displeasing was the complex control logic needed in the electron transport routine, `ELECTR`, in order to transport electrons by variable distances to interaction points or boundaries using only step lengths taken from a set of 16 discrete values. This procedure had been necessary in order to implement Nagel's discrete reduced-angle multiple-scattering scheme [24, 25, 26, 30] in a general multi-region environment. In addition, comparisons of backscattered photon fluence as computed by EGS2 versus unpublished HEPL data, as well as bremsstrahlung angular distribution calculations comparing EGS2 results with those of Berger and Seltzer using ETRAN [36], suggested that EGS2 might be predicting values in the backward direction that were low by up to a factor of two. For these reasons, and in order to achieve greater universality of application (*e.g.*, so that a monochromatic beam of electrons impinging on a very thin slab would have a continuous angular distribution on exit), Ford decided in the summer of 1976 to try to implement a multiple scattering-scheme that would correctly sample the continuous multiple-scattering distribution for arbitrary step lengths. After some thought, an extension of the method used by Messel and Crawford [12] was devised. Most of the code for this addition was written by Ford at Science Applications, Inc., and was brought to SLAC in August 1977 where it was debugged and tested by Nelson and Ford. The implementation of this system required some once-only calculations which were made using a stand-alone code called CMS (**C**ontinuous **M**ultiple **S**cattering)[3]. It should be mentioned that the version of PEGS brought to SLAC at this time had the same physics in it as Version 2, but had been partly rewritten in order to be more machine independent (*e.g.*, IBM versus CDC), its main remaining machine dependency being its use of `NAMELIST`. (`NAMELIST` is a common extension to Fortran employed by many Fortran compilers but is not part of the Fortran-IV or Fortran 77 standards.) Another option was added to the TESTSR code to allow testing of the new EGS multiple-scattering sampling routine, MSCAT.

These versions of EGS, PEGS, and TESTSR comprise what was called Version 3 of the EGS code system (*i.e.*, EGS3, PEG3, and TESTSR3). Subsequent comparisons of EGS3 calculations against experiments and other Monte Carlo results were made by the authors (*e.g.*, see SLAC-210 [1] and/or Jenkins and Nelson [37]) and others and the agreements clearly demonstrated the basic validity of the code.

The EGS3 Code System released in 1978 contained many features that distinguished it from Nagel's original code, SHOWER1, the most noteworthy being:

1. Showers could be simulated in any element (Z=1 through 100), compound, or mixture.
2. The energy range for transporting particles was extended so that showers could be initiated and followed from 100 GeV down to 1 keV for photons, and 1.5 MeV (total energy) for charged particles.
3. Photons and charged particles were transported in random rather than discrete steps, resulting in a much faster running code.
4. Positrons were allowed to annihilate either in-flight or at rest, and their annihilation quanta were followed to completion.
5. Electrons and positrons were treated separately using exact, rather than asymptotic, Møller and Bhabha cross sections, respectively.
6. Sampling schemes were made more efficient.
7. EGS3 became a subroutine package with user interface, allowing much greater flexibility and reducing the necessity for being familiar with the internal details of the code. This

[3]Logically, the CMS code should have been included as an option of PEGS, but this has never been done.

also reduced the likelihood that user edits could introduce bugs into the code.

8. The geometry had to be specified by the user by means of a user-written subprogram called `HOWFAR`. However, geometry utilities for determining intersections of trajectories with common surfaces (*e.g.*, planes, cylinders, cones, spheres and boxes) had also been developed and were made available.
9. The task of creating media data files was greatly simplified and automated by means of the PEGS3 preprocessing code, which created output data in a convenient form for direct use by EGS3.
10. PEGS3 constructed piecewise-linear fits over a large number of energy intervals of the cross-section and branching-ratio data, whereas PREPRO and SHINP both made high-order polynomial fits over a small number of intervals (as did SHOWER1 and SHOWER2).
11. In addition to the options needed to produce data for EGS3, options were made available in PEGS3 for plotting any of the physical quantities used by EGS3, as well as for comparing sampled distributions from the TESTSR user code with theoretical spectra. The `NAMELIST` read facility of FORTRAN was also introduced at this time.

In particular, for Version 3 versus Version 2

12. The multiple-scattering reduced angle was sampled from a continuous rather than discrete distribution. This was done for arbitrary step sizes provided that they were not too large to invalidate the theory. An immediate application of this was the following simplification to subroutine `ELECTR`.
13. The control logic in the charged-particle transport routine, `ELECTR`, was greatly simplified and modifications were made to both `ELECTR` and the photon transport routine, `PHOTON`, to make interactions at a boundary impossible.
14. The above changes to the control logic then made it possible for the user to implement importance-sampling[4] techniques into EGS without any furthers "internal" changes to the system itself. Examples that come to mind include the production of secondary electron beams at large angles, photon energy deposition in relatively small (low-Z) absorbers, and deep penetration (radial and longitudinal) calculations associated with shower counter devices.
15. Provision was made for allowing the density to vary continuously in any given region.
16. A new subroutine (`PHOTO`) was added in order to treat the photoelectric effect in a manner comparable to the other interaction processes. The main interest in this was to facilitate the development of a more general photoelectric routine, such as one that could produce fluorescent photons and/or Auger electrons for subsequent transport by EGS.
17. Additional calls to `AUSGAB`, bringing the total from 5 to 23, were made possible in order to allow for the extraction of additional information without requiring the user to edit the EGS code itself. For example, the user could determine the number of collision types (*e.g.*, Compton *vs.*photoelectric, *etc.*).

