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Using Pre-Computed Kernels to Accelerate Effects Calculations for AE9/AP9: A Displacement Damage Example

August 20, 2013

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Space Science Applications Laboratory
Physical Sciences Laboratories

Prepared for:

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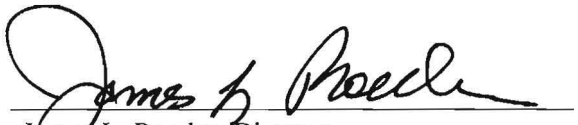

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Abstract

The AE9/AP9 trapped radiation climatology models represent model uncertainty by means of multiple static and dynamic environments that represent the statistical uncertainty in the models themselves and the temporal dynamics of the radiation environment. Radiation effects codes are used, in turn, to compute effects on parts and materials from AE9/AP9 particle fluxes. Many radiation effects codes cannot be run easily for the multiple cases provided by AE9/AP9, much less for the dynamic scenarios. It is desirable, therefore, to reformulate some of the slowest calculations in such a way that the part of the calculation that is generic, regardless of the input flux, is pre-computed and stored, so that only the final convolution of this effects "kernel" must be calculated for each case provided by AE9/AP9. We explore this technique in the context of a full-physics calculation of displacement damage in an idealized spherical aluminum shielding geometry with a silicon target. We show that the kernel approach can be used to obtain accuracy comparable to the full calculation with much shorter calculation times once the kernel is generated.

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1. Introduction

Whereas previous space radiation environment models, such as AP8 [Sawyer and Vette, 1976] and IGE-2006 [Sicard-Piet et al., 2008] attempted to provide individual spectra either for different conditions or for different safety levels, the AE9/AP9 [Ginet et al., 2013] models address model uncertainty and dynamics through Monte Carlo variation. Specifically, the AE9/AP9 model paradigm is to run the satellite orbit through the model 40 or more times, either through static environments representing possible values of the mean, or through dynamic environments that incorporate both uncertainty in the model and uncertainty in the dynamic series of events the spacecraft will actually see. One is then supposed to compute confidence values from these 40+ cases. The quick-and-dirty approach is to compute the desired confidence value (e.g., the 95th percentile) and feed that into the effects calculation of interest (e.g., dose vs depth). Statistically speaking, this approach is incorrect because the effects code combines data from different energies, and thus the percentiles must be computed after the effects code is run for each of the 40 cases. Thus, it becomes necessary to run an effects code many times.

Effects codes, such as ShielDose2 [Seltzer, 1994], are not built to run easily in batch mode over many cases. Some more elaborate calculations, such as a MULASSIS [Lei et al., 2002] displacement damage calculation, are so time consuming that one would not want to run them 40+ times. For those cases where the effect being computed is a linear function of the input flux spectrum, one can precompute a "kernel" that transforms the input spectrum to the desired output, such as ionizing dose or displacement damage vs depth of shielding. A kernel is simply a matrix, as large as the list of energies by the list of depths. The kernel is a discrete representation of the Green's function, or impulse response, of the effects code to input flux. This is, in fact, how many effects codes operate: they are kernels derived from a full physics simulation. However, in most cases, the kernel is not exposed to the user to exploit as such.

Calculating the kernel can itself be computationally intensive. Therefore, it is most beneficial when the problem is vey generic; e.g., displacement damage on a silicon target behind varying depths of spherical aluminum shields.

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2. Mathematical Representation of the Kernel

Many radiation effects are linear in the input flux or fluence (time-integrated flux). They can thus be described in terms of a convolution integral:

$$D(d) = \int_0^\infty S(E,d)\, j(E) dE \tag{1}$$

Damage *D* at depth *d* is given by the convolution of a transfer function *S* and the particle flux (or fluence) *j* over all energies *E*. In this case, *S* is the Green's function or impulse response function because

$$S(E,d) = \int_0^\infty S(E',d)\, \delta(E,E') dE'. \tag{2}$$

Although our example assumes damage versus depth, if one probes an arbitrary effects calculation with a sequence of delta functions (mono-energetic input flux), one can derive the corresponding *S*.

