Coupled Neutronics and Thermal-Hydraulics Simulations Using MCNP and FLUENT

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INTRODUCTION

High fidelity simulations for nuclear reactors have become more practical with the fast growing computing power and improved computational methods. Monte Carlo methods, more faithful in capturing neutron cross sections and domain geometries but computationally more expensive than deterministic methods, may soon be feasible for routine simulations. For example, MCNP, an advanced Monte Carlo neutron, photon transport code, is being increasingly used for reactor modeling [1]. It can calculate 3D neutron flux distribution with fine resolution in acceptable time limits. Simultaneous progress in thermal hydraulics modeling is seeing increasing use of 3D computational fluid dynamics (CFD) codes. For example, FLUENT and STAR-CD are two state-of-the-art CFD codes [2, 3]. These are versatile tools for various thermal-hydraulics applications, including multi-phase flows. Monte Carlo and CFD represent the current state-of-the-art in neutronics and thermal hydraulics. Hence, it is only natural for efforts to start toward the development of tools to analyze coupled neutronics-thermal hydraulics problems using these two approaches.

Seker et al. reported the successful coupling of MCNP and STAR-CD [4]. Work reported here is similar in spirit with minor deviations. Rather than STAR-CD, the CFD code FLUENT is used in this work. In addition, a more flexible mesh mapping scheme has been developed.

DESCRIPTION

Since the CFD code is a commercial code with no access to the source, the coupling designed is an explicit one, with an interface between the two codes. In this case, a Perl script has been created to execute MCNP and FLUENT in a cyclic fashion, and also to transfer the appropriate inputs and outputs from one code to another. Process is repeated until self-consistent converged results are obtained. To solve a specific nuclear coupled thermal hydraulics problem, separate MCNP and FLUENT models—a text input file for MCNP and a case file for FLUENT—are created. The case file includes all the information needed (materials and their properties, boundary conditions, etc.) to run the FLUENT model. For example, a model may be developed for a single fuel rod with the surrounding fluid (a unit cell), or a fuel bundle, etc. Then 2 text files, one for MCNP and one for FLUENT, are written to store the necessary information of every cell, e.g., cell number, cell center coordinates, material number, original temperature and density. After each run, FLUENT is directed to export a file with updated temperature and density of each cell. The Monte Carlo code MCNP is then executed to calculate power distribution (including fission power, neutron and gamma heating energy) over the entire geometry leading to one value for each cell in this case. Since results from MCNP calculation are normalized to per starting neutron, a subroutine is then called to convert MCNP results to real volumetric power distribution, given a power level for the whole reactor. A User-Defined-Function (UDF) is developed in FLUENT to read the converted power density distribution and then incorporate it as the heat source to the FLUENT model. FLUENT then calculates conjugate heat transfer and fluid transport etc. using the given heat source. It then exports temperature and density of every cell, which is used to update the neutron cross section through the cross-section processing code NJOY [5]. A subsequent MCNP run is carried out with a new input file, with updated cross section and density, followed by another FLUENT run with updated heat source. The process is repeated until the results are converged (the whole process is executed by the developed Perl script).

The need to transfer the power distribution from Monte Carlo calculations to the CFD code, and the temperature and density results from the CFD calculations to the Monte Carlo code requires that a mesh mapping or interpolation scheme between the meshes used in the two approaches be incorporated. Though several improvements are possible and are being studied, at this point a rather simple "closest cell" scheme is incorporated. [In general, CFD code requires a finer mesh than the Monte Carlo code.] The code finds the cell in the receiver code whose distance (from cell center to cell center) to the cell in the donor code is the smallest (and they should be of the same material of course). This scheme will offer more flexibility for mesh mapping as it is not based on any fixed cell information like cell number etc., and it will always find the best corresponding cell in the other model to exchange information.

RESULTS
A simple model was created to test this coupled code package. In this model, a nuclear fuel block (3% U235 enrichment) is sitting side by side with light-water channel. Figure 1 shows the grid of this model used in FLUENT (the dimension of the whole grid is 10 x 10 x 10 cm, and 4 x 4 x 4 cells, 64 cells in total). The fuel block has the exact same dimensions as the water channel (fuel occupies the left half of the whole geometry and water occupies the right one). Water flows in the +z direction. Same grid was used in MCNP model, with 32 cells for fuel and the other 32 cells for water (reflective boundaries were assumed). Though this grid may not be fine enough, for this proof of principal calculation, it was deemed sufficiently refined.

This calculation was performed on a Linux workstation (2.0 GHz AMD Turion processor and 2 GB RAM). Around one million particle histories were used in each MCNP run. Each FLUENT run had about 4,000 iterations. Default neutron cross sections (at room temperature) were used in the first run of MCNP. Volumetric heat source from fission, neutron and gamma heating was calculated using MCNP, and then was read into FLUENT through UDF. A new run of MCNP was carried out using updated neutron cross section (based on updated temperature in each cell). Neutron cross section of water was updated every 5 degree K and neutron cross section of fuel was updated every 100 degree K (since a much larger temperature variation in fuel is observed in this case). K-eff converges after only two cycles (changing from 0.93435 to 0.93271) because of the simplicity of the geometry. The problem took about 70 minutes of clock time.

Figure 2 shows the volumetric heat source calculated using MCNP over a z plane (z = -1.25 cm, the origin is at the center of the whole geometry). Higher heat source region is the fuel block. Heat source inside water channel comes from neutron and gamma heating.

Figure 3 shows the temperature contour calculated using FLUENT over y = 0 plane. The inlet velocity of water channel was assumed as 5 m/s. Small water temperature variation was observed because of the large specific heat and relatively high velocity.

In summary, in this work, a new explicit coupling scheme was developed, executed and tested. The results shows that these neutronics-thermal hydraulics coupled calculations are feasible and can be done within acceptable time frame. Future work will focus on further testing this package on much more complex geometry with many more cells, such as a fuel bundle with thousands of cells. Parallel computing of this coupling will also be developed.

REFERENCES
