Criticality Benchmarks for COG: A New Point-Wise Monte Carlo Code

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INTRODUCTION

COO is a new point-wise Monte Carlo code being developed and tested at LLNL for the Cray computer. It solves the Boltzmann equation for the transport of neutrons, photons, and (in future versions) charged particles. Techniques included in the code for modifying the random walk of particles make COG most suitable for solving deep-penetration (shielding) problems. However, *its* point-wise cross-sections also make it effective for a wide variety of criticality problems.

COO has some similarities to a number of other computer codes used in the shielding and criticality community. These include the Lawrence Livermore National Laboratory (LLNL) codes TART and ALICE, the Los Alamos National Laboratory code MCNP, the Oak Ridge National Laboratory codes 05R, 06R, KENO, and MORSE, the SACLAY code TRIPOLI, and the MAGI code SAM. Each code *is* a little different in its geometry input and its random-walk modification options.¹

Basically, COO includes:

- Cross-section data is described by the point data included on the LLNL ENDL and EGDL libraries. The current neutron library has data from 20 MeV to thermal. Photon cross sections are available from 100 MeV to lOOeV.
- To check the geometry, the user may calculate volumes and draw cross-sectional pictures.
- General fixed-source routines are available. A special option, WALK-SOURCE, will take a generated source particle and will force it to collide in one, two, or three specified regions before allowing it to start its random walk.
- Random walk modification techniques include splitting and Russian roulette at both collision sites and boundaries, path stretching, survival, scattered energy bias, forced collisions, weight control, and secondary production controL
- A summary of results for random walk events includes reaction type, boundary crossings, and energy depositions. COG also makes plots indicating the location of events in phasespace.

Validating COG consists in part of running benchmark calculations against critical experiments as well as other codes.

The objective of this paper is to present calculational results of a variety of critical benchmark experiments using COG, and to present the resulting code bias. Numerous benchmark calculations have been completed for a wide variety of critical experiments which generally involve both simple and complex physical problems. The COG results, which we report in this paper, have been excellent.

In addition, the results from COG are compared to results we calculated using several other Monte Carlo codes: MORSE-C² (which is an LLNL modified code based on the ORNL code MORSE³), KENO-IV⁴, KENO-Va⁵, and MCNP⁶; and the discrete ordinates code SAN which is an LLNL version of $ANISN^{18}$. For these calculations, the ENDL library of neutron cross sections² was used with COG. A 92 group set (N92GRP) of multigroup cross sections' derived from the ENDL library was used with MORSE-C and SAN. The 16 group Hansen-Roach cross section set¹⁰ and a modified set with potential scattering were used with KENO-IV. With KENO-Va, the 27, 123, and 218 group ENDF-B IV cross-sections^{11,12} were used. With MCNP the code's standard cross sections based on ENDF/B-V were used^{6,13}. The resulting biases calculated for these code and cross section set combinations are compared for various thermal and fast systems.

BENCHMARKS

Tables 1A and IB present a list of the benchmark problems and some general information about each. Detailed references and the multiplication factors calculated for each case using the computer codes COG, MCNP, MORSE-C. KENO-IV, KENO-Va and SAN are shown. Each benchmark case is identified by an ID designator.

Table 1A provides a list of the critical experiments used for this benchmark. The first column is an identification designator. This ID designator connects the information supplied in Table lA with both the information in Table 18 and the graphs in Figures 1 and 2. The second column identifies the fuel form. Next, the fuel isotope is shown followed by % of isotopic content and concentration. The sixth column shows the general fuel core configuration followed by reflector material and thickness. In column 9, the mean neutron energy in Mev is displayed. Finally, a reference number to the original critical experiment paper is listed. The appropriate reference at the end of this paper will lead the reader to greater detail of the experiment by the original experiment authors.

In Table 18, the calculation results of the codes for each identification designator, (associated with Table 1A) are listed by k-eff and the one standard deviation value.

This study has included many different types of critical experiments for the purpose of benchmark comparisons. From a neutron energy standpoint, these included both the fast metal and the thermalized solution systems. From a fissle system standpoint, it considers Pu-239, U-235, and U-233 systems. In addition, bare and reflected systems with metal or hydrogenous reflectors were considered. The geometries of these critical experiments also spanned from simple spheres to concentric cylinders, as well as annular cylindrical tanks and nuclear reactors.

To synthesis and analyze the computer results of these diverse cases, we grouped them into categories containing some common feature. We then examined whether specific biases or trends developed with each of these computational methods.

