Radiation Damage by Low Energy Neutrons with Geant4: A Review of Current Approaches and Results

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Introduction and Motivation

One possible outcome of high energy particles' (neutrons, photons and other charged particles) interaction with crystalline matter is the creation of lattice structure defects, arising from the transfer of energy to atoms of the crystal.

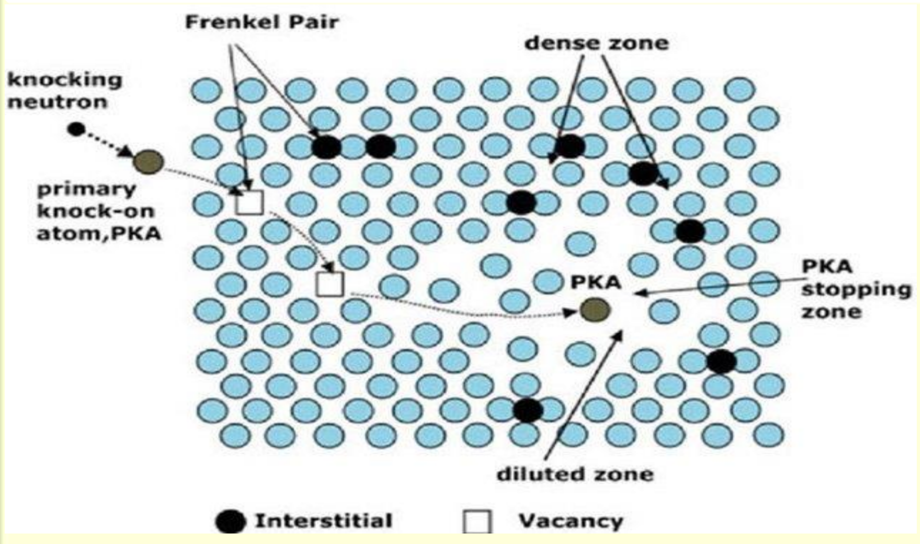


Figure. 1: Formation of Frenkel Pairs by neutrons (Dawson, 2018)

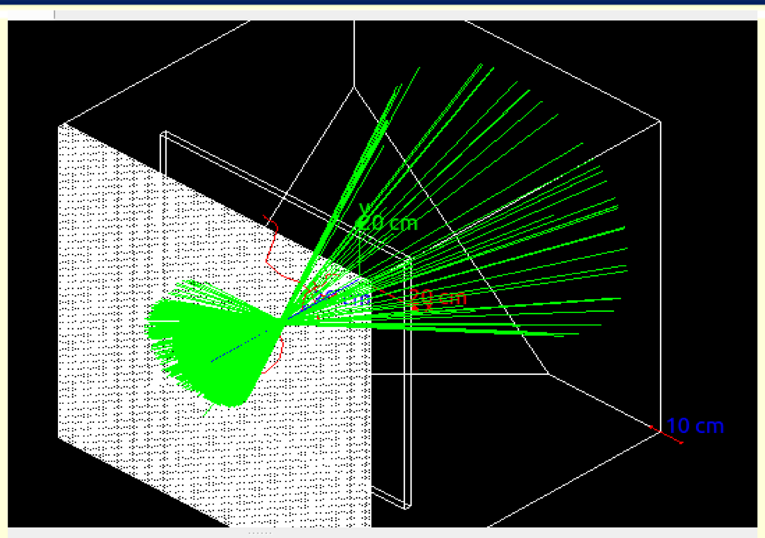
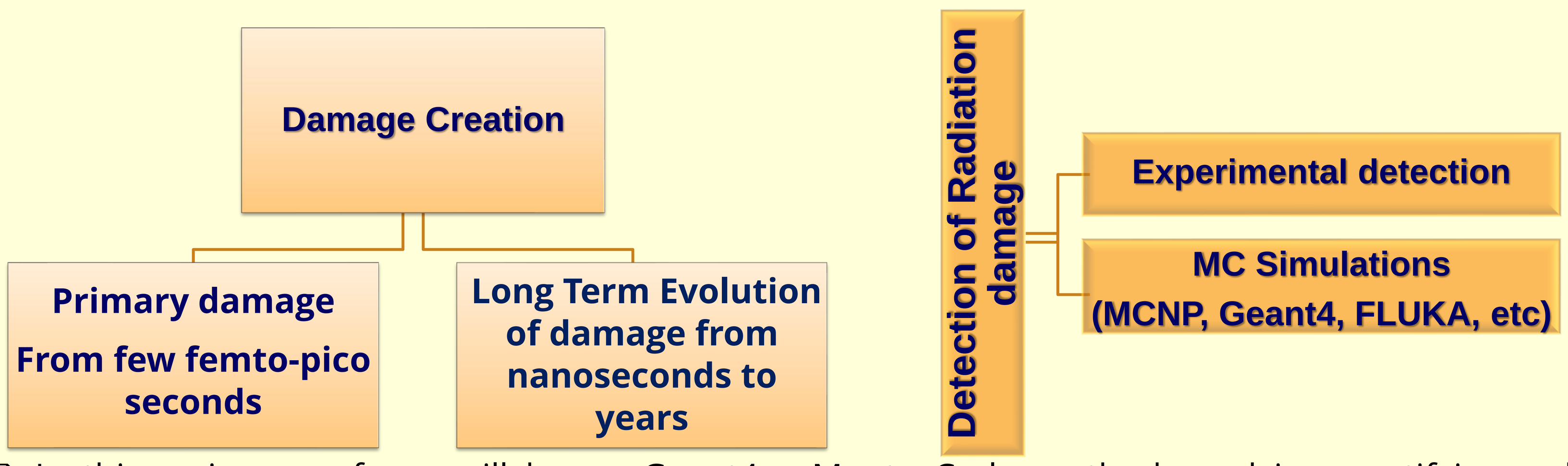


