The Application of MCNP6.2 Unstructured Mesh Geometry Capabilities to the Study of Heavy Ion Single Event Effect on Microelectronic Devices and the Reactor Physics Analysis

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Unstructured meshes allow irregular or complex geometries to be modeled precisely in Monte Carlo radiation transport codes. Through this capability, it is possible to share an unstructured mesh model between multiple codes that use unstructured mesh geometry and thus improving coupled multi-physics simulations. In this work, unstructured meshes are used to model energy deposition from heavy ion strikes for single event effects on microelectronic devices as well as neutron flux mapping of nuclear reactor configurations. In each case, MCNP6.2’s unstructured mesh functionality and applicability to the problem is demonstrated and analyzed.

I. INTRODUCTION

Unstructured meshes are used in a wide variety of codes and become especially important for many deterministic solvers using finite element methods. For these codes, mesh construction is critical for convergence to the solution. Both a properly shaped and adequately refined mesh is required for convergence or even for a simulation to complete. For Monte Carlo codes such as MCNP, the mesh (structured or unstructured) is used for tracking in order to tally spatial quantities. Therefore the mesh must be refined enough for the necessary spatial resolution, while features such as element types are less critical. Since Monte Carlo does not have strict mesh requirements, it can fundamentally accept any more highly constrained mesh utilized by a deterministic solver. Thus for coupled simulations, such as in multi-physics frameworks, a single mesh could be shared between different solvers. This allows high fidelity Monte Carlo results in areas such as particle transport to be coupled with a deterministic solver while eliminating data interpolation errors. This becomes increasingly important in cases where many codes are coupled or solving requires iterative data transfers between codes.

Unstructured mesh capabilities have been added to MCNP, making it more powerful for coupled simulations with other codes. This work studies MCNP6.2 unstructured mesh functionality for both heavy ion transport and reactor physics applications. Heavy ion transport is done in the context of space applications for microelectronic power devices. The reactor physics analysis considers neutron flux and criticality for a low power reactor critical facility.

I.A. MCNP6.2 Unstructured Meshes

Unstructured meshes were first introduced to MCNP in version 6.1.1 and were expanded to include heavy ions in MCNP6.2. This feature allows MCNP to use models and meshes created by the CAD program Abaqus to define the problem geometry and mesh. Unstructured meshes will contain elements of different size and shape, such as first- and second-order hexahedral and tetrahedral shapes in order to closely fit the geometry. Doing so permits complex or irregular geometry to be meshed comprehensively without the use of excess elements. Using unstructured meshes invokes a special set of routines that track particles across element boundaries in order to accomplish tallies similar to those of structured meshes¹. Unstructured meshes follow the same basic tally types used by the standard MCNP mesh tally FMESH, but have somewhat different statistical properties and thus are called elemental edits instead of tallies.

I.B. Single Event Effects

High radiation environments, such as space, pose a serious threat to SiC-based power devices². As devices are continuously downsized and run at higher powers and voltages, the risk of radiation induced failures becomes even greater. Space is full of energetic heavy ions which can induce significant amounts of ionization in a device leading to numerous effects. The reactions occurring from a single ion strike on a device are known as single event effects (SEEs), the most serious of these being a burnout (SEB). SEBs occur when the ion strike causes enough ionization to create runaway electro-thermal heating which results in the device burnout. Heating occurs due to the excess electrons and holes (positively charged vacant electron sites) flowing to the oppositely charged regions of the device and inducing excess current. The chances for SEB increase with incident ion linear energy transfer (LET) and the device’s operating voltage².

SEEs are generally modeled using the rudimentary heavy ion modules within electro-thermal simulators. Electro-thermal simulators are finite element based and thus require unstructured meshes to operate. MCNP6.2 offers a high fidelity transport based model for the heavy ion and electron interactions occurring from an ion strike.
Thus it is desirable to utilize a code such as MCNP6.2 for the radiation portion of the simulations. Doing so requires addressing many challenges in data compatibility and particularly working between Monte Carlo and finite element models operating on different meshes. By utilizing an unstructured mesh based Monte Carlo simulator, it is possible to circumvent the dilemma of different models34.

