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REACTOR SIMULATION WITH COUPLED MONTE CARLO AND COMPUTATIONAL FLUID DYNAMICS.

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ABSTRACT

This paper demonstrates the applicability of Monte Carlo analysis to perform nuclear reactor core simulations with thermofluid feedback from a computational fluid dynamics code. An interface program, McSTAR, was written to couple MCNP5 to the commercial computational fluid dynamics code STAR-CD. McStar is a Perl script which alternately executes MCNP5, STAR-CD and cross section update routines on multiprocessor Linux clusters. It also performs the necessary manipulations in the MCNP5 input and data files. Cross section libraries are generated using the sub-pin level temperature distribution calculated by STAR-CD, and MCNP input files are manipulated to reflect the moderator density distribution provided by STAR-CD. Using this feedback data, the MCNP simulation proceeds and determines the next approximation for the eigenvalue as well as the heat source distribution for the next CFD calculation. Several methods to update cross section library were investigated and are described in the paper. The coupled codes were tested using a single PWR pin-cell problem and 3x3 array of PWR fuel pins. The preliminary results are compared with those obtained from a STAR-CD calculation coupled with the deterministic transport code DeCART. Ongoing research is described to investigate more efficient acceleration and convergence methods, as well as more robust methods to validate the coupled calculation.

Key Words: Monte Carlo, thermal feedback, McStar, CFD, high-performance computing

1. Introduction

Increased computational capabilities and improvements in computational methods has accelerated interest in high fidelity modeling of nuclear reactor cores during the last several years. High-fidelity has been achieved by utilizing full core neutron transport solutions for the neutronics calculation and computational fluid dynamics solutions for the thermal-hydraulics calculation. Previous researchers have reported the coupling of 3D deterministic neutron

transport method to CFD and their application to practical reactor analysis problems [1,2,3]. One of the principal motivations of the work here was to utilize Monte Carlo methods to validate the coupled deterministic neutron transport and CFD solutions.
Previous researchers have successfully performed Monte Carlo calculations with limited thermal feedback. In fact, much of the validation of the deterministic neutronics transport code DeCART in [1,2,3] was performed using the Monte Carlo code McCARD [8] which employs a limited thermal feedback model. However, for a broader range of temperature/fluid applications it was desirable to couple Monte Carlo to a more sophisticated temperature fluid solution such as CFD. This paper focuses on the methods used to couple Monte Carlo to CFD and their application to a series of simple test problems.

2. Methods for Coupling MCNP and STAR-CD

In work here, the Monte Carlo code MCNP5 [4] was used to simulate the transport of neutrons through the system. Thermal-hydraulic feedback data was obtained from the commercial computational fluid dynamics (CFD) code STAR-CD [5], which solves the 3-D momentum and energy transport equations. Cross sections were generated by the NJOY [6] code using data from the CFD solution.

One of the principal decision in coupling multi-physics codes is choice of mapping of the fields and the mechanisms for data transfer. In the work here a simple approach was used in which an MCNP model was created with as many regions as CFD cells of the corresponding STAR-CD model. Each MCNP region represents a different material number and the flux or power is tallied separately in each region and matched to the CFD cell as a heat source. The one-to-one mapping is depicted in Figure 1.

