LLNL-AR-678519

Summary Report on LLNL Participation in US and International Analytic Methods Collaborations in FY-2015

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September 30, 2015

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Auspices

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Executive Summary

This document fulfills a specific analytic methods milestone given in the 2015 Five-Year Execution Plan for a summary report of LLNL participation in US and international analytical methods collaborations.

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0.0 Introduction

This document fulfills a specific analytic methods milestone given in the 2015 Five-Year Execution Plan for a summary report of LLNL participation in US and international analytical methods collaborations. Part 1.0 of the report addresses collaborative work with other elements of the Lawrence Livermore National Laboratory. Part 2.0 addresses collaborations with other US national laboratories, US universities, and foreign laboratories.

1.0 Internal Collaborations

1.1 OFFICE OF THE DIRECTOR

1.1.1 Environment, Safety and Health (ES&H)

LLNL analytic methods used to develop the databases for the delayed fission gamma (DFG) feature in COG11.1 under DOE NCSP auspices are also used to calculate the concentration of fission product isotopes per fission as a function of time. This data, together with fission product activities identified and measured by Dr. Dave Hickman (ES&H) in irradiated ^{235}U foils, was used to estimate Godiva-IV excursion yields in IER-147, and this important analytical methods capability will be maintained for use in FY-2016 to support IER-148 and IER-252, and IER-175, IER-252, IER-253, IER-268, and IER-406 in the out-years.

1.1.2 Institutional Quality Program

In FY-2015, the COG code development team continued to collaborate significantly with Darrel Whitney, LLNL Software Quality Assurance (SQA) Manager, to upgrade COG (risk level 3 with major developmental control) software to meet all Institutional Software Quality Assurance Program (ISQAP) requirements for compliance with 10CFR830, DOE O 414.1D and NQA-1. Per Whitney, COG is now fully compliant and well positioned for inclusion in the DOE Safety Software Quality Assurance Central Registry[1] as a "toolbox" code. In FY-2016, additional work may be required for compliance with changes to NAP-24, Weapon Quality Policy.

Note that MCNP and SCALE are not developed nor maintained to 10CFR830 or NQA-1 standards by LANL and ORNL, respectively, as confirmed directly with the code team leaders. Therefore, the NCS Division applied the LLNL NQA-1 program to qualify MCNP equivalent to commercial grade dedication. SCALE and TRIPOLI may be similarly qualified as time and funding permits.

1.2 ENGINEERING

1.2.1 Chief Electronics Engineer

In 2012, the Planet and Flattop critical assembly machines at NCERC experienced two control system anomalies resulting in uncommanded movements of the machines. Joe Galkowski, Chief Electronics Engineer, in collaboration with the NCS Division Leader, dispatched Albert Lee, Robert Reed, Mathew Brown and David Milhouse to trouble-shoot and fix the electronics and programmable logic control (PLC) systems enabling these machines to return to service[2]. In FY-

[1] http://energy.gov/ehss/safety-software-quality-assurance-central-registry

[2] Dr. Jerry McKamy, letter to Monya Lane, Associate Director for Engineering, August 28, 2012.

2015, Doug Modlin[3] replaced Joe as Chief Electronics Engineer. Should NCERC require LLNL electronics engineering support including software (i.e., analytic methods) relating to PLCs, the NCS Division Leader will coordinate this support through Doug.

1.2.2 Computational Engineering Division

Bob Ferencz, Computational Engineering Division Leader, in collaboration with the NCS Division Leader, continues to provide high-priority access to Soon Kim, John Scorby et al., on unclassified and classified Livermore Computing high performance machines. This access is essential for multi-physics simulations in support of IER-299, Kilowatt Reactor Using Stirling TechnologY, accident analysis, in addition to computationally challenging problems such as IER-126, Silene CAS Benchmark.

