AC 2008-657: TEACHING THE SN METHOD: ZERO TO INTERNATIONAL BENCHMARK IN SIX WEEKS

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Abstract

The discrete ordinates or S_N method is employed to solve the neutron transport equation in a number of code packages that are considered mainstays of reactor design and safety analysis. Yet students often begin using these codes without having gained the deep understanding of the S_N approach that stems from implementing the S_N algorithm in a computer code of their own design.

This paper presents a series of lectures and computing activities involving beginning graduate students having no prior transport theory experience. The students wrote three codes: a multigroup spatially homogenized code, an S_N code in one-dimensional slab geometry and an S_N code in two dimensional cartesian geometry. Accurate group cross sections and Legendre moments are essential for high-fidelity calculation; therefore, the students were also taught to use NJOY99[1] to generate appropriately weighted and energy self-shielded group constants. MATLAB code and NJOY99 script templates are presented for each of these activities.

The students validated their final S_N codes against an infinite-lattice pressurized water reactor (PWR) benchmark developed by the Organization for Economic Cooperation and Development Nuclear Energy Agency (OECD NEA). Good agreement – within a few percent on multiplication factors, spectra, and neutron interaction rates by species – was obtained. The students came away with self-authored, easily generalized S_N algorithms and, more importantly, deeper confidence and understanding when using commercial S_N codes in their own research.

1. Introduction

With the emergence of high-performance computing as an everyday, widely-used tool, Monte Carlo approaches to solving the neutron transport equation have become ascendant in both the classroom and the research arena. Monte Carlo codes offer the advantage of direct, exact solution of the transport equation with accuracy limited only by the fidelity of nuclear data and the availability of computing power. Hence other methods for solving the transport equation – discrete ordinates (S_N), collision probability and integral approaches – while still in wide use are perhaps no longer being as intensively developed. This shift extends to the classroom in the sense that it is often easier to teach students to use Monte Carlo code packages especially when the system being studied contains irregular geometries.

It can be argued that, since even PhD students will be unlikely to be called upon to develop their own deterministic transport software during the course of their careers, teaching these methods from other than a theoretical standpoint is not productive. On the other hand, it is very likely that these students will be called upon to make use of a 'legacy' deterministic transport code. A number of codes that use the discrete ordinates approximation to the transport equation remain in widespread use; this method remains a very strong choice when systems having regular lattice geometries or systems in which neutron populations in regions of space and/or energy vary by

many orders of magnitude. Given the considerable investments that have been made in perfecting these codes, and the range of applications for which they are considered standard tools, it is likely that they will continue to be used for decades. However the new generation of professionals, steeped in Monte Carlo approaches during their training, might find themselves stymied when confronted with such unfamiliar issues as mesh construction and spacing, ray effects, negative flux fix-up, and convergence acceleration techniques quite unlike those employed in Monte Carlo calculations. The young professional who has not had practical experience with the S_N method at the level of encoding and debugging his/her own algorithms, could struggle to develop an intuitive grasp of the tool. Experience has shown that code users who are not first code developers are prone to making errors that stem from the mathematics employed by the code being, to them, a black box.

This paper describes a six week module taught for the first time at The University of Texas at Austin in Fall, 2007. The module constituted about half of the Computational Methods in Radiation Transport class, a graduate-level elective. The class assumes a background in computer solution of the diffusion equation but no prior knowledge of deterministic transport methods, computational or otherwise. Students learned the theoretical basis for the solution the S_N equations for one and two dimensional geometries and practiced its implementation by completing three coding exercises. The coding exercises culminated in the reproduction of an international criticality benchmark calculation for a UO_2 fuelled water moderated pin-cell in an infinite square lattice. Students developed their own multigroup cross section libraries as well, thereby mastering another critical and generally poorly covered step in performing a transport calculation. Finally, the students were asked to devise an exercise inspired by their research and adapt their S_N code to analyze it. These exercises, which ranged in subject from an oil well logging problem to a study of the effects of homogenization in TRISO fuel kernels, were quite successful and will be used as case studies in future offerings of the class.

The remainder of this paper is structured as follows. Section 2, Curriculum, describes the materials covered during the six week module. In Section 3, Exercises, the three computational problems and one NJOY exercise assigned to the students are presented. Section 4, Projects, addresses the students' self-directed application of their S_N codes to problems germane to their research.

2. Curriculum

Since the module was to be presented in just six weeks, coverage of the material in the text (Lewis and Miller[2]) was necessarily abbreviated. Table 1 shows the schedule followed during the seven weeks of the module – six weeks devoted to transport theory and methods and one week spent covering preparation of multigroup cross sections in NJOY99.

Table 1. Course Schedule for Discrete Ordinates Module. L&M = Lewis and Miller.

