LA-UR 95-2058

CONF-9509100--21

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TITLE: VISUALIZATION AND ANALYSES OF MCNP CRITICALITY CALCULATION RESULTS

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SUBMITTED TO: The 5th International Conference on Nuclear Criticality Safety, Albuq., NM, 9/17-21/95

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FORM NO 836 R4
ST NO 2629 5/81

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VISUALIZATION AND ANALYSES OF MCNP CRITICALITY RESULTS

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INTRODUCTION

Careful assessment of the results of a calculation by the code itself can detect mistakes in the problem setup and execution. MCNP [1] has over four hundred error messages that inform the user of FATAL or WARNING errors that have been discovered during processing of just the input file. MCNP4A performs a self assessment of the calculated results to aid the user in determining the quality of the Monte Carlo results.

MCNP4A contains new built-in sensitivity analyses of the Monte Carlo calculation that provide the user with simple WARNING messages for both criticality and fixed source calculations. The goal of the new analyses described in this paper is to provide the MCNP criticality practitioner with enough information in the output to assess the validity of the k_{eff} calculation and any associated tallies. The results of these checks are presented in the k_{eff} results summary, several k_{eff} tables and graphs, and tally tables and graphs. Plots of k_{eff} at the workstation are also available as the problem is running or in a postprocessing mode to assess problem performance and results. Plots of the fission source by cycle supply valuable visual information, although they are not yet available in the production version of MCNP.

k_{eff} RESULTS SUMMARY

As a foundational check, MCNP determines if any fissionable cells were not sampled for source locations. Analysis is then provided about the apparent normality of the active cycle k_{eff} values for each of three MCNP k_{eff} estimators: collision, absorption, and track length. The normality of each of the three sets of active k_{eff} cycle data is checked at the 95 and 99% confidence levels. A printed line for each of the three k_{eff} estimators indicates the confidence level at which it passed. Any k_{eff} data set that does not pass at the 99% confidence level should be considered as not normally distributed. WARNING messages are printed for k_{eff} cycle sets that do not appear normal at the 99% confidence level. Perhaps this is a statistical occurrence, or perhaps more k_{eff} cycles should be skipped for improved convergence of the spatial fission source. The calculation should be examined further; e.g., by examining the behavior of the solution as function of the number of inactive cycles.

A box is then printed that contains the final estimated average k_{eff}, standard deviation, and three different confidence intervals. These averages are a statistical combination of the three k_{eff} estimators. If all three estimators appear nonnormal at the 99% confidence level, the final boxed k_{eff} confidence intervals are NOT printed. A WARNING message is printed in its place. (The final confidence intervals are available elsewhere in the output if the user insists on using them. Normality checks and confidence intervals for different numbers of inactive k_{eff} cycles are available in the k_{eff}-by-cycles-skipped table.) The final box is also NOT printed if fewer than thirty active k_{eff} cycles have been used in the calculation. Fewer than thirty cycles is not recommended because the quality of the spatial convergence of the fission source cannot be adequately assessed.

A conservative (toward large k_{eff} values)

[1] MCNP and Sabrina are trademarks of the Regents of the University of California, Los Alamos National Laboratory

average k_{eff} confidence interval is also estimated by assuming that the largest cycle k_{eff} value for each of the three estimators occurs on the next cycle. This range gives a conservative estimate of criticality.

BATCHED k_{eff} RESULTS

A table of batched (using more than one cycle) k_{eff} using more than one active cycle for each k_{eff} is now available. This table is useful in determining the impact of cycle-to-cycle correlations in the spatial fission source distributions on the estimated standard deviation. The table includes the k_{eff} results that would be found if the k_{eff} were taken in batch sizes greater than one. This table is included so that the user can evaluate the impact of different batch sizes on the combined k_{eff} estimator and the estimated standard deviation. This information is a built-in sensitivity study of the k_{eff} confidence intervals as a function of batch size.

