MONTE CARLO METHODS IN MATERIALS SCIENCE
BASED ON FLUKA AND ROOT

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Introduction

A comprehensive understanding of mitigation measures for space radiation protection necessarily involves the relevant fields of nuclear physics and particle transport modeling. One method of modeling the interaction of radiation traversing matter is Monte Carlo analysis, a subject that has been evolving since the very advent of nuclear reactors and particle accelerators in experimental physics. Countermeasures for radiation protection from neutrons near nuclear reactors, for example, were an early application and Monte Carlo methods[1-8] were quickly adapted to this general field of investigation.

The project discussed here is concerned with taking the latest tools and technology in Monte Carlo analysis and adapting them to space applications such as radiation shielding design for spacecraft, as well as investigating how next-generation Monte Carlos can complement the existing analytical methods[9] currently used by NASA. We have chosen to employ the Monte Carlo program known as FLUKA[10-11] (A legacy acronym based on the German for FLUctuating KAscade) used to simulate all of the particle transport, and the CERN developed graphical-interface object-oriented analysis software called ROOT.[12-13] One aspect of space radiation analysis for which the Monte Carlo's are particularly suited is the study of secondary radiation produced as albedoes[14] in the vicinity of the structural geometry involved.

This broad goal of simulating space radiation transport through the relevant materials employing the FLUKA code necessarily requires the addition of the capability to simulate all heavy-ion interactions from 10 MeV/A up to the highest conceivable energies. For all energies above 3 GeV/A the Dual Parton Model[15-16] (DPM) is currently used, although the possible improvement of the DPMJET event generator for energies 3-30 GeV/A is being considered. One of the major tasks still facing us is the provision for heavy ion interactions below 3 GeV/A. The ROOT interface is being developed in conjunction with the CERN ALICE (A Large Ion Collisions Experiment) software team through an adaptation of their existing AliROOT (ALICE Using ROOT) architecture. In order to check our progress against actual data, we have chosen to simulate the ATIC[14] (Advanced Thin Ionization Calorimeter) cosmic-ray astrophysics balloon payload as well as neutron fluences in the Mir spacecraft[17]. This paper contains a summary of status of this project, and a roadmap to its successful completion.

A Comparison of Monte-Carlo-based Codes

Since the 1960's many different radiation transport simulation codes[1-8] have been developed. Such diversity is a result of the wide variety of applications for which these codes are employed. Software strategies derive from both *analytic* methods[9] and *Monte-Carlo* methods[1-8,10-20]. Uses range from the estimation by NASA of flight crew radiation doses[17-22] and the related problem in cancer treatment

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of determining a delivered therapeutic radiation dose, to the evaluation of data in accelerator-based elementary particle physics experiments[1-2,4,8,11-16] and even extending to the design of instruments for use in cosmic-ray astrophysics[14]. The Monte Carlo method is adopted here, having become widely used in the field of experimental particle physics because it represents the best approach to include the widest range of physics and the greatest sensitivity to geometry.

The present project has as its goal the development of a new integrated Monte-Carlo software package specifically tailored for use in the simulation of the space radiation environment. It is intended to address design problems, astronaut dosimetry calculations, and astrophysical payload development. A principal goal is to determine the applicability of such a Monte-Carlo-based computer simulation of the space radiation environment to NASA's Human Exploration and Development of Space (HEDS) enterprise. The new code is based upon the melding together of two existing software packages, the FLUKA, [1,2,4,10-11] radiation transport program and the object-oriented physics analysis infrastructure ROOT[12-13]. We have reported elsewhere[17-20] on preliminary results and only recent developments are discussed here. The acronym for this investigation is FLEUR (FLUKA Executing Under ROOT) with additional information at our websites. [23]

An older Monte Carlo code known as GEANT (GEometry and ANalysis Tool) is still in use. This code was frozen by CERN approximately one decade ago as GEANT3.21, and a new object-oriented version known as GEANT4 is under current development. A recent CERN benchmark comparison of GEANT4 against hadronic interaction data,[24] however, suggests that its progress will be slow. Nevertheless, the AliROOT software concept we discuss below is being developed with the intent to seamlessly imbed GEANT3, GEANT4, and FLUKA within its architecture – allowing the user to select the desired transport engine as these become available. At the present time, only FLUKA has been modified to do the full heavy ion transport in an integrated way, although hybrid strategies are being used elsewhere such as at the RHIC[25] (Relativistic Heavy Ion Collider) where GEANT3.21 has been used in conjunction with the HIJING[8] event generator for limited collider applications.