1.3 GLOBAL SECURITY N-PROGRAM

The NCS Division and N-Program continue to collaborate in the application and development of analytical methods (i.e., SrcSim, BIGFIT, and their successor codes) to analyze experimental and simulated subcritical (multiplicity) benchmark count distributions including:

- IER-143, Benchmarking Multiplication Calculations with Neutron Multiplicity Measurements
- IER-160, Plutonium Sphere Reflected with Tungsten
- IER-161, Plutonium Sphere Reflected with Nickel (complete)
- IER-407, ISSA Subcritical Multiplicity Benchmark
- IER-422, Plutonium Sphere Reflected with Copper

In FY-2007, at the request of N-Program, the NCS Division[4] enabled sampling of the fission multiplicity distribution (as opposed to just nu-bar) in COG to enable analog Monte-Carlo calculations simulating the measured count distributions so that both measured and simulated data could be analyzed using the same analytical methods (e.g., BIGFIT). This approach utilized the user-specified source and user-specified detector options in COG. In FY-2016, these features will be reviewed and standardized with funding support from N-Program.

1.4 NIF AND PHOTON SCIENCE

The NCS Division continues to work with Dr. Jim Hall to add high-fidelity nuclear resonance fluorescence cross-sections for additional materials of interest and maintain "… COG, which is now the sole code that contains correct physical modeling for the accurate prediction of nuclear resonance fluorescence detection scenarios" as stated in the FY-2014 LDRD Annual Report, UCRL-TR-113717-14, pp. 299-301.

In FY-2016 and beyond, NIF is expected to continue to provide financial support to further develop COG as the "premiere nuclear photonics simulation tool."

[3] https://pao-int.llnl.gov/news/memos/2015/po-45.23.pdf
[4] http://cog.llnl.gov/UCRL-PROC-231582.pdf

1.5 PHYSICS AND LIFE SCIENCES

1.5.1 Equation of State and Materials Theory Group

In FY-2014, the NCS Division (John Scorby) collaborated with Phil Sterne et al. to develop new equations of state for uranium with detailed metal-metal phase transitions in support of the ROMEO Project. This capability may be required in future.

1.5.2 Nuclear Data and Theory Group

In FY-2015, the NCS Division (Dave Heinrichs) continued to collaborate with Bret Beck and Caleb Matoon on FUDGE, which is LLNL's advanced nuclear data processing code being developed in support of the proposed Global Nuclear Data (GND) format under WPEC SG38. Dave Brown (BNL) is also an active collaborator in this project.

1.5.3 Nuclear Security Physics Group

Essential N-Program (see Section 1.3) subject matter experts reside in the Nuclear Security Physics Group including Les Nakae (Deputy Group Leader), Greg Keefer, Phil Kerr, Jerome Verbeke and Sean Walston.

1.5.4 Rare Event Detection Group

Nathaniel Bowden (Deputy Group Leader) provides subject matter expertise in radiation detector design, manufacturing, development and deployment. In FY-2016, or in the out-years, the NCS Division will collaborate with Bowden to develop independent analysis software to support LLNL's long-term use of the new AWE-developed Passive Neutron Single Sphere Spectrometer, which will require Monte Carlo calculation of the detector response as a function of energy and development of spectrum unfolding software.

1.6 WEAPONS AND COMPLEX INTEGRATION

1.6.1 Nuclear Materials Technology Program

SBK-08-085, Memorandum of Understanding between the Nuclear Materials Technology Program (NMTP) and Nuclear Operations (NucOps), assigns responsibility for 10CFR830 software used in criticality safety evaluations supporting WCI nuclear facilities to the NCS Division Leader. A portion of the NMTP budget for criticality safety support is available for maintenance and limited development of COG and other analytical methods.

1.6.2 Weapons Simulation and Computing Program

The NCS Division (John Scorby) is working closely with computational physicists to develop, maintain and apply modern LLNL-developed multi-physics analytical methods on high-performance computing machines supporting:

- IER-268, PDV Measurements of Godiva for Validation of Multi-Physics Simulations
- IER-299, Kilowatt Reactor Using Stirling Technology

1.6.3 Weapon Technologies and Engineering Program

The Weapon Technologies and Engineering Program supports Directed Stockpile Work managed by the Defense Technologies Engineering Division. This work includes criticality safety evaluations for work involving nuclear weapons, nuclear weapon components, and their transport outside nuclear facilities, and in facilities at NNSS and other NNSA Defense Program sites. In FY-2016, NAP-24 is expected to be revised, which may require the LLNL ISQAP to be updated in which case the activity level SQAPs, SCMPs, etc., may need to be revised as well. In this case, the WTE Program should provide additional funding support.

