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TITLE: MCNP ANALYSES OF CRITICALITY CALCUALTION RESULTS

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MCNP ANALYSES OF CRITICALITY CALCULATION RESULTS

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1. INTRODUCTION

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

MCNP4A, which was released to RSIC in October 1993, contains new analyses of the MCNP Monte Carlo calculation that provide simple user WARNINGs for both criticality and fixed source calculations. The goal of the new analyses 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 page, 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.

2. Keff RESULTS SUMMARY PAGE

The MCNP k_{eff} results summary page begins with a line containing the title of the job and problem ID, followed by the numbers of inactive and active cycles and histories requested and run. The next two pieces of information address how acceptable the Monte Carlo solution appears to be. The first check is to determine if all cells with fissionable material had fission source points on any cycle. This serves as a geometry sampling check. If so, a line is printed to acknowledge that fact that all cells were sampled. Otherwise, a WARNING message is printed in the output and at the terminal to inform the user which fissionable cells had no tracks entering, and/or no collisions, and/or no fission source points.

Another check involves the behavior of the average k_{eff} versus active cycle number. It is highly unlikely that the average k_{eff} would increase or decrease monotonically during the last ten active cycles for a problem with a properly converged spatial fission source. A WARNING message is issued if there is a monotonic trend during the last ten average k_{eff} values. This message could indicate incomplete spatial convergence of the fission source.

Information 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 percent confidence levels. A printed line for each of the three k_{eff} estimators indicates the level of passage. WARNING messages are printed for k_{eff} cycle sets that do not appear normal at the 99% confidence level. Any k_{eff} data that does not pass at the 99 percent confidence level should be considered as not normally distributed. Perhaps this is a statistical occurrence or more cycles should be skipped. 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 less 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) 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 conservative average k_{eff} confidence interval can be used for extra conservatism for a correct calculation.

3. BATCHED Keff RESULTS PAGE

A table of batched (using more than one cycle) k_{eff}s 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}s were taken in batch sizes other 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. 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 other 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. (They are not independent because of fission source correlations from cycle to cycle.) The larger batches will have less correlation between the batches than the correlation between the individual k_{eff} cycles. The user can now assess the impact of different batch sizes on the k_{eff} confidence interval.

4. Keff RESULTS BY CYCLE TABLE

This table 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.

5. PRINTED PLOT OF THE COMBINED Keff BY CYCLE

This is the most important k_{eff} plot for the user. 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}.

6. Keff RESULTS BY CYCLES SKIPPED TABLE

This table tells the user what the values of the various k_{eff} estimators would have been for a different number of inactive cycles without having to rerun the problem. 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. WARNING messages are printed in the output and at the terminal if the 99 percent 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 of or even all of a calculation.

7. PRINTED PLOT OF THE COMBINED Keff BY CYCLES SKIPPED

This printed plot shows the combined k_{eff} confidence interval by cycle skipped. This plot can be used to visually assess how many cycles should have been skipped. An "*" on the plot vertical axes indicates how many active cycles were used in the original calculation. The number of cycles that should have been skipped can be estimated from this plot, the location of the minimum estimated variance of k_{eff} as a function of the number of cycles skipped, and the stabilization of the average k_{eff} printed plot.

8. GRAPHICAL Keff OUTPUT

MCNP has the capability to plot the individual and average k_{eff}s and their one standard deviation confidence intervals, as well as the average k_{eff} estimator, during a calculation or by postprocessing. These plots provide additional insights into the behavior of k_{eff} during the calculation.

9. 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 indicators for 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. 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 $f(x)$'s are printed in the output and can be plotted for detailed examination by the user. The track length estimator of k_{eff} can be done easily as a separate tally to apply 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.

10. SUMMARY OF MCNP CRITICALITY WARNING MESSAGES

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

1) no sampling of cells with fissionable material;
2) the average k_{eff} has a monotonic trend during the last ten active cycles;
2) k_{eff} sets that do not appear normal at the 99% confidence level;
3) all three k_{eff} sets do not appear normal at the 99% confidence level and the final boxed k_{eff} is not printed;
4) fewer than thirty active k_{eff} were run and the final boxed k_{eff} is not printed; 5) the k_{eff} confidence intervals for the first and second halves of the problem;
do not overlap at the 99% confidence level; and
6) 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.

11. EXPERIENCES WITH THE NEW CAPABILITIES

The new self assessment checks in MCNP have made an impact on the criticality user community. One non-LANL 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. 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% percent confidence level.

