DISCLAIMER:

This document does not meet the
current format guidelines of
the Graduate School at
The University of Texas at Austin.

It has been published for
informational use only.

Copyright
by
William Ladd Gurecky
2015

**The Thesis Committee for William Ladd Gurecky
Certifies that this is the approved version of the following thesis:**

**Development of an MCNP6 - ANSYS FLUENT
Multiphysics Coupling Capability**

**APPROVED BY
SUPERVISING COMMITTEE:**

Supervisor:

Erich Schneider

Steven Biegalski

**Development of an MCNP6 - ANSYS FLUENT
Multiphysics Coupling Capability**

by

William Ladd Gurecky, MSE

Thesis

Presented to the Faculty of the Graduate School of

The University of Texas at Austin

in Partial Fulfillment

of the Requirements

for the Degree of

Master of Science in Mechanical Engineering

The University of Texas at Austin

December, 2015

Acknowledgements

I acknowledge Andrew Godfrey, Ben Collins and Aaron Grahm for their guidance in the use of VERA-CS and insight into multiphysics coupling problems. I appreciated the lively and friendly atmosphere provided by those with whom I worked with at Oak Ridge National Laboratory (ORNL). Most importantly, this work would not have been possible without the direction and support of my primary academic advisor, Erich Schneider.

Funding for this work was provided by the Consortium for Advanced Simulation of LWR's (CASL), a DOE innovation hub based at ORNL (contract No. DOE-4000122526).

Abstract

Development of an MCNP6 - ANSYS FLUENT Multiphysics Coupling Capability

William Ladd Gurecky, MSME.

The University of Texas at Austin, 2015

Supervisor: Erich Schneider

This thesis presents a novel core multiphysics coupling method and its application to geometries and thermal hydraulic operating conditions typical of U.S. PWRs. Monte Carlo based radiation transport from the MCNP6 package and finite volume thermal hydraulic (TH) packages provided by ANSYS-FLUENT are combined to produce results with intra-pin resolved spatial resolution equivalent to state-of-the-art reactor physics and multi-physics suites. The Virtual Environment for Reactor Applications (VERA) whose development is spearheaded at Oak Ridge National Laboratory is one such example package. Benchmark and validation tasks performed as an integral part of the development of VERA demand intra-pin resolved pin power distributions as well as finely spatially resolved fuel burnups. This level of detail is not provided by most other lattice physics code packages. Intra-pin powers, for example, are reconstructed from lower fidelity model results using empirically derived shape functions. In addition, data sets from operating PWRs are sparse, resolved only at the inter-pin level, and prone to experimental error. With the proposed MCNP-FLUENT model, it is possible to provide within-pin/channel resolved power, temperature and moderator density field data. MCNP-FLUENT iteratively solves for multiple physical fields: flow velocity, temperature, energy deposition rate, and neutron flux. It does so by repeatedly passing information between dedicated solvers which independently handle the neutron transport and thermal hydraulic physics. The codes are linked by a Picard iteration scheme. Doppler and moderator density feedbacks are explicitly treated. In contrast to preceding generations of MCNP-FLUENT coupling implementations, the coupling framework described employs the latest unstructured mesh capabilities of the MCNP v6.1 code to achieve a new level of geometric and mesh tally generation flexibility. The coupling is demonstrated by a suite of test cases spanning planar 2D geometry, single pin and a 3x3 assembly at hot full power with TH feedbacks. Good power and eigenvalue agreement ($\pm 4\%$, 340[pcm] respectively) is achieved for the hot full power single pin case. Qualitative agreement in the predicted power profiles and fuel temperature distributions is seen in the 3x3 pin geometry.

Table of Contents

List of Tables	x
List of Figures	xii
CHAPTER 1.....	16
1.1 Introduction.....	16
CHAPTER 2.....	19
2.1 Prior Art	19
2.1.1 CASL	19
2.1.2 IDOM Nuclear Services.....	20
2.1.3 Supercritical Water Reactor Analysis	21
2.1.4 Pseudo Material Construct.....	22
2.1.5 Coupled Neutronics and TH Simulations using MCNP and FLUENT.....	23
2.1.6 MCNP5 – STAR-CCM+ Coupling.....	25
2.1.7 Coupled CFD and MOC Simulations	26
2.1.8 Coupled CFD and Monte Carlo Simulations	28
2.1.9 Literature Review Conclusion	29
2.2 Overview of Numerical and Physical Processes.....	30
2.2.1 Neutron Transport Theory	30
2.3 Core Programs	34
2.3.1 Neutron Transport: MCNP6.1	35
2.3.2 Thermal Hydraulics: ANSYS FLUENT	37
2.3.3 Meshing: GMSH.....	38
CHAPTER 3.....	39
Methodology	39
3.1 Coupling Procedure	39
3.1.1 Geometry Specification and Mesh Generation	41

3.1.2 MCNP	44
3.1.3 Grid to Grid Interpolation	46
3.1.4 Doppler Feedback	49
3.1.5 ANSYS FLUENT	50
3.1.6 Picard Iterations and Convergence	52
CHAPTER 4.....	56
Results.....	56
4.1 2D Unit Cell Hot Zero Power	56
4.2 2D Plane Wall	62
4.2.1 Plane Wall Setup.....	63
4.2.2 2D Plane Wall Results	66
4.2.3 Plane Wall Mesh to Mesh Interpolation Accuracy	73
4.2.4 Plane Wall Convergence Rate Study	74
4.2.5 Plane Wall Gamma Transport Sensitivity.....	78
4.2.6 Plane Wall Conclusions	80
4.3 Full Height Single Rod	81
4.3.1 Problem Setup.....	82
4.3.2 1x1, 75% Power Results	85
4.3.3 1x1, 100% Power Results	89
4.3.4 1x1 Pin Cell Mesh to Mesh Interpolation Accuracy.....	92
4.3.5 1x1 Pin Cell Conclusions.....	93
4.4 3x3 Fuel Rod Assembly.....	94
4.4.1 3x3 Fuel Rod Assembly Problem Setup	94
4.4.2 3x3, 100% Power Results	95
4.4.3 3x3 Pin Conclusions	100
4.5 Scalability Summary	101

CHAPTER 5.....	104
Conclusion	104
Appendix A.....	107
A-1: Thermophysical properties	107
A-2: UDF Code.....	109
Bibliography	112

List of Tables

Table 1) Summary of prior art.	30
Table 2) Unit cell problem specification.	57
Table 3) Unit cell eigenvalue results.	59
Table 4) MPACT solver settings [8].	59
Table 5) Corrected volume MCNP unit cell hot zero power results.	60
Table 6) Run time vs. number of F6 tally cells.	61
Table 7) Plane wall problem setup.	64
Table 8) Plane wall FLUENT settings.	65
Table 9) Coupling parameters.	65
Table 10) KCODE history for the plane wall case.	66
Table 11) MCNP and FLUENT mesh statistics for the 2D plane wall case.	66
Table 12) Eigenvalue results for plane wall case.	67
Table 13) Volume averaged mesh to mesh interpolation error for the plane wall case.	73
Table 14) KCODE sensitivity study case definitions.	75
Table 15) KCODE Convergence sensitivity study results.	77
Table 16) KCODE study compute time summary. Wall times summed over all outer iterations. 23 Cores used for FLUENT and MCNP calculations.	78
Table 17) Fraction of energy deposited in the moderator channel.	79
Table 18) Single Pin problem setup.	83
Table 19) Single full height pin coupling parameters.	83
Table 20) Single full height pin cell FLUENT parameters.	84
Table 21) Single pin mesh statistics.	84

Table 22) 1x1 KCODE history.	85
Table 23) 1x1 Full height pin cell computation time. Sum of all iterations.	85
Table 24) Eigenvalue and convergence history for the 1x1 75% power case.	88
Table 25) Eigenvalue and convergence history for the 1x1 100% power case.	92
Table 26) 1x1 pin cell volume averaged quantity comparison.	93
Table 27) 3x3 Case meshing summary.	94
Table 28) MCNP timing results derived from unit cell, plane wall and full height single fuel pin cases.	102

List of Figures

Figure 1: Comparison of the pseudo material mixing method with explicit Doppler broadened cross section data on the neutron multiplication factor of a VHTGR fuel pin. Reproduced from [11].	23
Figure 2: Coarse 4x4x4 cell meshed used in [12].	24
Figure 3: Volumetric energy deposition rates at the z+ midplane. [12]	24
Figure 4: STAR-CCM+ mesh (left). MCNP cells (right). Reproduced from [13].	25
Figure 5: STAR-CCM+ and DeCART meshes with high degrees of mesh parity. Reproduced from [14].	27
Figure 6: MCNP5 cell based geometry discreteization. Reproduced from [15].	28
Figure 7: MCNP-FLUENT coupling procedure overview.	40
Figure 8: Basic parts used to construct the problem geometry. Parameters defining the part geometry are presented alongside the part figures. From left to right: Rectangular prism, wedge, fluid quadrant.	42
Figure 9: MCNP UM Parts (a) and assembled problem geometry (b). Reproduced from MCNP UM guide [19].	42
Figure 10: A collection of rectangular prism parts constructed into a single assembly. The underlying mesh is visible in each part.	43
Figure 11: Unstructured mesh embedded in a traditional CSG container cell. Cells (distinct material regions) are differentiated by color.	44
Figure 12: Discrete temperature field data points superimposed on an MCNP cell.	47
Figure 13: Evaluation of a piecewise linear interpolation function at the centroids of tetrahedron inside a top view of a single hexahedral element. Many elements can comprise a single MCNP UM part.	48

