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Applications of the 3-D Deterministic Transport Attila® for Core Safety Analysis

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An LDRD (Laboratory Directed Research and Development) project is ongoing at the Idaho National Engineering and Environmental Laboratory (INEEL) for applying the three-dimensional multi-group deterministic neutron transport code (Attila®) to criticality, flux and depletion calculations of the Advanced Test Reactor (ATR). This paper discusses the model development, capabilities of Attila, generation of the cross-section libraries, and comparisons to an ATR MCNP model and future.

1.0 Introduction

The Idaho National Engineering and Environmental Laboratory operates and maintains the Advanced Test Reactor (ATR) for the Department of Energy (DOE). The ATR has produced much of the world's data on material response to reactor environments. It has nine flux traps in its core and achieves a close integration of flux traps and fuel by means of the serpentine fuel arrangement shown in Figure 1.0.

The ATR fuel region resembles a four-leaf clover (Figure 1.0 The nine flux traps within the four corner lobes of the reactor core are almost entirely surrounded by fuel, as is the center flux trap position. The remaining four flux trap positions have fuel on three sides. Experiments can be performed using test loops installed in some flux traps with individual flow and temperature control, or in reflector irradiation positions using the primary fluid as coolant. The serpentine fuel arrangement allows a closer proximity of the fuel to the test loops than is possible in a rectangular grid configuration. Five of the flux traps are equipped with independent test loops and four are used for drop-in capsules. Four of the independent test loops are pressurized water loops through which water circulates at pressures up to 2,500 psi. The fifth loop is used for increased temperature and pressure up to 680°F and 3,800 psi. Sample capsules are also irradiated in vertical holes in the neck shim housing, center flux trap baffle, beryllium reflector, and racks located on the outside of the reflector.

The ATR uses a combination of rotational control cylinders (shims), and neck shim rods that withdraw vertically to adjust power while maintaining a constant axial flux profile. The 16 shims (operated in four groups of four) are beryllium cylinders in the beryllium reflector surrounding the core. The shims have plates of hafnium (a neutron absorber) on 120 degrees of their outer surfaces. Rotating the hafnium away from the core raises the reactor power. The effect is uniform along the vertical dimension of the core. By independently positioning the shims, large power variations among the nine flux traps can be performed.