The grouping categories we selected for fast systems (Figure 1) are: (1) Plutonium-239, (2) Uranium-235, (3) Uranium-233, (4) bare core problems, (5) problems reflected by Beryllium, and (6) problems reflected by Tungsten.

The grouping categories we selected for thennal systems (Figure 2) are: (1) water reflected, low enrichment uranium fluoride solution, (2) bare high enrichment uranium nitrate solution, (3) plutonium nitrate solution, (4) water reflected PuO₂, (5) concrete reflected, high enrichment uranium nitrate, (6) water reflected, mixed nitrate solution, and (7) reactor core. We performed fewer thennal calculations and as a result, we had less data points for our comparisons within a thermal category.

RESULTS

Figures 1 and 2 display our synthesized results for fast and thennal systems respectively. In Figure 1 the critical experiment k -eff = 1 line is drawn. The y-axis shows k -eff. On the x-axis the averaged calculational results for each code for each composite group is displayed.

For example, at the top of the graph in Figure 1, Pu-239(12) shows that we grouped 12 critical experiments that were all fast and had similar characteristics. At the bottom of the graph, the ID designator C1-C12 refers back to Tables 1A and 1B information. We computed the average k-eff for these 12 experiments along with the composite standard deviation for each. As a result, the circle at the extreme left of the graph represents the average k-eff for 12 Pu-239 fast critical experiments with the composite standard deviation error bar shown for COO. The darkened circle next to it is the composite k-eff result for MCNP. Next, the open triangle shows the Keno IV results followed by a darkened triangle for MORSE-C.

The next colwnn on the graph in Figure 1 present the results for the four codes for 15 U-235 systems. This is followed by average values for 11 U-233 systems and so on.

Results of the fast-metal systems as calculated by these four codes are shown in Figure 1. It indicates a general agreement among the results of the four codes for the U-235, the Pu-239, and the bare systems considered. However, for the U-233 systems the MORSE-C/92 group consistently yields k-eff values 2% below critical. For metal systems reflected by beryllium and tungsten alloy, the KENO-IV/16 group consistently yields k-eff values 2.5 and 1.5% above critical, respectively. Such trends or systematic errors were not found in the point-wise Monte Carlo codes (i.e., MCNP and COO).

Results for the thermal systems shown in Figure 2 again demonstrate that the point-wise codes COO and MCNP gave good agreement with critical experiments. The group-wise code KENO-IV and MORSE-C continued to show an overall bias due to group-wise cross-sections. However, we do not have enough cases in the thermal systems examined to adequately represent a statistical sample for each of the selected categories.

Pointwise Monte Carlo methods, such as those employed by COG and MCNP, have not demonstrated a systematic bias, since the cross sections they use vary continuously with energy and inherently cover all ranges of neutron energy.

The COG results were excellent for the wide variety of thennal and fast critical problems we considered. The overall bias for COO was +0.00057, the bias for thermal systems was +0.00480, and the bias for fast systems was -0.00050. We found no abnormal trends for COO, while we found anomalous systematic trends for both KENO-IV and MORSE-C (for the cross-section sets selected). In general, we conclude that COG performed excellently and consistently.

Table 1A

List of Problems, Descriptions, and References

$Table 1B$

List of Problems and Results

Figure 1. Comparison of code Results of the Fast-Metal Systems (55)

