CRITICALITY SAFETY ENHANCEMENTS FOR SCALE 6.2 AND BEYOND*

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ABSTRACT

SCALE is a widely used suite of tools for nuclear systems modeling and simulation that provides comprehensive, verified and validated, user-friendly capabilities for criticality safety, reactor physics, radiation shielding, and sensitivity and uncertainty analysis. Since 1980, regulators, industry, and research institutions around the world have relied on SCALE for nuclear safety analysis and design. SCALE 6.2 provides several new capabilities and significant improvements in many existing features for criticality safety analysis. Enhancements are realized for nuclear data; multigroup resonance self-shielding; continuous-energy Monte Carlo analysis for sensitivity/uncertainty analysis, radiation shielding, and depletion; and graphical user interfaces. An overview of these capabilities is provided in this paper, and additional details are provided in several companion papers.

KEYWORDS Monte Carlo, cross sections, sensitivity, depletion

1. INTRODUCTION

SCALE is a widely used suite of tools for nuclear systems modeling and simulation that provides comprehensive, verified and validated, user-friendly capabilities for criticality safety, reactor physics, radiation shielding, and sensitivity and uncertainty analysis [1]. Since 1980, regulators, industry, and research institutions around the world have relied on SCALE for nuclear safety analysis and design. SCALE 6.2 provides several new capabilities and significant improvements in many existing features for criticality safety analysis. Many historical biases observed for SCALE calculations have been mitigated through improvements in nuclear data libraries and resonance self-shielding techniques. Continuous-energy (CE) Monte Carlo capabilities are expanded beyond eigenvalue calculations to also provide shielding, depletion, and sensitivity/uncertainty analysis, including problem-dependent temperature

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corrections and an initial capability for parallel computing. A new hybrid deterministic/Monte Carlo capability is available to enable rapid and accurate fission source convergence for challenging criticality applications, and a new capability is introduced to determine spent fuel characterization for burnup credit analysis. Uncertainty quantification techniques are expanded to include a stochastic sampling tool to determine the uncertainty and correlation in any computed quantities due to uncertainties in many types of nuclear data as well as physical parameters such as dimensions and concentrations. Additionally, a new graphical user interface (GUI) is introduced.

2. NUCLEAR DATA ENHANCEMENTS

AMPX is a cross-section processing software package that has been developed at Oak Ridge National Laboratory for more than 40 years and is completely independent of any other cross-section–processing software package [2]. AMPX is used to process Evaluated Nuclear Data File (ENDF) nuclear data evaluations as well as other data sources that use the ENDF format, and to provide nuclear data libraries for use in SCALE radiation transport calculations. AMPX provides CE and multigroup (MG) neutron and gamma cross-section data as well as cross-section covariance data. Recently, the development, maintenance, quality assurance, and deployment of AMPX has been synchronized with SCALE such that the distribution of SCALE 6.2 includes both code systems, marking the first time AMPX has been publicly released since 1977.

SCALE 6.2 includes updated nuclear data libraries developed with AMPX, including the introduction of ENDF/B-VII.1 data [3], new MG energy structures for neutron libraries, substantial improvements in the accuracy of CE data for ENDF/B-VII.0 and VII.1, and coupled neutron/gamma data for CE calculations. The SCALE 6.2 nuclear data libraries are listed in Table I, and the performance of these libraries is documented in a companion paper [4]. The primary conclusion of this work is that the MG and CE libraries in SCALE 6.2 provide generally lower k_{eff} biases than the libraries released with SCALE 6.1. In particular, SCALE 6.2 with the ENDF/B-VII.1 252-group library provides notable improvements compared to SCALE 6.1 and its ENDF/B-VII.0 238-group library for light-water-moderated lattices. A new 56-group broad group library provides reliable results for the water-moderated lattice systems for which it was optimized. Both the 56- and 252-group neutron libraries include Bondarenko factors with full-range intermediate resonance (IR) parameters to enable rapid resonance self-shielding [2]. Substantial improvements have also been made to the CE libraries, resulting in improved performance for fuel pin lattice applications [5].

