

COG11.1 Description, New Features, and Development Activities

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ABSTRACT

The latest COG code version, COG11.1BETA2, is described along with a summary of new features and ongoing and future development activities. This version is available from the Radiation Shielding Information Computer Center and Nuclear Energy Agency Data Bank.

Key Words: code, COG, criticality, Monte Carlo, transport

1 DESCRIPTION

1.1 Software Name:

COG

1.2 Most Recent Distributed Version:

COG11.1BETA2

1.3 Manual and Supplements:

UCRL-TM-202590 [Ref. 1], LLNL-SM-461824 [Ref. 2], LLNL-SM-635621 [Ref. 3]

1.4 Software Completion Date:

April 15, 2013

1.5 Short Title:

A Multiparticle Monte Carlo Transport Code

1.6 Author Names:

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1.8 Brief Description:

COG is a modern, full-featured, Monte Carlo radiation transport code, which provides accurate answers to complex shielding, criticality, and activation problems. COG was written to be state of the art and free of physics approximations found in earlier codes. COG is fully 3-D, uses point-wise cross-sections and exact angular scattering, and allows a full range of biasing options to speed up solutions for deep penetration problems. Additionally, COG has a criticality option for computing k-eff for assemblies of fissionable materials. Cross-section libraries in ENDL, ENDF-6 and ACE formats may be used.

1.9 Method of Solution:

COG uses Monte Carlo methods to solve the Boltzman transport equation for particles traveling through arbitrary 3-dimensional geometries. Neutrons, photons, electrons, and protons can be transported.

1.10 Computer(s) for which Software is Written:

LINUX PC/workstations
Mac OS X 10.6 Workstations
Windows 7 or Windows XP PC/workstations

1.11 Computer Software Requirements:

Bash, csh, and perl are required to run installation scripts. The code uses graphics routines from the PGPLOT subroutine library.

1.12 Computer Hardware Requirements:

The code system without the data libraries requires 35 MB of disk space. The standard data library set requires 1.6 GB. The optimum disk space for code system and the complete set of data libraries is 100GB.

1.13 Programming Languages Used:

FORTRAN77 (99%), C (1%)

1.14 Software Limitations:

Size of problems may be limited by computer memory.

1.15 Unique Features of the Software

Cross-sections – COG can use either LLNL ENDL cross-sections or any cross-sections in ENDF-6 or ACE formats; e.g., ENDF/B-VII.1.

Geometry – Analytic surfaces are used to describe geometric boundaries. Parts (volumes) are described by a method of Constructive Solid Geometry. Surface types include surfaces of up to fourth order, and pseudo-surfaces such as boxes, finite cylinders, and figures of revolution. Repeated assemblies need be defined only once using UNIT or LATTICE features. Parts are visualized in cross-section and perspective picture views.

Biasing options – Source and random-walk biasing techniques may be selected to improve solution statistics. These include source angular biasing, importance weighting, particle splitting and Russian roulette, pathlength stretching, point detectors, scattered direction biasing and forced collisions.

Criticality – For a fissioning system, COG will compute k-eff by transporting batches of neutrons through the system. Special features of interest to criticality safety practitioners have been published in conference proceedings [Ref. 4-6].

Activation – COG can compute gamma-ray doses due to neutron-activated materials, starting with just a neutron source.

Coupled problems – COG can solve coupled problems involving neutrons, photons and electrons.

User-specified Sources and Detectors – COG offers a large variety of radiation sources and detectors that can be selected for any problem. However, if a custom detector or source is wanted (e.g., an energy-angle correlated source), the user may write a routine which when called by COG returns the starting parameters of a source particle. This routine is compiled and loaded into a runtime library file that COG reads at startup.

Detectors - Reaction, tallies number of reactions within a specified volume; Boundary, tallies particles crossing a specified boundary; Point, estimates the particle flux at a point; Point Volume, estimates flux at points randomly selected within a volume; Pulse, simulates a counting experiment, with or without coincidence; and USRDET, allows user defined detectors.

High Performance Computing – COG is designed to run under the high performance and widely portable implementation of the Message Passing Interface (MPI) standard. It can also run under the InfiniBand, channel-based, switched fabric interconnect architecture environment. It is scalable to run on the LLNL Sequoia machine – one of the fastest super computers in the world. Actual performance results depend on the complexity of the problems and the number of nodes/processors.

1.16 Related and Auxiliary Software:

Uses graphics routines from PGPLOT subroutine libraries. Electron transport uses the EGS transport kernel.

1.17 Other Programming or Operating Information Restrictions:

None.