Upon release in 1978, the EGS3 Code System soon became the "industry standard" for designing shower detectors in high-energy physics. Looking back at this period of time several reasons can explain why EGS became so popular so quickly. Leading the list was the fact that the other codes mentioned above simply were not available; whereas, anyone could get EGS,

[4] For those who may be unfamiliar with the term, importance sampling refers to sampling the most important regions of a problem and correcting for this bias by means of weight factors (see, for example, the report by Carter and Cashwell [38].)

together with its documentation, free-of-charge from SLAC. Furthermore, the code had been successfully benchmarked and support was provided to anyone requesting help. These things provided the fuel for the fire. What ignited it, however, was the so-called November Revolution [34, 35] of particle physics and the resulting shift to the use of colliding-beam accelerators. In particular, there was an immediate need by the high-energy physics community for tools to aid in the design of shower counters for the large, vastly-complicated, 4π detector systems associated with the new colliding-beam storage-ring facilities under construction throughout the world. EGS was there at the right time and right place when this happened.

We would be remiss if we did not mention one other code that also was available during this time period, particularly since published results from it had been used as part of the benchmarking of EGS3 itself. We refer to the ETRAN Monte Carlo shower code written by Berger and Seltzer [36][5]. ETRAN treated the low-energy processes (down to 1 keV) in greater detail than EGS3. Instead of the Molière [40, 41] formulation, ETRAN made use of the Goudsmit-Saunderson [42, 43] approach to multiple scattering, thereby avoiding the small-angle approximations intrinsic to Molière. ETRAN also treated fluorescence, the effect of atomic binding on atomic electrons, and energy-loss straggling. Because of the special care taken at low energies, ETRAN, which was initially written for energies less than 100 MeV and later extended to 1 GeV [44], ran significantly slower than EGS3. However, in spite of its accuracy and availability, ETRAN went unnoticed in the world of high-energy physics during this period.

1.5 EGS4

EGS3 was designed to simulate electromagnetic cascades in various geometries and at energies up to a few thousand GeV and down to cutoff kinetic energies of 0.1 MeV (photons) and 1 MeV (electrons and positrons). However, ever since the introduction of the code in 1978 there had been an increasing need to extend the lower-energy limits—*i.e.*, down to 1 and 10 keV for photons and electrons, respectively. Essentially, EGS3 had become more and more popular as a general, low-energy, electron-photon transport code that could be used for a variety of problems in addition to those generally associated with high-energy electromagnetic cascade showers. It had many features that made it both general as well as versatile, *and it was relatively easy to use,* so there had been a rapid increase in the use of EGS3 both by those outside the high-energy physics community (*e.g.*, medical physics) and by those within. Even though other low-energy radiation transport codes were available, most notably ETRAN [36, 45, 46] and its progeny [39, 47], there had been many requests to extend EGS3 down to lower energies and this was a major, but not the only, reason for creating EGS4. The various corrections, changes and additions, and new features that were introduced in the 1985 release of the EGS4 Code System [3] are summarized below.

1.5.1 Summary of EGS3 to EGS4 conversion

As with any widely used code, there had been many extensions made to EGS3 and many small errors found and corrected as the code was used in new situations. The following lists the most significant differences between EGS3 and EGS4.

- Major Changes and Additions to EGS3.
  - Conversion from Mortran2 to Mortran3.

[5] A later version of this programme, which contained a fairly general geometry package, was known as SANDYL [39] and was also available at this time.

  - Corrections to logic and coding errors in EGS3.
  - Extension of electron transport down to 10 keV (kinetic energy).
  - Improved Sternheimer treatment of the density effect.
  - Improved definition of the radiation length at low atomic numbers.
- New Options and Macros.
  - Macro templates for introduction of weighting and biasing techniques.
  - Pi-zero option.
  - Rayleigh scattering option.
  - Compton electron stack position preference (macro).
  - Positron discard option (macro) for creation of annihilation gammas.
- Auxiliary Subprograms and Utilities.
  - Geometry subprograms and corresponding macro packages.
  - Miscellaneous energy conservation and event counter utility routines.
  - Fixed fractional energy loss subroutines.
- New Applications and Examples.
  - Leading-particle biasing macro to increase efficiency.
  - Fluorescent-photon transport capability.
  - Charged-particle transport in magnetic fields.
  - Combinatorial Geometry package.
  - Coupling of hadronic and electromagnetic cascade codes.

The most significant changes were made to subroutine `ELECTR` to correct problems which occurred when lower-energy charged-particle transport was done. The most significant change in this regard was first brought to attention in the paper *Low energy electron transport with EGS* by Rogers [48]. Many of the difficulties with the low-energy transport related to the fact that electron transport sub-steps (multiple scattering and continuous energy loss are modeled at the endpoints of these steps) were too large and various approximations that were valid for high-energy transport (above 10–20 MeV) were invalid for low-energy. Rogers modified the EGS code to allow the user to control the electron step-size in two ways, one by specifying a maximum allowable energy loss to continuous energy-loss processes (`ESTEPE`) and a geometric step-size control (`SMAX`) that restricts the electron step-size to be no larger than some user-specified distance. This allowed low-energy electron transport to be calculated with some degree of confidence although the user was required to study the parametric dependence of applications on these two parameters, `ESTEPE` and `SMAX`.

