



INEEL/CON-04-1628
PREPRINT

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April 25 – 29, 2004

PHYSOR2004

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Investigating the Use of 3-D Deterministic Transport for Core Safety Analysis

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Abstract

An LDRD (Laboratory Directed Research and Development) project is underway at the Idaho National Laboratory (INL) to demonstrate the feasibility of using a three-dimensional multi-group deterministic neutron transport code (Attila[®]) to perform global (core-wide) criticality, flux and depletion calculations for safety analysis of the Advanced Test Reactor (ATR). This paper discusses the ATR, model development, capabilities of Attila, generation of the cross-section libraries, and comparisons to experimental results for Advanced Fuel Cycle (AFC) concepts, and future work planned with Attila.

1. Introduction

The Idaho National Laboratory maintains and operates the Advanced Test Reactor (ATR). The ATR began operation in 1967 and is expected to continue operating for several decades. The ATR is the world's premier test reactor, offering high thermal neutron flux and large test volumes for performing irradiation services. A major spin-off is the production of radioisotopes for medical, industrial, environmental, agricultural, and research applications. It has produced much of the world's data on material response to reactor environments. The ATR was originally designed to study the effects of intense radiation on reactor material samples, especially fuels. 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.

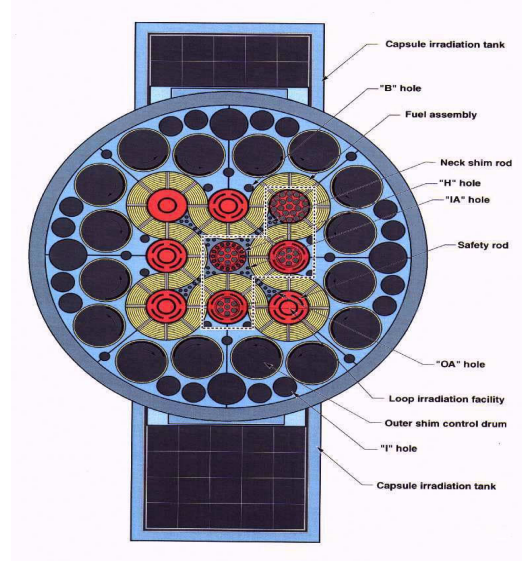


Fig. 1. Horizontal Cross-Section View of ATR Core

As shown above, the ATR fuel region resembles a four-leaf clover. There are nine flux trap positions, which are used as the test regions. The 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.

One of the advantages of the ATR is the precision with which the power level (or neutron flux) can be controlled for the individual test positions. The ATR uses a combination of control cylinders, which rotate, and neck shim rods, which withdraw vertically to adjust power. The 16 control cylinders (operated in four groups of four) are beryllium cylinders in the beryllium reflector surrounding the core. The cylinders have plates of hafnium (a neutron absorber) on 120 degrees of their outer surfaces. Power is raised by rotating the hafnium away from the core, the effect is uniform along the vertical dimension of the core. By independently positioning the control cylinders, large power variations among the nine flux traps are possible.

The ATR's power level (or neutron flux) can be adjusted at the various flux trap positions to meet irradiation requirements, each of which can be varied or held steady during the operation cycle. The efficient arrangement of fuel around the flux traps allows intense irradiation of experiments, saving time in testing. As a result, effects from years of irradiation in a normal power reactor can be duplicated in months or even weeks in the ATR. Between each fuel cycle, which is approximately 42 days, test capsules can be inserted or removed from the reactor. The maximum total power is 250 MW (thermal). With a balanced maximum ATR full power distribution, 50 MW would be produced in each lobe. However, power shifting allows for maximum and minimum lobe powers of 60 and 17 MW, respectively.

