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AN ULTRA-FINE GROUP SLOWING DOWN BENCHMARK

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ABSTRACT

We suggest a new solution to the neutron slowing down equation in terms of multi-energy panels. Our motivation is to establish a computational benchmark featuring an ultra-fine group calculation, where the number of groups could be on the order of 100,000. While the **CENTRM** code of the **SCALE** code package has been shown to adequately treat this many groups, there is always a need for additional verification. The multipanel solution principle is simply to consider the slowing down region as sub regions of panels, with each panel a manageable number of groups, say 100. In this way, we reduce the enormity of dealing with the entire spectrum all at once by considering many smaller problems. We demonstrate the solution in the unresolved U^{238} resonance region.

Key Words: slowing down, ultra-fine groups, multipanels

1. INTRODUCTION

Generation of multigroup cross sections lies at the heart of reactor physics methods. This is especially true in light of new reactor designs proposed for **NGNP** and **PBMR**. The process, generally performed in three steps, is quite involved and its proper implementation essential to the subsequent reactor physics analyses. A crucial first step is access to cross section data and creation of intermediate cross section libraries from which multigroup cross section sets emerge. In the past, intermediate cross section sets did not carry any spatial information about the reactor subassemblies. However, as data processing rates continue to increase through parallel computing, greater fidelity regarding the incorporation of cross section data into reactor physics analyses becomes possible. For example, to treat resonance self-shielding as neutrons moderate to thermal energies, approximations employing the Dancoff correction for fuel pin shadowing was the accepted methodology. Now, because of increased computational efficiency, we are able to view resonance self-shielding from first principle slowing down theory. The **CENTRM** spectrum code, a part of the **SCALE** code system, is one of the first and most well known of the ultra-fine group class of cross section processing codes. The algorithm contained in the **CENTRM** code is designed to treat many thousands of energy groups in an efficient and accurate fashion. In addition, one dimensional neutron transport in the three fundamental geometries has been integrated into the algorithm. Below 100*ev*, where relatively sparse resonances occur, the **CENTRM** code has been verified against **MCNP** for slowing down in an infinite medium – but what about in the resolved resonance region with its thousands of resonances? This region is arguably the most crucial when constructing a weighting spectrum to produce representative multigroup cross section libraries for a lattice code. Accurately predicting the spectral/spatial neutron flux distribution in fuel assemblies is central to predicting proper steady state and transient reactor behavior and remains a reactor physics challenge.

While the **CENTRM** code is state of the art, there is always a need for its verification and improvement with respect to current and future application. The emphasis here is on the establishment of an independent verification of the ultra-fine group spectral flux representation as determined by the **CENTRM** module with an eye toward a future algorithm. For this purpose, we will describe and demonstrate an entirely independent method of treating a large number of groups, on the order of 100,000, in a "multipanel" format.

2. THE THEORY OF MULTIPANEL SLOWING DOWN

The key feature of the multipanel approach is the decomposition of a large number of groups into a smaller, more manageable number. In this way, N groups, where N could be on the order of 100,000 required in the resolved resonance region to capture enough spectral detail, are decomposed into a sequential collection of G groups, where $G << N$.

2.1 Multigroup Slowing Down Equation

In essence, pointwise **ENDF/B** data live on a group structure because of the energy uncertainty associated with their measurement. So all **ENDF/B** cross sections are representable in terms of groups. To begin, one specifies an overall energy group structure from **ENDF/B** and then decides on an appropriate paneling strategy. The panels, of size G groups, are a subset of the overall energy group structure and may or may not be representative of specific the cross section variations one may investigate. Here, we take G to be a single value throughout the energy grid, but this is not required as we can arrange the panels to emphasize any particular energy region. We then perform the entire calculation in the usual multigroup format within each panel.

