

GNES-R: Global Nuclear Energy Simulator for Reactors

Task 1: High-Fidelity Neutron Transport

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Abstract

A multi-laboratory, multi-university collaboration has formed to advance the state-of-the-art in high-fidelity, coupled-physics simulation of nuclear energy systems. We are embarking on the first-phase in the development of a new suite of simulation tools dedicated to the advancement of nuclear science and engineering technologies. We seek to develop and demonstrate a new generation of multi-physics simulation tools that will explore the scientific phenomena of tightly-coupled physics parameters within nuclear systems, support the design and licensing of advanced nuclear reactors, and provide benchmark quality solutions for code validation. In this paper, we have presented the general scope of the collaborative project and discuss the specific challenges of high-fidelity neutronics for nuclear reactor simulation and the inroads we have made along this path.

The high-performance computing neutronics code system utilizes the latest version of SCALE to generate accurate, problem-dependent cross sections, which are used in NEWTRNX - a new 3-D, general-geometry, discrete-ordinates solver based on the Slice-Balance Approach. The Global Nuclear Energy Simulator for Reactors (GNES-R) team is embarking on a long-term simulation development project that encompasses multiple laboratories and universities for the expansion of high-fidelity coupled-physics simulation of nuclear energy systems.

KEYWORDS: NEWTRNX, SCALE, High Performance Computing, 3-D General-geometry Transport, Coupled-Physics

1. Introduction

A multi-laboratory, multi-university collaboration has formed to advance the state-of-the-art in high-fidelity, coupled-physics simulation of nuclear energy systems. Through united Laboratory Directed Research and Development funds at Idaho National Laboratory (INL) and Oak Ridge National Laboratory (ORNL), along with a grant from the Science Alliance at the University of Tennessee, we are embarking on the first phase multi-physics simulation tools that

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in the development of a new suite of simulation tools dedicated to the advancement of nuclear science and engineering technologies. We seek to develop and demonstrate a new generation will explore the scientific phenomena of tightly-coupled physics parameters within nuclear systems, support the design and licensing of advanced nuclear reactors, and provide benchmark quality solutions for code validation.

The underlying phenomena during nuclear reactor operation and transient conditions are often a result of a complex multi-physics, multi-scale system behavior. Therefore, the long-range vision for the GNES-R code system includes the:

- Simulation of severe accident transients not amenable to experimentation,
- Simulation of long-term effects on materials in a high-temperature, high-radiation field environment,
- Optimization of nuclear designs to improve experimental and commercial facilities, and
- Exploration of scientific phenomena of tightly-coupled physics parameters within nuclear systems.

1.1 Developing the State-of-the-Art

To be able to model this vast array of scenarios, a suite of interoperable codes within the domain of several disciplines is required, namely, radiation (neutron/gamma) transport, fluid-structure elasto-plastic mechanics, impact dynamics, multi-scale materials processing, multi-phase chemically-reactive non-isothermal fluid dynamics, and conjugate heat transfer.

The initial phase of GNES-R integrates the expertise at three national laboratories (INL, ORNL, and Argonne National Laboratory(ANL)) and two universities (Georgia Institute of Technology and University of Tennessee at Knoxville) in an effort to develop and couple two of the most significant physics packages for the simulation of nuclear systems: fluid dynamics and heat transfer (EMPRESS [1]) with neutron/gamma transport (NEWTRNX) within a united multi-physics scientific computing backplane with associated geometry and mesh generation tools.

Coupled high-fidelity simulation is extremely challenging because the requirements of each physics simulation tools can be in conflict: some require extensive computational speed (computational fluid dynamics and conjugate heat transfer), others massive memory resources (neutron transport with thousands of energy groups), and still others that are accurate and efficient on single processors with limited memory (isotopic depletion and decay).

Each software component that requires high-performance computing systems for a high-fidelity solution will be designed specifically for efficient use of thousands of processors using the latest advances in mathematical and scientific computing tools and algorithms. Software components that do not require substantial computational resources must still conform to the conventions of the scientific computing backplane to ease interoperability of independently-derived software.