2.0 External Collaborations

2.1 US NATIONAL LABORATORIES

2.1.1 Bettis Atomic Power Laboratory (BAPL)

LLNL (Dave Heinrichs) and Bettis Atomic Power Laboratory (Mike Zerkel) are partners with North Carolina State University (Ayman Hawari) in developing new thermal scattering laws and associated data processing tools under the Nuclear Data element of the DOE NCSP; however, testing the new data is performed under the Analytical Methods element.

In FY-2015, NCSU developed a new thermal scattering law for poly-methyl-methacrylate (PMMA) (or $C_5H_8O_2$ with trade names: Lucite, Plexiglas, Acrylite, Perspex). This data has been provided by NCSU to LLNL and Bettis for testing using COG and MC21. Preliminary analyses identified no ICSBEP benchmarks sensitive to the thermal scattering law. This was a surprise! However, pulsed neutron data is available which ranges from no sensitivity in (large) low leakage systems to very high sensitivity in (small) high leakage systems. MC21 is unsuitable for analyzing experiments of this type; hence, COG is being relied upon for testing this data in ACE and ENDF-6 File 7 formats.

Preliminary results indicate the most thermal TEX experiment is sensitive to the thermal scattering law. Consequently, it may be desirable to compare this TEX configuration with polyethylene to a similar configuration where Lucite replaces the polyethylene, as the necessary procurements should be relatively inexpensive.

In FY-2016, preliminary thermal scattering law data and testing results will be presented at the NDAG meeting at BNL on November 4, 2015, at the request of chairman. Final testing results will be presented to WPEC SG42, when available.

In FY-2016, LLNL will test the thermal scattering law developed by BAPL for solid water (i.e., ice) against measured pulsed neutron die-away experiments.

2.1.2 Brookhaven National Laboratory (BNL)

LLNL (Dave Heinrichs, Chuck Lee, and Ed Lent) is collaborating with BNL (Dave Brown) on the Automated Data Verification and Assurance for Nuclear Calculations Enhancement (ADVANCE) Project[5]. In FY-2015, LLNL provided BNL with COG11.1 and the COG Library Maker Codes together with 503 ICSBEP HEU and PU benchmarks to get started.

[5] https://ndclx4.bnl.gov/gf/project/checkendf/

2.1.3 Los Alamos National Laboratory (LANL)

LLNL (Dave Heinrichs, Ed Lent) are collaborating with LANL (Forrest Brown) to resolve issues associated with the Ganapol analytic benchmarks. In FY-2015, issues associated with the half-space problems 3.2.2a, 3.2.2b and 3.2.3 were resolved as published by Forrest Brown in ICNC 2015 and provided in a draft document by E. Lent to the NCSP Analytical Methods Working Group Meeting at ICNC 2015.

In FY-2016, LLNL hopes Barry Ganapol will continue to work with Forrest Brown and Ed Lent to resolve the significant discrepancies identified by Lent for problems 3.1.5a, 3.1.5b, 5.1.3a and 5.1.3b; and, resolve or clarify the minor issues associated with problems 2.1.2 (at high lethargy), 3.1.1 (near $x \approx 0$). Note that LLNL results for problems 2.1.3b, 2.1.4, 3.1.2a, 3.1.2b, 3.1.3, 3.1.6, 3.2.2a, 3.2.2b, 3.2.3, 3.3.1a, 3.3.1b, 3.3.2a, 3.3.2b, 5.1.1, 5.1.2, 5.1.4a, and 5.1.4b are in excellent agreement.

Los Alamos also plans to publish additional (new) analytic benchmark results based on original recent work by Gonzales. LLNL is very interested in this work.