Ongoing FLUKA modifications
The FLUKA authors are committed to the development of a version of the code that includes the complete range of heavy-ion interactions that are needed to simulate the propagation of heavy cosmic rays. However, they presently require manpower assistance to facilitate that implementation in a timely fashion and they have agreed to allow us to provide such assistance. As a result of our support, FLUKA is now available with an embedded version of the heavy ion event generator known as DPMJET which is based on the Dual Parton Model.[15-16] Above 30 GeV/A and on up to air shower energies, we are satisfied that this version of FLUKA well represents the physics. However, the transition region between 3-30 GeV/A is still potentially subject to some improvement in terms of fits to existing data, and below 1-3 GeV/A there are currently no reasonably acceptable comprehensive models.

The current version of FLUKA, which provides a full simulation of heavy-ion inelastic collisions with lab energies above 3 GeV/A, will be further improved by either modifying the existing DPMJET software now present in FLUKA as Version II.5,[16] or the version of FLUKA containing DPMJET III.0 that is about to be released.[23] The simulation of collisions below 3 GeV/A is more problematic and will require considerable effort as part of the NASA Code U investigation of nuclear fragmentation and spallation physics at those energies during the next decade. We hope to participate as part of this future collaborative effort with other groups in the development of accurate models based upon a careful assessment of all of the existing data.[26-27]

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In the interim, in order to deal with the lower-energy heavy-ion interactions, we are currently exploring the accuracy with which the RQMD (Relativistic Quantum Molecular Dynamics) code[29] replicates the existing data down to the limit for inelastic nuclear collisions. If RQMD is deemed to do an acceptable job at these energies, then it will be incorporated into FLUKA in the same fashion as DPMJET has been. We have already determined that such an incorporation can be accomplished, although there are reservations about some of the neglect of nonlocal quantum mechanics used in RQMD's derivation and a lack of understanding of light-cone physics for relativistic Hamiltonians. In the event that RQMD is found to have unacceptable inaccuracies, our fall-back solution would be to extend the Pre-Equilibrium model called PEANUT, which is already employed internally by FLUKA to generate the interactions of singly-charged incident particles on nuclear targets. Both options (PEANUT and RQMD) will probably be made available to the user.

Beyond the physics enhancements needed for heavy ion transport, there has also been substantial progress in the development of 3-D geometry software technology since FLUKA was first designed. Driven by computer graphics developments and ray-tracing applications, many new 3-D geometry packages are now available. There is also considerable room for improvement in the user-friendliness of the procedures required to input geometry information into the existing FLUKA input formats. Going beyond such utility changes, one of the potential benefits that may be realized by incorporation of a totally new and different geometric representation includes an increase in the calculation speed during transport propagation simulations, along with the additional bonus of easy access to industry-standard input and graphic display formats. As described below, this task has the potential to take advantage of FLUKA's structure to facilitate such an implementation, once the optimum geometry package is identified.

The major reason FLUKA is not more widely used today is the relatively awkward nature of the present user interface to the code. To address these limitations, one major thrust of our present project is to meld FLUKA together with the recently released physics analysis infrastructure software known as ROOT. This task will require an intimate access to the FLUKA data structures as opposed to the grafting of one code to another as, for example, was required to incorporate the DPMJET code within FLUKA.

In the interim, while we are pursuing an integrated solution, we are supporting several enhancements to the existing software. In particular to aid with the FLUKA input geometry problem, we have been successful at designing a set of software assisted procedures for translating geometry inputs originally coded for use with the more widely used, but less accurate GEANT3.21 directly into FLUKA geometry inputs. This effort was undertaken because GEANT3.21 is so widely used, for example as it is by the RHIC experiments at BNL (Brookhaven National Laboratory).[25] It was felt that providing the utility of enabling previous GEANT studies to be converted into FLUKA analyses would be greatly appreciated. With this capability the rich heritage of GEANT3.21 research can now be run with FLUKA[14].

