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Importances for MCNP Calculations on a Shield with a Penetration

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INTRODUCTION

This work was motivated by experience of shielding calculations on fusion-related facilities such as ITER and IFMIF using MCNP4C.[1] These shielding calculations are very demanding, particularly due to the presence of penetrations along which neutrons can stream for a few meters. The work reported here can be considered a continuation of that reported by the author at the RPS2002 meeting.[2]

The main tool for variance reduction in MCNP calculations of this kind is importances or weight windows, and the main conclusion of the previous work was that the weight window generator in MCNP4C is useful. The weight windows it provides gave a greater variance for a fixed number of histories than the manually chosen importances, but the time per history was so much shorter that the net result was a substantially better figure of merit.

However, this by no means obviates the need for manual variance reduction. There are two problems that need to be addressed:

(1) How should the shield be subdivided into cells for optimum performance? (If mesh-based rather than cell-based weight windows are used, the same question applies to the mesh.)

(2) Good starting importances are necessary for the weight window generator to give useful results. Even if the step-wise method is used, first generating weight windows for a tally somewhere inside the shield, then using these to take the neutrons farther into the shield and so on, good starting importances will help.

A possible solution to this problem is to use deterministic calculations to estimate importances, as has been described by many authors. However, this also involves difficulties. If two fully separate programs are used for the deterministic importance calculation and the actual (MC) flux calculation, the geometry must be modeled twice, which is prohibitive when even modeling it once may require many person-months or even years. If the two programs form a program system capable of using the same input file, this difficulty is avoided, but we do not have such a system in use at VTT. In any case, deterministic methods have difficulties in coping with streaming through long and narrow penetrations. Therefore, there remains an incentive to find a way of estimating importances that take streaming into account properly.

We consider the longitudinal variation of the importances (along the streaming direction) a nearly solved problem (see Appendix A). However, how to handle the transverse variation (the spatial dependence of the importances at right angles to the streaming direction) was not clear, and solving this problem was the goal of this work.

METHOD

The geometry we used for our test calculations was two-dimensional, with a steel + water shield (80 volume % stainless steel 316 L(N), ITER grade and 20 % water at a density of 0.9 g/cm^3) 240 cm in thickness, penetrated by a plane slit 2 cm high. On the left side of the shield was a surface source of 14-MeV neutrons, and the neutron current on the right side was the main quantity to be tallied. In most cases we tallied only the current above 1 or 0.1 MeV, since, in the fusion applications we are interested in, most of the gamma radiation after shutdown is caused by activation reactions in this energy range.

In the direction of neutron streaming, the shield was divided into 7.5 cm thick layers, so that there were 32 such layers. In the lateral direction, the cell boundaries were set at 0.001, 0.002, 0.004. 0.008, 0.016, 0.032, 0.064, 0.125, 0.25, 0.5, 1, 2, 3, 4, 6, 8, 11.2, 16, 22.4 and 32 cm from the slit, with a void boundary condition beyond the last cell.

The calculations were performed with MCNP4C on a Linux cluster. The cross sections were taken from JEF2.2.03.

The program was set to generate weight window lower boundaries, which constituted the actual quantities of interest. These were then translated back into importances by dividing the weight window lower boundary for the reference cell (which was always set to 0.4) with the corresponding boundary for each cell. These importances, and in particular their lateral distributions, were then investigated. Two kinds of importance ratios were calculated: the ratio of the importance in a cell immediately adjacent to the slit (a "wall cell") to that in the slit itself, and the ratios of the importances in cells farther away from the slit to that in the wall cell.

In practical problems it will be unfeasible to use such a fine cell structure. We generally aim to use 3 lateral layers, with importances reduced by a factor of 4 and 16, respectively, from the cells adjacent to the penetration. Therefore we determined the locations at which the generated importances dropped below ¼ and 1/16 of the values in the wall cells.

To get good results, we typically ran hundreds of millions of histories. Longitudinal starting importances calculated as described in Appendix A were used, but mostly no lateral variations were present in the starting importances. Even so it sometimes happened that the cells farthest from the slit and about halfway along the shield thickness did not get any generated weight windows. However, these difficulties were limited to a few cells, so they do not detract from the usefulness of the results presented here.