2.1.4 Oak Ridge National Laboratory (ORNL)

In FY-2015, LLNL provided the following software to the Radiation Safety Information Computational Center (RSICC) for external distribution as Export Control Information:

- CCC-829, COG11.1 Multiparticle Monte Carlo Code System for Shielding and Criticality Use
- PSR-607, COG LibMaker - Data Conversion Utility

Also in FY-2015, LLNL (Soon Kim) provided independent COG11.1 calculational results to ORNL (Thomas Miller) in support of IER-126, SILENE CAS Benchmark, approved for publication in the 2015 edition of the ICSBEP Handbook as ALARM-TRAN-AIR-SHIELD-001, Neutron Activation Foil and Thermoluminescent Dosimeter Responses to a Bare Pulse of the CEA Valduc SILENE Critical Assembly. Note that the COG11.1 calculations were unbiased "one step" criticality and shielding calculations with and without delayed fission gammas (DFG).

In FY-2016, LLNL plans to provide similar calculational results for additional SILENE CAS benchmarks in which the SILENE reactor is shielded with lead or (cadmium-lined) polyethylene.

Note that a new criticality detector variance detector variance reduction (CritDetVR) feature was added by Rich Buck to COG11.1 to enable "one step" calculation interleaving unbiased criticality batches with biased shielding cycles (enabling use of all variance reduction options). While this feature is working correctly in serial mode, it needs full parallelization to be of practical use.

2.1.5 Sandia National Laboratories (SNL)

In FY-2015, Bettis Atomic Power Laboratory (Mike Zerkel) introduced LLNL (Dave Heinrichs) to a United Kingdom counterpart at Rolls-Royce[6] (James Lam) at ICNC-2015. Dr. Lam expressed interest in IER-407, ISSA Subcritical Multiplicity Benchmark, and its associated detectors, data acquisition system, and count distribution (multiplicity) analysis methods. In

[6] http://www.rolls-royce.com/customers/nuclear/submarine-nuclear-propulsion.aspx

addition to the low multiplication ($M \leq 20$) measurements at ISSA, Dr. Lam was interested in applying these techniques for higher multiplication measurements. Consequently, Heinrichs and Gary Harms (SNL) discussed the possibility of deploying LLNL instrumentation for use with 7uPCX at SNL. This work, if performed, would follow completion of IER-407.

The analytical methods needed to analyze the experimental (and simulation) results include BIGFIT and its successor codes developed by Sean Walston, LLNL, N-Program, for another Government Program Manager (see Sections 1.3 and 1.5.3).

2.2 US UNIVERSITIES

2.2.1 North Carolina State University (NCSU)

As noted in Section 2.1.1, LLNL and BAPL are collaborating with Professor Ayman Hawari (NCSU) to develop new thermal scattering laws for moderator materials. In FY-2015, a new thermal scattering law was completed for Lucite and work began on polyethylene complimenting experimental work by Rensselaer Polytechnic Institute.

In FY-2016, new collaborative work will begin to develop modern analytical methods for generating thermal scattering law data from physical parameters that are more general and accurate than current processing codes (e.g., AMPX and NJOY).

2.2.2 South Carolina State University (SCSU)

In FY-2016, LLNL plans to continue work with Dr. Kenneth Lewis, Dean of the College of Science, Mathematics, and Engineering Technology, to identify a summer student interested in performing Criticality Slide Rule calculations as part of an AWE-IRSN-LLNL-ORNL collaboration.

2.2.3 Texas A&M University (TAMU)

TAMU is a university partner for the LLNL NIF and Photon Science Directorate using COG11.1 for "nuclear photonics" simulations under the auspices of another GPM (see Section 1.4).

2.2.4 University of Arizona

Professor Barry Ganapol, University of Arizona, Department of Aerospace and Mechanical Engineering, published the compendium "Analytic Benchmarks for Nuclear Engineering Applications: Case Studies in Neutron Transport Theory," which is available from the OECD NEA Databank as NEA No. 6292 (© 2008) and on-line[7].

In FY-2015, Ed Lent (LLNL) and Forrest Brown (LANL) corresponded with Professor Ganapol to resolve calculational discrepancies identified by Lent for the half-space problems. The cause of the discrepancies was confusion relating to boundary conditions and the equivalent source specification as now published by Forrest Brown in ICNC 2015.

It is hoped the remainder of the discrepancies identified in Section 2.1.3 can be resolved for these valuable (exact) analytic benchmarks in FY-2016.

[7] https://www.oecd-nea.org/databank/docs/2008/db-doc2008-1.pdf

2.2.5 University of Michigan (UM)

Professor Sara Pozzi, or a student under her supervision, is a possible analytic methods participant in IER-407, ISSA Subcritical Multiplicity Benchmark, using MCNPX-PoliMi[8].