In order to facilitate this conversion capability, as well as to improve the native FLUKA geometry input constraints, we have also contributed to the enhancement of the logical operations that may be specified in the combinatorial geometry input format. While this effort may eventually become moot for our project if an entirely different geometry scheme is ultimately employed, such a change is most likely several years away, and in the interim, our contribution will have a substantial positive impact.

ROOT, A Data Analysis Infrastructure

ROOT is based upon Object-Oriented (OO) data structures, a utilization of OO programming that allows many difficult tasks with multiple functions to be done only once. For example, after the work of introducing the complex geometry of an object such as the International Space Station (ISS) is complete, that same information can be used seamlessly as the input for subsequent Monte Carlo calculations. The same data structure can also be applied to visualizations of individual Monte Carlo events in a fly-through 3-D event viewer (Figure 1a), or for choosing regions to provide plots of individual summed quantities of interest. It can be employed for analysis or display applications that need to specify or depict some portion of the geometry involved, or the entire structure. A strong feature of ROOT is that much of the manipulation is provided via GUI (Graphical User Interface) menus, displays, and simple editing features (Figure 1b). Furthermore, when special features need to be added, ROOT uses C++ as a scripting language. This implementation of the scripting language allows the user to create structures and functions that blend naturally into the ROOT architecture, while providing the user a customized extension of the system. In addition, an intelligent pre-processor completely solves the problem of persistency of objects in disk storage. ROOT features and examples can be viewed on the Web (http://root.cern.ch), and that site contains the downloadable software with accompanying tutorials.

Within C++, one is allowed to define transportable data structure objects called classes. One advantage of adopting ROOT is that the large and growing community of users is continually developing new classes. These are distributed in an open source model similar to that employed by the developers of the Linux operating system. This permits users to incorporate the new developments of others rapidly into their own customized codes. As different groups begin to utilize this software structure for space radiation simulation, it is anticipated that an exchange of well-documented libraries containing such additions will become commonplace.

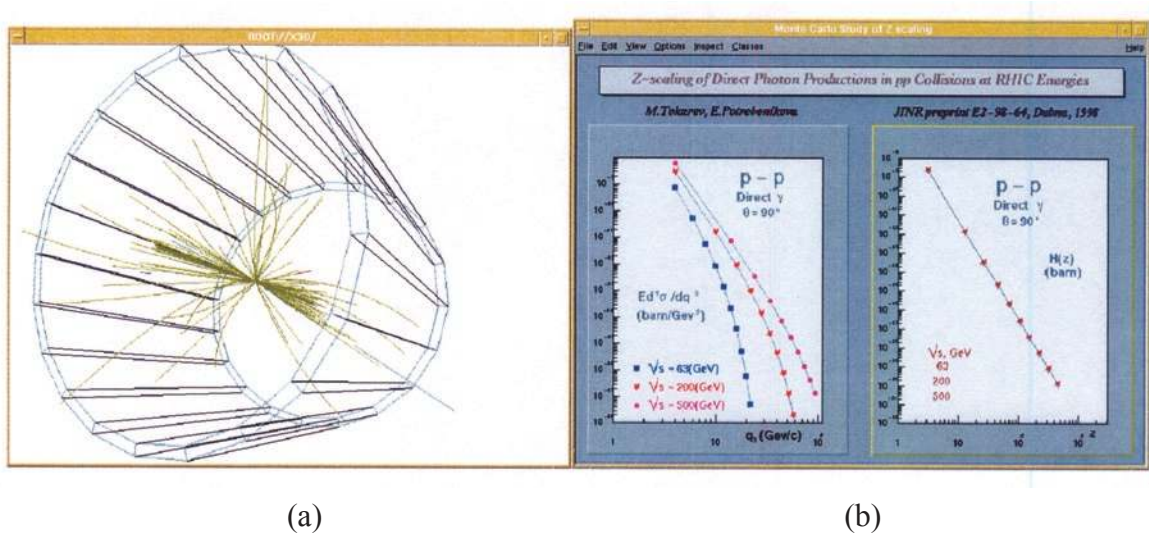(a)   (b)

Figure 1. (a) Example of a 3-D event viewer of ATLAS produced by a Monte Carlo simulation (FLUKA/ROOT) with full rotation and zoom capability using only a mouse. (b) Examples of log-log plotting and fitting of data in ROOT.