Since integration is itself a linear operation, it is possible to discretize the integral to convert Eq. (1) to a matrix-vector operation:

$$\vec{D} = \underline{\underline{K}}\vec{j} \tag{3}$$

where

$$D_i = D(d_i) \tag{4}$$

$$j_k = j(E_k) \tag{5}$$

$$K_{ik} = S(E_k, d_i)\Delta E_k, \tag{6}$$

and ΔE_k represents the weight from a numerical integration technique (e.g., ΔE_k can simply be $(E_{k+1} - E_{k-1})/2$). The matrix $\underline{\underline{K}}$ is the kernel.

With the kernel $\underline{\underline{K}}$ in hand, it is necessary only to store it to disk along with the list of energy and depth grid points. One can then interpolate any new spectrum onto the kernel's energy grid, multiply by $\underline{\underline{K}}$, and, if necessary, interpolate that result onto the user's depth grid. In fact, these interpolation procedures can themselves be performed in a linear formulation so that $\underline{\underline{K}}$ can be easily recast onto any other desired grid. It is often the case, however, that one wishes to use a non-linear interpolation (e.g., log-log), in which case that should be done before and after utilizing the pre-computed $\underline{\underline{K}}$.

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3. Example: A Displacement Damage Kernel

Displacement damage is an effect most often encountered with photovoltaic, photosensitive, or optical components of spacecraft. It arises from the displacement of nuclei of solid-state or optical materials (e.g., the focal plane of a star tracker). Protons are by far more effective at displacing nuclei, but electrons can do it, also.

For the purposes of this demonstration, we will focus on the displacement damage effects of protons on a silicon target inside spherical aluminum shields of varying thickness. To compute the damage, we will use MULASSIS, which is itself a wrapper for GEANT4 [Agostinelli et al., 2003]. GEANT4 manages the physics of individual protons traversing the aluminum shields and interacting with the silicon target. MULASSIS handles the launching of particles and tabulates the resulting energy deposit. MULASSIS provides options for defining shielding material and geometry, target material, and the input species and spectrum. In our case, the input species is protons and the spectrum is a monoenergetic beam.

3.1 MULASSIS Runs

We ran MULASSIS as described in TOR-2013(3906)-52 [Kwan and O'Brien., 2013] for the following proton energies: 0.1, 0.2, 0.4, 0.6, 0.8, 1, 2, 4, 6, 8, 10, 15, 20, 30, 50, 60, 80, 100, 150, 200, 300, 400, 700, 1200, and 2000 MeV. This list is based on the energy channels used by AP8 and AP9.

For each of the energies, we ran MULASSIS for spherical aluminum shielding of 1 to 10,000 mils in thickness, logarithmically spaced with 10 depths per decade, as in: 1, 1.26, 1.58, …10,000. mils.

The spherical target volume of silicon had a radius equal to 0.1 of the shielding thickness. We ran one million protons for each energy and shielding thickness combination. It took 2 to 3 weeks to run all the energies and thicknesses.

3.2 Conversion to a Kernel

After the extensive MULASSIS runs, we realized that we had not, in fact, sampled the energy grid in enough detail. Therefore, we had to perform some fitting and interpolation to generate a kernel suitable for use in a numerical integral like Eq. (3).

The MULASSIS calculation did not yield any response at depths of 1 mil Al or more for protons with less than 2 MeV incident energy. One convention in the displacement damage field is to convert displacement damage dose to equivalent 1 MeV neutrons, and we have adopted that convention here. From 2 to 400 MeV, we fit the equivalent neutron fluence $J^{(n)}$ as a function of depth d at each incident energy to a function of the form:

$$J^{(n)}(d) = \begin{cases} 0 & d < d_0 \\ a + b\exp(d - d_0)/L & d > d_0 \end{cases} \quad (7)$$

The parameters a, b, d_0, and L are determined separately for each energy. We note that d_0 is approximately the range in aluminum of a proton with the specified incident energy. Above 400 MeV, we simply used the mean value of $J^{(n)}$ since the response is flat across all depths for incident particles above 400 MeV. Figure 1 shows the calculations and the resulting fits.