Figure 2: Simulations

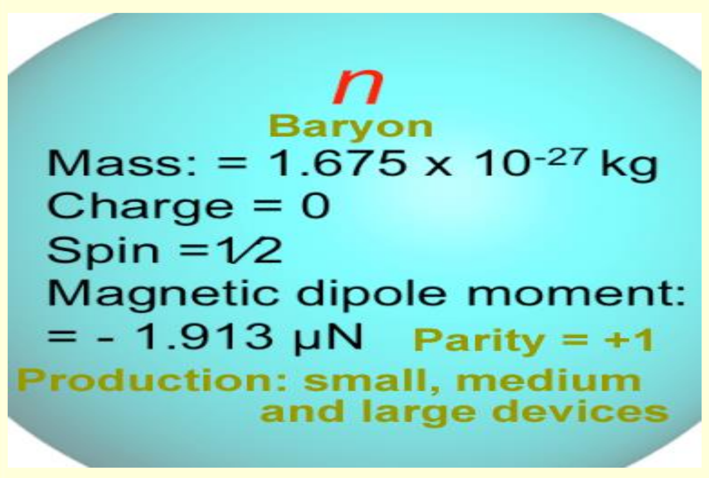
- ❑ Radiation damage can be essentially a permanent displacement of the atomic structure in solids, brought about by high energy particles.
- ❑ As radiation interacts with solids, a progression of atomic displacements may emerge, producing damage in materials that affects the properties of the material (Nordlund *et al*, 2018).



- ❑ In this review our focus will be on Geant4 a Monte Carlo method used in quantifying radiation damage by low energy Neutrons in matter.