The averages of the three individual k_{eff} estimators are the same for all batch sizes, but the estimated statistical standard deviations and the combined k_{eff} confidence intervals are not. Batch sizes greater than one may reflect a better estimate of the true deviation because the k_{eff}s are assumed to be independent from cycle-to-cycle when the statistical uncertainties are calculated [2]. However, they are not independent because of fission source correlations from one cycle to the next. The correlation between larger batches will be less than the correlation between the individual k_{eff}s with a batch size of one cycle. The user can now assess the impact of different batch sizes on the k_{eff} confidence interval.

k_{eff} RESULTS BY CYCLE

The table of k_{eff} results by cycle lists the neutron histories, individual, cumulative average, and cumulative combined k_{eff}s by cycle. The table is a relisting of the cycle-dependent prints (with deviations instead of relative errors) in a more convenient form. The figure of merit, which is an indicator of problem efficiency and stability, is also included as a convergence rate check for k_{eff}. The largest and smallest active values of k_{eff} are printed for each estimator to indicate the spread of values sampled so far in the calculation

PRINTED PLOT OF THE COMBINED k_{eff} BY CYCLE

The most important k_{eff} plot for the user is the plot of the combined k_{eff} by cycle. A trend in k_{eff} relative to the final value and the estimated standard deviation can be quickly determined visually. The estimated one standard deviation confidence intervals that are printed for each line are useful for helping to spot meaningful trends in the behavior of the average k_{eff}.

k_{eff} RESULTS BY CYCLES SKIPPED

The table of results by cycles skipped tells the user what the values of the various k_{eff} estimators would have been for different numbers of inactive cycles without having to rerun the problem. This information is another built-in sensitivity study of the k_{eff} confidence intervals as a function of the number of k_{eff} cycles skipped. The normality for each of the three sets of k_{eff} data are calculated and printed for each number of active cycles. The active cycle number where the minimum standard deviation of the combined k_{eff} occurred is printed. If this cycle is an inactive cycle, the number of cycles skipped was probably adequate. If the number of inactive cycles is significantly less than this cycle, it may indicate that not enough cycles were skipped.

The first and second active halves of a valid k_{eff} calculation should have nominally the same k_{eff} and estimated standard deviation of the average value of k_{eff}. MCNP calculates and prints the combined k_{eff} and the statistical uncertainty for the first half and second active halves of the problem. This comparison is a built-in sensitivity analysis of the two active halves of the calculation. WARNING messages are printed in the output and at the terminal if the 99% confidence intervals do not overlap or the estimated standard deviations do not appear to be statistically the same. Either or both might indicate that the normal spatial mode was not achieved during the early part, or even all of a calculation. Systems that have a difficulty converging the source are typified by high dominance ratios, the ratio of the second eigenvalue to the dominant eigenvalue (k_{eff}). Large systems or ones with many isolated elements tend to have high dominance ratios.

PRINTED PLOT OF THE COMBINED k_{eff} BY CYCLES SKIPPED

The combined k_{eff} confidence interval by cycles skipped is shown in a printed plot. By visually locating the minimum standard deviation in this plot, the number of cycles that should have been skipped can be estimated. The minimum standard deviation results from enough inactive cycles to converge the source and sufficient remaining active cycles to give good statistics.

GRAPHICAL k_{eff} OUTPUT

MCNP has the capability to plot the cycle values and the cycle-averaged values of the individual and combined k_{eff} estimators, along with their one standard deviation confidence intervals. The plots are available both during a calculation and postprocess These plots provide additional insights into the behavior of k_{eff} during the calculation. (Examples are shown below in Figures 2, 6, 7, and 8.)