Figure 14: Linear and log law of the wall velocity profiles as a function of y^+ . Reproduced from [20].	52
Figure 16: Left: Top view of a pin cell finite element geometry displayed in quarter symmetry. 6 azimuthal segregations per quartile are shown. The discrepancy between the FE mesh and the CSG geometry is shown on the right.	58
Figure 17: 2D unit cell energy deposition rate. Arbitrary scaling.	61
Figure 18: Side view of plane wall geometry. 2.11% enriched fuel is shown in red. The moderator is colored blue. Reflecting surfaces are shown as dotted lines.	63
Figure 19: Left: Energy Deposition [W/m^3]. Center: Temperature [K]. Right: Moderator density [g/cc]. Geometry not to scale.	68
Figure 20: Left: Velocity magnitude profiles. Right: Zoom of velocity profiles with viscous sub layer and buffer zones removed. Centerline at 0.005 [m].	69
Figure 21: Plane wall moderator temperature profiles.	70
Figure 22: Fuel-Moderator interface axial temperature profile.	70
Figure 23: Plane wall FLUENT convergence behavior. Five outer iterations shown.	71
Figure 24: Normalized energy deposition rate inside the fuel region.	72
Figure 25: Left: Volume averaged fuel temperature. Right: Volume averaged moderator temperature in the coolant channel as a function of distance to the bottom of the active fuel.	72
Figure 26: Comparison of the plane wall energy deposition with gamma transport enabled and disabled in MCNP.	79

Figure 27: Top view of MCNP single fuel rod geometry in quarter symmetry. ...	82
Constituent pseudo-cells differentiated by color.	82
Figure 28: Coolant channel plots for the full height single pin case operating at 75% power. Left: Moderator temperature profile. Right: Moderator density profile.....	86
Figure 29: MCNP-FLUENT vs. MPACT-CTF Power distribution comparison. Single full height pin operating at 75% power conditions.....	86
Figure 30: MCNP-FLUENT vs. MPACT-CTF average fuel temperature comparison. Single full height pin operating at 75% power conditions.	87
Figure 31: 1x1 pin cell CFD convergence behavior.	89
Figure 32: Coolant channel plots for the full height single pin case operating at 100% power. Left: Moderator temperature profile. Right: Moderator density profile.	90
Figure 33: MCNP-FLUENT vs. MPACT-CTF Power distribution comparison. Single full height pin operating at 100% power conditions.....	91
Figure 34: MCNP-FLUENT vs. MPACT-CTF average fuel temperature comparison. Single full height pin operating at 100% power conditions.	91
Figure 35: 3x3 case with zoned enrichment and empty central guide tube.	95
Figure 36: Normalized pin power plot for 3x3 case. MPACT-CTF result shown as broken black lines.	96
Figure 37: Average moderator temperature in each pin cell as a function of axial position.....	97
Figure 38: Average fuel temperature as function of axial position.	98

Figure 39: Energy deposition rate [W/m^3] in the 3x3 assembly. 3.1% enriched pins are in front.....	98
Figure 40: Moderator density [g/cc] (left) and temperature [K] scalar fields for the 3x3 assembly.....	99
Figure 41: Viscosity of water at 2250[psia].....	107
Figure 42: Density of water at 2250[psia].	108
Figure 43: Isobaric specific heat of water at 2250[psia].....	108

CHAPTER 1

1.1 Introduction

The advent of widely available High Performance Computing (HPC) facilities enables numerical investigation of transport phenomena underlying nuclear reactor operation with fidelity unobtainable when the majority of the currently operating reactor fleet in the U.S. was constructed. This provides economic benefit the nuclear power industry by helping to incrementally improve existing pressurized water reactor (PWR) designs and to stimulate the development of entirely new reactor concepts.

To characterize reactor performance under full power conditions demands knowledge of the spatial distribution of thermal energy generated within the core, the transport of thermal energy through the core geometry and how the energy is utilized in generation-side components. This work focuses on characterizing the behavior of the reactor core at steady state (SS), hot full power (HFP) conditions.

Power distribution calculations are a precursor to reactor design and optimization. The goal is often to achieve greater fuel utilization, and provide a sound engineering assessment of existing reactor designs to verify and license proposals for power up rates. Computing the power distribution in an operating PWR requires coupling radiation transport and thermal-hydraulic (TH) physics. With the aid of modern computational tools, this task may be accomplished with high fidelity and in a reasonable time. In all cases, a tradeoff is made between retaining underlying physics and computational time.

In this work lattice geometries typical of operational U.S. PWRs are investigated to demonstrate a novel core physics coupling methodology. Monte Carlo based radiation transport performed by MCNP v6.1 [18] and finite volume computational fluid dynamics (CFD) methods provided by ANSYS FLUENT v14.0 [20] are combined to achieve a

spatial resolution equivalent to state-of-the-art reactor physics and multi-physics suites. The Virtual Environment for Reactor Applications (VERA) [8] whose development is spearheaded at Oak Ridge National Laboratory is one such example package. Simplifications are made in the coupling routines to decrease computation time and algorithmic complexity. Scaling of the presented coupled solution method will be demonstrated by moving through a series of increasingly complex geometries.

In contrast to preceding generations of MCNP-FLUENT coupling implementations, the coupling framework described in this thesis employs the latest unstructured mesh (UM) capabilities of the MCNP v6.1 code to achieve geometric and mesh tally generation flexibility that was previously extraordinarily difficult to obtain. The current method is thus not constrained to PWR-lattice geometries. Future work could utilize the new coupling method in applications that demand the inclusion of unstructured geometry which is not easily modeled by traditional constructive Boolean geometry. Advanced applications may include characterizing thermal performance of highly irradiated laboratory apparatus, such as the target at the Spallation Neutron Source [1], cold neutron generators [2, 3], and thin foils [4]. Other potential applications include predicting the power and temperature distribution in exotic fuel geometry, such as that found in the High Flux Isotope Reactor at Oak Ridge National Laboratory.

This thesis is structured as follows. An overview of the key physical phenomena to be modeled along with a description of numerical packages employed to simulate them in a coupled fashion are presented in Chapter 2. A description of the coupling methodology developed for this work is given in Chapter 3. Finally, results of the coupling procedure are discussed in Chapter 4 for a variety of reactor geometries. Results from the MCNP-FLUENT coupling framework are compared and contrasted to a

deterministic solution provided by the MPACT-COBRA-TF (MPACT-CTF) package available in VERA.

CHAPTER 2

2.1 Prior Art

Investigating previous neutron transport and TH coupling efforts illustrates the difficulties encountered and overcome the pursuit of scalable and comprehensive reactor multiphysics computations. Numerical procedures which are employed in past reactor physics coupling investigations are useful for adoption in the current work.

2.1.1 CASL

A primary emphasis of the Consortium for the Advanced Simulation of Light Water Reactors' (CASL) technical portfolio is the coupling neutron transport and thermal hydraulics codes. An array of such coupled transport codes are collimated in the Virtual Environment for Reactor Applications (VERA) [5]. A strong focus on memory efficiency and parallel scalability is present in CASL's work. Though Monte Carlo neutron transport and finite volume based CFD packages are present in CASL's portfolio by way of SHIFT and HYDRA-TH respectively, these codes are not typically employed at the full-core geometric complexity level. Full core reactor simulation favors deterministic neutron transport and nodal TH codes informed by high fidelity simulation and experimental data. By applying simplifications in the treatment of neutron and fluid transport drastic reductions in computational requirements are achieved. MPACT employs a 2D radial lattice - 1D axial solver methodology, splitting up the 3D transport problem into a conglomerate of 2D MOC problems and 1D P1 transport calculations which reduce the computational requirement when compared to a full core 3D MOC calculation while retaining acceptable accuracy in axial and radial flux profiles. The thermal hydraulic workhorse of the VERA-Core Simulator is nodal based code: COBRA-TF (recently rebranded to CTF), the effects of turbulence, inter-pin mixing, and

subcooled boiling are incorporated into the nodal code by the use of empirically or numerically derived correlations from higher fidelity models [6]. Reduced runtimes for a single state point improve the prospect of carrying out core optimization exercises spanning fuel shuffling and full-core pin-resolved burnup calculations [7].

A multitude of deterministic transport codes in VERA, operating in either a standalone or coupled TH mode, are driven by a single unified ASCII input deck [8]. The VERA input format supports reactor lattice geometries. Problem geometries which may be identically represented in VERA and in the current MCNP-FLUENT framework offer an avenue for benchmarking and validation of the coupling method explored in this thesis. To this end, the method of characteristics transport code MPACT coupled with COBRA-CTF will be used. Though the solution procedures employed in VERA-CS differ from the current work, the comparison of results between the two methods can reveal strengths of finely resolved CFD and Monte-Carlo neutron transport, particularly in cases where strong neutron absorbers are present in the problem and in cases where macroscopic turbulent cross flow between coolant channels becomes important.

