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Title

RAPTURE: A 1-D Radiation Effects Analysis Tool

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Abstract

RAPTURE is a coupled photon-electron radiation effects analysis tool for 1-D slab geometries. Built on the SCEPTRE radiation transport code using CEPXS cross sections, RAPTURE is a modern alternative to the legacy code ADEPT.

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RAPTURE: A 1-D Radiation Effects Analysis Tool

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***Abstract*—RAPTURE is coupled photon-electron radiation effects analysis tool for 1-D slab geometries. Built on the SCEPTRE radiation transport code using CEPXS cross sections, RAPTURE is a modern alternative to the legacy code ADEPT.**

I. RAPTURE OVERVIEW

RAPTURE is a coupled photon-electron radiation-effects analysis tool for one-dimensional slab geometries developed to serve as a modern alternative to the legacy code ADEPT. RAPTURE is applicable to a variety of radiation effects problems, uses a straightforward and verbose input format, runs on Windows, Linux, and Apple systems, and is actively supported by developers in the Radiation Effects Theory Department at Sandia National Laboratories (SNL) and the Radiation Science Group at the Atomic Weapons Establishment (AWE).

RAPTURE is built upon the SCEPTRE deterministic transport code [1][2] and the photon-electron cross-section generation code CEPXS [3], inheriting the extensive history of verification and validation efforts associated with these codes. Modern software design practices including version control, unit and regression testing, and a portable release system distinguish RAPTURE from the legacy code ADEPT and its predecessors [4][5][6]. RAPTURE, SCEPTRE, and CEPXS are production codes that are actively supported by developers at SNL and AWE.

The RAPTURE input file uses the verbose XML format which emphasises clarity and avoids ambiguity in the problem description. The input file describes the problem to be solved, specifying the problem geometry, the materials present in the geometry, the radiation source that drives the problem, and the quantities of interest (QoIs) desired by the user. The problem geometry is characterized in terms of thicknesses. Materials are described by density and the mass fraction of the constituent elements. Radiation sources may be monoenergetic, constant in energy, or a spectrum defined by a probability density function (PDF) or cumulative density function (CDF). RAPTURE supports a variety of QoIs, including energy deposition, charge deposition, or kerma in a region of interest, reflected or transmitted spectra, or response functions for energy deposition or kerma. Comprehensive error checking and verbose error messages alert the user to mistakes in the input file before calculations begin.

Discretization and solution of the problem specified in the input file is automatically performed by RAPTURE. RAPTURE generates a spatial mesh, a multigroup energy discretization and multigroup cross sections, and an angular discretization based upon the radiation source and the QoI(s). The radiation transport problem is solved using these physics-informed space, angle, and energy discretizations. The discretization of the phase space is iteratively refined until all QoIs converge to a user-specified tolerance. The physics-based rules in RAPTURE are similar to the heuristic rules found in ADEPT but the addition of a convergence study improves the reliability and accuracy of the RAPTURE results as compared to results generated by ADEPT.

RAPTURE produces as output text files and plots of the QoI(s) requested by the user and a collection of the input files necessary to rerun the fully-converged SCEPTRE problem to reproduce the reported solution. The input and the output files produced during the final, converged calculation are collected and presented alongside the RAPTURE output.

The CEPXS and SCEPTRE input and mesh files created by RAPTURE for a particular problem may be the output desired by the user rather than the files containing the user-specified QoI. A user's objective when running RAPTURE could be, for example, to determine the resolution necessary in the spatial or energy mesh in order to resolve the physics of interest for a particular problem. This information can inform the discretization of a 2-D or 3-D SCEPTRE calculation along 1-D slices of the multi-dimensional geometry. Alternatively, a user wishing to perform an uncertainty quantification analysis of a 1-D problem might use RAPTURE to generate a set of input files that adequately resolve the nominal problem. From these files an ensemble of problems can be assembled by replicating and perturbing the nominal SCEPTRE input files. The ensemble of input files might contain perturbed values of the spectrum of the radiation source, the dimensions of the material stackup, or the densities of the materials in the problem. The meshes produced by RAPTURE should be valid for minor perturbations to the problem of interest and the ensemble of problems can be run with SCEPTRE without needing to perform a convergence study on each realization.

RAPTURE is released under a commercial copyright from Sandia National Laboratories. The licence is free. RAPTURE is released via Docker, a free commercial product that enables cross-platform portability [7]. RAPTURE and all necessary libraries are compiled and installed by the development team and packaged as a Docker Image. Users install RAPTURE by downloading and installing Docker, obtaining the RAPTURE Docker Image from SNL, and then loading the RAPTURE

Docker Image in Docker. No compilation is required on the part of the user. This release method supports users that wish to run RAPTURE on Linux, Windows, and Apple computers.