2 Overview of the EGS4 Code System – vintage 1985

The following is a summary of the main features of the EGS4 Code System, including statements about the physics that has been put into it and what can be realistically simulated.

- The radiation transport of electrons (`+` or `-`) or photons can be simulated in any element, compound, or mixture. That is, the data preparation package, PEGS4, creates data to be used by EGS4, using cross section tables for elements 1 through 100.
- Both photons and charged particles are transported in random rather than in discrete steps.

- The dynamic range of charged-particle kinetic energies goes from a few tens of keV up to a few thousand GeV. Conceivably the upper limit can be extended higher, but the validity of the physics remains to be checked.
- The dynamic range of photon energies lies between 1 keV and several thousand GeV (see above statement).
- The following physics processes are taken into account by the EGS4 Code System:
  - Bremsstrahlung production (excluding the Elwert correction at low energies).
  - Positron annihilation in flight and at rest (the annihilation quanta are followed to completion).
  - Molière multiple scattering (*i.e.*, Coulomb scattering from nuclei). The reduced angle is sampled from a continuous (rather than discrete) distribution. This is done for arbitrary step sizes, selected randomly, provided that they are not so large or so small as to invalidate the theory.
  - Møller (e^-e^-) and Bhabha (e^+e^-) scattering. Exact rather than asymptotic formulae are used.
  - Continuous energy loss applied to charged-particle tracks between discrete interactions.
    * Total stopping power consists of soft bremsstrahlung and collision loss terms.
    * Collision loss determined by the (restricted) Bethe-Bloch stopping power with Sternheimer treatment of the density effect.
  - Pair production.
  - Compton scattering.
  - Coherent (Rayleigh) scattering can be included by means of an option.
  - Photoelectric effect.
    * Neither fluorescent photons nor Auger electrons are produced or transported in the default version of subroutine `PHOTO`.
    * Other *user-written* versions of `PHOTO` can be created, however, that allow for the production and transport of K- and L-edge photons.
- PEGS4 is a stand-alone data preprocessing code consisting of 12 subroutines and 85 functions. The output is in a form for direct use by EGS4.
  - PEGS4 constructs piecewise-linear fits over a large number of energy intervals of the cross section and branching ratio data.
  - In general, the user need only use PEGS4 *once* to obtain the media data files required by EGS4.
  - PEGS4 control input uses the `NAMELIST` read facility of the FORTRAN language (in Mortran3 form).
  - In addition to the options needed to produce data for EGS4, PEGS4 contains options to plot any of the physical quantities used by EGS4, as well as to compare sampled distributions produced by the UCTESTSR User Code with theoretical spectra.
- EGS4 is a package of subroutines plus block data with a flexible user interface. The division between user-interface and EGS4 is shown in Figure 1.
  - This allows for greater flexibility without requiring one to be overly familiar with the internal details of the code.
  - Together with the macro facility capabilities of the Mortran3 language, this reduces the likelihood that user edits will introduce bugs into the code.