2.3 FOREIGN LABORATORIES

2.3.1 Atomic Weapons Establishment (AWE)

In FY-2015, AWE (Richard Jones, Chris Wilson – JOWOG30 CS POCs) requested COG user training and the latest version of COG, COG11.1. Due to funding constraints, LLNL deferred training to a later date but will deliver COG11.1 software to Leo Clark (AWE) by hand at the KRUSTY meeting scheduled for October 27-28, 2015, at the University of California Washington Center in Washington, DC.

LLNL is collaborating with AWE in analytical methods and other areas as identified in the JOWOG30 Criticality Safety Task Specification and NCSP Five-Year Execution Plan. These activities include development of an updated criticality accident slide rule as part of an AWE-IRSN-LLNL-ORNL consortium.

2.3.2 Canadian Nuclear Laboratories (CNL)

In FY-2015, LLNL (Dave Heinrichs, Ed Lent) began to collaborate with CNL (Danil Roubtsov) on testing a new thermal neutron scattering law for heavy water[9] (D_2O) developed by CAB (see Section 2.3.3) for CNL. Face-to-face meetings occurred at CSEWG and WPEC SG42.

2.3.3 Centro Atomicó Bariloche (CAB)

LLNL (Dave Heinrichs, Ed Lent) is collaborating with José Ignacio Márquez Damián (CAB) under the auspices of WPEC SG42. In FY-2015, LLNL (Ed Lent) created the libraries T.CAB and T.CAB.ACE containing CAB thermal scattering laws for H_2O and D_2O[10] and commenced testing the D_2O scattering law using the same ICSBEP benchmarks as Roubtsov (CNL). This work will continue throughout FY-2016 until complete.

2.3.4 Commissariat à l'Énergie Atomique (CEA)

In FY-2015, in his capacity as an ICSBEP Internal Reviewer, Soon Kim (LLNL) collaborated with Evaluators from ORNL (Thomas Miller), CEA-Saclay (Yi-Kang Lee, Emmanuel Gagnier), and CEA-Valduc (Nicolas Authier, Jerome Piot, Xavier Jacquet and Guillaume Rousseau) to complete IER-126, "Silene CAS Benchmark," published in the ICSBEP Handbook as ALARM-TRAN-AIR-SHIELD-001, "Neutron Activation Foil and Thermoluminescent Dosimeter Responses to a Bare Pulse of the CEA Valduc Silene Critical Assembly."

In FY-2016, LLNL (Dave Heinrichs, Jerome Verbeke) may begin evaluation of the CEA code TRIPOLI for possible qualification and inclusion in the LLNL 830 safety software registry.

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[8] http://dnng.engin.umich.edu/mcnpx-polimi-training-workshop/

[9] https://www.oecd-nea.org/science/wpec/sg42/Meetings/2015_May/SG42_8_DR.pdf

[10] https://www.oecd-nea.org/science/wpec/sg42/Meetings/2015_May/SG42_3_JIM.pdf

2.3.5 International Atomic Energy Agency (IAEA)

Dr. Dermott "Red" Cullen develops and maintains the PREPRO nuclear data processing code for IAEA. In FY-2015, LLNL (Chuck Lee) assisted Dr. Cullen in testing PREPRO baselines on various hardware/software computational platforms prior to the release of a new software baseline, PREPRO2015[11].

In future, LLNL (Dave Heinrichs) may provide additional support to Dr. Cullen for using the PREPRO software to independently process nuclear data parameters (from ENDF/B, JEFF, JENDL, etc.) into useable cross-section libraries at various temperatures in ENDF-6 format. The latest ENDF/B-VII.1 libraries are available for download from IAEA as the POINT2015 Data[12].

Note that the LLNL Nuclear Theory and Data Group have incorporated Cullen's RECENT and SIGMA1 codes (from PREPRO) in their FETE[13] (production) data processing code. AMPX and NJOY also use SIGMA1.