NEW STATISTICAL CHECKS FOR MONTE CARLO TALLIES

Two new statistical diagnostics for tallies have been developed and included into MCNP: 1) the relative variance of the variance; and 2) the empirical history score probability density function f(x). Statistical studies have shown that these two quantities are excellent for detecting false convergence of difficult Monte Carlo tallies. These and other quantities have been incorporated into ten statistical checks involving the estimated mean, relative error, relative variance of the variance, figure of merit, and the logarithmic "slope" of the largest f(x) values [3]. These ten checks for one tally bin of each MCNP tally are made and the user is given a "yes" or "no" for satisfying the test criteria. The empirical f(x) values are printed in the output and can be plotted for detailed examination by the user. The user can request a tally that is equivalent to the track length estimator, and therefore use these new techniques to assess k_{eff} convergence. The MCNP user now has much more information about the statistical quality of a tally result than just the value of the estimated relative error and its behavior as a function of the number of histories.

SUMMARY OF MCNP CRITICALITY WARNING MESSAGES

MCNP provides the following WARNING messages based on analyses of the results of a criticality calculation:

- no sampling of cells with fissionable material
- the average k_{eff} has monotonic trend during the last ten active cycles
- k_{eff} sets that do not appear normal at the 99% confidence level
- all three k_{eff} sets do not appear normal at the 99% confidence level and the final boxed k_{eff} is not printed
- fewer than thirty active k_{eff} were run and the final boxed k_{eff} is not printed
- the k_{eff} confidence intervals for the first and second active halves of the problem do not overlap at the 99% confidence level
- the estimated standard deviations for the first and second halves of the problem do not appear to be the same

The appearance of one or more of these WARNING messages is reason for additional scrutiny of the calculation. The calculation may be continued for any number of additional active cycles desired.

FISSION SOURCE VISUALIZATION

Two methods to visualize the fission source by cycle are under development. One way involves a visualization package, such as PAW (Physics Analysis Workstation) [4], where the fission source density in cells of a regular grid overlaying the geometry are plotted. The other way is Sabrina's [5] rendering of fission source points with data gathered from MCNP's ptrac file [6]. Sabrina can plot the source points together with the geometry. Both methods are versatile and in color. They give users an indication of the calculation's adequacy of sampling and convergence of the fission source, especially when used in conjunction with MCNP's other capabilities and statistical checks.

EXPERIENCES WITH THE NEW CAPABILITIES

The new self assessment checks in MCNP have made a positive impact on the criticality user community. One user commented that the cell sampling check showed a cell that had not been sampled. The reason was that an object had been mistakenly placed far out of position and no neutron histories ever reached it. The object location was corrected and the calculation proceeded normally with an increased value of k_{eff}. The normality checks of the k_{eff} sets have the capability to find problems with a poor (too small) number of inactive k_{eff} cycles. Deliberately not skipping enough cycles has resulted in all three k_{eff} data sets not appearing to be normally distributed at the 99% confidence level.

We have run the "k_{eff} of the world" array problem [7] with 729 4.7 cm radius spheres containing Jezebel plutonium (0.037047 atoms/b-cm Pu-239, 0.001751 Pu-240, 0.0001 Pu-941, and 0.001375 Ga), spaced at 60 cm surrounded by a thick water reflector. The 4.7 cm radius is much smaller than the 6.385 cm radius of Jezebel required for criticality. The calculation uses a uniform volume source in the array for the initial spatial distribution 1000 neutrons per cycle skipping 20 cycles and running a total of 120 cycles. The value of 1000 neutrons per cycle was used because this is probably a lower limit for most criticality calculations today with the availability of fast PCs and workstations. Sampling of the array is poor on a per-object basis because there are only about 1.4 histories per object. The fact that the objects are identical makes this calculation tenable with only 1000 neutrons per cycle The 99% k_{eff} confidence interval for this system is 0.918 to 0.933. There were no WARNING messages, and all three k_{eff} data sets appeared normally distributed at the 95% confidence level. The first and second active half 99% confidence intervals were 0.913 to 0.933 and 0.915 to 0.940. All aspects of the calculation were well behaved.