Neutrons in Geant4

- ❑ Low energy neutrons in Geant4 are classified under QGSP_BERT_HP class



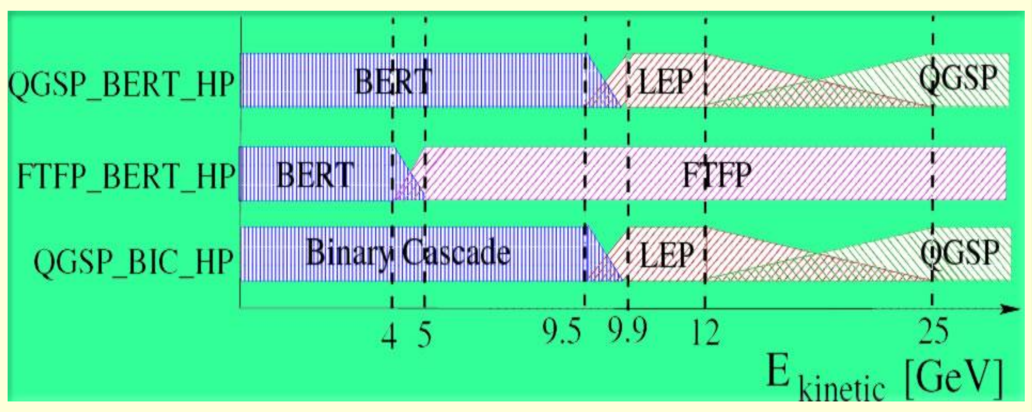


Figure3: Geant4 Hadronic PhysicsList

Monte Carlo Simulation with Geant4

- ❑ The Monte Carlo (MC) method is a stochastic method for numerical solution of mathematical problems. A technique that utilizes random sampling to simulate the real-world problems or phenomena.
- ❑ In neutron transport studies, MC methods are employed to look at the interaction of neutrons with matter. Codes mentioned above are used to achieve this
- ❑ Geant4 is a MC based simulation toolkit that is used for the geometry and tracking of particle's transport through matter. (Mudau, 2013).

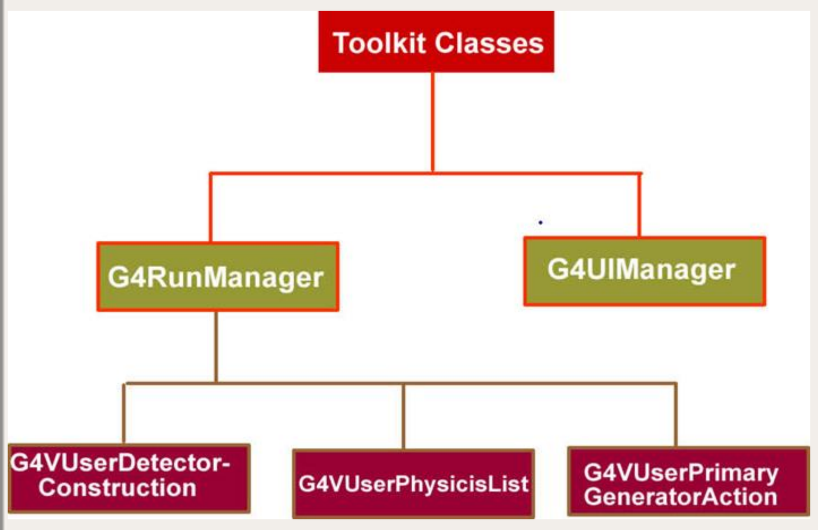


Figure 4: Geant4 toolkit classes

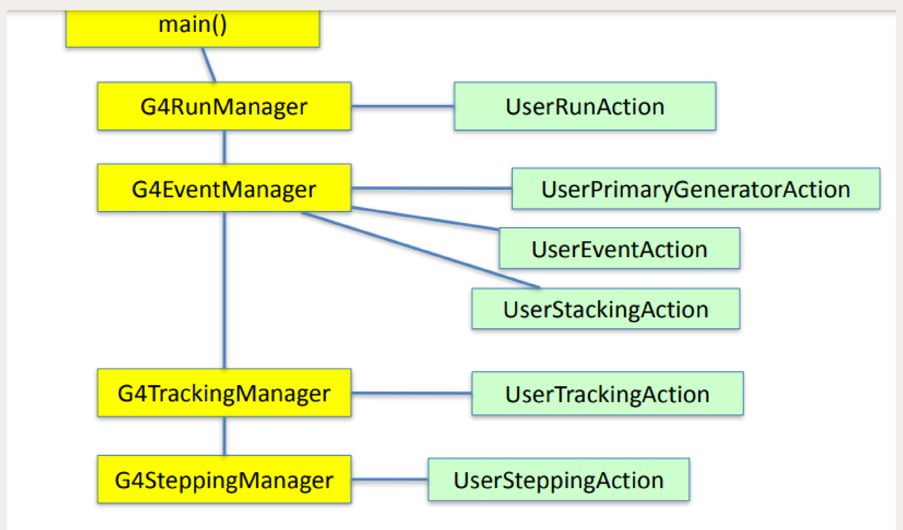


Figure 5: Geant4 Sequential mode

- ❑ Geant4 has two main classes which are the G4RunManager and the G4UIManager (see figure 4) and Subprograms includes SteppingAction, TrackingAction, EventAction added to the main program in a sequential mode shown in figure 5.
- ❑ The G4UImanager on the other hand creates pointers to the interface. The User Interface is created in order for the user to supply commands to Geant4. (Mudau, *et al*, 2013).