I.C. Reactor Physics Modeling

As with SEEs, reactor systems are strongly coupled multi-physics systems. Current codes for analyzing advanced reactor systems such as BISON for fuel performance5 and Nek5000 for thermal hydraulics6 both rely on finite element methods. By using finite elements, all these codes require unstructured meshes to operate on the intricate geometries of a reactor system. To complete the multi-physics framework, these codes need to be combined with a reactor physics code, such as PROTEUS7 or MCNP6.2. With the unstructured mesh feature of MCNP6.2, it is possible to maintain spatial consistency with the finite element codes in a coupled multi-physics analysis. This is also highly needed in a recent development effort for the DOE NEAMS integration product line program8. In this work, neutron flux mapping over unstructured mesh geometry for a cluster of fuel pins is demonstrated using the unstructured mesh feature.

II. HEAVY ION AND DELTA RAY PHYSICS

Heavy ions are dangerous to electronic devices due to the high level of ionization they induce. This is due to the Coulomb interactions between strongly positive incident ion and the orbital electrons in the host material. At higher energies (at least tens of MeV/amu), the incident ion so energetic and ionized that it will pass through the host material while transferring its energy through inelastic collisions with orbital electrons9. The electrons stripped from their orbits are themselves energetic enough to cause further ionization and are known as delta rays. This interaction is highly probable and will occur along the entire ion track. Although by the end of the ion track, any secondary electrons produced will be too low energy to be considered delta rays.

Once the ion loses enough energy to delta ray generation, it will begin to pick up electrons and become less ionized. As electrons are accumulated, the ion’s LET will increase up until a Bragg peak is reached. The LET increases because as the ion energy and charge decrease, its reaction probability increases. It gradually becomes incapable of zipping through a material leaving free electrons in its wake. The Bragg peak is the inflection point for the previously increasing LET. Upon reaching the peak, nearly all of the ion’s energy has been deposited and therefore its LET will drop sharply. After the Bragg peak, the ion has minimal charge and penetrative ability and will promptly come to rest after a short straggling distance. Straggling refers to the statistical variation in the final portion of the distance the ion will travel. While a small variation, each ion will ultimately reach a slightly different range. During this time, the ion energy is low enough that it will undergo elastic collisions with host nuclei instead of the inelastic collisions with electrons as before. These elastic interactions are capable of creating secondary heavy ions from host material atoms9.

II.A. Heavy Ion Transport

To model heavy ion transport and energy loss, MCNP6.2 uses a continuous slowing down approximation (CSDA). Using CSDA breaks the ion’s energy loss into energy steps which are then further divided into substeps10. Realistically the ion would constantly be interacted upon by Coulomb forces, but this becomes very computationally intensive to model especially across a large energy range. Instead steps are used to discretize the energy loss. Energy steps are based on a percentage loss of the particle’s current kinetic energy at each step while substeps are the number of steps taken within each energy step. The more substeps used, the closer the model is to being continuous and thus is more realistic.

Heavy ion interactions in MCNP6.2 are modeled with the low energy SPAR model (up to 1.31 MeV/amu) and the Bethe-Bloch formula for higher energies (above 5.24 MeV/amu). For energies between 1.31 MeV/amu and 5.24 MeV/amu, the results are interpolated between the two models11. Additionally, DBCN option 33 may be used to increase the interpolation range. This option makes the results more accurate for higher Z heavy ions4.

Of the two energy models, the higher energy Bethe-Bloch formula is of greater consequence for SEE simulations since this is where the inelastic delta ray generation occurs. Delta ray generation is a new feature introduced in MCNP6.2 where any charged particle is capable of creating secondary electrons through inelastic collisions. It should be noted that delta ray production (DRP) is not activated by default. Without DRP delta ray energies are still accounted for, but will all be locally deposited instead of generating an electron to be transported5. The form of the Bethe-Bloch equation used in MCNP6.2 is given by (1) and (2) [ref 11].

\[
\frac{1}{\rho} \frac{dE}{dx} = \frac{4\pi r_e^2 m c^2}{\beta^2} \sum_i Z_i f_i \frac{1}{u} \sum_i A_i f_i z^2 L(\beta)
\]

(1)

\[
L(\beta) = \frac{1}{2} \ln \left( \frac{2mc^2\beta W_{\text{max}}}{1 - \beta^2} \right) - \beta^2 - \frac{\sum_i Z_i f_i \ln l_i}{\sum_i Z_i f_i} - \frac{\sum_i c_i f_i}{Z_i} \delta(\beta, z, l) \frac{1}{2}
\]

(2)
where the last two terms are the shell and density correction factors respectively. $W_{\text{max}}$ is the maximum energy transferred to a delta ray which is given in (3) [ref 12]. All variables from (1) to (3) are listed in Table I.

$$W_{\text{max}} = \frac{2\tau(\tau + 2)m_e c^2}{1 + 2(\tau + 1)\left(\frac{m_e}{m}\right) + \left(\frac{m_e}{m}\right)^2}$$ (3)

From (3), it is shown that delta ray energies are directly related to the incident ion energy. For an ion of a given mass, a higher initial energy will yield delta rays of a higher maximum energy.

