A Review of Nuclear Computational Information

B. L. Kirk

Radiation Safety Information Computational Center (RSICC)
Oak Ridge National Laboratory (ORNL), Oak Ridge, Tennessee USA

Abstract

The Radiation Safety Information Computational Center (RSICC) and the Organisation for Economic Co-operation and Development (OECD) Nuclear Energy Agency Data Bank (NEADB) work together to acquire sets of computer codes, nuclear data, and integral experiments relevant to shielding and dosimetry applications for fission, fusion, and accelerator applications. To keep up with advances in computing technology, international researchers continue to develop nuclear software. Collection centers like RSICC and NEADB serve the community and play a role in advancing nuclear science and technology research.

Background

Since the first meeting in Arlington, Texas, in 1994, the Nuclear Energy Agency Data Bank (NEADB) and the Radiation Safety Information Computational Center (RSICC) have been working together to continue the series of meetings to stay abreast of advances in computer software technology for accelerators, targets, and other radioactive environments. There have been nine meetings on the Shielding Aspects of Accelerators, Targets and Irradiation Facilities (SATIF):

- SATIF-1, Arlington, Texas (1994)
- SATIF-2, Geneva, Switzerland (1996)
- SATIF-3, Sendai, Japan (1997)
- SATIF-4, Knoxville, Tennessee (1998)
- SATIF-5, Paris, France (2000)
- SATIF-6, Stanford, California (2002)
- SATIF-7, Sacavém, Portugal (2004)
- SATIF-8, Pohang, South Korea (2006)
- SATIF-9, Oak Ridge, Tennessee (2008)

During the last 15 years, software developers have submitted either newly developed or updated computer codes to NEADB and RSICC. The two centers continue to work together in collecting computer codes and data for distribution to the scientific community.

New Software Updates since SATIF-9

The following section describes the software that has been updated or newly contributed to the centers. A more detailed listing is found in Table I.

RSICC CODE PACKAGE CCC- 657

BETA-S 6: A Code System to Calculate Multigroup Beta-Ray Spectra

DATA LIBRARY

ENSDF-95: Beta-decay transition data based on the Evaluated Nuclear Structure Data Files maintained by National Nuclear Data Center (NNDC0 at Brookhaven National Laboratory

CONTRIBUTORS

Oak Ridge National Laboratory, Oak Ridge, Tennessee

CANDU Owner Group, Toronto, Ontario, Canada

Atomic Energy of Canada Limited, Whiteshell Laboratories, Manitoba, Canada

BETA-S[1, 2] calculates beta-decay source terms and energy spectra in multigroup format for time-dependent radionuclide inventories of actinides, fission products, and activation products. Multigroup spectra may be calculated in any arbitrary energy-group structure. The code also calculates the total beta energy release rate from the sum of the average beta-ray energies as determined from the spectral distributions. BETA-S also provides users with an option to determine principal beta-decaying radionuclides contributing to each energy group. The SCALE code system must be installed on the computer before installing BETA-S, which requires the SCALE subroutine library and nuclide-inventory generation from the ORIGEN-S code. This release is compatible with SCALE Versions 5.0, 5.1 and 6. The following enhancements were completed in this version:

- The BETA-S source code was converted to modern Fortran 90 standard.
- Dynamic memory allocation was implemented.
- The free-format input reading routines were replaced with reading modules in SCALE 5.
- The capability to obtain beta-decay branching data from either a binary- or card-image-format ORIGEN data library (required for compatibility with ORIGEN-ARP) was added.
- An error associated with spectral calculation in the highest energy group was corrected.
- The spectrum calculation was improved by normalizing spectral energy to evaluated beta energy.
- The capability to generate plot files compatible with the PlotOPUS program was added.

RSICC CODE PACKAGE CCC-726

CNCSN: One-, Two- and Three-Dimensional Coupled Neutral and Charged Particle SN Code System

AUXILIARY CODES Included in the CNCSN Package

KATRIN-2.0: Three-dimensional neutral and charged particle transport

KASKAD-S-2.5: Two-dimensional neutral and charged particle transport

ROZ-6.6: One-dimensional neutral and charged particle transport

ARVES-2.5: Preprocessor for the working macroscopic cross-section FMAC-M format for transport calculations

MIXERM: Utility for preparing mixtures on the basis of multigroup cross-section libraries in ANISN format

CEPXS-BFP: A version of Sandia National Laboratories' multigroup coupled electron-photon cross-section-generating code CEPXS, adapted for solving the charged particle transport in the Boltzmann-Fokker-Planck formulation with the use of discrete-ordinates method

SADCO-2.4: Institute for High-Energy Physics modular system for generating coupled nuclear data libraries to provide high-energy particle transport calculations by the multigroup method

KATRIF: Postprocessor for KATRIN code

KASF: Postprocessor for KASKAD-S code

ROZ6F: Postprocessor for ROZ-6 code

ConDat 1.0: Code for converting by the tracing algorithm the combinatorial geometry presentation to the bit-mapped one

MCU Viewer: Code for combinatorial geometry visualization

Maplook: Script for SURFER to automate geometry visualization on the basis of material maps given as atlas boundary (*.bna) files

SYNTH: Utility for construction of an approximate solution of 3D transport equation in vicinity of reactor pressure vessel by the synthesis method

CONTRIBUTOR

Keldysh Institute of Applied Mathematics, Moscow, Russia

KATRIN, KASKAD-S, and ROZ-6[3] solve the multigroup transport equation for neutrons, photons, and charged particles in 3D (x, y, z and r, ϑ, z), 2D (x, z, r, z and r, ϑ), and 1D (plane, spherical, and cylindrical) geometries, respectively. The transport equation for charged particles can be solved with direct treatment of the continuous slowing-down (CSD) term; for 1D plane and spherical geometries, the Bolzmann-Fokker-Plank equation can be solved with direct treatment both CSD and continuous scattering terms. The scattering anisotropy can be treated in the P_L approximation. The adjoint solution of the problem can be also obtained (for neutral particles only). The principal application is solving of deep-penetration transport problems, typical for radiation protection and shielding calculations. Fission problems (subcritical boundary value and k_{eff}), problems with upscattering (thermalization, etc.), electron-photon, and hadron cascade problems can also be solved.