Time	Topic / Activity	Assignment
Week 1: 8/30/07	Introduction; preliminaries: what is the S_N theory? Derivation of the transport equation	L&M Ch 1
Week 2: 9/4, 9/6	Transport equation, scattering distribution, Legendre polynomials, spherical harmonics	L&M Ch 1 and Appendix A

Week 3: 9/11, 9/13	Energy and time discretization: multigroup formulation, multiplying systems	L&M Ch 2
Week 4: 9/18, 9/20	Implementation and acceleration of multigroup calculations. Interlude: NJOY99	L&M Ch 2
Week 5: 9/25, 9/27	P_N and S_N methods in one dimension: spatial differencing in Cartesian and curvilinear coords.	L&M Ch 3
Week 6: 10/2, 10/4	S_N methods in one dimension, cont'd: implementation and acceleration	L&M Ch 3
Week 7: 10/9, 10/11	Multidimensional S_N method: quadrature sets, Cartesian, curvilinear, hexagonal geometries	L&M Ch 4

The lectures were prepared entirely in PowerPoint; classes were videotaped and made available for online viewing using the distance learning classroom facilities at (Unversity). The lecture slides are available from the author upon request.

The text presents theoretical material and derives relevant sets of difference equations. The class significantly departed from the text in that it focused heavily on practical implementation of the methods by the students themselves. To that end a number of animations were prepared to aid the students in visualizing the practical elements that come into play when solving the discrete ordinates equations numerically.

As an example of the use of an animation to illustrate putting a concept into practice, consider the problem of solving the one-dimensional discrete ordinates equations in slab geometry subject to reflecting boundary conditions. Figure 1 shows how an animation helps explain the concepts of iterating on the scattering source, assembling the angular fluxes $\psi_{i,ng}$ for each mesh point i, ordinate n and group g via successive left-to-right and right-to-left sweeps, and banking scattered and reflected neutrons for use in the next iteration.

In the animation, of which only a snapshot can be depicted in this paper, a source of reflected neutrons is present at the left-hand edge of the slab of transporting material (yellow). The animation shows how the reflected neutron field is used to determine the ordinate fluxes for the rightward-directed ordinates at the first mesh boundary point $x_{1/2}$. The animation shows how these fluxes, plus a known inscattering source that has been already calculated for each mesh element, are used to solve for the ordinate fluxes at the first mesh center point x_1. The animation then propagates the calculation of the rightward-directed ordinate fluxes until the sweep reaches the right-hand edge of the material. Subsequently, the rightward-directed ordinate fluxes at the final boundary point $x_{I+1/2}$ are saved for use as specularly reflected incoming fluxes during the next iteration, and the right-to-left sweep for the remaining ordinate fluxes begins. Further animations show how the converged flux distribution is obtained by summing the results obtained from each scattering source iteration.