Our investigation is initially concerned with the following infinite medium slowing down equation for the scalar flux $\phi(E)$:

$$\Sigma(E)\phi(E) = \sum_{j=1}^{J} \int_0^{E_0} dE' \Sigma_{sj}(E', E)\phi(E') + \\ + \chi(E) \int_0^{E_0} dE' \nu(E') \Sigma_f(E') \phi(E') + Q(E). \tag{1a}$$

At this point, there is no restriction on the scattering law so Eq(1a) is valid for slowing down in resonances or in the thermal regime alike. In addition, the fission contribution can be eliminated and re-considered after the multigroup equations have been solved since

$$F \equiv \int_0^{E_0} dE' \nu(E') \Sigma_f(E') \phi(E') \tag{1b}$$

to give for Eq(1a)

$$\Sigma(E)\phi(E)=\sum_{j=1}^{J}\int_{0}^{E_0}dE'\Sigma_{sj}(E',E)\phi(E')+ \\ +\sum_{j=1}^{J}\int_{E_0}^{E_0/\alpha_j}dE'\Sigma_{sj}(E',E)\phi(E')+Q(E) \tag{2a}$$

where

$$Q(E)\rightarrow F\chi(E)+Q(E). \tag{2b}$$

We recover the fission source F after solving the slowing down equation and introducing the flux into Eq(1b). In addition, we assume neutrons are slowing down to the energies of interest from above E_0. The second term on the RHS of Eq(2a) represents the slowing down source from higher energies. Further, if we assume a $1/E$ flux of strength q_0 above E_0, Eq(2a) becomes

$$\Sigma(E)\phi(E)=\sum_{j=1}^{J}\int_{0}^{E_0}dE'\Sigma_{sj}(E',E)\phi(E')+Q(E), \tag{3a}$$

with the external and slowing down sources combined into

$$Q(E)\rightarrow\sum_{j=1}^{J}q_0\int_{E_0}^{E_0/\alpha_j}dE'\frac{\Sigma_{sj}(E',E)}{E'}+Q(E). \tag{3b}$$

The numerical evaluation of Eqs(3) can take several forms. For the most appropriate form, we should consider the information that is available and in what sense the balance equation is to be satisfied as well as our level of effort. For example, we may have multigroup cross sections for a given group structure and therefore we would consider solving the multigroup form of Eqs(3). Alternatively, we may have pointwise data and therefore it would be appropriated to solve Eqs(3) in a pointwise sense on a given energy grid. In addition, do we require point or group fluxes and how accurately? Four numerical approaches to address these issues have been investigated including, the multipoint, multigroup, multigroup-quadrature, and multipoint-interpolation, leading to the following multigroup-like equation for all cases:

$$\Sigma_g\bar{\phi}_g=\sum_{j=1}^{J}\sum_{g'=1}^{N}\Sigma_{sjgg'}\bar{\phi}_{g'}+\bar{Q}_g. \tag{4}$$

Here $\bar{\phi}_g$ is the multigroup flux in group g and Σ_g and $\Sigma_{sjgg'}$ are the group interaction cross sections.

While this equation seems easy enough to solve by matrix inversion, the challenge emerges when N is 70,000, requiring a computational effort proportional to N^3. This is true even for elastic scattering where $\Sigma_{sjgg'}$ is banded. For this reason, we seek an alternative solution algorithm.

2.2 Multigroup Slowing Down Equation

Our approach is to decompose the solution to the full problem into a series of smaller ones-- each for only a fraction of the number of the N groups. At this point, we must clarify notation. For the entire slowing down region, the number of groups or points will be N as above. The number of groups for the lower dimensional problems, defined in a panel, is G. Effectively, we are taking a large linear problem and decomposing it into a series of smaller easier to solve multipanel problems. Figure 1 depicts the multipanel concept with the upper panels serving as sources to the lower panels. The source comes from the neutrons above a given panel able to reach the upper boundary of the adjacent panel and is therefore known since we are considering only down scatter. For instance, the source for panel l, originates in the energy region (or higher)

$$E_{l-1G} \le E \le E_{(l-1)G} / \min\left(\alpha_j\right)$$

of panel l-1. For panel l

$$E_{lG} \le E \le E_{(l-1)G},$$

we can write the exact slowing down equation as

$$\begin{aligned}\Sigma(E)\phi(E) = &\sum_{j=1}^{J} \int_{E_{lG}}^{E_{(l-1)G}} dE'\Sigma_{sj}(E',E)\phi(E') + \\ &+ \sum_{j=1}^{J} \int_{E_{(l-1)G}}^{E_{(l-1)G}/\alpha_j} dE'\Sigma_{sj}(E',E)\phi(E') + Q(E).\end{aligned} \tag{5}$$