RSICC CODE PACKAGE CCC-755

CINDER Version 1.05: Code System for Actinide Transmutation Calculations

AUXILIARY CODES

ACTIVATION**:** Script to automate the coupling between CINDER'90 and the MCNPX code (also available through RSICC), geared for accelerator-driven applications

GAMMA_SOURCE**:** Script to format gamma spectral intensities from CINDER'90 into a source definition for MCNPX

CONTRIBUTORS

Los Alamos National Laboratory, Los Alamos, New Mexico, USA

Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

Argonne National Laboratory, Argonne, Illinois, USA

Paul Scherrer Institut, Villigen, Switzerland

The CINDER 1.05[4, 5] package includes the CINDER'90 code Version 7.4.2, ACTIVATION 1.0, GAMMA_SOURCE 1.0. CINDER'90 is the latest in the sequence of data and code evolutions built upon the original work of T. England at Bettis Atomic Power Laboratory (BAPL) in the early 1960s. It is used to calculate the inventory of nuclides in an irradiated material. Utilizing a self-contained nuclear data library, CINDER'90 calculates the atom density (atoms per unit volume) and activity density (curies per unit volume) of each and every nuclide present at a specified time. Though always providing a nuclide inventory, its functional identity depends upon the application. In nuclear reactor applications, such a code is commonly called a "burnup code," since it follows the temporal burnup of fissionable material and the associated production of fission products. It may also be called an "activation code" since it well describes the conversion of stable nuclides to radioactive nuclides by particle bombardment. In keeping with more recent vernacular, the code is identified as a transmutation nuclide inventory code, since the code follows all paths of nuclide transmutation — the conversion of a nuclide to a different nuclide by particle absorption and/or radioactive decay. Nuclide evolution code has recently become the more popular terminology, perhaps linked to R- and S-process applications in astrophysics.

The CINDER'90 library of 63-group cross sections describes 3400 nuclides in the range $1 \leq Z \leq 103$. The code requires a multigroup neutron flux for $E_n \leq 20$ MeV and nuclide production rates for reactions at higher neutron energies or for additional particles. Although developed for accelerator-driven problems, the code is applicable to any transmutation problem for which simulation calculations of particle reactions are available.

RSICC CODE PACKAGE CCC-744

EASYQAD: A Visualization Code System for Gamma and Neutron Shielding Calculations, Version 1.0

CONTRIBUTORS

Innovative Technology Center for Radiation Safety (iTRS) and Nuclear Reactor Analysis Laboratory at Hanyang University, Seoul, Korea

EASYQAD, Version 1.0[6], is a standalone Windows XP code system that facilitates gamma and neutron shielding calculations with user-friendly graphical interfaces. It is used to analyze radiation shielding problems and includes

- 8 kinds of geometry types,
- various flexible source options,
- common material library,
- various detector types.

Through intuitive windows and their interactions inside EASYQAD, the user can specify the dimensions of 3D shapes, their material compositions, their densities, the type of radioactive sources, the locations of the sources, and the type and positions of detectors. With the ease of using these sequences, shielding problems will become simpler and more clearly understandable.

Furthermore, the error-checking system can prevent users from making mistakes by automatically debugging the user inputs and giving modal dialog windows. The included Atomic Energy of Canada Limited (AECL) implementation of QAD-CGGP-A, Version 95.2 (C00645/MNYCP/00), is run from the user interface.

RSICC CODE PACKAGE CCC-745

ERANOS 2.0: Modular Code and Data System for Fast Reactor Neutronics Analyses.

CONTRIBUTORS

DER/SPRC/LEPh, CEA-Cadarache, France, through the OECD Nuclear Energy Agency (NEA) Data Bank, Issy-les-Moulineaux, France; NEA Package ID: NEA-1683/01

The European Reactor ANalysis Optimized calculation System, ERANOS[7], has been developed and validated with the aim of providing a suitable basis for reliable neutronic calculations of current as well as advanced fast reactor cores. It consists of data libraries, deterministic codes, and calculation procedures that have been developed within the European Collaboration on Fast Reactors over the past 20 years or so, in order to answer the needs of both industrial and R&D organizations. The whole system counts roughly 250 functions and 3000 subroutines totaling 450,000 lines of Fortran-77 and ESOPE instructions.

ERANOS is written using the ALOS software, which requires only standard Fortran compilers and includes advanced programming features. A modular structure was adopted for easier evolution and incorporation of new functionalities. Blocks of data (SETs) can be created or used by the modules themselves or by the user via the LU control language. Programming and dynamic memory allocation are performed by means of the ESOPE language. External temporary storage and permanent storage capabilities are provided by the GEMAT and ARCHIVE functions, respectively. ESOPE, LU, GEMAT, and ARCHIVE are all part of the ALOS software. This modular structure allows different modules to be linked together in procedures corresponding to recommended calculation routes ranging from fast-running and moderately accurate “routine” procedures to slow-running but highly accurate “reference” procedures.

RSICC CODE PACKAGE CCC-728

GENII-LIN: Multipurpose Health Physics Code System with a New Object-Oriented Interface, Release 2.1

CONTRIBUTORS

Laboratorio di Montecuccolino, Bologna University, Bologna, Italy

Based on Genii-1.485 developed at Pacific Northwest Laboratory, Richland, Washington

The goal of the GENII-LIN[8] project was to develop a multipurpose health physics code running on a Linux platform. The general features of the GENII-LIN system include

- capabilities for calculating radiation dose both for acute and chronic releases, with options for annual dose, committed dose and accumulated dose, and
- capabilities for evaluating exposure pathways, including direct exposure via water (swimming, boating, fishing), soil (buried and surface sources), and air (semi-infinite cloud and finite cloud model), inhalation pathways, and ingestion pathways.