Figure 1 shows an MCNP 2-D plot of the water-reflected array geometry with Jezebel at the center instead of the 4.7 cm radius sphere. Inserting Jezebel with a radius of about 6.385 cm in the center of the array changed the behavior of the problem drastically, but not the final confidence interval. The final 99% k_{eff} confidence interval result was 0.942 to 0.958, which is far from the correct critical value. Two WARNING messages were produced:

- the k_{eff} results were monotonically increasing over the last ten active k_{eff} cycles
- the first and second half k_{eff} cor[illegible] intervals appeared to be different a[illegible] 99% confidence level

The 99% confidence interval for the first half was 0.922 to 0.940 and the that for the second half was 0.960 to 0.978. Figure 2 shows an MCNP plot of the average k_{eff} by cycle number. It is clearly evident that k_{eff} is increasing. This trend is caused by more and more fission source points being created in Jezebel as additional k_{eff} cycles are run because the Jezebel array element is so much more reactive than the other elements. The well-behaved array problem without Jezebel (labeled "No Jezebel") is shown for comparison in Figure 2. The three k_{eff} sets appeared normal at the 99% level, but not 95%. This result is not necessarily a strong indicator of non-normal behavior, but could indicate a problem. The figure of merit decreased by 30% during the last twenty active cycles, showing that statistical error in k_{eff} was not decreasing as the inverse of the square root of the number of historia during the last portion of the active calculation. One of the ten statistical checks failed on the separate tally of the track length k_{eff}; the mean was monotonically increasing during the last active half of the problem. The quality of this solution is CLEARLY unacceptable and further investigation is required. Further investigation may involve examining the output more closely, running more cycles, or possibly starting over with a different computational parameter set, such as a better source guess or a different random number sequence.

Fission source visualization provides further insight to the unacceptability of this calculation. Figure 3 shows a Sabrina plot of the fission source points at cycle 120 for each of the 9 planes. Jezebel is in the center plane and is showing more source points. However, the spheres on the periphery are not all sampled.

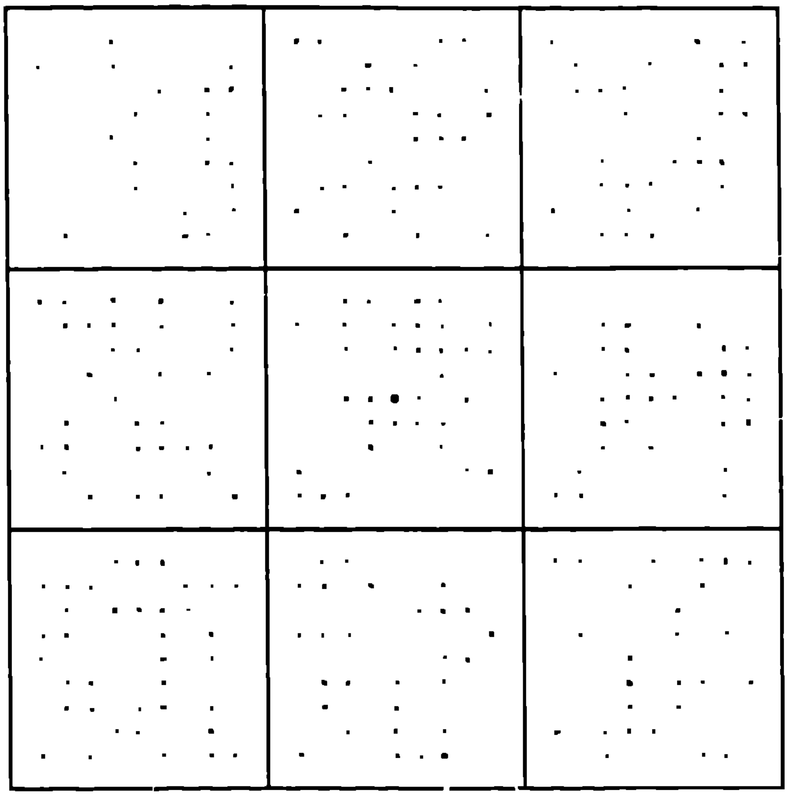

Figure 3: From left to right and top to bottom, the 9 frames show the fission source points in each plane at cycle 120 for 1000 histories per cycle.

