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Final Report

NAG 9 - 803

DEVELOPMENT OF A SPACE RADIATION MONTE CARLO COMPUTER SIMULATION

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Preamble

This Final Report is submitted in partial fulfillment of the performance of the tasks under NASA Regional Universities Grant NAG 9 - 803. The work performed was completed on April 15. 1997 and pursuant to the originally proposed task, a proposal was submitted to NASA Headquarters, Life Sciences Division. Unfortunately, the P.I. was informed by personnel in the Space Radiation Program within that division, that they were not considering proposals to do physical science, including the development of radiation simulation codes, but were restricting their funding to biological experiments only. The P.I. has requested funding from the 1997 R.U.G. program to continue this effort, and to search for other constituencies within the present NASA program.

Abstract

The ultimate purpose of this effort is to undertake the development of a computer simulation of the radiation environment encountered in spacecraft which is based upon the Monte Carlo technique. The current plan is to adapt and modify a Monte Carlo calculation code known as FLUKA, which is presently used in high energy and heavy ion physics, to simulate the radiation environment present in spacecraft during missions. The initial effort would be directed towards modeling the MIR and Space Shuttle environments, but the long range goal is to develop a program for the accurate prediction of the radiation environment likely to be encountered on future planned endeavors such as the Space Station, a Lunar Return Mission, or a Mars Mission. The longer the mission, especially those which will not have the shielding protection of the earth's magnetic field, the more critical the radiation threat will be. The ultimate goal of this research is to produce a code that will be useful to mission planners and engineers who need to have detailed projections of radiation exposures at specified locations within the spacecraft and for either specific times during the mission or integrated over the entire mission. In concert with the development of the simulation, it is desired to integrate it with a state-of-the-art interactive 3-D graphics-capable analysis package known as ROOT, to allow easy investigation and visualization of the results. The efforts reported on here include the initial development of the program and the demonstration of the efficacy of the technique through a model simulation of the MIR environment. This information was used to write a proposal to obtain follow-on permanent funding for this project.

1. Introduction

This proposal originally requested funding to support an effort to begin the process of developing a full Monte Carlo based simulation of the radiation environment within spacecraft. The intention was to allow a sufficient demonstration of the capabilities to allow a more formal proposal for permanent funding to be submitted. Such a proposal has been submitted to NASA Headquarters Life Sciences Division. However, in conversations with Dr. Walter Schimmerling it has become clear that the Life Sciences Division, which did support this kind of work when the grant reported on here was initially funded, they are no longer funding what they consider physical science efforts. Rather they are only funding work on the biological aspects of the problem. This report will paraphrase the proposal as submitted in accordance with the original intent of the present grant. We are now seeking to continue this effort by finding other constituencies within NASA who may be interested in funding it, and an additional R.U.G. to allow the seamless continuation during the ensuing period.

The project as presently proposed would adapt and participate in the evolution of the current Monte Carlo code known as FLUKA [1]-[8] to a form that is useful to simulate the spacecraft environment. In addition, it is proposed to amalgamate the software infrastructure known as ROOT [9]-[11], which is currently being developed at CERN (the European Laboratory for Particle physics located in Geneva, Switzerland) into a single package capable of providing a complete state of the art analytical framework in which to explore predictions of the radiation environment within spacecraft.

Much prior effort has gone into both measuring and predicting the radiation environment is spacecraft [12]-[20]. This is of course especially true for manned spacecraft because of the potential health risks to the crews posed by the radiation, but also in this era of decreasing scale size for individual components within Large Scale Integrated Circuits, there is an interest in predicting the environment with some degree of specificity for use in predicting other kinds of injury.

Perhaps the longest continuous effort to address the problem is the program of Wilson and Townsend and their collaborators at NASA, Langley [18]. They have chosen a pseudo-analytic type transport (shielding) calculation in one-dimension (using the straight ahead approximation). In essence, rather than follow the transport of individual particles through a medium, they solve the diffusion equation for a function representing the total analytic flux of particles. They have assembled a semi-

empirical reaction cross section data base which concentrates on nucleons and nuclear fragments typically using the abrasion and ablation models to augment the data. They do not treat the production of secondary particles such as mesons and antibaryons, nor do they include electromagnetic cascades to any significant degree. They calculate the integrated dose in tissue equivalent material behind a particular type of shield layer. They indicate that they hope to evolve this ultimately into a full three-dimension calculation which would also attempt to incorporate the reactions not yet included as noted above. This effort resulted in the HZETRN code and its modification BRYNTRN [20]. These codes have been used to fit data from prior missions with significant success. However, they do not afford the ability to evaluate the effects that the geometric details of a spacecraft might have upon the environment, and they cannot as easily incorporate all of the accurate details of the known physics.