The release scenarios considered are the following

- acute release to air, from ground level or elevated sources, or to water;

- chronic release to air, from ground level or elevated sources, or to water; and
- initial contamination of soil or surfaces.

GENII-LIN is the result of implementing the GENII-1.485 software package on the Linux platform. [Note that GENII-1.485 was distributed as RSICC package identifier C00601IBMPC02 and has been replaced in the RSICC collection with GENII 2.06 from Pacific Northwest National Laboratory (PNL) (C00737PC58600).] The GENII portion of the GENII-LIN package contains the program that was developed to incorporate the internal dosimetry models recommended by the International Commission on Radiological Protection (ICRP) into the environmental pathway analysis models used at Hanford. GENII is a coupled system of six programs (ENV, ENVIN, DOSE, INTDF, EXTDF, DITTY) and the associated data libraries that comprise the Hanford Dosimetry System (Generation II) to estimate potential radiation doses to individuals or populations from both routine and accidental releases of radionuclides to air or water and residual contamination from spills or decontamination operations.

GENII-LIN 2.0 came with a new set of programs (ENV13, INTDF13, EXTDF13, DOSE13) and associated data libraries. It retains all the capabilities of GENII-1.485 and incorporates into the existing environmental pathway analysis models the more recent internal dosimetry models recommended by the ICRP 72 and the radiological-risk-estimating procedures of FGR13.

GENII-LIN-2.1 is primarily a maintenance release with several bug fixes and improvements.

RSICC CODE PACKAGE CCC-742

GES_MC: Gamma-electron Efficiency Simulator, Version 3.1

CONTRIBUTORS

Radiation Department, Institute of Public Health, Cluj-Napoca, Romania

GES_MC (Gamma-electron Efficiency Simulator Monte Carlo)[9] is written entirely in Java and is based on the EGSnrc (Electron Gamma Shower) source code. Although GES_MC is designed especially for the computation of the response function and peak efficiency for gamma detectors, it can also be used in various studies concerning photon or electron interactions with the matter in any cylindrical (RZ) geometry. This application is designed mainly for computation of detector peak efficiency and detector total efficiency (whole spectrum) involved in gamma spectrometry. It can also compute detector efficiency for beta radiation (electrons and positrons), absorbed dose and kerma in any cylindrical (RZ) geometry, attenuation, and scatter fraction of radiation in detector walls. Furthermore, it can be used for some radiological applications such as the evaluation of scattered X radiation (secondary radiation) at a user-defined distance from the patient. GES_MC is based on the radiation transport theory and algorithms (routines taken from EGSnrc software) developed by the Stanford Linear Accelerator Center, USA (SLAC) and the National Research Council, Canada (NRC). The original EGSnrc system of computer codes is a general-purpose package for the Monte Carlo simulation of the coupled transport of electrons and photons in an arbitrary geometry for particles with energies above a few keV up to several hundreds of GeV. See the GES_MC developers' website for additional information [2]http://tensp.academic.ro/download/fulea/.

RSICC CODE PACKAGE CCC-740

MCNP5/MCNPX: Monte Carlo N-Particle Transport Code System Including MCNP5 1.51 and MCNPX 2.6.0 and Data Libraries

The CCC-740 package contains MCNP5 1.51, MCNPX 2.6.0, and MCNPDATA.

AUXILIARY PROGRAMS Included in the Distribution

MAKXSF: Prepares MCNP cross-section libraries, now with Doppler broadening.

ONEGXS: Creates one-group cross sections with P0 or P1 scattering in ACE format.

VISED 22S: Visual Editor for interactively constructing and visualizing MCNP geometry (runs on Windows PCs only). More VISED information is on the web at the Visual Consultants website http://www.mcnpvised.com/.

RELATED DATA LIBRARY

MCNPDATA: Standard Neutron, Photoatomic, Photonuclear, and Electron Data Libraries for MCNP5 and MCNPX

CONTRIBUTOR

Los Alamos National Laboratory, Los Alamos, New Mexico.

MCNP5[10-12] is a general-purpose Monte Carlo N-Particle code that can be used for neutron, photon, electron, or coupled neutron/photon/electron transport, including the capability to calculate eigenvalues for critical systems. Some of the new features of MCNP5 1.51 include the following

- variance reduction with pulse height tallies,
- new VAR input card added to control variance-reduction methods,
- annihilation gamma tracking,
- Doppler broadening added to the *makxsf* utility code,
- improved S(α,β) thermal scattering,
- large lattice enhancements,
- direct RSSA file reading for distributed multiprocessing,
- improved Compton scattering PSC calculation for detectors and DXTRAN, and
- web-based documentation.

MCNPXTM[13] is a general-purpose Monte Carlo radiation transport code that tracks virtually all particles at almost all energies. The official release date of MCNPX 2.6.0 is April 30, 2008. MCNPX began in 1994 as a code-merger project of MCNP 4B and LAHET 2.8. It was first released to the public in 1999 as version 2.1.5. In 2002, MCNPX was upgraded to MCNP 4C, converted to Fortran 90, enhanced with 12 new features, and released to the public as version 2.4.0. The release of version 2.6.0 includes many new features described in the document, "MCNPX Extensions Version 2.6.0," which is provided with the MCNPX distribution. The depletion/burnup capability is based on CINDER'90 and MonteBurns. MCNPX depletion is a linked process involving steady-state flux calculations in MCNPX and nuclide depletion calculations in CINDER'90. Currently, the depletion/burnup/transmutation capability is limited to criticality (KCODE) problems. Physics improvements include a new version of the Cascade-Exciton Model (CEM), the addition of the Los Alamos Quark-Gluon String Model (LAQGSM) event generator, and a substantial upgrade to muon physics. Current physics modules include the Bertini and ISABEL models taken from the LAHET Code System (LCS), CEM 03, and INCL4. Many new tally source and variance-reduction options have been developed. MCNPX is released with libraries for neutrons, photons, electrons, protons, and photonuclear interactions. In addition, variance-reduction schemes (such as secondary particle biasing) and new tallies have been

created specific to the intermediate- and high-energy-physics ranges. The “mesh” and “radiography” tallies were included for two- and three-dimensional imaging purposes. Energy deposition received a substantial reworking based on the demands of charged-particle high-energy physics. An auxiliary program, GRIDCONV, converts the mesh and radiography tally as well as standard MCTAL-file results for viewing by independent graphics packages. The code may be run in parallel at all energies via PVM or MPI. Information about MCNPX development can be found on the following web site: http://mcnpx.lanl.gov/.