1.2 Creating the Foundation for Complete High-Fidelity Nuclear Energy Simulation

The fruit of this initial collaboration will produce the capability to:

- Build a model of a nuclear energy system using a standard CAD package,
- Mesh that geometry with an advanced tetrahedral mesh generation tool,
- Partition the spatial domain onto thousands of processors using advanced mesh generation and load balancing software,

- Utilize NRC-qualified nuclear cross sections processing tools to define accurate space-, time-, temperature-dependent multi-group (or point-wise) cross sections,
- Calculate the spatial distribution of the heat generation source from a 3-D deterministic neutron/gamma transport solver,
- Calculate the spatial distribution of the temperature and density field utilizing the latest 3-D computational fluid dynamics and conjugate heat transfer solver,
- Perform transient analyses to simulate hypothetical accident scenarios in that system.

1.3 Leveraging Existing Software and Expertise

Substantial effort and expertise has been invested in many software applications for high-performance computing, geometry and mesh generation, nuclear data processing, and transport and fluids simulation. One cannot simply discard the substantial effort that has been incorporated into the array of software for these purposes. However, it can be immensely difficult to retrofit existing software to perform efficiently, let alone interchangeably, on high-performance computing architectures in a modular framework. Therefore, we must strike a balance between leveraging existing tools and developing entirely new components.

For many tools and applications, there is no need to develop new software. For instance, a commercial CAD software package (SolidWorks [2]) is being used to define the geometry. The Scientific Discover through Advanced Computing (SciDAC [3, 4]) initiative of the Office of Science has produced and supported many tools and interfaces to couple a host of CAD software with advanced mesh generation tools like those we are using: CUBIT [5] and GRUMMP [6]. We also plan to take advantage of ZOLTAN, developed by Sandia National Laboratory, which is a parallel processing and load balancing toolset for high-performance computing architectures [7, 8]. The SCALE nuclear analysis software package from ORNL was developed and maintained jointly by the Nuclear Regulatory Commission (NRC) and the DOE Office of Nuclear Energy, Science, and Technology [9]. SCALE is the NRC-qualified nuclear analysis software package for multigroup cross section generation and depletion/decay analysis, among other things. However, the computational requirements for the CFD and neutron transport solutions require high-performance computing to produce a high-fidelity solution for many problems of interest.

There is no readily available, three-dimensional, general-geometry, open-source neutron-transport software package that is capable of running on thousands of processors and producing an accurate solution on an unstructured grid. Many codes meet several of those requirements and a few theoretically meet all, but have not been tested for scalability to thousands of processors [10] or have not fully integrated the tallying requirements for unstructured grids [11].

1.4 Scope and Focus of this Publication

The scope of this paper is limited to the neutronics solver being developed at ORNL, in collaboration with Georgia Tech and the University of Tennessee. It will not discuss the scientific computing backplane (infrastructure), geometry and mesh generation tools, parallel computing tools, or the computational fluid dynamics and conjugate heat transfer solver. A future journal article will report on the full structure of the code and present more comprehensive results.

2. High-Fidelity Neutronics

The SCALE code system [9], initially developed at ORNL for the U. S. Nuclear Regulatory Commission (NRC), is a recognized world leader for analysis of nuclear systems and facilities. Present reactor analysis methods in SCALE use a three-step approach to modeling the core of a nuclear reactor:

1. Cross section processing:
 - a. Fine-mesh, one-dimensional neutron transport on a small subset (pincell or fuel particle) of the core with an accurate representation of the energy resolution.
 - b. The solution is used to weight the high energy resolution cross sections and formulate a (sometimes homogenized) multi-group set of cross sections;
2. Lattice physics:
 - a. Coarser-mesh, two-dimensional neutron transport on a larger subset of the core (assembly or lattice) with a coarse (multi-group) energy resolution.
 - b. The solution is used to weight the multi-group cross sections and homogenized the larger subset to formulate a single effective material with a few-group set of cross sections; and
3. Core physics (performed externally from SCALE using PARCS/TRACE [12]):
 - a. Very coarse, three-dimensional neutron diffusion in the full core with a very coarse energy resolution
 - b. Coupling with thermal-hydraulic feedback is integrated into this step
 - c. The fine-mesh solution is reconstructed using the core physics magnitude and a shape function (form factor) from the lattice physics (and possibly the cross section processing) step.

Petascale (and beyond) parallel computing brings about the opportunity to combine the following elements defining *high-fidelity* radiation transport simulations in nuclear reactors heretofore not possible:

- Detailed description of the *full geometry* of all components in the core of a nuclear reactor;
- Detailed account of energy-dependent interactions of neutrons with matter.