In multigroup form, this equation becomes

$$\Sigma_g \bar{\phi}_g^l = \sum_{j=1}^{J}\sum_{g'=1}^{G} \Sigma_{sjgg'}\bar{\phi}_{g'}^l + \sum_{j=1}^{J}\sum_{r=(l-1)G}^{(l-1)G-R} \Sigma_{sjgr'}\bar{\phi}_{r'}^{l-1} + \bar{Q}_g. \tag{6}$$

Note that we are now only concerned with a G-group slowing down problem in a single panel Note also that contributions to a panel may come from any or all contiguous panels above.

This method of solution enables a variety of well-known solution techniques since it greatly reduces the effort especially when spatial transport is included. The second to last term on the

right hand side represents the source from panel *l*-1 (or above) slowing down into panel *l*. In this way, we cover the entire energy range of interest sequentially through the linking of panels. We

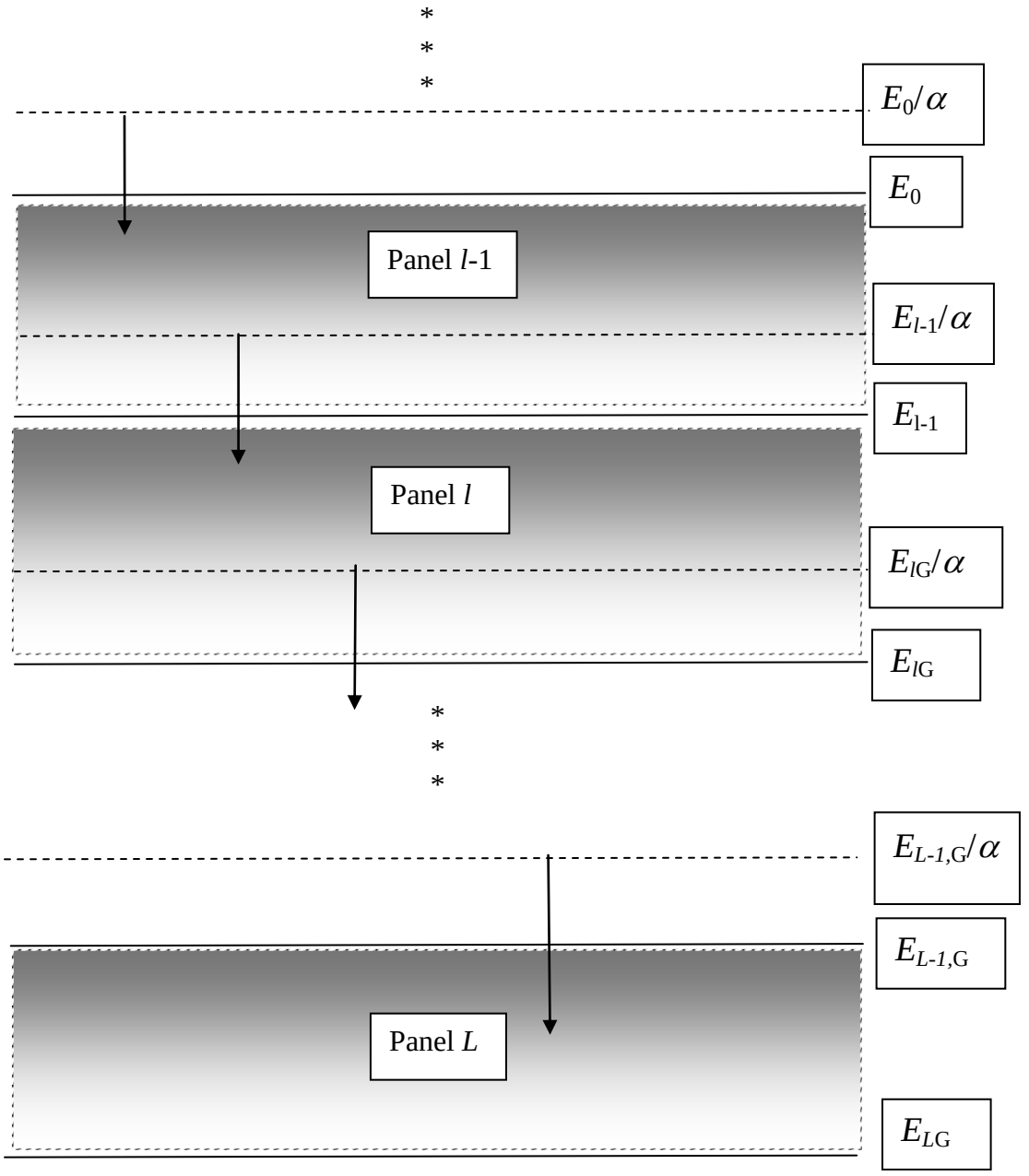

Fig. 1 Panels cover the energy range

can find a numerical solution to the slowing down equation through the continuous analytical continuation (CAC) formulation [1]. The solution, embedded in a fictitious time-dependent problem, results when we assume a source steady in time. Further, we resolve the resulting equation through a Taylor series expansion, converged to high accuracy.

3. A DEMONSTRATION OF MULTIPANEL SLOWING DOWN

As a first demonstration, Fig. 2 shows convergence with respect to number of groups N up to 18,000 for 38 ^{238}U-simulated resonances in carbon. N is decomposed into panels, each of (G =) 20 groups. The multigroup parameters were determined analytically for each material at zero temperature [2]. As is evident, for the modest ultra-fine group calculations of N = 512 and 1125, the multigroup approximation is generally poor near thermal energies. This poor performance is a clear demonstration of the importance of an ultra-fine group calculation required to capture resonance effects. The entire calculation required less than 6 min on a 1.2 GHz Gateway PC for unoptimized coding. A full 18,000-group calculation without paneling would have taken several hours on the same platform, hence the advantage of the multiplanel approach.