RSICC CODE PACKAGE CCC-760

PARTISN 5.97: Time-Dependent, Parallel Neutral Particle Transport Code System

CONTRIBUTOR

Los Alamos National Laboratory, Los Alamos, New Mexico

PARTISN (PARallel, TIme-Dependent SN)[14] is the evolutionary successor to CCC-547/DANTSYS. The PARTISN code package is a modular computer program package designed to solve the time-independent or time-dependent multigroup discrete-ordinates form of the Boltzmann transport equation in several different geometries. The modular construction of the package separates the input-processing, the transport-equation-solving, and the post-processing (or edit) functions into distinct code modules: the Input Module, the Solver Module, and the Edit Module, respectively. PARTISN is the evolutionary successor to the DANTSYSTM code system package. The Input and Edit Modules in PARTISN are very similar to those in DANTSYS. However, unlike DANTSYS, the Solver Module in PARTISN contains one-, two-, and three-dimensional solvers in a single module. In addition to the diamond-differencing method, the Solver Module also has Adaptive Weighted Diamond-Differencing (AWDD), Linear Discontinuous (LD), and Exponential Discontinuous (ED) spatial differencing methods. The spatial mesh may consist of either a standard orthogonal mesh or a block adaptive orthogonal mesh. The Solver Module may be run in parallel for two- and three-dimensional problems. One can now run one-dimensional problems in parallel using Energy Domain Decomposition (EDD, triggered by Block 5 input keyword npeg>0). EDD can also be used in two or three dimensions with or without our standard Spatial Domain Decomposition.

Both the static (fixed-source or eigenvalue) and time-dependent forms of the transport equation are solved in forward or adjoint mode. In addition, PARTISN now has a probabilistic mode for Probability of Initiation (static) and Probability of Survival (dynamic) calculations. Vacuum, reflective, periodic, white, or inhomogeneous boundary conditions are solved. General anisotropic scattering and inhomogeneous sources are permitted. PARTISN solves the transport equation on orthogonal (single-level or block-structured AMR) grids in 1-D (slab, two-angle slab, cylindrical, or spherical), 2-D (X-Y, R-Z, or R-T) and 3-D (X-Y-Z or R-Z-T) geometries.

RSICC CODE PACKAGE CCC-756

PENELOPE2008.1: Code System for Monte Carlo Simulation of Electron and Photon Transport

CONTRIBUTORS

Facultat de Fisica (ECM), Universitat de Barcelona and Universitat Politècnica de Catalunya de Barcelona, Spain, through the Nuclear Energy Agency Data Bank, Issy-les-Moulineaux, France

PENELOPE[15] performs Monte Carlo simulation of coupled electron-photon transport in arbitrary materials and complex quadric geometries. A mixed procedure is used for the simulation of electron and positron interactions (elastic scattering, inelastic scattering and bremsstrahlung

emission), in which “hard” events (i.e., those with deflection angle and/or energy loss larger than preselected cutoffs) are simulated in a detailed way, while “soft” interactions are calculated from multiple scattering approaches. Photon interactions (Rayleigh scattering, Compton scattering, photoelectric effect, and electron-positron pair production) and positron annihilation are simulated in a detailed way. PENELOPE reads the required physical information about each material (which includes tables of physical properties, interaction cross sections, relaxation data, etc.) from the input material data file. The material data file is created by means of the auxiliary program MATERIAL, which extracts atomic interaction data from the database of ASCII files.

PENELOPE mailing list archives and additional information about the code can be found at http://www.nea.fr/lists/penelope.html.

The following features are specific to the 2001 and later versions of the code:

1. The simulation parameters (Eabs, C1, C2, Wcc, and Wcr) are defined independently for each material. This allows the user to specify regions of interest where the simulation is performed in greater detail.
2. The argument DSMAX of subroutine JUMP specifies the maximum allowed path length between hard interactions of electrons and positrons. By selecting a suitably small value for this parameter, the user can control the number of hinges in thin regions (which must be larger that ten or so, to ensure accuracy). This argument is also used for simulating the transport of charged particles in the presence of static external electric and magnetic fields. DSMAX has no effect when set equal to a very large number (e.g., 10**35).
3. The structure of the common /TRACK/ differs from previous versions. The variable ILB(5), which describes the origin of secondary particles, can be used to study partial contributions from particles originated by a given process.

RSICC COMPUTER CODE PSR-158

SAMMY-8.0.0: Code System for Multilevel R-Matrix Fits to Neutron and Charged Particle Cross Section Data Using Bayes’ Equations

AUXILIARY CODES

Seventeen auxiliary codes are provided along with the SAMMY code. These codes aid with such processes as preparing input, plotting results, or studying statistical properties of resonance parameters. A complete list and description of the auxiliary codes is provided in Section X of the SAMMY users’ manual.