We have run the k_{eff}-of-the-world array problem with 729 4.7 cm radius spheres containing Jezebel plutonium (0.037047 atoms/b-cm Pu-239, 0.001751 Pu-240, 0.000117 Pu-241, 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 the identical makes this calculation tenable with only 1000 neutrons per cycle. The 99% k_{eff} confidence interval for this system is 0.920 to 0.932. 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 0.919 to 0.937 and 0.916 to 0.932. All aspects of the calculation were well behaved.

Figure 1 shows a 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: 1) the k_{eff} results were monotonically increasing over the last ten active k_{eff} cycles; and 2) the first and second half k_{eff} confidence intervals appeared to be different at the 99% confidence level (the first half was 0.922 to 0.940 and the second half was 0.960 to 0.978). The MCNP plot of the average k_{eff} versus cycle number CLEARLY showed the increasing trend, as is shown in Fig. 2. 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 jez") is shown for comparison in Fig. 2. The three k_{eff} sets appeared normal at the 99% level, but not 95%. This result is not necessarily a strong indicator of nonnormal 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 histories 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 more calculations need to be done.

Continuing the problem for a total of 520 active cycles supplies the correct result, but not as the 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). The minimum estimated standard deviation 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 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 Figs. 3 and 4.

If the problem were run for only thirty active cycles and 1000 neutrons per generation, there would be no clue to the difficulties. 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. Thirty cycles is simply not enough to adequately calculate the proper spatial source distribution. Figure 5 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.

12. SUMMARY

The above statistical and geometry sampling checks, WARNING messages, and yes/no indicators provide the MCNP user with more information to assess that a problem has been calculated properly. 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 appears to have an unsatisfactory spatial source convergence based on the k_{eff} normality checks or less than thirty active k_{eff} cycles, the final boxed k_{eff} confidence intervals will not be printed. These WARNINGs 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.

Although these statistical and geometry sampling checks of the calculation results lessen 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 judgement.

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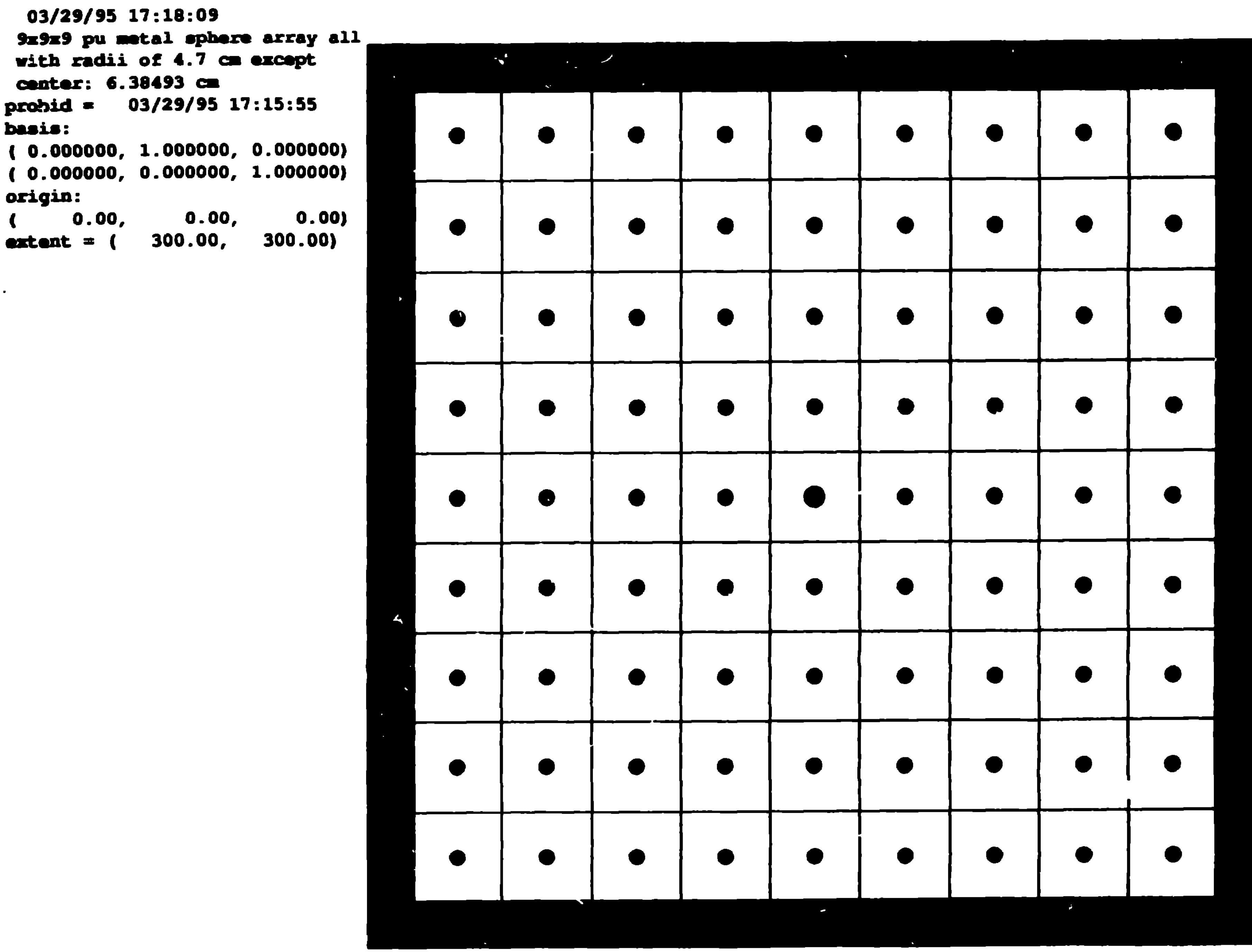