A new SCALE cross-section covariance data library has been generated based on ENDF/B-VII.1 data where possible, and is presented in the 56-group energy structure. These data are mostly consistent with the previous 44-group covariance data file distributed with SCALE 6.0–6.1, with a notable exception for a reduction in the uncertainty of $\bar{\nu}$ for ²³⁹Pu where the ENDF/B-VII.1 uncertainties are reduced relative to the ENDF/B-V uncertainties used in the previous SCALE covariance library. The performance of this new library for a wide range of applications is documented in a companion paper [6].

| Mnemonic names | Primary data source/format | | |
|---------------------------------------|--|--|--|
| v7-238 ; v7-238n ; v7.0-238n | ENDF/B-VII.0 238-group neutron library | | |
| v7.1-252n | ENDF/B-VII.1 252-group neutron library | | |
| v7.1-56n | ENDF/B-VII.1 56-group neutron library | | |
| v7.1-200n47g | ENDF/B-VII.1 200-group neutron/47-group gamma library | | |
| v7-200n47g ; v7.0-200n47g ; v7-200g47 | ENDF/B-VII.0 200-group neutron/47-group gamma library | | |
| v7.1-28n19g | ENDF/B-VII.1 28-group neutron/19-group gamma library | | |
| v7-27n19g ; v7.0-27n19g | ENDF/B-VII.0 27-group neutron/19-group gamma library | | |
| ce_v7.1_endf | ENDF/B-VII.1 Continuous-energy neutron and gamma library | | |
| ce_v7; ce_v7_endf; ce_v7.0_endf | ENDF/B-VII.0 Continuous-energy neutron and gamma library | | |

Table I. SCALE 6.2 cross-section data

3. MULTIGROUP RESONANCE SELF-SHIELDING

The migration of SCALE 6.1 capabilities to advanced methods in the modern SCALE framework began with MG cross-section resonance self-shielding codes, which have historically required substantial intermediate file input/output and operated only for serial calculations. These features are used in a majority of SCALE calculations as they provide the foundation for all MG transport calculations for criticality, shielding, depletion, and sensitivity calculations. The preparation of problem-dependent MG cross sections is now integrated into a modern module called XSProc. XSProc implements capabilities for problem-dependent temperature interpolation, calculation of Dancoff factors, resonance self-shielding using Bondarenko factors including IR theory, and use of CE resonance self-shielding in the resolved resonance region. Cross sections can be provided as microscopic data for each nuclide or as macroscopic data for each material in the original group structure. Additionally, a flux-weighting spectrum can be applied to collapse to a coarser group structure and/or to integrate over volumes for homogenized cross sections. The flux-weighting spectrum can be input by the user or calculated using one-dimensional coupled neutron/gamma transport.

XSProc integrates and enhances the capabilities previously implemented independently in BONAMI, CENTRM, PMC, WORKER, ICE, and XSDRNPM, with some additional capabilities that were provided by MIPLIB and SCALELIB. Integrating these capabilities into a single module has a number of benefits, including maintainability, extensibility, and the ability to easily replace the entire module with a future implementation with updated features with very little effort. The use of the modern XSProc instead of individual legacy codes of previous versions of SCALE generally results in the preparation of cross sections in about one-third the time, but a speedup of 1800 times was realized for a complex model with hundreds of detailed compositions, even when run as serial calculations (parallel capabilities are not currently implemented). Additionally, the memory requirements of XSProc are substantially improved by generating only the data needed for a particular calculation instead of generating a general-purpose library.

The benefits of XSProc over the legacy implementation are shown in Table II, where the computational times required to prepare MG cross sections for a typical burnup credit calculation with 18 axial zones of spent fuel are shown using SCALE 6.1 and SCALE 6.2 with XSProc with various options and libraries. When applying the same 238-group library and the same techniques as SCALE 6.1, XSProc produces equivalent results four times faster. When the new BONAMI-IR approach is applied, the calculation completes nearly 18 times faster, even with a finer group structure. Currently, the IR factors in the MG libraries are provided for light water reactor analysis, and their use in more general analyses is not recommended.

| Table II. Time required to generate resonance self-shield cross sections for a burnup credit calculation wi | th |
|---|----|
| 18 axial zones of spent fuel | |

| Options | SCALE 6.1 (minutes) | SCALE 6.2 - XSProc (minutes) | Speedup (6.1 238-group CENTRM/6.2) |
|---------------------|------------------------|---------------------------------|--|
| 238-group CENTRM | 112.1 | 27.4 | 4.1 |
| 252-group CENTRM | n/a | 33.4 | 3.4 |
| 252-group BONAMI-IR | n/a | 6.3 | 17.9 |