ANGODF: Convert PLOT file from energy/angle to angle/energy

CONVRT: Convert from REFIT input to SAMMY or vice versa

SAMAMR: Add, mix, or recover variables in COVariance file

SAMAMX: Alter the value of one nonvaried parameter in the COVariance file after completion of an analysis

SAMCPR: Compare SAMMY calculations to those from other sources

SAMDIS: Calculate statistical distributions for resonance parameters

SAMFTZ: Modify the experimental energies with t0 and L0

SAMORT: Plot the ORR resolution function

SAMPLT: Alternative form for plot files

SAMQUA: Generate resonance quantum numbers for particle pairs

SAMRML: Read ENDF File 2, calculate cross sections and derivatives

SAMRPT: Plot RPI resolution function

SAMRST: Plot Gaussian plus exponential resolution function

SAMSMC: Perform Monte Carlo calculation of multiple scattering corrections

SAMSTA: Generate staircase plots of resonance widths

SAMTHN: Thin experimental data

SUGGEL: Estimate quantum numbers for resonances

CONTRIBUTOR

Oak Ridge National Laboratory, Oak Ridge, Tennessee

The purpose of the SAMMY[16] is to analyze time-of-flight cross-section data in the resolved and unresolved resonance regions, where the incident particle is either a neutron or a charged particle (p, α, d,..). Energy-differential cross sections and angular-distribution data are treated, as are certain forms of energy-integrated data.

In the resolved resonance region (RRR), theoretical cross sections are generated using the Reich-Moore approximation to R-matrix theory (and extensions thereof). Sophisticated models are used to describe the experimental situation: data-reduction parameters (e.g., normalization, background, sample thickness) are included. Several options are available for both resolution and Doppler broadening, including a crystal-lattice model for Doppler broadening. Self-shielding and multiple-scattering correction options are available for analysis of capture cross sections. Multiple isotopes and impurities within a sample are handled accurately.

Cross sections in the unresolved resonance region (URR) can also be analyzed using SAMMY. The capability was borrowed from Froehner's FITACS code; SAMMY modifications for the URR include more exact calculation of partial derivatives, normalization options for the experimental data, increased flexibility for input of experimental data, and introduction of user-friendly input options.

In both energy regions, values for resonance parameters and for data-related parameters (such as normalization, sample thickness, effective temperature, resolution parameters) are determined via fits to the experimental data using Bayes' method (see below). Final results may be reported in ENDF format for inclusion in the evaluated nuclear data files. The new features added to SAMMY include the following:

- The value of ν (nu) for η (eta) calculations can now be energy dependent.
- Extensive revisions have been made to the self-shielding multiple-scattering (ssm) module.
- Tabulated values (from Monte Carlo calculations) can be used instead of SAMMY-generated double-plus scattering corrections.
- The "simple" resolution function may include a Gaussian curve whose width is a linear function of energy.
- Input resonance parameters can now be presented as reduced-width amplitudes γ instead of partial widths $\Gamma = 2P\gamma\ 2$.
- For transmission measurements, the sample thickness may be nonuniform.

- SAMMY now produces a third type of output file from which plots may be made—an ASCII file (with extension “LST”) is created.

RSICC CODE PACKAGE CCC-750

SCALE 6: Standardized Computer Analyses for Licensing Evaluation Modular Code System for Workstations and Personal Computers, including ORIGEN-ARP

CONTRIBUTOR

Oak Ridge National Laboratory, Oak Ridge, Tennessee

The following items highlight new capabilities that are included in SCALE 6:[17].

- Continuous energy (CE) capability in KENO V.a and KENO-VI
- CE and 238-group ENDF/B-VI.8 and ENDF/B-VII.0 (latest ENDF release) cross-section libraries with full-range Bondarenko factors in multigroup libraries
- MAVRIC/Monaco 3-D Monte Carlo shielding modules with automated variance reduction
  - Uses SCALE Generalized Geometry Package (same as KENO-VI)
  - Flexible source description: separable spatial, energy, and directional distributions
  - Tally options: region tally, point detectors, and mesh tally
  - Uses CADIS methodology to perform automated 3-D variance reduction
  - Creates a biased source distribution and weight windows in space and energy
  - Uses FW-CADIS (Forward-Weighted CADIS) to optimize multiple tallies simultaneously or produce mesh tallies with more uniform relative uncertainties
  - Graphical displays of mesh tallies, weight windows, source distributions, intermediate flux files, and tally convergence with Java viewer
- ENDF/B-VII coupled neutron/gamma shielding cross-section libraries for use with MAVRIC/Monaco (200 neutron/47 gamma groups and 27 neutron/19 gamma groups)
- Criticality accident alarm system (CAAS) analysis using CSAS6/KENO-VI criticality sequence and MAVRIC/Monaco shielding sequence
- TRITON/NEWT enhancements
  - Depletion with doubly heterogeneous unit cells (e.g., pebble-bed or prismatic fuel)
  - Automatic group collapse for depletion calculations
  - Extended limits for number of depletion materials and depletion steps
  - Improved treatment of depletion by flux vs depletion by power for nonpower rods
  - Full support for fixed-source calculations
  - Improved treatment for sigma-transport calculations (current weighted)
  - Improved accuracy in calculations where critical buckling is supplied
  - Addition of arbitrarily high order product quadrature set
  - New fast reactor ORIGEN-S library for fast reactor analysis with TRITON

    - Tracking of trace element nuclides in TRITON depletion calculations
    - Full support for all OPUS capabilities including stacked OPUS specifications within a single TRITON calculation
- TSUNAMI-3D with KENO-VI (SCALE 5.1 used only KENO V.a with TSUNAMI)
- Flexible mesh grids in KENO V.a and KENO-VI for TSUNAMI or criticality accident alarm system (CAAS) analyses
- HTML output for KENO-VI (SCALE 5.1 included HTML output for KENO V.a)
- Covariance library with data for more than 300 materials based on
    - Los Alamos National Laboratory (LANL) covariance data for light nuclei up to and including F-19
    - "Integral method" in thermal and resonance range for other nuclides [Oak Ridge National Laboratory (ORNL)]
    - Nuclear model techniques in fast range for other nuclides [Brookhaven National Laboratory (BNL), LANL]
- TSURFER sensitivity/uncertainty (S/U) data adjustment tool to examine measured and calculated data and adjust integral experiment values within uncertainties to produce consistency between measured and calculated results
- Reactivity sensitivity analysis tool, TSAR
- New USLSTATS (**U**pper **S**ubcritical **L**imits **STAT**istic**S**) entirely rewritten in Java with integrated user interface for input, output, and plotting
- VIBE (Validation, Interpretation, and Bias Estimation) Java user interface to filter TSUNAMI files and sort/filter sensitivity data
- ExSITE (**Ex**tensible **S**CALE **I**ntelligent **T**ext **E**ditor) Java user interface for TSUNAMI-IP, TSURFER, and TSAR
- STARBUCS burnup-credit cask-loading curve search
- MCDancoff (Monte Carlo Dancoff) control module to calculate Dancoff factors in complicated 3-D geometries using Monte Carlo integrations in a modified version of KENO-VI called "KENO_Dancoff"