The cosmic ray group at the U.S. Naval Research Laboratory in Washington, D.C. which has a long and impressive history of notable contributions in the field of cosmic ray propagation [19], has also considered in this problem. Their most recent work is also based on a pseudo-analytic, one-dimensional treatment similar to the Langley approach. This effort has evolved into the program of Adams, Silberberg, and Tsao [21]. One significant difference from the Langley calculation is the use of the NRL developed code UPROP and in particular the long evolving tabulation of cross sections by Silberberg and Tsao [22]. In addition to this effort, Letaw who worked at NRL before moving to the Severn Communications Corporation, Severna Park, MD, did an analysis employing UPROP and HETC (see the discussion in the next paragraph) type calculations [23].

The Department of Energy and its precursors have had a historical interest in the evaluation of radiation hazards of all kinds. One Monte Carlo code developed there to deal with the general problem of particle transport in three-dimensions is HETC (High Energy Transport Code) [24]. HETC has evolved as a shielding code since 1967 and uses the intranuclear cascade code to internally calculate the reactions with nuclei [25]. In its most recent version it has become a rather useful tool, but tends to be based on nuclear physics applications driven by lower energy considerations where high multiplicity hadronic showers are not of concern. At present, the breadth of the physics capabilities of the original HETC code have been considerably added to by the present state-of-the-art Monte Carlo codes in use in high energy physics. FLUKA, the code that is proposed as the basis for the project here, incorporates a version of HETC nuclear evaporation model within it [1].

What the code that is proposed here offers in contrast to these other efforts is a full three-dimensional simulation that is easily adaptable via industry standard CAD formats to any complex spacecraft design, and which includes all of the known physics at a reasonably precise level. Further, the code is planned to be easily modifiable in the future to include updates in the data as they become available.

II. The FLUKA Monte Carlo Code

The heart of the physics simulation and transport code proposed for this effort is an evolution of the present version of the FLUKA Monte Carlo code [1] & [36] - [42]. FLUKA is less well known that GEANT [4], which has for many years been the de facto standard Monte Carlo Code in high energy physics. FLUKA has been chosen for use here because of its superior representation of the physics and its imminent amalgamation with the ROOT infrastructure which is described in the next section. FLUKA has recently been selected for use over GEANT by both the ATLAS and ALICE collaborations at CERN [4]. These large experiments approximate the complexity and physics interests of a space radiation simulation reasonably closely, and also serve to insure the continued development and support for these codes into the foreseeable future. A tutorial for FLUKA is currently available on the World Wide Web at http://rita02.ge.infn.it:8000/fluka/indice.html (note: address should all be lower case). FLUKA has been used to simulate a wide variety of different problems and in fact is no stranger to simulating cosmic ray fluxes [28] - [29].

Most Monte Carlo codes are "analog" codes, in that they attempt to simulate all of the physics processes as closely as possible to their natural way of occurrence. Another way of looking at these codes is that the statistical weight of each occurrence modeled is equivalent. GEANT is an analog code and FLUKA is certainly capable of running in a strictly analog mode. However, FLUKA is at its core a "biased' code. That is, FLUKA allows the use of statistical variance reduction methods to bias the weight of rare events. Using this technique, such rare events can be simulated with higher frequency to build statistical significance orders of magnitude faster than for analog codes. The use of these biases are intimate to the code and can include not only the obvious biases in the input fluxes, but the biasing of the subsequent reactions which occur within the transport processes. The proper accounting is done automatically within the code so that the output may be evaluated rescaled to proper relative values. Note that such biasing can be done with a wide range of variability, so that one can ignore many processes and lower energy limits in geometric volumes that are not of

much interest, while exploring building balanced statistics and tracking things down to the code limits in other areas. At present the code will handle detailed tracking of charged particles and photons down to 10 KeV, and neutrons down to thermal energies. Note that it is possible to save accurate records of these particles for volumes of interest and then consider their further transport with other micro-Monte Carlo codes. Such micro-Monte Carlo codes are presently being developed to track knock-on electrons down to atomic and molecular binding energies and explore the damage to individual DNA molecules[34].

FLUKA is a fully integrated code which uses a common transport for all of the propagation. As mentioned above, the HETC nuclear evaporation model is employed along with a drastically improved and expanded version of the EGS4 ElectroMagnetic cascade code. FLUKA employs several different models for hadronic interactions, depending upon the energy regime being simulated. A considerable effort has gone into carefully comparing the output of the code with the existing data to insure an accurate representation where there is good data for comparison. One of the more notable strengths of FLUKA in comparison to its competitors is its ability to accurately handle neutrons at low energies. Special cross section data for 50 elements and isotopes at different temperatures allows very accurate simulation of the transport down to thermal energies.

FLUKA is currently maintained by a group at the INFN section at the University of Milan in collaboration with the code's original architect, Johannes Ranft of the University of Leipzig [1] - [8]. The adoption of FLUKA by major experiments at CERN and its use in this country at Los Alamos, SLAC, and FERMILAB, serve to bolster its long term viability. Presently FLUKA is running under VMS and UNIX, and is in principle portable to any operating system that will support FORTRAN. The most recent version of the FLUKA code is currently installed and running at the University of Houston.