O COG
• MCNP Δ KENO-IV **MORSE-C**

REFERENCES

- 1. T.P. Wilcox, Jr. and E.M. Lent, "COG: Particle Transport Code Designed to Solve the *Boltzman Equation for Deep-Penetration (Shielding) Problems,"* Lawrence Livennore National Laboratory (April 1989).
- 2. T.P. Wilcox, *"MORSE-C. A CDC-7600 Program Designed to Solve Nuclear Criticality Problems by Using the Monte Carlo Method,"* UCID-18993, Lawrence Livennore National Laboratory (January 30, 1981).
- 3. E.A. Straker, P.N. Stevens, D.C. Irving and V.R. Cain, *"The MORSE Code A Multigroup Neutron and Gamma-Ray Monte Carlo Transport Code,"* ORNL-4585, Oak Ridge National Laboratory (September 1970).
- 4. L.M. Petrie and N.F. Cross, *"KENO-IV An Improved Monte Carlo Criticality Program,"* ORNL-4938, Oak Ridge National Laboratory (November 1975).
- *5.* L.M. Petrie and N.F. Cross, *"KENO-Va: An Improved Monte Carlo Criticality Program with Supergrouping,"* NUREGICR-0200, ORNL/NUREG/CSD-2, Vol. 2, Sec. Fll, Oak Ridge National Laboratory (November 1985).
- 6. J.P. Briesmeister, ed., *"MCNP - A General Monte Carlo Code for Neutron and Photon Transport,"* LA-7396-M, Rev. 2, Los Alamos National Laboratory (September 1986).
- 7. W.W. Engle, Jr., *"A User's Manual for ANISN: A One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering,"* K-1693, Oak Ridge Gaseous Diffusion Plant (1967).
- 8. K.D. Lathrop, *"The S Method,"* Y-CDC-11, Union Carbide Corp. (1970).
- 9. M.A. Gardner and RJ. Howerton, *"ACIL: Evaluated Neutron Activation Cross-Section Library- Evaluation Techniques and Reaction Index,"* UCRL-50400, Vol. 18, Lawrence Livermore National Laboratory (October 1978).
- 10. G.E. Hansen and W.H. Roach, *"Six and Sixteen Group Cross Sections for Fast Intermediate Critical Assemblies,"* LAMS-2543, Los Alamos Scientific Laboratory (1961).
- 11. N.M. Greene, et al., *"AMPX: A Modular Code System for Generating Coupled Multigroup Neutron Gamma Libraries from ENDF/B," ORNL/TM-3706, Oak Ridge National Laboratory* (1976).
- 12. W.E. Ford, et al., *"A 218-Group Neutron Cross-Section Library in the AMPX Master Interface Format for Criticality Safety Studies,"* ORNLJCSD/fM-4, Oak Ridge National laboratory (July 1976).
- 13. R. Kinzey, *"Data Formats and Procedures for the Evaluated Nuclear Data File, ENDF,"* BNL-NCS-50496 (ENDF 102) 2nd Edition (ENDF/B-V), Brookhaven National Laboratory (October 1979).
- 14. H.C. Paxton, *"Los Alamos Critical-Mass Data,"* LA-3067-MS, Rev., Los Alamos Scientific Laboratory (November 1975). (a) Table IAl, case 2, (b) Table IAl, case 1, (c) Table IC3, case 10, (d) Table IC3, case 12, (e) Table IC4a, case 2, (f) Table IC2, case 8, (g) Table IC2, case 4, (h) Table IC1, case 3, (i) Table IC1, case 4, (j) Table IB1, case 5, (k) Table IB1, case 4, (m) Table ffil, case 2, (n) Table ffil, case 1, (p) Table IV, case 1, (q) Table IV, case 8, (r) Table IV, case 7, (s) Table IV, case 6, (t) Table IV, case 5, (u) Table IV, case 4, (v) Table IV, case 3, (w) Table VA, case 9, (x) Table VA, case 10, (y) Table VA, case 11, (z) Table DIAl, case 1, (aa) Table IIIAl, case 11, (bb) Table IIIAl, case 8, (cc) Table VA, case 1, (dd) Table IIIAl, case 6, (ee) Table IIIAl, case 4.
- 15. G.E. Hansen and H.C. Paxton, *"Reevaluated Critical Specifications of Some Los Alamos Fast-Neutron Systems,"* LA-4208, Los Alamos Scientific Laboratory, (June 1969). (a) p.9, 5.74 ± 0.03 kg $U^{23}(98.13 \text{ wt\%})$, (b) p.12, 5.79 kg \pm 0.5% sphere of Pu²³⁹(94.5%).
- 16. H.C. Paxton and N.L. Pruvost, "Critical Dimensions of Systems containing ²³⁵U, Pu²³⁹, and U²³³, *1986 Revision,"* LA-10860-MS, Los Alamos National Laboratory, (July 1987). (a) Table 16, line 3, 6.6±0.2cm sphere.
- 17. *"Argonne Code Center: Benchmark Problem Book,"* ANL-7416, Argonne National Laboratory, (July 16, 1968). (a) Problem 1.