2.0 Model Development

The geometric and material information for the Attila model, including initial atom mixture densities and atom fractions, was obtained from previous ATR core calculations using MCNP [1]. The geometry for the Attila calculations was generated using Solidworks®, a widely used solid-modeling computer aided design (CAD) system. The CAD assembly was parametrically created to facilitate both test section modifications and control drum repositioning. The model included 12 inches of water on the top, bottom and perimeter of the reactor core. To compare with previous simulations, the 19 radial plate fuel elements were homogenized into 3 radial sections. In all cases, the CAD assembly was exported to Attila through the Parasolid® format. Through this process, Attila preserves the original CAD component names in the translation, which facilitates the assignment of region-wise material properties. The Attila graphical user interface (GUI) was used for the full analysis setup, including mesh generation, material assignments and the creation of post processing edits. The computational model for Attila included approximately 3 million tetrahedral elements with 27 axial layers. Figures 2 and 3 provide illustrations of the computational mesh used for the analyses.

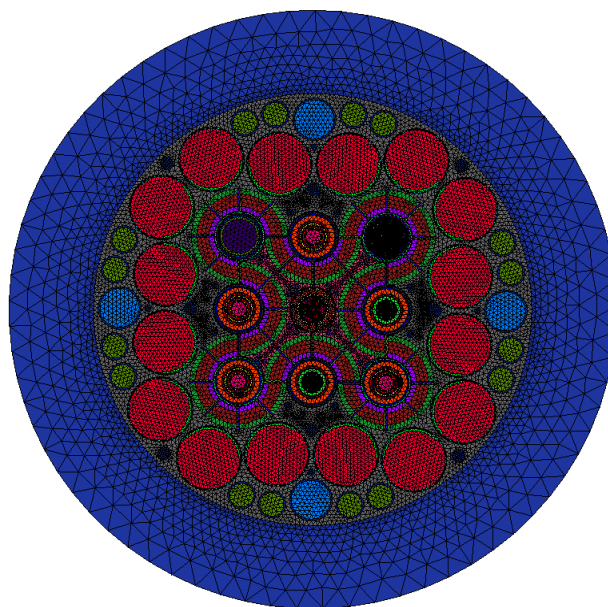


Fig. 2. Attila computational mesh

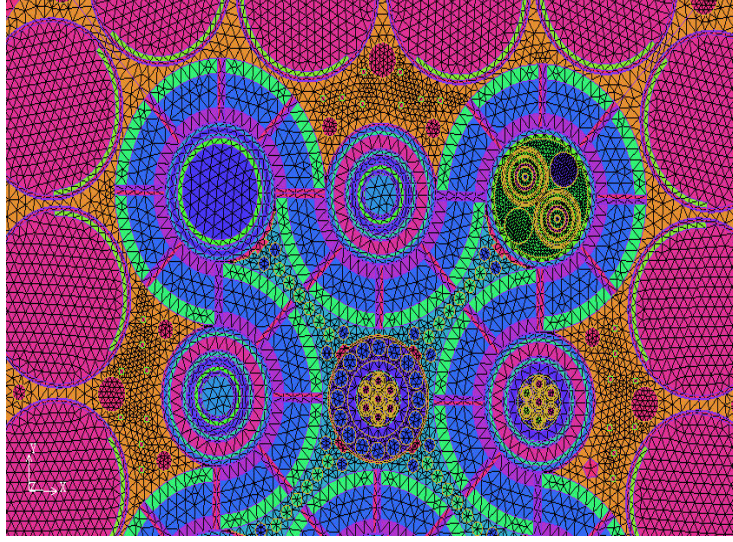


Fig. 3. Close-up of the Attila computational mesh

3.0 Attila Problem Solving Capabilities

Attila solves the standard first order form of the steady state, linear Boltzmann transport equation [3]:

$$\frac{d}{ds} \psi(\vec{r}, E, \hat{\Omega}) + \sigma_t(\vec{r}, E) \psi(\vec{r}, E, \hat{\Omega}) = Q_s(\vec{r}, E, \hat{\Omega}) + Q_f(\vec{r}, E, \hat{\Omega}) + q(\vec{r}, E, \hat{\Omega}) \quad (1)$$

where

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

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

and where ψ denotes the angular flux, d/ds denotes 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 $\hat{\Omega} \circ \nabla$. Making this substitution equation 1 becomes:

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

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.