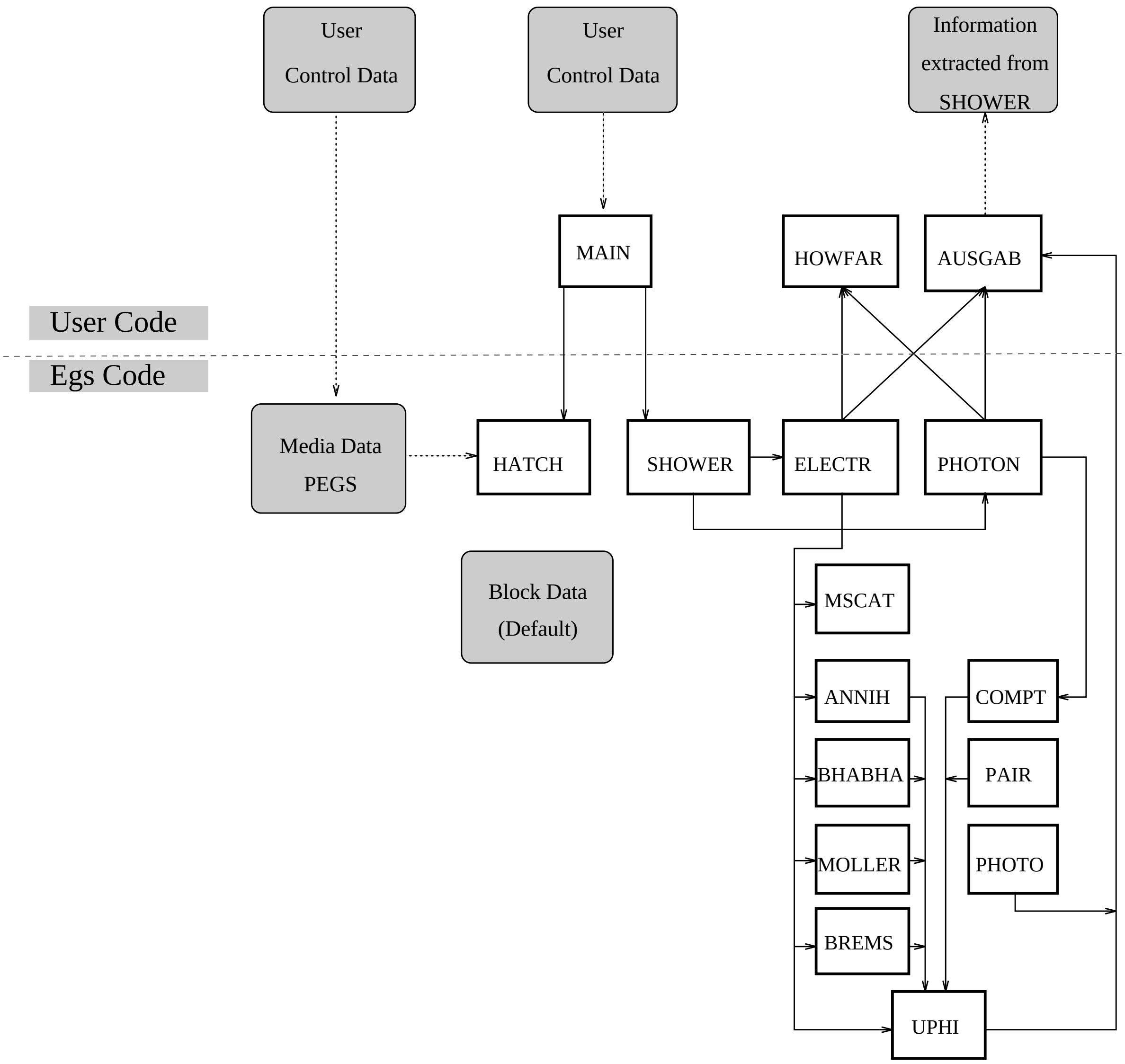

Figure 1: Division between user-interface and EGS4.

  - EGS4 uses material cross section and branching ratio data created and fit by the companion code, PEGS4.
- The geometry for any given problem is specified by a *user-written* subroutine called `HOWFAR` which, in turn, can make use of auxiliary subprograms.
  - Auxiliary geometry routines for planes, cylinders, cones, spheres, *etc.*, are provided with the EGS4 Code System for those who do not wish to write their own.
  - Macro versions of these routines are also provided in the set of defining macros (*i.e.*, in the EGS4MAC file) which, if used, generally result in a faster running simulation.
  - The MORSE-CG Combinatorial Geometry package can be incorporated into `HOWFAR` (*e.g.*, see the UCSAMPCG file on the EGS4 Distribution Tape). However, experience indicates that a much slower simulation generally results (of the order of at least a factor of four).
  - Transport can take place in a magnetic field by writing a specially designed `HOWFAR` subprogram, or in a more general manner (*e.g.*, including electric field) by making use of Mortran3 macro templates that have been appropriately placed for that purpose in subroutine `ELECTR`.
- The user scores and outputs information in the *user-written* subroutine called `AUSGAB`.
  - Auxiliary subprogram `ECNSV1` is provided in order to keep track of energy for conservation (or other) purposes.
  - Auxiliary subprogram `NTALLY` is provided in order to keep track of the number of times energy has been scored into the `ECNSV1` arrays (*i.e.*, an *event counter*).
  - Auxiliary subprogram `WATCH` is provided in order to allow an event-by-event or step-by-step tracking of the simulation.
- EGS4 allows for the implementation of *importance sampling* and other variance reduction techniques (*e.g.*, leading particle biasing, splitting, path length biasing, Russian roulette, *etc.*).
- Initiation of the radiation transport:
  - An option exists for initiating a shower with two photons from pi-zero decay (*i.e.*, use `IQI=2` in the `CALL SHOWER` statement).
  - The user has the choice of initiating the transport by means of a monoenergetic particle, or by sampling from a known distribution (*e.g.*, a synchrotron radiation spectrum).
  - Transport can also be initiated from sources that have spatial and/or angular distributions.

3 Improvements to EGS4 since 1985

In this section the improvements to EGS since the Version 4 release in December 1985 are described briefly. Only marginal detail is provided and the interested reader is encouraged to consult the references cited for deeper explanation. Most of the improvements/enhancements that are mentioned are supplied with the UNIX version (see below) or can be obtained by contacting the authors of the references. These enhancement are all <u>options</u> and must be "switched on" either through the use of flags (that are documented in the references given below) or by including macros in user codes that become active after recompilation.

3.1 Improvements/enhancements to EGS4 physics modeling

3.1.1 PRESTA

Following Rogers' low-energy work with EGS4 [48], an almost completely new algorithm called PRESTA (**P**arameter **R**educed **E**lectron **S**tep **T**ransport **A**lgorithm) for electron transport was introduced to EGS [49, 50, 51]. This new way of executing electron transport makes changes to three principle areas:

1. A refined calculation of the average curvature of the electron sub-step (between points of deflection by multiple elastic scattering) was developed. (Standard EGS4 overestimates the curvature correction by up to a factor of 2!)
2. A lateral correlation algorithm was introduced. This introduces an extra lateral component to the sub-step correlating it to the multiple-scattering angle selected at the end of the sub-step. (Standard EGS4 ignores this, underestimating lateral diffusion.)
3. A boundary crossing algorithm was introduced. This algorithm causes electron sub-steps to become shorter in the vicinity of boundaries insuring that no transport artefacts will occur near interfaces.