### Table I. List of Variables for (1) to (3) [refs 11,12]

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho$</td>
<td>Material density</td>
<td>g/cm$^3$</td>
</tr>
<tr>
<td>$dE/dx$</td>
<td>Stopping power</td>
<td>MeV/c</td>
</tr>
<tr>
<td>$r_e$</td>
<td>Classical electron radius</td>
<td>cm</td>
</tr>
<tr>
<td>$m$</td>
<td>Ion mass</td>
<td>MeV</td>
</tr>
<tr>
<td>$c$</td>
<td>Speed of light</td>
<td>m/s</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Ratio of ion velocity to speed of light</td>
<td>-</td>
</tr>
<tr>
<td>$u$</td>
<td>Atomic mass unit</td>
<td>-</td>
</tr>
<tr>
<td>$Z_i$</td>
<td>Atomic number for element $i$</td>
<td>-</td>
</tr>
<tr>
<td>$f_i$</td>
<td>Atomic fraction for element $i$</td>
<td>-</td>
</tr>
<tr>
<td>$A_i$</td>
<td>Atomic weight for element $i$</td>
<td>-</td>
</tr>
<tr>
<td>$z$</td>
<td>Ion charge</td>
<td>-</td>
</tr>
<tr>
<td>$W_{\text{max}}$</td>
<td>Maximum possible energy transferred to delta ray</td>
<td>eV</td>
</tr>
<tr>
<td>$l_i$</td>
<td>Mean excitation energy</td>
<td>eV</td>
</tr>
<tr>
<td>$C_i$</td>
<td>Shell correction</td>
<td>-</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Density correction</td>
<td>-</td>
</tr>
<tr>
<td>$m_e$</td>
<td>Electron mass</td>
<td>MeV/c$^2$</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Ratio of ion kinetic to rest mass energy</td>
<td>-</td>
</tr>
</tbody>
</table>

### III. Simulation Setup

#### III.A. Heavy Ion Strikes

The microelectronic device being modeled is a JBS diode which is shown in Fig. 1. Its structure is primarily SiC with dopants along with two metal layers on top of the SiC. For purposes of electro-thermal simulations, only an energy deposition profile within the SiC is required. It has also been determined that while electrically significant, the doping levels are too low to be relevant for energy deposition and therefore only a homogeneous SiC slab is used. The slab size used was 12 x 12 x 80 µm. The incident ion was centered on the top surface of the slab and aimed perpendicularly into the slab. A 1289 MeV Ag ion was used based on having an LET know to induce SEB$^{13}$. The slab geometry was constructed in Abaqus and then meshed with elements of multiple sizes. DBCN option 33 is enabled along with a DRP of 10 keV. To tally the energy deposition, type 6 elemental edits are used for both heavy ions and electrons. The edits have native units of MeV/g which were converted into pure energy units based on the material density and element volumes. Additionally a standard energy deposition cell tally was used to validate the total energy deposition on the mesh.
III.B. Fuel Pin Flux Profile

A set of four fuel pins were modeled based on pins used at the Rensselaer Polytechnic Institute Walthousen Reactor Critical Facility (RCF). RCF pins have an active length of 91.44 cm (36 in) and use stainless steel cladding. The fuel is enriched to 4.81 wt% U235 with a helium filled fuel-cladding gap region.

The cluster of four pins was modeled as a 2.54 cm segment in moderator (light water) with reflecting boundaries on all sides using a square lattice pitch of 0.8128 cm. Each material region was constructed as a separate part and then merged into a single part while maintaining boundaries between materials. This configuration was meshed with a 0.06 cm global seed size using first order hexahedral elements. The global seed size defines the target element size in Abaqus. For example, the size used here will cause elements to be 0.06 x 0.06 x 0.06 cm if possible. Deviations from this size occur as needed to best fit the geometry. Such a small seed size was used to ensure smooth meshing around the curved fuel pin surfaces. Merging into a single part ensures conformity of the mesh elements as shown in Fig. 2 with a detailed view in Fig. 3. Mesh conformity prevents gaps between elements of different parts which may cause irregularities in the elemental edits (lost particles in the worst case). In Fig. 3, it can be seen that elements in the narrow gap region appear stretched in order to link the element edges between the fuel and cladding.