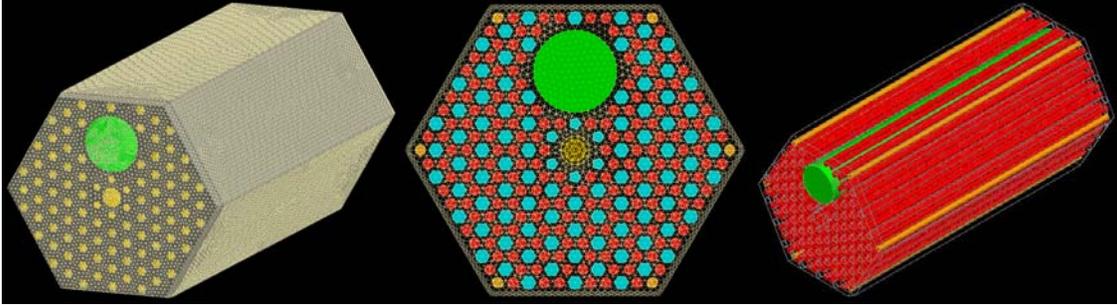
The purpose of this project is to incorporate these elements in one computational tool and begin the process of eliminating the multi-step approach and its inherent approximations. *The successful implementation of this new computational analysis capability will circumvent two of the most significant sources of error in present-day reactor analysis methods: poor geometric resolution and poor approximation of the energy dependency of neutron transport.*

2.1 High-Fidelity Geometric Resolution

Advances in computational geometry and mesh generation in supercomputers make it possible now to model (geometrically) the entire core of a nuclear reactor. However the task remains a challenge, because resolving a standard prismatic fuel element on the GT-MHR (gas-turbine modular helium reactor) to an 1-cm scale level requires a 1.6-million-tetrahedral cell model (Figure 1). The coarseness of the model is limited by the accurate representation of the geometry, therefore, further coarsening of the mesh would not substantially reduce the total number of cells required. In fact, a 600-MW GT-MHR design by General Atomics calls for 720 prismatic graphite elements, arranged radially and stacked as columns inside the core of the

reactor. Geometrically similar elements are also used for control and reserve shutdown. Taking all elements into consideration, a minimum of 1.2-billion-tetrahedral-element model is needed to resolve the core alone. If the reflector blocks, and other shielding and structural elements that make up the interior of the reactor are included, an estimated 3-billion-cell model is needed to resolve linear dimensions of 1 cm inside the reactor. Tools developed within the SciDAC center (Terascale Tools and Simulation Technologies [4]) are being extended and used to meet the challenge of generating combined geometry and mesh generation for Gen-IV and GNEP reactors.

Figure 1: Standard prismatic fuel element on the GT-MHR with mesh resolution of 8 mm. Left and center: Mesh with 1.6M tetrahedra. Right: fuel rods inside the element.



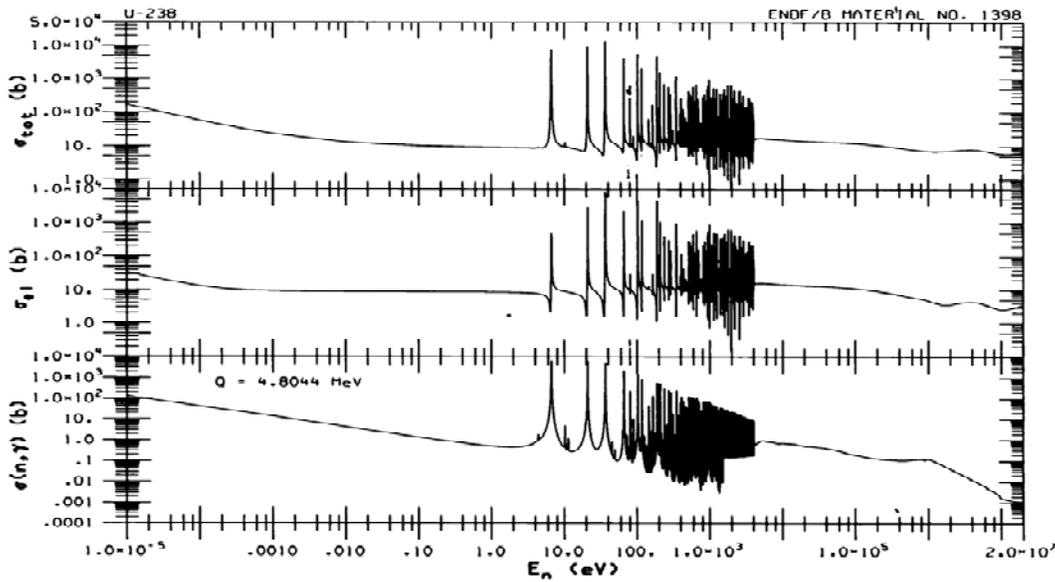
Leveraging the development of the most advanced present-day reactor analysis methods for step 2 of the three-step approach, the required number of mesh can be substantially reduced by allowing arbitrary polyhedra cells with re-entrant surfaces using the ‘Characteristic Form’ of the neutral-particle transport equation [13]. This discretization has successfully been implemented for two spatial dimensions in the NEWT [14] code within SCALE and will allow accurate solutions for both neutron and photon transport. The successful extension of this discretization to three-dimensions with arbitrary polyhedra cells and arbitrarily high-order accuracy will allow the solution to be accurately resolved with substantially less cells (at least an order of magnitude) for the entire reactor core, reflector and pressure vessel. *Successful achievement of this goal defines the first element of high-fidelity simulation – the ability to obtain full geometric resolution.*