2.3.6 Institut de Radioprotection et de Sûreté Nucléaire (IRSN)

In FY-2015, in his capacity as an ICSBEP Internal Reviewer, Soon Kim (LLNL) collaborated with Evaluators from ORNL (Thomas Miller), CEA (see Section 2.3.4) and IRSN (Matthieu Duluc, Francois Trompier, Marie Anne Chevallier, Sylvain Beytout) to complete IER-126, "Silene CAS Benchmark," published in the ICSBEP Handbook as ALARM-TRAN-AIR-SHIELD-001, "Neutron Activation Foil and Thermoluminescent Dosimeter Responses to a Bare Pulse of the CEA Valduc Silene Critical Assembly."

In FY-2015, LLNL (Dave Heinrichs) provided IRSN (Eric Letang) with an (unlimited) multi-user license for COG11.1 for inclusion in IRSN's PROMÉTHÉE software application and use in criticality accident slide rule calculations. LLNL (Heinrichs) also provided COG11.1 criticality safety training to IRSN users.

In FY-2016, LLNL (Chuck Lee, Jerome Verbeke) and IRSN (Gregory Caplin) will utilize COG11.1 and other analytical methods in analyzing IER-407, ISSA Subcritical Multiplicity Benchmark, experimental and simulated data.

2.3.7 Japan Atomic Energy Agency (JAEA)

LLNL (Song Huang) corresponded with JAEA (Toshiro Yamamoto) for assistance in obtaining, modifying and using the RHEINGOLD[14] two-dimensional higher-harmonic analysis code under Institutional (G&A) auspices. Note that this software may be useful in analyzing ISSA (IER-407).

2.3.8 Organisation for Economic Co-operation and Development (OECD)

In FY-2015, Dave Heinrichs (LLNL) continued to liaise with OECD (Jim Gulliford, Ian Hill, John Bess, Lori Scott) regarding NCSP contributions to ICSBEP and DICE. This included

[11] https://www-nds.iaea.org/public/endf/prepro/
[12] https://www-nds.iaea.org/point/
[13] http://nuclear.llnl.gov/CNP/fete/userguide.pdf
[14] http://www.tandfonline.com/doi/pdf/10.1080/18811248.2003.9715336

writing a joint paper with Ian Hill on "New NCSP Contributions to ICSBEP and DICE" to be published in the proceedings of the ANS Winter Meeting in November 2015.

Also in FY-2015, Dave Heinrichs (LLNL) participated in the kick-off meeting of WPEC SG42[15] with subsequent correspondence furthering this project on "Thermal Scattering Kernel S(α,β): Measurement, Evaluation and Application."

Due to funding constraints, LLNL did not participate in FY-2015 in any of the OECD Nuclear Energy Agency (NEA) Working Party on Nuclear Criticality Safety (WPNCS[16]) Expert Groups including those on Advanced Monte Carlo Techniques, Criticality Excursions Analyses, and Uncertainty Analyses for Criticality Safety Assessment. Similarly, no NCSP funds were used to participate in WPEC SG38[17] activities pertaining to "Beyond the ENDF format: A modern nuclear database structure."

In FY-2015, Dave Heinrichs (LLNL) discussed inclusion of COG11.1 in the NDEC Project with Carlos Javier (OECD). NDEC is similar to ADVANCE (see Section 2.1.2) with the exception that its focus is on JEFF rather than ENDF/B data.

2.3.9 Rolls-Royce

In FY-2015, LLNL entered into discussions with Rolls-Royce as described in Section 2.1.5.

3.0 Meetings

In addition to site visits, the following meetings have been useful venues for technical information exchanges:

- American Nuclear Society Annual Conference (in June)
- American Nuclear Society Winter Conference (in November)
- Cross Section Evaluation Working Group Meeting (in November)
- International Criticality Safety Benchmark Evaluation Project Meeting (in April/May)
- JOWOG30 (Criticality Safety)
- NCSP Nuclear Data Advisory Group Meeting (in November)
- NCSP Analytical Methods Working Group Meeting
- OECD NEA WPNCS Expert Group Meetings
- OECD NEA WPEC SG38 and SG42 Meetings

[15] https://www.oecd-nea.org/science/wpec/sg42/
[16] https://www.oecd-nea.org/science/wpncs/
[17] https://www.oecd-nea.org/science/wpec/sg38/