SENSITIVITY STUDIES

Since real applications will differ in many ways from the cases studied here, we set out to study how the results were affected by changes in geometry, source spectrum, the energy range of interest and the shield material. Although we could not carry out an exhaustive investigation of this in view of the limits on time and funding, we could draw at least some tentative conclusions, which will be expressed here in terms of how steeply the generated importances decline with increasing distance from the penetration.

- Changing the geometry, to a slit 7 cm in height or to a duct of circular cross section with a diameter of 20 cm made the decline slightly steeper, but the change was minor. For a circular duct with a diameter of 2 cm the generated importances actually increased with increasing distance from the duct, but this was probably an erroneous result caused by extremely poor statistics. We conclude that changes in the geometry of the shield penetration apparently do not make a big difference.

- We did not study the effect of changing the shield thickness, but we do not believe that it would change the results presented here, so long as the thickness is sufficient to make streaming dominate over bulk transport.
- The effect of changing from a 14 MeV source to a fission spectrum is small. Near the slit the decline of the importances becomes slightly steeper, farther away less steep, but these changes are not significant.
- Going from a cutoff energy of 1 MeV to 10^{-5} eV makes essentially no difference near the slit, but farther out the decline becomes less steep. The z boundary where the importance decreases by a factor of 16 from the wall cell moves out from 0.25 cm near the middle of the shield to about 1 cm.
- Changing the shield material made a big difference. For this reason we tested several different materials. The results are described below.

MATERIAL CHOICE

Four of the materials chosen were intended as extremely simplified versions of possible shield materials. These were water, quartz (as a simplified version of concrete), iron and tungsten. Light concrete, as specified for ITER, was also used, as was stainless steel 316 L(N) ITER grade, with and without 20 volume % water. A comparison of these seven materials led to the following conclusion: The importance drops off much more sharply with increasing distance from the slit for the most effective shielding materials than for the least effective ones.

This is physically reasonable. In a poor shielding material, even a neutron far from the slit may have a significant chance to reach the tally surface, but not in a good shielding material.

The extremely poor performance of pure iron in this respect was particularly noteworthy. We attribute it to cross section windows. Even though the cutoff at 0.1 MeV which we used eliminates the effects of the notorious window at about 25 keV, the windows above 0.1 MeV are apparently still enough to have a major influence.

RESULTS

The results are presented here for all materials, but only for the 2 cm slit with a 14 MeV source and for the energy range above 0.1 MeV, since only the material choice made a big difference.

Fig. 1 shows the importances in the slit itself, both estimated with the "handy method" of Appendix A ("est.imp.") and calculated from the generated weight windows for different materials. The agreement is as good as one can hope reasonably hope for, with most of the calculated importances agreeing with the estimates within about a factor of 2. As the stair-like "est.imp." curve shows, we didn't even try for greater accuracy.

The biggest differences are found for pure iron. Obviously the handy method underestimates the transport through the bulk shield in this case, where the cross section windows have a strong influence. For pure iron the flux halving length of 7.5 cm is too short.