Present Work

- ❑ Evidence shown the versatility in opting for Geant4 to estimate radiation damage in nuclear materials with low neutron energies within the range of the Nuclear fission reactor.
- ❑ Preliminary simulations have been performed for Indium Arsenide (InAs) with results shown in figures 6a-c.

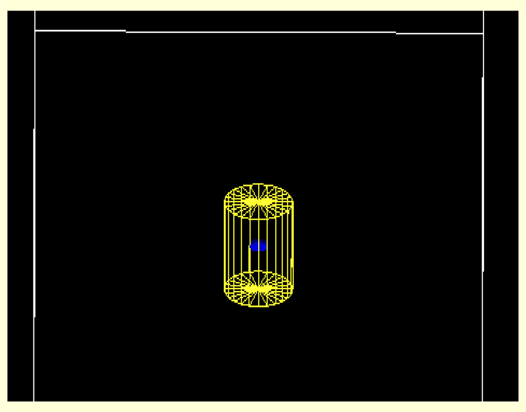


Figure 6a: Geometry

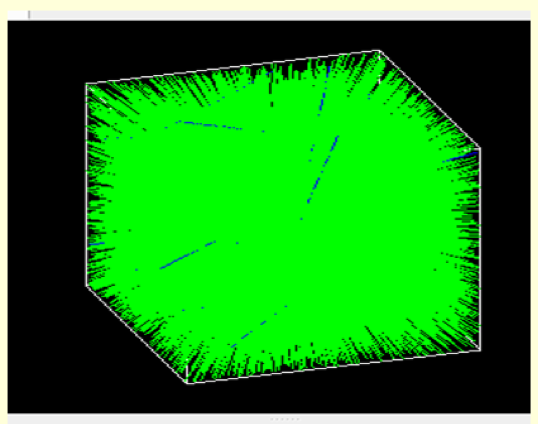


Figure 6b: Simulation

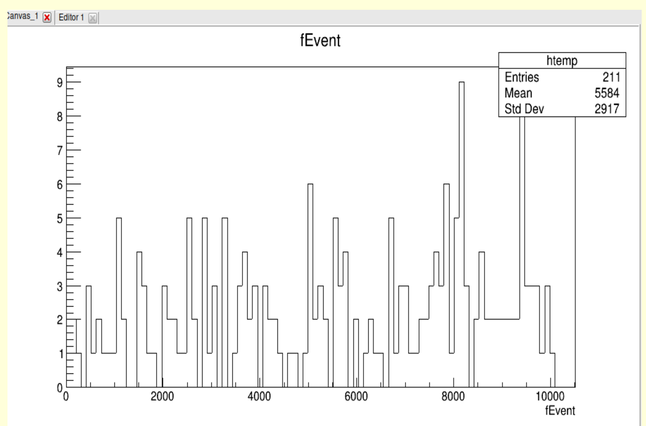


Figure 6c: Neutron hits on InAs

What were the approaches and Results in previous researches?

(a) Liu *et al* 2019: simulated radiation damage for Silicon Drift Detector

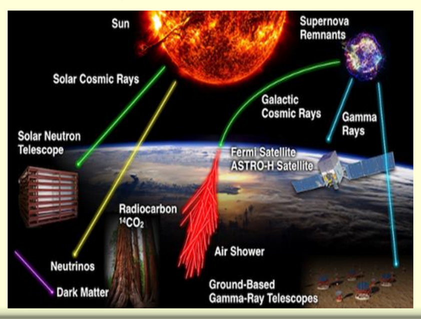
- ❑ Norgett-Robinson-Torrens model was used for displacement damage and Ionization damage was part of the methods to estimate damage.

$$N_d(E) = \begin{cases} 0, & E < E_d \\ 1, & E_d \leq E < 2.5E_d \\ \frac{0.4E_d(E)}{E_d}, & E \geq 2.5E_d \end{cases}, \quad where E_D(E) = \frac{E}{1+k_d g\left(\frac{T}{E_d}\right)},$$ N_d number of offsite atoms produced by PKA, E_D damage energy of PKA.