A small correction for the PRESTA's energy-loss averaging process was given by Malamut, Rogers and Bielajew [52] with further discussion and examples provided by Rogers [53]. It has also been noted that the "path-length-correction" provided by PRESTA only specifies information regarding the average endpoint along the direction of initial motion after a multiple scattering event. Its use to predict the total path executed by electrons going through thin foils in a single step is inappropriate[54].

3.1.2 Bremsstrahlung angular distribution

Bielajew *et al.* [55] modified EGS4 to allow for angular distributions employing the Schiff formula from a review article by Koch and Motz [56]. Standard EGS4 makes the approximation that the angle of the bremsstrahlung photon with respect to the initiating charged particle's direction is $\Theta = 1/E_0$ where E_0 is the initiating charged particle's energy in units of the electron rest mass energy. It was acknowledged that this may be a bad approximation for thin-target studies, but it was expected that there would be no effect in thick-target studies since multiple scattering would "wash-out" the initial bremsstrahlung angular distribution and that an average value would be sufficient. However, thick-target studies in the radiotherapy range showed dramatic evidence of this approximation as a calculation artefact [57]. Angular distributions near the central axis changed by as much as 40%!. Thick-target studies at diagnostic energies also showed the artefact which was eliminated through use of the new sampling technique [58].

3.1.3 K and L-shell fluorescence

Standard EGS4 does not create or transport fluorescent photons. However, a substitute sampling routine `SUBROUTINE PHOTO` allows for the generation of K_{α_1} and K_{β_1} fluorescent photons. It, along with the auxiliary subroutine `EDGSET` (extended by Keith Weaver of the University of California at San Francisco to 100 elements) are provided with the EGS4 distribution in the example code `UCEDGE.MOR[TRAN]` . Software switches must be enabled to activate this feature. This version of `SUBROUTINE PHOTO` is used as the standard in the UNIX and PC distributions described below.

Del Guerra *et al.* [59] have developed a K and L-edge sampling scheme for compounds. Conti *et al.* [60] have used this scheme for investigating the response of HgI_2 and CdTe photon detectors in the diagnostic range.

3.1.4 Electromagnetic field transport

As mentioned in the previous section, the electron transport subroutine `ELECTR` contains the necessary macro replacement templates to permit the user to effect transport in magnetic and electric fields of any configuration. The user must supply macros or subroutines that describe the spatial configuration of the magnetic field and/or the electric field with its associated scalar potential.

This was first done for a dosimetry study [61] which investigated the effect of electron storage in plastic targets on depth-dose profiles. A more general theoretical treatment was given subsequently [62] which studied the feasibility of coupling the equations for electron transport in external EM fields with the other physics affecting the transport and commented on how to guarantee the accuracy of electron transport. One application made a preliminary study on how electron and photon external beam radiotherapy would benefit from the use of strong longitudinal magnetic fields to control the lateral spread of beams, making them more geometrical in character [63].

3.1.5 ICRU37 collision and radiative stopping powers

Duane *et al.* [64] modified PEGS4 to give collision stopping powers identical to those of ICRU Report 37 [65, 66]. The NBS (now NIST) database EPSTAR [67] which was used to create the ICRU tables was employed. The modifications also allow the user to input easily an arbitrary density-effect correction. This change is relatively small but crucial if one is doing detail stopping-power-ratio studies [52, 68].

In a related work, Rogers *et al.* [69] adapted PEGS4 to make the radiative stopping powers ICRU37-compliant using the NIST database ESPA [67]. Effectively, this modification globally renormalises EGS4's bremsstrahlung cross section so that the integral of the cross section (the radiative stopping power) agrees with that of ICRU Report 37 [65, 66]. This improvement can lead to noticeable changes in the bremsstrahlung cross section for particle energies below 50 MeV [57] and significant differences for energies below a few MeV where bremsstrahlung production is very small [58].

3.1.6 Improved photon cross sections

The standard EGS4 photon cross section data is based on the library compiled by Storm and Israel [33]. Sakamoto [70] updated the photon cross sections to the more modern PHOTX library [71]. As discussed by Sakamoto, the principal change is to the low energy photoelectric cross section. Although the attenuation coefficients between the two photon libraries are different, the effect on exposure buildup factors is small.

3.1.7 Photoelectron angular distribution

In standard EGS4, a photoelectron, the electron produced when a photon is absorbed by an atom by the photoelectric effect, is set in motion in the same direction as the incident photon. In order to try an refine the comparison with low-energy TLD experiments, Bielajew and Rogers [72] employed the theory of Sauter [73] and made it an option for EGS4. Although

Sauter's theory is a relativistic one, ($v \approx c$), it was adopted universally even though Fischer's non-relativistic theory [74] may be more appropriate in the ($v << c$) region. However, Davisson and Evans [75] have shown that Sauter's theory is accurate down to 92 keV ($v/c = 0.092$). In the cases studied it did not have a major effect [72].

