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

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INTRODUCTION

COG 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.

COG 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, COG 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 100eV.
- 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^{7,8}. For these calculations, the ENDL library of neutron cross sections² was used with COG. A 92 group set (N92GRP) of multigroup cross sections⁹ 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 1B 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 1A with both the information in Table 1B 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 1B, 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 thermal 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 PuO_2 , (5) concrete reflected, high enrichment uranium nitrate, (6) water reflected, mixed nitrate solution, and (7) reactor core. We performed fewer thermal 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 thermal 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 COG. 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 column 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 COG).

Results for the thermal systems shown in Figure 2 again demonstrate that the point-wise codes COG 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 thermal and fast critical problems we considered. The overall bias for COG 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 COG, 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

| ID | Fuel | | | | | Reflector | | MFE | Reference | |
|----------------|------------|-------|-------|---------|----------|-----------|--------|----------|----------------|--|
| | | | | | | | ****** | | | |
| | Form | Iso | Iso | U or Pu | Shape | Material | Thick | | | |
| | | | [wtt] | [g/cc] | | | [cm] | [MeV] | | |
| | | | | | | | | 1 15.00 | 14- 15 | |
| Al | metal | 0235 | 93.9 | 18.810 | sphere | None | | 1.12+00 | 148,15 | |
| A2 | metal | U235 | 93.7 | 18.740 | sphere | None | | 1.02+00 | 140,10 | |
| A3 | metal | U235 | 94.6 | 18.750 | sphere | None | | 1.1E+00 | 1/2.3/ | |
| A4 | metal | U235 | 93.9 | 18.500 | sphere | Be | 4.70 | 8.1E-01 | 14c,18 | |
| A5 | metal | U235 | 93.6 | 18.600 | sphere | Be | 11.79 | 5.9E-01 | 14d, 16, 18 | |
| A6 | metal | U235 | 93.2 | 18.490 | sphere | Be | 20.27 | 4.7E-01 | 19a | |
| A7 | metal | U235 | 93.9 | 18.700 | sphere | C | 10.16 | 8.9E-01 | 14e.20 | |
| 84 | matal | U235 | 93.8 | 18.380 | sphere | N1 | 4.94 | 9.4E-01 | 14f,15,18 | |
| A9 | matal | U235 | 94.0 | 18.430 | sphere | Cu | 10.56 | 8.1E-01 | 14g,15,18 | |
| A10 | matal | U235 | 93.9 | 18.750 | sphere | W | 5.08 | 8.6E-01 | 14h, 16, 18 | |
| A11 | metal | U235 | 93.9 | 18.750 | sphere | W | 10.16 | 7.9E-01 | 141.18 | |
| 112 | maral | 11235 | 93.9 | 18,700 | sphere | U238 | 1.77 | 1.1E+00 | 141,15,16 | |
| A12 | meral | 11235 | 94 0 | 18 670 | sphere | U238 | 4.47 | 1.1E+00 | 14k.15.16 | |
| ALD | metal | 11235 | 03 0 | 18 690 | enhara | 11238 | 9 98 | 1 1E+00 | 14m.15.16.21 | |
| AI4 | metal | 11225 | 03.2 | 18 620 | sphere | 11238 | 18 01 | 1 25+00 | 14n.15.16 | |
| ALS | metal | 17235 | 03 1 | 0.020 | sphere | None | 10.01 | 3 25-08 | 22= 23 24 | |