In order to demonstrate the potential use of FLUKA, a simple simulation was undertaken of the exposure of the tissue equivalent proportional counter (TEPC) which was flown on the MIR space station [20]. Figure 1 shows the MIR shielding distribution in Aluminum equivalent thickness as seen by the detector, and of a simplified representation of that distribution as three dimensional cylinder of variable aluminum wall thickness with air inside and a model of the TEPC in the center. A cross sectional view of the cylinder is depicted. A CAD drawing of the MIR was unavailable, so this simple shape was used for demonstration purposes only. This ersatz spacecraft was subjected to an isotropic proton flux incident in the plane of symmetry with an energy

distribution mimicking a primary cosmic ray spectrum having a lower energy cutoff at 300 MeV. Again, just as a demonstration of what is possible with such codes, Figure 2 shows the dose in Grays per incident particle in a cross sectional view integrated for each pixel. Note the ability to include the albedo of the spacecraft so that the dose including the splash back from the interactions in the spacecraft material is also modeled.

Figure 3 depicts the charged particle fluence, and Figures 4 and 5 depict the photon and neutron fluences. Notice how the charged particle fluences peak in the lower shielded regions where as the photon and neutron fluences peak in the heart of the shielding. Note also the differences in the albedo distributions between the charged particles and the neutrals, and note also the differences between the charged particle fluence distributions and the dose form Figure 2. Just to illustrate further the ability to segregate out information as desired, Figure 6 shows the charged pion fluence by itself. It is not suggested that these simple examples of the use of FLUKA represent very accurately the actual conditions inside the MIR spacecraft, but rather are meant only as simplistic examples of the technique itself. It would be very tedious to attempt to model a complex geometry from mechanical drawings for example. However, the use of CAD files makes the inputting of complex geometry a relatively painless exercise. Note that the ATLAS experiment geometry consists of over 11 million individual distinct shapes and volumes. This is likely to be comparable to or greater than the geometric complexity in something like the space shuttle or even the space station.

Figure 7 shows the spectrum of energy deposited per primary particle in the tissue equivalent gas of the TEPC. Also shown are the results of the simulation of this measurement by the BRYNTRN code and the results of the simplistic calculation done here. I emphasize that the present simulation did not include any other particles except protons in the incident flux. This exercise, was intended to merely demonstrate the prospects.

One question of central interest when Monte Carlo codes are run is the amount of CPU time required to obtain reasonable results. When running on a single DEC Alpha™ with a 266 MHz CPU clock, FLUKA in its present incarnation can handle on the order of 10⁵ events per hour with reasonably complex geometries (similar to that of the Space Shuttle) and reasonably low limits for the energy cutoffs.

The technique proposed here would employ an initial run to produce a database of "pseudo-incident" particles for the next more detailed step. As an example consider a simulation of the Space Shuttle. An initial run would only

consider the propagation of the external incident flux up to the inner surface of the crew compartment walls, creating a database of the flux at that boundary. Then to evaluate the detailed conditions at some specific location within the crew compartment, a second order calculation can be made, using the database calculated in the initial run as an incident flux. This process can be repeated for example to produce a second database of the flux incident to the skin of a crewmember in a certain location. A third order calculation can then be made, following the particles down to very low energy levels and scoring the dose as desired. Note that the process can be biased at each level so that each incident particles ultimate source can be identified at each level. This means that a generic calculation can be done at the higher level, with many different lower level runs being possible, such as biasing for different mission profiles on the second and subsequent level runs without the need to rerun the higher level. It should be noted that there are projects underway to assemble CAD-like models of the human body for both sexes at all stages of life [35].

One can estimate the number of events that would have to be simulated in a baseline high level run to provide the lookup database for further runs. One method is to base the estimate upon the external surface of the volume to be simulated. Consider Figure 3 once again. The incident flux was 5 * 10⁵ protons and the scale is normalized per proton. The pixels are 1 cm * 1 cm and the effective incident area is on the order of several square meters. Even the most heavily shielded regions have a fluence of several particles in this unbiased calculation. To be safe one would likely want to have an order of magnitude more particles than this. Assume then that we need 10⁶ particles per square meter. Taking the volume of interest to be roughly bounded by and area of 100 square meters we would need to simulate on the order of 10⁸ incident events. At 10⁵ events per hour, that seems to imply the need for 1000 hours of dedicated Alpha™ time, not to mention the 10 GB of disk space to store the data base!