4. EIGENVALUE ANALYSIS ADVANCEMENTS

SCALE provides separate Monte Carlo capabilities for eigenvalue neutronics and fixed-source coupled neutron-gamma calculations in the KENO and Monaco codes, respectively [7,8]. Two variants of KENO provide identical solution capabilities with different geometry packages. KENO V.a uses a simple and efficient geometry package that is sufficient for modeling many systems of interest to criticality safety and reactor physics analysts. KENO-VI uses the SCALE Generalized Geometry Package, which provides a quadratic-based geometry system with much greater flexibility in problem modeling. Additionally, KENO implements grid geometry for accumulating data or communication of data into or out of a calculation. Grid geometries can be used for source or biasing parameter specifications as well as for tallying results from a calculation. KENO V.a and KENO-VI perform eigenvalue calculations for neutron transport primarily to calculate multiplication factors and flux distributions of fissile systems in both CE and MG modes. Both codes allow explicit geometric representation with their respective geometry packages. KENO provides a MG adjoint capability, which is especially useful for sensitivity analysis.

4.1. Improved Continuous-Energy Capabilities

The CE Monte Carlo capabilities provided in SCALE 6.0–6.1 [7] have large memory requirements such that routine criticality experiment modeling could require tens of gigabytes of random access memory (RAM), and spent fuel or reactor systems could require hundreds of gigabytes of RAM. Those capabilities are of limited value for practical analysis. In addition, large biases have been observed for some applications in the CE data previously generated with AMPX. As documented in recent publications [5, 9], CE Monte Carlo capabilities are substantially improved for SCALE 6.2 in terms of both accuracy and efficiency. Updates in the AMPX processing, especially of thermal scattering data, as well as updates to the CE physics methods themselves have minimized biases observed with previous calculations [3]. Refinements in data storage and use strategies have enabled the modeling of critical systems and even complex spent fuel or reactor systems with only 2 GB of memory instead of the tens or hundreds of gigabytes required by the previous implementation. Additionally, as part of the overall strategy for SCALE modernization [10], the CE data and physics have been developed as independent modules for

integration into the next-generation Monte Carlo code, Shift [11], which is quickly evolving but is not scheduled for release with SCALE 6.2.

4.2. Problem-Dependent Doppler Broadening

In SCALE 6.0–6.1, CE calculations are performed only at temperatures available on the data libraries distributed with SCALE, which contain a limited number of cross-section temperatures per isotope (typically five). Previously, when temperatures of isotopes in the KENO model were different from those present on the CE library, KENO would select the nearest temperature, which often differs from the desired temperature and may produce results that vary significantly from those that would be produced at the correct temperature.

New for SCALE 6.2, the cross sections are updated to the user-requested temperature as the problem initiates [12]. A finite difference method is used for Doppler broadening of the pointwise data in the resolved resonance region, and interpolation methods are implemented for thermal scattering data and probability table treatments in the unresolved resonance region. The eigenvalues computed for a typical fresh pressurized water reactor (PWR) pin cell using the nearest selected CE temperature and problem-dependent CE temperature treatments are shown in Figure 1. The previous approach of rounding to the nearest temperature in CE calculations is seen to produce unrealistic, step-like behavior in the problem eigenvalue estimates and eigenvalue biases that exceed 1000 pcm in some cases.



Figure 1. Eigenvalues Computed for a PWR Pin Cell with Different Temperature Treatments.

