June 28, 2002

Summary
To be published in ***TRANSACTIONS***
Track 4L

Nuclear Science and Technology Division (94)

New Two-Dimensional Deterministic Criticality Safety Capabilities in SCALE 5

M. D. DeHart

Oak Ridge National Laboratory,*
PO Box 2008,
Oak Ridge, TN 37831-6370 USA
(865) 576-3468
Email: dehartmd@ornl.gov

Submitted to the
American Nuclear Society 2002 Winter Meeting
"Building the World Nuclear Community — Strategies for the Deployment of New Nuclear Technologies",
November 17–21, 2002,
Washington, D.C.
Omni Shoreham Hotel

The submitted manuscript has been authored by a contractor of the U.S. Government under contract No. DE-AC05-00OR22725. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

---

* Managed by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy.

New Two-Dimensional Deterministic Criticality Safety Capabilities in SCALE 5

M. D. DeHart

Oak Ridge National Laboratory,*
P.O. Box 2008,
Oak Ridge, TN 37831-6370
E-mail: dehartmd@ornl.gov

Introduction

With the impending release of Version 5 of SCALE (**S**tandardized **C**omputer **A**nalyses for **L**icensing **E**valuations) [1] at Oak Ridge National Laboratory (ORNL), several significant new modules and sequences for criticality safety analysis will be publicly available. These include the NEWT [2] (**NEW** **T**ransport algorithm) functional module, for two-dimensional (2-D) discrete-ordinates analysis, and the SAS2D control module [3], which provides automated sequences for 2-D criticality safety analyses and 2-D depletion. NEWT is unique in the domain of discrete ordinates methods because it is based on a non-orthogonal, flexible mesh scheme that allows accurate representation of complex geometric configurations that are normally impossible to model with discrete ordinates methods without significant approximations. SAS2D brings to NEWT the automated and simplified approach for setting up and performing complex sets of calculations, a hallmark of the SCALE system.

Capabilities of NEWT

Using a discrete ordinates approximation to the transport equation on an arbitrary grid, NEWT provides a robust and rigorous deterministic solution for non-orthogonal configurations. In the past, analyses in this problem domain have been limited to Monte Carlo simulations or lower-order deterministic approximations. While each of these techniques has its own strengths and is the most appropriate selection for certain types of analysis, they also have shortcomings that are answered by NEWT's capabilities. For example, the stochastic nature of Monte Carlo solutions can provide a very good estimate of the global neutron multiplication factor for a system; however, flux distributions and small differential quantities cannot be accurately determined. Such data are important in certain types of sensitivity/uncertainty analysis and in depletion calculations. Lower-order deterministic methods typically applied in lattice analyses (e.g., integral transport and collision probability methods) do not provide the angular resolution necessary to treat strongly anisotropic fluxes, such as those in the vicinity of strong absorbers or in high-leakage cores. This limitation may be exacerbated in mixed oxide fuels due to the

---

* Managed by UT-Battelle, LLC, under contract DE-AC05-00OR22725 with the U.S. Department of Energy.

increased sensitivity of such fuels to the thermal spectrum. NEWT has already been used to demonstrate the effect of minor assumptions on the thermal spectra of MOX fuels [4].

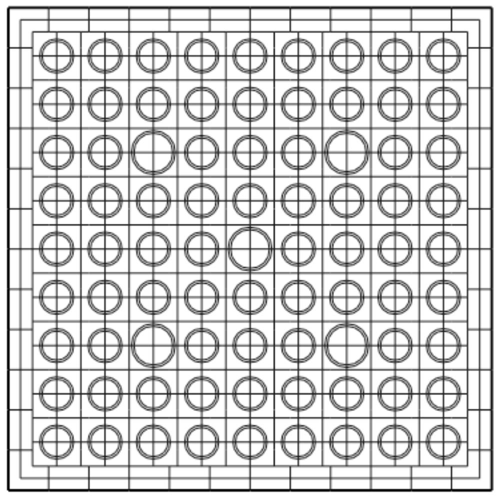
NEWT offers several calculational options. It may be used to calculate the eigenvalue of a system, to perform a fixed source calculation, or to calculate the critical (x-y) buckling of a lattice. It allows the specification of an axial buckling or calculates an axial buckling from a specified height, to account for axial leakage effects. NEWT can collapse cross sections to an appropriately weighted group structure subset, in the form of an AMPX working-format library. NEWT calculates the transport-corrected cross-section and diffusion coefficient for each energy group that can be used in diffusion calculations.