3.1.8 Pair angular distributions

Bielajew [76] also modified [6] EGS4 to sample the angular distribution of the electron and positron emanating from pair production according to the Schiff formula as given in the review article by Motz *et al.* [78]. A simplified and faster executing form of this angular sampling, similar to that employed by ETRAN [79, 80], is also available as an option. These angular distributions have a noticeable effect at large energies where the pair interaction dominates the photon cross section and the scoring regions of interest are small enough that multiple scattering does not "wash out" the effect of the initial pair distribution.

3.1.9 Low-energy electron cross section modeling

Standard EGS4, having been designed originally for high-energy applications, makes the assumption that as electrons lose energy the cross section for discrete interaction always decreases. This assumption is exploited by introducing a "fictitious" discrete interaction event, a no-scattering event that retains the incident particle's phase space, to account for cross section decrease with energy loss. This is a good assumption in the relativistic regime, since both bremsstrahlung production and Møller/Bhabha interactions increase with energy. However, in the non-relativistic regime, the Møller interaction cross section begins to rise as electrons and positrons slow down and have more probability to scatter inelastically from atoms. The rise is enough to overtake the fall off in the bremsstrahlung cross section. Ma and Nahum [81] introduced a linear-variation model to account for this low-energy behaviour, and recommend its use for electron kinetic energies below 1 MeV with Møller creation thresholds below 20 keV. They noted differences of 1–2% in the peak region of depth-dose curves for 10 keV – 1 MeV electrons incident on water and larger differences in fluence distributions in the 100–300 keV range.

3.1.10 More accurate trigonometric functions

Particle tracking algorithms make frequent use of sines and cosines. In order to save execution time (as much as 45% overall [82]), standard EGS4 employs look-up tables for the sine function and relates the cosine to the sine using the trigonometric relation, $\cos\theta = \sin(\frac{\pi}{2} - \theta)$. For problems where accurate small-angle modeling is crucial, EGS4 provides macro replacements to recover the trigonometric functions that are intrinsic to the native FORTRAN compiler, at the cost of increased CPU time. However, one application noted the shortcomings of the default table look-up approach [83] and a further investigation accomplished small-angle accuracy while retaining the look-up table method and speed [82].

[6] Development of the pair-angle sampling scheme was motivated by a high-energy physics experiment at SLAC [77]. A secondary result of this effort was the discovery (and correction) of a bug in subroutine `UPHI` that occurs at energies above 50 GeV and shows up at small angles.

3.1.11 Single elastic scattering

The Molière multiple-scattering theory [40, 41] is employed in standard EGS4 to account for elastic multiple scattering of electrons and positrons from nuclei. There are several shortcomings with this approach. The Molière formalism employs the small-angle form of the screened Rutherford cross section and couches it in a small-angle formalism. Moreover, Molière made analytic approximations [41] that make angular distributions unstable for short electron sub-steps [50, 84, 85]. In order to study the effect of these assumptions, Bielajew *et al.* [86] modified EGS4 to allow for single elastic scattering using partial-wave cross sections calculated by Berger and Wang [87]. A subsequent theoretical study [85] has resolved the small step-size difficulty of the Molière formalism and is being prepared for a future release of EGS4.

3.1.12 Binding effect in the Compton interaction

In its treatment of Compton scattering, standard EGS4 treats the electrons in the atomic clouds of the target atoms as "free", ignoring the binding of the atomic electrons to the nucleus. This is a good approximation for photon energies down to 10's of keV for most materials. The lower bound where this approximation works reasonably well is defined by the K-shell energy, although the effects can have significant influence above it, particularly for the low-Z elements. Namito and Hirayama have included binding effects in the Compton interaction model taking into account the change in photon cross section as well as the angular distribution of the emergent particles [88]. The bound Compton modeling was shown to have noticeable effect in low-energy gamma-ray buildup factors in various materials at low energy (40–200 keV) with the effect being stronger at the lower energies studied [89].

3.1.13 Doppler broadening and linearly-polarised photon scattering

In addition to neglecting the binding of the electrons in the Compton interaction, standard EGS4 also ignores the motion of the electrons in the atomic cloud. Since this motion is represented by a distribution of momenta, the electrons from a Compton interaction acquire a distribution called Doppler broadening. This detail has been taken into account by Namito *et al.* [90] who demonstrate improved calculations of 40 keV photon scattering measurements.

Standard EGS4 considers all particles to be unpolarised, using cross sections that have been summed over incident and out-going particle polarisations. Namito *et al.* [91] have introduced polarised Compton and Rayleigh scattering and made comparisons with low-energy experiments where gamma ray build-up factors and attenuation coefficients in water, iron and lead were studied in the energy range 40–250 keV [92]. The effects of binding, doppler broadening and polarisation have pronounced effect in the lower energy range studied [7].

