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Automated Acceleration and Convergence Testing for Monte Carlo Nuclear Criticality Safety Calculations

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INTRODUCTION

Monte Carlo (MC) methods have been used for over 60 years to solve nuclear criticality safety (NCS) problems [1-5]. Figure 1 summarizes a number of advances in MC methods and capabilities in the *mcnp* code [6] over the past 20 years.

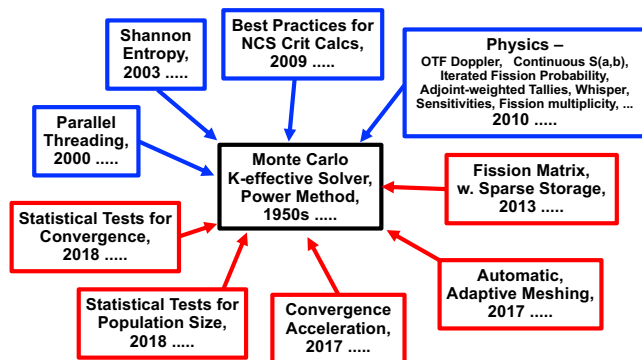


Fig. 1. Recent advances in MCNP MC methods

The red boxes in Figure 1 have recently been used to automate the acceleration of the MC iterative solution method and to statistically determine when the iterations have converged. With these advances, *mcnp6* will converge to steady-state faster and will provide statistical evidence for convergence. The methods significantly reduce the burden on *mcnp6* end-users by eliminating the needs for: trial calculations, examining Shannon entropy plots to determine the number of cycles required for convergence, modifying input files, and rerunning calculations. The new methods are fully automated and do not require any additional user input.

METHODS

The new methods from Figure 1 have been consolidated and automated in a modified version of *mcnp6.2*. An adaptive mesh is automatically constructed with spacing based on the RMS distance from birth to subsequent fission in a generation, and is used for computing the Shannon entropy and for tallying the fission matrix [7,8]. The fission matrix is tallied during inactive cycles and beyond to provide a reference solution for the global fission distribution using compressed row storage (CRS) to alleviate memory storage constraints. The adaptive mesh and fission matrix CRS are

automatically expanded when necessary. It should be noted that the eigenfunction of the fission matrix provides a global reference solution that is not subject to source renormalization bias (as is the neutron distribution). The fission matrix reference solution may be used for importance sampling of the fission neutron source to accelerate convergence of the iteration process. Further details on the adaptive meshing, the fission matrix method, and convergence acceleration may be found in [9].

After the source and fission matrix tallies have stabilized, blocks of cycles are run (default is 10 cycles/block), and 11 statistical checks are performed at the end of a block to assess whether the eigenvalue iteration scheme has converged to steady-state. Seven of the tests involve a “slope test” on different metrics, and the other 4 tests involve Shannon entropy or goodness-of-fit tests on the fission distribution vs the fission matrix reference solution. The slope test involves taking a metric (e.g., the pathlength estimate of k_{eff}) for each cycle in the block, computing a least-squares estimate of the slope and standard deviation of the slope for the set of metrics in the block, and then testing whether the slope is less than $t_{0.025} \cdot \sigma$. If so, the slope for that metric is statistically indistinguishable from zero, indicating steady-state at the 95% confidence level. Otherwise, the test fails. The metrics tested with the slope-test include

- Slope for the cycle pathlength estimate of k_{eff} ,
- Slope for the cycle collision estimate of k_{eff} ,
- Slope for the cycle absorption estimate of k_{eff} ,
- Slope for the cycle Shannon entropy, H ,
- Slope for the cycle H_x , the Shannon entropy of the marginal distribution in x of the fission source,
- Slope for the cycle H_y , entropy y marginal,
- Slope for the cycle H_z , entropy z marginal.

An additional metric test is performed comparing the average Shannon entropy for the block of neutron cycles to the Shannon entropy of the fission matrix reference eigenfunction.

Three goodness-of-fit statistical checks are performed comparing the fission neutron distribution to the fission matrix reference solution:

- Kolmogorov-Smirnov test at the 95 level,
- Chi-square 2-point test at the 95% level,
- Relative entropy (Kullback-Liebler discrepancy) at the 95% level.

Further details on the statistical testing for convergence may be found in [10,11].

If the none of the 11 tests fail, then convergence is declared (within statistics) and active cycles for tallies are begun with the next cycle. Results for all 11 statistical tests are provided as evidence of convergence. Convergence is then locked-in, such that if on subsequent cycles some statistical checks are not passed, convergence is not rescinded. (Typically some of the statistical checks may later fail, and then later pass on most cycles.)