ROOT is a software package whose scope and capability is much more easily understood by example rather than be a textual description. The following section describes AliROOT (ALICE using ROOT), which is an example of an adaptation of ROOT to control and evaluate Monte Carlo simulations of the

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ALICE experiment at CERN. This existing code is serving as a starting point for the FLEUR space radiation simulation code.

AliROOT and the Virtual Monte Carlo Interface
Given ROOT's strengths as a data analysis infrastructure, it is natural to consider developing a general Monte Carlo radiation transport interface. One can break down the general problem of simulating the transport of radiation through a complex geometry into six basic steps:

a) Inputting the geometry including the specification of the material elemental composition of each sub-volume;
b) Inputting the incident flux form;
c) Setting up the desired scoring;
d) Initializing the transport code as required for the materials and options to be used;
e) Specifying the number of incident particles to be included in the run;
f) Executing an event transport cycle for each incident particle during which the specified scoring is done as required.

The information needed by the last cycle, the transport cycle, from the earlier input steps is typically included in one or more files. ROOT is ideally designed to allow the construction of GUI-based tools to accomplish these steps. AliROOT has introduced the concept of a VIRtual Monte Carlo Interface, and it
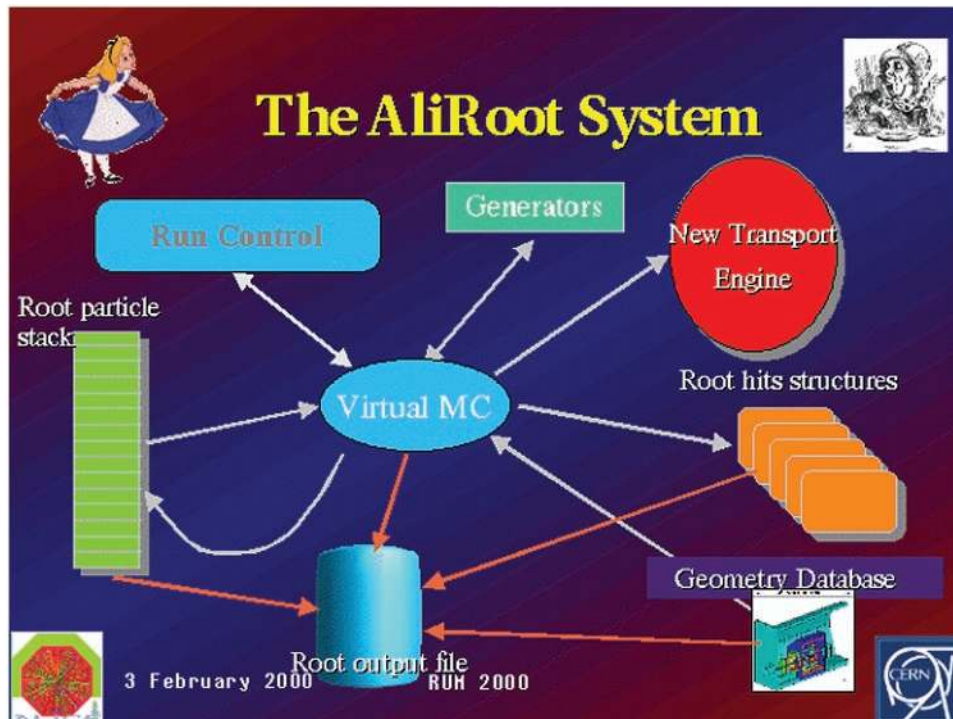

Figure 2. Functional schematic of the ALIROOT architecture.

is in the last step that the features of VIRMCI come into play (Figure 2). During the transport process, as particles move from one sub-volume to another, interactions are determined by reference to known cross-sections appropriate for the composition of each sub-volume. When secondary particles are produced in these interactions, they are pushed onto a stack for subsequent transport after the original incident primary is followed to its eventual end. In each sub-volume, any desired scoring can be done. As an example, the

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total energy deposited in that sub-volume by the current particle can be calculated and added to the output data bin for that sub-volume.