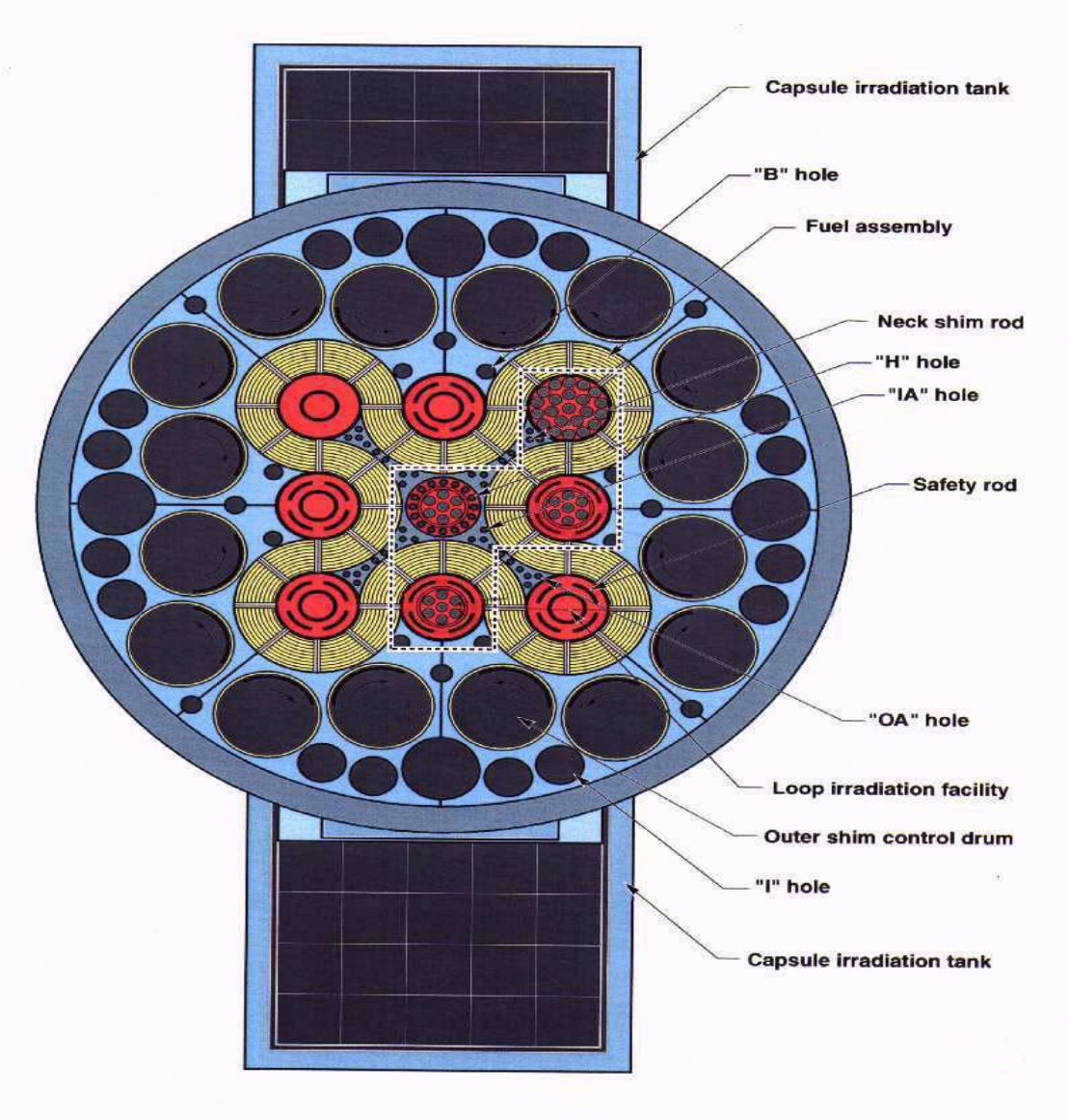

Figure 1.0 ATR Core Horizontal Cross-Section View

The power level (or neutron flux) of the flux trap positions in ATR can be adjusted for irradiation requirements. Each power level can be operated in steady state or varied during the cycle of operation. The arrangement of fuel around the flux traps results in focused irradiation of the experiments, saving testing time. Effects from years of irradiation in a normal power reactor can be duplicated in months or even weeks. Between fuel cycles, vary in duration from 2 to 60 days, test capsules can be irradiated, inserted or removed from the reactor. Maximum total power is 250 MW (thermal) in ATR. Balancing maximum ATR full power distribution results in as much as 50 MW produced in each lobe. Power shifting allows for a maximum and minimum lobe power of 60 and 17 MW.

2. Model Development

Geometric and material information for the Attila model, which includes atom mixture densities and atom fractions, were obtained from ATR core calculations using the ATR MCNP [1] model. Geometry parameters for the Attila calculations were generated using Solidworks®, a computer aided design (CAD) system. The CAD assembly allowed test section modifications and control drum (shim) rotations. The ATR Attila model included the structure of the reactor on the top, bottom and perimeter of the reactor core. In order to compare the Attila ATR model with MCNP, the 19 radial plate fuel elements were homogenized into 3 radial sections. The CAD assembly was exported to Attila through the Parasolid® format. Attila preserves the original CAD component names in the translation, aiding the assignment of region-wise material properties. Attila's graphical user interface (GUI) was used for the full analysis, including mesh generation, material assignments and the creation of post processing edits. The code can be executed in the GUI setup or separated as a solver. The computational model for Attila included approximately 2 million tetrahedral elements with 13-16 axial layers, since the mesh is unstructured. Figures 2.0 and 3.0 provide illustrations of the solid geometry for the ATR and the computational mesh.