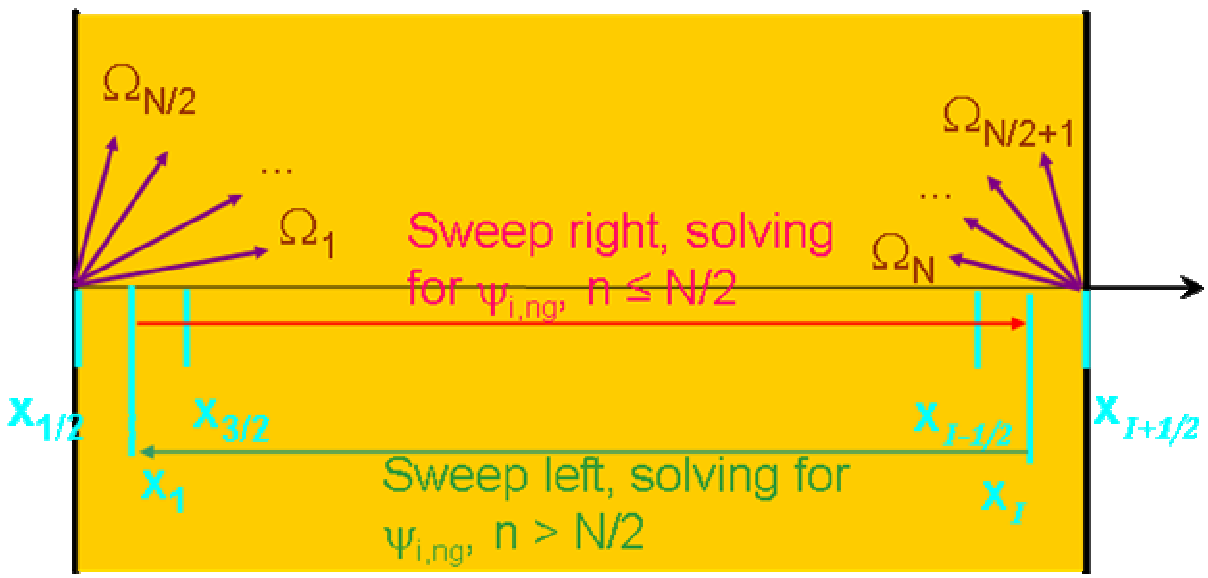

Figure 1. Typical Animated Illustration from Online Lecture Materials

A second animation, shown in Figure 2, displays the steps associated with assembly of a first collision source ($s^1_{i,n}$, neutrons scattering from the beam in mesh interval i and traveling in direction n) to be used in subsequent transport calculations given a monodirectional beam of incident neutrons. The animation shows the calculation of the scattering rate from the incident beam so generate a local scattering source magnitude for each mesh interval. The next frame in the animation cannot be seen in the figure; it shows the reconstruction of the scattering kernel from the Legendre moments of the scattering cross section. The final frame in the animation shows the assignment of the individual source terms for neutrons traveling in the direction associated with each ordinate from the collision density and scattering kernel.

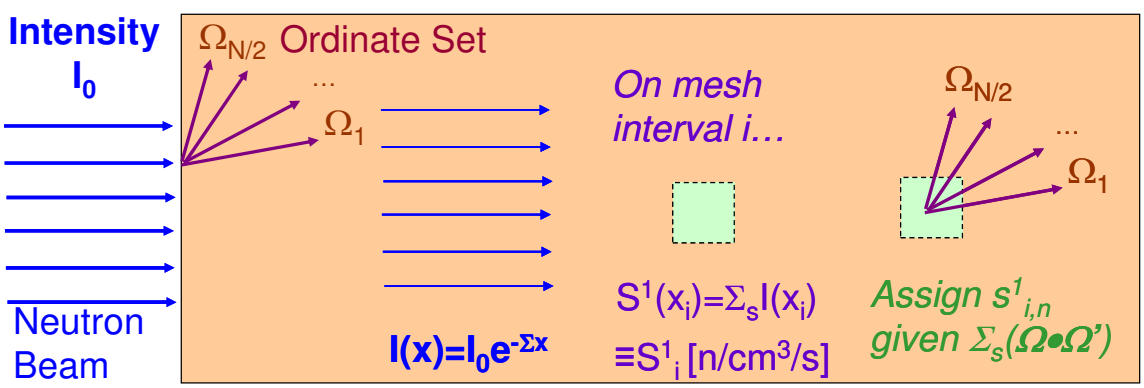

Figure 2. Animated Illustration: Generation of First Collision Source

Further visualization tools included methods for depicting the ordinate fluxes themselves. Students showed a tendency to be uncomfortable with the ordinate fluxes, ψ_n, as compared to the angle-integrated flux ϕ which they had seen many times before. The class found compass

diagrams that associated the ordinate fluxes with their directions, as shown in Figure 3, to be helpful. This visualization tool became particularly valuable when the time dependent transport equation was being solved. A graphical illustration of ordinate fluxes directed outward toward the edges of a bare slab decaying with time more quickly than fluxes pointed along the axis of the slab in a transient problem, for instance, was considered by the students to be a powerful illustration of a phenomenon that cannot be reproduced using diffusion theory.

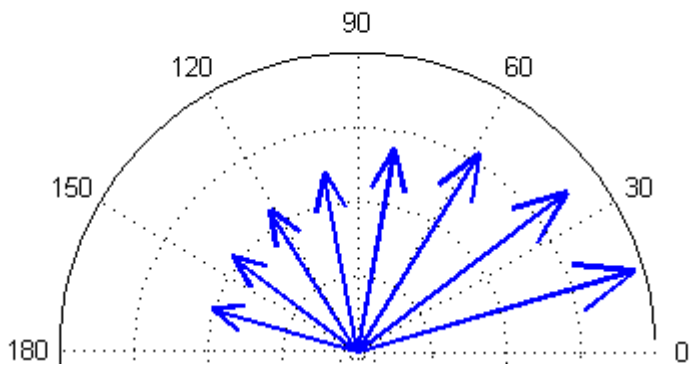

Figure 3. Compass Plot of Ordinate Fluxes

Other animated graphics included flowcharts depicting the logical progression of an S_N transport calculation. One such flowchart is shown in Figure 3. This flowchart shows the iterative process for an eigenvalue calculation in one dimension, beginning with initial guesses for the ordinate group fluxes and multiplication factor. The outer (eigenvalue) and inner (scattering source) iterations are shown, as are the sweeping loops. These animations proved popular with the students as a valuable complement to the more theoretically oriented treatment of the subject in the text.