Fig. 1. MCNP plot of a cross section of the water-reflected array problem with Jezebel in the center.

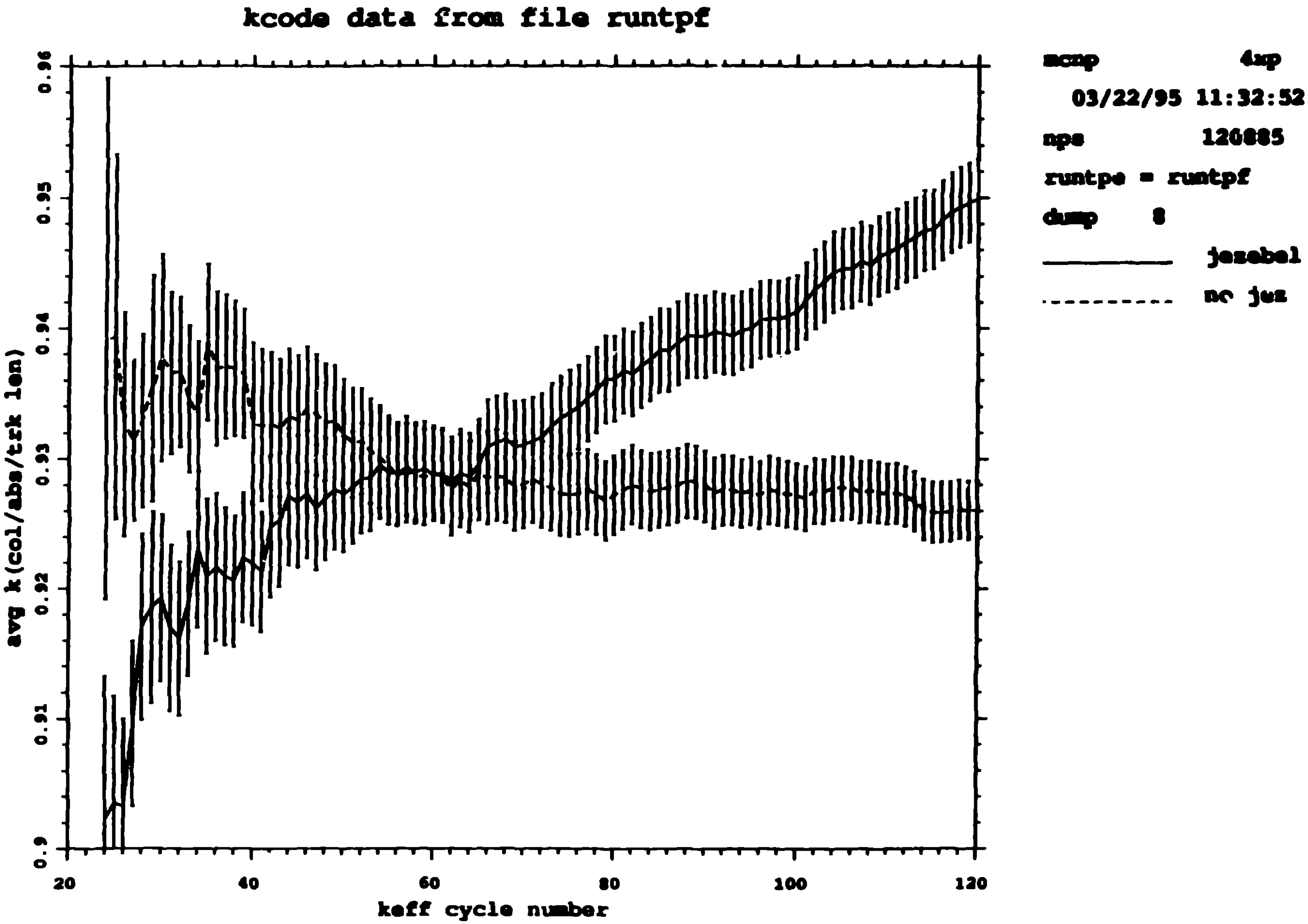

Fig. 2. One standard deviation confidence intervals for the average keff of the array with and without Jezebel for 120 cycles.