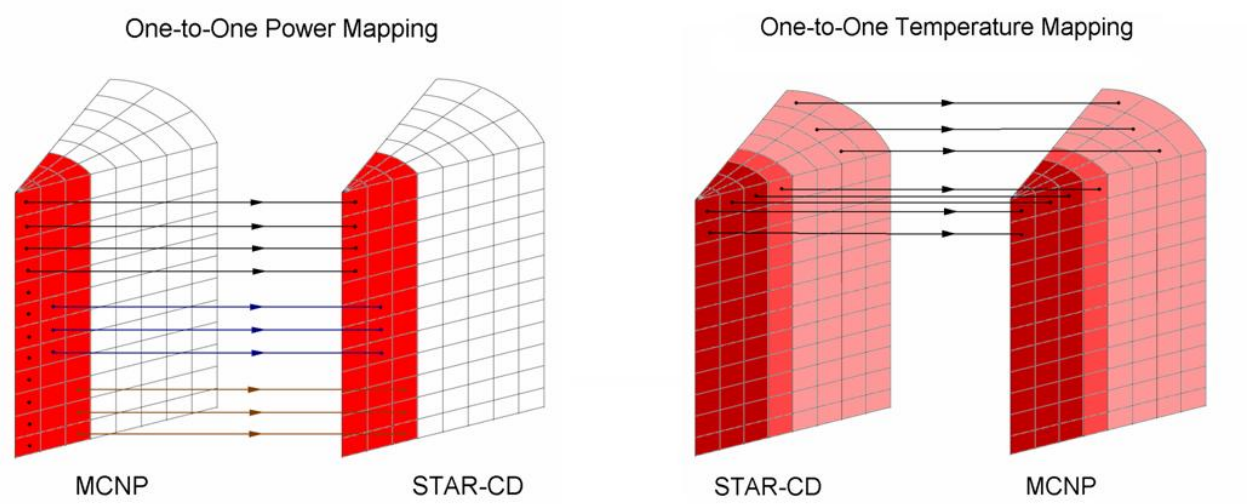


Figure 1: Data mapping

The cross sections that MCNP uses for the transport calculation are generated by the NJOY code from ENDF-B data in which the cross sections for each nuclide are stored in a table format with

continuous energy grid at a certain temperature. Once the temperature of each region is obtained in the MCNP model, the cross sections are then updated at the new temperature. The following section will describe the various methods investigated to treat the cross section update in McSTAR.

2.1. Cross Section Update

Three techniques for updating the cross sections with the available temperature field data were considered in this study. The most accurate way of updating the cross sections would be perform an NJOY calculation for each nuclide in each region at the temperature of that region. The second approach would be to pre-generate a library for each nuclide with a small temperature increment (2K-5K) between the range of minimum and maximum temperatures that can be observed during the calculations.[7] The cross section table having the temperature nearest the local region temperature would then be used in the calculation. The third technique would be to again pre-generate a library, but with a larger temperature increment (25K-50K). Then, with the use of an interpolation method the cross sections lying between the temperature intervals could be approximated. Although it is most accurate, the first option is not practical because of the excessive computation time required to generate a cross section for every nuclide at every temperature. The second option is the most practical and applicable of the three methods. However, there would be an inherent error depending on the size of the temperature increment.

The third option is also practical one and depending on the size of the temperature interval of the library, could potentially produce more accurate results than the second option. For example a library was used with a temperature increment of 50K for a single PWR pin problem. The interpolated cross sections resulted in only a 30pcm difference in eigenvalue from the same calculation performed with the cross sections generated by NJOY at the actual temperature.

2.2 McStar: The Coupling Interface

In order to perform the calculations described earlier, an interface program to couple the MCNP and STAR-CD codes was written. This program, which is named McStar, is a Perl script which alternately runs each of the three programs until the eigenvalue and flux are converged. McSTAR performs several necessary functions. After completing the update of the cross section library, a few manipulations to the MCNP input are performed in McSTAR to reflect the temperature effect in the Monte Carlo calculation. The “xsdir” file is rewritten with the new generated cross section identifiers, temperatures, library names and library paths. The MCNP input file is then modified by replacing the calculated temperatures and cross section identifiers with the previous ones. All these processes are performed in McSTAR.

Prior to the iterative coupled calculation, a standalone STAR-CD calculation is performed with an initial power profile to obtain an initial temperature distribution for the MCNP cross section library. MCNP is also run with a standard library to obtain an initial source file. The iterative calculation begins with the MCNP calculation in which tallies are normalized with the power given as an input and the distribution is written on “mcnp2star.dat” file. This file is then read by the user subroutines of STAR-CD to update the power profile in the CFD calculation. These user

subroutines also generate the "star2mcnp.dat" file which contains the temperature, density and volume of each cell along with cell indexes of MCNP and STAR-CD models. The information in this file is used to generate the new cross section library, and to update the MCNP input file with new densities and temperatures. To update the cross sections the user can choose either of the last two options described in the previous section.