Several comments need to be made here. First, the newer versions of the AlphaTM machines in existence today are already capable of performing several times faster than the benchmarks quoted here, and they are also available in mainframe versions with multiple processors and multi-processor operating systems that allow very efficient parallel processing of calculations such as these. Thus, with the hardware we are proposing to acquire (and not taking into account any anticipated advances in the state-of-the-art), the time can be reduced by a factor of 100! Thus, for example every 10 hours one can generate and propagate 100 particles per square cm incident upon the entire 100 square meter surface area of the enclosed Space Shuttle

crew compartment volume. It should be further pointed out that these since these calculations lend themselves to really massive parallel processing, the recently announced advances in such techniques and the current plans to develop national centers to explore their uses, have the potential to enhance these estimated event rates by several orders of magnitude more.

In short, the hardware to make such calculations accessible is in existence, and for most actual applications, biasing and clever use of layering, can reduce the demands upon the hardware quite substantially. If fact, it is the goal of this project to develop an end product that can produce significant practical results typically in overnight runs on hardware that costs less than \$50k.

III. The ROOT Infrastructure

One key element of the proposed project is to participate in the immersion of the FLUKA code into the ROOT infrastructure. ROOT is basically an object-oriented data class framework or software infrastructure which is designed to handle arbitrarily complex polymorphic data structures [9] - [11]. It is intended to provide the framework on which to implement the next generation of physics workstation analysis applications. For a view of what is presently incorporated into ROOT and examples of the simulation analyses that can be accomplished, the ROOT home page on the World Wide Web is an excellent resource at http://hpsalo.cern.ch/root/Welcome.html (note, the address may be case sensitive). Rather that attempt to put several full color examples of graphics outputs from ROOT into this proposal as figures, it is perhaps better to refer the reader to this web site. Figure 8 includes an image of a 3-dimensional representation of a particular Pb-Pb collision generated by the VENUS code. A version of this image is available for viewing at the ROOT web site. In this example, each of the individual tracks may be color coded by particle type, or dE/dx, or by any other identifiable parameter or combination thereof. In addition, when viewed interactively within ROOT, the image can be rotated and zoomed, and further, one can click on individual tracks to have their full parameter set displayed as shown in the insets to Figure 8. This example is just an illustration of the detail of graphic presentation which will be routinely available. This same power can be brought to bear on more conventional analysis techniques such as sequential cutting and binning of data.

The data that is generated by FLUKA can be produced as ROOT data structures which would allow immediate access to many varied forms of analysis including full

real-time graphics integration. From the ability to explore single events in microscopic detail to a full combinatorial analysis of several integrated runs, the ROOT infrastructure will allow quick integration and visualization of the data generated by FLUKA simulations of actual spacecraft. As a practical matter what this means is that one does not have to contemplate every conceivable question that might be asked about the results, before running the simulation. The data structures will preserve a vast amount of information which may then be easily and quickly retrieved, filtered, and then visualized in many different formats within the ROOT infrastructure. Thus for example if after the fact one wanted to know the spectrum of neutrons traversing a particular volume such as the actual silicon wafer of a memory integrated circuit located is some specific place, such a plot could be done quickly from within ROOT. Likewise if you wanted to generate a three-dimensional image of a human organ (presuming that the volume of interest was identified within the original FLUKA calculation) and superimpose the predicted dose profiles in a color v. intensity code, rotatable interactively by the user on the workstation screen for full 3-dimensional viewing effect, ROOT can provide that as well. It is a tool that will enable the results of the simulation to be rapidly evaluated and understood, as well as communicated to others.

The ROOT project was initiated at CERN as part of NA49, one of the major heavy ion experiments being performed there. The motivation grew from the archaic nature of the existing workstation analysis packages and the demands placed on them by the massive data sets generated in these experiments where a single event buffer can easily exceed 30 MB. Looking ahead to the L/C collider experiments such as ALICE, it was clearly foreseen that the present software would be inadequate. There has been a commitment from both CERN and several of these experiments to finish the full development of ROOT and to sponsor and encourage the conversion of FLUKA's internal data structures to be compatible with ROOT for analysis. ROOT is presently running on DEC, HP, and Sun hardware along with versions for PCs that run Linux and Windows NT or Windows 95. It is rapidly becoming a mature software system, and will shortly integrate OpenGL formats.

The combination of FLUKA and ROOT to be developed for this project will provide investigators with the tools to not only simulate the space radiation environment with unprecedented accuracy, but to subsequently be able to rapidly explore the detailed character of those predictions. Because mundane examples of simple graphs or even pseudo 3-dimensional plots do not do justice to the full color animated interactive graphics that will routinely be available from the proposed

package, they have not been included here, and the reader is again referred to the ROOT web page which itself is even a poor substitute for the reality.

IV. The Future Project as Proposed and to be Continued

The FLUKA code as it presently exists needs several significant modifications to make it suitable as a state-of-the-art simulator of the space radiation environment. Among these are: the inclusion of the event generators to allow propagation of heavy ions up to and including Uranium through any and all of the materials likely to be present in spacecraft; the selection and implementation of a standard CAD format-geometry interface; and the blending of the ROOT infrastructure into the FLUKA formats. All of these modifications are in fact underway, and it is proposed here that they all be monitored and aided as part of the present effort. The motive to undertake such intimate collaboration with the development and evolution of the code from this point is to insure that it will be available in a form that is most useful for simulation of the space radiation environment as it emerges from these modifications.