2.2 High-Fidelity Energy Resolution

A salient feature of neutron transport in nuclear reactors is the highly energy-dependent probability of interaction of neutrons with matter (Figure 2). Here the total microscopic cross section, $\sigma_t(^{238}\text{U})$, varies widely with the energy of the neutron. The microscopic cross section is a material property that has been measured for numerous isotopes as a function of energy for up to hundreds of thousands of incident neutron energy values. Total cross section data enter the governing equation of particle transport on the left side of equation (1) through the corresponding macroscopic cross section $\Sigma_t(\vec{r}, E, T, t)$. In addition, a related quantity, the total macroscopic double-differential cross section, $\Sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}, T, t)$, accounts for interactions wherein the energy and direction of the scattered neutron depends on the energy and direction of the initiating neutron. This information enters the right side of equation (1) in integral form and considerably complicates the task of solving the neutron transport equation due to its non-local character, both in physical direction and energy spectrum.

Through work for the NRC, National Nuclear Security Administration (NNSA), and DOE/NE, the CENTRM [15] code was developed and incorporated within SCALE as step 1 of the three-step method for present reactor analysis calculations. This experience in developing strategies for incorporating the fine energy spectrum of cross-section data into the solution of the governing transport equation (1) will be leveraged. The treatment of the double-differential cross-section is treated analytically for every isotope independently via the fundamental physics of neutral-particle collision kinematics for the elastic, inelastic, and bound scattering regimes. This is a unique procedure for accurate calculation of the neutron distribution in nuclear reactors that ORNL has developed and maintained. However, this methodology does require the complete space-angle distribution of the solution at 10^4 to 10^5 discrete energy points. *The method is referred to as a continuous-energy treatment of cross section properties and it defines the second element of high-fidelity simulation.*

Figure 2: ^{238}U microscopic total cross section $\sigma_t^{238\text{U}}$ showing the resonance peaks.



$$\begin{aligned} & \frac{1}{v(E)} \frac{\partial \psi}{\partial t} + \bar{\Omega} \cdot \bar{\nabla} \psi + \Sigma_t(E, T) \psi(E, \bar{\Omega}) \\ & = S_{ext}(E, \bar{\Omega}) + \int_0^\infty dE' \int_0^{4\pi} d\Omega' \left[\Sigma_s(E' \rightarrow E, \bar{\Omega}' \rightarrow \bar{\Omega}, T) \psi(E', \bar{\Omega}') \right] \end{aligned} \quad (1)$$

2.3 High-Fidelity Resolution is Currently Unattainable

Combining these two requirements leads to a minimum of 10^9 spatial elements and 10^4 discrete energy points, which is several orders of magnitude larger than the latest computers can store in memory. However, creating a new code and developing it to production quality with rigorous validation and verification is a process that generally takes more than five years and the highest quality software tends to stay in service for decades. Therefore, one should develop computational tools that surpass the limits of today's computing power so that we will be able to

fully realize the goal of complete high-fidelity simulation when the fastest computers in the world can catch up.