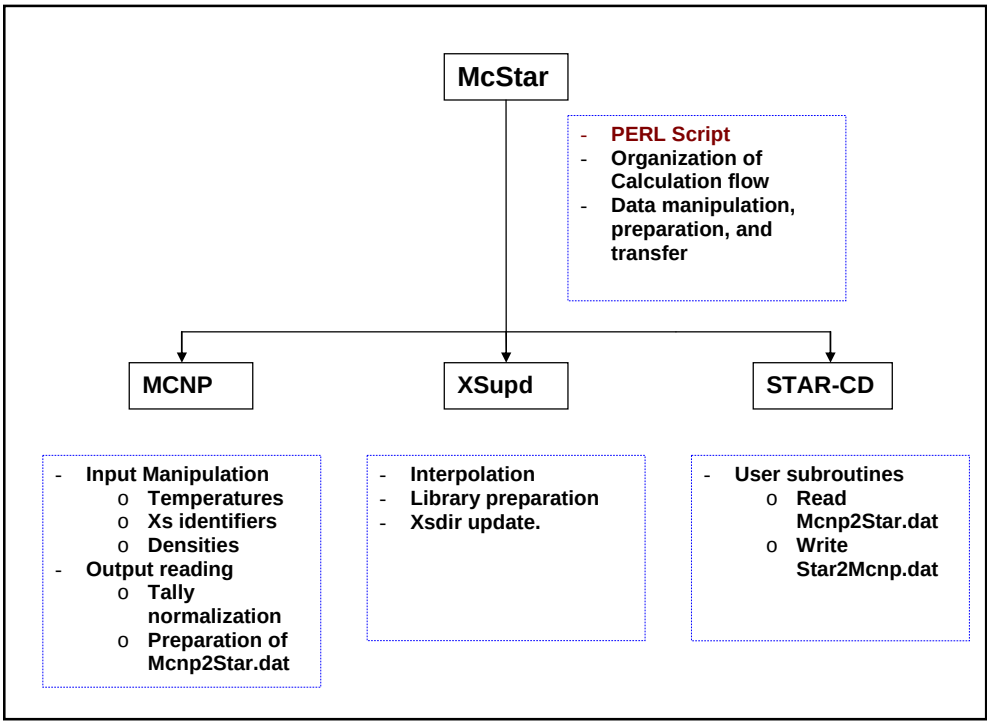


Figure 2. Calculation scheme

3. Example Problems

Two test problems were performed to investigate the methods developed here to couple MCNP5 and STAR-CD. A model of a single 3D PWR pin cell and then are a larger 3X3 array of PWR fuel pins were developed with both MCNP5 and STAR-CD. Initial comparisons were made with the same calculation performed using the deterministic code DeCART coupled to STAR-CD.

3.1. Problem I: A 3D PWR Pin Cell

The pin-cell model includes a UO_2 fuel pin with the surrounding coolant and moderating water. A1/8th symmetric 3D model was developed in both MCNP and STAR-CD as shown in Figure 3. The STAR-CD model consisted of 24 radial cells, 9 of which are in the fuel region and 600 axial cells. The number of radial cells was consistent in the STAR-CD and MCNP models. However, for simplicity the number of axial cells was reduced to 12.