In particular, the need to ask many different questions at different times argues for a system of recording raw calculation results which can be used subsequently to investigate detailed questions without the necessity to rerun the bulk of the simulation. This will save substantial amounts of computer time and make may detailed applications feasible at a reasonable cost.

In addition to the collaboration on the evolution of the FLUKA/ROOT code, an incident flux generator needs to be developed that will allow simulation of any desired space radiation environment. It is proposed to include not only the primary cosmic ray flux as modulated in the solar environment, but also the trapped radiation flux and even solar flare events [30] - [33]. Thus, it should be possible to evaluate any possible mission from low altitude equatorial earth orbit to extended Mars missions which might experience various solar flare possibilities. The simulation possibilities will not only be limited to spacecraft. Surface and subsurface lunar habitats will also be within the capabilities of the code to simulate. Finally, given the neutron simulation possibilities of FLUKA, accurate modeling of the effects of artificial sources such as reactors and thermal neutron power sources are also possible, integrated with the effects of the external sources of radiation.

Some mention of the physics involved in the inclusion of heavy ion reactions in the FLUKA code needs to be made. There are a number of event generators that will produce the results of collisions from a given pair of heavy ions under specified conditions. It is not proposed as part of this effort to become intimately involved in designing such a generator. Rather, as the various heavy ion experiments gather data these generators will naturally evolve under the direction of their mentors, and will in turn be ported to FLUKA. Present plans call for the use of the most recent update to the VENUS event generator [26] - [27] in the initial version of the space radiation simulation code. In the interim, the full simulation of the physics of light ion transport including He and deuterium within FLUKA is planned for this year.

A. Near Term Objectives (1st year)

A post-doctoral fellow will be requested in this proposal and will be directly involved along with the P.I. in the task of aiding the integration of FLUKA and ROOT with the goal of insuring the compatibility of the final code with the needs of the proposed space radiation simulation. In addition, the work initiated previously to model the MIR results will be continued as an initial milestone in the project. This will include:

- Monitoring and evaluation of the integration of the ability to use CAD format inputs to the FLUKA code;
- 2) Development of a more accurate geometric model of the MIR spacecraft (by creating simplified CAD models of the MIR if necessary);
- 3) Integration and use of He and Deuterium in the FLUKA code as incident flux constituents:
- 4) Initiation of the general incident flux generator which includes primary cosmic ray spectra, solar modulation effects, and solar flare simulation;
- 5) Full simulation of the MIR experiment with the more correct geometry and incident flux., and exploration of the use of ROOT to analyze the results.

B. Long Term Objectives (2nd & 3rd years)

It is proposed to continue the evolution of the codes towards a version that will allow the construction of a fully adaptable software package that is capable of simulating the space radiation environment in spacecraft for a wide variety of near earth and interplanetary missions. The code will be immediately adaptable to existing spacecraft as well as future design concepts through the use of CAD inputs. The intention is to develop and publish a stand alone code that can be made available for

use of any interested party, within NASA or otherwise, and to deliver the initial version of such a code within the grant period. That final version will include the representation of the effects of the full cosmic ray, solar, and trapped spectra.

V. Summary

We have initiated a substantial effort under the present funding and carried out a demonstration of the capabilities of the FLUKA code. This effort did result in the writing and submission of a formal proposal to NASA Headquarters, Life Sciences Division as originally intended. That continued project as proposed has been outlined here along with a description of the results of the model simulation. A proposal to obtain funds from the 1997 NASA Johnson Space Center Regional Universities Grant program has also been submitted to allow the continuation of this effort and to search out additional constituencies within NASA for permanent support in light of the present direction taken by the Space Radiation program of the Life Sciences Division.

VIII. References

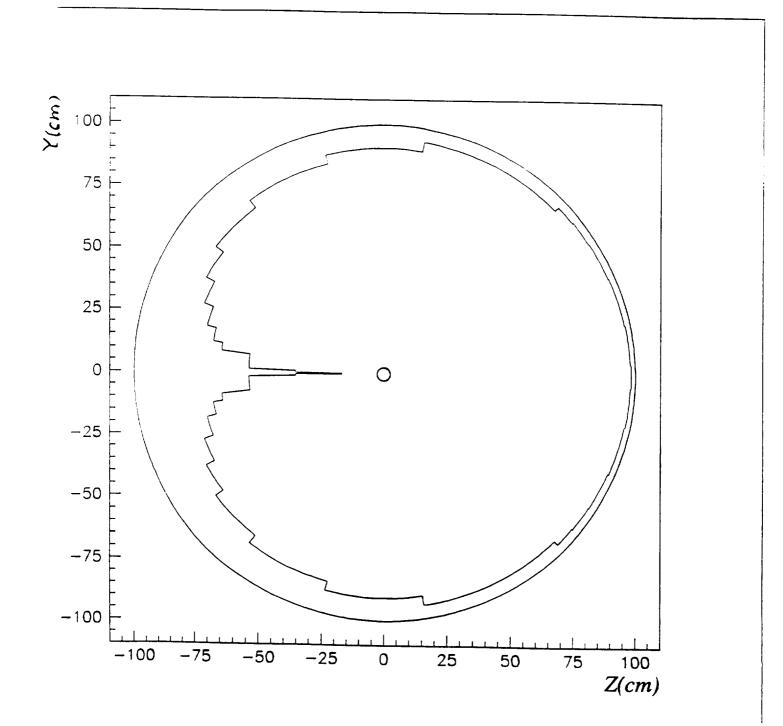
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Figure Captions