| A16 | U02(N03)2 | 0235 | 93.1 | 0.020 | sphere | None | 20 00 | 3 65-08 | 25 260 | |
| A17 | U02F2 | 0235 | 4.9 | 0.728 | cylinder | 120 | 20.00 | 3.05-00 | 25,265 | |
| A18 | UO2F2 | 0235 | 4.9 | 0.650 | cylinder | HZO | 20.00 | 3.46-08 | 25,200 | |
| A19 | UO2(NO3)2 | U235 | 93.2 | 0.357 | annular | Concrete | 20.32 | | 364 | |
| A20 | U02 | U235 | 2.5 | 9.007 | reactor | | | | 338 | |
| | | | | | | | | | | |
| | | | | | | | | | | |
| | | 11233 | 98 1 | 18 420 | sphere | None | | 1.3E+00 | 140.15.16 | |
| BI | metal | 11233 | 08 2 | 18 620 | anhere | Re | 2 04 | 1.2E+00 | 140.16.27 | |
| 82 | Betal | 11233 | 08 2 | 18 640 | sphere | Be | 4 20 | 1 1E+00 | 14r.16.27 | |
| 83 | metal | 0233 | 00.4 | 10 620 | sphere | 17 | 2 44 | 1 25+00 | 14e 16 27 | |
| B 4 | metal | 0233 | 90.2 | 18.620 | sphere | | 5 70 | 1 15+00 | 14+ 16 27 | |
| B5 | metal | 0233 | 98.2 | 10.040 | sphere | W | 3.75 | 1.125.00 | 14. 16 27 | |
| B6 | metal | 0233 | 98.2 | 18.620 | spnere | 0238 | 2.30 | 1.52700 | 14. 16 27 | |
| B7 | metal | U233 | 98.2 | 18 640 | sphere | 0238 | 5.31 | 1.46+00 | 140,10,27 | |
| B8 | metal | U233 | 98.1 | 18.420 | sphere | 0238 | 19.89 | 1.5E+00 | 108,10 | |
| B9 | metal | U233 | 98.1 | 18.620 | sphere | 0235(93.2 |) 1.21 | 1.3E+00 | 140,15,27 | |
| B10 | metal | U233 | 98.1 | 18 640 | sphere | 0235(93.2 |) 1.99 | 1.2E+00 | 14x,15,27 | |
| B11 | metal | U233 | 97.9 | 17 780 | sphere | U235(93.2 |) 4.82 | 1.1E+00 | 14y | |
| B12 | UO2(NO3)2 | U233 | 98.4 | 0 017 | sphere | None | | 3.2E-08 | 226,23,24 | |
| | Contra des | | | | | | | 1 45.00 | 14- 15 16 28 | |
| C1 | metal-d | Pu239 | 92.0 | 15 450 | sphere | None | | 1.42+00 | 142,13,10,20 | |
| C2 | metal-a | Pu239 | 94.5 | 19 740 | sphere | H20 | 20.00 | 1.1E+00 | 150 | |
| C3 | metal-d | Pu239 | 94.8 | 15.620 | sphere | Be | 3.69 | 1.2E+00 | 1444,16,27 | |
| C4 | metal-d | Pu239 | 93.7 | 15 800 | sphere | Be | 5.25 | 1.1E+00 | 16,29a | |
| C5 | metal-d | Pu239 | 93.7 | 15 800 | sphere | C | 3.83 | 1.3E+00 | 16,29b | |
| C6 | metal-d | Pu239 | 93.7 | 15 800 | sphere | Ti | 8.00 | 1.4E+00 | 16,29c | |
| 67 | matalad | Pu239 | 94.8 | 15 620 | sphere | W | 4.70 | 1.2E+00 | 14bb, 16, 27 | |
| 68 | matel d | P1230 | 94 8 | 15 620 | sphere | U235(93 2 |) 1.66 | 1.3E+00 | 14cc.15.27 | |
| 68 | metal-d | D | 03 7 | 15 800 | sphere | 11238 | 1.93 | 1.4E+00 | 16.29d | |
| C9 | metal-d | Pu237 | 04. 9 | 15 620 | sphere | 11238 | 4 13 | 1 45+00 | 14dd. 15.16.27 | |
| C10 | metal-d | Pu239 | 94.0 | 15 800 | spuere | 11238 | 6 74 | 1 55+00 | 16 29e | |
| C11 | metal-d | Pu239 | 93.1 | 15 800 | spuere | 11230 | 10 61 | 1 58400 | 1400 15 16 | |
| C12 | metal-d | Pu239 | 94.8 | 13 360 | sphere | 0238 | 19.01 | 1.32400 | 20- | |
| C13 | Pu(NO3)4 | Pu239 | 97.4 | 0 009 | sphere | None | | 3.8E-08 | 304 | |
| C14 | Pu(NO3)4 | Pu239 | 95.4 | 0 039 | sphere | None | | 4.9E-08 | 32a | |
| 0.000 | | | | | | | | | | |
| | | | | | | | | | 31 . 32 | |
| C15 | Pu(NO3)4 | Pu239 | 95.4 | 0 1.00 | sphere | 120 | 15.00 | 3 05-00 | 33.0 | |
| C16 | Pu(NO3)4 | Pu239 | 94.0 | 0 012 | cylinder | H20 | 15.00 | 3.95-08 | | |
| and the second | UO2(NO3)2 | U235 | 0.7 | 0 0 30 | | | | | 14- | |
| C17 | Pu02 | Pu239 | 100.0 | 9 960 | sphere | H20 | 30.48 | /.3E-01 | 108 | |