We then interpolated the fit parameters onto a fine energy grid with 300 points logarithmically spaced from 2 to 2000 MeV. We then evaluated the parameters on the original depth grid to obtain $J^{(n)}(E,d)$, the equivalent 1 MeV neutron fluence for a given incident proton energy and intensity of 1 proton/cm^2/MeV. The kernel is then given by:

$$K_{ik} = J^{(n)}(E_k, d_i)\Delta E_k \quad (8)$$

We selected ΔE_k based on the logarithmic grid spacing as:

$$\Delta E_k = \begin{cases} \sqrt{E_{k+1}E_k} - E_k & k = 1 \\ \sqrt{E_{k+1}E_k} - \sqrt{E_k E_{k-1}} & 1 < k < 300. \\ E_k - \sqrt{E_k E_{k-1}} & k = 300 \end{cases} \quad (9)$$

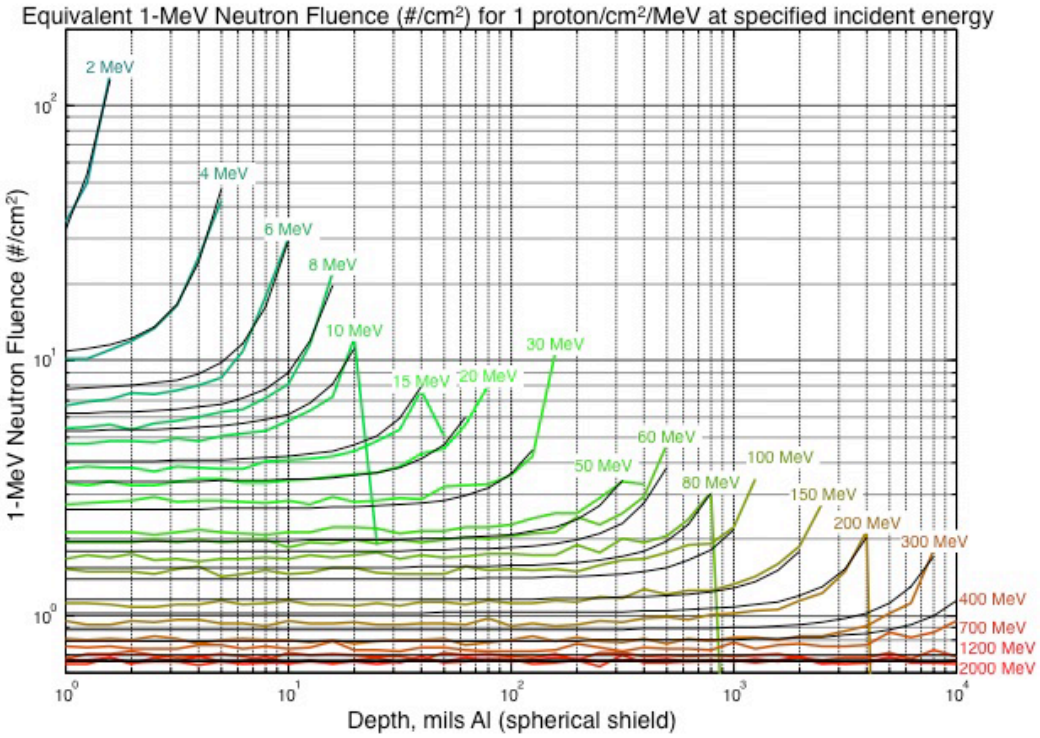

Figure 1. Calculated (color) and fitted (black) impulse response: equivalent 1 MeV neutron fluence to monoenergetic protons.

3.3 Validation

To validate our kernel calculation, we compare to a full MULASSIS run with an input proton spectrum appropriate to a long mission geostationary orbit (see TOR-2013(3906)-52). MULASSIS can be run with a spectrum instead of a monoenergetic beam, and we have used that capability to generate four examples of the "Slow" calculation. We used the same four input spectra to perform the equivalent calculation using the kernel described in Subsection 3.2. We used nonlinear (log-log) interpolation to put the input spectrum onto the kernel grid.

Figure 2 shows the comparison of the two calculations. As expected, the full MULASSIS calculation extends to slightly lower depths (due to the limitations of our kernel pre-calculation). Somewhat unexpected is the fact that the statistical noise in the full MULASSIS calculation (e.g., the spike at 40 mils depth in the black 95th percentile curve) is smoothed out in the kernel calculation (red). This smoother result arises because we ran more test particles per unit energy when generating the kernel.