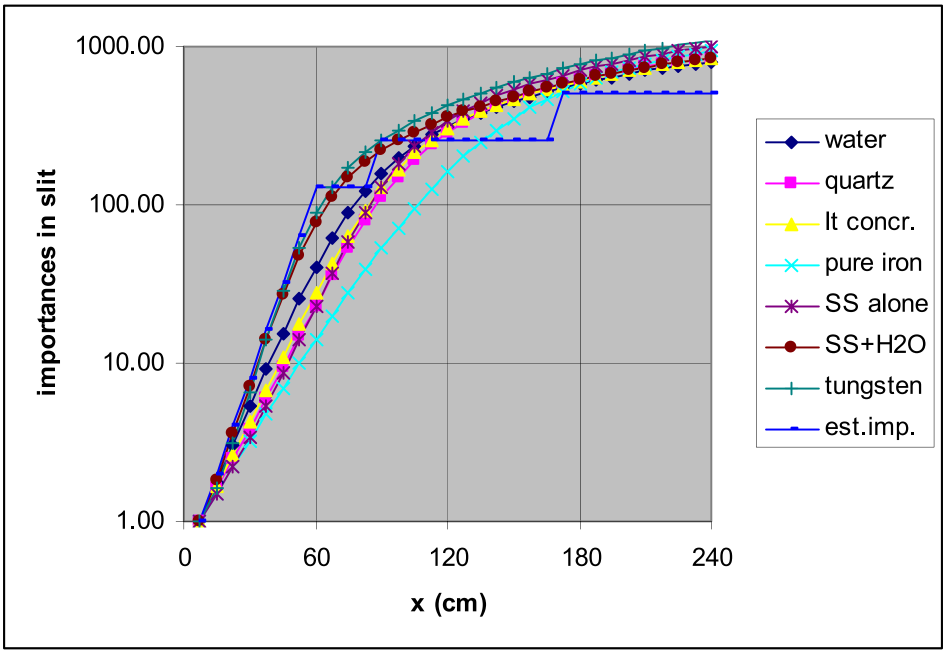

Fig. 1: Importances in the slit itself as functions of the longitudinal coordinate x

In any case, the importance in the void cells of the slit itself is of little relevance, since MCNP doesn't split particles in a void. The above results justify the use of the "handy method" for estimation of the longitudinal importance distribution in the slit, but we also need to investigate the lateral distribution.

First let us note that the lateral dependence of the importance is very flat in the rightmost layer of cells, 232.5 cm < x < 240 cm. This is easy to understand, since any particle in this layer has a good chance of reaching the tallying surface at x = 240 cm, regardless of its proximity to the slit. This dependence is also relatively flat in the leftmost cells, 0 < x < 7.5 cm. In between, the lateral variation of the importance is very pronounced.

Fig. 2 shows the ratio of the importance in the first 0.001 cm of the wall to the slit itself as a function of x (the position along the slit). This value is remarkably small in most of the shield. A reasonable approximation of this ratio would start at 1/16, then drop gradually to 1/128 at one quarter of the shield thickness, increase to 1/64 at half the thickness, remain there to three quarters of the thickness and then rise gradually to 1. We don't know where the breakpoints should be located in a shield with a thickness different from 240 cm, however. And this recommendation is obviously not valid for pure iron.

The above gives us the importances in the cells immediately adjacent to the slit. There remains the question of determining the cell structure and importances farther from the slit. Fig. 3 shows how the importance declines with increasing distance from the slit surface in the middle of the shield.

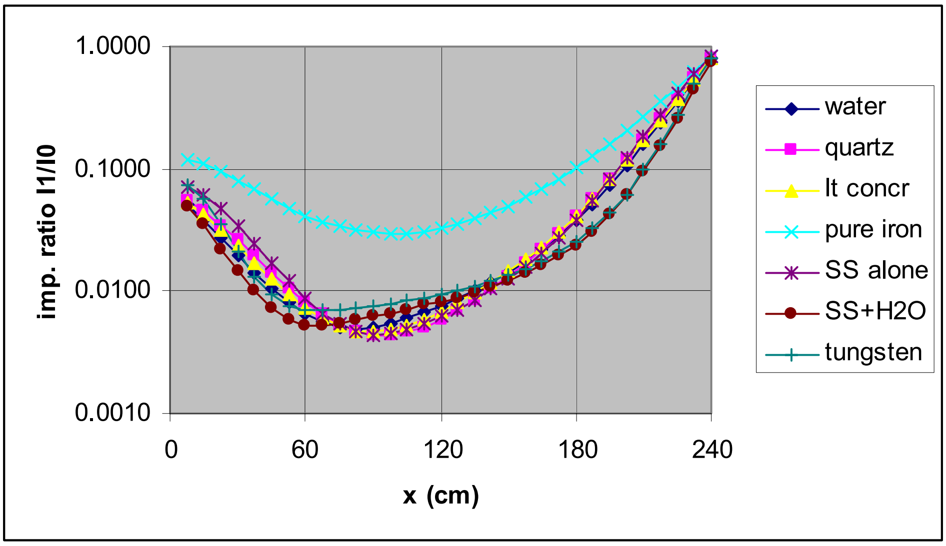

Fig. 2: Ratios of importance in the first 0.001 cm of the wall (I1) to that in the slit (I0) as functions of the longitudinal coordinate x