As a second demonstration, consider the 200 randomly simulated resonances shown in Fig. 3a. For this case, a direct matrix inversion numerically resolves Eq(6). We have assumed 50 group panels. It should be emphasized that the direct inversion calls for an inversion of a $G\times G$ matrix N/G times and not the full $N\times N$ matrix. Figures 3b and 3c show the group flux for N = 100, 500, 1000, 5000 and 10,000. Near convergence over the 200 resonances requires about 1000 groups, but full convergence as shown in the zoom frame of Fig. 3c is achieved at 10,000 groups.

4. DISCUSSION: ADVANTAGES OF PANELING

In first encountering the panel method, its advantages are not obvious. After all, the pure infinite medium slowing down problem is just a lower diagonal matrix requiring only the recurrence of Eq.(4) – what could be simpler. However, complications arise with recurrence for ~100,000 groups since roundoff accumulation will eventually destroy the calculation. On the other hand, direct inversion of the full $N\times N$ matrix when N is large is not convenient either, even in today's computational environment. However, conjugate gradient methods with preconditioning certainly present possibilities. Thus, reformulating the solution of the slowing down problem in terms of N/G lower order problems seems a reasonable approach.

In principle, by recasting a large slowing down calculation into many smaller ones, the number of groups we can consider is unlimited. While we are considering N on the order of 100,000 here, with faster sequential processors and parallel computing strategies, we could conceive of millions of groups in the future.

In addition, since we track the slowing down source as neutrons down scatter, we can include this source via input into an existing multigroup code, which then treats each panel independently by stacking. This is also true even when spatial variation is included. Thus, we can use routine multigroup transport or diffusion codes without modification to generate ultra-fine weighting spectra for down scattering using the multiplanel method.