A Sabrina animation can show the source locations changing from cycle to cycle. Figure 4 shows the center plane for cycles 1, 2, 4, 5, 10, and 100. The particles have started finding Jezebel sometime after cycle 5, but other indications from MCNP suggest the the source is not converged, even at 100 active cycles.

Figure 5 is PAW's projection of fission source density from all 9 planes, accumulated over the active cycles. In grayscale, it shows that the center region has accumulated about two orders of magnitude more fissions than the surrounding columns of spheres. A view perpendicular to any of the sides would isolate the higher fission density in the center sphere. Figures 5 and 4 indicate to the user the importance of the center of the system, and, combined with other statistical checks, that the ter may have not been adequately sampled over all the cycles.

Continuing the problem to 500 active cycles (520 total cycles) supplies the correct result in the k_{eff}-by-cycles-skipped table, but not as the boxed final answer, which is 0.986 to 0.994 at the 99% confidence level. This problem produced one WARNING message: the first and second half k_{eff} confidence intervals appeared to be different at the 99% confidence level (the first half was 0.973 to 0.985 and the second half was 0.997 to 1.005). This message should be interpreted as NOT being able to accept the final boxed k_{eff} result because the confidence intervals are so far apart. The minimum estimated standard deviation in the k_{eff}-by-cycles-skipped table occurs with 108 inactive cycles and 412 active cycles, producing a 99% confidence interval of 0.996 to 1.003. Examination of the two printed k_{eff} plots confirms the quality of the result based on the behavior of k_{eff} by both the average and by cycles skipped as shown in the MCNP plots in Figures 6 and 7.

If the problem were run for only thirty ac-

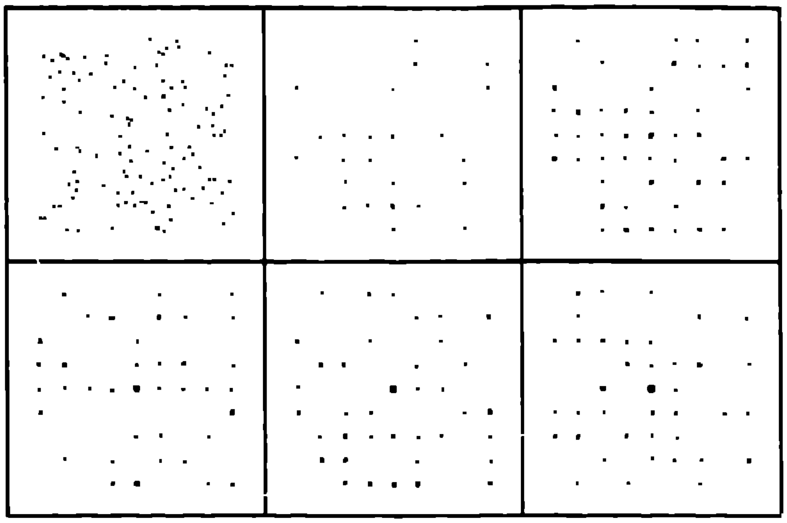

Figure 4: The fission source points in the center plane for cycles 1, 2, 4, 5, 10, and 100 for 1000 histories per cycle and an initial random uniform source.

Figure 5: The projected fission source from all 9 planes accumulated over [illegible] active cycles. The grayscale on the right indicates the fission source density.

tive cycles with 1000 neutrons per generation, there would be no WARNING message to suggest calculational difficulties. The only clue is that thirty cycles and about one neutron per object per k_{eff} cycle is simply not enough to adequately calculate the proper spatial source distribution for such a complex heterogeneous configuration. Using 5000 neutrons per cycle produces the WARNING that the first and second half k_{eff} confidence intervals appeared to be different at the 99% confidence level (0.946 to 0.964 for the first half and 0.990 to 1.001 for the second half). Figure 8 is an MCNP plot that shows the expected faster rate of convergence for 5000 histories per cycle compared with 1000 histories per cycle because there is more sampling of the Jezebel element during each k_{eff} cycle.