3.2 Development of tools and techniques

3.2.1 Forcing photon interactions

EGS4 is an analogue code, transporting particles through media whether or not they interact with the target until they escape the target or degrade in energy below the cut-offs. In some simulations, for example photons passing through a thin target, it is wasteful to track photons that do not interact with the target. The technique of "forcing photon interactions" may be

[7] A recent paper by Flöttmann [93] has introduced polarisation into EGS4, by means of the additional-calls-to-`AUSGAB` feature, in order to investigate the development of high-intensity positron sources for future linear colliders.

employed [94, 95] to eliminate this waste. This technique is included here because it may be employed in a completely *application-independent* fashion unlike some techniques which rely upon some detailed knowledge of the target. This technique employs the geometry routine written by the user, `HOWFAR`, to extract all the information it needs. Thus, no matter how the target is shaped or how transparent or opaque it appears to the incident photons, the incident photons can be made to interact with the target and the particle "weights" adjusted accordingly. The technique, as described in the above references, should only be employed when the unscattered photon fluence is not important in the application.

Developments by Rogers *et al.* [96, 97] have refined this technique, creating "fictitious photons" that carry the non-interacting photon characteristics beyond the interaction point but with a weight that is reduced to account for its attenuation. This allows the fictitious photon to contribute to fluence scoring and also allows the photon to produce interactions in more than one place in the target, making efficient use of the tracking algorithms in EGS4.

3.2.2 Graphics tools

There are several general-purpose graphics packages that have been developed to provide graphical output of particle tracks and geometries of EGS4 simulations. They are:

- `SHOWGRAF` from SLAC, developed by Cowan and Nelson [98],
- `SHOW` from NRCC developed by Mangin and Bielajew.
- `EGS_Windows Version 1` from NRCC developed by Wiebe and Bielajew [99],
- `EGS_Windows Version 2` from LBL (Lawrence Berkeley Laboratory) developed by Chatterjee and Donahue,
- `EGS_Windows Version 3` from NRCC developed by Zurawski and Bielajew.

These packages have different functions and require different hardware and software libraries. More details can be found in another reference [100].

3.2.3 Bremsstrahlung splitting

In applications where the production of bremsstrahlung is being studied, Bielajew *et al.* [55] introduced a variance reduction technique to improve the statistics associated with the scoring of bremsstrahlung-related quantities. Instead of setting one bremsstrahlung photon in motion, one may set N photons in motion, giving each photon a weight of $1/N$ but re-sampling for each photon in terms of energy and direction. To preserve the full-energy straggling of the initiating electron, only the energy of <u>one</u> of the photons (the first) is deducted from the electron's total energy. This violates specific interaction-by-interaction energy conservation but energy is conserved on average. Faddegon *et al.* [101] employed this technique at radiotherapy energies using multiplication factors of $N = 5$–30. Namito *et al.* [58] used multiplication factors as high as 300 in a low-energy study to reduce calculations taking many hours on an IBM mainframe computer to about an hour.

3.2.4 Range rejection

Range rejection is a technique whereby electrons that cannot reach a region of interest within a target are discarded "on the spot". A full discussion of the approximations involved is given by Bielajew and Rogers [95]. Rogers *et al.* [97] have developed methods for integrating the restricted stopping powers provided by PEGS4 to provide accurate restricted range tables employed in this technique. Range rejection is quite powerful, saving as much as a factor of 4 in computing time in the calculation of ion chamber response [102].

3.2.5 Long sequence random number generators

Standard EGS4 comes with two default random number generators, one specific to IBM mainframe architecture [103] and one based on the same generator but recoded for generic 32-bit 2's-complement integer arithmetic. This random number generator is based on the multiplicative congruential method [104] and has a sequence length of 2^{30} which is inadequate for most studies that execute for more than one hour on a modern workstation-class computer. Bielajew [105] proposed a 64-bit multiplicative congruential random number generator that has a sequence length of 2^{62}. This multiplier is architecture dependent and relatively slow (it slows down a typical calculation by about 20%) since it must mimic 64-bit integer arithmetic in software. (There is some hope for this generator in modern newer architectures that can perform 64-bit integer arithmetic.) This generator has been replaced by modern generators that are machine-independent and easily adaptable to parallel implementations of Monte Carlo [106, 107]. The version now distributed with the UNIX system (see below) was taken from a review article by James [108]. This random number possesses a sequence length of about 10^{43}, effectively infinite for any calculation, and has about 10^{9} independent sequences that can be selected from initial conditions. Compared to the 32-bit generic random number generator described above, this generator slows down a typical calculation by no more than 5%.

3.2.6 PEGS tools

To generate PEGS4 data files, the user must create input files that describe the medium, execute PEGS4, concatenate the output data files and finally store them for routine execution by EGS4. This is a fairly easy procedure, involving only a few input cards that are read in by PEGS4. Recently an interactive tool has been developed [109] that performs all these tasks automatically, includes the ICRU37 stopping powers described previously, and maintains a database of 100 elements and over 300 commonly-used compounds.

Nevertheless, it is very important to completely understand the quality of the PEGS4 output that will be used by EGS4. The EXAMIN user code was developed at the NRCC for just this purpose. Although it has been distributed since 1985 as part of the EGS4 Code System, it is an important PEGS tool and we mention it here for completeness.