Table 1B

List of Problems and Results

| ID | COG | MCNP | MORSE-C | KENO | SAN |
|-----|---------------|---------------|---------------|----------------------|--------|
| | | | | | |
| | K-eII GK-eII | K-eff dk-eff | k-eff dk-eff | k-eff dk-eff Version | k-eff |
| 41 | 1 0002 0 0029 | 0 9954 0 0037 | 0 9990 0 0020 | 1 0006 0 0034 79.076 | 1 0000 |
| 12 | 0 9987 0 0028 | 1 0031 0 0033 | 1 0033 0 0030 | 1.0006 0.0034 17/16 | 1.0029 |
| 13 | 1 0009 0 0029 | 1.0031 0.0033 | 0.0007 0.0030 | 1.0045 0.0036 17/16 | 1.0030 |
| A. | 0 9967 0 0025 | 1 0005 0 0035 | 1 0039 0 0030 | 1.0003 0.0030 10/16 | 1.0030 |
| 45 | 0 9957 0 0026 | 0 9935 0 0037 | 0 0000 0 0000 | 1.0244 0.0034 19/16 | 1.0110 |
| 16 | 0 9961 0 0037 | 0.7733 0.0037 | 0.0046 0.0029 | 1.0250 0.0041 19/16 | 0.9900 |
| A7 | 1 0056 0 0078 | 1 0265 0 0033 | 1 0010 0 0030 | 0 9871 0 0041 11/16 | 1.0024 |
| 48 | 0 9964 0 0027 | 0 9971 0 0035 | 1 0162 0 0030 | 0.9065 0.0030 77/16 | 1.0024 |
| 49 | 1.0084 0.0028 | 0.9906 0.0028 | 1.0186 0.0030 | 0 9992 0 0037 10/16 | 1 0184 |
| A10 | 0.9986 0.0027 | 1.0142 0.0036 | 1.0016 0.0030 | 1 0158 0 0037 TV/16 | 1.0040 |
| A11 | 1.0002 0.0028 | 1.0074 0.0027 | 1.0054 0.0030 | 1 0119 0 0031 77/16 | 1 0020 |
| A12 | 0.9978 0.0028 | 1.0071 0.0044 | 1 0041 0 0030 | 1 0001 0 0031 17/16 | 1 0066 |
| A13 | 1.0012 0.0027 | 1.0054 0.0030 | 1.0135 0.0030 | 1 0045 0 0033 TV/16 | 1 0117 |
| A14 | 1.0013 0.0027 | 1.0026 0.0028 | 1 0061 0 0030 | 1 0031 0 0038 TV/16 | 1 0094 |
| A15 | 1.0004 0.0033 | 1.0073 0.0030 | 1.0014 0.0030 | 1 0022 0 0031 TV/16 | 1 0056 |
| A16 | 0.9917 0.0045 | | 1.0069 0.0030 | 1 0085 0 0104 TV/16 | 0 9980 |
| A17 | 1.0010 0.0030 | 1.0033 0.0035 | 0.8198 0.0029 | 0 9950 0 0035 TV/16 | 0.7700 |
| A18 | 1.0015 0.0064 | 1.0010 0.0039 | 0.8467 0.0029 | 0 9971 0 0030 TV/16 | |
| A19 | 0.9935 0.0063 | | | 0 9941 0 0063 TV/16 | |
| A20 | 1.0032 0.0124 | | | 0 9790 0 0038 Va/27 | |
| | | | | 1 0008 0 0040 Ve/123 | |
| | | | | 0.9789 0.0045 Va/218 | |
| 81 | 0.9952 0.0028 | 0.9925 0.0035 | 0.9801 0.0030 | 1 0052 0 0040 10/16 | 0 9792 |
| 82 | 0 9984 0 0027 | 0 9942 0 0033 | 0 9770 0 0030 | 1 0080 0 0044 17/16 | 0.9792 |
| 83 | 1.0034 0.0022 | 0.9925 0.0048 | 0.9854 0.0031 | 1 0199 0 0045 77/16 | 0 9884 |
| 84 | 0.9992 0.0027 | 1.0011 0.0047 | 0.9756 0.0031 | 1 0200 0 0044 TV/16 | 0 9800 |