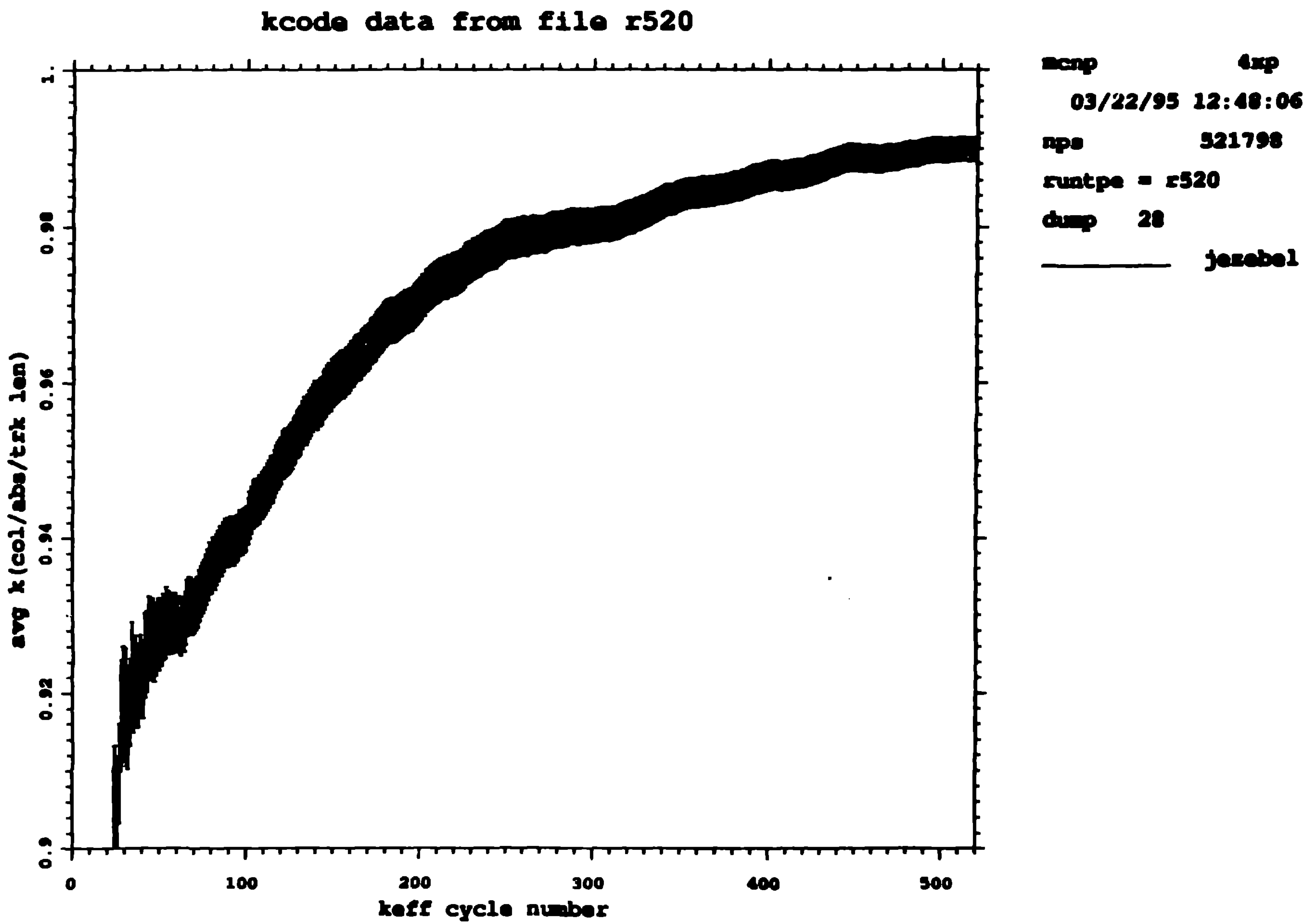

Fig. 3. One standard deviation confidence interval for the average keff of the array with Jezebel for 520 cycles.

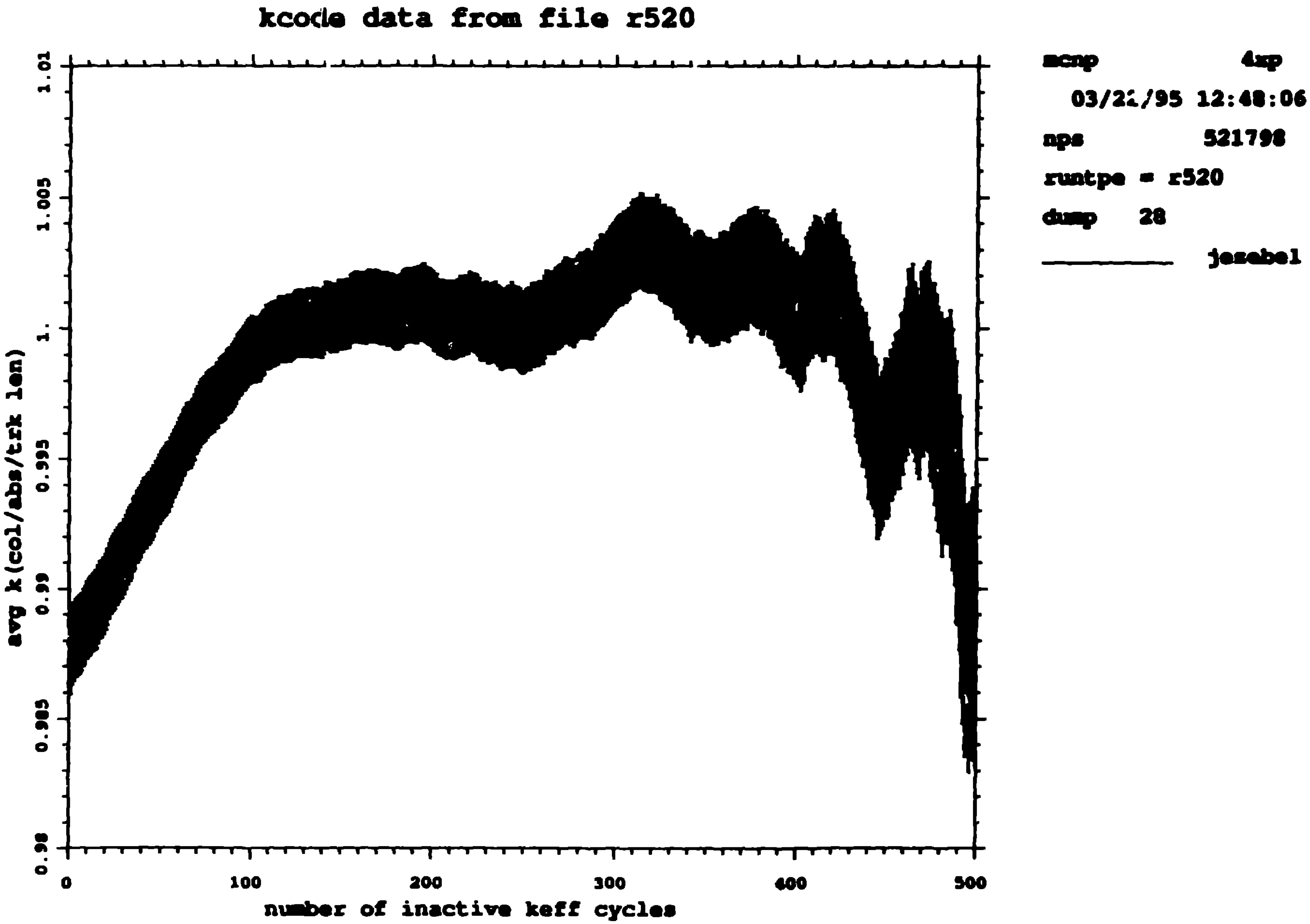

Fig. 4. One standard deviation confidence interval for the average keff of the array with Jezebel as a function of the number of cycles skipped (inactive cycles).