The dominance ratio of the "k_{eff} of the world" problem is about 0.92, as estimated by a nonproduction fission matrix patch [8] to MCNP. This is a fairly large dominance ratio and signals slow source convergence. The earlier calculations began with a uniform source that, coupled with poor sampling due to Jezebel's relatively small volume fraction, required over 100 cycles to converge.

Motivated by the indications from MCNP's checks and the graphical analyses, we reran the problem with 1000 initial source points all beginning in the center sphere. Figure 9 shows the center plane for cycles 1, 2, 4, 5, 10, and 120. The center sphere is well sampled, but the outer subcritical spheres are inadequately sampled, as in the case of a uniform initial distribution. Starting all the source points in the center sphere is a good source guess, such that, even with 1000 histories per cycle, the source appeared converged after 16 cycles. After 10 inactive cycles and 100 active cycles the 99% k_{eff} confidence interval was 0.994 to 1.011. Note, however, that a good initial source guess will not eradicate cycle-to-cycle correlations. Detection of such correlations is possible with the batch statistics.

Assuming no prior knowledge of the converged fission source shape, the prudent user would be best served by determining the k_{eff}s of the different individual elements of a loosely coupled system such as the "k_{eff} of the world" problem. Such knowledge would be beneficial when investigating the system as a whole.

SUMMARY

The above statistical and geometry sampling checks, built-in sensitivity analyses, WARN-

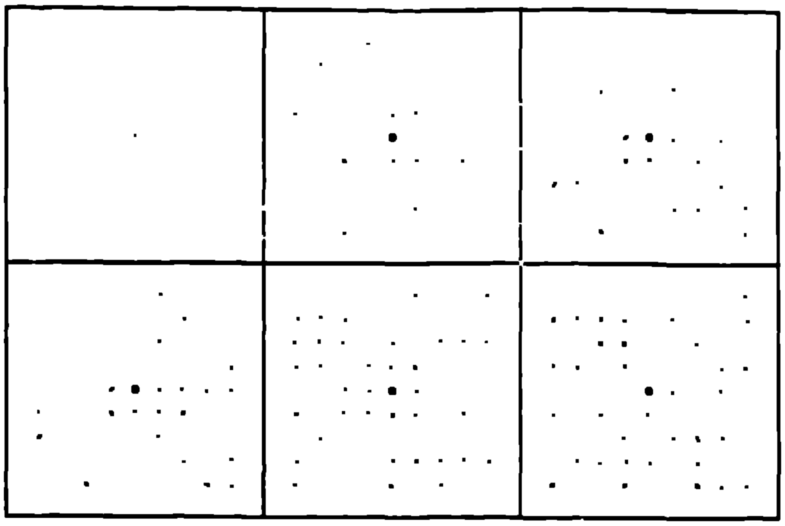

Figure 9: The fission source points in the center plane for cycles 1, 2, 4, 5, 10, and 100 for 1000 histories per cycle and all initial source points in Jezebel.

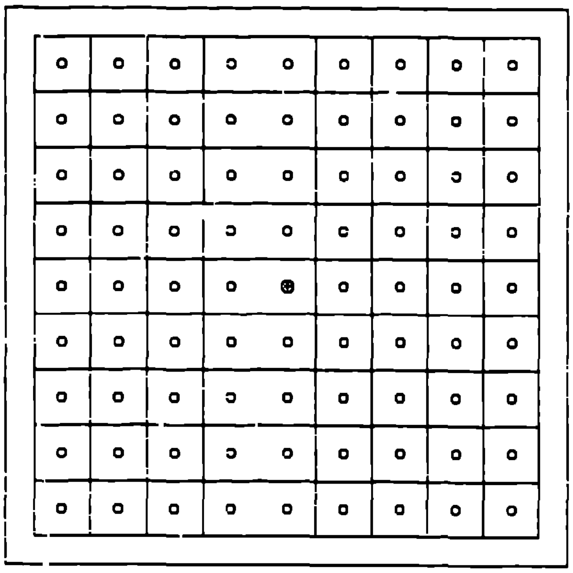

Figure 1: MCNP plot of a cross section of the water-reflected array problem with Jezebel in the center