RSICC CODE PACKAGE CCC-757

SERPENT 1.1.7: Continuous Energy Monte Carlo Reactor Physics Burnup Calculation Code

DATA LIBRARIES

Serpent 1.1.7 cross-section library based on ENDF/B-VI.8

Serpent 1.1.7 cross-section library based on ENDF/B-VII

Serpent 1.1.7 cross-section library based on JEF-2.2

Serpent 1.1.7 cross-section library based on JEFF-3.1.1

Serpent 1.1.7 thermal scattering libraries based on JEF-2.2, JEFF3.1, ENDF/B-VI.8, and ENDF/B-VII

CONTRIBUTORS

VTT Technical Research Centre of Finland

SERPENT[18] is a three-dimensional continuous-energy Monte Carlo reactor physics burnup calculation code specifically designed for lattice physics applications. The code uses built-in calculation routines for generating homogenized multigroup constants for deterministic reactor simulator calculations. The standard output includes effective and infinite multiplication factors, homogenized reaction cross sections, scattering matrices, diffusion coefficients, assembly discontinuity factors, point-kinetic parameters, effective delayed neutron fractions, and precursor group decay constants. User-defined tallies can be set up for calculating various integral reaction rates and spectral quantities.

Internal burnup calculation capability allows SERPENT to simulate fuel depletion as a completely stand-alone application. Extensive effort has been put into optimizing the calculation routines, and the code is capable of running detailed assembly burnup calculations similar to deterministic lattice codes within a reasonable calculation time. The overall running time can be further reduced by parallelization.

SERPENT can be used for various reactor physics calculations at pin, assembly, and core levels. The continuous-energy Monte Carlo method allows the modeling of any critical reactor type, including both thermal and fast neutron systems. The suggested applications of SERPENT include group-constant generation; fuel cycle studies; validation of deterministic lattice physics codes; and educational, training, and demonstration purposes.

A complete description of the project is found at the SERPENT website, http://montecarlo.vtt.fi.

RSICC DATA LIBRARY DLC-237

SINBAD-2009.02: Shielding Integral Benchmark Archive and Database, Version February 2009

CONTRIBUTORS

OECD Nuclear Energy Agency Data Bank, Issy-les-Moulineaux, France

Oak Ridge National Laboratory, Oak Ridge, Tennessee

Many of the organizations that contributed to this benchmark compilation are listed in the index file SINBADIS.htm.

SINBAD[19] began in 1992–93, prompted by the continued closure of experimental facilities worldwide. The loss of benchmark experimental facilities jeopardizes the future of new shielding data. Further, because of the loss of lab notes and/or logbook records from poor document storage and/or aging, together with the loss of guidance from the retirement of key research staff who were conducting the experiments, complete benchmark data become a premium under today's strict quality assurance needs. The decision was made to collect, recompile, and distribute benchmark information in formats acceptable to the international community in an attempt to preserve and disseminate the information. The data integrity was checked and reference sources examined for self-consistency. At times, full benchmark information was gathered from multiple sources including personal contacts and laboratory logbooks.

The guidelines developed by the Benchmark Problems Group of the American Nuclear Society Standards Committee (ANS-6) on formats for benchmark problem description have been followed. SINBAD data include benchmark information on (1) the experimental facility and the source; (2) the benchmark geometry and composition; and (3) the detection system, measured data, and an error analysis. A reference section is included with the data. Relevant graphical

information, such as experimental geometry or spectral data, is included. All information that is compiled for inclusion with SINBAD has been verified for accuracy and reviewed by two scientists.

The data in the RSICC SINBAD-2009.02 package were received through the NEADB and correspond to Data Bank packages as follows:

- NEA-1517 SINBAD REACTOR (abstract last modified 11-FEB-2009)
- NEA-1552 SINBAD ACCELERATOR (abstract last modified 6-FEB-2009)
- NEA-1553 SINBAD FUSION (abstract last modified 10-FEB-2009)

RSICC CODE PACKAGE CCC-747

TRIPOLI-4.4: Code System for Coupled Neutron, Photon, Electron, Positron, 3-D, Time Dependent, Monte-Carlo, Transport

DATA LIBRARIES

GALILEE 0.2 processed libraries in a TRIPOLI-4 specific format based on JEFF31, FENDL21, JENDL33, ENDFB7R0, and EPDL97. Also included are libraries produced using NJOY in a TRIPOLI-4-specific format based on JEF2, ENDFB6R4, and ENDL.

CONTRIBUTORS

Commissariat à l'Énergie Atomique, CEA/Saclay, Cedex, France, through the OECD Nuclear Energy Agency

TRIPOLI-4[20] is a general-purpose radiation transport code. It uses the Monte Carlo method to simulate neutron and photon behavior in three-dimensional geometries. The main areas of applications include, but are not restricted to, radiation protection and shielding, nuclear criticality safety, fission and fusion reactor design, and nuclear instrumentation. In addition, it can simulate electron-photon cascade showers.

New features available in TRIPOLI-4 version 4 include the following:

1. New biasing features: It is possible to store and reuse importance maps. Biasing with a plane or spherical surface has been added. (Cylindrical was already available.)

2. Neutron collision in multigroup homogenized mode: Anisotropy up to the order 3 in the Legendre polynomial expansion (P3).

3. Display of the collision sites.

4. ENDF format evaluations: Mixed representation of the anisotropy from file 4: Legendre format used at low energy and tabulated probability distributions at high energy (e.g., O16 from ENDFB6R8). cf ENDF-102 Data formats and procedures for the evaluated nuclear data file ENDF-6. 07/1990, revised 04/2001.