3.2.7 Workaround to PEG4 limitations

In going from PEGS3 to PEGS4 a limitation was imposed on the operation of PEGS4 restricting the material creation to one set at a time. PEGS4 would have to be restarted for each material. Previously, users could create as many materials as desired without having to restart PEGS. A workaround was reported by Nick Hammond of EDS-Scicon, United Kingdom, and it is available from the authors of this report.

3.3 Systems and other support

At the time Version 4 of EGS was released, there was support given for only two types of machines, IBM/VM(CMS) and VAX/VMS. This support came in the form of example scripts (*i.e.*, exec files, command procedures, *etc.*) for running and compiling user codes within the EGS4/PEGS4 system. This original distribution is still available either from SLAC (contact

WRN) or through the Radiation Shielding and Information Center at Oak Ridge. However, interest in these two computer systems has waned (Alpha/VMS is making a comeback) and general distributions for PC's and UNIX systems are now available. These are described below. General information on getting EGS4 is given in References [110] and [111], contacting one of the authors of this report, or by posting a question to the EGS4 discussion list (egs4-l@slac.stanford.edu).

3.3.1 PC distributions

At the time when PC's became available with Intel-386/387 processors there was a surge of interest in using EGS4 on these machines since they executed EGS4 about as fast as a VAX 11/780/FPA minicomputer. At this time Walker *et al.* [112, 113, 114] volunteered to manage and distribute the EGS4 code on PC's. Details on how to get the PC version is given elsewhere [111].

3.3.2 UNIX distributions

The fastest growing architecture for scientific computing is the workstation-class computers which is dominated by the UNIX operating system. To satisfy the growing demand, Bielajew [115, 110] developed the UNIX-distribution for EGS4. Most of the enhancements/improvements described in this report are included as part of the UNIX distribution. Details on how to get the UNIX version is given elsewhere [110, 111].

3.4 Timing benchmark database

The best way of comparing the performance of computers is to make direct comparisons of one's own application. To this end, a standard timing benchmark targeted for radiotherapy calculations was introduced [116] and comparisons for a variety of computers from PC's to supercomputers was given. A separate PC comparison using the same benchmark code was also published at the same time [114]. These studies contain contributions from many colleagues and the latest combined results are posted in the anonymous ftp servers described below.

High energy timing benchmarks were discussed extensively by Yasu *et al.* [117] for a wide variety of computers. EGS4 calculations using example codes as well as the radiotherapy benchmark mentioned above were compared to the standard CERN [118] and SSCL [119] benchmarks.

3.4.1 Listserv and anonymous ftp support

The EGS-community has grown dramatically. Fortunately, common Internet access has made the EGS community a self-help enterprise. In order to promote discussion on EGS4-related issues, a discussion list has been started by Rick Donahue of Lawrence Berkeley Laboratory (RJDonahue@lbl.gov). Users post questions to this list that can be answered by the EGS-community-at-large. Sign-on instructions are given elsewhere [110]. Distribution of the UNIX system is most conveniently done via anonymous ftp. The current anonymous ftp sites are nrcnet0.nrc.ca [132.246.160.2] and academic.lbl.gov [128.3.12.48]. More details are given in the reference [110].

These anonymous ftp sites are dynamic and should be browsed periodically by interested EGS users. Besides distributions of the EGS system and graphics-support code, there are also contributions from users, PostScript reprints of EGS-related papers and reports (including many mentioned in the reference list herein) as well as the most recent timing benchmark studies.

3.4.2 Courses and Users' Meetings

In addition to the self-directed training outlined above, formal training courses in EGS, including laboratory sessions are provided. The courses that have been given or are planned to be given are: National Research Council, Ottawa (Feb. 1986, Feb. 1987, Sept. 1990), National Physical Laboratory, London (Sept. 1989, Sept. 1993), Institute of Applied Physiology and Medicine, Seattle (Mar. 1992), University of Ferrara, Italy (June, 1994), Lanzl Institute, Seattle (Mar. 1995). These courses are run "at cost", are limited to about 30 students, and have proven to be effective in getting researchers into the productive phase of using Monte Carlo calculations.

There have also been EGS-specific users' meetings in Japan (Jul. 1991, Jul. 1992, Jul. 1993) and these have resulted in Proceedings [120, 121, 122]. These documents are an important source of new capabilities of EGS as well as a description of interesting applications.

Acknowledgment

It is clear from this historical account that many people have contributed to the development of the EGS Code System. We hope that we have properly recorded the sequence of events and have referenced all of the contributions. However, EGS is truly "the child of a thousand mothers and fathers" and doubtlessly we have failed to cite some contributions and enhancements to the EGS code. These omissions ought to be blamed on nescience alone as no one can claim ownership of public-domain software that is intrinsically "open" in design. We would like to consider this report to be a "working document" to be updated periodically as new information is made available to the authors and new capabilities are built into the software distributions.

A proper acknowledgment of all the people who have helped along the way would add too much to the length of this report. We appreciate all of the help and thank you for it. We do wish to single out several individuals: Hans-Helmutt Nagel for starting it all, David Nicoli for his important early contributions, Richard Ford for his generalisations and beautiful programming, Yoshihito Namito (KEK, Japan) for his many contributions to the low-energy physics modeling and Sue Walker (Lanzl Institute, Seattle) and Richard Donahue (LBL, Berkeley) for helping with distributions.

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