| 85 | 0.9926 0.0028 | 1.0033 0.0032 | 0.9679 0.0030 | 1 0105 0 0038 19/16 | 0 9779 |
| 86 | 0.9992 0.0029 | 0.9977 0.0034 | 0.9827 0.0031 | 0.9948 0.0039 TV/16 | 0.9855 |
| 87 | 1.0084 0.0028 | 0.9975 0.0037 | 0.9869 0.0030 | 0 9962 0 0042 TV/16 | 0 9888 |
| 88 | 0.9983 0.0027 | 1.0034 0.0035 | 0.9836 0.0030 | 0 9893 0 0039 TV/16 | 0 9879 |
| 89 | 1.0078 0.0028 | 0.9872 0.0040 | 0.9854 0.0030 | 1.0027 0.0044 TV/16 | 0.9860 |
| B10 | 0.9947 0.0027 | 1.0005 0.0038 | 0.9870 0.0030 | 1.0012 0.0048 TV/16 | 0.9919 |
| B11 | 0.9960 0.0027 | 0.9991 0.0029 | 1.0081 0.0030 | 1.0061 0.0037 TV/16 | 1.0054 |
| B12 | 0.9984 0.0027 | | 1.0082 0.0029 | 1.0041 0.0085 IV/16 | 1.0140 |
| C1 | 1.0011 0.0030 | 0.9951 0.0034 | 1.0001 0.0031 | 1 0001 0 5000 TV/16 | 1 0029 |
| C2 | 1.0104 0.0088 | | 0.9940 0.0048 | 0.9912 0.0038 TV/16 | 0.9710 |
| C3 | 1.0002 0.0030 | 0.9907 0.0038 | 1.0033 0.0032 | 1.0121 0.0049 IV/16 | 1.0052 |
| C4 | 0.9964 0.0030 | 0.9982 0.0041 | 0.9988 0.0032 | 1.0256 0.0045 IV/16 | 1.0039 |
| CS | 1.0055 0.0042 | 0.9905 0.0038 | 0.9996 0.0030 | 0.9921 0.0042 TV/16 | 1.0049 |
| C6 | 0.9864 0.0042 | 0.9752 0.0043 | 0.9785 0.0034 | 0.9846 0.0044 IV/16 | 0.9905 |
| C7 | 0.9959 0.0032 | 1.0068 0.0040 | 0.9950 0.0030 | 1.0100 0.0044 IV/16 | 0.9973 |
| C8 | 1.0074 0.0028 | 1.0016 0.0037 | 1.0060 0.0030 | 1.0083 0.0046 IV/16 | 1.0038 |
| C9 | 0.9947 0.0028 | 0.9939 0.0032 | 0.9944 0.0031 | 0.9951 0.0044 IV/16 | 0.9974 |
| C10 | 0.9931 0.0029 | 0.9985 0.0051 | 1.0098 0.0030 | 1.0008 0.0039 IV/16 | 1.0056 |
| C11 | 0.9991 0.0047 | 0.9909 0.0039 | 0.9926 0.0030 | 0.9930 0.0042 IV/16 | 1.0019 |
| C12 | 0.9952 0.0032 | 1.0027 0.0033 | 1.0036 0.0030 | 0.9914 0.0031 IV/16 | 1.0028 |
| C13 | 1.0164 0.0047 | | 1.0208 0.0028 | 1.0191 0.0020 IV/16 | 1.0230 |
| C14 | 1.0018 0.0030 | | 1.0219 0.0030 | 1.0081 0.0029 TV/16 | 1.0216 |
| | | | | 1.0300 0.0050 Va/27 | |
| | | | | 1.0360 0.0049 Va/123 | |
| | | | | 1.0211 0.0050 Va/218 | |
| C15 | 1.0380 0.0047 | | 1.0098 0.0049 | 1.0547 0.0032 IV/16 | 1.0170 |
| C16 | 1.0042 0.0066 | | 1.0141 0.0029 | 1.0233 0.0017 IV/16 | |
| | | | | | |
| C17 | 1.0018 0.0153 | | 0.9988 0.0030 | 1.0227 0.0055 TV/16 | 0.9789 |



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

COG
 MCNP
 KENO-IV
 MORSE-C

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