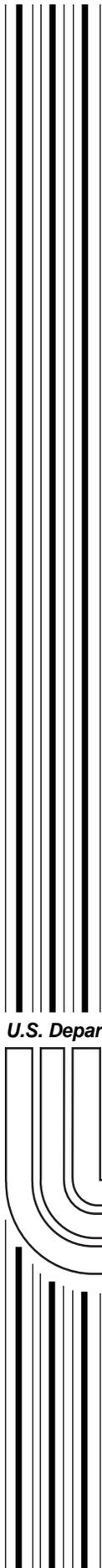


**TART:
Monte Carlo Radiation Transport in
Industrial Applications**

D. E. Cullen

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Lawrence
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TART: Monte Carlo Radiation Transport in Industrial Applications

by
Dermott E. Cullen
University of California
Lawrence Livermore National Laboratory
P.O. Box 808/L-128
Livermore, CA 94550

Telephone: 925-423-7359
E.mail: cullen1@llnl.gov
Website: <http://www.llnl.gov/cullen1>

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What is TART?

TART¹ is a coupled neutron-photon, 3D combinatorial geometry, fully time dependent Monte Carlo transport code, that runs on virtually any type of computer: mainframes, UNIX, IBM-PC/Windows/Linux, PowerMAC – you name it, TART runs on it. Compared to similar codes TART is incredibly fast, and yet still very accurate. While other codes may claim to use the most accurate nuclear data, TART takes things one-step further by also using the most appropriate nuclear engineering methods. It is this approach that makes TART suitable for use in such a wide variety of applications. It can perform criticality calculations: both static and dynamic. It can also perform neutron and/or photon source calculations.

Scope of TART

TART does what I call our bread and butter applications: those involving neutron and/or photon transport. The lion's share of our application only involve coupled neutron-photon calculations. Recently other codes have expanded to handle other types of particles, while TART has concentrated on improving its treatment of neutron and photons. TART uses continuous energy particles. In the case of photons it uses

continuous energy cross sections over the energy range 100 eV to 1 GeV. In the case of neutrons it uses multi-group, multi-band² cross sections, over the energy range 10⁻⁵ eV to 1 GeV (currently only implemented up to 20 MeV). Groups are equally spaced in lethargy [$\log(E)$], 50 per energy decade, for a total of 700 groups.

Not just one Code: a System

Rather than being one code that only performs Monte Carlo calculations, TART is a system of codes that helps you prepare and check input parameters, obviously allows you to run Monte Carlo transport calculations, and then helps you analyze your output. Interactive graphics are heavily used in this system. For example, the interactive graphics code TARTCHEK allows you to see your geometry in 2D and 3D, and to check for errors before you run TART. It also allows you to overlay your results on your geometry immediately after running TART. With this approach you can be very confident as to the accuracy of your TART input before you run TART, and rather than being faced with a large stack of output that could take you many days to analyze, within minutes you can see your results and get a global feel for variations in flux, energy

deposit, dose, etc., throughout your geometry.

Figures 1 and 2 illustrate the use of graphics. Figure 1 is a 3-D view of the geometry of a simple experimental set-up. We have a spherical photon source to the lower left. There is a cylindrical lead filter in the middle. Finally there is a cylindrical detector to the upper right. Figures such as this help to easily visualize our geometry, but even more useful is to see your results overlaid onto your geometry, as shown in figure 2. For this example I have used a photon source directed at the detector and having a 20 degree angular spread. Here I illustrate energy deposition. With the absolute scale at the lower right of the figure we can read directly off the plot how the deposition is varying. Note the high deposition in the lead filter (as we would expect in a high Z material), and the lower deposition in the detector. We can also see the spatial variation of deposition in the detector. With figures similar to this it is very easy to design experimental set-ups. For example, you can quickly check to see if this is really the thickness of lead filter you should use to achieve a given response in the detector. You can also check on other features that might not otherwise be obvious to you. For example, note the relatively high deposition on the side of the lead filter closest to the detector and outside of the photon source. This indicates a lot of backscatter from the detector, which might lead you to re-position the lead filter relative to the detector - something you might never have noticed when reading a long output listing - here you can see it minutes after you have run the TART calculation.