The VIRMCI requires that the transport code have the ability to break out at each point where scoring needs to be accomplished to allow that it be done in ROOT data structures. This process can be facilitated if the core data structures of the transport program itself can be mapped directly into ROOT. In the case where the Monte Carlo code is written in FORTRAN, as is FLUKA, utilities exist to enable the direct conversion of FORTRAN common blocks into C++ classes. This means a great saving in execution speed because the internal Monte Carlo values do not have to be passed back to the ROOT-based routines as arguments. Rather, the ROOT-based code will have direct access to any of the transport code's data structures for use in scoring. Thus, one can employ the FLUKA transport code to simulate the physics, and use ROOT-based code to set up the needed FLUKA input files as well as to score the parameters of interest during the simulation. The additional benefit is that the scored events can be examined in ROOT in real-time during the execution of the simulation and the power of ROOT is available to conduct any desired analysis.

In FLUKA, it turns out that the geometry is also dealt with in a sufficiently modular way that it can be broken out and analyzed externally to do the physics calculations. This is because at each spatial step, FLUKA enters a specific set of routines that simply advise the physics calculations what material the present sub-volume is composed of and how far the current particle can go in that sub-volume, given its direction of travel, before its trajectory intersects a boundary of that sub-volume. This allows one to potentially substitute an external geometry package for the internally provided FLUKA geometry package. Currently, such substitute packages exist that allow FLUKA to be run using GEANT4 geometry files internally for these distance calculations. Since translators exist to convert GEANT3.21 geometry into GEANT4 geometry, one can already effectively choose to run FLUKA with any of these geometries. ALIROOT takes advantage of these capabilities, and we hope to be able to explore the possibility of additional geometry packages optimized for particle transport to increase the execution speed of the code. In combination with the GEANT3.21-to-FLUKA converter mentioned earlier, there exist several techniques for translating the geometry databases into the Virtual Monte Carlo shown in Figure 2.

In the current version of AliROOT, the major effort is directed at the creation of generic scoring capabilities. Little attention has gone into input interfacing. Typically, one still edits the original input file with a text editor and then specifies that file through a ROOT macro. Our intention is to add the capability to edit the contents of the required input files directly from ROOT GUI menus and dialogue boxes. This will free the user from having to learn the input file syntax, and can insure that mutually conflicting choices are protected against.

Although not strictly part of the Monte Carlo codes themselves, analysis and display of the data are another strong attribute of AliROOT. Event displays can plot depictions of the trajectories superimposed on the geometry. Full 3-D images can be zoomed, rotated, and edited (Figure 1a), allowing for strong visual analysis tools. Conventional histogramming where the plotted events can be subjected to any number of filters is also routinely possible. These and other tools are a natural consequence for AliROOT and are planned for FLEUR.

Status of the Current Project Including Recent Testing, and Validation

We have made substantial progress in the forging of the final simulation tool to be produced for NASA. The incorporation of the highest energy nucleus-nucleus interactions within FLUKA has been accomplished and interim solutions at the lowest energies are being actively worked on. We anticipate having a version of FLUKA that includes a first attempt at such an interim solution by the end of the current calendar year. The more general problem of providing an event generator to simulate interactions for all heavy ions of interest in the cosmic-ray flux is formidable. The very fact that NASA has embarked on an associated program to take the experimental measurements necessary for modeling heavy-ion transport and nuclear fragmentation below 1 GeV/A energies is indicative of the importance of addressing this problem. The timeframe for this ambitious project is ~10 years. While the use of an interim solution is not perfect, it will allow us to begin exploring the possibilities with the available resolution and based on the currently available data. As the long-term NASA project unfolds, such improvements will be introduced into future releases of our FLEUR software.