The calculation using the "slow" method was 4 h. The calculation time for the "quick" method, using the kernel, is a fraction of a second on a modern computer. Of course, this speed-up is only achievable because we could invest 2−3 weeks pre-computing the kernel. The kernel can, however, be applied to any new input proton spectrum, at a cost of less than a second of additional computing time, so long as the shielding geometry is spherical aluminum and the target is silicon.

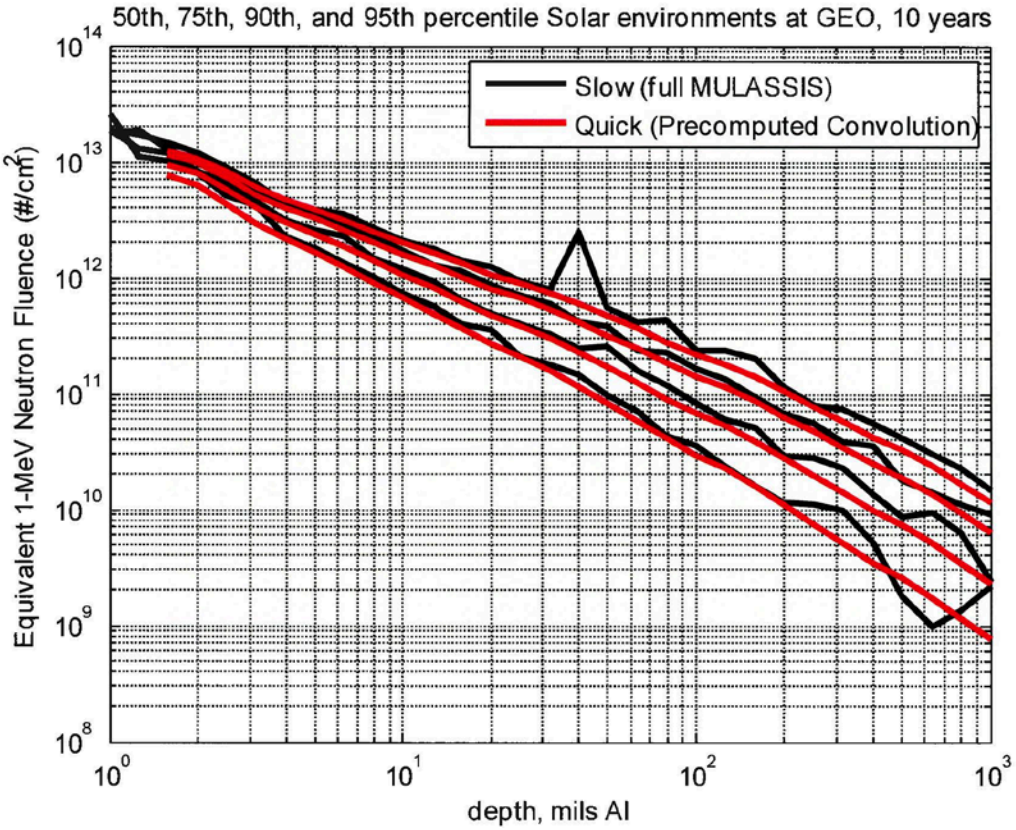

Figure 2. Comparison of full MULASSIS calculation and pre-computed kernel calculation for 4 percentiles of the solar proton environment at geostationary orbit.

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4. Summary

We have described a method for speeding up effects calculations in the new paradigm of multiple cases provided by the AE9/AP9 trapped radiation models. This technique involves representing a linear radiation effect as a linear operator (matrix) derived from the impulse response (or Green's function) of the full physics effect calculation. We have demonstrated this "kernel" approach using displacement damage computed from the MULASSIS code. The kernel approach can reproduce the longer calculation, and more quickly, once the pre-computation is done. The need for pre-computation means that the kernel approach is likely limited to the most generic cases of shielding geometry target material, or target part. However, such generic cases are often the starting point for radiation analysis and satellite system design.

The kernel approach can be applied to any effect that is linear in the incident particle spectrum. Such effects include total ionizing dose, displacement damage, single-event effects, and some kinds of sensor noise and backgrounds. If the definition of a kernel is abstracted into a standard or conventional file format, then it would be possible to develop a library of such kernels for use with radiation environment and effects modeling software such as ESA's widely-used SPENVIS [Kruglanski et al., 2009].

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