The Picard method is implemented in VERA to provide an iterative solution procedure to the multiphysics coupling problem. The Picard iteration scheme is adopted in this work due to its simplicity and ability to treat each component of a multiphysics suite as a black box. No Jacobian information is needed in the Picard iteration method.

2.1.2 IDOM NUCLEAR SERVICES

ANSYS FLUENT – MCNP5/MCNPX coupling routines have been implemented by IDOM Nuclear Services [9]. A traditional structured MCNPX mesh tally was utilized to store energy deposition rate. The energy deposition rate was mapped to the ANSYS

Fluent grid and inserted as a source term into ANSYS Fluent through the user of a User Defined Function (UDF). IDOM cites interpolation error encored at the interface of material regions when projecting the MCNP energy deposition results onto the irregular CFD mesh as a primary challenge. Two sources of error are reported to arise in grid to grid interpolation:

- Inexact geometry representations in the CFD mesh result in small errors in the part volumes.
- Unphysical smearing of the volumetric heat source when interpolating between grids with different node densities.

IDOM's implementation focuses on spent fuel storage and wall heating computations for the ITER project, though their approach could be applied to steady state reactor performance calculations.

The IDOM results imply that to combat mesh-to-mesh interpolation errors a high degree of grid parity should be sought between the two codes. Significant improvements over IDOM's coupling procedure can be made both in ease of mesh tally generation and complex geometry representation in MCNP by employing the latest version of the MCNP code. MCNP v.6.1 may import unstructured meshes in the ABAQUS format [18, 19]. Interpolation error can be minimized if the MCNP mesh tally nodes lie at the same location as the TH nodes.

2.1.3 SUPERCRITICAL WATER REACTOR ANALYSIS

A 3D Monte Carlo / nodal TH coupling scheme has been developed between MCNP and the OpenFOAM finite volume PDE framework [10]. The problem geometry consisted of a single full height Supercritical Water Reactor (SCWR) pin cell. The

problem was subdivided into 80 axial regions via an F6 energy deposition tally. The linear heat rate [W/m] data computed by normalizing the F6 tally data was passed to a nodal OpenFOAM TH model which computed the moderator density, temperature, and velocity fields. Thermo-physical properties of the coolant were found by NIST-based table look-up. The two codes were linked by the method of successive substitutions and were iterated until a 5% relative change was seen in the axial power profile. The nodal TH model relied upon a modified Dittus-Boelter equation to compute cladding-to-coolant heat transfer rates. To better address the large density gradients inside of the SCWR coolant channel a 3D TH coupling with a standard $K-\epsilon$ turbulence model was proposed by the authors as future work. The MCNP-FLUENT coupling methodology will maintain applicability to a wide variety of reactor designs, such as the SCWR concept, as steep density gradients and turbulent mixing effects on the flow and temperature field can be resolved by the CFD package.

2.1.4 PSEUDO MATERIAL CONSTRUCT

A MCNP5 and a nodal TH RELAP coupling was achieved to explore the performance of the pseudo material mixture method for Doppler feedback in a Very High Temperature Gas Reactor (VHTGR). This work was conducted by Jeremy Collin et. al [11]. Doppler feedback was implemented via pseudo material mixing in which cross section data was interpolated at the appropriate temperature by weighting cross section data libraries that were evaluated at temperatures which bracketed the desired material temperature. A comparison between the pseudo material method and explicitly generated temperature dependent cross sections is given in Figure 1.

Figure 1: Comparison of the pseudo material mixing method with explicit Doppler broadened cross section data on the neutron multiplication factor of a VHTGR fuel pin. Reproduced from [11].

In this figure, the pseudo material mixing procedure is shown to give similar results when compared to explicitly Doppler broadened cross section treatment. In Collin's implementation, the energy dependent microscopic cross sections are weighted by the square-root temperature distance to the bounding temperatures. This weighting scheme is consistent with the energy dependence of the Doppler broadened cross section resonance integral. This method of cross section interpolation is adopted in the present work. An explanation of the pseudo material mixing procedure is given in chapter 3.

2.1.5 COUPLED NEUTRONICS AND TH SIMULATIONS USING MCNP AND FLUENT

Work conducted at the University of Illinois, Urbana by Jianwei Hu and Rizwan-uddin resulted in another coupling of MCNP5 to ANSYS FLUENT [12]. FLUENT's

User-Defined-Function (UDF) capability allowed volumetric energy deposition data from MCNP to be read into the CFD mesh. The mesh used in FLUENT was identical to the F6 heating mesh in MCNP, allowing a 0th order interpolation scheme to map volumetric heating rates to the FLUENT mesh. Doppler broadening feedback was implemented by nearest neighbor cross section interpolation with a temperature resolution of 100K.

Figure 2: Coarse 4x4x4 cell meshed used in [12].

Figure 3: Volumetric energy deposition rates at the z+ midplane. [12]

Shown in figures Figure 2 and Figure 3, implementation of the coupling methodology was limited to the relatively simple 2D slab geometry coarsely discretized by as 4x4 grid. This geometry does not give rise to many of the coupling challenges encountered in full scale reactor physics calculations. Regardless, the work proved the feasibility of using user defined C functions (UDFs) to ease field data transfer and interpolation in FLUENT and implementing an external Perl wrapping script of MCNP and ANSYS FLUENT.

2.1.6 MCNP5 – STAR-CCM+ COUPLING

A masters project conducted by Jefferey Cardoni at the University of Illinois at Urbana-Champaign demonstrated a 3D coupling of MCNP5 and STAR-CCM+ [13]. Identical to the aforementioned coupling methodologies, the method of successive substitutions iteration scheme was employed to solve to coupled problem.

The energy deposition field was discretized using an extremely large number of traditional MCNP cells each with an associated F7 fission heating rate tally. 7,489 individual elements were used in a single pin case and 67,401 elements in a 3x3 pin case. The MCNP input deck was generated algorithmically. Each cell was assigned a unique ID, such that it could be mated with its TH cell counterpart.

Figure 4: STAR-CCM+ mesh (left). MCNP cells (right). Reproduced from [13].

Shown in Figure 4, the TH mesh was constructed such that a high degree of mesh parity was obtained, though an exact match was not pursued. A nearest neighbor interpolation scheme was used to map volumetric heat data from MCNP to STAR-CCM. A Perl script linked each MCNP cell with a TH cell according to a minimum distance criterion. Neutron and gamma heating in the coolant was neglected as ~97% of the

recoverable fission energy is claimed to be deposited in the fuel. Therefore the author did not tally heating rates inside the moderator or cladding.

The TH mesh was not refined near the cladding-coolant interface. In order to obtain a convective heat transfer rate, law-of-the-wall approximations were employed by STAR-CCM at the interface to approximate the temperature and velocity gradients at the wall. This decision was likely made to conserve computational resources while demonstrating the initial functionality of the coupling. Furthermore, allowing flexible mesh cell spacing would require modification of the Perl script responsible for mesh generation and cell linking. To avoid complications and geometric inflexibility induced by cell-to-cell linking, the method employed in this thesis will instead employ a volume averaging scheme to map the finely resolved TH field data into larger MCNP cells.

2.1.7 COUPLED CFD AND MOC SIMULATIONS

Work performed by a Michigan Ann Arbor, Oak Ridge National Lab and Westinghouse Electric Company consortium coupled a method of characteristics transport code with a CFD thermal hydraulics code to obtain high resolution pin power and velocity profiles for a 3x3 PWR lattice geometry [14]. This work fulfilled the CASL milestone: “Apply a baseline transport (DeCART) and CFD (STAR-CCM+) capability with loose coupling to a PWR 3x3 fuel pin with a spacer grid to demonstrate feedback coupling” in the Advanced Modeling Applications (AMA) CASL Focus Area (FA). This work is distinguished from other coupling attempts because the spacer grid present in the assembly is resolved explicitly in the TH mesh, however the spacer grid is homogenized in the neutronics model.

The method of successive substitutions was used to couple the two codes together. Convergence was obtained when the L1 neutron multiplication factor norm and the L2 fission source distribution and temperature distribution norms reached a satisfactorily stationary value.

Data transfer was handled by writing heating tally, temperature and density distribution results to files on the hard disk which are subsequently read. Mesh conformance was only required at the interface of two different materials. Inside the DeCART material cell bounds however, the CFD mesh may be unstructured and refined. Figure 5 displays the mesh parity between the two codes with some mesh refinement present in the STAR-CCM+ mesh. Cell centroids were used to map the CFD field data to the appropriate DeCART material cell.

Figure 5: STAR-CCM+ and DeCART meshes with high degrees of mesh parity. Reproduced from [14].

The authors suggest the future application of this work may be to better predict cladding surface temperatures and thus, obtain estimates for the axial position at which departure from nucleate boiling (DNB) occurs. Leveraging 3D CFD rather than a nodal TH approach allows resolution of turbulent mixing effects on the flow field downstream of spacer grids that locally suppresses the cladding temperatures and delays the onset of

DNB. Subcooled boiling rates are important to accurately predict when studying CRUD deposition rates and TH reactor safety margins [35].