Our efforts to begin to provide ROOT-based tools to support interacting with FLUKA is also actively proceeding, although full-fledged incorporation of a version of FLUKA within AliROOT is still some distance away. In the interim, ROOT input aids will be made available and ROOT analysis tools will be provided as well.

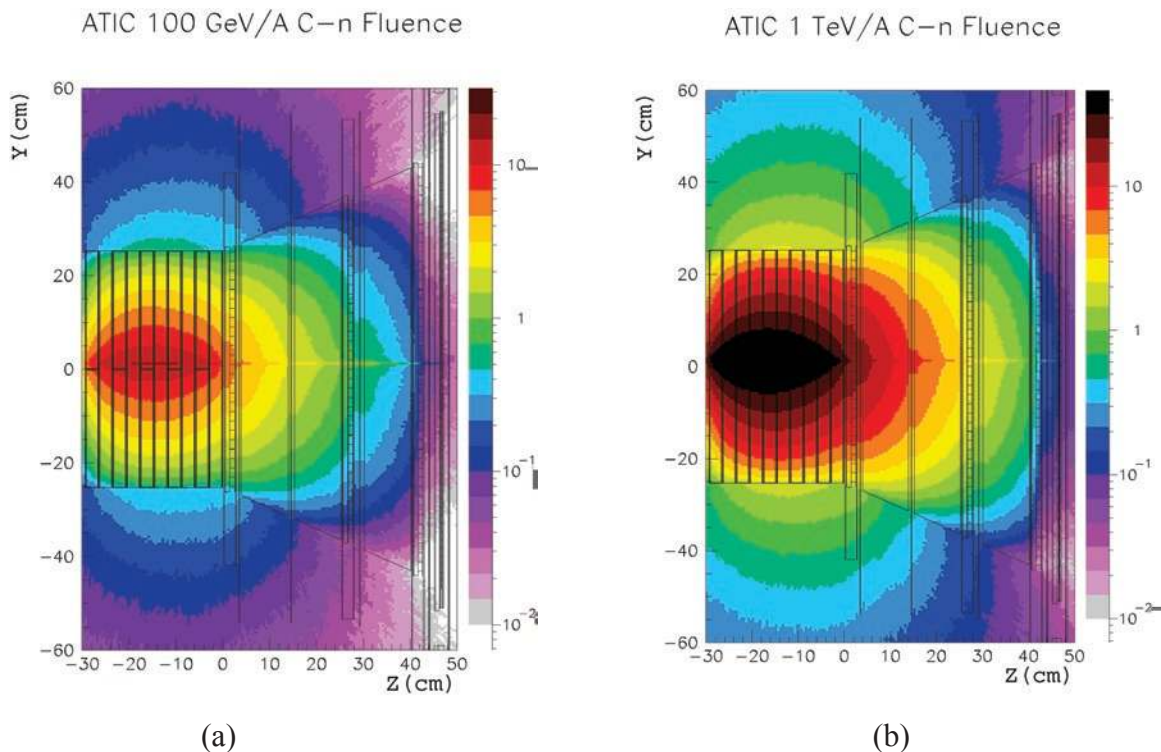(a)   (b)

Figure 3. Color plots of neutron fluences due to (a) 100 GeV/A and (b) 1 TeV/A incident carbon in the ATIC experiment as calculated with FLUKA/DPMJET II.5.

In order to validate the present version of FLUKA incorporating the DPMJET code, in order to begin testing the products we have produced we have chosen to perform simulations of the ATIC experiment, a cosmic-ray astrophysics collaboration under the lead of Louisiana State University's Department of Physics and Astronomy.[14] ATIC is a balloon-borne instrument designed to look at the cosmic-ray

composition in the 100 GeV/A to 10 TeV/A range. It consists of a telescope of silicon strip detectors on top of a set of carbon interaction targets followed by a BGO (Bismuth-Germanium-Oxygen, $Bi_4Ge_3O_{12}$) calorimeter, with triggering scintillators interspersed at various points. The experiment was flown near the top of the atmosphere for an extended time in Antarctica during January 2001. Our interest is in determining if FLUKA with DPMJET is sufficient to simulate the actual flight data accurately, and to develop in the process some of the initial ROOT-based analysis tools that will become part of the eventual final package.