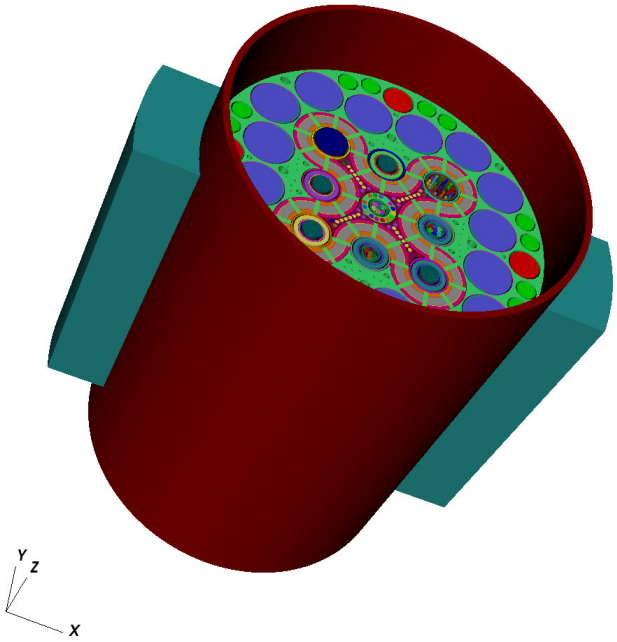

Figure 2.0 ATR Solid Geometry

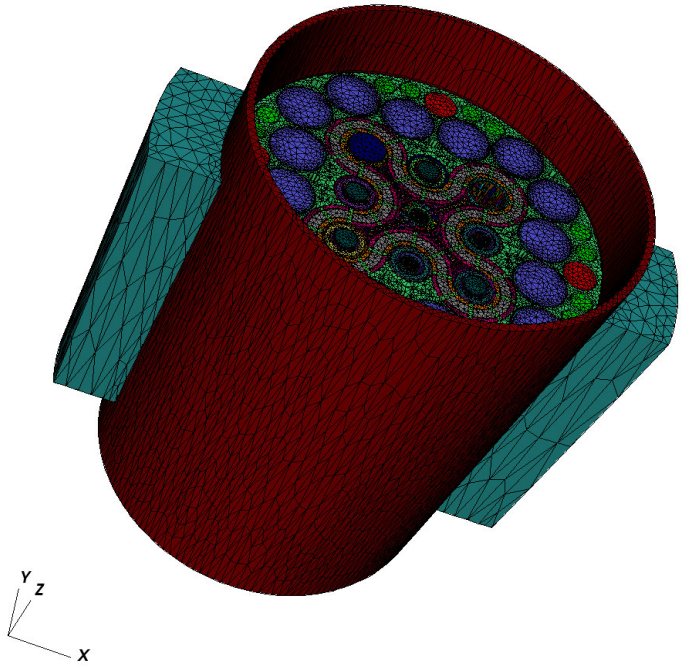

Figure 3.0 Computational Mesh

3.0 Attila Problem Solving Capabilities

Attila uses the standard first order steady state form of the linear Boltzmann Transport Equation (BTE) [2]:

$$\frac{d}{ds}\psi\left(\vec{r},E,\hat{\Omega}\right)+\sigma_t\left(\vec{r},E\right)\psi\left(\vec{r},E,\hat{\Omega}\right)=Q_S\left(\vec{r},E,\hat{\Omega}\right)+Q_f\left(\vec{r},E,\hat{\Omega}\right)+q\left(\vec{r},E,\hat{\Omega}\right) \qquad (1)$$

where

$$Q_S\left(\vec{r},E,\vec{\Omega}\right)=\int_0^\infty\int_{4\pi}\sigma_s\left(\vec{r},E'\rightarrow E,\ \hat{\Omega}\circ\hat{\Omega}'\right)\psi\left(\vec{r},E',\hat{\Omega}'\right)d\hat{\Omega}'dE' \qquad (2)$$

and

$$Q_f\left(\vec{r},E,\vec{\Omega}\right)=\frac{\chi(E)}{k}\int_0^\infty\nu\sigma_f\left(\vec{r},E'\right)\int_{4\pi}\psi\left(\vec{r},E',\hat{\Omega}'\right)d\hat{\Omega}'dE' \qquad (3)$$

where ψ denotes the angular flux, d/ds is the directional derivative along the particle flight path, $\hat{\Omega}$ is a unit vector denoting the particle direction, σ_t denotes the total macroscopic interaction cross section (absorption plus scattering), σ_s denotes the differential macroscopic

scattering cross section, χ is the fission spectrum, σ_f denotes the fission macroscopic cross section, ν is the mean number of fission neutrons produced in a fission and q denotes a fixed source.