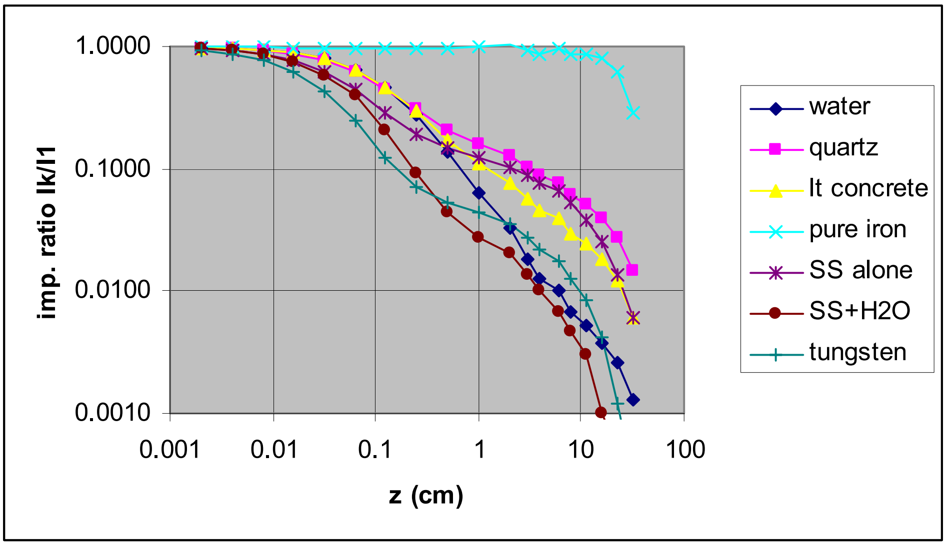

Fig. 3: Ratios of importance in the k'th cell (Ik) to that in the first 0.001 cm of the wall (I1) as functions of the lateral coordinate z in the interval 112.5 cm < x < 120 cm (in the middle of the shield).

Since the geometries we typically deal with are complex enough already (some thousands of cells), we prefer not to use a large number of cells in the lateral direction.

We consider three layers of cells, each with an importance lower by a factor of 4, to be reasonable. From Fig. 3 one can conclude that for the best shielding materials, such as tungsten or a combination of 80 % stainless steel with 20 % water, the importance drops by a factor of 4 in the first 0.1 cm or less and by a factor of 16 at about 0.35 cm. For light concrete, the corresponding distances are about 0.3 and 2.5 cm, for stainless steel 0.16 and 6 cm. Pure iron behaves in its own idiosyncratic way.

Fig. 4 shows how the lateral importance distribution, expressed as the ratio of the importance at z to that at the slit surface z = 0, varies longitudinally through the shield for a single material, the 80 volume % stainless steel + 20 % water mixture. As was pointed out above, the distribution is quite flat at i = 32, the end of the shield, and also relatively flat at the beginning, steeper in between.

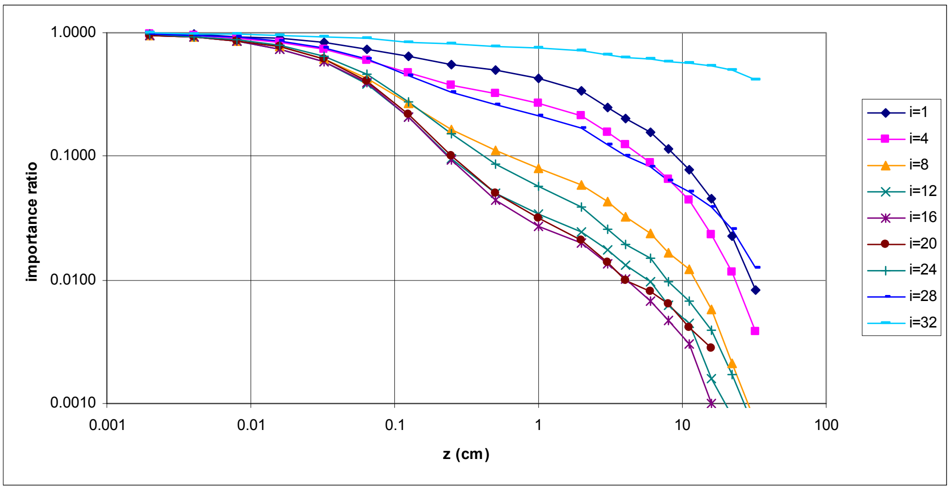

Fig. 4: Ratios of importance in the k'th cell to that in the first 0.001 cm of the wall as functions of the lateral coordinate z at different longitudinal locations for 80 % SS + 20 % water. i = 1 is the first layer of the shield, i = 32 is the last.