As an example of this simulation testing, Figure 3 displays a fluence plot of some of the FLUKA results for a study of the neutron backscatter albedo within ATIC. [14] It represents the total neutron fluence through a raster of pixels due to 1000 simulated 100 GeV/A carbon nuclei normally incident along the central axis of the experiment, and 1600 similar events at 1 TeV/A. An outline of the ATIC hardware geometry is superimposed on the plot. The color-coded levels are logarithmic and represent 6 levels per decade. Fluence is the net flux (time integral of flux) and is expressed as the total path-length density of neutrons
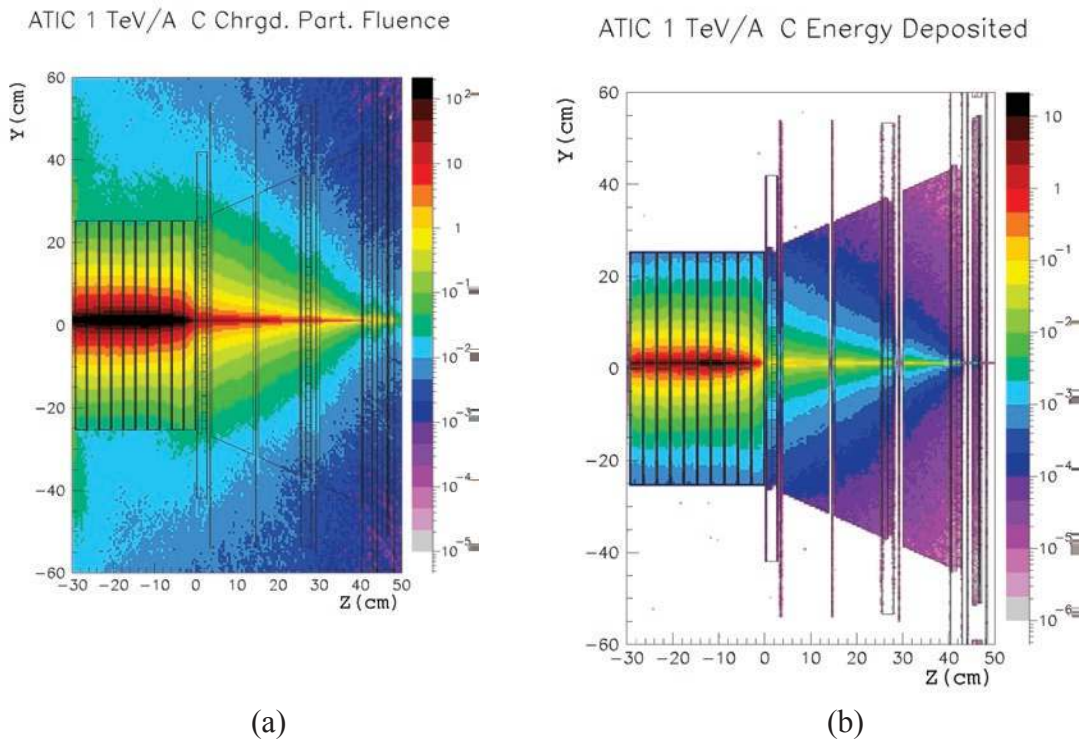

Figure 4. Color plots of (a) charged particle fluences and (b) energy deposited for 1 TeV/A incident carbon in the ATIC experiment as calculated with FLUKA/DPMJET II.5.

of all energies through each pixel. One can use this plot to evaluate the possibility for neutron backscatter contamination in the entire detector from events of this type. Such contamination represents a potential background that must be accounted for in the design of the instrument and it may affect triggering schemes as well as the interpretation of certain data. Additional FLUKA plots from the ATIC study are shown in Figure 4.