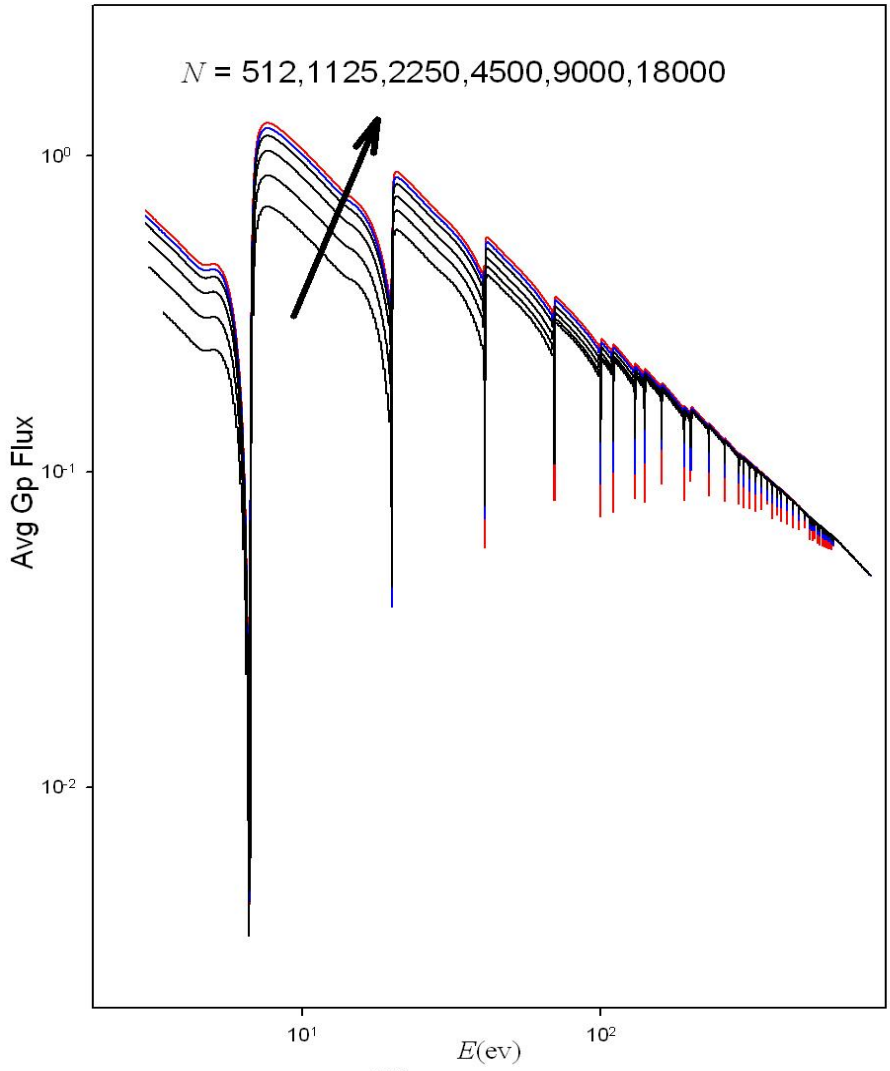

Fig 2 Simulation of ^{238}U resonances in 3ev<E<800ev with 38 resonances

algorithm should be appropriate for the even larger slowing down problems of the future.