AN APPLICATION

To demonstrate and test how these importances work, we carried out some calculations with them. For comparison we also did some calculations with old importances, the way we would have done before this investigation.

When using the old importances, we set the z boundaries at 2 and 8 cm from the slit surface; with the new importances, we set them at at 0.064 and 0.5 cm. (In practice all 4 boundaries were present, but the importances were changed only at the appropriate boundaries.)

The tables show the importances for different cells in both the x and z directions. The first case used no lateral importance variations whatever, only longitudinal importances. The second and third cases used lateral variations also, in the old way. In the second case the importances were separable in the x and z directions, which is sometimes necessary when using universes. In the third case, the importances were modified to give a laterally flat distribution at the end of the shield, which is more realistic though unfortunately not always feasible.

With the new importances we also had both a separable and a non-separable case. For the separable case, we first divided the importances in the slit by 64 to get the importances in the cells immediately adjacent to the slit, on the basis that this seems like a reasonably representative average of what Fig. 2 shows. Then there were two further reductions by a factor of 4, going farther from the slit. In the non-separable case, we took into account the x dependencies shown by Figs. 2 and 4.

There was a further change, compared with the old method. If we had used an importance of 1 in the first cell in the slit, as we would traditionally have done, the importances of the cells at the left end of the shield and far from the slit would have been very small (1/1024 in the separable case), which would have involved an inordinate amount of Russian roulette for newly started neutrons. Instead we renormalized the importances so that we got more reasonable values in the material-filled cells at the start of the shield. This way the importances in the slit were quite large, but this has no practical significance, since MCNP doesn't split particles in a void.

The importances used in each calculation, the figure of merit and fractional standard deviation for the total current exiting the shield and the number of histories per minute are shown in Tables I through V. The fractional standard deviations (fsd's) are comparable, because each calculation ran for 525 minutes on a single processor in a Linux PC.

i (x location index)	I (importance)
1	1
2	2
3	4
4	8
5	16
6	32
7	64
8-11	128
12-22	256
23-32	512
FOM	16.34
histories/min	96,973
fsd	0.0107

Table I: Calculation with old, exclusively longitudinal importances

The first calculation, using importances depending only on the x coordinate (Table I), worked fairly well. Introducing our old guesses concerning the lateral variation of the importances (Tables II and III) actually made things worse, decreasing the figure of merit by more than a factor of 2. Whether separable or non-separable importances were used made no significant difference.

Table II: Calculation with old separable importances

z intervals (cm)	-1…0	0…2	2…8	8…32
Material	void	80 % SS + 20 % water		
i (x location index)	I (importances)			
1	1	1	0.25	0.0625
2	2	2	0.5	0.125
3	4	4	1	0.25
4	8	8	2	0.5
5	16	16	4	1
6	32	32	8	2
7	64	64	16	4
8-11	128	128	32	8
12-22	256	256	64	16
23-32	512	512	128	32
FOM	7.808			
histories/min	45,820			
fsd	0.0155			

Table III: Calculation with old non-separable importances

z intervals (cm)	-1…0	0…2	2…8	8…32
Material	void	80 % SS + 20 % water		
i (x location index)	I (importances)			
1	1	1	0.25	0.0625
2	2	2	0.5	0.125
3	4	4	1	0.25
4	8	8	2	0.5
5	16	16	4	1
6	32	32	8	2
7	64	64	16	4
8-11	128	128	32	8
12-22	256	256	64	16
23-28	512	512	128	32
29	512	512	128	64
30	512	512	256	128
31	512	512	256	256
32	512	512	512	512
FOM	7.921			
histories/min	46,416			
fsd	0.0155			

Changing to the new separable importances (Table IV) resulted in a slight improvement over Tables II and III but the figure of merit did not reach the same level as when using only longitudinal importances.

Table IV: Calculation with new separable importances

z intervals (cm)	-1…0	0…0.064	0.064…0.5	0.5…32
Material	void	80 % SS + 20 % water		
i (x location index)	I (importances)			
1	256	4	1	0.25
2	512	8	2	0.5
3	1024	16	4	1
4	2048	32	8	2
5	4096	64	16	4
6	8192	128	32	8
7	16384	256	64	16
8-11	32768	512	128	32
12-22	65536	1024	256	64
23-32	131072	2048	512	128
FOM	9.475			
histories/min	73,697			
fsd	0.0142			

However, the new non-separable importances (Table V) worked signifiantly better, giving the best figure of merit, improved over Table I by a factor of 2.