- ❑ Recoil atoms distribution by neutrons in SDD was uniform and found in low energies.
- ❑ Secondary particles produced by neutrons had large energy loss in inelastic scattering and energy deposition with γ was linear with SDD.

(b) Pioch, 2012: Measurement and simulation of the Radiation Environment in the Lower Atmosphere for Dose Assessment.

- ❑ Validation of response functions of the spectrometer was done with Geant4 and experiments for the different intra-nuclear cascade (INC) models applied (Bertini and Binary).



- ❑ Estimation of damage in Be was done using displacement per atom (dpa),

$\sigma_{dpa}(E) = \frac{0.8}{2}(E)$, where, E_d - displacement energy σ_D- damage energy cross-section

- ❑ Damage caused by He atoms is about thrice less the damage caused by Be
- ❑ PKAs. 70% of the damage occur at Be energies below 100 KeV,

Comparison of Geant4 with MCNP, FLUKA and FISPACT II

(a) A comparison of neutron scattering in Geant4 and MCNP (Madau, et al, 2013)

- ❑ In this study neutron interaction with materials such as water, Beryllium, uranium and Aluminium was considered. Results for water shown in fig.7

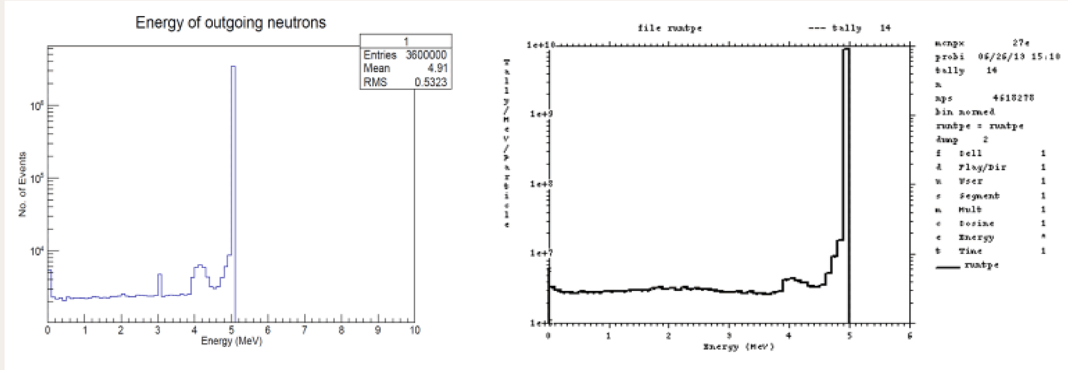


Figure 7: Comparison of neutron scattering in Geant4(left) and MCNP(right)

- ❑ Findings revealed that calculated total scattering cross sections are similar,
- ❑ This validates the Geant4 use of ENDF/B-VII cross sections. Although the scaling of the histograms is different, the number of particles with exit MeV are proportional in both the codes.

(b)Validation of the thermal neutron physics in GEANT4.9.3 and MCNPX (Garcia, *et al*, 2013)

