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Expansion of the Monte Carlo Integrated Tiger Series Validation Suite

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INTRODUCTION

The Integrated Tiger Series (ITS) program is a Monte Carlo code for simulating Coupled Electron-Photon transport [1,2]. It is used normally to assess the radiation hardness of complex systems, such as components for satellites in space. The ITS code is currently maintained by Sandia National Laboratories. This work's goal is to discuss the current status and potential areas of improvement for the validation suite in the Integrated Tiger Series code. This validation suite is used to confirm the accuracy of ITS simulations, and at present consists of seven examples with three methods of transport per example. Significant gaps in validation coverage exist for photons and electrons in the >1 eV and <10 MeV energy range – to address these gaps, additional experimental data will be sought out, simulated, and then added to the validation suite to create a more robust test suite.

The aforementioned seven cases are tested for three different forms of transport algorithms – the condensed-history method, a hybrid multigroup/continuous-energy method, and a single-scattering, analog type method. All three methods use the bremsstrahlung production and spectra cross sections from Seltzer. These seven experiments have been summarized in the table below and are discussed in greater detail by Franke and Kensek in Reference 1.

Representative Tests in the ITS validation suite [1]

TABLE I. Current Coverage by Validation Suite

Experiment	Energy	Material	Assessments and Observations
Lockwood Electron Albedo [3]	0.032 - 1 MeV	Uranium	Error increases for more glancing angles. Analog issues above 256 keV.
Hanson Electron Angular Scattering [4]	15.7 MeV	Gold	Could the parameter studies be cast in terms of convergence studies (in some useful metric)? Could a sub-step size be added for condensed history? Analog fails to capture peak.
Tabata Charge Deposition [5]	14.9 MeV	Beryllium	Analog misses depth location of peak energy depositions, and slight distortion of shape.
McLaughlin Energy Deposition [6]	3 MeV	Aluminum	Analog misses depth location of peak and shape of distribution.
McLaughlin Energy Deposition [6]	100 keV	Polystyrene	All methods miss the measured tail. Cannot properly assess how well any method captures the peak.
Sanford Radial Dose Profile from Bremsstrahlung [7]	750 keV	Carbon	Difficult to assess how far off the last measurement is. Analog has issues.
Dolan Electron emission from Photons [8]	50 keV endpoint Bremsstrahlung spectrum	Tantalum	Disagreement between all models and experiments under 20 keV for all methods.

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These seven experiments ultimately show disagreement with analog data, with no quantitative assessment in the reporting of comparisons, or their accuracies. The current understanding of the benchmark data solely resides in graphs that, on a majority of the occasions, miscalculate the depth location of energy deposition peaks and fail to highlight the distortion of the overall energy deposition distributions with the expected distributions [1]. When viewing the plots in the Franke and Kensek paper, there is no quantification of numerical error for the data, some plots lack error bars, and those that do have error bars on the plots don't effectively demonstrate what those confidence intervals are (i.e. one sigma, three sigma, or some other decided interval). The goal of any validation program should include an output of quantitative data.

The question is raised: are there gaps in the validation suite that could potentially be expanded? This paper aims to identify the limitations of the validation suite, and to explore how ITS's validation benchmarks can be expanded to better understand and quantify the accuracy of the physics models.

CURRENT ITS TRANSPORT METHODS

Currently, the ITS validation suite includes seven physical benchmark examples, and utilizes three forms of transport in each of the seven examples. The three methods ITS is concerned with are the condensed-history method, a hybrid multigroup/continuous-energy method, and a single-scattering method [1]. All three methods use similar cross-sectional data. When looking at the single-scattering method, a high-energy factorization is used in ITS for a screened Mott representation while the Riley distribution is used for curve fitting with a concern for energies between 1 and 256 keV [1]. The condensed-history and hybrid multigroup/continuous-energy methods use high energy factorization above 256 keV using a modified screening parameter due to the transition. The single-scattering uses the same factorization method when dealing with energies at 10 MeV and higher, with a logarithmic cubic spline to fill in the gap for the entirety of the total elastic cross section. However, the gap is left unfilled for the elastic differential angle to then rely on user-implemented interpolation for that selected set of data. For bremsstrahlung production, the condensed history uses angular distributions from the Bethe-Heitler theory, and the multigroup/continuous energy use a simpler model, which is similar to that in MCNP. When examining the relaxation cascades, they are similar for both the multigroup and condensed, however there are slight differences between the two. The single-scatter method (which can also be referred to as the analog method) uses a complete set of subshell data for the relaxation cascades.

All three methods in ITS have a different energy-loss model and vary in their treatment of both large and small energy-loss interactions. For the condensed history method, it works off of a pre-computed energy-loss, as well as a pre-computed set of angular-scattering distributions. Electron tracking is separated into sub steps, with collisional energy loss sampling at the start of each step. Angular scattering is computed over a sub step centered in the middle of a step with the use of Goudsmit-Saunderson expansion. Angular deflection in part of inelastic-scattering is accounted for by adjusting the elastic-scattering distribution with the assistance of a (Z+1)/Z correlation [9]. Energy loss is sampled over a step from the Blunck-Leisegang distribution with a Seltzer [10] distribution correction. The Jordan-Mack algorithm is used for boundary crossings. Bremsstrahlung photon production, knock-on electron production, and ionization events are sampled for each sub step.