A k-code simulation was run for the pin cluster along with an elemental edit for neutron flux across all energy groups.

IV. RESULTS AND DISCUSSION

IV.A. Heavy Ion Strikes

The purpose of modeling the heavy ion strikes was to pass the energy deposition profiles to an electro-thermal simulator in order to model the SEB process. This would be done using a conversion script, to convert the simulator’s native mesh file into an Abaqus file so that MCNP6.2 could run on the same mesh. Afterwards, the energy deposition results could then be translated to a charge density on the same mesh in the electro-thermal simulator. For a reference energy distribution, a high fidelity (0.2 x 0.2 x 0.2 µm elements) type 3 TMESH tally was used on a constructive solid geometry (CSG) model of the SiC slab which is shown in Fig 4. The delta rays form a funnel shaped cloud around the linear ion track which narrows as the ion depth increases. The funnel is widest near the ion entry point due to those delta rays being the highest energy and thus traveling the furthest from the ion track. The ion track itself will remain a consistent width up until the very end where it widens slightly due to larger scattering angles occurring once the ion’s energy has decreased. The highest energy central line is the ion track while the lower energy radial contributions are from the delta ray cloud. The ion has a total track length of about 74 µm which is comparable to results from SRIM ion range tables. The delta rays travel about 3 µm radially. While this is not a particularly long range, it is more than enough for the delta rays to traverse micro or nanoscale devices and create charges in sensitive regions. A break in the smooth distribution can be seen about 41 µm, however this is from a 1% error cutoff for the data and is not a physical phenomenon.
It had been determined that the electro-thermal simulator’s results were quite sensitive to mesh size with as small as nanometer sized elements being desirable in certain regions. Thus multiple Abaqus meshes were created to determine the optimal element size and quantity for reasonable runtimes. The coarsest mesh used for the electro-thermal simulations has elements using a 0.8 µm global seed size so this was the baseline size used for MCNP6.2. The meshes used are hereafter referenced by their global seed size.

Figs. 5 and 6 show the heavy ion and electron energy deposition, respectively, for the 0.8 µm mesh. The heavy ion is seen to deposit its energy along a straight track which broadens as it traverses the region. Its total range is 74 µm as was shown in Fig. 4. Even as the track broadens, the most significant energy deposition occurs in elements falling along the center of the track. The delta rays follow the funnel shape as described previously and are not present over the total ion range. This is due to the DRP energy setting a lower limit for delta ray production to 10 keV [ref 12]. Here the $W_{max}$ is about 26 keV which is equivalent to 3380 electron hole pairs in SiC (7.8 eV per electron hole pair) for a maximum energy delta ray. This causes $1.5 \times 10^{5}$ electrons to be generated with energies up to 26 keV. Any delta rays that would have been produced below the DRP become locally deposited as part of the heavy ion energy deposition. The delta ray cloud energy deposition can be seen to be about two orders of magnitude lower than that of the heavy ions. Energy is still primarily deposited in elements along the central ion track while some delta rays move several elements (a few micrometers) away. These results follow the expected distribution and proper total energy deposition. Total energy deposition results are shown in Table II.

<table>
<thead>
<tr>
<th>TABLE II. Total Energy Deposition</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
</tr>
<tr>
<td>F6 Cell Tally</td>
</tr>
<tr>
<td>(both meshes)</td>
</tr>
<tr>
<td>0.8 µm Mesh EMBEE6</td>
</tr>
<tr>
<td>0.6 µm Mesh EMBEE6</td>
</tr>
</tbody>
</table>

