

## REACTOR PHYSICS SIMULATIONS WITH COUPLED MONTE CARLO CALCULATION AND COMPUTATIONAL FLUID DYNAMICS

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### ABSTRACT

A computational code system based on coupling the Monte Carlo code MCNP5 and the Computational Fluid Dynamics (CFD) code STAR-CD was developed as an audit tool for lower order nuclear reactor calculations. This paper presents the methodology of the developed computer program "McSTAR". McSTAR is written in FORTRAN90 programming language and couples MCNP5 and the commercial CFD code STAR-CD. MCNP uses a continuous energy cross section library produced by the NJOY code system from the raw ENDF/B data. A major part of the work was to develop and implement methods to update the cross section library with the temperature distribution calculated by STAR-CD for every region. Three different methods were investigated and implemented in McSTAR. The user subroutines in STAR-CD are modified to read the power density data and assign them to the appropriate variables in the program and to write an output data file containing the temperature, density and indexing information to perform the mapping between MCNP and STAR-CD cells. Preliminary testing of the code was performed using a 3X3 PWR pin-cell problem. The

preliminary results are compared with those obtained from a STAR-CD coupled calculation with the deterministic transport code DeCART. Good agreement in the  $k_{\text{eff}}$  and the power profile was observed.

### INTRODUCTION

Increased computational capabilities and improvements in computational methods have 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.

## DESCRIPTION OF THE ACTUAL WORK

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.

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 to 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.

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 FORTRAN90 program which utilizes two PERL scripts that execute MCNP and STAR-CD alternately 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. The simplified algorithm of McStar is depicted in Figure 1.

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.

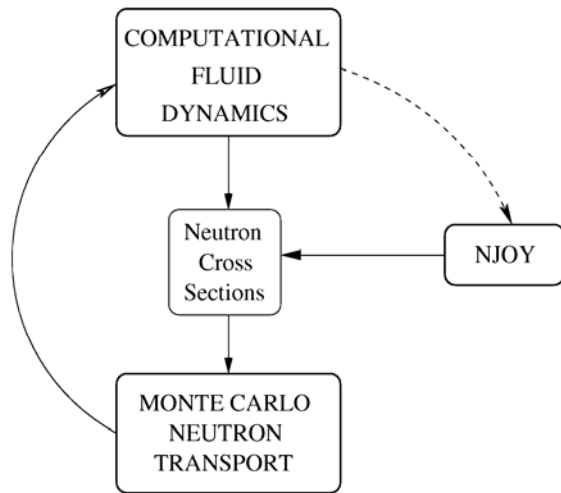


Figure-1 McStar Algorithm

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  $600 \times 2240 = 1,344,000$  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 3 and 4 show the radial meshing of the STAR-CD and MCNP models, respectively.

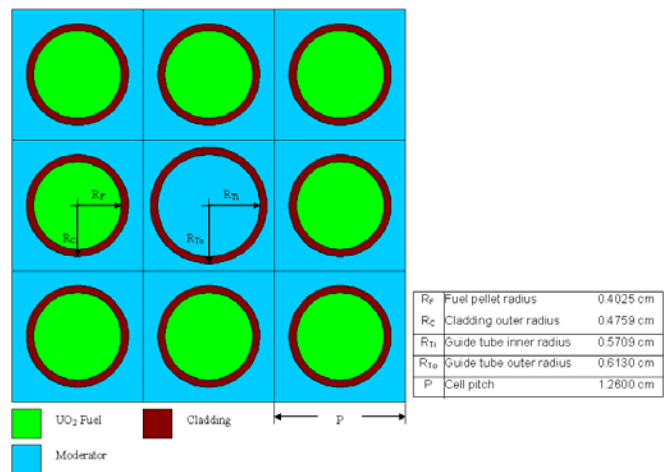


Figure-2 3X3 array of PWR fuel pins

## RESULTS

A model of a 3D 3X3 array of PWR fuel pins was developed with both MCNP5 and STAR-CD. The model consisted of 8  $UO_2$  fuel pins surrounding a central guide tube as shown in Figure 2. The active fuel is 200 cm in height and with 20 cm of water above and below the active fuel. The cladding is zircaloy and the moderator is liquid water. Initial comparisons were made with the same calculation performed using the deterministic code DeCART coupled to STAR-CD.