2.1.8 COUPLED CFD AND MONTE CARLO SIMULATIONS

Preceding the work of the aforementioned DeCART/STAR-CCM+ coupling, V. Seker et. al. completed a loose coupling between MCNP5, NJOY, and STAR-CCM+ which was named McSTAR [15]. Doppler feedback was handled by interpolating pre-computed cross sections in each material region. Discretization of the fuel and moderator in MCNP was accomplished using standard MCNP cells depicted in an overhead view in Figure 6. The cell geometry generation procedure was scripted to simplify the construction of PWR lattice geometries.

Figure 6: MCNP5 cell based geometry discretization. Reproduced from [15].

To demonstrate the preliminary MCNP and STAR coupling capability the solution produced by McSTAR was compared against a coupled DeCART/STAR simulation for a 3x3 pin problem. A maximum pin power difference of 4% was reported between the DeCART and MCNP coupled calculations. The authors reported that 300 active cycles were utilized per outer iteration with 5e5 neutrons histories simulated per

cycle. A total of 12 outer Picard iterations were performed requiring approximately 100 hours of simulation time on 120 cores.

The authors recognized that due to large computation times required to reduce uncertainty in the estimated parameters Monte Carlo neutron transport was not expected to displace deterministic transport for large scale core design and optimization applications. Instead, the proposed targeted use case for the MCNP5-STAR-CCM+ was to provide an audit tool for simple, few-pin coupled PWR problems. The MCNP-FLUENT coupling is expected to be limited to similar small-geometry applications.

2.1.9 LITERATURE REVIEW CONCLUSION

A weakness present in the majority of the coupling methods, with the notable exception of IDOM Nuclear Services' implementation of an MCNPX-Fluent coupling, was the requirement for conformal CFD and heating tally meshes. This weakness is present to reduce mesh to mesh interpolation algorithmic complexity and to reduce the computational requirement associated with estimating volume integrals and/or computing a mapping matrix required for a generic mesh to mesh coupling scheme. Furthermore, enforcing mesh conformity alleviates concerns of interpolation error. A review of prior art is presented in Table 1.

Table 1) Summary of prior art.

Project	Neutron Transport	Thermal Hydraulics	Outer Iteration Method	Mesh to Mesh Capability	Doppler Feedback
CASL (MPACT-COBRA-TF)	Deterministic: MOC	Nodal: COBRA-TF	Picard	- 3D Lattice Geometry Only. - Refinement possible in nodal TH mesh	True OTF Doppler Broadening.
UMich, WEC, ORNL	Deterministic: MOC	CFD: STAR-CCM+	Picard	- 3D - Conformal. - Refinement possible in CFD mesh.	N/A (Not Available in Published Literature)
Jefferey Cardoni (MULTINUKE)	Monte Carlo: MCNP5	CFD: STAR-CCM+	Picard	- 3D - Conformal - Mesh Parity Required - No refinement possible in CFD.	N/A
Jianwei Hu Et. al. (Uillinois)	Monte Carlo: MCNP5	CFD: ANSYS FLUENT	Picard	- 3D - Conformal	Nearest neighbor
Jeremy Collin (UMich)	Monte Carlo: MCNP5	Nodal: RELAP	Picard	- Structured - Conformal - 3D neutronics / 1.5D TH.	Pseudo Material Mixture
IDOM Nuclear Services (Proprietary)	Monte Carlo: MCNP5	CFD: ANSYS FLUENT	N/A	- 3D - Unstructured - Conformal recommended	N/A
Current Work (MCNP-FLUENT)	Monte Carlo: MCNP6.1	CFD: ANSYS FLUENT	Picard	- 3D - Unstructured - Non-conformal <i>allowed</i> . Conformal recommended	Pseudo Material Mixture

2.2 Overview of Numerical and Physical Processes

2.2.1 NEUTRON TRANSPORT THEORY

The continuous energy time dependent neutron balance for a multiplying medium in differential form is shown in equation 1.

$$\begin{aligned}
& \frac{1}{v} \frac{\partial \psi}{\partial t} - \mathbf{\Omega} \cdot \nabla(\psi) - \Sigma_t(x, E)\psi + \int_0^\infty \int_0^{4\pi} \Sigma_s(x, \mathbf{\Omega}' \cdot \mathbf{\Omega}, E' \rightarrow E) \psi d\mathbf{\Omega}' dE' \\
& + \frac{\chi(x, E)}{4\pi} \int_0^\infty \int_0^{4\pi} \nu(x, E') \Sigma_f(x, E') \psi d\mathbf{\Omega}' dE' + \frac{S}{4\pi} = 0
\end{aligned} \tag{1}$$

$$\psi = \psi(x, \mathbf{\Omega}, E)$$

The first term represents the streaming of neutrons through a point in space. The second term is the net neutron removal rate when considering all possible neutron interactions. The third term accounts for scattering events which redistribute the neutrons in energy and direction. The fourth term represents neutron born in fission events. The final term includes non-fission included neutron sources. All neutrons born from fission are assumed to be promptly emitted. No delayed neutron contribution to the rate equation is considered for simplicity.

In the problem of interest in this thesis, in which a fissile material provides neutron multiplication and no fixed source is present, the time derivative may be eliminated by scaling the neutron production rate from fission by a factor of $1/k$.

$$\begin{aligned}
& \mathbf{\Omega} \cdot \nabla(\psi) - \Sigma_t(x, E)\psi + \int_0^\infty \int_0^{4\pi} \Sigma_s(x, \mathbf{\Omega}' \cdot \mathbf{\Omega}, E' \rightarrow E) \psi d\mathbf{\Omega}' dE' \\
& + \frac{\chi(x, E)}{k4\pi} \int_0^\infty \int_0^{4\pi} \nu(x, E') \Sigma_f(x, E') \psi d\mathbf{\Omega}' dE' = 0
\end{aligned}$$

The inclusion of the neutron multiplication factor results in a pseudo steady state neutron balance. The pseudo steady state multiplying medium transport equation may be discretized in energy, producing a set of coupled equations known as the multigroup transport equations. The multigroup transport equation may be represented concisely in matrix form:

$$\mathbf{H}\psi = \frac{1}{k} \chi f^T \int_{4\pi} d\mathbf{\Omega} \psi$$

The multigroup transport operator $\mathbf{H}$ acts on the multigroup neutron flux vector ψ to redistribute neutrons in energy due collisions and to remove neutrons due to absorptions:

$$\mathbf{H}_{gg'} = \delta_{gg'}[\mathbf{\Omega} \cdot \nabla + \Sigma_t(x)]_{gg} + \int_0^{4\pi} \Sigma_{s_{gg'}}(x, \mathbf{\Omega}' \cdot \mathbf{\Omega}) d\mathbf{\Omega}$$

The discrete energy fission probability distribution and fission multiplicity row vectors are defined respectively:

$$\chi = \{\chi_{g_1}, \dots, \chi_{g_N}\}$$

$$f^T = \left\{ \nu \Sigma_{f_{g_1}}, \dots, \nu \Sigma_{f_{g_N}} \right\}^T$$

For compactness it is useful to define a neutron production rate vector:

$$F(x) = f^T \int_{4\pi} d\mathbf{\Omega} \psi$$

Multiplying by the inverse of $\mathbf{H}$ and operating on ψ on both sides of transport equation with $f^T \int_{4\pi} d\mathbf{\Omega}$ yields:

$$k f^T \int_{4\pi} d\mathbf{\Omega} \psi = \chi f^T \int_{4\pi} d\mathbf{\Omega} \mathbf{H}^{-1} f^T \int_{4\pi} d\mathbf{\Omega} \psi$$

Using the definition of $F(x)$ we obtain:

$$kF = \chi f^T \int_{4\pi} d\mathbf{\Omega} \mathbf{H}^{-1} F$$

$$\mathbf{A} = \chi f^T \int_{4\pi} d\mathbf{\Omega} \mathbf{H}^{-1}$$

We arrive at a k-eigenvalue problem:

$$kF = \mathbf{A}F$$

This equation may be numerically solved by the method of power iteration [16]. The power iterations are carried out by repeatedly applying the operator $\mathbf{A}$ to an initial guess for the angle integrated multigroup fission distribution shape, F_0 . At each iteration i , the vector is updated according to:

$$F_n = \prod_{i=0}^{i=N} k_i^{-1} \mathbf{A}^n F_o$$

And the neutron multiplication factor is updated according to:

$$k_{i+1} = \frac{\int F_{i+1} dV}{(1/k_i) \int F_i dV} = \frac{\int \mathbf{A} F_i dV}{\int F_i dV}$$

Where V is the reactor volume.