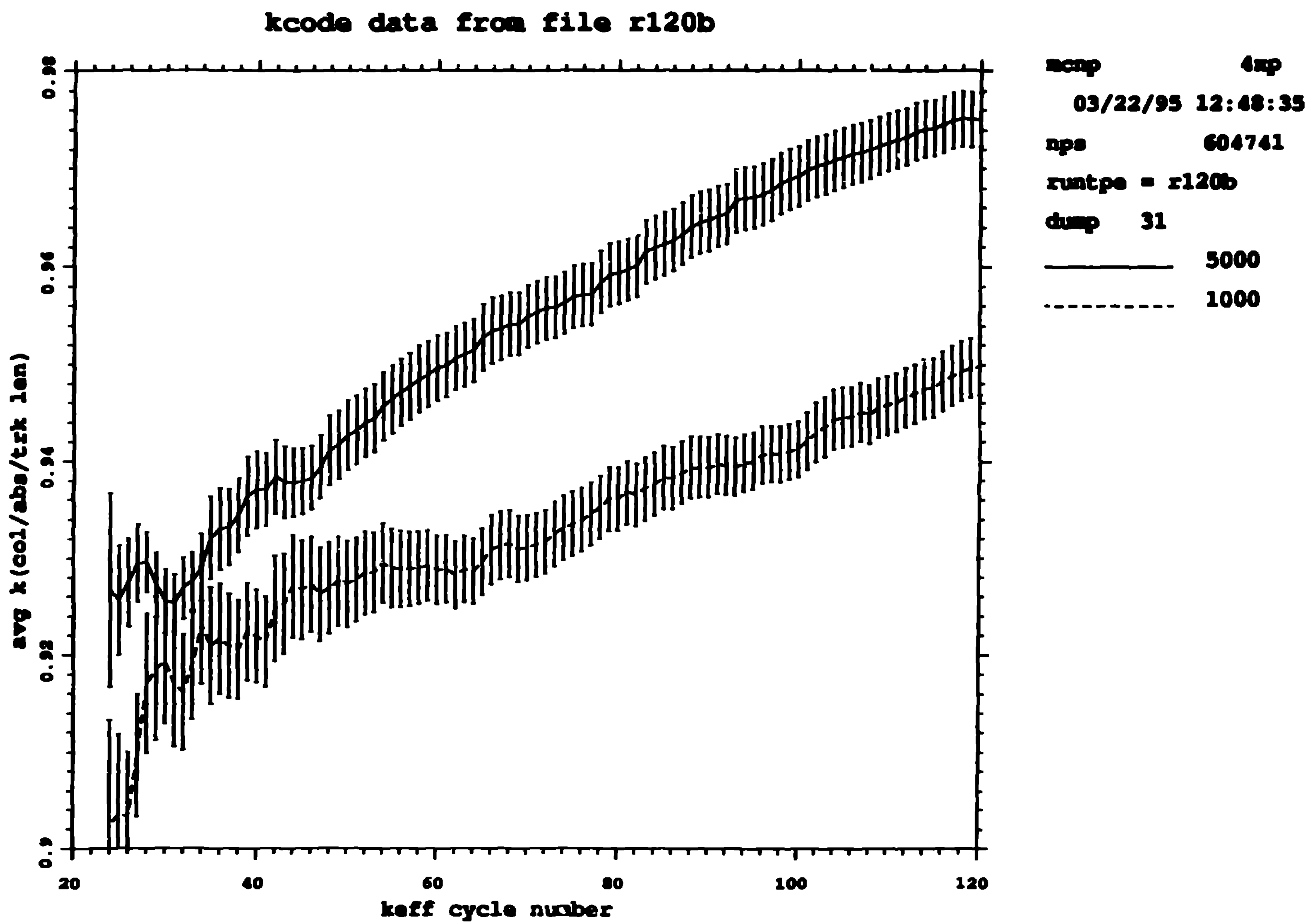

Fig. 5. One standard deviation confidence intervals for the average keff of the array with Jezebel for 5000 and 1000 neutrons per cycle for 120 cycles.