ING messages, and yes/no indicators provide the MCNP user with more information to assess whether a problem has been properly calculated. The MCNP4A documentation including the MCNP4A Manual (LA-12625-M) and the new MCNP Criticality Primer (LA-12827-M) have been updated to describe these new features. If a criticality calculation ap-

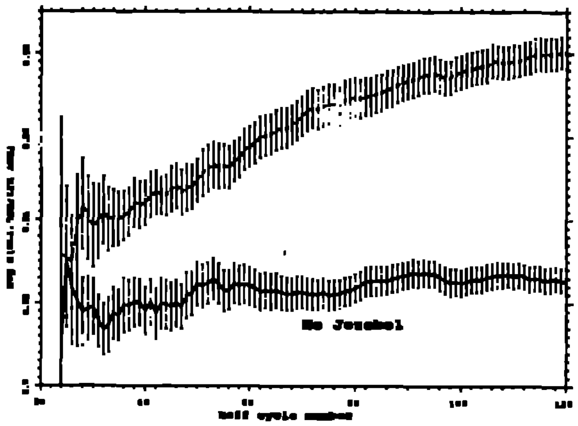

Figure 2: One standard deviation confidence intervals for the average k_{eff} of the array, with Jezebel (top curve) and without Jezebel (bottom curve), for 120 cycles.

pears to have an unsatisfactory spatial source convergence based on the k_{eff} normality checks or fewer than thirty active k_{eff} cycles, the final boxed k_{eff} confidence intervals will not be printed. These WARNING messages have caught real user errors and are effective for the "k_{eff} of the world" problem as long as at least 100 active cycles are run. Graphical analyses available in future versions of MCNP will supply an additional and invaluable tool.

Although these statistical and geometry

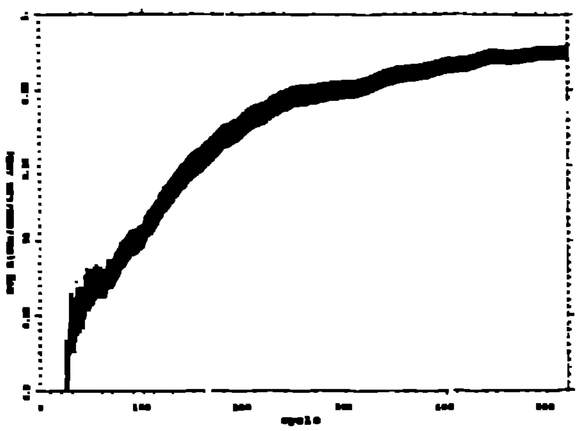

Figure 6: One standard deviation confidence interval for the average k_{eff} of the array with Jezebel for 520 cycles.

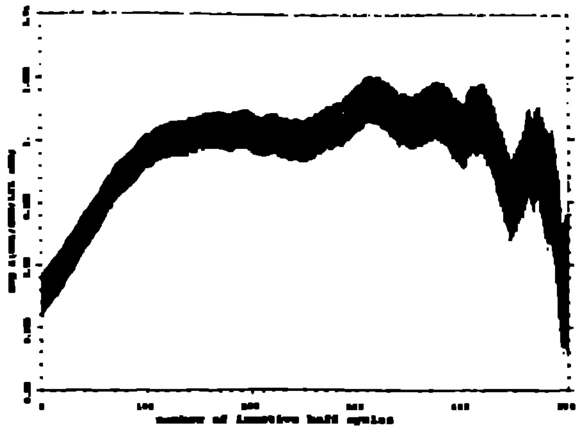

Figure 7: One standard deviation confidence interval for the average k_{eff} of the array with Jezebel as a function of the number of cycles skipped (inactive cycles).