Assume there are l eigenvalues and eigenvectors each representing a possible solution to the eigenvalue problem shown in equation 2.

$$\mathbf{A} F^l = \lambda_l F^l \quad (2)$$

The initial guess F_0 is some linear combination of the solution eigenvectors:

$$F_0 = \sum_l \alpha_l F^l$$

Applying $\mathbf{A}$ a total of n times produces:

$$\mathbf{A}^n F_o = \sum_l \lambda_l^n \alpha_l F^l = \alpha_1 \lambda_1^n F^1 + \sum_{l>1} \lambda_l^n \alpha_l F^l \quad (3)$$

Assuming atleast one positive real eigenvalue exists, and there are no duplicate eigenvalues (all solution eigenvectors are linearly independent) then there is an ordered sequence of eigenvalues that satisfies $\lambda_1 > \lambda_2 > \lambda_3 \dots$. According to equation 3, as n becomes large the largest eigenvalue and corresponding eigenvector will dominate the fission source distribution, F . This eigenvector is termed the fundamental harmonic of the fission source distribution. The rate at which a stationary solution is achieved by power iteration is dependent on the ratio λ_2/λ_1 . If this ratio is small then $(\lambda_l/\lambda_1)^n$ tends to 0 in relatively few power iterations. It can be shown that in cases where the root-mean-squared distance a neutron travels before causing a fission is much smaller than the dimensions over which the fissile material is spread gives rise to slow convergence [16].

Non fundamental mode eigenvectors may persist in the solution estimate over many power iterations. This case has the potential to arise in PWR criticality calculations as the axial and radial dimensions are large.

Briefly, there are a variety of acceleration methods available to combat slow convergence to the fundamental mode when using power iteration to solve the k -eigenvalue problem. The Coarse-Mesh Finite Difference (CMFD) technique is commonly employed to damp the higher harmonics of the fission source distribution by rebalancing the neutron population in space according to lower order approximations to the neutron transport equation. This method has shown to be an effective means to accelerate a variety of transport codes, including MPACT [7, 8]. Despite their attractiveness, acceleration techniques for k -eigenvalue power iterations are not a focus of this thesis however, incorporating a CMFD acceleration step into the MCNP KCODE solution updates is an active area of research [17].

For every power iteration the inverse of the multigroup transport operator $\mathbf{H}$ must be computed. This operation often requires iterative procedure such as the Gauss-Seidel method to be invoked. From the perspective of MCNP, the inversion of the transport operator is carried out implicitly by simulating many particle histories, though there is no exact analogy to the matrix inversion operation in Monte Carlo transport methodology.

2.3 Core Programs

In this section a brief background of the code packages selected to perform radiation transport, thermal hydraulic analysis and mesh generation is provided. Key features and solver algorithms present inside the code packages which are used in the MCNP-FLUENT multiphysics framework are highlighted.

2.3.1 NEUTRON TRANSPORT: MCNP6.1

The Monte Carlo N-Particle transport package MCNP v.6.1 is leveraged for radiation transport [18]. This package is capable of Continuous Energy (CE) neutron and photon transport. Monte Carlo methods in radiation transport reduce the number of simplifications applied to the physics of simulation of particle transport at the expense of providing only an approximate solution to the transport equation. The simulated particles' aggregate behavior solves the transport equation exactly in the limit as the number of simulated particle histories approaches infinity. Interaction probabilities are derived from experimentally obtained nuclear physics cross section data when available. User generated cross section data can be supplied in the ACE format via the cross section processing tool NJOY.

MCNP will be used in the KCODE mode to solve the k-eigenvalue problem presented in equation (2). In this mode, an initial guess for the spatial neutron fission source distribution is provided. With each simulated neutron generation, an improved estimate for the true fission source distribution is obtained by releasing neutrons from the previous source locations, simulating their lifetimes and finally updating the source distribution according to the updated fission event spatial distribution. Given enough neutron generations are simulated, the fission source distribution converges to the true shape. The solution method is essentially the method of power iteration as described in section 2.2.1 Neutron Transport Theory, with similar drawbacks of slow convergence for large, loosely coupled multiplying geometries.

MCNP allows the problem domain to be spatially discretized for reaction rate tallying enabling the end user to obtain an estimate for the local energy deposition inside a given volume embedded in the model, for example. With the release of v6.0, MCNP gained the capability to import unstructured meshes supplied in the ABAQUS ASCII

mesh file format. The unstructured mesh can be used to define a mesh tally, though the output scalar field data is written in the EEOUT file format which significantly differs from a MCTAL file. Detailed information on the EEOUT format may be found in the MCNP unstructured mesh manual [19]. In addition, user specified regions in the unstructured mesh can be treated as traditional MCNP cells in which material composition and temperature may be assigned. This capability enables highly complex geometry involving multiple materials to be easily defined and meshed. Before the advent of this capability, individual MCNP macrobodies could have been combined to form a mesh using traditional cell based reaction rate tallies. Other coupling methodologies relied upon traditional structured mesh tallies superimposed over constructive solid geometry cells.

When coupling equation 1 with thermal and fluid transport PDEs as is the case in reactor calculation of interest, the energy deposition rate due to fission events must be computed. In MCNP an F6 tally can be used to compute the local energy deposition due to all particle iterations. The F6 tally estimates the integral given by equation 4 [18].

$$F_6 = \frac{N}{V\rho} \iiint_{V,t,E} H(E)\phi(x,V,t)dVdt dE \quad (4)$$

Where V is the volume of the F6 tally cell, ρ is the mass density, N is the atomic density, E is energy, and t is time. The heating response function $H(E)$ is strongly dependent on the microscopic fission cross section in instances when energy deposition due to fission events is of primary interest with other minor contributions from neutron collision and gamma heating. ϕ is the angle integrated scalar flux. The F6 tally produces results in $[MeV/gram/source\ particle]$ [18]. To provide a volumetric heating rate to a coupled thermal hydraulic code requires scaling the raw F6 tally by the mass density of the

material and by a scalar quantity C_i determined by the power normalization given in equation 5:

$$Q_i = F_6 \rho_i C_i [\text{Watts}/\text{cm}^3]$$

$$\text{Reactor Power} = Q_{tot} = \sum_{cells} Q_i V_i \quad (5)$$

Where the scalar C_i has units of $[1/\text{s}]$.

2.3.2 THERMAL HYDRAULICS: ANSYS FLUENT

The following capabilities were desired from the TH modeling software:

- Ease of field data transfer to and from the simulation package
- Heat transport in solid bodies
- Buoyancy driven flow
- Arbitrarily complex geometry
- Ability to include turbulence effects in a Buoyancy driven flow model

ANSYS FLUENT v. 14.0 was adopted as the TH code of choice. ANSYS FLUENT is capable of performing all of the tasks listed above [20]. This package is capable of conjugate heat transfer and provides built in methods to read and write field-data to ASCII files. The package contains a multitude of turbulence models to choose from which are compatible with buoyancy driven flow models. FLUENT is a finite volume based Computational Fluid Dynamics (CFD) package. Multiple discretization schemes and solution methodologies are available to the user. The Semi-Implicit Method for Pressure Linked Equations (SIMPLE) pressure-velocity coupling scheme will be employed in this thesis. Overviews of the finite volume discretization method for PDEs and the SIMPLE solution algorithm may be found in [21].

FLUENT's conjugate heat transfer capability allows the energy balances written for cells inside the solid regions in the problem to be directly coupled with the energy balances equations in the fluid portions of the mesh. This results in only one matrix equation for the thermal energy balance to be solved per TH iteration. This reduces overall computation time as it alleviates the need for a separate solid heat transport solver and an additional solution coupling procedure.

2.3.3 MESHING: GMSH

The task of mesh generation is appropriated to GMSH, a GPL licensed finite element mesh generation program [22]. The GMSH program can be driven by an internal scripting language which enables cell dimensions and mesh parameters to be changed pragmatically. This capability is utilized to automate the MCNP geometry and tally generation process. GMSH can output mesh data in the ABAQUS ASCII file format, which is accepted by both MCNP6.1 and ANSYS FLUENT after minor modification of the mesh output files.

CHAPTER 3

Methodology

The coupled physics framework simultaneously solves for multiple physical fields, in this case flow velocity, temperature, energy deposition rate, and neutron flux. It does so by repeatedly passing information between dedicated solvers which independently handle the neutron transport and thermal hydraulic physics. The codes are linked by the method of successive substitutions, or a Picard Iteration scheme which is discussed in section 3.1.6 Picard Iterations and Convergence and is referred to as the outer iteration scheme. This chapter describes the outer iteration scheme as well as the implementation of the dedicated solvers which it brings together.

3.1 COUPLING PROCEDURE

Figure 7 illustrates the iterative multiphysics coupling procedure. The problem geometry must first be defined, meshes constructed for FLUENT and MCNP, and temperature dependent cross section data generated before the automated outer Picard iterations begin. Scripts developed in the Python language handle all data transfer to and from MCNP and FLUENT in addition to automating the generation of MCNP input decks and FLUENT journal files.

Figure 7: MCNP-FLUENT coupling procedure overview.

Following the problem setup, the automated iteration loop is initiated, first, computing the temperature and density in each component of the MCNP problem geometry according to the initial conditions provided in the problem setup. MCNP is responsible for computing the energy deposition scalar field. The energy deposition data is passed to an preprocessor which applies a normalization to the energy deposition field such that the total thermal power produced the be problem domain is equivalent to a user set value.