The RAPTURE release contains a User's Manual which includes a brief overview of RAPTURE, extensive instructions on constructing RAPTURE input decks, running problems in RAPTURE, and interpreting RAPTURE output, and an overview of a collection of test problems. The test problems were run with RAPTURE, TIGER (1-D ITS) [8], and ADEPT, and where possible are compared with experimental data. Input decks for the test problems are included in the RAPTURE release. These test problems cover the span of the RAPTURE problem space and form a useful set of templates for the user. The following section includes plots from the User's Manual comparing the RAPTURE results against results calculated with TIGER and ADEPT. The full suite of test problems will be displayed and performed at the code demonstration during the March HEART meeting.

The RAPTURE and SCEPTRE codes are under active development. Incremental RAPTURE releases during calendar year 2020 will add the explicit treatment of positrons, allow the user to specify radiation sources incident at non-normal angles, and support user-provided space and energy meshes. As new sources of multigroup cross-sections become available they will be included in RAPTURE, including sub-keV cross sections generated with the SNL- and AWE-developed code SKEPTXS. Improvements to SCEPTRE will be inherited by RAPTURE and may include novel discretization schemes in energy and angle. Feature requests, bug reports, and requests for support will be accepted at rapture-support@sandia.gov.

II. Selected RAPTURE Output

A selection of problems are presented to motivate the use of RAPTURE. The problems presented include photon and electron sources, mono-energetic and spectrum sources, energy-deposition, charge-deposition, and spectrum quantities of interest, and demonstrate both forward and adjoint (response function) modes of running RAPTURE. For each problem the results are plotted for a scaled source of one particle per square centimeter (p/cm^2). The RAPTURE input file allows users to scale the source by any number of particles and a future release of RAPTURE will allow the user to scale the source by total incident energy or by the number of incident particles.

The first figure plots the energy deposition profile produced by 6 MeV photons normally incident on the left face of a 4 cm slab of tungsten. Figure 1 contains solutions generated with RAPTURE, TIGER, and ADEPT, showing excellent agreement between RAPTURE and TIGER and good agreement between those two codes and ADEPT. Table 1 highlights the differences in the space, angle, and energy discretizations used by RAPTURE and ADEPT to solve this problem.

Several differences between the RAPTURE and ADEPT discretization schemes are evident in Table 1. Spatial meshes produced by RAPTURE are feathered near problem boundaries and material discontinuities and grow exponentially with depth into homogeneous material regions. The ADEPT spatial mesh also varied throughout the slab but was much coarser than the RAPTURE mesh. RAPTURE uses a Gauss-Lobatto quadrature set which includes the directions with cosines $\mu = -1$ and $\mu = 1$ allowing the source to be exactly normally incident on the problem. ADEPT uses the Gauss-Legendre quadrature set and places the source in the angle closest to normal. Finally, for problems that contain a mono-energetic source RAPTURE creates an energy group centered at the source energy with a width equal to one percent of the source energy. While ADEPT chooses the energy bounds of the highest-energy group such that the average energy in that group is equal to the mono-energetic source energy, ADEPT does not control the width of that energy group.

The problem displayed in the second figure uses the same geometry as the problem in the first figure. These plots show response functions for energy deposition in a 4.0 cm slab of tungsten by photons incident on the left face of the slab. The four curves in the figure show the response function for the total energy deposition in the slab, the energy deposition in the the first cm of the slab, the middle cm of the slab, and the final cm of the slab, respectively. This figure is a compilation of four RAPTURE calculations as each adjoint calculation must be performed independently.

The third figure plots charge deposition as a function of depth for 1 MeV electrons incident on a slab of plastic. The

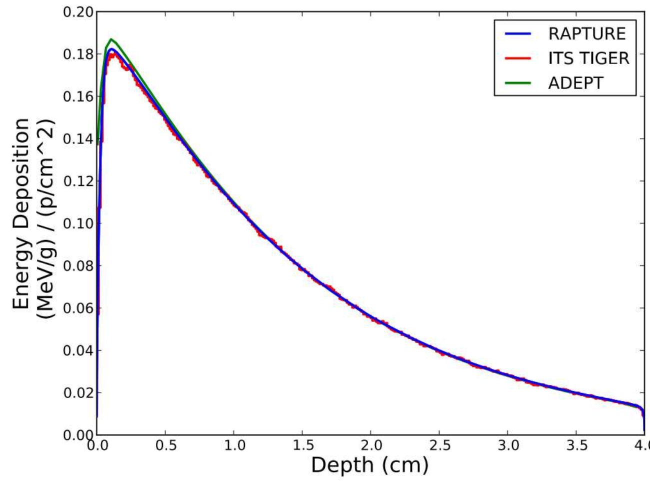

Fig. 1. Energy deposition for 6 MeV photons normally incident on the left face of a 4.0 cm of tungsten.