To this end, we have are developing a tool that will be able to utilize the latest innovation for cross section processing (step one of the three-step process) and solve the (multi-group) transport equation on the full geometry with tens or hundreds of groups so that we can produce a useful tool that can address the challenging problems of today. We are also implementing the high-fidelity (point-wise) energy treatment to begin testing on smaller subsets of the core so that we can utilize the computational resources of tomorrow.

3. Nuclear Cross Section Generation

The solution to the transport equation is only as accurate as the data supplied. Because we cannot utilize the near-continuous-energy treatment for the entire spatial domain, we must (for many simulations) rely on cross section processing tools. Nuclear cross section data is stored on evaluated nuclear data files for many reactions on the order of 10^5 discrete energy points. To produce a multi-group cross section library (independent of the number of groups) requires a weighting function (equation 2). The analytically correct weighting function is the space-, angle-, energy-dependent solution of the problem. However, decades of research have produced methods to define approximate weighting functions that are used to collapse these discrete energy libraries into a set of multi-group macroscopic cross section tables for most nuclear energy systems.

$$\Sigma_g(\bar{r}, \bar{\Omega}, t) = \frac{\int_{\Delta g} dE' [\Sigma(\bar{r}, E', \bar{\Omega}, t) \Psi(E')]}{\int_{\Delta g} dE' [\Psi(E')]} \quad (2)$$

3.1 The SCALE Code System

“SCALE (Standardized Computer Analyses for Licensing Evaluation) is a modular code system that was originally developed by Oak Ridge National Laboratory at the request of the U.S. Nuclear Regulatory Commission. It is maintained and enhanced under joint sponsorship of the NRC and the U.S. Department of Energy. The SCALE system utilizes well established computer codes and methods within standard analysis sequences that ... automate the data processing and coupling between modules and provide accurate and reliable results. System development has been directed at problem-dependent cross-section processing and analysis of ... depletion/decay.”

Abstract of Reference [9]

Over twenty-five years of development have lead to a validated, verified, and benchmarked system of tools, with NRC qualification, for generating problem-dependent multi-group cross sections, using those cross sections with a variety of transport codes to determine the rate of fission and capture reactions, and simulation of the depletion and decay of isotopic concentrations.

3.2 SCALE Cross Section Processing

Most of the codes within SCALE are computationally inexpensive, as they were developed and maintained for single-processor architectures. In addition, only ten of the codes are required to create the cross section library and model the depletion/decay of isotopes, each of which takes less than one minute on a single CPU. However, this must be done for every material (a region with a given temperature, density, and isotopic concentration) in the problem – which could theoretically equal the number of spatial elements, but likely would be limited to thousands.

The basic components of the SCALE code system that this project will require include all of the components that are used to model doubly-heterogeneous fuel and the depletion and decay of materials. This consists of 9 independent codes (BONAMI, WORKER, CENTRM, PMC, ICE, CHOPS, CAJUN, AJAX, and ORIGEN-S) that currently run in series as system-call executables controlled with a driver code. The first task of the driver code is to read the general input file and create a set of input files for each of the independent code. Each independent code reads an input file, performs its task, and writes a data file that the next code in the sequence will read.

This modular framework using system-calls is an extremely-portable, nearly-passive backplane that has been exceptionally useful for the independent development of each code within SCALE and the interoperability on various single processor computer systems, including Windows. However, several challenges exist when attempting to port this to high-performance computing architectures.

Many high-performance computing architectures have limited I/O nodes, therefore, large amounts of reading and writing would make each execution of the series a substantially larger portion of the execution time than on single-processor machines. In addition, performing a system-call to an executable prevents any of the data within that code from being accessible to other modules on the backplane without the I/O.

3.3 SCALE – Now as a Subroutine

Because of these challenges, we plan to replace the FORTRAN main of each code with a FORTRAN module so that the data will be accessible to other modules (multigroup transport solvers). In addition, we will be working with the SCALE team to begin to remove the I/O from each code and provide the opportunity to store the necessary data in memory.

Thus far, we have replaced the driver code with a module that is connected to the backplane through a series of ports. Therefore, the cross section processing sequence of SCALE may be called as a subroutine by a driver code to provide accurate multigroup cross sections that can fully account for the double-heterogeneity of fuel. This will greatly simplify the portability of our code system to be able to incorporate additional transport solvers as the tools are developed.