- 18. G.E. Hansen, H.C. Paxton and D.P. Wood, *"Critical Masses of Oralloy in Thin Reflectors,"* LA-2203, Rev., Los Alamos Scientific Laboratory, (July 16, 1958).
- 19. H.R. Ralston, *"Critical Masses of Spherical Systems of Oral/oy Reflected in Beryllium,"* UCRL-4975, University of California Radiation Laboratory, Livermore, (October 10, 1957), (a) Table I, case 1.
- 20. E.C. Mallary, *"Oralloy Cylindrical Shape Factor* and *Critical Mass Measurements in Graphite, Parafm, and Water Tampers,"* LA-1305, Los Alamos Scientific Laboratory (October 27, 1951).
- 21. G.E. Hansen and D.P. Wood, *"Precision Critical Mass Determinations for Oralloy and Plutonium is Spherical Tuballoy Tampers,"* LA-1356, Los Alamos Scientific Laboratory {February 1, 1952).
- 22. Alan Staub, D.R. Harris, and Mark Goldsmith, *"Analysis of a Set of Homogeneous U-H20 Spheres,"* Nucl. Sci. and Eng., 34 (1968) 263-274. (a) Experiment number 1, (b) Experiment number 5.
- 23. R. Gwin and D.W. Magnuson, *"Critical Experiments for Reactor Physics Studies,"* ORNL-60-4- 12, Oak Ridge National Laboratory (1960).
- 24. R. Gwinn and D.W. Magnuson, "Determination of Eta by Comparison of $\pi\sigma$ for U^{23} and Pu^{239} with \overline{r} *for U²³⁵* in a Flux Trap Critical Assembly," Nucl. Sci. & Eng., 12 (1962) 359-363.
- 25. S. Morioka, Y. Hariyama, H. Kadptani, M. Senda, K. Tamura and K. Saito, *"Criticality Safety Analysis with the Monte Carlo Code MCNP,"* International Seminar on Nuclear Criticality Safety, Tokyo, Japan (October, 1987) 335-339.
- 26. E.B. Johnson and D.F. Cronin, "Critical Dimensions of Aqueous UO₂F₂ Solutions Containing *4.9% usu-Enriched Uranium,"* ORNL-3714, Oak Ridge National Laboratory (Dec. 1964) 31-33. (a) Table 2.2.1, case 3, (b) Table 2.2.1, case 4.
- 27. E.A. Plassmann and D.P. Wood, "Critical Reflector Thicknesses for Spherical U^{23} and Pu^{230} *Systems,"* Nucl. Sci. & Eng., 8 (1960) 615-620.
- 28. G.A. Jarvis, G.A. Linenberger, J.D. Ornfoff and H.C. Paxton, *"Two Plutonium-Metal Critical Assemblies,"* Nucl. Sci. & Eng., 8 (1960) 525-531.
- 29. F.A. Kloverstrom, *"Spherical and Cylindrical Plutonium Critical Masses,"* UCRL-4957, University of California Radiation Laboratory, Livermore (September 1957). (a) Table II, case 7, (b) Table II, case 3, (c) Table II, case 5, (d) Table II, case 1, (e) Table II, case 6.
- 30. R.C. Lloyd, RA. Libby, and B.D. Clayton, *"The Measurement of Eta and the Limiting* Concentration of the Pu²³⁹ in Critical Aqueous Solutions," Nucl. Sci. & Eng., 82 (1982) 325-331. (a) Table I, case 4.
- 31. C.R. Richey, *'Theoretical Analyses of Homogeneous Plutonium Critical Experiments,"* Nucl. Sci. & Eng., 31 (1968) 32-39. (a) Table III, 11.5-in. diameter, 140 gPu/1.
- 32. R.C. Lloyd, C.R. Richey, E.D. Clayton and D.R. Skeen, *"Critical Studies with Plutonium Solutions,"* Nucl. Sci. & Eng., 25 (1966) 165-173. (a) Table I, footnote d, HJPu = 668.
- 33. R.C. Lloyd and E.D. Clayton, *"Criticality of Plutonium-Uranium Nitrate Solution Containing 30* wt% *Pu,"* Trans. ANS, 17 (1973) 269-270. (a) Table I, 12.4 gPu/1 case.
- 34. R.C. Lloyd and B.D. Clayton, *"Effect of Fixed and Soluble Neutron Absorbers on the Criticality of Uranium-Plutonium Systems,"* Nucl. Sci. & Eng., 62 (1977) 726-735.
- 35. M.N. Baldwin, G.S. Hoovler, R.L. Eng and F.G. Welfare, *"Critical Experiments Supporting Close Proximity Water Storage of Power Reactor Fuel, Summary Report,"* BAW-1484-7, Babcock & Wilcox Co., Lynchburg, VA, (1979). (a) case XIIIa.
- 36. Robert E. Rothe, *"Criticality Safety of an Annular Tank for Fissile Solution,"* Trans. Am. Nucl. Soc., 39 (1981) 525-527. (a) Table I, configuration I, 0.8% boron-loaded concrete "interior", 559mm x 415mm.
- 37. R.E. Peterson and G.A. Newby, *'ltn Unreflected UVS Critical Assembly,"* Nucl. Sci. & Eng., 1 (May 1956) 112.

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