In Cartesian coordinate systems d/ds can be expressed as $\hat{\Omega} \circ \nabla$. Using this substitution equation (1) is:

$$\hat{\Omega} \circ \nabla \psi\left(\vec{r}, E, \hat{\Omega}\right) + \sigma_t\left(\vec{r}, E\right)\psi\left(\vec{r}, E, \hat{\Omega}\right) = Q_S\left(\vec{r}, E, \hat{\Omega}\right) + Q_f\left(\vec{r}, E, \hat{\Omega}\right) + q\left(\vec{r}, E, \hat{\Omega}\right) \quad (4)$$

This is the basic form of the transport equation solved by Attila. Attila uses multi-group energy, discrete-ordinate angular discretization and linear discontinuous finite-element spatial differencing (LDFEM). Based on user-supplied input, these equations are solved to produce a particle distribution function in space, angle, and energy. From this particle distribution function, user edits can be produced as desired. The LDFEM spatial discretization is third-order accurate for integral quantities and provides a rigorously defined solution at every point in the computational domain. Since it allows for solution discontinuities between element faces, LDFEM will capture sharp gradients with a much larger element size than would be needed for lower order S_n methods. The general solution technique within Attila is source iteration. Source iteration can converge slowly for problems where scattering is dominant, a known problem for discrete-ordinates methods. To mitigate this, Attila incorporates an efficient diffusion synthetic acceleration (DSA) algorithm which can greatly reduce the number of iterations required for convergence and hence can significantly reduce the CPU time for problems with substantial within-group scattering. Both k-eigenvalue and fixed source modes are supported, including coupled neutron-gamma calculations.

4.0 Cross-Section Libraries

The COMBINE [3] code was used to develop a four group ENDF-5 and ENDF-6 set of cross-section libraries for Attila in Data Table Format (DTF). All data processing with COMBINE used an ATR energy spectrum combining the fast and thermal regions in COMBINE. Resonance treatment was used for those materials that have resonance data in the ENDF-5 and ENDF-6 cross-section sets. A Fortran program was written to place the selected ANISN output format for cross-sections in DTF. Testing was performed on the cross-section libraries for assurance of reasonable values compared to the Hansen-Roach cross-section library and comparisons using the Venus Reactor test provided with Attila. Radion Technologies also supplied two cross section sets that are being used for comparisons.

5.0 Calculations

The calculations presented here incorporate 4 energy groups, 24 angular (S_4 quadrature) unknowns, and 4 spatial unknowns per cell. This results in over one billion unknowns solved in the complete model. A 2-CPU AMD Opteron was used for the k_{eff} (eigenvalue) and flux distribution calculations. The k eigenvalue typically converges in five outer iterations, which takes approximately 5 hours on the Opteron for the two million-cell model.

6.0 Comparison to the ATR MCNP Model

The goal of this project is a comparison of the Attila ATR model to that of the MCNP model. To this end, values for the atom fractions and densities were taken from the MCNP input deck, placed on a spreadsheet and used in the Attila input. The COMBINE generated

four-group library was limited to natural instead of isotopic values for some elements. In addition, some of the geometric regions were “lumped” in order to obtain results in a reasonable amount of time. The eigenvalue generated by Attila was 1.029 for 20 outer iterations compared to 1.001198 for MCNP. MCNP uses a continuous cross-section library while Attila has been limited to four groups for this comparison. Figures 4.0 and 5.0 illustrate the total flux distribution for a top and axial view.