At the mesh size of 0.6 µm, the energy deposition profiles change quite notably. This is shown in Figs. 7 and 8. In Fig. 7, it is apparent that the energy deposition is significantly lower than what was seen previously for the heavy ions in Fig. 5. Some reduction is due to the smaller elements, but Fig. 7 shows much lower values for all elements and very little change in energy deposition along the ion track. The result is a total energy deposition of about only 3% of the 0.8 µm mesh value. This is a striking difference considering only the element size has been changed. Additionally, results from the standard cell tallies do not reflect this reduced energy deposition. Looking at Fig. 8 interestingly shows that the delta ray energy deposition is largely unaffected by the questionable heavy ion results. Between the meshes, there is less than 1% difference in the delta ray energy deposition. At this time there is not a definitive explanation for the heavy ion energy deposition error. It have been suggested that it may be caused by an issue
where heavy ions passing through vertices of the mesh are effectively lost\textsuperscript{4}. When the mesh becomes too fine, too many particles directly pass through a vertex and discrepancies occur in the tallied quantity. This was further tested by positioning the source in the center of an element (instead of the center of the surface). Doing so causes the source particle to enter through an element face instead of a vertex. This results in energy deposition of around 1000 MeV, which is much closer to the total value than the 100 MeV shown for the 0.6 µm mesh in Table II. However, this “fix” becomes completely ineffective for more complex meshes or for problems where larger scattering angles are more probable. The “fix” also becomes less effective as the number of histories are increased and therefore to make use of it statistical certainty must be sacrificed. For this problem, $10^4$ histories were found to be effective for the fix while it failed at $10^5$ histories.

The energy deposition discrepancy was found to occur with any global seed size below 0.8 µm even for slabs of different dimensions. Therefore this currently the minimum element size for unstructured meshes used with heavy ions. This size limitation makes unstructured meshes unsuitable for heavy ion induced SEE modeling considering the significantly smaller elements that are required. Small elements are required to accurately capture the energy peak which occurs along the ion track. The peak value is critical for inducing runaway charge production and heating necessary to cause SEB. Equivalent integral energy deposition over a larger area will not induce the same event.

Fig. 5. Heavy Ion Energy Deposition on 0.8 µm Mesh
Fig. 6. Delta Ray Energy Deposition on 0.8 µm Mesh

Fig. 7. Heavy Ion Energy Deposition on 0.6 µm Mesh
IV.B. RCF 4 Pin Cluster Flux

For the four RCF pin cluster, a k-code calculation based on 500 active cycles yields a $k_{inf}$ value of $1.40588 \pm 2$ pcm. For an equivalent CSG model, $k_{inf}$ is calculated to be $1.40677 \pm 2$ pcm. The difference of about 100 pcm is larger than what would typically be expected for a merged part model\textsuperscript{15}. The difference in $k_{inf}$ values may be related to how the problem’s reflecting boundaries were applied. Reflecting boundaries are not necessarily compatible with unstructured meshes, but should function normally with CSG geometry in the same problem\textsuperscript{16}. The reflecting boundaries were applied by creating a separate CSG cell encompassing the unstructured mesh based geometry that was minutely offset from the mesh surface. It is thought that the reflecting boundaries may still be close enough to the
Fig. 11. Fast Neutron Flux for RCF 4 Pin Cluster

mesh to cause an issue. In future work, a full RCF core model may be modeled to see if the discrepancy persists.

Fig. 9 shows the flux profile (for all energy groups) plotted on the unstructured mesh for the four pins. The flux follows the expected trends with it being lowest in the fuel pins and peaking in the moderator. In Figs. 10 and 11 the flux is plotted for the thermal and fast groups respectively. Here the threshold between the two groups is set to 1 eV. These figures show that the fast flux peaking in the fuel while thermal flux is highest in the most heavily moderated regions. Agreement can also be seen between the magnitude of the total flux and the sum of the group fluxes.

V. CONCLUSIONS

The unstructured mesh features of MCNP6.2 present a strong opportunity for coupled simulations using deterministic codes that rely on a mesh for computation. Using the unstructured mesh feature, MCNP6.2 may be run with meshes from other codes by converting the meshes to an Abaqus format. Doing so is advantageous in areas where maintaining the spatial distribution of data is critical, such as reactor physics or SEE modeling. However there are still some notable limitations of unstructured meshes in MCNP6.2 which make them unusable for certain coupled simulation applications. For scenarios involving heavy ions, the global seed size for the mesh cannot be less than 0.8 μm. While not an issue for a large scale problem, it greatly limits the usefulness of unstructured meshes for microelectronics modeling where nanoscale elements are more ideal. In the case of reactor physics models, unstructured meshes exhibit some deviation from CSG results for small geometries using reflecting boundaries. This is not expected to carry over to larger models such as those for a full core.

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REFERENCES