5. Computation of the gamma source produced by neutrons.

6. Output format for all results: The -a execution option allows even zero results to be displayed in the output. Although the standard deviation is infinite in this case, for reason of compatibility with the rest of the code, the output file also gives a zero value for the standard deviation.

7. Verbose level for output warnings: The code now gives only the most important information to the user. The -v option allows the warnings; the -D option gives the same verbose level as previous versions.

8. Photon reaction rates: In the RESPONSES command, interaction code 100 (coherent scattering), 101 (incoherent scattering), 102 (photoelectric effect), 103 (pair production), and 106 (total photon) are now available.

9. XML format output: In the SIMULATION command, the “XML_EXPORT” keyword allows the user to get an XML-format output file. Any post-processing tool that can cope with XML format may be used to process this file.

10. ENDF format evaluations:

- By default, evaluations produced by NJOY99 (version 81) are used.
- It is possible to use jeff3.1, endfb7, and jendl3.3 evaluations:
    - The maximum order of Legendre polynomials is no longer limited to 21.
    - ENDF-format 2D interpolation “unit-base” (file 6) is now supported.

11. Combinatorial geometry checks: It is now possible to choose the number of points for the non-overlapping tests of combinatorial volumes. The keyword is “TEST_GENERATED_POINTS n” (200 by default).

The keyword may be written

- only once, at the beginning (after the TITLE keyword), or
- as many times as necessary in the GEOMETRY command, just before a VOLU keyword. (For each combinatorial volume, the number of generated points refers to the last TEST_GENERATED_POINTS keyword.)

12. Green's functions files.

13. Neutronics-shielding coupling.

14. Responses, scores, biasing names: It is possible to give names (instead of giving a number) to responses and scores. It is necessary to give names to responses, scores, and biasings for neutronics-shielding coupled simulations.

15. Units: The -u execution option allows the code to output scores with their units.

RSICC CODE PACKAGE CCC-759

TITAN 1.19: A Three-Dimensional Deterministic Radiation Transport Code System

AUXILIARY CODES

PENMSHXP 2.64b: Mesh Generator to Build TITAN or PENTRAN Input Deck with the DISLIN graphic library

PENMSHXP 2.61a: Mesh Generator to Build TITAN or PENTRAN Input Deck without the DISLIN graphic library

CONTRIBUTORS

University of Florida, Gainesville, Florida

TITAN[21, 22] is a time-independent deterministic radiation transport simulation code in 3-D Cartesian geometry. The hybrid approach in the TITAN code allows different transport solvers (Sn or ray racing) to be applied in different regions. TITAN solves both the k-effective and fixed-source forward/adjoint problems. It has been benchmarked on a number of OECD/NEA benchmark problems:

- 3-D radiation transport benchmarks for simple geometries with void regions (Kobayashi problem),
- benchmark on deterministic transport calculations without spatial homogenization mixed-oxide (MOX) fuel assembly 3-D extension case (C5G7 MOX), and
- benchmarks on the accuracy of solution of 3-D transport codes and methods over a range in parameter space.

The extra sweep with the fictitious quadrature technique enables TITAN to simulate the SPECT (single photon emission computed tomography) projection images that are generally produced by Monte Carlo codes. A benchmark using the TITAN code on a torso phantom has been established. In the TITAN SPECT simulation, collimators are not explicitly simulated. Instead, a technique called "circular ordinate splitting" is used to simulate the collimator blurring effects.

RSICC CODE PACKAGE CCC-754

VIM 5.1: Continuous Energy Neutron/Photon Transport Code System

AUXILIARY CODES

XSEDIT2 edits or performs binary conversion of processed physics data.

RETALLY repeats the statistical analysis of tally data, optionally collapsing energy groups and/or spatial regions or skipping early generations.

KEFCODE repeats the statistical analysis of keff tallies.

ISOVIM produces multigroup VIM material files from COMPXS or ISOTXS interface files or from CASMO ASCII output.

REBATCH regroups tally records to encompass more generations to permit assessment of serial correlation of reaction rate and flux estimates.

Slicer, a C++ program, generates color 2D snapshots of a specified VIM geometry.

CONTRIBUTOR

Argonne National Laboratory, Argonne, Illinois

VIM[23] is a continuous-energy criticality, reactor physics, and shielding code. It solves the transport problem for neutrons or photons, including thermal neutron scattering effects, either in the eigenvalue mode or for photon or neutron fixed source. VIM features flexible geometry and neutron physics data carefully constructed from ENDF/B data. Special neutron physics capabilities in VIM include unresolved resonance probability tables and direct treatment of resolved resonances described with Reich-Moore parameters. VIM has been extensively benchmarked using both experiments and other accurate codes.

VIM solves the steady-state neutron or photon transport problem in any detailed three-dimensional geometry using either continuous-energy-dependent ENDF nuclear data or multigroup cross sections. Neutron transport is carried out in a criticality mode or in a fixed-source mode (optionally incorporating subcritical multiplication). Photon transport is simulated in the fixed-source mode. The geometry options are infinite medium, combinatorial geometry, and hexagonal or rectangular lattices of combinatorial geometry unit cells and rectangular lattices of cells of assembled plates. Boundary conditions include vacuum, specular, and white reflection, as well as periodic boundaries for reactor cell calculations.

The VIM 5.1 (April 2009) release includes data from ENDF/B-IV, ENDF/B-V, ENDF/B-VI, and ENDF/B-VII.0. ASCII data libraries and a convenient means to convert them to binary on a target machine are included.