3.0 Cross-Section Libraries

The COMBINE [4] 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 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 ENDF5 and ENDF6 cross-section sets. A Fortran program was written to place the selected ANISN output format for cross-sections in DTF. Testing was done on the cross-section libraries to assure reasonable values compared to the Hansen-Roach cross-section library and comparisons using the Venus Reactor test provided with Attila.

4.0 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. Several hardware platforms were tested, including a Cray YMP and an AMD Opteron. For the Cray, the vectorized multiprocessor version of Attila run time was 10 hours. The single processor run time using the Opteron was approximately 17 hours.

5.0 Comparison to Experimental Data for the Advanced Fuel Cycle Test

The Advanced Fuel Cycle (AFC) test is part of the DOE Advanced Fuel Cycle Initiative (AFCI) launched in fiscal year 2003. A key roadblock to development of additional nuclear power capacity is the concern over the nuclear waste produced by the plants, which requires disposal. AFCI is developing the technology base for waste transmutation (the nuclear transformation of long-lived radioactive materials into short-lived or non-radioactive materials), and will demonstrate its practicality and value for long-term waste management.

The AFC test consisted of a Cadmium basket with additional materials for irradiation in the ATR in order to assess various designs for producing shorter-lived radioactive materials. The experiments irradiated in the ATR flux traps with an absorber filter, such as the Cadmium (Cd) basket can have a perturbation on the ATR core axial fuel power distribution. In order to assess this affect a separate experiment was performed in the ATRC (Advanced Test Reactor Core facility) in order to obtain axial flux data to ascertain that the experiment was in the safety limits for testing the AFC assembly in ATR. The ATRC is a low-power, full-size nuclear duplicate of the ATR, designed to test prototypical experiments before irradiation of the actual experiments in the ATR. The ATRC provides valuable reactor physics tests, including (a) control element worths and calibrations, (b) excess reactivities and charge lifetimes, (c) thermal and fast neutron distributions, (d) gamma heat generation rates, (e) fuel loading requirements, (f) effects of inserting and removing experiments and experiment void reactivities, and (g) temperature and void reactivity coefficients. The ATRC is a pool type reactor located in an extension of the ATR canal. Normal power level is about 100 W; maximum power is 5 kW. Thermal neutron distributions and fission rate values are obtained with the ATRC by measuring the activation of uranium-aluminum wires.

The purpose of analyzing the Advanced Test Reactor Critical Facility [ATRC] flux run data is to evaluate the potential impact the AFC test would have on the fuel axial profile in the Advanced Test Reactor. Experiments to be inserted in the ATR must be assessed to assure that the reactor safety basis is maintained. One of the parameters that is influenced by an inserted experiment is the axial fission profile in the ATR fuel. Experiments that could potentially impact the fuel performance are typically inserted and measured in ATRC prior to being approved for insertion at ATR. Acceptable axial fission profile results from ATRC measurements assure acceptable axial fission distributions in the ATR fuel when the reactor is operated with the associated experiment installed. The safety category that will govern the performance of the calculations for this analysis is 'safety significant', because the consequences of operation with the experiment must be bounded by the assumptions made concerning fuel performance in the ATR safety basis. This analysis is performed to provide assurance that the reactor response with the experiments inserted meets the established safety envelope. A cross-sectional view of the computational mesh used in the calculation is shown in Figure 4.