The impact of Doppler broadening is expected for reactor temperatures, especially the broadening of the resolved resonance region. What may not be so obvious is the impact of temperature changes in $S(\alpha,\beta)$ data for thermal solution criticality systems. For example, in the recent criticality accident alarm system (CAAS) benchmark experiments at the SILENE Facility [13], the fissile solution temperature is elevated several degrees above the default 293 K value provided by KENO. The necessity of using problem-dependent temperatures is shown in Table III, where a reactivity difference of 655 pcm is realized for this system.

| Temperature (K) | Temperature difference (K) | k _{eff} | ∆k _{eff} (pcm) | Relative uncertainty |
|--------------------|----------------------------------|-------------------------|----------------------------|-------------------------|
| 293.0 | 33.8 | 1.022831 | -655 | 0.000057 |
| 326.8 | | 1.016286 | | 0.000055 |

Table III. Impact of temperature on SILENE fissile solution system

4.3. Hybrid Method for Starting Source Distribution

As the fidelity of criticality models continues to increase, especially for storage and transportation systems, the ability of the Monte Carlo codes to consistently provide a converged fission source can be challenged. Studies have shown that using a starting fission distribution that is similar to the true fission distribution can both reduce the number of skipped generations required for fission source convergence and significantly improve the reliability of the final k_{eff} result [14,15]. The Sourcerer sequence introduced in SCALE 6.2 uses the solution from the Denovo [16] discrete-ordinates code as the starting fission source distribution in a KENO Monte Carlo calculation.

For many criticality safety applications, the additional step of performing a deterministic calculation to initialize the starting fission source distribution is not necessary. However, for challenging criticality safety analyses, such as as-loaded spent nuclear fuel transportation packages with a mixed loading of low-and high-burnup fuel, even a low-fidelity deterministic solution for the fission source produces more reliable results than the typical starting distributions of uniform or cosine functions over the fissionable regions, as demonstrated in a recent study [17]. In that study, a cask containing 24 spent fuel assemblies was examined using a uniformly distributed starting source and a deterministically calculated starting source. Multiple KENO simulations were run with different random number seeds for various numbers of skipped cycles, and the number of calculations that produced incorrect k_{eff} estimates was tabulated. As shown in Figure 2, using a precomputed deterministic starting source can significantly increase the k_{eff} reliability of the eigenvalue calculation.



Figure 2. Fraction of Results Failing to Agree with the Reference k_{eff} Value by within Three Standard Deviations for KENO Calculations with Different Starting Sources (Figure 4 from Ref. [17]).

4.4. Reaction Rate Tallies

In SCALE 6.2, a new reaction tally feature has been added for CE calculations in KENO. The reaction data block is available only in CE mode and provides the specifications for reaction rate, neutron flux, and reaction cross-section tallies. For MG KENO calculations, users can continue to use the KMART module, which provides a similar functionality as a postprocessing code.

5. SENSITIVITY AND UNCERTAINTY ANALYSIS ADVANCEMENTS

Sensitivity coefficients describe the fractional change in a system response that is induced by changes to system parameters and nuclear data. The Tools for Sensitivity and Uncertainty Analysis Methodology Implementation (TSUNAMI) code within the SCALE code system makes use of eigenvalue sensitivity coefficients for an extensive number of criticality safety applications, such as quantifying the data-induced uncertainty in the eigenvalue of critical systems, assessing the neutronic similarity between different critical systems, and guiding nuclear data adjustment studies [18].

5.1. Eigenvalue Sensitivity Capability

With SCALE 6.2, the MG eigenvalue sensitivity and uncertainty analysis methods that use KENO for transport analysis are extended to provide CE capabilities through the implementation of the Contribution-Linked Eigenvalue Sensitivity/Uncertainty Estimation via Tracklength Importance Characterization (CLUTCH) and Iterated Fission Probability methods [19, 20]. CLUTCH is an efficient methodology that has been demonstrated to provide high-fidelity results with manageable runtimes and memory requirements, and both of these state-of-the-art sensitivity methods make CE sensitivity calculations easier to learn and use than MG in several ways. For example, CE calculations do not require resonance self-shielding calculations to determine implicit sensitivity effects, separate adjoint transport calculations to determine importance functions, or spatial meshes to quantify fluxes and flux moments. In a companion paper [21], the application of these methods is demonstrated for numerous criticality safety systems.

5.2. Generalized Response Sensitivity Capability

In SCALE 6.2, the TSUNAMI-3D sensitivity capabilities have also been extended to calculate sensitivity coefficients for generalized neutronic responses using the Generalized Adjoint Response in Monte Carlo (GEAR-MC) methodology [20, 22]. Rather than calculate sensitivity estimates for eigenvalue responses, the GEAR-MC methodology uses Generalized Perturbation Theory to calculate the sensitivity of the ratio of two neutronic reaction rates to perturbations in system parameters. Some commonly used ratios for this technique include production/destruction of isotopes and capture or fission rates at different energy ranges. Quantification of the sensitivity of these reaction ratios to each energy-dependent reaction cross-section in the model enables the uncertainty assessment for safety analysis, similarity assessment for validation, and model calibration where measured reaction rate ratios are available. Additionally, these sensitivity coefficients can be used in the design of optimized processes for target irradiations such as foil activation or isotope production.