Figures 3 and 4 illustrate more complicated geometries; in this case, the TART input model for the entire National Ignition Facility (NIF), a seven story building, some 30 meters high. Figure 3 shows a different color for each spatial zone, and figure 4 shows a different color for each material.

User Friendly

One of the features of TART is that it is designed to be user friendly, and easily used by anyone. Unlike other codes where a user is expected to be an expert in radiation

transport, using TART doesn't require any background in this area. I have tried to keep it simple and intuitively obvious, so that almost anyone can productively use it.

For example, TART has an array of options for importance sampling, unfortunately as with all codes of this type, if you are not an expert and really understand what this implies, you can really screw yourself by trying these options. Instead, because TART is so fast and we have so much cheap computer power available, I recommend that users not use importance sampling, and instead overwhelm their problems with more histories; below, I'll discuss how many histories. This way users can concentrate on what they know best, such as an accurate model of their geometry and sources, and let TART concentrate on what it knows best, which is quickly supplying an accurate, easy to understand answer.

Why use Monte Carlo?

In principle Monte Carlo is the only method that can accurately model our applications. Other methods are limited in their ability to model complicated geometry; this point is well known, but there are many other advantages to Monte Carlo, that I'll cover in detail below. Here I'll only mention that other methods are also limited in their ability to accurately model reaction kinematics; this point is less well known. For example, if we consider even the simple cases of neutron elastic scattering, and photon Compton scattering, where there is an exact correlation between the scattering angle and secondary energy of a particle, this exact correlation cannot be accurately modeled by deterministic methods, whereas it is relatively simple to do using Monte Carlo. If this is important in your applications, is there any question that you should be using Monte Carlo.

The Advantages of Monte Carlo

The ability of Monte Carlo to model complex geometry is usually quoted as "THE" advantage of Monte Carlo over deterministic methods. In fact this is but one of many advantages of Monte Carlo. I'll briefly describe this and other advantages of Monte

Carlo, with emphasis on how TART attempts to use these to its own best advantage.

In order to insure that TART makes the most of the advantages of Monte Carlo it allows geometry to be defined in terms of 3-D, combinatorial geometry. As with most 3-D Monte Carlo codes, TART allows the surfaces of spatial zones to be defined in terms of combinations of first degree surfaces (planes) and quadratic surfaces (spheres, cylinders, cones, etc.), but TART also allows surfaces to be defined by cubic and quartic surfaces; an example of a quartic surface is a torus. The extensions to cubic and quartic surfaces makes it possible to define very complicated surfaces as smoothly varying, similar to what automobile manufacturers can do in designing the profile of an automobile.

Monte Carlo has another advantage over deterministic methods in that it can exactly model kinematics, for example it is simple for Monte Carlo to model the exact correlation between secondary energy and scattering cosine for neutron elastic scattering and photon Compton scattering. In comparison take a close look at how an S_N code models these kinematics using a P_L expansion of the scattering and multi-group transfer matrices; you may be shocked to see how crude this is modeled.

Another advantage of Monte Carlo is its ability to model continuous energy particles, as opposed to multi-group particles. Here TART takes advantage of this by using continuous energy neutrons and photons, and continuous energy kinematics for each reaction. But in the case of neutrons it takes things a step further by using multi-group cross sections; I'll discuss this point of continuous energy neutrons using multi-group cross sections in more detail below.

Yet another advantage of Monte Carlo is its ability to edit or tally almost any quantity of interest. In the case of TART output always includes for each spatial zone both analog and expected energy deposition, and reactions, versus energy and time, as well as integrals over energy and time. In addition for each zone the user may request one of 21 different types of derived analog and/or expected results, such as scalar flux

or current, angular distributions, etc. These output options used in combination with TART's utility codes, allows user to quickly define and in most cases use graphics to see their results.

I'm not finished yet – another advantage of Monte Carlo is its ability to use multiple processors to solve problems. Here the TART system includes the codes MULTIPRO and TARTSUM to allow you to use as many different processors, on as many different computers as you can get your hands on. With TART's approach, you can make all of these runs at the same time, or a series of runs, and you can still combine all of your results to define your final answer.