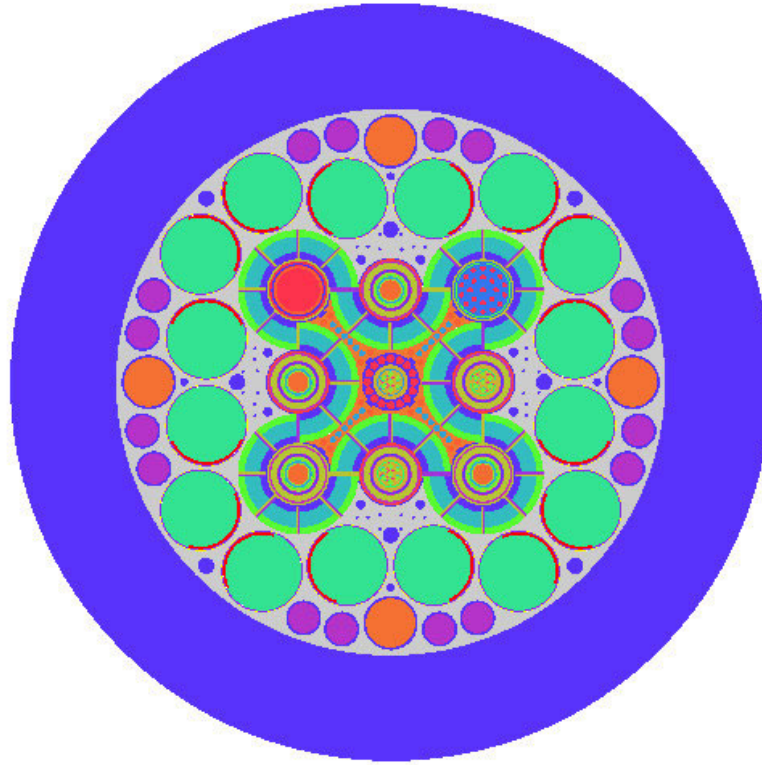


Fig. 4. Cross-sectional view of AFC test (computational mesh shown without grid lines)

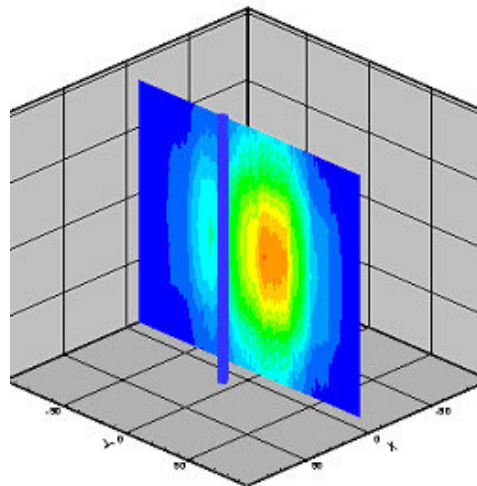


Fig. 5. AFC Test Flux Profile

Flux profiles for the Attila calculation are shown in Figures 5 and 6. The section plane in Figure 5 shows an axial cut through the AFC test section. It should be noted that the plots in Figures 5 and 6 are node based contours derived from cell-wise average values, and they are intended more for qualitative analysis than for rigorous data extraction.

The local to average flux values were compared for fuel element 22 channel 6 data, relatively close to the AFC Cadmium basket. Figure 7 shows a plot of experimental data from the AFC test in the ATRC compared to the Attila results.