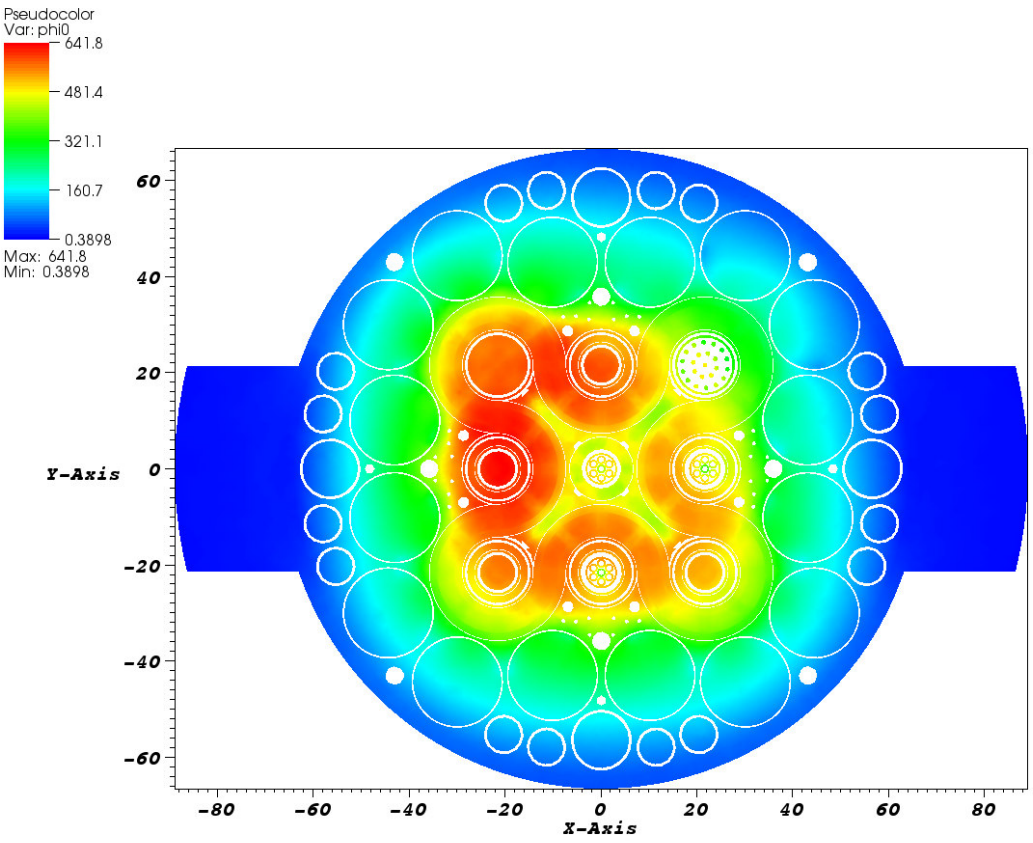

Figure 4.0 Top Cross-Sectional View of Flux Distribution

It should be noted that the plots in Figures 4.0 and 5.0 are node based contours derived from cell-wise average values, and they are intended more for qualitative analysis than for rigorous data extraction. The plots in this report were constructed using Visit[4], a plotting package available from LLNL.

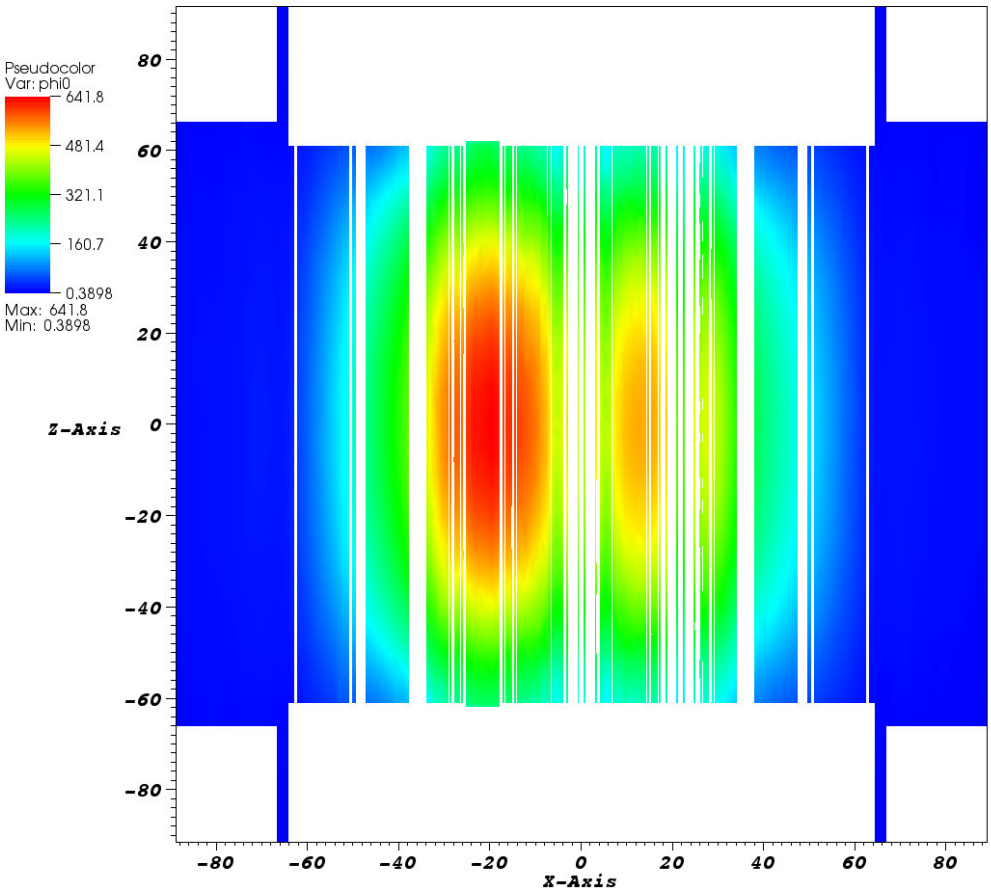

Figure 5.0 Axial View of Total Flux

7.0 Future Work

For complete cycle analysis a safety analysis code must perform isotope depletion computations. INEEL is presently collaborating with Radion Technologies to implement this capability into Attila.