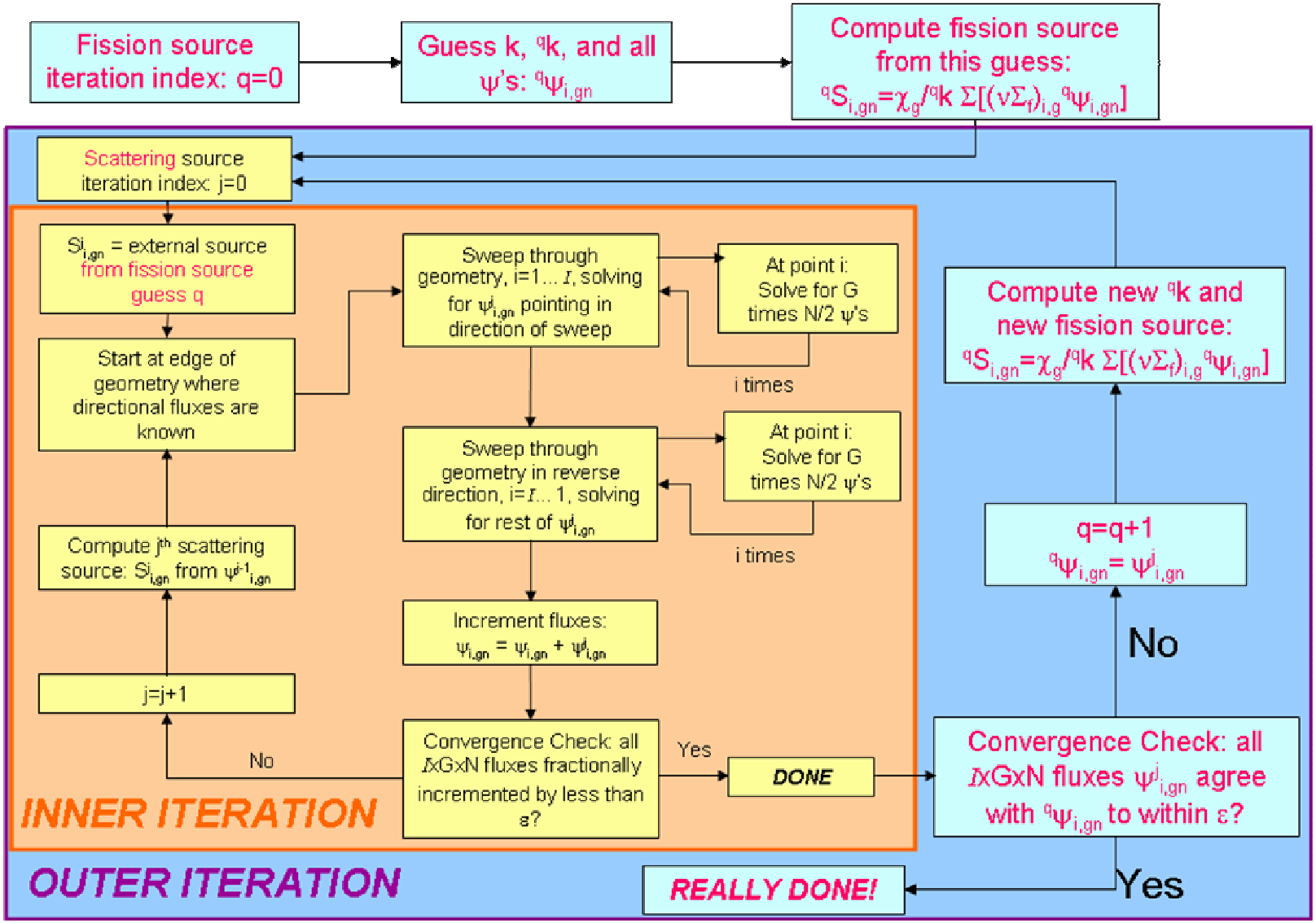

Figure 3. Animated Flowchart: Progression of an S_N Calculation

3. Exercises

The three coding exercises – two preliminary exercises followed by the benchmark case – were completed by the students during the final four weeks of the module. Students were free to complete the exercises in the language of their choice; in the event, most students chose MATLAB with the remainder working in C++. The first of the preliminary exercises, a multigroup calculation in an infinite medium, was intended to allow the students to design the necessary data structures and to read in and initialize the cross section database they constructed in NJOY99. This database exercise is discussed further below.

The second coding exercise involved a neutron beam incident on a nonmultiplying slab of borrated graphite. Students added one-dimensional discrete ordinates transport to their multigroup code; as an aside, several incident neutron beam energies were considered. The graphite scattering kernel, nearly isotropic at low energies, becomes highly forward-directed at higher energies while the cross section remains roughly the same. This exercise offered dramatic illustrations of the dependence of angular flux distributions, and therefore the transmission probability through the slab, upon the angular distribution of scattered neutrons.