TABLE I
Comparison of the discretization schemes used in the deterministic ADEPT and RAPTURE codes to solve the problem displayed in Figure 1.

Discretization	**ADEPT**	**RAPTURE**
Spatial Cells	78	264
Cell Containing Peak Dose	4	104
Discrete Ordinates Order	16	12
Source Angle (degrees)	8.3	0.0
Energy Groups	56	104
Width of Source Group (keV)	300	60

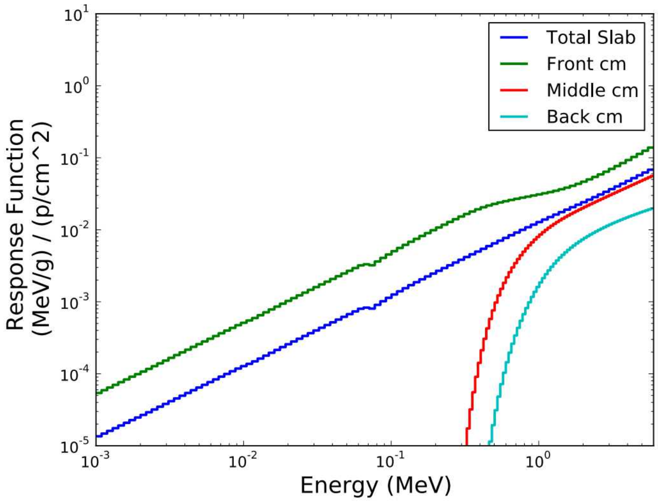

Fig. 2. Response functions for energy deposition in various regions of a 4.0 cm tungsten slab for particles normally incident on the left face of the slab.

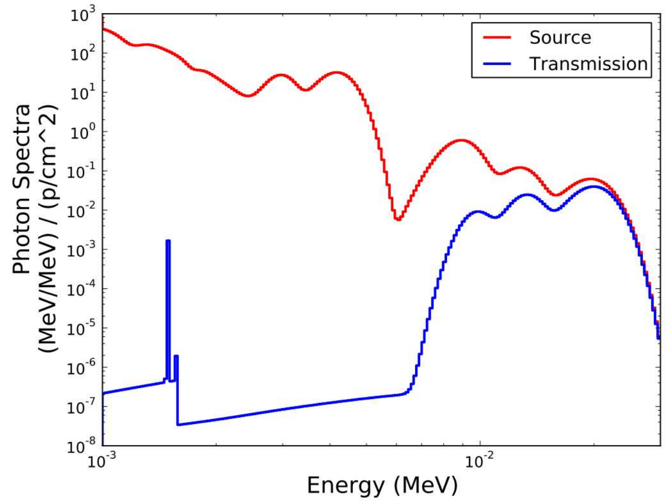

Fig. 4. Photon spectra produced by NIF source normally incident on 0.05 cm of aluminum.

RAPTURE show excellent agreement with results calculated with TIGER.

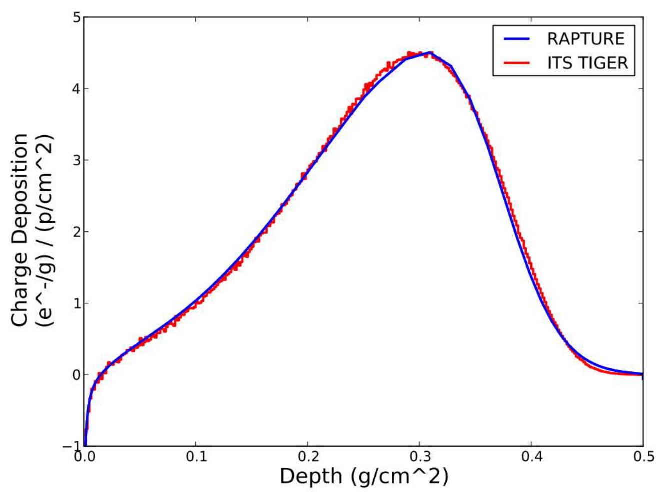

Fig. 3. Charge deposition profile for 1 MeV electrons incident on a slab of plastic.

The fourth figure highlights RAPTURE's ability to process complex radiation sources. This problem models a spectrum produced by the National Ignition Facility at Lawrence Livermore National Laboratory impinging upon a 0.05 cm sheet of aluminum. The desired QoI is the photon spectrum transmitted through the aluminum layer. The driving spectrum is described by a CDF containing 30,000 data points. Figure 4, produced by RAPTURE, shows both the source spectrum and the spectrum transmitted through the aluminum layer.

Additional test problems are contained in the RAPTURE release and will be demonstrated during a computer demonstration during the HEART meeting in March.

Acknowledgment

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