Given boundary conditions and a volumetric heat source distribution, ANSYS FLUENT approximately solves a coupled energy, mass, and momentum balance throughout the problem domain to obtain solution field variables – temperature and density – which feed back to the neutron transport calculations. The TH solution data is

passed into interpolation routines which compute the temperature, density and material composition in each MCNP cell.

After MCNP is executed (for the second time), scaled residuals are computed and checked against a converge tolerance. The process is repeated until the convergence criteria are met or a maximum number of outer iterations are performed. The remainder of this section explains each step of the process in detail.

3.1.1 Geometry Specification and Mesh Generation

The fundamental geometric component in MCNP is a cell. Traditionally, an MCNP cell is defined by Boolean combinations of spatial regions. This is the constructive solid geometry (CSG) approach to geometry specification. The current work departs from the use of CSG techniques in favor of the flexible UM geometry construction paradigm. To maintain consistency with standard MCNP UM terminology, geometric components used to construct the problem are referred to as UM *parts*. A variety of parts typically employed to build PWR lattice geometries are provided in Figure 8. Figure 9 shows that assemblies are constructed from a collection of simple parts. Each part is located in Cartesian space by specifying the part origin. In addition, each part contains unique parameters which fully define its geometry.

Figure 8: Basic parts used to construct the problem geometry. Parameters defining the part geometry are presented alongside the part figures. From left to right: Rectangular prism, wedge, fluid quadrant.

Figure 9: MCNP UM Parts (a) and assembled problem geometry (b). Reproduced from MCNP UM guide [19].

Since each part is defined as a distinct entity, GMSH can be used to adjust meshing parameters which control mesh density or whether to enable a structured or unstructured meshing algorithm on a per part basis.

Figure 10: A collection of rectangular prism parts constructed into a single assembly. The underlying mesh is visible in each part.

MCNP UM parts are used to define pseudo-cells in the MCNP input. Pseudo-cells are analogous to traditional MCNP cells with minor restrictions that are irrelevant to this work. Example input cards utilizing the MCNP unstructured meshing capability may be found in the MCNP UM users guide [19]. Each pseudo-cell is associated with unique material, density, and temperature information so that the cell properties may be updated throughout the iterative solution procedure. Henceforth the prefix “pseudo” will be dropped when referring to a region of space inside the MCNP geometry which is assigned unique material and temperature information. MCNP UM pseudo-cell’s will be referred to simply as cells. In addition to material properties, a Boolean is assigned to each cell indicating whether it contains a multiplying medium so that the flagged cell can be specified as a source region inside MCNP using the special VOLUMER keyword on the SDEF card.

A plane wall assembly that is ready for MCNP or FLUENT import is shown in Figure 10. MCNP pseudo-cells are differentiated by color, and the unstructured mesh is shown as yellow lines. The mesh can be used as an F6 heating mesh tally definition within MCNP. The same mesh can be imported into ANSYS FLUENT using the built in

ABAQUS mesh import functionality. In contrast to constructive solid geometry (CSG) MCNP specification, implementation of the unstructured mesh geometric representation technique allows one to obtain identical meshes in both MCNP and ANSYS FLUENT, helping to eliminate grid-to-grid interpolation error issues. This is a primary benefit of taking advantage of MCNP6.1 unstructured mesh support for multiphysics coupling applications.

3.1.2 MCNP

All UM pseudo-cells are collected into a single assembly which is placed into a conventional MCNP container cell. The container cell is a traditional MCNP constructive geometry cell which is used as the problem's bounding box. Boundary conditions are specified on the container cell faces and particle importances are set to null outside of the container.

Container Cell

Figure 11: Unstructured mesh embedded in a traditional CSG container cell. Cells (distinct material regions) are differentiated by color.

Figure 11 displays the unstructured mesh placed within the container cell. In the figure pseudo-cells are denoted by color. Each cell is associated with a corresponding material definition in the MCNP input deck. Since each cell is tagged with a material name, and the density of the material inside the cell is known, the appropriate material and isotopic vector can be selected from a global inventory dictionary, e.g. a cell with a material name “lwtr” will be assigned hydrogen and oxygen isotopes in their proper proportions.

In each cell’s material definition, MCNP requires isotopes to be associated with continuous energy cross section libraries. Assigning the correct cross section library to each isotope inside a given cell depends upon the cell temperature. The cell average temperature is computed by integrating the temperature scalar field data provided by FLUENT simulation results inside of the cell in question. The procedure is discussed in detail in section 3.1.3. Given the cell temperature, an approximate method known as pseudo material mixing is used to handle Doppler feedback. Interpolation of the cross section libraries bracketing the average cell temperature is performed. Cross section data libraries are weighted by the relative distance to bounding cross section temperature abscissa. This pseudo material mixing procedure is discussed in section 3.1.4.

An F6 heating tally is generated using the collective assembly mesh. The F6 tally measures the energy deposited per unit mass due to locally deposited fission gammas, and from neutron collisions and absorptions [18]. The raw F6 heating tally is normalized according to equation 6 to obtain volumetric heating rates.

$$E_i = \frac{C \rho_i F_i V_i}{\sum_{i=0}^N \rho_i F_i V_i} \quad (6)$$

Where i is the cell index, E is the total energy deposition in [Watts]. F is the raw F6 tally values [eV/gram/source particle], ρ is the volume averaged material density in the cell, and E_i/V_i is the volumetric heating rate inside a given MCNP mesh element. C is a user defined scaling parameter with units of [Watts] that scales the energy deposition tally to yield the specified amount of power when integrated over the entire problem.

It should be noted that a MCNP “continue run” operation is not permitted when material compositions change within the problem between outer iterations due to the pseudo material mixing procedure. Following the first Picard iteration, the previous fission source distribution is available for use as the fission source initial guess in the current iteration. This is accomplished with the MCNP fission source import command line argument accompanied by a SRCTPE file [18].

3.1.3 Grid to Grid Interpolation

Field data must be exchanged between the MCNP and the FLUENT meshes. The resolution at which material, temperature, and density information is tracked within MCNP is only cell-resolved. Within FLUENT, temperature and density scalar fields are comparatively finely resolved. The CFD temperature and density fields are supported at the CFD mesh element centroids. An interpolation scheme must be employed to map the finely resolved temperature and density scalar field information onto the coarsely resolved Cell-based geometry description in MCNP.

Figure 12: Discrete temperature field data points superimposed on an MCNP cell.

Discrete temperature and density field data is passed from the FLUENT computation to MCNP. In the following example, the temperature field data is considered. In Figure 12 an MCNP cell is presented with origin $O\{x_0, y_0, z_0\}$ alongside discrete temperature data as received from a mesh-cell centered FLUENT data set, shown as T_i . Red points indicated data which lie inside of the cell, blue data points lay outside of the cell. A piecewise continuous linear interpolating function, ψ , is constructed upon the discrete temperature data set. In equation (7) this function is integrated over the cell volume to obtain an average temperature within the cell. The integration limits and cell volume are easily determined from the cell parameters $(O, \Delta x, \Delta y, \Delta z)$ in the case of a rectangular prism cell. In the case of more complex cell geometry the volume integral in equation (7) is not trivial to compute.

$$\overline{T_{cell}} = \frac{1}{V_{cell}} \int_V \psi dV \quad (7)$$

This piecewise linear interpolation procedure is particularly susceptible to interpolation errors when large second derivatives exist in the field data. Refining the

number of cells in the MCNP domain reduces interpolation error at the expense of computing time to resolve the field at a greater fidelity.

For MCNP cells of arbitrary shape a novel procedure was developed to compute equation 7. Consider a single UM part in the MCNP geometry, for example a quarter-cylindrical ring shaped region in the fuel. The underlying finite element mesh generated by GMSH is comprised of simple geometric *elements* (arbitrary shaped hexahedron) which are guaranteed to be convex. A 2D representation of a hexahedral element is provided in Figure 13.

Figure 13: Evaluation of a piecewise linear interpolation function at the centroids of tetrahedron inside a top view of a single hexahedral element. Many elements can comprise a single MCNP UM part.

Each element in the MCNP UM part is subdivided into tetrahedra using the Delaunay triangulation algorithm [23]. The piecewise linear field interpolant, ψ , is evaluated at the centroids of the Delaunay tetrahedra. The resultant interpolated values, $T_{fine_{ij}}$, are weighted by their respective tetrahedral volume, V_{ij} . The vector is summed over M Delaunay tetrahedra in each of the N elements to produce an estimate for the volume averaged cell quantity in equation 8.

$$T_{cell} = \frac{1}{V_{cell}} \sum_i^N \sum_j^M V_{ij} T_{fine_{ij}} \quad (8)$$

This volume integral estimation method is applicable regardless of the FLUENT mesh density, shape of the MCNP parts, mesh scheme implemented in each MCNP part, or how few MCNP parts make up the problem geometry.