4. NEWTRNX – 3D, General-Geometry Transport

This team has embarked on a journey to develop a new three-dimensional transport code for analysis of nuclear energy systems, with a focus on the core of a nuclear reactor. This need is driven by the lack of readily-available, three-dimensional, general-geometry, open-source neutron-transport codes that are capable of running on thousands of processors and producing an accurate solution on an unstructured grid.

4.1 Requirements of the Transport Solver for Reactor Analysis

The requirements for a new computational tool should be considered before development begins. For any given method of solving the transport equation, a problem could be conceived that would render it inefficient and often inaccurate. Several aspects of a nuclear reactor lead to the specification of a method that will most-often produce accurate results efficiently.

As this section will likely render much debate, we do not claim that any single method (or code) will produce the most accurate and efficient solution for every conceivable problem, nor do we claim that the method we have chosen is the only (or ideal) method for the problem described. However, it is important that we explore and understand the specific challenges of the problem (high-fidelity, coupled-physics reactor simulation) to ascertain the standards to which our code must perform.

4.1.1 Complete Spatial Resolution

The challenge of creating a code that will produce high-fidelity spatial resolution for an entire nuclear reactor is daunting for many reasons. Many safety-significant parameters are required on the fine-mesh solution (peak pin power, peak clad temperature, etc.) and these can expand further with advanced reactor designs (peak fuel particle temperature). In addition, for coupling with other physics, such as a CFD and heat transfer code, it is imperative that we know the solution on the fine-mesh, unstructured-grid geometry (i.e. we cannot homogenize materials).

Tabulating a Monte Carlo solution on an unstructured-mesh has been explored [16], but has not been applied for a billion-mesh geometry and would likely overload memory requirements and lead to excessive execution times due to the additional overhead. Continuous-energy Monte Carlo methods are also challenged by the memory requirements when hundreds of isotopes are utilized at many different temperatures.

Structured-grid Cartesian-mesh transport solvers have been shown to be robust and readily available for high-performance computing, but would require substantially more mesh, with respect to an unstructured-grid, to accurately resolve the geometry of air-gaps and cladding in nuclear reactors with a Cartesian block mesh.

The geometric size of many materials in the core are very small (such as cladding thickness and air-gaps), therefore complete resolution of the geometry will always result in a fine-spatial mesh. However, each of these cells tends to be very small in optical thickness (well under one mean-free-path). Therefore, even low-order of accuracy methods, such as step characteristics, generally produce highly accurate solutions.

4.1.2 Reduced memory requirements

The geometry and energy resolution requirements lead to a memory-limited problem. Therefore, nuclear reactor simulations require a method that will minimize the memory requirements, especially for problems with hundreds (or thousands) of energy groups (or points).

The Method of Characteristics has been used in lattice physics codes with great success because information is stored on a coarse, angle-integrated mesh (often with the exact spatial representation). This coarse, angle-integrated mesh can include re-entrant surfaces (the entire air-gap can be a single cell), because the inversion of the angle-dependent streaming plus collision operator may be performed on an angle-dependent fine mesh structure (this will be discussed further in Section 4.2).

4.1.3 Accuracy in Near-Voids

Many advanced nuclear reactor designs, both fast and thermal, utilize gas (BWR, GT-MHR, GFR) as a coolant and almost all designs must consider multi-phase coolant flow in a transient scenario. Therefore, it is imperative that a general reactor analysis tool be accurate and efficient in the presence of a near-voided material – an inherent limitation in any method that uses the 2nd order (even/odd-parity) form of the transport equation.

4.2 The Slice-Balance Approach and Method of Characteristics

The Method of Characteristics and Slice-Balance Approach separate the right-hand side (RHS) and left-hand side (LHS) of the transport equation and solve their equations on an independent (though hierarchical) mesh. The scalar flux and higher order angular moments that are used to calculate the source for a given ordinate direction are stored on a substantially reduced mesh, as compared to the mesh on which that the angular flux is being calculated.