Table I: Software and Data Updates since the SATIF-9

Software	Description
ACAB-2008	ACtivation ABacus Inventory Code System for Nuclear Applications
ALICE-2008	Statistical Model Code System to Calculate Particle Spectra from HMS Precompound Nucleus Decay
ANGELO-LAMBDA	Covariance Matrix Interpolation and Mathematical Verification
BETA-S 6	Code System to Calculate Multigroup Beta-Ray Spectra
BOT3P-5.3	Code System for 2D and 3D Mesh Generation and Graphical Display of Geometry and Results for Radiation Transport Codes
BOXER	Fine-flux Cross Section Condensation, 2D Few Group Diffusion and Transport Burnup Calculations
BULK_C-12	Code System to Estimate Neutron and Photon Effective Dose Rates from Medium Energy Protons or Carbon Ions through Concrete or Concrete/Iron
CINDER 1.05	Code System for Actinide Transmutation Calculations
CNCSN	One-, Two- and Three-Dimensional Coupled Neutral and Charged Particle SN Code System
DANESS V1.0	Dynamic Analysis of Nuclear Energy System Strategies
DWBA07/DWBB07	Code System for Inelastic and Elastic Scattering with Nucleon-Nucleon Potential
DWUCK-CHUCK	Nuclear Model Code System for Distorted Wave Born Approximation and Coupled Channel Calculations
EASY-2005.1	Inventory Code System for Neutron Activation Analysis
EASY-QAD 1.0	Visualization Code System for Gamma and Neutron Shielding Calculations
ERANOS 2.0	Modular Code and Data System for Fast Reactor Neutronics Analyses
GANAPOL-ABNTT	Analytical Benchmarks; Case Studies in Neutron Transport Theory
GENII 2.09	Environmental Radiation Dosimetry Software System
GENII-LIN 2.1	GENII-LIN Multipurpose Health Physics Code System with a New Object-Oriented Interface, Release 2.0
GES_MC	Gamma-electron Efficiency Simulator, Version 3.1
IRDF-2002	The International Reactor Dosimetry File
JDL-IMPORTANCE	Adjoint Function: Physical Basis of Variational and Perturbation Theory in Transport and Diffusion Problems
JDL-REACTOR-KIN	Nuclear Reactor Kinetics and Control
JDL-THERMODYNAM	Thermodynamics: Frontiers and Foundations
LAPUR6	BWR Core Stability Measurements
MATJEFF31.BOLIB	Fine-Group Cross-Section Library Based on JEFF3.1 for Nuclear Fission Applications
MCNP5/MCNPX	Monte Carlo N-Particle Transport Code System including MCNP5 1.51 and MCNPX 2.6.0 and Data Libraries (Source & Executables)
MCNP5/MCNPX-EXE	Monte Carlo N-Particle Transport Code System including MCNP5 1.51 and MCNPX 2.6.0 and Data Libraries (Executables—No Source)
MGA8	Code System to Determine Pu Isotope Abundances from Multichannel Analyzer Gamma Spectra
MURE	MCNP Utility for Reactor Evolution
NRCDOSE 2.3.15	Code System for Evaluating Routine Radioactive Effluents from Nuclear Power Plants with a Windows Interface
NUCHART	Nuclear Properties and Decay Data Chart of Nuclides
PARTISN 5.97	Time-Dependent, Parallel Neutral Particle Transport Code System
PENELOPE2008.1	Code System to Perform Monte Carlo Simulation of Electron Photon Showers in Arbitrary Materials
PHOBIA	Photon Buildup Factors to Account for Angular Incidence on Shield Walls

Software	Description
PLOT-S	Plotting Program with Special Features for Windows Environment
POINT2009	A Temperature-Dependent Linearly Interpolable Tabulated Cross Section Library Based on ENDF/B-VII.0
PR-EDB	Power Reactor Embrittlement Data Base, Version 3
PUFF-IV	Code System to Generate Multigroup Covariance Matrices from ENDF/B-VI Uncertainty Files, Version 6.0.1
RASCAL 3.0.5	Radiological Assessment for Consequence Analysis for Windows
RSAC7	Radiological Safety Analysis Code System
SAMMY-8	Code System for Multilevel R-Matrix Fits to Neutron and Charged-Particle Cross-Section Data Using Bayes' Equations
SCALE 6	Modular Code System for Performing Criticality and Shielding Analyses for Licensing Evaluation with ORIGEN-ARP (Source and Executables)
SCALE 6-EXE	Modular Code System for Performing Criticality and Shielding Analyses for Licensing Evaluation with ORIGEN-ARP (Executables—No Source)
SCAMPI	SCAMPI: Collection of Codes for Manipulating Multigroup Cross-Section Libraries in AMPX Format
SELFS-3	Self-Shielding Correlation of Foil Activation Neutron Spectra Analysis by SAND-II
SERPENT	Continuous Energy Monte Carlo Reactor Physics Burnup Calculation Code
SINBAD 2009.02	Shielding Integral Benchmark Archive and Database, Version February 2009
SUSD3D	Multidimensional, Discrete-Ordinates-Based Cross-Section Sensitivity and Uncertainty Analysis Code System
TALYS 1.0	Nuclear Model Code System for Analysis and Prediction of Nuclear Reactions and Generation of Nuclear Data
TENDL-2008-ACE	TALYS-Based Cross Section Library for Use with MCNP(X)
THYDE-B1/MOD2	Computer Code for the Analysis of Small-Break Loss-of-Coolant Accident of Boiling Water Reactors
THYDE-P2	Computer Code for PWR LOCA Thermohydraulic Transient Analysis
TITAN 1.19	A Three-Dimensional Deterministic Transport Code System
TRIPOLI 4.4	Code System for Coupled Neutron, Photon, Electron, Positron, 3-D, Time-Dependent, Monte Carlo, Transport Calculations
VARSKIN 3 V3.1. 0	Code System for Assessing Skin Dose from Skin Contamination, Version 3.1.0
VIM 5.1	Continuous Energy Neutron and Photon Transport Code System, April 2009 Release
VITENEA-J	AMPX 175-n,42-g Multigroup X-section Library for Nuclear Fusion Applications
VITJEFF31.BOLIB	A JEFF-3.1 Multigr Coupled (199n + 42g) X-Section Lib. in AMPX Fmt for Nuclear Fission Applications

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