3.1.4 Doppler Feedback

As a component of problem setup, the nuclear data processing code, NJOY, is executed to obtain ACE formatted Doppler broadened cross sections for every isotope present in the problem at 50K intervals [24]. The fuel material temperatures considered range from 300K to 1400K. Cross sections for the isotopes present exclusively inside the moderator are generated from 300K to 700K. Equation (9) illustrates that cross sections for the isotopes in a cell are weighted by the square root temperature distance to bounding cross section temperature abscissa. This is consistent with the temperature dependence of the Doppler broadened resonance integral [13, 25].

$$\Sigma_{cell} = w_c \Sigma_c + (1 - w_c) \Sigma_h \quad (9)$$

With weight:

$$w_c = \left(\frac{\sqrt{T_h} - \sqrt{T_{cell}}}{\sqrt{T_h} - \sqrt{T_c}} \right)$$

T_c & T_h are the bounding hot and cold temperatures for which Doppler-broadened XS data exists. Σ represents the macroscopic cross section of the mixed material in a

cell. Expanding macroscopic cross sections in equation 10 exposes the number density of the j^{th} isotope inside the mixture:

$$\Sigma_{cell} = \sum_j N_j [w_c(\sigma_j)_c + (1 - w_c)(\sigma_j)_h] \quad (10)$$

The weighted isotopes, $w_c N_j$ and $w_h N_j$, correspond to bounding lower and upper cross sections $(\sigma_j)_c$ and $(\sigma_j)_h$ respectively. The microscopic cross sections, σ_j , are continuous functions of energy. According the MCNP material specification format, cross sections for the same isotope at different temperatures may be uniquely identified by library suffix tags. The appropriate cross section libraries can thus be selected from a pre-generated list and the number densities can be appropriately weighted before being written to a MCNP material card.

3.1.5 ANSYS FLUENT

After a mesh is imported into FLUENT, boundary conditions, solver options, and material composition must be specified to complete the TH problem setup. At the inlet, a mass flow rate and static pressure are specified. A free outflow boundary is specified at the fluid region outlet. Symmetry boundary conditions are enforced at the radial problem boundaries. Adiabatic boundary conditions are employed at the top and bottom of the fuel region.

The SIMPLE iterative scheme for solving pressure velocity coupling is utilized to solve the steady state Reynolds-averaged Navier-Stokes (RANS) equations. The RANS formulation requires relationships to describe turbulent shear stresses in order to close the

system of equations describing momentum and mass conservation [20]. A widely used closure relationship is provided by the K- ϵ turbulence model.

When using the standard K- ϵ wall treatment, care must be taken to ensure that the mesh density near the fluid-cladding interface is adequate to resolve the log-law of the wall region of the boundary layer. ANSYS recommends $60 < y^+ < 100$ is satisfied when using the standard K- ϵ wall treatment [20]. y^+ is a dimensionless distance to the wall given in by equation 11. It is used to parameterize the law-of-the wall approximations to the velocity profile in close proximity to a no slip boundary.

$$y^+ = \frac{yu_\tau}{\nu} \quad (11)$$

Where ν is the kinematic viscosity and y is the distance from the wall. The shear velocity u_τ is given by:

$$u_\tau = \sqrt{\frac{\tau_w}{\rho}}$$

Where τ_w is the wall shear stress.

Enhanced wall treatments are enabled inside the FLUENT model to take advantage of high near-wall mesh density to more accurately resolve velocity and temperature gradients near the no-slip boundary [20]. The enhanced wall treatment smoothly blends the linear log of the wall region with the log law of the wall relationship at y^+ values between $5 < y^+ < 60$. The boundary layer velocity magnitude scaled by u_τ is shown in Figure 14.

Figure 14: Linear and log law of the wall velocity profiles as a function of y^+ .
Reproduced from [20].

To take advantage of the enhanced wall treatment's improved boundary layer representation, the cell closest to the fluid-cladding boundary is ensured to have a $y^+ \leq 30$ at all axial locations and for all fuel pin configurations.

3.1.6 Picard Iterations and Convergence

In this thesis, a steady state solution to the coupled neutron transport and thermal hydraulics problem is desired. The coupling of several steady state balance equations can be cast as a fixed point problem. A fixed point iteration scheme may be represented by relation 12.

$$x_{n+1} = G(x_n) \quad (12)$$

The system variables of interest which comprise the solution vector x are the energy, space and direction dependent neutron flux, ψ , the temperature and density scalar fields, T and ρ respectively, and the moderator velocity field, $\mathbf{v}$. The fission reaction rate inside the fuel, a key response of interest, is dependent on these system variables.

The Picard iteration scheme is outlined in the following steps for this particular multiphysics application.

The Picard Iterative Method

Requires: Initial guess for ψ, T, ρ and $\mathbf{v}$

$k=0$

While Not Converged **do**:

$k+=1$

MCNP solve steady state (SS) transport. $f_\psi(\psi^k, r(\rho^{k-1}, T^{k-1}))=0$ for ψ^k

Obtain heating rate $H = H(\psi)$

Scale and under relax heating. $S^k = c ((1 - \omega)H^k + \omega H^{k-1})$

TH SS solve. $f_{TH}(\rho^k, T^k, \mathbf{v}^k, r(S^k)) = 0$ for $\rho^k, T^k, \mathbf{v}^k$

Where f_ψ represents the nonlinear steady neutron rate balance equation, f_{TH} represents the coupled TH system of equations: the momentum balance, energy balance, and mass balance PDEs. A scaling parameter, c , is included to obtain the volumetric heating scalar field, S . The function r represents a solution mapping from one code to another. In this instance, this is the mesh to mesh interpolation routines. The Picard iteration scheme under optimum conditions is expected to converge to the steady state system values at a linear rate. Since in the current coupling method f_ψ contains inherent Monte-Carlo noise in its solution, a linear convergence rate is not expected to hold true [26, 27].

To facilitate convergence of the Picard iterations it is common to use an under relaxation scheme which incorporates some portion of the previous iterations solution vectors into the current iteration. A power under relaxation factor, ω , is included in the

Picard solution in the current application. This has the effect of damping oscillations in the power profile that may be present between solution updates.

Two factors influence oscillations in the power profile between solution updates in the current coupled system. The first is due to the repeated application of an approximate Picard solution update procedure to system of coupled non-linear equations. Oscillations are damped if the system has sufficient negative feedbacks, provided in the cases investigated in this thesis by negative thermal reactivity coefficients or by introducing artificial dampening by under relaxation. Secondly, small fluctuations due to residual Monte Carlo noise persist in the heating tally result vector despite a slight reduction in magnitude by under-relaxation. These small fluctuations can be defeated by either running more particle histories in MCNP per Picard iteration or by averaging together many past energy deposition solution vectors into the current iterate by a weighted averaging process.

It is of interest to consider fixed point numerical methods with improved convergence characteristics over the basic Picard iteration scheme. Principle among them are Newton based iterations in which an approximate Jacobian computation must be performed. If the Jacobian is computationally costly or prohibitively difficult to estimate, motivation remains to use Jacobian free methods. To this end, the application of Anderson acceleration to fixed point problems that arise in core simulation calculations is an active field of research [28]. In some circumstances Anderson acceleration may be viewed as a direct upgrade to the Picard iteration scheme. Few modifications to the Picard algorithm, and thus the implementation in code, are required to adopt its use in multiphysics applications. Shown in equation 13, Anderson acceleration attempts to find a linear combination of the previous M solution vector differences, F_k .

$$F_k = G(x_k) - x_k \quad (13)$$

that minimize the L2 norm:

$$\{\alpha^{(k)}\} = \min_{\alpha} \left\| \sum_{i=0}^M \alpha_i F_{k-M+i} \right\| \quad (14)$$

With the constraint:

$$\sum_{i=0}^M \alpha_i = 1$$

Where k is the current iteration number and $M = \min(\{k, m\})$ where m is a user set max solution vector storage depth. In an Anderson scheme with no additional under relaxation (sometimes referred to as mixing), the solution is updated by equation 15:

$$x_{k+1} = \sum_i^M \alpha_i^{(k)} G(x_{k-M+i}) \quad (15)$$

This is akin to the minimal residual method for solving coupled linear equations known as GMRES. It can be shown that Anderson acceleration does not perform as intended if significant noise in the solution is introduced by the mapping of the old solution vector to the new, such in the case of using Monte Carlo methods [27]. Noise in the solution update affects the ability to meaningfully and accurately solve the Anderson minimization problem. Despite not being able to employ Anderson acceleration directly in the current work, it provides a good starting point for the implementation of an improved under-relaxation strategy in future Monte Carlo – CFD style couplings.

CHAPTER 4

Results

In this chapter MCNP-FLUENT is applied to suite of progressively more challenging geometries and operating conditions to demonstrate the accuracy and scalability of the coupling method. First, a unit fuel cell at hot zero power conditions is studied to quantify error induced in the neutron multiplication factor by using a first-order finite element representation of the geometry in MCNP rather than the traditional, exact constructive solid geometry (CSG) representation. Following the zero power case, a 2D plane wall geometry three meters in height with a moderator to fuel ratio of 1:1 is studied at full power conditions. A degree of geometric complexity is added by simulating a single PWR fuel pin at full and 75% nominal power conditions. Finally, a 3x3 fuel pin assembly without spacer grids is modeled and the coupled solution is contrasted against results provided by the MPCAT-CTF package available in VERA.