The Method of (Long) Characteristics produces a fine angular dependent mesh by placing a series of rays that track across the domain and are calculated using a characteristics approximation from the incident to the exiting boundary of the angle-integrated coarse-mesh (defined by the exact geometry). The Method of (Long) Characteristics then uses a step approximation perpendicular to the direction of travel for the volume integration and restriction to the coarse angle-integrated mesh, thus it does not solve the problem on the exact geometry, but merely stores information based on the exact geometry. The Method of (Long) Characteristics (generally) creates global rays that track from one boundary surface to another (though it is not required). Therefore, if one domain of the problem requires a fine distribution of rays, then that fine-mesh must be propagated across the entire domain.

The Slice-Balance Approach meshes the exact geometry with an arbitrary polyhedral mesh, rather than the exact geometry. The fine angular-dependent mesh is formulated as a subset of the polyhedral mesh and the volume integration and restriction to the coarse angle-integrated mesh is performed with a trapezoidal approximation, rather than step. This allows for a substantially more coarse angle-dependent mesh. In addition, the mesh is derived locally, so refining the mesh in one region does not affect the global mesh – greatly simplifying adaptive mesh refinement techniques. A more comprehensive comparison of the Slice-Balance Approach with the Method of Characteristics is provided in reference [17].

Therefore, NEWTRNX utilizes the Slice-Balance Approach. The initial implementation is based on a step-step characteristics approximation where the analytic solution in a slice is calculated with an average incident surface flux and source and produces an average solution in the slice and on the exiting surface. The initial geometry generation package that has been implemented produces a tetrahedral mesh. However, we are in the process of implementing a linear-linear characteristics method and will soon begin to solve on an arbitrary polyhedral mesh.

4.3 Initial results

We have developed a series of test problems for initial verification and version control testing. Many test cases have been developed and analyzed with simple geometries to ensure that analytic solutions are reproduced for infinite medium k-eigenvalue and source-driven problems. In addition, symmetry and conservation principles are ensured. We are in the process of performing a comparison of results with KENO-VI [18] (multi-group Monte Carlo) using identical cross sections from SCALE for a set of problems on a more realistic geometry – the results of which will be presented at the conference and published in a future journal article.

5. Conclusions and Future Direction

A multi-laboratory, multi-university collaboration has formed to advance the state-of-the-art in high-fidelity, coupled-physics simulation of nuclear energy systems. Through united Laboratory Directed Research and Development funds at INL and ORNL, along with a grant from the Science Alliance at the University of Tennessee, we are embarking on the first-phase in the development of a new suite of simulation tools dedicated to the advancement of nuclear science and engineering technologies. We seek to develop and demonstrate a new generation of multi-physics simulation tools that will explore the scientific phenomena of tightly-coupled physics parameters within nuclear systems, support the design and licensing of advanced nuclear reactors, and provide benchmark quality solutions for code validation. In this paper, we have presented the general scope of the collaborative project and discuss the specific challenges of high-fidelity neutronics for nuclear reactor simulation.

High-fidelity neutronics simulation entails solving the neutron transport problem with an accurate representation of the entire nuclear reactor geometry and utilizing the temperature-modified point-wise nuclear data directly. This leads to a minimum of 10^{13} angle-integrated unknowns, which will require at least peta-byte memory storage. Therefore, the grand computers of tomorrow will be able to simulate transport of neutrons within the entire nuclear reactor geometry to produce a fine-spatial mesh solution that may be coupled with other physics.

The SCALE code system is an exceptional foundation to integrate within a coupled physics simulation suite because of the NRC-qualified multi-group cross section and depletion/decay codes that have been rigorously tested and qualified for an array of applications. Modifications have been made to a limited number of routines to integrate the required code suite within a single FORTRAN module so that NEWTRNX, or any other transport code, may call the SCALE cross section generation sequence as a subroutine. Therefore, our code suite is able to utilize the NRC-qualified nuclear data processing, which includes a double-heterogeneity treatment.

NEWTRNX is a new 3-D, general-geometry, discrete-ordinates transport solver, based on the Slice-Balance Approach and designed specifically for high-performance computing architectures. It has been designed to minimize memory storage requirements and initial testing has shown excellent agreement with simple test problems with analytic solutions. Advanced acceleration methods, a higher-order solver, and a more general-geometry capability will be implemented in the following year.

In conclusion, the Global Nuclear Energy Simulator for Reactors (GNES-R) team is embarking on a long-term simulation development project that encompasses multiple laboratories and universities for the expansion of high-fidelity coupled-physics simulation of nuclear energy systems.

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