Garbage in, Garbage out!

It is extremely important for code users to understand that any radiation transport code is only as good as the nuclear and atomic data that it uses. It cannot be stressed enough that regardless of how modern and easily useable today's codes are, if the nuclear and atomic data they use are not the best available, you can be in a "Garbage in, Garbage out" situation. It is amazing to me how many hotshots are interested in writing codes to perform transport calculations, and yet they totally ignore the importance of the data they use. Therefore, before deciding to use any radiation transport code you should know the pedigree of the nuclear and atomic data it is using. In the case of TART, it always uses the most recently available ENDF/B data for both neutrons and photons. Currently TART uses the ENDF/B-VI, release 7, neutron data³, and our EPDL97 photon data⁴ (now adopted as the ENDF/B standard photon data).

Most Appropriate Nuclear Engineering

As an example of using the most appropriate nuclear engineering methods, I'll discuss the difference between the multi-group, multi-band cross sections used by TART, and so called continuous energy cross section codes.

First let me state that none of the codes presented in this session; namely, VIM, MCNP, and TART, exclusively use

continuous energy cross sections. All of these codes use a multi-group method in the unresolved resonance region: VIM and MCNP use the probability table method, and TART uses the multi-band method². In all cases the objective is similar, in trying to account for the effect of resonance self-shielding in the unresolved resonance region.

TART takes this a step further by using multi-groups and the multi-band method at all energies to account for self-shielding. Why don't I follow the current trend and simply extend TART to use continuous energy cross sections; it wouldn't be hard to do. Why? Because for my problems I do not think it is a good idea, in that continuous energy cross sections can actually introduce more problems than they solve.

For example, an interesting question to ask is: how many codes are really using accurate continuous energy cross section; here I stress the word "accurate"? I use one code that claims to use continuous energy cross sections. When I examined in detail what it is doing I discovered that for U-238 it is using cross sections tabulated at about 3,200 energy points; this is claimed to be ENDF/B-VI data. In contrast when I reconstruct the ENDF/B-VI U-238 to a modest of accuracy of within 0.5 %, I need over 83,000 energy points (see, ref. 3); and, when I reconstruct to high accuracy in order to define data for use by TART I have over 250,000 energy points. 3,200 versus 250,000 energy points? This makes me question how accurate are the cross sections used by this continuous energy cross section code; as I stated above, your answers can only be as accurate as the nuclear data you are using.

TART does not use continuous energy cross sections because it: 1) makes codes run much, much longer, to run the same number of neutron histories, 2) convergence due to uncertainty introduced in sampling in the cross sections can be incredibly slow, meaning that we have to run many more neutron histories to reach convergence, and 3) most important: for my problems, I can get the same answer, to the same accuracy, in much less time, using multi-group, multi-band cross sections. The approach used by

TART is to start from the best available cross sections, represented to high precision, and to then use the most appropriate nuclear engineering methods to apply the methods we were taught in graduate school. This approach allows me to account for resonance self-shielding over the entire energy range by using the multi-band method. Compared to a continuous energy cross section data, this approach allows TART to run the same number of histories much faster, and virtually completely eliminates the problem of convergence due to cross section sampling, and when I compare answers, mine are the same or better than what I get from continuous energy cross section codes. How can my answers be better? They are often better because I would have to run the other code for an incredibly long time in order to achieve convergence in cross section sampling.

To illustrate my point concerning cross section sampling, consider an array of fuel pins in water. Fission produces fast neutrons which leak from the fuel pins into the water, where they slow down, and then try to find their way back into the fuel. Consider just a small part of this problem: neutrons with keV like energies are trying to find their way back into U-238. To appreciate the problem that faces a code using continuous energy cross section, figure 5 illustrates the U-238 total cross section over the energy range 1 to 2.15 keV. We can see that the cross section varies over a range of about a factor of a hundred, and has numerous narrow peaks and valleys. My question is: how many neutrons does the code have to sample in order to have a good estimate of:

the average cross section

$$\int_1^{2.15} S(E) \cdot \Sigma t(E) \cdot dE / \int_1^{2.15} S(E) \cdot dE ;$$