5.3. Stochastic Sampling of Uncertainties

Sampler is a new "super sequence" that performs general uncertainty analysis by stochastically sampling uncertain parameters that can be applied to any type of SCALE calculation, propagating uncertainties throughout a computational sequence.[23] Sampler treats uncertainties from two sources: (1) nuclear data and (2) input parameters. Sampler generates the uncertainty in any result generated by any computational sequence,

each with a randomly perturbed sample of the requested uncertain quantities. The mean value and uncertainty in each parameter are reported along with the correlation in uncertain parameters where multiple systems are simultaneously sampled with correlated uncertainties.

Used in conjunction with nuclear data covariances available in SCALE, Sampler is a general technique to obtain uncertainties for many types of applications. SCALE 6.2 includes covariances for MG neutron cross-section data as well as for fission product yields, radioactive decay data, and gamma yields. The availability of this wide range of covariance libraries allows uncertainty calculations to be performed for most MG computational sequences in SCALE. At the present time, nuclear data sampling cannot be applied to SCALE CE Monte Carlo calculations, although the fundamental approach is still valid.

Sampler enables a new class of uncertainty calculations that were not previously available in SCALE. For example, Sampler can be applied to spent fuel characterization with the Transport Rigor Implemented for Transient Depletion with ORIGEN (TRITON) sequences [24] to quantify the uncertainty in isotopics due to uncertainties in the nuclear data used throughout the calculation, as shown in Figure 3 [25].



Figure 3. Uncertainty in Plutonium Isotopics as a Function of Burnup Computed with Sampler and TRITON.

Used in conjunction with uncertainties in input data, Sampler can determine the uncertainties and correlations in computed results due to uncertainties in dimensions, densities, distributions of material compositions, temperatures, or any quantities that are defined in the user input for any SCALE computational sequence. This methodology was especially developed to produce uncertainties and correlations in criticality safety benchmark experiments, as documented in a companion paper [26], but it has a wide range of applications in numerous scenarios in nuclear safety analysis and design. The input sampling capabilities of Sampler also include a parametric capability to determine the response of a system to a systematic variation of an input parameter.

6. DEPLETION AND SPENT FUEL SOURCE TERM CHARACTERIZATION

SCALE 6.1 provides one-, two-, and three-dimensional (1D, 2D, 3D) depletion capabilities within the TRITON sequences, where problem-dependent MG cross sections are provided to deterministic neutron transport calculations in 1D and 2D or KENO Monte Carlo calculations in 3D. The Oak Ridge Isotope

Generation and Depletion Code (ORIGEN) [27] is employed to update isotopic compositions at each time step. Libraries of ORIGEN cross-section data can be archived for specific reactor types, configurations, conditions, and burnup for use in subsequent ORIGEN calculations to efficiently quantify specific isotopic compositions for burnup credit calculations as well as source terms for decay heat and shielding analysis.

6.1. Spent Fuel Characterization

The ORIGEN Assembly Isotopics (ORIGAMI) code is introduced to SCALE 6.2 for determining assembly isotopics using multiple ORIGEN calculations [28]. Here the parameterized ORIGEN reactor libraries generated with TRITON are interpolated as functions of enrichment, burnup, moderator density, and other variables. ORIGAMI can compute 1D axially varying isotopics radially averaged over the fuel assembly, or it can compute a full 3D isotopic distribution for all fuel pins, using an input power shape. Nuclide concentrations for each axial depletion zone are output as ORIGEN binary concentration files and in a text file formatted for direct use by KENO and/or the Monte Carlo N-Particle (MCNP) code [29] for criticality calculations. The neutron and gamma decay heat source is computed for use in thermal analysis and has been applied in the COBRA-SFS code to analyze spent fuel containers [30].