If convergence is not attained, then the acceleration scheme [12] is activated based on source importance sampling weights for each fission bank neutron determined by $S_{FM}(m)/S_{neuts}(m)$, where $S_{FM}(m)$ is the fission matrix reference solution and $S_{neuts}(m)$ is the fission neutron distribution for region m in the adaptive mesh containing the potential fission site.

After convergence and the start of active cycles, additional statistical tests are performed at the end of each block of cycles. These tests examine the relative entropy between the fission neutron distribution and the eigenfunction of the fission matrix, and the average entropy for the block of cycles and the fission matrix eigenfunction to assess whether adequate neutrons/cycle are being used to prevent bias in k_{eff} and the shape of the fission distribution [13]. If the 2 tests are not passed, warning messages are issued that more neutrons/cycle should be used.

TESTING

The automated acceleration and convergence testing methods have been applied to an assortment of criticality problems, including:

- the MCNP *validation_criticality* suite, containing 31 ICSBEP benchmark problems,
- the MCNP *validation_crit_extended* suite, containing 119 ICSBEP benchmark problems,
- a fully-detailed 2D model of a commercial PWR,
- the AGN-201 research reactor at the University of New Mexico,
- the ATR (advanced test reactor) at INL,
- the ACRR burst reactor at Sandia,
- the OECD-NEA Hoogenboom-Martin 3D reactor computer-performance benchmark,
- the 3D C5G7 U-Mox OECD-NEA benchmark problem,
- the ICSBEP benchmark case LEU-COMP-THERM-078 (a Sandia experiment),
- a large 3D storage pool with checkerboard arrangement (OECD-NEA EG on source convergence benchmark #1),
- a 400 cm tall single reactor fuel-pin unit cell with reflecting boundary conditions,
- the Whitesides problem (k_{eff} of the world),
- a 3D Triga reactor model,

- the OECD-NEA source convergence benchmark #4, *test4s*, and
- the Godiva HEU sphere

For all of these cases, standard *mcnp6* input files were used with ENDF/B-VII.1 nuclear data. The only additional input supplied consisted of commands to activate the fission matrix treatment, automated convergence testing, and fission source acceleration:

```
kopts      fmat=      yes
           fmatconvr= yes
           fmataccel= yes
```

Figure 2 shows some results from testing on the *test4s* problem (OECD-NEA Source Convergence benchmark #4). The upper plots of k_{eff} (for neutrons, fission matrix, and cumulative) and H (for neutrons and fission matrix) are from a typical traditional calculation, where a short trial run is made to determine the number of inactive cycles based on plots of k_{eff} and H_{neut} , and then a final run is made after manually setting the number of inactive cycles in the *mcnp6* input file. The number of inactive cycles is somewhat arbitrary, and typical conservative-minded users would choose 150-200 inactive cycles. The lower plots of k_{eff} and H show results from the automated acceleration and convergence methods, with convergence achieved after 31 cycles with no additional user input or trial runs. In all cases tested, the acceleration and diagnostic tests were effective. Following the warning advice, increasing the number of neutrons/cycle to larger values resulted in passing the population size tests (no warning issued). Figure 3 shows the quantitative evidence reported when the statistical tests for convergence are all passed.

Regarding robustness and reliability of the automated methods, all of the 163 test problems performed as expected, with no false positives for convergence or false negatives (which would not affect results, but would increase computer time). When run using conventional methods, the 31 problems in the *validation_criticality* suite required 108 minutes of run time with *mcnp6* using 12 threads. Using the automated acceleration and convergence, the same suite of 31 problems required only 70 minutes to complete correctly. These and other results demonstrate that the combination of automated methods provides effective acceleration and reduces unnecessary conservatism in the number of inactive cycles.

CONCLUSIONS

The convergence acceleration typically reduces the number of initial inactive cycles by factors of 2-10 times, and the use of 11 statistical checks for convergence has proven to be extremely robust and reliable. In the future, *mcnp6* users will not have to make trial runs, plot k_{eff} and H vs cycle, manually edit the input file to adjust the *kcode* card parameters, and

then rerun the problem. Common user pitfalls and annoyances have been removed by the automated convergence and statistical testing methods, and quantitative evidence of convergence is provided. That quantitative evidence is extremely important in today's regulatory environment – “eye-balling the plots” is difficult to defend, whereas documented evidence of passing 11 statistical tests is clear cut. Further work in progress includes the automated generation of the initial guess for the fission neutron distribution.