That non-separable importances work better than separable ones is easy to understand, since separable importances cannot match the way the optimal importance distribution scrunches up near the penetration in the middle of the shield but spreads out near the end. The surprising thing is the absence of any signifiant difference between the old separable and non-separable importances. This may be due to the different cell subdivisions. Near the end of the shield, there are likely to be few fast neutrons farther from the slit than 2 cm, so the importance used in this region doesn't matter much, while that between 0.064 cm and 0.5 cm and even that beyond 0.5 cm does matter.

The observation that using longitudinal importances alone worked so well is interesting and, at the moment, unexplained.

CONCLUSIONS

We have shown that, in shields constructed of a good shielding material, the cell boundaries needed to define the lateral distribution of importances or weight windows around a penetration should be quite close to that penetration, of the order of a few millimeters or less. We have also found a way of manually constructing importances that are probably close to optimal for the geometry considered here, and this method is expected to be applicable to many other geometries with a shield penetrated by slits or ducts. These importances are, however, only intended for use as a starting point, allowing efficient generation of cell-based weight windows. These weight windows will presumably further improve the calculation efficiency. Unfortunately we did not have time to test that before the deadline for completion of this paper.

Table V: Calculation with new non-separable importances

Case	nnos2 (new, non-separable imortances)			
z intervals (cm)	-1…0	0…0.064	0.064…0.5	0.5…32
Material	void	80 % SS + 20 % water		
i (x location index)	I (importances)			
1	32	2	1	0.5
2	64	4	2	1
3	128	4	2	1
4	256	8	2	1
5	512	8	2	1
6	1024	16	4	1
7	2048	16	4	1
8-11	4096	32	8	2
12-16	8192	64	16	4
17-22	8192	128	32	8
23-26	16384	256	64	16
27	16384	512	128	64
28	16384	1024	256	128
29	16384	2048	1024	512
30	16384	4096	2048	2048
31	16384	8192	4096	4096
32	16384	16384	16384	16384
FOM	32.82			
histories/min	222,910			
fsd	0.0076			

For maximum efficiency, a non-separable importance distribution is required. In some cases the geometry model does not allow this. Our results suggest that, in such instances, one might as well make the lateral importance distribution flat and use only the longitudinal distribution. It seems likely that the optimal longitudinal distribution in that situation would not be the one calculated for the penetration itself as described in Appendix A but the product of that and the ratio shown in Fig. 2, i.e., the importance distribution for the walls of the penetration. The reason for this is that the importance in a void has no significance in MCNP.

Appendix A: Estimation of Longitudinal Importances

To estimate the importance as a function of position in the direction of streaming (longitudinal position), we follow the principle that the number of tracks should be roughly constant as one goes from the source to the tally. For this we estimate neutron transport through the bulk material and the streaming separately.

For the transport through bulk material, we assume that the neutron current attenuates exponentially. Based on ITER experience, we assume a halving of the flux for each 7.5 cm. Thus the importance doubles for each 7.5 cm. (This is the reason why we generally use cells with a thickness of about 7.5 cm in the direction of the neutron current, especially at the beginning of a shield.)

For streaming through voids, we assume that the neutron current is proportional to the solid angle subtended by the beginning of the duct as seen from the location under consideration. Thus the importance increases in inverse proportion to this solid angle.

We then choose the lower of these two importances, so that the importance is inversely proportional to the dominant part of the current. This usually means that, near the beginning of the shield, the importance will increase in the exponential fashion dictated by bulk attenuation. Farther on the streaming is well collimated, so it will dominate and the importance grows much more slowly.

As a final step, we calculate the nearest power of 2 that does not exceed the estimated importance, and then use this as the final importance.

This method is closely related to the "Handy Method" of Iida et al.[3] for estimation of flux or current in a shield. It is not quite identical, but close enough that we borrow that name for this method. One difference is that Iida used the sum of the bulk transport and streaming, while we use the greater of the two. The conversion to a power of 2 is also, of course, missing from Iida's method, since it makes sense only for importances. It means that that the ratio of importances is always an integer, which ensures conservation of weights in each individual splitting event (when using MCNP), not just averaged over all splits at a given surface.

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