A new nuclear transmutation code "Fornax" (Latin for "laboratory furnace") has been written by Radion Technologies (~13,000 lines of C++). This code is based on the algorithms and methods used in the ORIGEN transmutation code developed at ORNL. Links between Fornax and the Attila transport code have been implemented (~1500 lines of F90). Initial testing has been completed with good results. Burn problems are controlled through a few simple keywords in the Attila input deck. Attila calls Fornax on behalf of the user and the results are stored in a separate directory for each time-cycle.

Fornax Capabilities

Fornax solves the fully coupled equations for the production, depletion, and decay of nuclides using a series expansion approximation to the matrix exponential solution. Short time constant products are treated separately using the same algorithm as in the ORIGEN code. Fornax independently tracks an arbitrary number of isotopic atom densities for actinides, fission products and activation products. A single input XML file describes the nuclear properties of each participating nuclide, including cross sections for [(n,2n), (n,3n), (n, gamma), (n,d), (n,t), (n,a), (n,f)] reactions, half-lives (with branching fractions for negatron-positron decay, alpha decay, internal transition and spontaneous fission), and fission product yields.

Fornax supports an arbitrary number of fissile species. Separate data for up to 99 metastable states are supported for a given nuclide. Default data for 1307 nuclides, including half lives, three group reaction cross sections, and fission product yields are provided in an XML data file (fornax.xml, 30,000 lines) based on an ORIGEN-S data set. Options are provided to specify a replacement data file of the user's choice, as well as to replace cross sections with multi-group data from the Attila Data Table Format (DTF) file.

Special DTF cross sections files were developed to support the burn, including detailed KERMA values for power normalization and cross sections for the individual capture reactions. For representative problems Fornax typically solves 20-75 burn zones per second on a single CPU 2.0 GHz Athlon Linux system.

Attila Capabilities – Depletion

Attila Links to the Fornax transmutation code via an isotopic atom density file and a flux file. It calls Fornax on behalf of the user and burns each cell in a problem independently using cell specific atom densities and spatial and energy flux shape without "burn-zone" averaging. Fornax is extremely accurate in space and energy with the ability to specify an arbitrary number of duration and power level time cycles, including "zero-power" cycles to simulate cool-down periods. Its material assignments can be changed during the course of a problem in order to simulate shim motion and changing Boron shim concentrations. The results are stored for each time cycle in a separate directory. The user can specify which time cycle directories to retain in order to conserve disk space. Fornax automatically calculates new flux shapes in space and energy at every cycle or configuration change. It normalizes results to the user specified power levels using KERMA data from a cross section set for a link to Fornax. Fornax provides for an edit of results and data at every time cycle. The user can specify any of the usually available Attila edits, as well as new edit capabilities that allow for the display of any isotopic atom density in the problem.

Documentation

The Attila user’s manual contains a new chapter, Chapter 11, entitled “Transmutation" that describes the setup and execution of burn problems in tandem with Fornax. New input keywords and arguments for control of the burn options are described in detail. A Fornax manual is currently under preparation.

Testing

The unit testing on Fornax is complete. Perfect agreement has been obtained when Fornax is compared with analytic results on a spreadsheet. Integration testing of Fornax with Attila has also been completed. A comparison of Fornax with SCALE results are within a few percent for simple single pin problems of both high and low enriched Uranium. BUCR1B NEA light water reactor benchmark problems are producing reasonable results.

8.0 Summary

In summary, preliminary results indicate the feasibility of using the Attila deterministic transport code for core safety analysis. Through a combination of CAD based modeling and arbitrary body fitted tetrahedral elements, the capability of Attila to efficiently model reactors having highly complex geometries has been verified. Flux profiles and core eigenvalues computed with Attila for an ATR reference case compare favorably to other codes using a four-group cross-section set.

Acknowledgements

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