The second coding exercise also offered a platform for demonstration of convergence acceleration techniques, in particular coarse mesh rebalance. These techniques proved to be much easier for students to grasp if they were implemented and their results graphically presented. An example of a coarse mesh rebalance step is shown in Figure 4; in practice, this is displayed in class as an animation where students can observe the rebalance taking place in each coarse mesh interval.

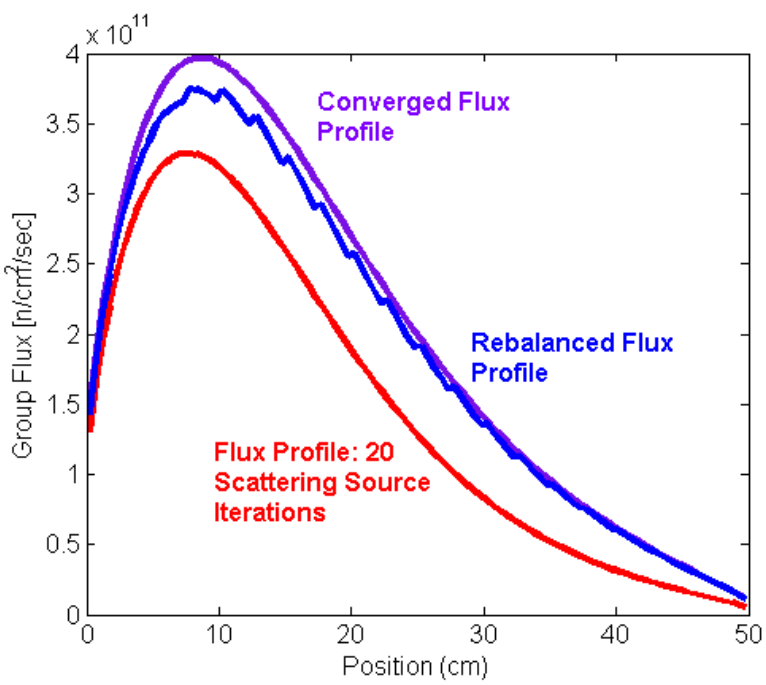

Figure 4. Illustration of Coarse Mesh Rebalance Process

The final coding exercise was to reproduce the calculation of reaction rates, flux spectra and multiplication factor presented for an infinite lattice of pin cells in the first phase of the OECD Burnup Credit Criticality Benchmark[3]. The benchmark case considered uranium oxide fuel in with an infinite array of simple pressurized water reactor unit cells. To limit the number of cross sections to be prepared, only the fresh fuel configuration was considered. Given the square lattice, the problem would be tractable in two-dimensional Cartesian as well as quasi one-dimensional cylindrical geometries. The decision to perform a two-dimensional Cartesian calculation was made because students could easily adopt their earlier codes which used one-dimensional Cartesian geometry.

Students were able to reproduce the benchmark results quite well. Figure 5 shows one student's result for the 10 group flux spectrum averaged over the fuel region as compared to the benchmark value. The greatest source of error in the calculation can be divined from this figure: a large number of scattering source iterations requiring significant computation time (at least for students coding in MATLAB) were required to obtain good convergence. Students who obtained an inadequate near-Maxwellian thermal peak had generally not carried out enough iterations.