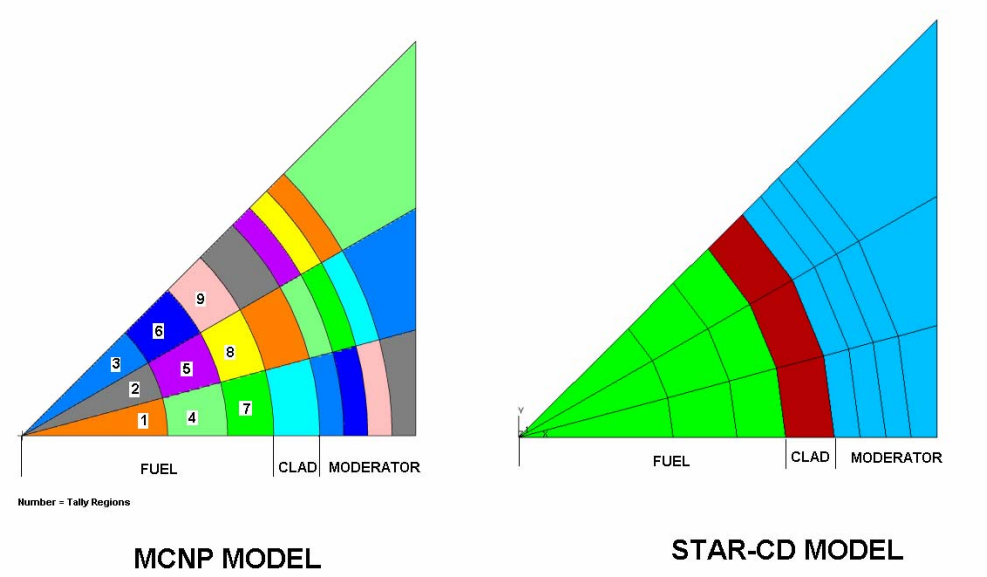


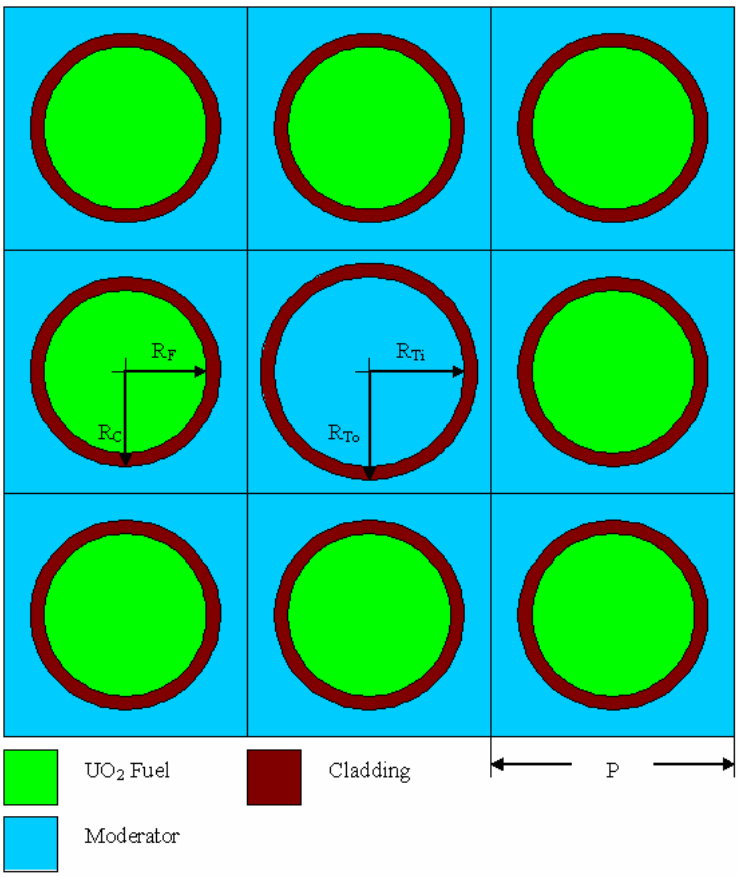
Figure 3. MCNP and STAR-CD models

All the fuel cells in the MCNP model are tallied to extract the power density for STAR-CD calculation. At each iteration of McSTAR, a total of 220 MCNP cycles were performed. Parametrics were performed on the number of histories per cycle to investigate convergence performance.

3.2. Problem 2: A 3x3 Array of PWR pins

The second model consisted of 8 UO_2 fuel pins surrounding a central guide tube as shown in Figure 4. The active fuel is 200 cm in height and with 20 cm of water above and below the active fuel. The cladding is zicaloy and the moderator is liquid water.

In the CFD model, the 240 cm height of the domain is discretized into 600 layers of 0.4 cm tall prismatic hexahedral cells. The discretization in the radial directions is the same for each layer (e.g., the same meshing is used in the reflector region and fuel region), with 2240 cells in each layer, yielding a total of 600 x 2240 = 1,344,000 CFD cells. The azimuthal meshing of the MCNP model is reduced to 8, furthermore, the axial meshing is again reduced to 12 in order to reduce the computational time. The total number of MCNP cells for this problem is 6720 with tallies performed in the 1920 cells located in the fuel region. Figure 5 shows the radial meshing of the STAR-CD and MCNP models.



R_F	Fuel pellet radius	0.4025 cm
R_C	Cladding outer radius	0.4759 cm
R_{Ti}	Guide tube inner radius	0.5709 cm
R_{To}	Guide tube outer radius	0.6130 cm
P	Cell pitch	1.2600 cm