One of the most significant changes in SCALE 5 is the use of truly dynamic runtime memory allocation. NEWT relies heavily on this capability to be able to allocate memory specific to the needs of any grid, angle, and energy specification. The limit of a problem size is determined only by the limits of physical memory on a given platform. Data is organized in terms of data structures that are dynamically allocated, to tailor memory on a cell-by-cell basis for an arbitrary number of sides, thereby most effectively utilizing memory. Other memory management techniques were utilized to minimize data storage requirements by eliminating unused data space. This allows calculations of very large grids with high order quadrature and P_n scattering expansions within the memory capacity of most modern computers.

NEWT's automated grid-generation scheme, based on the placement of simple bodies within a problem domain, allows rapid development of a model without the need to manually input a complex and irregular grid structure. However, NEWT permits a manually specified grid if desired,. Additionally, NEWT generates PostScript-based graphic files to allow a user to examine the computational grid generated by NEWT and to refine or alter as necessary. Figure 1 is an example of a graphic generated by NEWT for a hypothetical fuel assembly. Note that this model contains no curved surfaces, but instead consists of arbitrary polygons computed by NEWT in which volumes are conserved. The simplicity of the input specification required to describe this configuration is demonstrated by the input listing shown to the right of the graphic.

Capabilities of SAS2D

The SAS2D control module currently supports three analytic sequences. The *SAS2N* sequence may be used to create a problem specific cross-section library and mixing table for a subsequent NEWT calculation. The *SAS2K* sequence combines cross-section processing with a NEWT transport calculation using an embedded NEWT input model, and is similar in concept to the *CSAS25* sequence used for automated KENO V.a calculations. The *SAS2D* sequence is used to iteratively perform NEWT transport calculations and ORIGEN-S depletion calculations to rigorously track the depletion of materials in the transport model according to a user specified burnup history. The depletion capabilities of SAS2D are described in more detail in Ref. 3.



```
read geom
domain 10.0 10.0 12 12
boundary 1 1 1 1
  rectangle 2 0.25 0.25 9.75 9.75 ’outer
material 1 square region’ end
subgrid 1 1.0 1.0 2 2
  circle 3 0.5 0.5 0.4 ’inner water’ end
  circle 2 0.5 0.5 0.45 ’guide tube’ end
subgrid 2 1.0 1.0 2 2
  circle 1 0.5 0.5 0.3 ’fuel rod’ end
  circle 2 0.5 0.5 0.35 ’cladding’ end
array 0.5 0.5 9 9
2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2
2 2 1 2 2 2 1 2 2
2 2 2 2 2 2 2 2 2
2 2 2 2 1 2 2 2 2
2 2 2 2 2 2 2 2 2
2 2 1 2 2 2 1 2 2
2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2
end geom
```

Figure 1. PostScript rendering (left) of NEWT geometry input (right).

Summary

The release of NEWT and SAS2D, within Version 5 of SCALE, will herald a new set of tools for nuclear system analysis. Not intended as a replacement for other analysis techniques, NEWT is intended to provide specific capabilities not available elsewhere in SCALE. NEWT’s generalized geometry capabilities lend it to a wide variety of applications. SAS2D provides an automated method to execute NEWT for a single transport solution, and also provides a more realistic method for modeling multidimensional depletion of nuclear fuels. Additions and improvements for both codes are ongoing, and future releases of SAS2D will include additional analysis capabilities.

References

1. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 6 (ORNL/NUREG/CSD-2/R6), Vols. I, II, and III, May 2000. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.
2. M. D. DeHart, “An Advanced Deterministic Method for Spent-Fuel Criticality Safety Analysis,” *ANS 1998 Annual Meeting and Embedded Topical Meeting,* June 7–11, 1998, Nashville, TN. *Trans. Am. Nucl. Soc*. **78**, 170–172 (1998).
3. M. D. DeHart, “SAS2D – A Two-Dimensional Depletion Sequence for Characterization of Spent Nuclear Fuel,” 35583.pdf in *Proc. of 2001 ANS Embedded Topical Meeting on Practical Implementation of Nuclear Criticality Safety*, November 11–15, 2001, Reno, NV [ANS Order No.: 700284; ISBN: 0-89448-659-4].
4. M. D. DeHart, “A Deterministic Study of the Deficiency of the Wigner-Seitz Approximation for Pu/MOX Fuel Pins,” pp. 689–699 in *Proc. of M&C’99-Madrid, Mathematics and Computations Meeting*, September 27–30, 1999, Madrid, Spain.