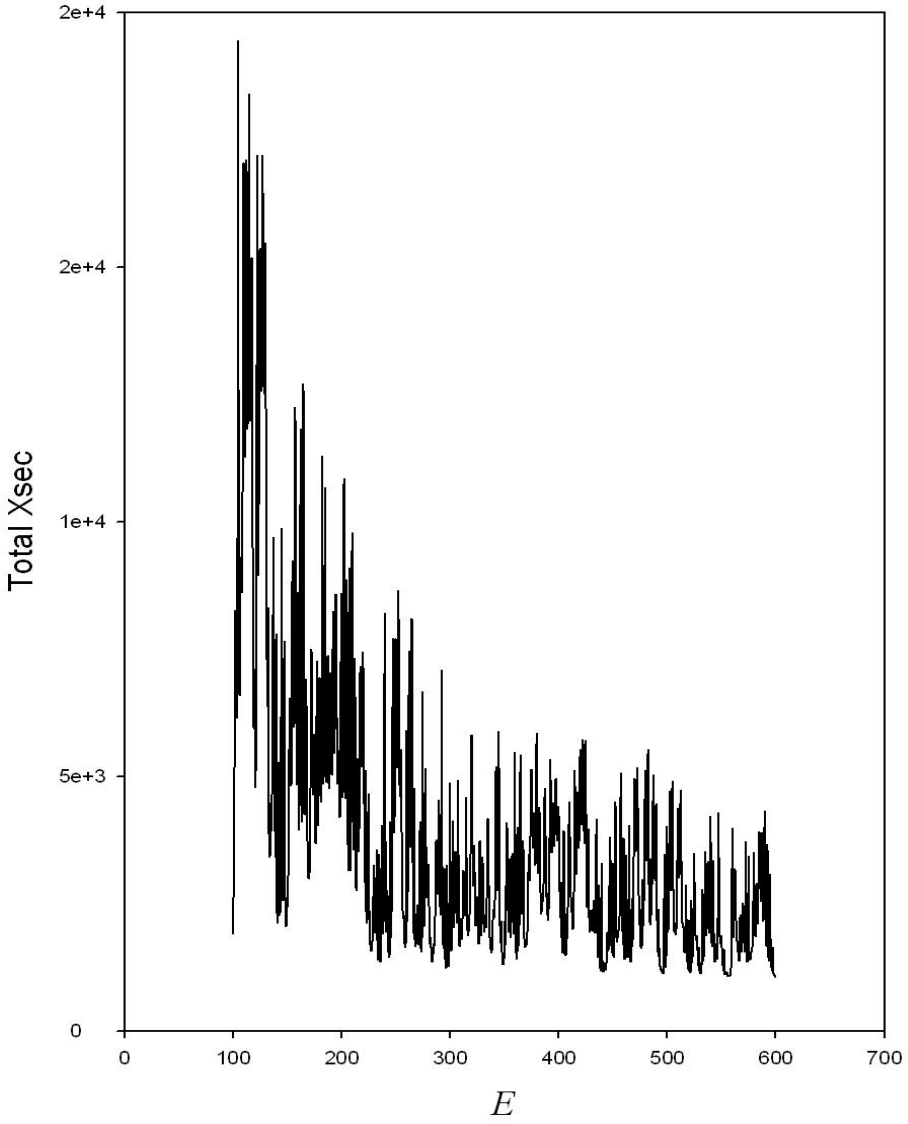

Fig. 3a Total Xsec variation for 200 simulated resonances

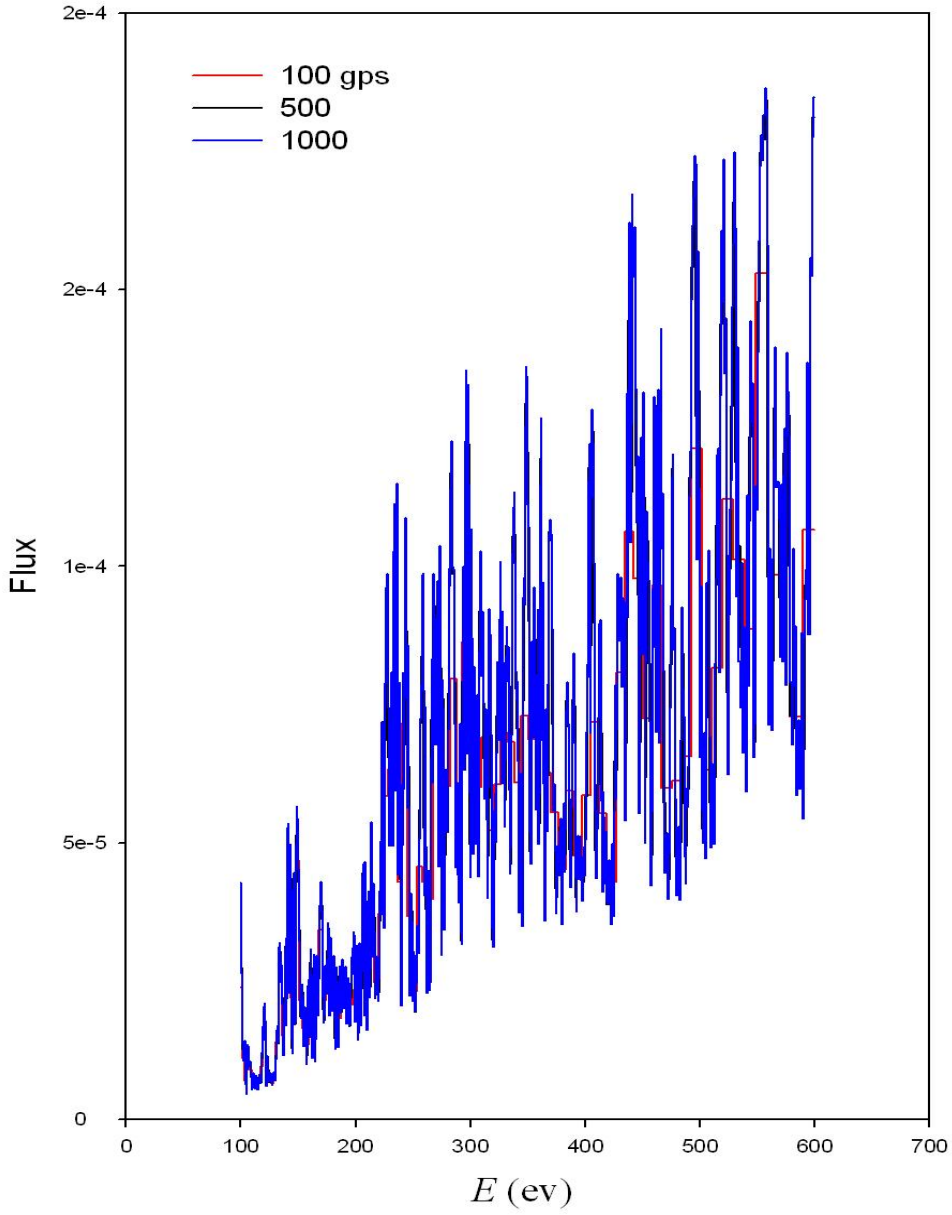

Fig. 3b FLux variation for 200 simulated resonances

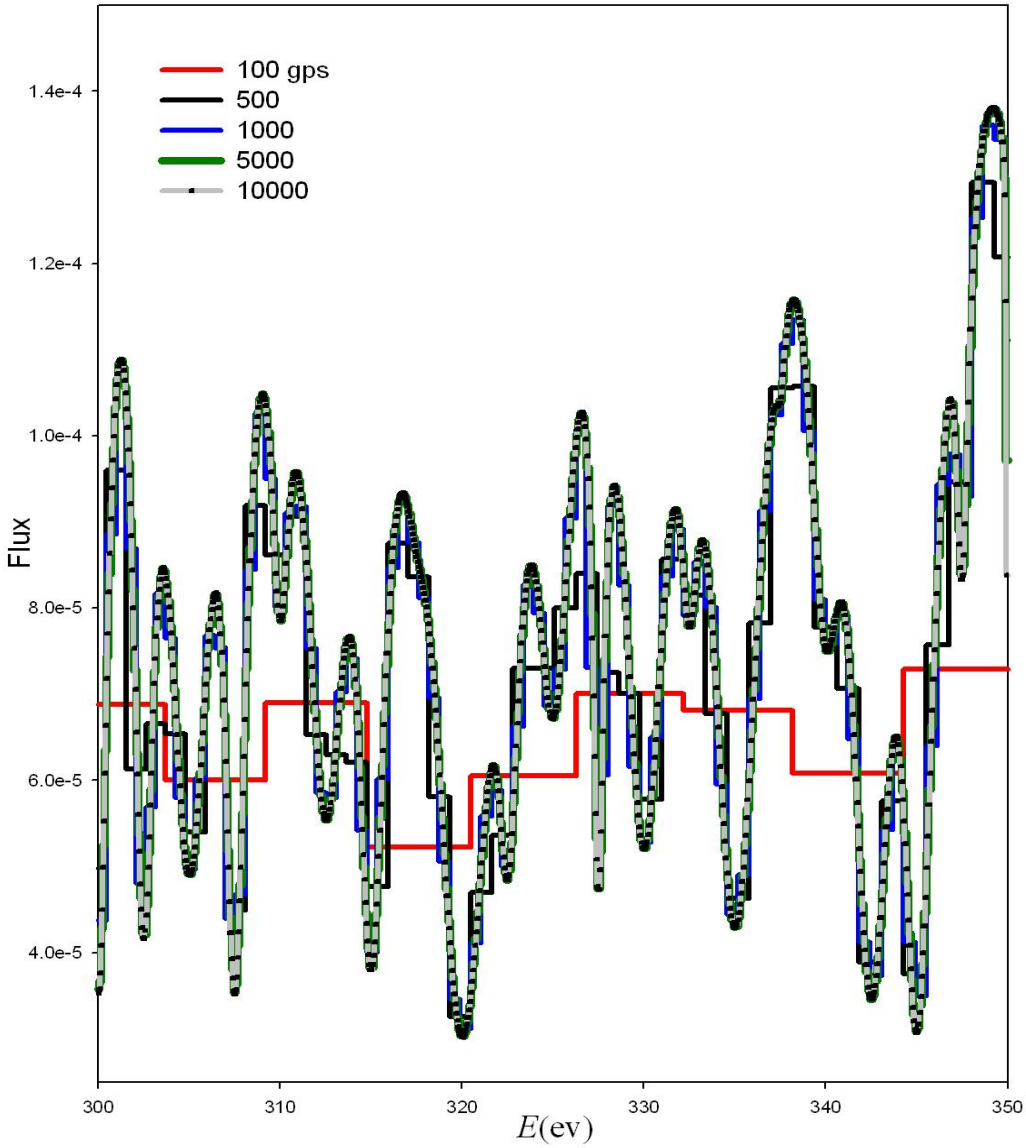

Fig. 3c Zoom of convergence over simulated resonances

5. SOME FINAL THOUGHTS

5.1. Improved Matrix Solver

An obvious improvement of the panel method is the inclusion of an efficient matrix multigroup solver. The **THERM/INL** solver used presently is not particularly well suited to slowing down without upscattering. However, the this solver is appropriate for the thermal energy region, which includes upscatter and becomes possible through interation. This requires that the upper triangular portion of the scattering contribution be evaluated iteratively since it is known at each iterate beforehand. We then apply the multipanel algorithm. The challenge lessons since we would need to consider only several thousand groups in the thermal region rather than 70,000.