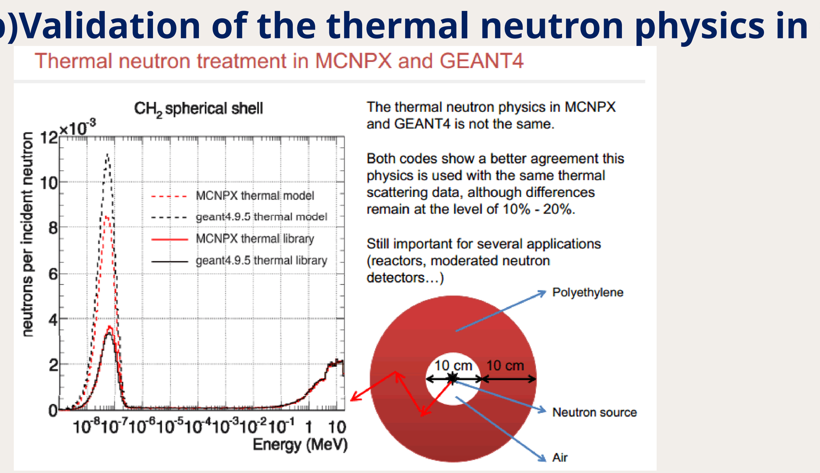


Figure 8: Thermal neutron treatment in Geant4 and MCNP

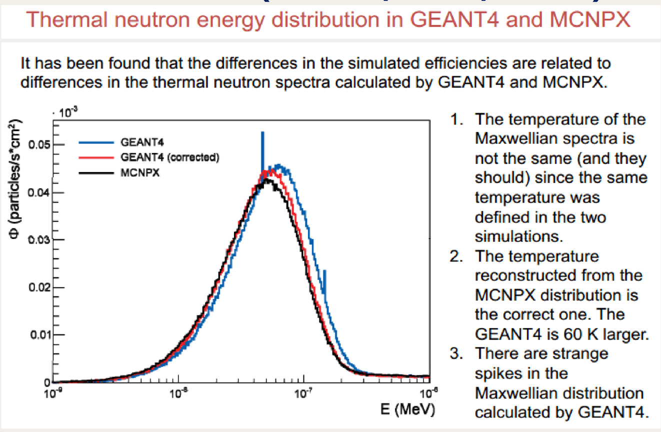


Figure 9: Thermal neutron distribution in Geant4 and MCNP

Comparison of Geant4.9.3 with MCNPX shows agreement. However, there was a deviation of 10-20%

(c) Geant4.10.03 and MCNP6.2 modeling of fast-neutron detectors based on single-crystal chemical vapor deposition diamond (Green *et al*, 2020)

- ❑ The macroscopic cross-section was compared in MCNP and Geant 4. shown in table 1

Table 1: Geant4 and MCNP neutron crossection results

Interaction with 14.1 MeV Neutrons	Calculated Σ (cm^{-1})	MCNP Σ (cm^{-1})	Geant4 Σ (cm^{-1})
^{12}C Elastic	1.37E-01	1.40E-01	1.44E-01
^{12}C Inelastic	9.32E-02	8.74E-02	8.41E-02
^{12}C Total	2.29E-01	2.28E-01	2.28E-01
^{12}C Elastic	1.49E-03	1.87E-03	1.20E-03
^{12}C Inelastic	1.28E-03	1.61E-03	1.29E-03
^{12}C Total	2.77E-03	3.12E-03	2.49E-03
Total	2.32E-01	2.31E-01	2.31E-01

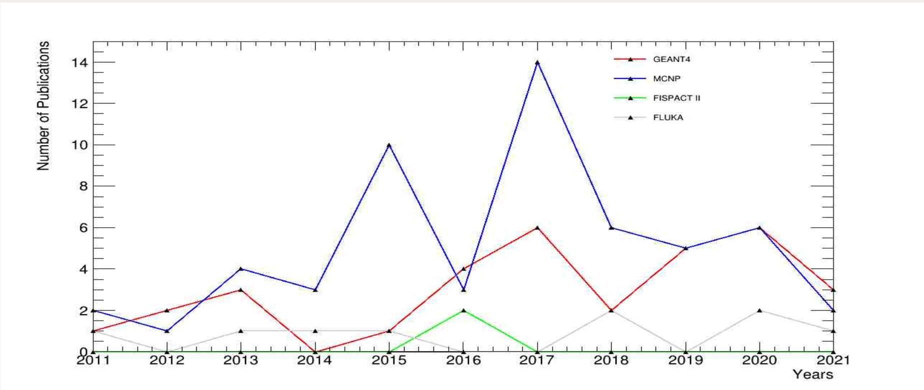


Figure 10: Neutron radiation damage publications (Scopus)

- ❑. In figure10, preference has been given to MCNP from 2011 to 2018, but beyond 2018 the usage of Geant4 started increasing and even more as of August 2021.
- ❑ Higher deviations from the experiments noticed for Geant4 than MCNP

Conclusion

- ❑ Geant4 has been used for simulation of neutron radiation damage in materials for low energies in other studies.
- ❑ Results obtained approximates closely experimental data and agrees reasonably with MCNP. Recent evolution in Geant4 to include G4TENDL files promises improved results for low energy neutrons.
- ❑ Geant4 has the potential of becoming a viable alternative MC simulation toolkit for the future since it has features that supports Machine Learning /Artificial Intelligence.
- ❑ Currently we are working on comparing nuclear material damage results obtained in Geant4 with experiments and other MC simulation codes for low energy neutrons.

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