6.2. Continuous-Energy Monte Carlo Depletion

In addition to the existing MG depletion KENO/ORIGEN Monte Carlo capability, a new CE-based depletion capability has been developed for SCALE 6.2 [31]. CE depletion is especially useful for models with complex geometry where it is difficult to obtain accurate resonance self-shielded MG data and for models with many depletion regions where the runtime needed to generate and store the resonance self-shielded cross-section data for each material is prohibitive.

In some cases, MG depletion suffers from the inadequacies of the MG approximations, such as an inadequate group structure or the inability to properly shield the cross sections for the problem using the 1D resonance self-shielding modules available in SCALE. Additionally, the requirement to update the resonance self-shielding at each depletion step can present a large computational burden that makes calculations impractical or impossible because the storage of independent sets of MG data for thousands of depletion materials can require excessive amounts of memory. To alleviate issues associated with the MG technique while maintaining components of the current depletion infrastructure of SCALE, a few-group or one-group microscopic reaction cross-section calculation capability is now available for CE calculations in KENO.

Results are shown in Table IV for a benchmark based on destructive isotopic assay data for sample MKP109-P of assembly D047 irradiated in the Calvert Cliffs PWR to a burnup of 44 GWd/MTU [32]. The percentage differences from the calculated to experimental (C/E) values are shown to be similar between MG and CE calculations on the same KENO models. However, for CE depletion, it is not necessary to compute and track resonance self-shielded cross sections for each depletion region separately. For models with hundreds or thousands of depletion regions, the previously described advancements in CE calculations provide substantially reduced memory requirements, enabling high-fidelity calculations that were not previously possible.

| | MG | CE | | MG | СЕ |
|-------------------|--------|--------|-------------------|-------|-------|
| ²³⁴ U | 4.03 | 3.37 | ¹³³ Cs | 0.67 | 0.53 |
| ²³⁵ U | 5.34 | 5.04 | ¹³⁵ Cs | 4.42 | 4.32 |
| ²³⁶ U | 1.82 | 1.65 | ¹³⁷ Cs | -2.76 | -2.76 |
| ²³⁸ U | -0.15 | -0.15 | ¹⁴³ Nd | 2.09 | 1.98 |
| ²³⁸ Pu | -10.38 | -10.15 | ¹⁴⁴ Nd | -3.22 | -3.15 |
| ²³⁹ Pu | 7.05 | 5.70 | ¹⁴⁵ Nd | -3.01 | -3.09 |
| ²⁴⁰ Pu | 3.15 | 2.82 | ¹⁴⁶ Nd | 0.18 | 0.29 |
| ²⁴¹ Pu | 0.72 | -0.05 | ¹⁴⁷ Nd | -0.03 | -0.01 |
| ²⁴² Pu | -7.40 | -6.91 | ¹⁵⁰ Nd | 2.58 | 2.60 |
| ²³⁷ Np | 2.33 | 2.39 | | | |
| ²⁴¹ Am | -6.56 | -7.35 | | | |

Table IV. C/E -1 (%) for Spent Fuel Assay Data for a PWR Assembly

7. DISTRIBUTED MEMORY PARALLELISM VIA MESSAGE PASSING INTERFACE

Although KENO has been applied by thousands of users and has been continually updated since the 1960s, it has only operated for serial calculations. To efficiently perform calculations with the numerous advanced features described above, parallel computation capabilities have been implemented to provide reductions in wall clock time, especially for sensitivity/uncertainty analysis or Monte Carlo depletion on computing clusters [9]. Due to its use in safety analysis calculations, the parallel strategy for KENO was designed to preserve the same solution regardless of the number of processors used in a calculation. Meeting this objective requires substantial communication between generations, and parallel performance diminishes above 100 cores. However, for a user community that is accustomed to calculations only executing on one core, the use of a few dozen cores represents a substantial improvement in performance. Additionally, SCALE users generally have access to desktop computers or small Linux clusters with dozens of processors.

The parallel performance of KENO as used in a CE calculation for a graphite-moderated reactor model is shown in Figure 4. The tests were conducted on a heterogeneous Linux cluster much like the clusters that SCALE users may encounter in practice, in which the size of the nodes varies from 4 to 16 cores with differing processor speeds. Tests were conducted with systematically increasing numbers of particles per generation, and various combinations of options were enabled to develop the distributions of speedups for each number of Message Passing Interface (MPI) processes shown in Figure 4. With larger numbers of particles per generation, KENO provides nearly linear speedup on the 64 processors tested here and has been successfully demonstrated on hundreds of processors.