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

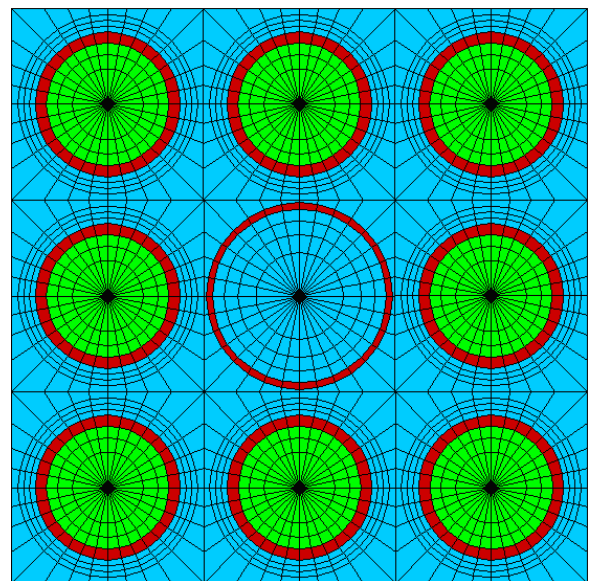


Figure-3 STAR-CD Meshing

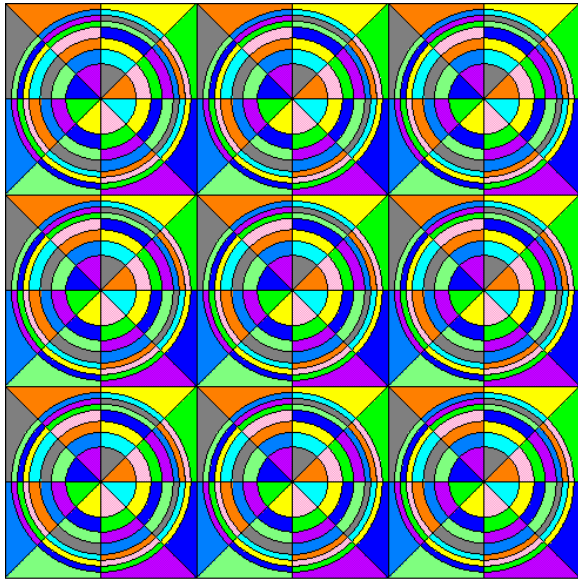


Figure-4 MCNP Meshing

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-I 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-II 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 5 and 6 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 I. Eigenvalue comparison for Problem-2 at fixed temperature**

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

**Table II. Eigenvalue comparison for Problem-2**

CODE	$k_{eff}$ (3x3 pins)
McStar	1.41555 ( $\pm 0.00006$ )
DeCART/STAR-CD	1.41489 (-66 pcm)

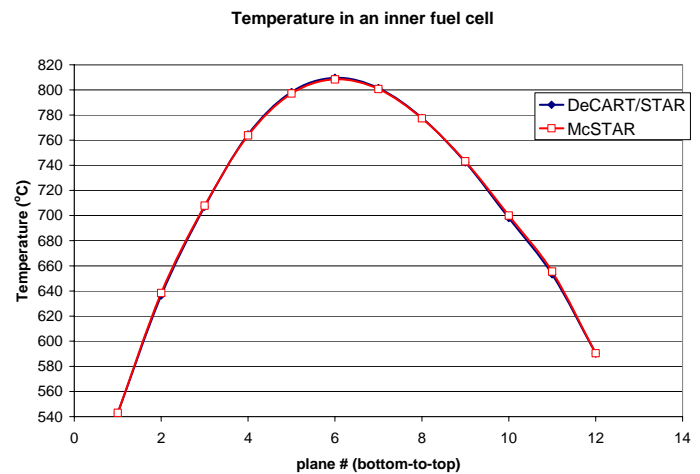


Figure 5 – Temperature profile for problem 2

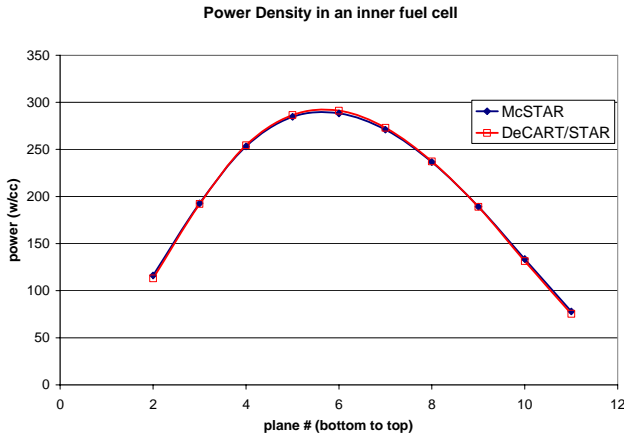


Figure 6 – Axial power density profile

## CONCLUSION AND FUTURE WORK

A methodology was developed to couple the Monte Carlo code MCNP5 to the Computational Fluid Dynamics code STAR-CD. The preliminary results for a simple PWR test problem 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.].

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