and distance to collision

$$\int_1^{2.15} S(E) / \Sigma t(E) \cdot dE / \int_1^{2.15} S(E) \cdot dE .$$

In an attempt to answer this question, I assumed neutrons were entering the fuel randomly in this energy range, i.e., I assumed S(E) is constant. I first analytically calculated the average cross section and distance to collision, and then randomly sampled energies and tallied the total cross

sections that I selected. Figure 6 shows the per-cent error in the average values versus the number of neutrons sampled. After 1,000 samples there is about a 10 % error in the sampled averages, by 10,000 it is reduced to about 3 %, and by 100,000 to less than 1 %. As we can see this a very slowly convergent process, and this is just one small energy range, and the cross section for only one material, so you can imagine how long it takes to converge in general. In contrast with multi-band parameters these averages are accurately defined within a hand full of samples, because this uses appropriate nuclear engineering methods, instead of just starting from scratch with the basic energy dependent cross sections.

More Information and Availability

Documentation for the entire TART system is now available at my website. TART2000 CD is now available through code centers throughout the world; this CD contains TART for use on mainframes, UNIX, IBM-PC/Windows/Linux, and PowerMAC. For details on obtaining TART2000 CD, see my website, <http://www.llnl.gov/cullen1>

Conclusion: Can you afford to use Monte Carlo?

In the past, the main reason that Monte Carlo radiation transport was not used more often was that it was considered to be prohibitively expensive and not practical if we wish to obtain an accurate answer in a reasonable period of time. It wasn't too long ago that we thought of Monte Carlo radiation transport calculations as limited to a few thousands of particle histories, e.g., track a few thousand photons. This is no longer the case. In just the last, few years the tremendous increase in inexpensive available computer power has allowed us to go from thousands, to millions, to billions of histories. For example, today a relatively inexpensive \$1,000 PC can be used with TART to process several billion photon histories per day; something we would have never even thought possible just a few short years ago. If you are a high roller with more computer resources you can push things even further. For example, with today's multi-processor computers that have

thousands of processors, you can use TART to process over a trillion (that's right, a trillion, 10^{12}) histories per day.

As an example of the recent tremendous increase in available computer power, consider that in 1996 the time required to run the set of 68 test problems distributed with TART on the fastest personal computer then available was 18,437 seconds, whereas today it is 89 seconds; an incredible decrease by a factor of 207; for details see, <http://www.llnl.gov/cullen1/speed.htm>

This means problems that took an entire 9 to 5, eight-hour workday in 1996, takes 2.3 minutes to run today. There has been a corresponding increase in the size of computers. A few years ago we were happy to have a few megabytes of memory; today even my laptop has 2 gigabytes of memory. All this increase in computer speed and size has been achieved while at the same time decreasing the cost of today's computers. That is absolutely incredible! Today we routinely run problems we would not have considered practical just a few short years ago.

Today, not only can TART run problems faster, but it has also kept up with the tremendous increase in available memory, by allowing problems of any size to be run. Just a few years ago TART was restricted to problems of a thousand or fewer spatial zones. Today, users can routinely run problems involving a million spatial zones.

The bottom line is that it is now practical to efficiently and quickly use Monte Carlo radiation transport to obtain very detailed and accurate answers. With the number of histories that we can now process, results have little, if any, statistical uncertainty. In addition Monte Carlo is the only method available to us that can accurately model the increased detail in our currently available data bases, e.g., exact correlated kinematics. Today we are to the point where the major cost in our applications is your salary; not the cost of computers. Therefore the question really should be: **Can you afford NOT to use Monte Carlo?**

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4) D. E. Cullen, J. H. Hubbell, and L. Kissel, "EPDL97: the Evaluated Photon Data Library, '97 Version," UCRL-50400, Vol. 6, Rev. 5, Lawrence Livermore National Laboratory, Livermore, CA, (September 1997); now available on-line at, <http://www-nds.iaea.org/epdl97/>