The parallel capabilities have recently been demonstrated in a series of high-fidelity physics test simulations for the AP1000[®] PWR [33]. A typical model used in this work was generated with 688,000 units and was simulated with 50 billion particle histories on 180 cores of a computational cluster, exercising many of the enhancements available in an early release of SCALE 6.2. Sample relative power distribution generated in this study is shown in Figure 5; many more details are provided in Ref. [33]. In this calculation, the parallel efficiency on 180 processors approached 50%, reaching the limit of KENO's parallel capabilities. However, a similar calculation with Shift using modular SCALE physics capabilities demonstrates strong scaling with parallel efficiencies of 97% to 100% on 150,000 processors and produced results equivalent to KENO's [11].



Figure 4. Speedup for Parallel KENO-VI Calculations for a Graphite-Moderated Reactor Model.



Figure 5. Relative Power Distribution in the AP1000[®] PWR.

8. SHIELDING ANALYSIS ENHANCEMENTS

Monaco is a fixed-source Monte Carlo shielding code that calculates neutron and photon fluxes and response functions for specific geometry regions, point detectors, and mesh tallies [8]. Monaco contains variance reduction capabilities to maximize the efficiency of shielding calculations, including source biasing and weight windows, which can be automated via the Monaco with Automated Variance Reduction using Importance Calculations (MAVRIC) sequence. MAVRIC performs radiation transport on problems that are too challenging for standard, unbiased Monte Carlo methods, such as facility-wide dose rates for sites with spent fuel canisters [34] and CAAS analysis [35].

Prior to SCALE 6.2, the MAVRIC/Monaco capabilities relied on the MG approach for radiation transport. The MG approach is suitable for many applications but can be problematic for others. For example, for deep penetration through iron shielding, the MG-averaged cross-section for capture resonances may not accurately represent the true transmission of neutrons due to fine "windows" through (i.e., minima in) the cross-section. Additionally, MG calculations cannot adequately resolve discrete gamma emission lines, such as those of ⁶⁰Co. The CE treatment introduced in SCALE 6.2 allows for improved solution fidelity by enabling Monaco calculations to use SCALE CE physics [5]. The generation of CE nuclear data and the implementation of CE physics in Monaco are based on a first-principles approach, where the simulation is represented as realistically as possible. This approach will lead to higher-fidelity results, but runtimes may be substantially increased over more approximate methods.

Additional enhancements in Monaco include the ability to directly import multiple used-fuel composition data files generated with ORIGAMI and to import gamma-line and yield data from ORIGEN, further facilitating high-fidelity simulation.

9. MODERN SCALE GRAPHICAL USER INTERFACE

Fulcrum is a cross-platform GUI designed to create, edit, validate, and visualize SCALE input, output, and data files. Historically, SCALE has provided several special-purpose GUIs that operate only on specific platforms and are loosely integrated with SCALE's computational and data components. Fulcrum, in contrast, is intended to provide a single user interface that directly integrates with SCALE's internal resources to provide a consistent experience between Fulcrum and SCALE's command line interface. Fulcrum will replace the previous GUIs GeeWiz, OrigenArp, KENO3D, Javapeño, PlotOpus, MeshView, and ChartPlot.

The layout of panels in Fulcrum is highly configurable to accommodate the preferences of many users. An example layout for a spent fuel cask analysis is shown in Figure 6.



Figure 6. Fulcrum View of Spent Fuel Storage Canister.

10. CONCLUSIONS

SCALE 6.2 continues a 35-year legacy of nuclear systems modeling and simulation by providing comprehensive, verified and validated, user-friendly capabilities for criticality safety, reactor physics, spent fuel and radioactive source term characterization, radiation shielding, and sensitivity/uncertainty analysis. The new capabilities within SCALE 6.2 provide significant advances over the previous versions, especially with enhancements in nuclear data; MG resonance self-shielding; CE Monte Carlo analysis for sensitivity/uncertainty analysis, radiation shielding, and depletion; and a new GUI.

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