The hybrid multigroup model estimates adjoint fluxes by transposing the group-to-group matrix already present within the code. What this allows for in this particular transport method is calculating a very specific quantity of interest (an example would be dose in one volume or point) and gets the answers for a variety of sources of different energies, spectra, or directions. This is accomplished by using the inner product as a multidimensional integral over phase space, where the operator for this would be the forward Monte Carlo transport code [11]. This model is coupled with the CEPXS code, which takes cross sectional data and integrates it over each particular group. Sixty-three scattering angles are used in this process.

The single-scattering transport is based on the LLNL EDL. The EDL data is represented in tabulation with mostly prescribed interpolation schemes. The EDL (electron data library) deals with four types of cross sections: ionization, excitation, elastic scatter, and bremsstrahlung. These are all tabulated as a function of the incident energy of the electron, with different grids used for each set of energy data. The single-scatter algorithm for elastic and inelastic electrons makes electron transport computationally expensive, but it can be reasonably applied to low-energy problems. The relaxation model that is present in this is far more detailed than anything in ITS presently and is still a rather recent implementation to the code that requires further testing.

Current Benchmark Validation Suite

The seven problems that use these three methods are the Lockwood Albedo, Hanson Angular Scattering, Tabata Charge Deposition, McLaughlin Energy Deposition in Aluminum, Sanford Bremsstrahlung Converter, McLaughlin Energy Deposition in Polystyrene, and Dolan Photoemission.

The Lockwood Albedo test deals with the experimental results for the Lockwood electron charge-deposition in uranium [3]. The experiment looked at the charge deposition, but the report contained the albedo as the result. Analog results have issues above 256 keV due to the sparse elastic angular-scattering data, but apart from that, there is consistency in the trends of the comparison between computational results and experimental results. It is known that in the condensed-history algorithm that the results are underestimated due to straight sub step mechanics. The error of the model in ITS shows that error increases for more glancing angles.

In the Hanson Angular Scattering data, it compares the experimental measurements of Hanson [4] for angular distribution of perpendicular 15.7 MeV electrons passing through gold foil. The condensed history results are good in agreement with the experimental data. However, the foil thickness is smaller than a sub step, which may be the reason for this. The analog results underestimate the electron transmission at small angles. However, there are some signs that show a potential for inaccuracy in the angular distribution at 10 MeV. The multigroup transport method also agrees well but required two changes from the default settings for cross-section generation. Because the problem was so thin, it was necessary for the electrons to undergo a large amount of interactions to avoid artifacts due to uncollided electrons. The Fokker-Planck scattering model is of limited accuracy for the forwarded-peaked electron elastic scattering [1].

With regard to the Tabata Charge Deposition experiment, the computational results of all three transport methods are compared against the data of Tabata for 14.9 MeV electrons incident perpendicularly on Beryllium [5]. There is a wide uncertainty in this experimental model. The condensed-history and multigroup results give reasonable agreement with the experimental data. However, once again, the analog simulation is inaccurate as it fails to clearly show the depth location of the peak of the deposition of charge within the material.

The McLaughlin Energy Deposition in Aluminum deals with 3 MeV electrons normally incident on a slab of aluminum [6]. The condensed-history and multigroup calculations are in good agreement with the experimental data, and the disagreement of the analog simulations may be due to the interpolation over a wide energy range from the 256 keV Riley distribution up to the 10 MeV Mott distribution.

The Sanford Bremsstrahlung Converter experiment consisted of carbon and an incident electron beam at 750 keV, with the carbon shaped into a 1 cm (radius) cylinder and 0.48 cm thick [7]. This design was to prevent source electrons from being transmitted. Because there are photons created by the electrons through bremsstrahlung and fluorescence, the carbon is said to “convert” the electrons to photons. Both the condensed-history and multigroup transport methods agree with the experimental data, with some level of underestimation. The analog data severely overestimates the forward-directed bremsstrahlung production. This is most likely because an angular model is required to accurately simulate this experiment.

The McLaughlin Energy Deposition in Polystyrene centers around a 100 keV electron beam incident on polystyrene in which there is a good agreement in all of the methods and data [1]. There is a slight disagreement with the experimental results in the tail end of the distribution with experimental results in the deep end of the polystyrene.

The Dolan Photoemission experiment dealt with reverse photoemission from tantalum [8]. All of the results have disagreement between all models and experiments under 20 keV for all methods of transport.

CONCLUSIONS AND FUTURE WORK

This work investigated the present ITS validation suite, identified potential drawbacks and limitations of the suite (such as gaps in the benchmark particle energy ranges). It is clear that more experimental data should be included in the ITS validation suite to make the suite more robust. The seven current validation problems all experience some inaccuracy in analog data, and while there are reasons surmised as to why in the article by Franke and Kensek, more data is required to verify their reasoning. As previously mentioned, it is also quite clear that the validation suite fails to provide what a validation suite should: quantitative results regarding both the outcomes of the experiments that were modeled, as well as the overall error in that model, with that error being consistent across all of the models in the validation suite. Additionally, it would be ideal to add a model that covers the gap between 256 keV and 10 MeV. This would assist in highlighting potential errors that may exist between that energy range for the already-present validation suite, whether it be in how the data was modeled or the use of a particular model itself. Different materials are also being explored that are relevant for the nuclear engineering field for use at low energy levels (under 256 keV) and higher energy levels (above 10 MeV). The larger problem surrounding that task however is the fact that there is not a large, well-maintained electron data library that contains all of the information we would like to include in the suite, so it must first be found and compiled into one that we can used for this purpose.

Currently, a limited database from the National Nuclear Data Center ran by BNL is being explored for data of interest, but it appears that other data may need to be located from other sources such as other papers regarding different benchmark data for other electron/photon transport codes, or that there may be another database online that is yet to be discovered.

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