Figure 4. 3x3 PWR Model Geometry

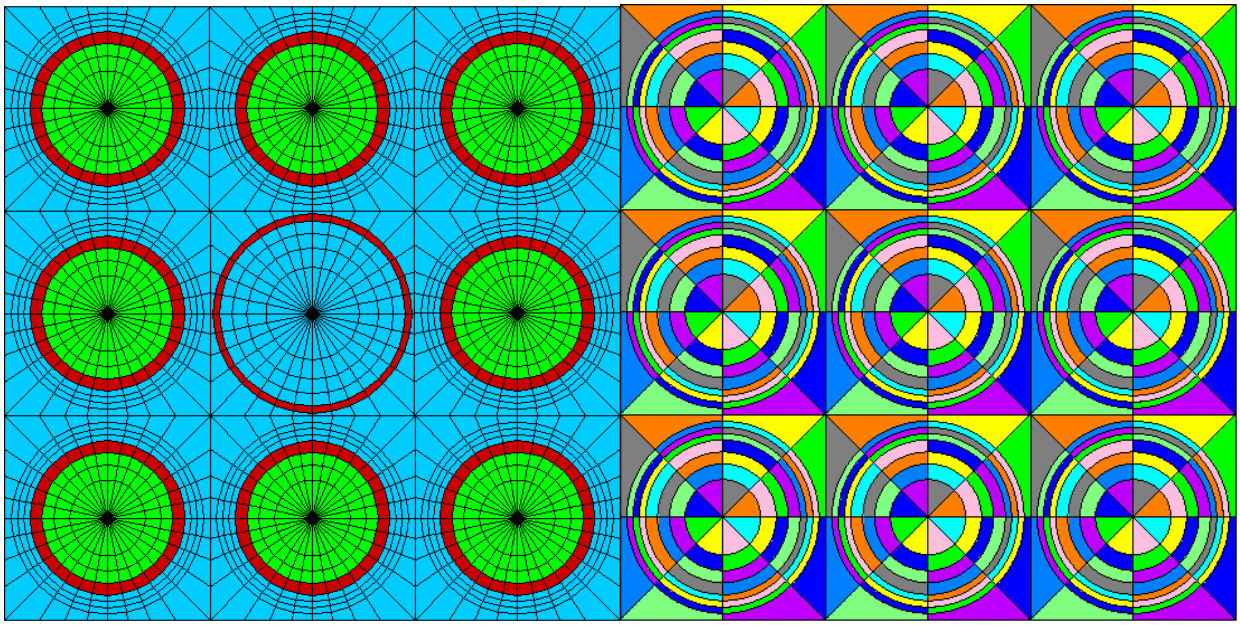


Figure 5. STAR-CD and MCNP Meshing for the 3x3 PWR Model

4. RESULTS

As a preliminary basis of comparison, the same test problems were modeled and analyzed with DeCART/ STAR-CD coupled code which has already been well validated for PWR applications [3].

4.1. Problem I:

A parametric study on the number of neutrons per cycle was performed to analyze the convergence behavior of the coupled calculation for Problem-1. Figure 6 shows the convergence of the eigenvalue for different numbers of iterations. As the number of histories is increased, the standard deviation of the eigenvalue decreases and a better convergence is obtained. The obvious disadvantage of using very high number of neutrons per cycle is that the run time is directly proportional to the number of histories. When 3 million histories were used in the MCNP calculation for the single pin cell problem, a total run time of 28 hours was required on 30 nodes with 3.4 GHz Pentium 4 processors on the ANL *Reserv* linux cluster.

As shown in Table-1 the eigenvalues calculated by McStar and DeCART/STAR-CD are in good agreement. The axial power density profiles of McStar and DeCART/STAR-CD, as shown in Figure-7, also compare well with each other.