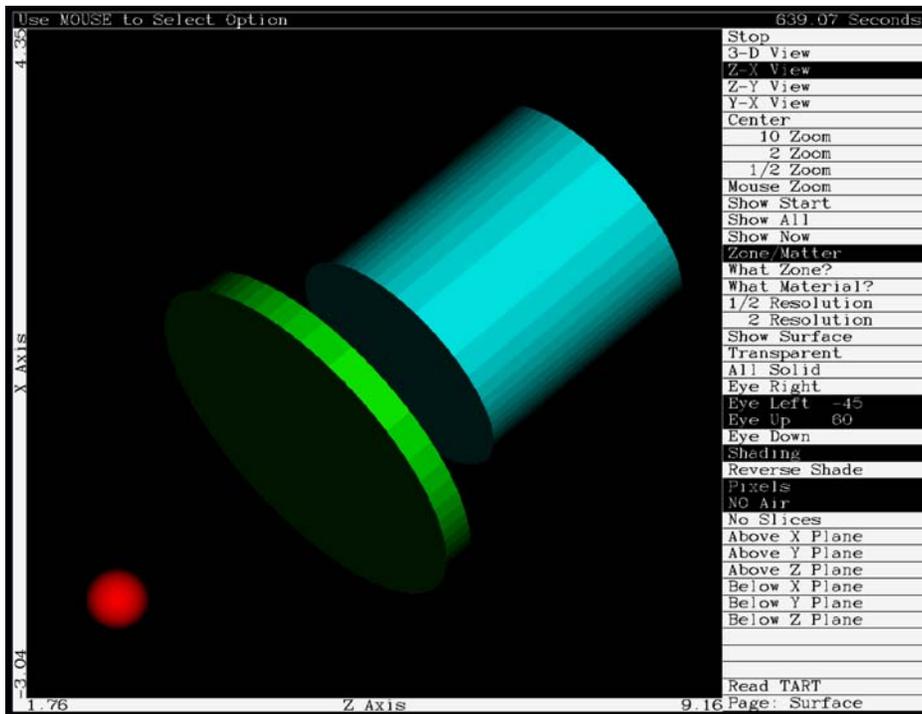


Fig 1: A simple experimental set-up.