As another illustration of the utility of Monte Carlo methods, Figure 5 depicts results from our study already published. [17] These early studies utilized FLUKA for the purpose of producing radiation dosimetry

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fluences in a phantom model of the Russian MIR spacecraft. The MIR was represented by a surrounding cylinder of variable thickness, and the shielding was defined as a probability of equivalent thickness of aluminum (an "Al-equivalent") as seen from the location of NASA, Johnson Space Center's TEPC, or Tissue Equivalent Proportional Counter. [21-22]

Conclusions

With the advent of new information technology, the tools available for space radiation analysis have shown remarkable improvement. For Monte Carlo methods in particular, what once may have taken weeks to calculate on a large mainframe computer can now be accomplished overnight on an office desktop. The utility of Monte-Carlo-derived fluences illustrated in Figures 3 and 4 becomes evident when one asks the mitigation question: Where is the safe haven from space radiation? In Figure 5, the neutral particles (Figure 5a are neutrons), and the charged particles (5b) are mirror images; if you move to get away from the charged particles then you are bathed by neutrons. Therefore, heavy shielding such as aluminum is not necessarily the answer. Of course, this observation has been known for some time using analytical methods. But the graphics helps us see it. Indeed, the challenge for materials science to come up with materials that will allow the most efficient shielding configurations is a formidable one.

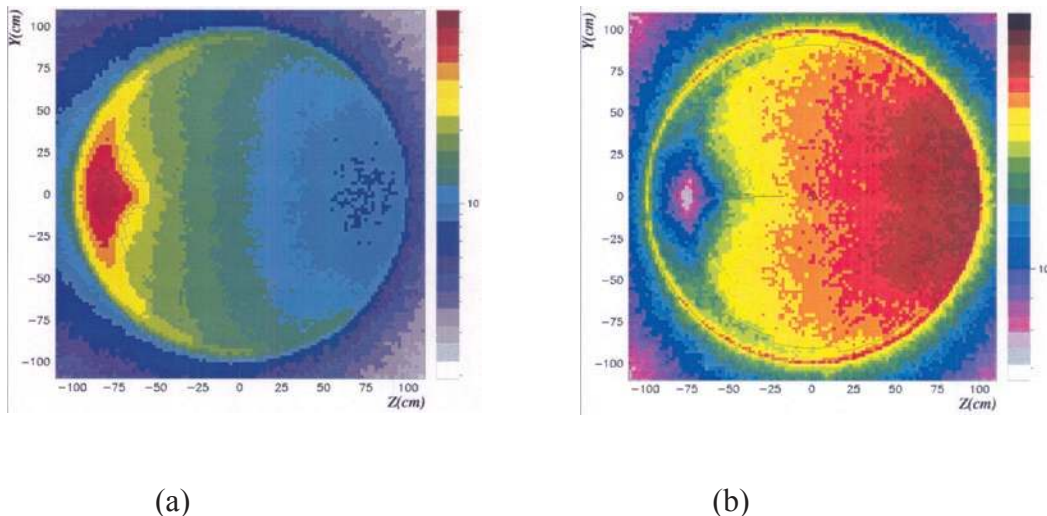(a)   (b)

Figure 5. Radiation fluences within and about an Aluminum-equivalent shielding model of the Mir spacecraft, as simulated (in color) by FLUKA and ROOT. (a) On the left is the neutron fluence, and (b) on the right is the charged particle fluence [Ref. 17].

The FLEUR collaboration will continue to adapt the tool of choice in high-energy physics, the Monte Carlo method, to space radiation analysis as our understanding of nuclear fragmentation evolves. In the process, we hope to contribute to the development of mitigation measures for particle radiation by providing a rigorous simulation of all of the relevant physics processes in a full detailed 3-D geometric simulation. As an example, a 10^{15} eV hydrogen ion at the "knee" in the cosmic-ray spectrum is rare (1 event/m^2/ster/year), but for the area of the ISS (>365 m^2) these events are happening every day. It is not just the primary, incident particle that poses a hazard but also the hadronic cascade with its shower of generations of lower-energy secondary particles that precipitate. The high-energy accelerators such as Fermilab and CERN deal with this subject daily, and we hope to bring their tools into the arena of space exploration as these are being developed.

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