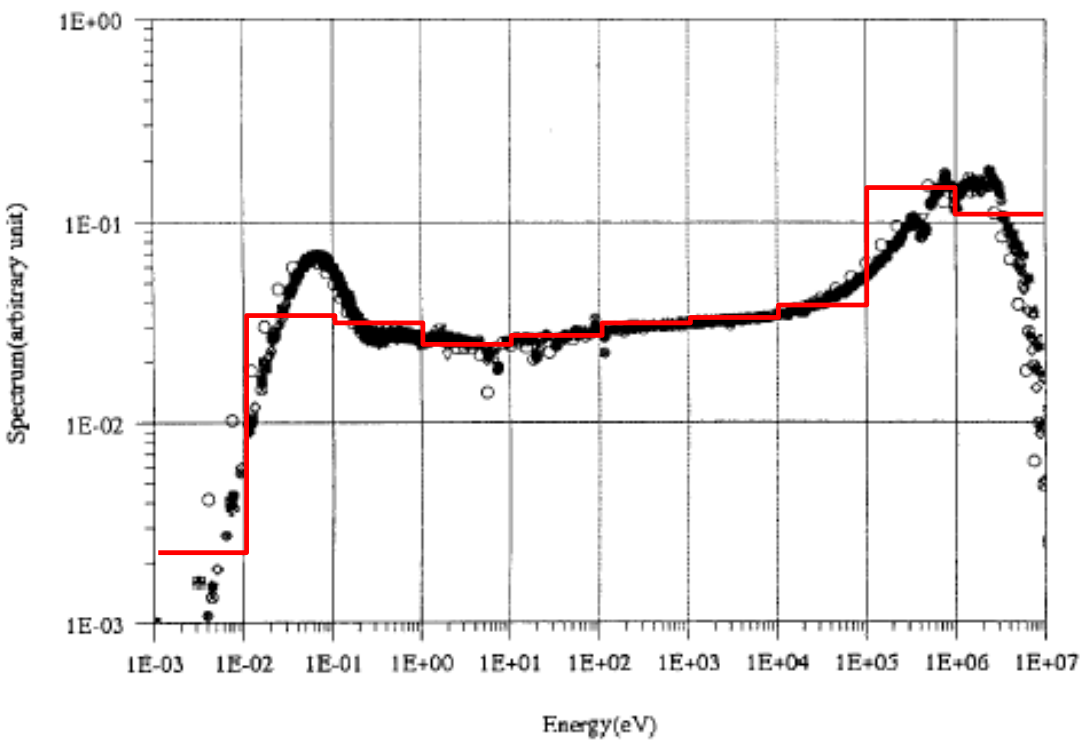

Figure 5. Comparison of Spectra, 10 Group S_8 (Red), Benchmark (Black)

Figure 6 shows student S_N results of the flux distribution in one quarter of the unit cell for representative fast and thermal energy groups. In the figure the geometric center of the fuel element is located at the (0,0) coordinate point. Figure 7 displays MCNPX results for analogous regions of space and energy. Agreement was seen to be excellent, although some error can be seen in the moderator region of the fast group where the S_N flux distribution shows a slight peak.

The peak is due to both ray effects and negative flux fix-up and can be reduced by decreasing the mesh spacing. Ordinate scales in all figures are arbitrary.

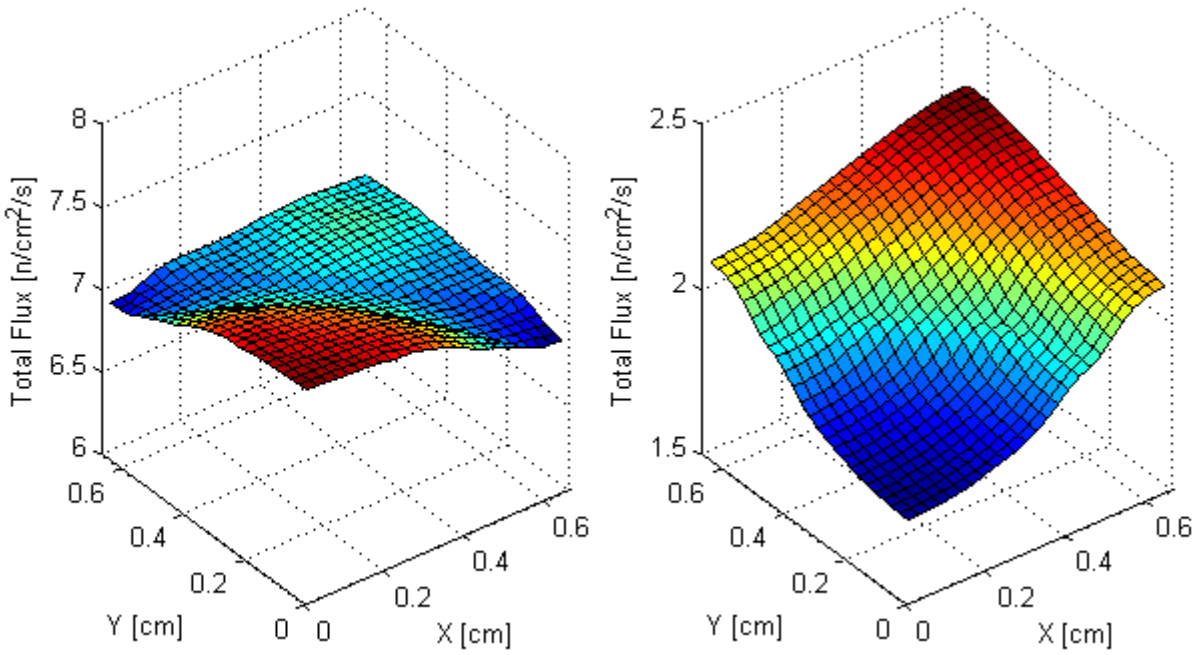

Figure 6. Flux Distribution, 10 Group S_8, 100 keV – 1 MeV Energy Group (Left) and 0.01 eV – 0.1 eV Group (Right). Pin Centerpoint is Located at (X=0 cm, Y=0 cm).