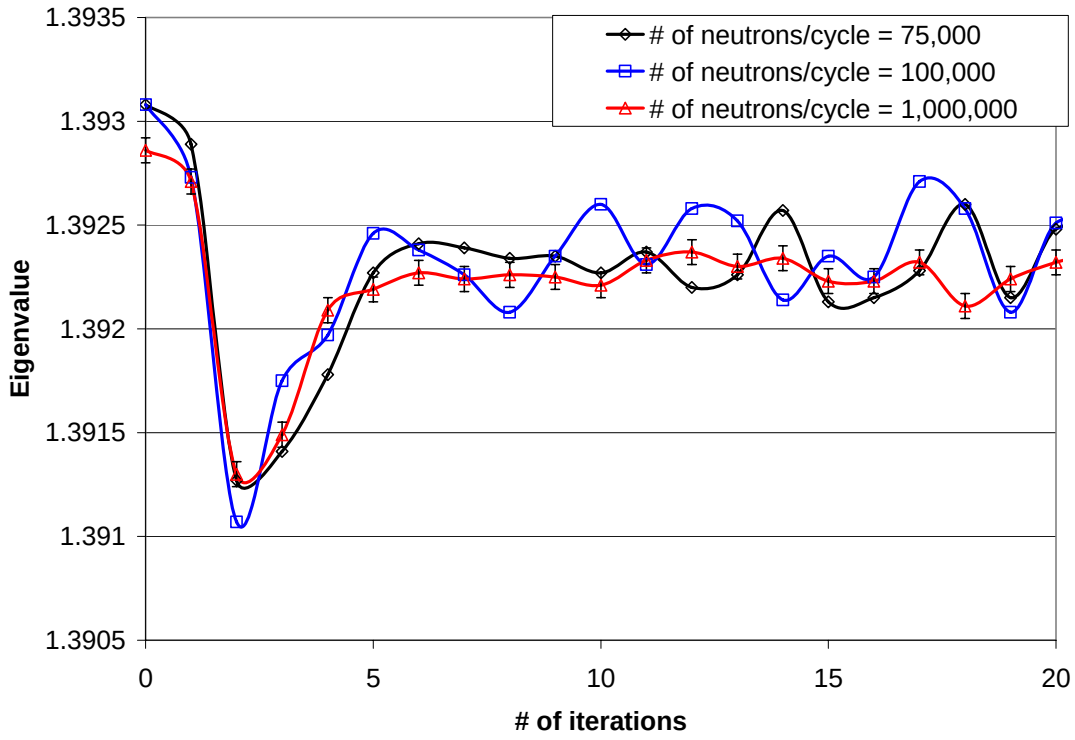


Figure 6. Convergence of eigenvalue for Problem-1

Table I. Eigenvalue comparison for Problem-1

Codes	k_{eff}
McSTAR	1.39224 (±0.00006)
Decart/StarCD	1.39276 (+52 pcm)

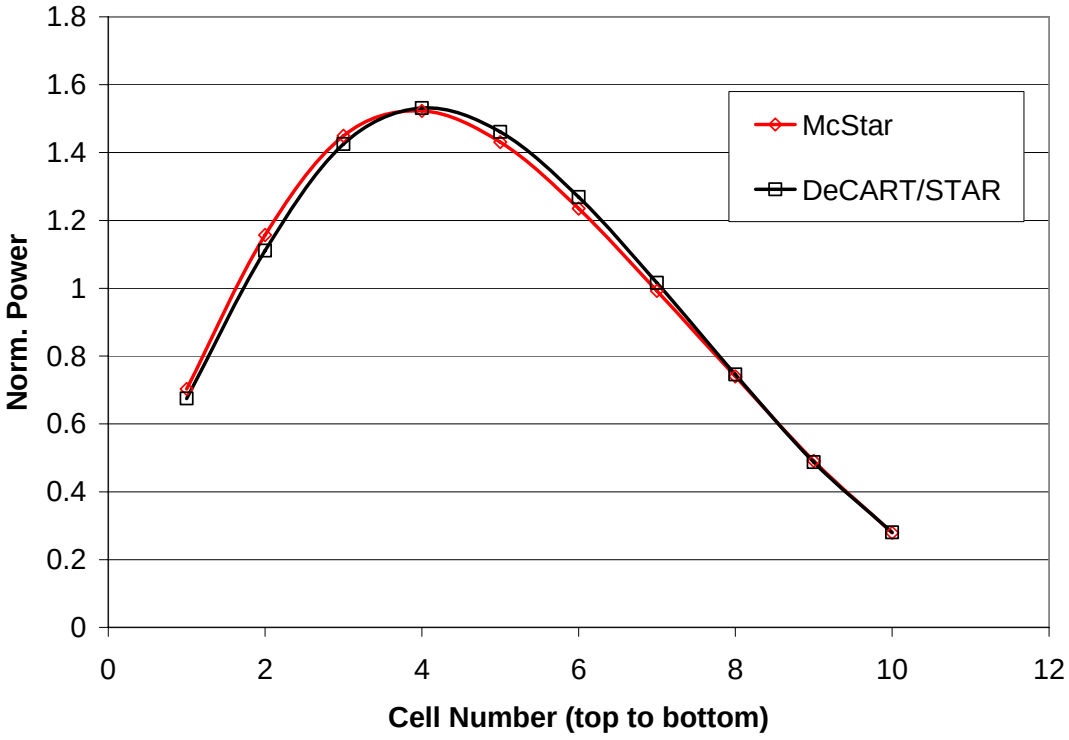


Figure 7 – Axial power density profile for problem 1.

4.2. Problem II:

The 3x3 problem was then performed with both DeCART-STARCD and McStar. The run-time for a single MCNP calculation with 300 active cycles and 500K neutrons per cycle is about 6 hours on 30 compute nodes of Purdue University's *Hamlet* linux cluster which consists of 3Ghz Pentium 4 processors with 2 GB memory. The total runtime for 12 iterations was about 100 hours.