1.18 Time Requirements:

Running time on a particular computer will vary widely, depending on geometric complexity, number of materials, and number of particles to be followed. For many problems, runs of tens of minutes may give an approximate solution. For a statistically precise solution, hours of computation may be necessary. Parallel processing is available using MPI.

2 NEW FEATURES

2.1 CritDetVR

COG has many techniques for variance reduction of detector scores. Though all differ, in general they act by attempting to sample important regions of the problem's phase space preferentially, thereby causing a greater fraction of computer time to be spent tracking particles that score, improving detector statistics and accelerating convergence to a solution.

Although these techniques can work well in shielding problems, difficulties arise in their application to criticality eigenvalue problems. To the extent that they modify the collision density in the fissioning system, the K eigenvalue will deviate from the correct value.

CritDetVR, the Crit Detector Variance Reduction mode, was introduced to allow variance reduction methods to be employed in a criticality eigenvalue problem without biasing in any way the outcome of the k-eff calculation. COG interleaves crit batches with shielding cycles in such a way that each shielding cycle transports the source neutrons generated by the preceding criticality batch.

There is no “feedback” from the shielding cycle to the eigenvalue calculation, so the computed k-eff is an unbiased result. Each shielding cycle treats the last computed criticality source as a sample of the problem's “settled source” and can employ any of the WALK-XX random-walk variance reduction methods available to enhance scoring statistics at the problem's detectors.

2.2 Delayed Fission Gammas

This feature simulates the production and tracking of delayed fission gammas. In the detector output, both a (total) prompt and delayed (between times t1 and t2) photon component is scored. Also included is the delayed fission gamma rate at t2.

2.3 Nuclear Resonance Fluorescence

Nuclear resonance fluorescence (NRF) reactions are the result of nuclear absorption and emission of photons. When a near resonance energy photon strikes the nucleus, the nucleus becomes excited. The excited nucleus subsequently decays to its ground state, releasing one or more discrete energy photons. The data needed to do nuclear resonance fluorescence calculations in COG are contained in the COG library COGNRF and consists of 8 elements, 15 isotopes, and 22 lines (7Li, 89Y, 140Ce, 142Ce, 142Nd, 144Nd, 152Sm, 152Sm, 154Sm, 154Gd, 156Gd, 156Gd, 156Gd, 156Gd, 158Gd, 158Gd, 160Gd, 235U, 238U, 238U, 238U, and 239Pu). The data provided, by Dr. James Hall of LLNL, are cross sections, branching ratios, and emission energies.

2.4 Radiation Simulation

Many applications require the calculation of an ideal theoretical radiation spectrum resulting from the natural decay of radioactive elements. The Radiation Simulation (RadSrc) option is designed to fill that need. COG computes the concentrations of decay products given an initial concentration and age, and photon radiation due to the continuing decay of those products.

2.5 COGLEX

The definitions in the COG dictionary COGLEX have been expanded to provide an approximate thermal treatment for many materials. For dictionary materials that have ‘water-like’ Hydrogen bonds, a corresponding definition has been included where the Hydrogen is replaced by Hydrogen bound in water; e.g., in addition to a definition for Blood we now have a definition for (Blood), where the ()’s indicate a thermal scattering treatment. We made similar additions for those materials that had ‘CH₂-like’ bonds, e.g. Acetone and (Acetone).

3 DATA LIBRARIES

3.1 Neutron Activation Library:

ACTL92 – LLNL’s ACTL-1992

3.2 Photon Libraries

COGGXS – Defaults to EPDL97

EPDL89 – LLNL’s EPDL-1989

EPDL97 – LLNL’s EPDL-1997

3.3 Nuclear Resonance Fluorescence Library

COGNRF – developed by LLNL’s Dr. J. M. Hall (new)

3.4 Photonuclear Libraries

COGPNUC – defaults to IAEAPNUC

IAEAPNUC – IAEA

PN.ENDFB7R1 – ENDF/B-VII.1 (new)

PN.MCNP.70u – MCNP’s.70u (new)

3.5 Radiation Simulation Library

COGRS – developed by LLNL’s Dr. E. M. Lent (new)

3.6 Delayed Fission Gamma Libraries

DFG.ENDFB7R1 – developed by LLNL’s Dr. E. M. Lent (new)

DFG.JEFF3.1.1 – developed by LLNL’s Dr. E. M. Lent (new)

DFG.JENDL4 – developed by LLNL’s Dr. E. M. Lent (new)