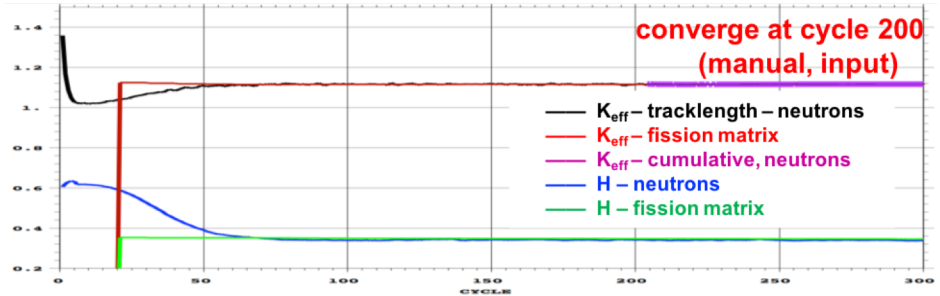
ACKNOWLEDGEMENTS

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50,000 neut/cycle
no acceleration
no auto-converge
k = 1.1164 (2)



50,000 neut/cycle
acceleration
auto-converge
k = 1.1165 (2)

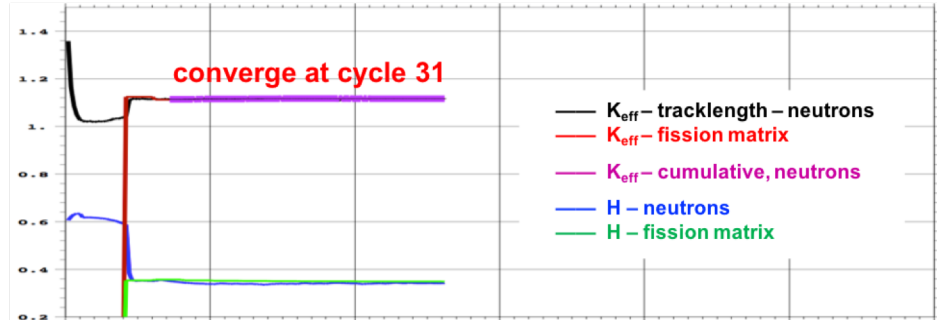


Fig. 2. K_{eff} and H by cycle for problem *test4s*, without/with automated acceleration & convergence

```

31  1.11257      1.12  0.35069                                680
      fmatrix keff= 1.11187, DR= 0.91653, iters=  138
      CONVERGENCE INFO & CHECKS:          (based on last  10 cycles)
      entropy for fmatrix eigenvector      =  0.35656
      entropy for neutron last cycle       =  0.35069      dif=  -1.65%
      relative entropy for last cycle      =  0.00972

      slope of keff (tracklen)             =  4.2E-03, target: < 5.1E-03  PASS
      slope of keff (collide)             =  4.6E-03, target: < 4.9E-03  PASS
      slope of keff (absorb)              =  4.6E-03, target: < 4.9E-03  PASS
      slope of entropy                    = -1.4E-02, target: < 1.6E-02  PASS
      slope of entropy X marginal          = -1.8E-02, target: < 1.9E-02  PASS
      slope of entropy Y marginal          = -1.8E-02, target: < 1.9E-02  PASS
      slope of entropy Z marginal          =  1.3E-03, target: < 1.6E-03  PASS
      entropy dif, neut vs fmat           = -9.1E-04, target: < 1.0E-02  PASS
      Kolmo-Smirnov, distrib, stat        =  2.5E-03, target: < 9.1E-02  PASS
      Chi-square, distrib, stat           =  9.0E+01, target: < 5.1E+02  PASS
      rel-h-block, distrib, stat          =  2.8E-03, target: < 5.1E-03  PASS

      *****
      *****
      ** FISSON SOURCE HAS CONVERGED, based on last  10 cycles **
      ** Metrics:
      **   slope of keff (tracklen)         is 0 (within uncert) **
      **   slope of keff (collide)         is 0 (within uncert) **
      **   slope of keff (absorb)          is 0 (within uncert) **
      **   slope of entropy                 is 0 (within uncert) **
      **   slope of entropy X marginal      is 0 (within uncert) **
      **   slope of entropy Y marginal      is 0 (within uncert) **
      **   slope of entropy Z marginal      is 0 (within uncert) **
      **   entropy dif, neut vs fmat        is 0 (within uncert) **
      ** Distribution checks:
      **   Kolmo-Smirnov, distrib, stat,   neut vs fmat (within conf) **
      **   Chi-square, distrib, stat,      neut vs fmat (within conf) **
      **   rel-h-block, distrib, stat,     neut vs fmat (within conf) **
      *****
      *****
      Convergence is locked-in, even if some tests fail in future cycles ←
      Active cycles will begin with cycle =  32 ←
      Active cycles will end with cycle =  131
      Total active cycles to be run =  100
  
```

Quantitative
Evidence
For
Convergence

Quantitative
Evidence
For
Convergence

Fig. 3. Automated convergence reporting for problem *test4s*