In order to assess the adequacy of the temperature dependent cross section modeling in McSTAR, the 3x3 problem was first performed with a constant temperature distribution and

results were compared to the DeCART model. Table-2 compares the eigenvalue results of MCNP and DeCART at constant temperature. The eigenvalue calculated with MCNP is 74 pcm higher than one obtained with DeCART at constant temperature. Table-3 shows MCNP and DeCART results when coupled to STAR-CD. The difference in eigenvalues is consistent with the one obtained at constant temperature. The maximum power density difference between MCNP and DeCART at constant temperature is about 3.2% which is similar to the accuracy of the power density with a variable temperature which is about 4%. Figure 8 and 9 show the axial temperature and power profile for an inner pin cell calculated with McStar and DeCART/STAR-CD. As indicated there is a good agreement in the solutions.

Table II. Eigenvalue comparison for Problem-2 at fixed temperature

CODE	k_{eff} (3x3 pins) @300C
MCNP	1.42852 (±0.00006)
DeCART	1.42778 (-74 pcm)

Table III. Eigenvalue comparison for Problem-2

CODE	k_{eff} (3x3 pins)
McSTAR	1.41555 (±0.00006)
DeCART/STAR-CD	1.41489 (-66 pcm)

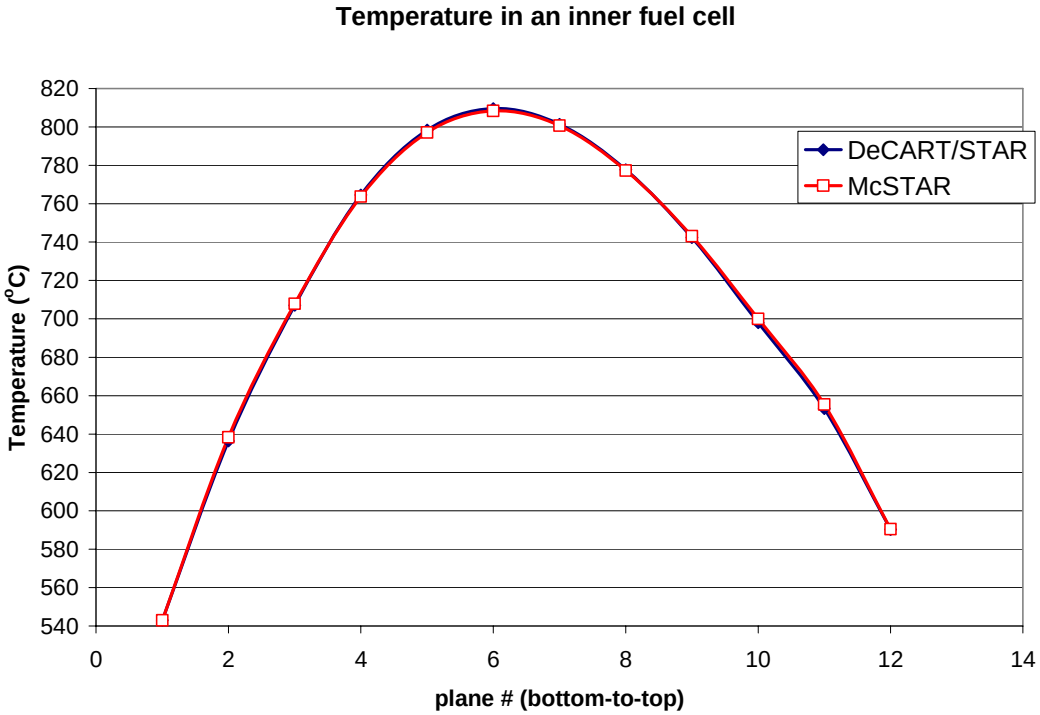


Figure 8 – Temperature profile for problem 2

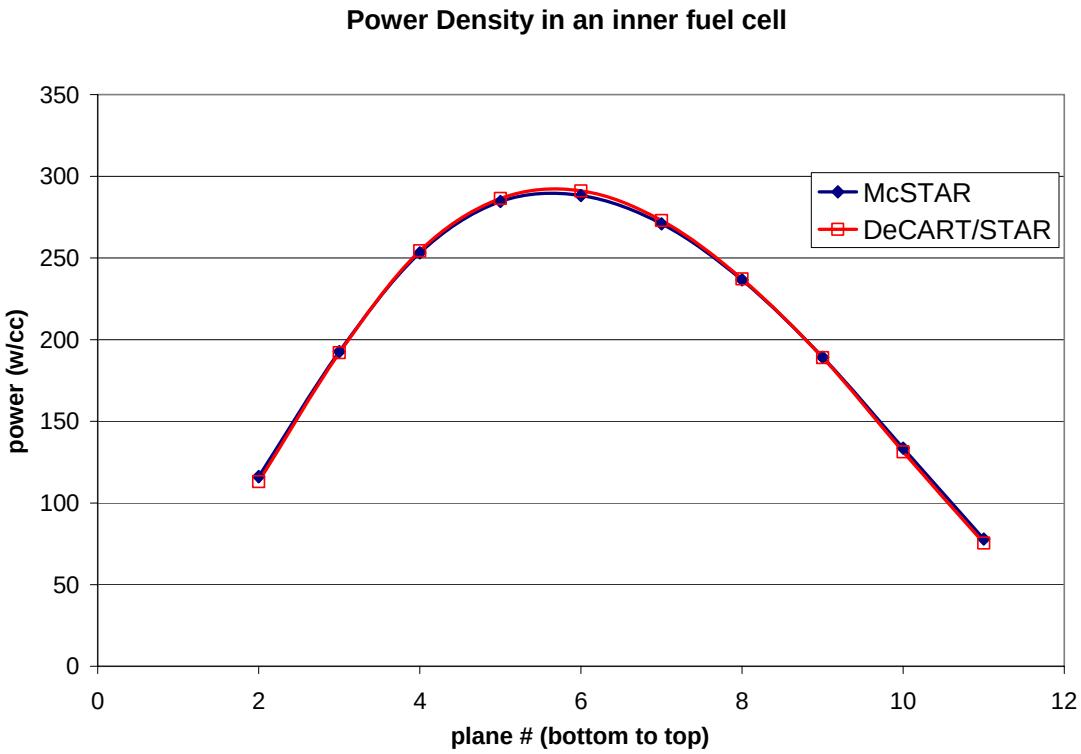


Figure 9 – Axial power density profile for problem 2

5. CONCLUSIONS

A methodology was developed to couple the Monte Carlo code MCNP5 to the Computational Fluid Dynamics code STAR-CD. The preliminary results for two simple PWR test problems demonstrate the feasibility of coupling Monte Carlo to CFD. Preliminary validation of the cross section update methodology was performed to assess the accuracy of the 5K increment tables for these problems. Studies are ongoing to reduce the computational time by developing methods to optimize the number of histories using variance reduction techniques.