- Figure 1. The cross section of an aluminum cylinder, 1 m in external diameter is shown. The variable wall thickness approximates the shielding thickness probability distribution of the MIR spacecraft as seen from the location of the TEPC as described in Ref. 20. A model of the TEPC was included in the center of the cylinder and the volume between the TEPC and the wall was filled with air at STP. The cylinder modeled was arbitrarily limited to 2 m length with open endcaps. The incident flux was isotropically distributed in both position and initial direction within the angles heading towards the cylinder from a ring source of 2 m radius surrounding the cylinder in a plane perpendicular to the axis of the cylinder and passing through its center. This simple model is intended only as a demonstration of the technique.
- Figure 2. The dose in Grays per incident particle is depicted for an incident flux of protons possessing a cosmic ray energy spectrum with a lower cut off of 300 MeV. The color code represents the dose per 1 cm x 1 cm pixel projected onto the plane perpendicular to the axis of the cylinder.
- Figure 3. The total fluence per pixel per incident particle is shown for all charged particles. The valued color coded is actually the total path length of charged particles in the pixel per incident particle.
- Figure 4. This is a plot similar to Figure 3, but for the fluence of photons.
- Figure 5. This is a plot similar to Figures 3 & 4 but for the fluence of neutrons.
- Figure 6. This is a plot similar to Figures 3, 4 & 5, but for the fluence charged pions.
- Figure 7. This is a plot taken from Ref. 20 with the predicted results of this example code superimposed. The points plotted were arbitrarily normalized.
- Figure 8. This is a screen shot of a 3-dimensional image which represents an event produced by the VENUS code and displayed by ROOT. As indicated in the text, the actual image is interactively rotatable and zoomable. Further, the individual tracks are color coded in this case by particle type, and may be clicked upon to obtain full readouts of their properties as shown in the inset example parameter panels.