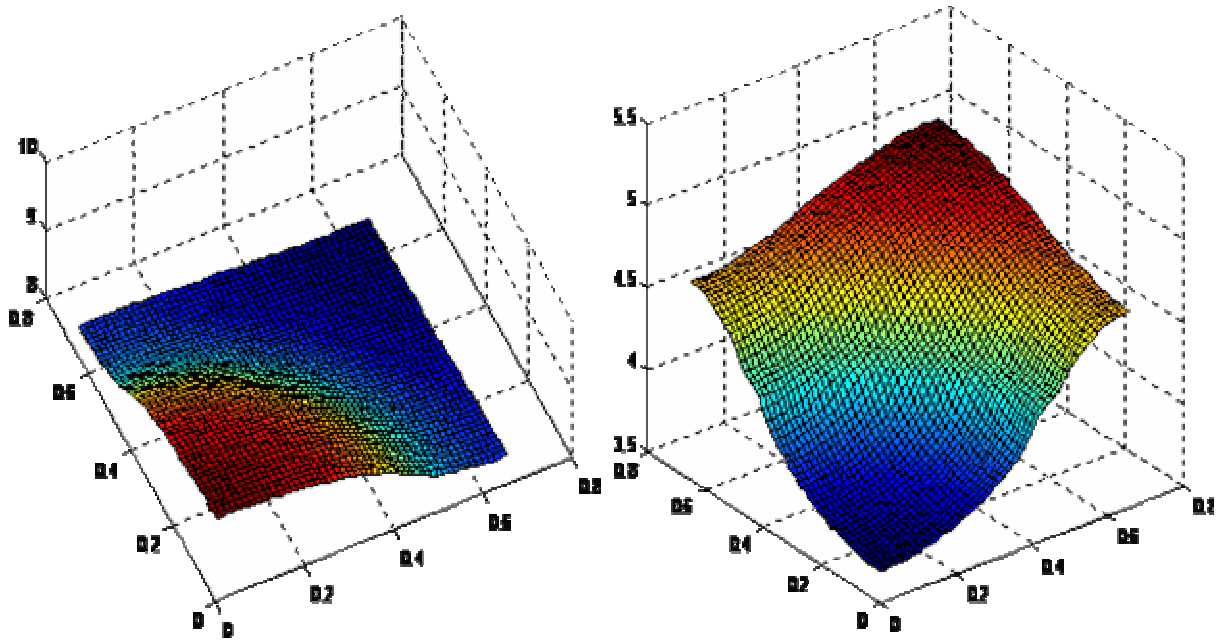

Figure 7. Flux Distribution, MCNPX, 100 keV – 1 MeV Energy Group (Left) and 0.01 eV – 0.1 eV Group (Right).

Multiplication factors and per-species relative production and destruction rates also agreed well. The multiplication factor of 1.465 obtained by the student should be compared against the benchmark value of 1.439 +/- 0.017. Similarly, the benchmark reported that 73.3% neutrons absorbed in the fuel were absorbed in ^{235}U, while this student computed 74.5%. Neutron production rates were in even better agreement; the benchmark result for the fraction of neutrons produced from ^{235}U fission was 94.5% while this student predicted 94.7%.

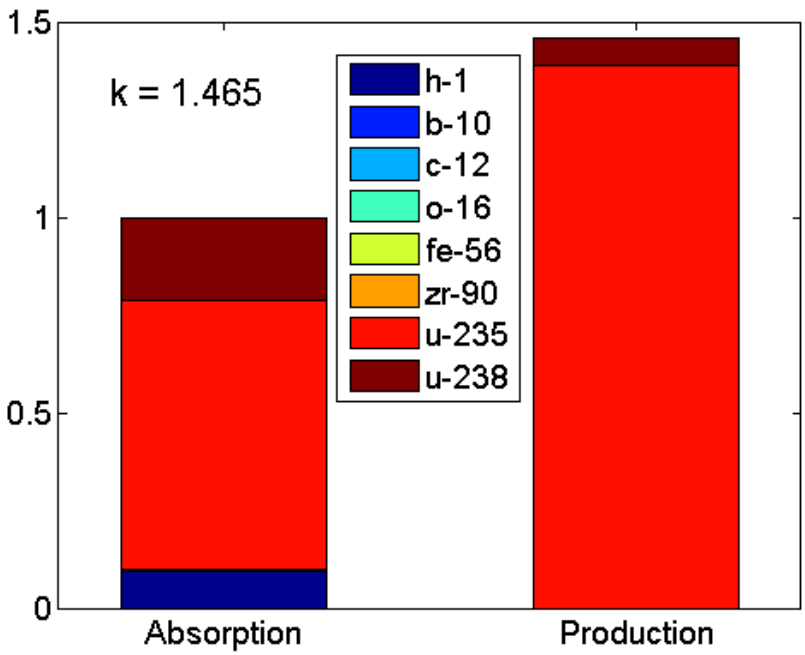

Figure 8. Neutron Absorption and Production Rates in Benchmark Cell, Normalized to Unit Absorption Rate