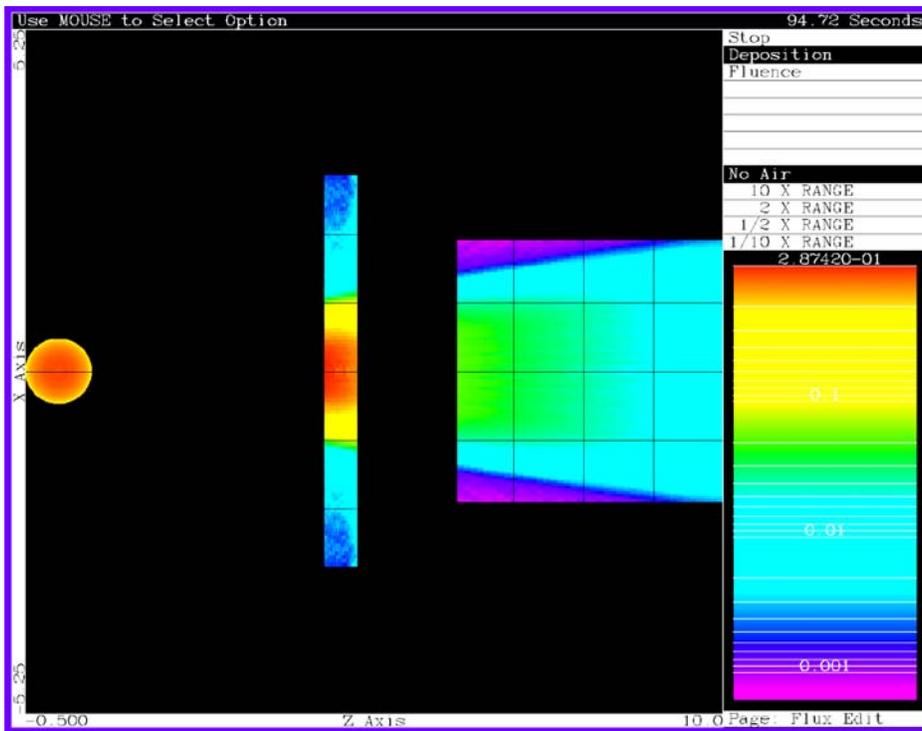


Fig 2: Overlay of energy deposition on geometry

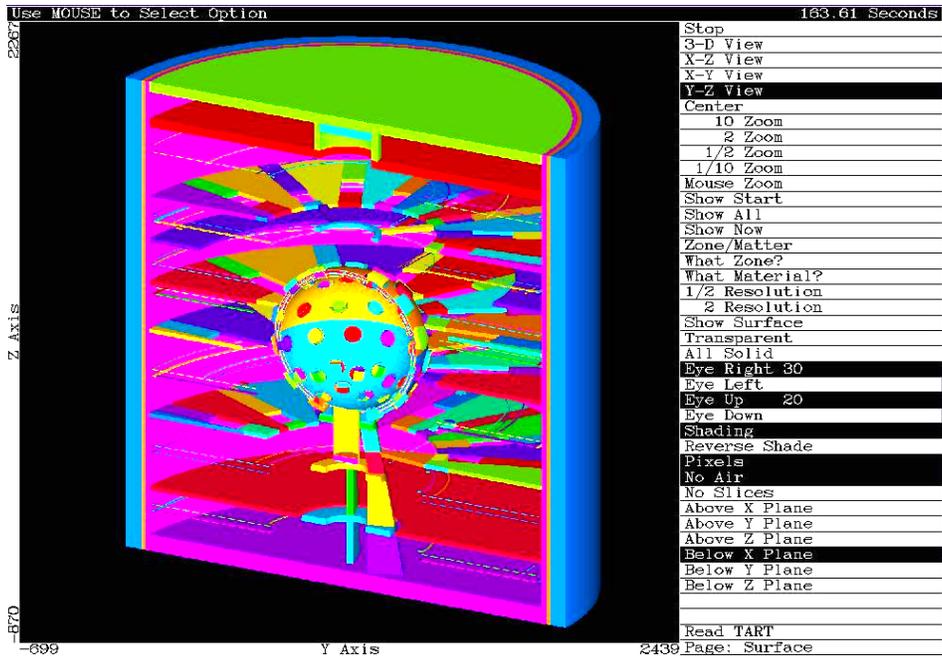


Fig 3: 3-D view of the National Ignition Facility (NIF) showing zones

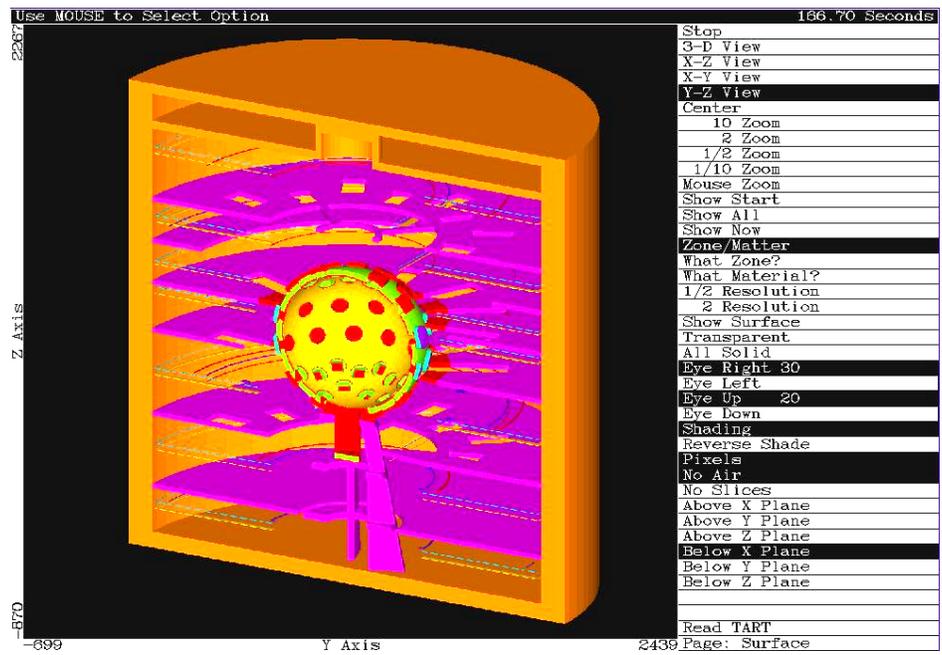


Fig4: 3-D view of the National Ignition Facility (NIF) showing materials