3.7 Neutron Libraries

ENDFB6R7	– ENDF/B-VI.7 developed by LLNL’s Dr. D. E. Cullen
ENDFB6R8	– ENDF/B-VI.8 developed by LLNL’s Dr. D. E. Cullen
ENDFB7R0	– ENDF/B-VII.0 developed by LLNL’s Dr. D. E. Cullen
ENDFB7R0.BNL	– ENDF/B-VII.0 developed by Brookhaven National Laboratory
ENDFB7R1	– ENDF/B-VII.1 developed by LLNL’s Dr. D. E. Cullen (new)
ENDFB7R1.BNL	– ENDF/B-VII.1 developed by Brookhaven National Lab. (new)
ENDL90	– LLNL’s ENDL-1990
ENDL99	– LLNL’s ENDL-1999
JEFF3.1	– JEFF3.1
JEFF3.1.1	– JEFF3.1.1
JEFF3.1.2	– JEFF3.1.2 (new)
JENDL3.3	– JENDL3.3
JENDL4	– JENDL4 (new)
MCNP.50c	– MCNP’s .50c
MCNP.51c	– MCNP’s .51c
MCNP.55c	– MCNP’s .55c
MCNP.66c	– MCNP’s .66c
MCNP.70c	– MCNP’s .70c
RED2002	– Hybrid ENDF/B-ENDL library by LLNL’s Dr. D. E. Cullen (2002)

3.8 Probability Table Libraries

PT.ENDFB7R0.BNL	– BNL’s ENDF/B-VII.0
PT.ENDFB7R1.BNL	– BNL’s ENDF/B-VII.1 (new)
PT.JEFF3.1	– JEFF3.1
PT.JEFF3.1.1	– JEFF3.1.1
PT.JEFF3.1.2	– JEFF3.1.2 (new)
PT.MCNP.66c	– MCNP’s .66c
PT.MCNP.70c	– MCNP’s .70c

3.9 Thermal Scattering Libraries

T.ENDFB3R0	– ENDF/B-III.0
T.ENDFB6R0	– ENDF/B-VI.0
T.ENDFB6R2	– ENDF/B-VI.2
T.ENDFB7R0	– ENDF/B-VII.0
T.ENDFB7R0.BNL	– BNL’s ENDF/B-VII.0
T.ENDFB7R0.LANL	– LANL’s ENDF/B-VII.0
T.ENDFB7R1	– ENDF/B-VII.1 (new)
T.ENDFB7R1.BNL	– BNL’s ENDF/B-VII.1 (new)
T.JEFF2.2	– JEFF2.2
T.JEFF3.0	– JEFF3.0
T.JEFF3.1	– JEFF3.1
T.JEFF3.1.1	– JEFF3.1.1
T.JEFF3.1.2	– JEFF3.1.2 (new)

3.10 Dosimetry Libraries

IRDF2002	– IRDF-2002
IRDF1.02	– IRDF Release 1.02

4 Ongoing and Future Development Activities

4.1 New Data Libraries

Laboratory development versions of the COG11.1 code have implemented the ENDL2008, ENDL2011, JEF2.2 and MCNP.71nc neutron libraries; the PT.MCNP.71nc probability table library; and the T.ENDFB71.LANL and T.IAEA2007 thermal scattering libraries. A joint research and development effort is planned to develop additional nuclear photonics and thermal scattering law data with collaborators at Texas A&M University and North Carolina State University, respectively. As new data libraries become available, they will be implemented in future code or supplemental data releases.

4.2 Automated Data Testing

Brookhaven National Laboratory and Lawrence Livermore National Laboratory [Ref. 7] have begun a project to automate the process that begins when a nuclear data evaluation is updated, followed by the processing of the revised evaluation parameters into cross-sections, followed by additional formatting into application-specific libraries, then testing of the data with the application (e.g., COG) using relevant benchmark calculations and inter-comparisons to other code results. The COG code development team is planning to participate in these efforts, which requires distribution of those auxiliary codes, which prepare and assemble the various COG application-specific libraries from source data in a variety of formats. As part of this effort, the COG benchmark suite will also be tested in the ARDRA [Ref. 8], an LLNL-developed massively parallel 3-D Sn code, which contains the COG geometry package and an automatic mesh generation feature. It is anticipated that ARDRA solutions may also be used as a starting source for accelerated convergence or for variance reduction in complex COG simulations.

4.3 Next Code Release

The next public release of the COG code is planned to coincide with the 2015 International Conference on Nuclear Criticality.

5 CONCLUSIONS

The Nuclear Criticality Safety Division of the Lawrence Livermore National Laboratory maintains COG as “safety software” for use in criticality safety and other research applications. Please visit our website at <http://cog.llnl.gov> for further details.

6 ACKNOWLEDGMENTS

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