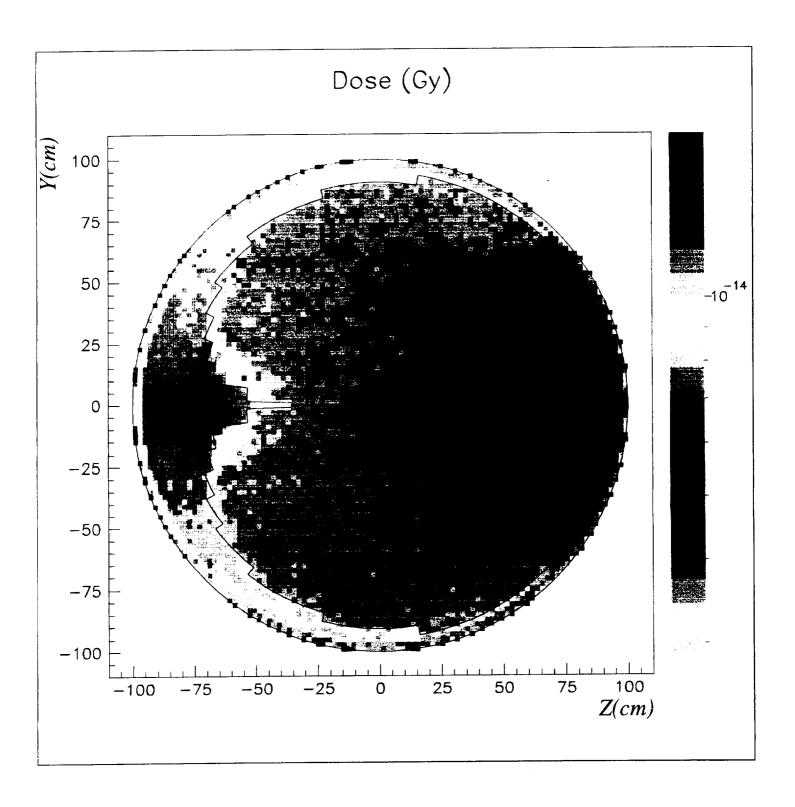


FIGURE 3

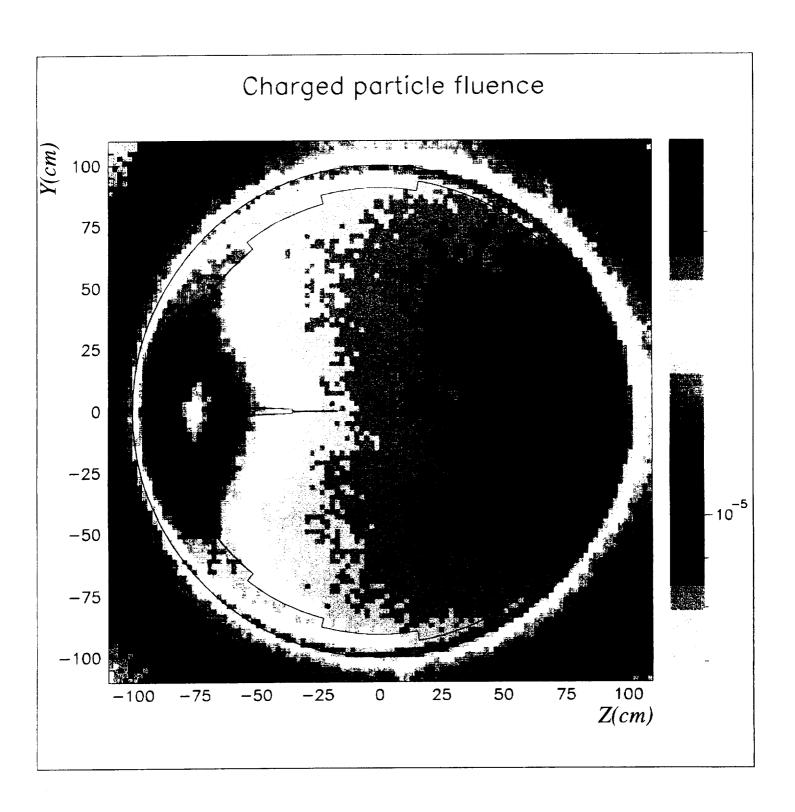


FIGURE 4

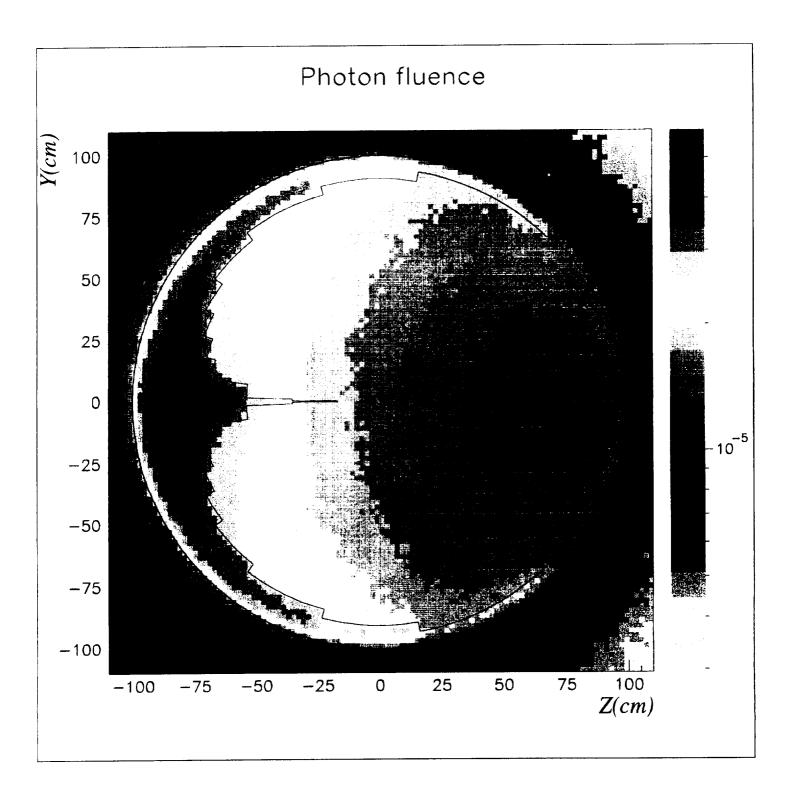