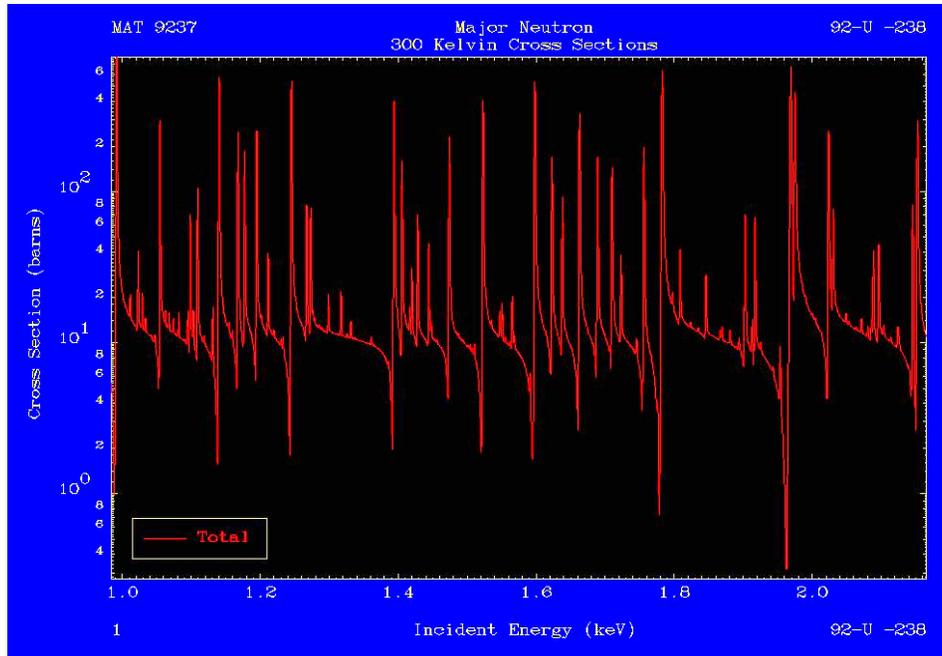


Fig. 5: U-238 Total cross section, 1 to 2.15 keV

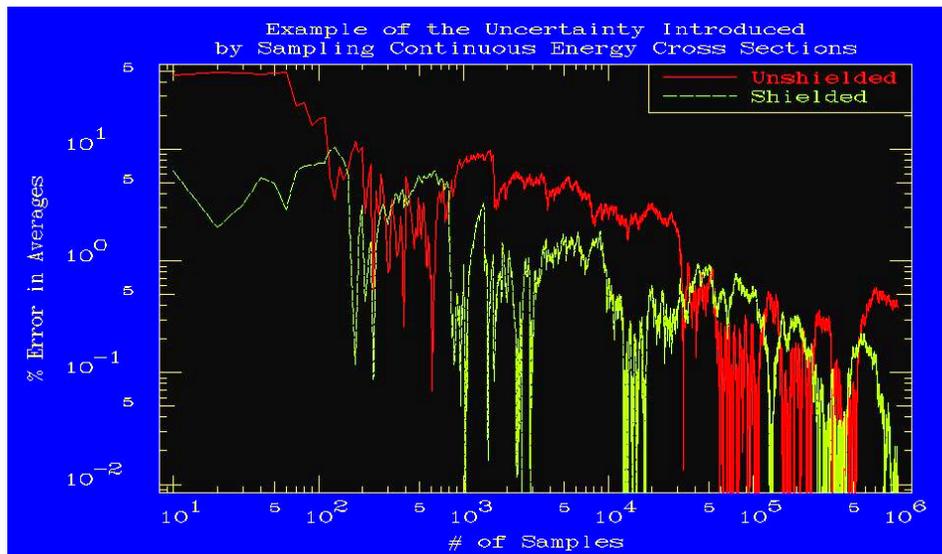


Fig 6: Error in Sampled Averages

University of California
Lawrence Livermore National Laboratory
Technical Information Department
Livermore, CA 94551