In general, coupled Monte Carlo/CFD appears feasible. However, because of the considerable computational burden to track large numbers of histories to obtain a reasonable standard deviation in the estimated parameters, it is not anticipated that coupled Monte Carlo/CFD will replace coupled deterministic/CFD for practical analysis of large reactor problems. Rather it is anticipated the principal role for Monte Carlo based coupled methods will be as an audit tool for specific problems. McStar is now being applied to advanced BWR fuel assemblies with strong axial heterogeneities to verify the accuracy of the 2D/1D solution methods in DeCART.

REFERENCES

1. D.P. Weber, *et.al*, "*The Numerical Nuclear Reactor - A High Fidelity Integrated Neutronic, Thermal-Hydraulic and Thermo-Mechanical Code*", Proceedings of Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Applications. Avignon, France, Sep 2005.
2. D.P. Weber, *et .al,*, "*Coupled Calculations Using the Numerical Nuclear Reactor for Integrated Simulation of Neutronic and Thermal-Hydraulic Phenomena*", PHYSOR 2004, Chicago, IL, April 2004.
3. D.P. Weber, et a.l, "High Fidelity LWR Analysis with the Numerical Nuclear Reactor, *Nuclear Science and Engineering*, **155**, 1 (2007).
4. X-5 Monte Carlo Team, "MCNP — A General Monte Carlo N-Particle Transport Code, Version 5", LANL, 2003
5. CD-adapco Group, STAR-CD, Version 3.26, Melville, NY
6. ORNL, NJOY99, Code System for Producing Point-wise and Multi-group Neutron and Photon Cross Sections from ENDF/B Data.
7. H.G. Joo, *et .al,*, " *Consistent Comparison of Monte Carlo and Whole-Core Transport* Solutions for Cores with Thermal Feedback", PHYSOR 2004, Chicago, IL, April 2004.