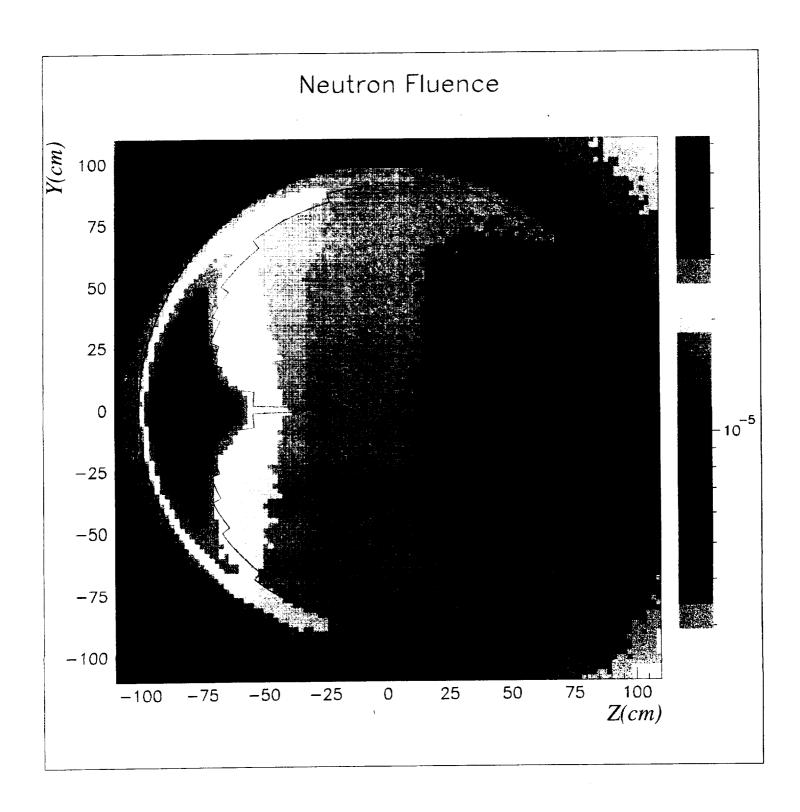
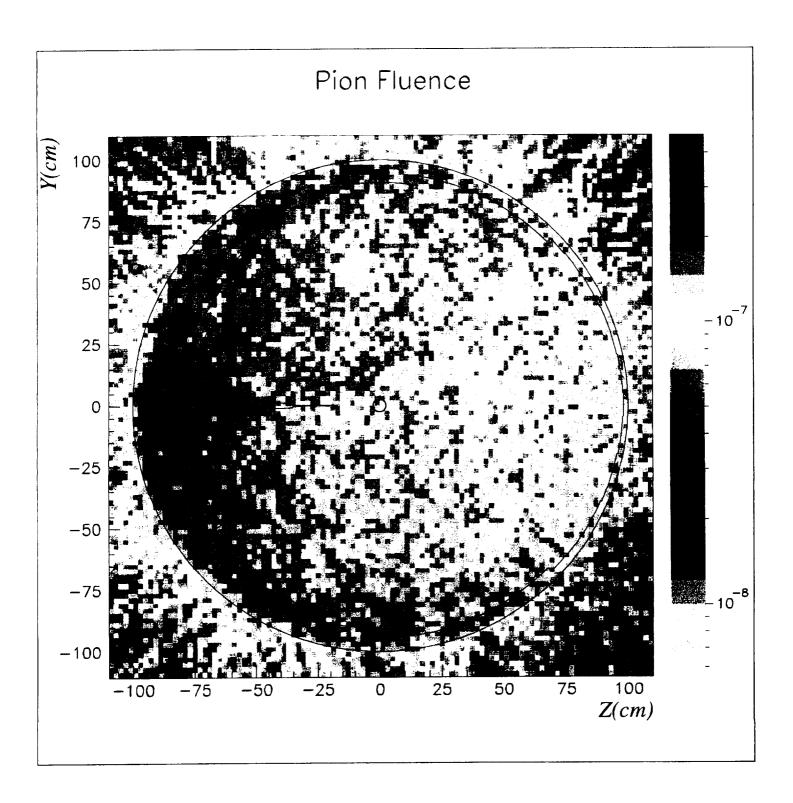


FIGURE 5





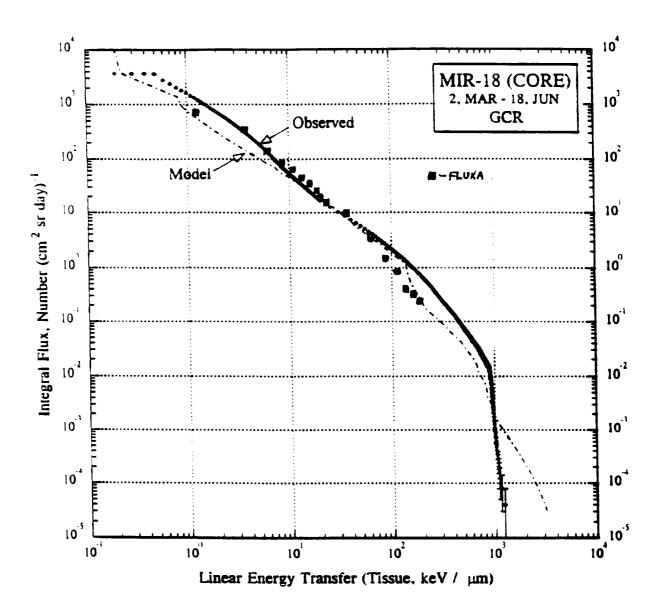


FIGURE 8