sampling checks of the calculation results reduce the likelihood of a user accepting a poorly executed MCNP calculation, it would be foolish to assume that these checks, by themselves, can prevent all erroneous Monte Carlo criticality estimates. These checks are important tools to aid the criticality expert in evaluating MCNP results. They are NOT intended as a substitute for criticality expertise and judgment.

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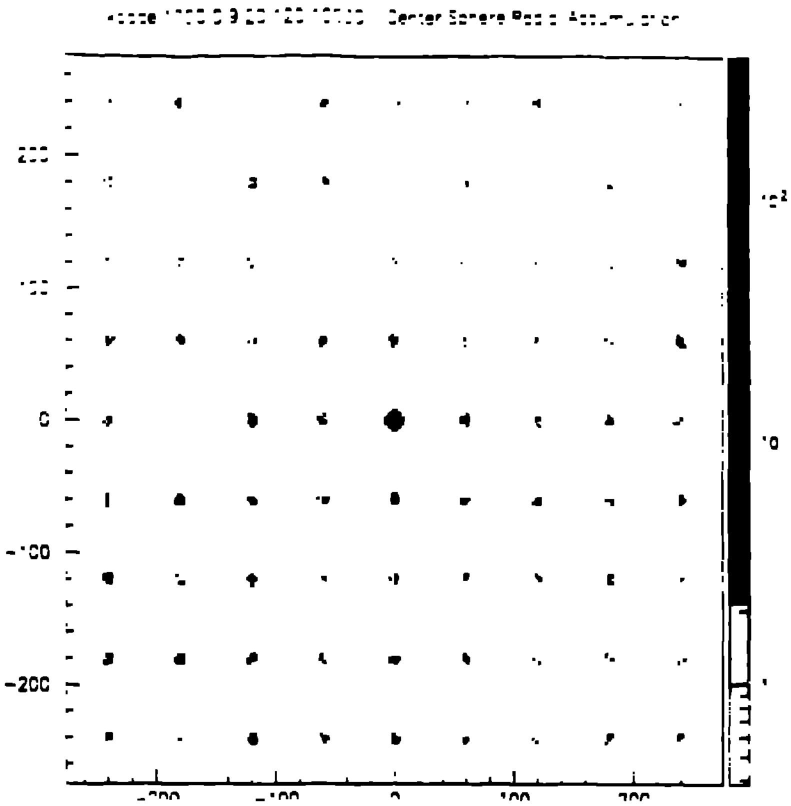

Figure 5: The projected fission source from all 9 planes accumulated over the active cycles. The grayscale on the right indicates the fission source density.

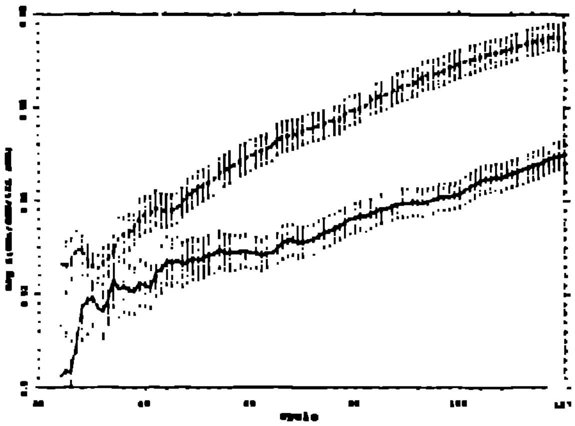

Figure 8: One standard deviation confidence interval for the average k_{eff} of the array with Jezebel for 5000 and 1000 histories per cycle for 120 cycles.