Of course, the central reason that the results are of good quality is that care was taken in creating the cross section libraries. During week 4 of the module students constructed these libraries using NJOY99 and adjusted them later to account for energy self shielding in the actual benchmark problem. Students were asked to create libraries of specified format from the NJOY results, which were to include scattering kernel Legendre orders of up to eight. The greatest difficulty in this portion of the class was not instructing students in the use of NJOY to create doppler-broadened temperature dependent group constants. Rather it was in the explanation of the critical importance of problem-dependent and energy-dependent background cross sections. Demonstrating to the students that the use of unselfshielded cross sections led to errors of 50%, rather than ~2%, in the multiplication factor for the benchmark case was convincing, albeit after the fact.

4. Projects

In lieu of a final exam the students were assigned a project. Students were responsible for choosing their own problem, ideally one drawn from their research, to which they would apply an S_N theory calculation. The text below is excerpted from the project assignment sheet.

"Purpose: apply NJOY99 and/or discrete ordinates theory to a problem you determine yourself. The problem would ideally be relevant to your own research, however this is not required. I would like you to think about this over the next few days and write a brief (less than 1 page) proposal.

My expectations: the project should require reasonable additional work beyond what we have already done, e.g.,

- preparation of additional cross section libraries,
- alteration of 1-D discrete ordinates code to include more regions, more materials, additional boundary conditions, and/or multiplying material,
- alteration of 2-D discrete ordinates code to address nonmultiplying material with fixed sources, additional materials, and/or other boundary conditions. Beware of choosing a too-complex problem here!
- alteration of 1-D discrete ordinates code to use a convergence acceleration method other than the one discussed in class.

What you should do:
There is no firm length requirement on what you should turn in; however it should be in the format of a report or technical paper. Here are some things you should include:

- A problem statement including motivation, definition of goals, simplifying assumptions made.
- A methodology section including enhancements or changes made to the code(s) you developed for class
- The results section should include sufficient numerical and graphical results to constitute a reasonably complete depiction of the radiation field you have calculated – what constitutes 'sufficient results' is left to you to determine as part of this exercise
- Code and input deck listings should be attached as appendices.

In addition to a report, I would also like each of you to plan on making a 15 minute presentation of your project, methodology and results."

The topics chosen by the students for the projects included:

- *Comparative Results of 2D Discrete Ordinates and Monte Carlo Methods in a Simple Neutron Logging Problem*
- *Use of 2D Discrete Ordinates to Calculate One Group Fuel Cross Sections for ORIGEN Burnup Calculations of Recycled Uranium Fuel*
- *Modeling the University of Texas TRIGA Reactor Hexagonal Lattice Using a Discrete Ordinates Transport Code with Triangular Coordinate System*
- *Effects of Spatial Homogenization in Random Media Transport Problems using One-Dimensional Discrete Ordinates*
- *Using The Time Dependant One Dimensional Transport Equation to Model the Propagation of a Pulse*
- *Comparison of MCNPX and Deterministic Transport for Active Neutron Interrogation of Shielded SNM*

In the event, the projects were so successful that the department chose to bind them into a package for publication and distribution as publicity material.

5. Conclusions

Although written student comments were not yet available as of this writing, feedback from the class was largely positive. The most often voiced complaint is that too much material was omitted; for instance, non-Cartesian coordinates were not covered, and only one acceleration technique was addressed in detail. The second half of the course as it was taught in Fall, 2007 focused on Monte Carlo methods and the option of breaking this offering into two courses is being considered so that each may be presented in more detail.

The projects were generally viewed favorably, although some students struggled to find a problem that was both tractable to ground-up modeling within a two week time frame and relevant to their research.

However, given that most of the students in the class will not likely be called upon to write a discrete ordinates transport code again, the most important question posed by the evaluator was in regard to the relevance of the class. Here the response was clearly in favor of retaining the module in the curriculum. Verbal communication with the students indicated that they felt their understanding of neutron transport phenomena to have been considerably advanced by the class, and that the coding exercises were definitely responsible for this positive effect. Students indicated that their level of confidence and comfort when using commercial transport codes was significantly improved by "getting inside the black box." Therefore, student coding exercises, omitted in earlier offerings of transport classes at the University of Texas at Austin as well as many other institutions, will be further emphasized in upcoming offerings of this class.

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