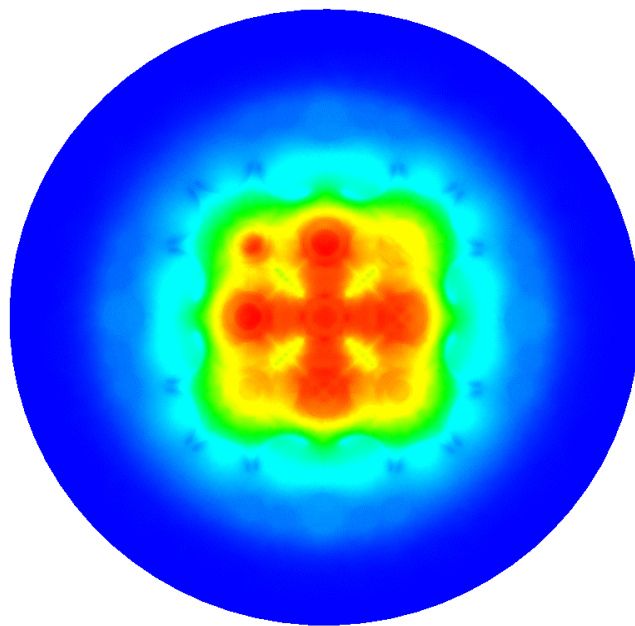
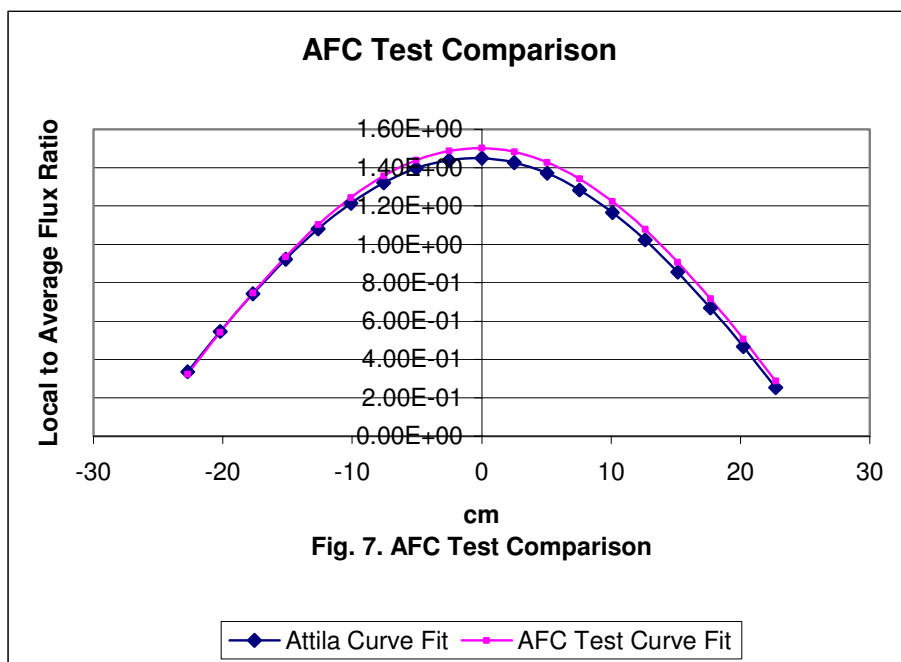


Fig. 6. Flux distribution



6.0 Future Work

For complete cycle analysis (ATR cycles run between 2 and 60 days in length), a safety analysis code must perform isotope depletion computations. INEL is presently collaborating with Radion Technologies to implement this capability into Attila.

7.0 Summary

In summary, preliminary results indicate the feasibility of using a three-dimensional 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 experimental results.

Acknowledgements

The authors wish to acknowledge Rick McCracken and Keith Penny of ATR and Robert Bush and Jerry Mariner of Bettis for their support of this work.

References

- 1) S. S. Kim and R. B. Nielson, "MCNP Full Core Modeling of the Advanced Test Reactor," NRRT-N-92-021, INEL, EGG Idaho Inc.
- 2) Attila User's Manual, Version 4.0
- 3) T. A. Wareing, J. M. McGhee, J. E. Morel, and S. D. Pautz, "Discontinuous Finite Element *Sn* Methods on 3-D Unstructured Meshes," Nuclear Science and Engineering, 138:1-13, 2001.
- 4) David W. Nigg, et. al "Combine/PC A Portable ENDF/B Version 5 Neutron Spectrum and Cross-Section Generation Program," EGG-2589, Rev. 1, February 1991.