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MAINTAINING SCALE AS A REALIABLE COMPUTATIONAL SYSTEM FOR CRITICALITY SAFETY ANALYSIS

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Accurate and reliable computational methods are essential for nuclear criticality safety analyses. The SCALE (Standardized Computer Analyses for Licensing Evaluation) computer code system (Ref. 1) was originally developed at Oak Ridge National Laboratory (ORNL) to enable users to easily set up and perform criticality safety analyses, as well as shielding, depletion, and heat transfer analyses. Over the fifteen-year life of SCALE, the mainstay of the system has been the criticality safety analysis sequences that have featured the KENO-IV (Ref. 2) and KENO-V.a (Ref. 1) Monte Carlo codes and the XSDRNPM (Ref. 1) one-dimensional discrete-ordinates code. The criticality safety analysis sequences provide automated material and problem-dependent resonance processing for each criticality calculation.

The objective in the development of SCALE was to use a set of well-established computer codes within standard analytic sequences that

- utilize simplified free-form input,
- automate data processing and coupling between codes, and
- provide accurate and reliable results.

Continuing to achieve these objectives in the fast-changing world of digital computing requires a thorough yet straightforward quality assurance (QA) plan (Ref. 3) that includes configuration management and validation and verification (V&V) plans and procedures. In addition, these plans must accommodate portability between different computing platforms.

Configuration management is essential because SCALE consists of more than 25 computer codes (referred to as modules) that share libraries of commonly used subroutines. Changes to a single subroutine in some cases affect almost every module in SCALE! Controlled access to program source and executables and accurate documentation of modifications are essential to maintaining SCALE as a reliable code system. The modules and subroutine libraries in SCALE are programmed by a staff of approximately ten Code Managers. The SCALE Software Coordinator maintains the SCALE system and is the only person who modifies the production source, executables, and data libraries. All modifications must be authorized by the SCALE Project Leader prior to implementation.

One important purpose of configuration management is to preserve configuration identification and integrity. Identification of the SCALE system baseline is maintained by the Software Coordinator through the use of configuration control lists for source, executables, and data. The program source is stored by individual subroutines, grouped by modules and subroutine libraries. The configuration management software used to store and modify the production source preserves archives of all previous versions of each subroutine. Each production executable module is identified by a unique name and version number that are displayed in the code output for user verification.

Modifications to the software are controlled by a configuration management plan (Ref. 4).

The software modification process is controlled and documented by revision reports, which are monitored by the Software Coordinator. A Code Manager modifies the software, performs testing, and documents these modifications in the revision report. The revision report is reviewed by an independent Technical Reviewer for technical validity and adequacy of the verification and documentation. The Software Coordinator updates the production software and performs testing to verify that the updated software performs consistently with the Code Manager's test version. Updates and tests of the new production software are documented on the revision report, which is logged and filed by the Software Coordinator. Users are notified of the update via an electronic bulletin board maintained by the Software Coordinator.

The benefits of the configuration management plan include not only configuration identity and integrity, but also traceability and reproducibility. If a user discovers that the results of a problem calculated previously give different results with the present version of the software, we can identify the changes that caused those differences and when they occurred. Likewise, when a discrepancy is identified, we can notify users of the circumstances under which it occurs and how long it has existed in the software. Quick resolution of discrepancies and the ability to continually enhance our software while maintaining system integrity are the goals of our configuration management plan.

As part of software QA, V&V are obviously essential for computer codes that are used for performing scientific calculations. A V&V plan (Ref. 5) has been implemented as part of the SCALE QA program. Each module in SCALE has one or more standard sample problems that

have been developed to verify that the module functions properly. Validation of the SCALE modules and data libraries is divided into the four analytical categories of SCALE modules: criticality, shielding, depletion and isotopics, and heat transfer. A set of benchmarks with known solutions (either measurements or analytical) has been identified for each analytical category. Validation is performed by a qualified analyst who compares the calculational results of the prescribed benchmarks to the known solutions. The validation is reviewed by a qualified independent technical reviewer. An extensive amount of validation had been performed for the criticality modules and cross-section libraries prior to the implementation of the V&V plan, as evidenced by the more than 20 criticality validation reports listed in Section F11.F of Ref. 1.

For SCALE to be useful to as many criticality safety analysts as possible, the codes must be portable to a wide range of computing platforms. The program source is written and maintained in Fortran, with comment codes for different machine types and operating systems that can be activated and deactivated automatically through a simple conversion program. In addition, some routines are programmed in Assembler for IBM mainframes or C for UNIX machines. SCALE is currently installed on an IBM MVS 3090 mainframe and an IBM RS/6000 AIX workstation at ORNL. The Fortran source contains comment codes for the following machines/operating systems: IBM MVS, VAX, UNIX, UNICOS Cray, DEC ULTRIX workstations, and IBM AIX workstations. SCALE has also been successfully installed on SUN and DEC Alpha workstations. We have also developed a Fortran-only version that runs on MS-DOS personal computers.

To maintain a complex code system such as SCALE and ensure that it is accurate, reliable, and has state-of-the-art capabilities cannot be achieved by good configuration

management and V&V unless you have adequate funding and qualified personnel. We would be remiss if we failed to acknowledge the SCALE sponsors at the Nuclear Regulatory Commission and the Department of Energy and the committed SCALE development staff at ORNL.

REFERENCES

- 1. SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation, NUREG/CR-0200 (ORNL/NUREG/CSD-2/R4), Vols. I, II, and III (Draft February 1990). Available from Radiation Shielding Information Center as CCC-545.
- 2. L. M. Petrie and N. F. Cross, "KENO IV An Improved Monte Carlo Criticality Program,"

 Section F5 of SCALE: A Modular Code System for Performing Standardized Computer Analyses

 for Licensing Evaluation, NUREG/CR-0200 (ORNL/NUREG/CSD-2), Vol. 2 (October 1981).
- "Quality Assurance Plan for the SCALE Computational System," QAP-X-90-WMRD-029,R3,
 Oak Ridge National Laboratory (June 1994).
- "Configuration Management Plan for the SCALE Code System," SCALE-CMP-001, Rev. 4, Oak
 Ridge National Laboratory (June 1994).
- "Verification and Validation Plan for the SCALE Code System," SCALE-CCV-001, Rev. 0, Oak
 Ridge National Laboratory (August 1994).