5.2. Including Spatial Transport Theory

To be comparable with **CENTRM**, we, of course, will need to implement 1D transport solvers in planar and curvilinear geometries. For planar geometry, two methods initially present themselves. The first choice is the ***Fn*** method [3], which is a spectral method based on singular integral equation representations of the exiting flux from a plane medium. The method features expansion in shifted Legendre polynomials and its relative simplicity of implementation. We can apply the method to heterogeneous and anisotropic media of any order.

With some modification, the same method is applicable in cylindrical and spherical geometries with isotropic scattering. Application to heterogeneous media with anisotropic scattering will require additional development however.

The second numerical method we investigate will be the discrete ordinates (***Sn***) solution. This method should be equally applicable across all 1D geometries. Here, we use the converged ***Sn*** method (***CSn***) [4], which is a modification of the method currently implemented in **CENTRM**. In this way, we can easily provide benchmark accuracy.

Finally, we note that the multipanel solution is especially appealing for the inclusion of spatial transport in either of the above numerical forms. In particular, we have tested the ***Fn*** and ***Sn*** methods on multigroup transport calculations characteristic of a panel showing exceptional performance

5.3. Benchmarking CENTRM

Future focus will be on developing a reliable benchmark for application to verify the **CENTRM** module. This will entail extensive internal as well as external verification. We will include the method of manufactured solutions to independently verify the multigroup and multipanel approximations. If possible, we will embed the benchmark as a diagnostic in the **CENTRM** module to provide optimal benchmarking capability.

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