The collective suite of results provides data necessary to assess the scalability of the multiphysics coupling method. Run time versus number of cells present in the MCNP and FLUENT simulations is charted in section 4.5.

4.1 2D UNIT CELL HOT ZERO POWER

The purpose of this case is to study the reactivity worth of using MCNP's unstructured mesh capability to represent PWR fuel geometries with respect to the constructive solid geometry representation of the same geometry. In addition, run time as a function of number of elements included in the mesh is recorded.

The temperatures and moderator density for this problem are specified in Table 2 below.

The MCNP model cell shown in

Figure 15 is 5 [cm] in height with reflective boundary conditions on all external walls. No thermal hydraulic feedback is featured in this case. A moderator temperature of 600 [K] was chosen to remove possible bias from using interpolated cross sections. Light water cross section libraries were available at precisely at this temperature. For the same reason, a constant fuel temperature of 900 [K] was selected.

Figure 15: 2D Unit cell geometry.

Table 2) Unit cell problem specification.

Moderator Temperature	600 [K]
Moderator Density	0.8 [g/cc]
Fuel Temperature	900 [K]
Clad Temperature	600 [K]
Boron Concentration	0 [ppm]
Pin Pitch	1.26 [cm]
Fuel Radius	0.4096 [cm]
Outer Clad Radius	0.475 [cm]
Inner Clad Radius	0.418 [cm]
Clad Material	Zircaloy 4
Gap Material	Void
Fuel Enrichment	2.11%
Fuel Density	10.24 [g/cc]

Figure 16: Left: Top view of a pin cell finite element geometry displayed in quarter symmetry. 6 azimuthal segregations per quartile are shown. The discrepancy between the FE mesh and the CSG geometry is shown on the right.

The pin dimensions, given in Table 2 are consistent with typical Westinghouse PWR fuel design [29]. Shown in Figure 16 an approximation of the true geometry by first order cells gives rise to differences in both the fuel and moderator volume. This geometry discrepancy impacts neutron moderation near the cladding moderator boundary and the amount of fissile material in the problem. A reactivity difference of 52 [pcm] relative to the CSG base case is seen using sixteen azimuthal fuel segments per quadrant. Eigenvalue results for the unit cell case are presented in Table 3.

Table 3) Unit cell eigenvalue results.

Case	Azimuthal Segregations Per Quartile	k_{eff}	k_{eff} Diff [pcm] ($k - k_{\text{Base}}$)*1e5	Cylindrical Volume Relative Error
MCNP Base	Inf.	1.24657(± 10 pcm)	--	--
MCNP FE 6	6	1.24893 (± 20 pcm)	+236	1.15%
MCNP FE 10	10	1.24755 (± 20 pcm)	+98	0.41%
MCNP FE 16	16	1.24709 (± 20 pcm)	+52	0.16%
MPACT	Inf.	1.24511	-146	0.00%

The first order finite element representation of the geometry is shown to have significant effect on the eigenvalue with a sensitivity of approximately +200[pcm] per percent relative cylindrical volume error for an infinitely repeating pin cell lattice geometry. A moderate though acceptable discrepancy (-146 [pcm]) is seen between the MPACT deterministic result and the MCNP CSG result. Details of the MPACT solver parameters for this case and all subsequent cases are provided in Table 4.

Table 4) MPACT solver settings [8].

MPACT VERA-IN Parameter	Value
Cross Section Library	Declib56g_e7_09042013_p0mixed.fmt
Scattering Treatment	P2
MOC Ray Spacing	0.05 [cm]
Angular flux Quadrature Set	Chebyshev-Yamamoto
Polars/Octant	16
Aximuthals/Octant	8
Aximuthally flat source regions	8
Eigenvalue tolerance	1e-6

For the 56 group cross section library employed in the MPCAT simulation, MPACT is known to exhibit an eigenvalue bias of -294 [pcm] for a similar case based on Watts Barr

Nuclear Unit 1 pin cell geometry at elevated fuel temperatures ($\geq 900\text{K}$) when compared to KENO-VI and MCNPX Monte Carlo continuous energy results [29].

Fuel and moderator volume discrepancies can be corrected by artificially increasing the fuel and cladding radius such that all volumes are conserved between the CSG and finite element representations. The unit cell calculations were repeated with corrected radii. The results are presented in Table 5.

Table 5) Corrected volume MCNP unit cell hot zero power results.

Case	Azimuthal Segregations Per Quartile	k_{eff}	k_{eff} Diff [pcm] ($k - k_{\text{Base}}$)*1e5	Corrected fuel radius. (True R=0.4096)
MCNP Base	Inf.	1.24657($\pm 10\text{pcm}$)	-	-
MCNP FE 4	6	1.24689 ($\pm 20\text{pcm}$)	+32	0.41194
MCNP FE 6	10	1.24651 ($\pm 20\text{pcm}$)	-6	0.41044
MCNP FE 9	16	1.24659 ($\pm 20\text{pcm}$)	+2	0.40993

The use of ten azimuthal segments per quartile will be adopted for all subsequent cases along with the corrected fuel radius, 0.41044[cm], in place of the nominal 0.4096[cm] value. Utilizing the corrected radii in the MCNP-FLUENT geometry specification alleviates some error induced by a coarse representation of the geometry. A compromise between geometric accuracy and compute time must be made. MCNP run time sensitivity as a function of number of underlying F6 tally cells is provided in Table 6. A total of 11e6 particles were run in each MCNP simulation. 220 neutron generations were simulated. The first 65 generations were utilized only to converge the fission

source distribution and did not contribute to tally counts. A walltime of 7.5 hours on 23 cores was reported when using 4400 F6 tally cells.

Table 6) Run time vs. number of F6 tally cells.

Axial Segments	azimuth segments per quartile	F6 Cells	wall time (23 cores) [hrs]	CPU time [hrs]
10	6	1200	4.53	104.1
10	10	2000	5.81	133.6
10	16	3200	6.73	154.7
10	20	4400	7.50	172.1

Finally the unit cell case, though run without thermal hydraulic feedback, can be used to exercise the unstructured F6 tally meshing capabilities of MCNP in preparation for the application of this technique to larger geometries. Shown in Figure 17, the fission reaction rate is largest near the fuel outer surface. This is expected for fresh fuel. Fission gammas were assumed to deposit energy locally.

Figure 17: 2D unit cell energy deposition rate. Arbitrary scaling.

4.2 2D PLANE WALL

The purpose of this case is to exercise all components of the coupling methodology using thermal hydraulic conditions and energy densities similar to a PWR operating at low power while reducing the geometric complexity of the problem. A convergence study was conducted for this case in which the number of MCNP particle histories simulated per outer iteration was altered and the impact on convergence rate on the power distribution was recorded. In addition section 4.2.5 investigates the sensitivity of the coupled solution to the treatment of photon transport. Since this case consists of a 2D planar geometry, runtimes are kept to a minimum while the results of the sensitivity studies remain relevant to the 3D full-height pin cell case.

This case also provides an opportunity to check for expected trends, such as fission reaction rate depression in regions of low moderator density near the top of the reactor geometry, effectively compressing the thermal energy production of the reactor towards the bottom of the core slightly. The resolution of more detailed physics is also demonstrated. A higher fission reaction rate is expected near the moderator-fuel boundary where the thermal neutron population is largest in the fuel. A growing boundary layer should be visible when studying velocity profiles as a function of axial position in the moderator channel. Confidence in the software implementation of the coupling methodology is built by successfully predicting expected trends with a straightforward 2D case.

4.2.1 Plane Wall Setup

The geometry for the 2D plane wall case is presented in Figure 18. Details of the problem setup are given in

Table 7. Moderator reflector regions of 30 [cm] in thickness were included in the MCNP model to realistically treat axial neutron leakage. The reflector regions were not included in the CFD model. Cladding was not modeled in this problem to simplify the case further. The fuel and moderator's thermophysical properties were obtained from NIST and IAEA data tables [33, 34]. Details of the thermophysical data used in FLUENT are provided in Appendix A.

Figure 18: Side view of plane wall geometry. 2.11% enriched fuel is shown in red. The moderator is colored blue. Reflecting surfaces are shown as dotted lines.

The inlet coolant state of 500[K], 2250 [psia] is well within the subcooled regime. This inlet condition ensures no boiling occurs on the fuel-moderator interface near the top

of the coolant channel where temperatures are greatest. Ensuring boiling does not occur simplifies the CFD calculation and problem setup by negating the need for a subcooled boiling model.

Table 7) Plane wall problem setup.

Moderator Inlet Temperature	500 [K]
Pressure	2250 [psia]
Moderator Inlet Mass Flux	1200 [kg/m ² s]
Moderator Reflector height	30 [cm]
Boron Concentration	0 [ppm]
Fuel and Moderator Half-Width	0.5 [cm]
Fuel Enrichment	2.11%
Fuel Density	10.24 [g/cc]
Active Fuel Height	3 [m]
Average Volumetric Heating (Power density)	6.0e7 [W/m ³]

The parameters used in the FLUENT thermal hydraulic model are provided in Table 8. A value of 3.4% turbulence intensity was used at the inlet as determined the empirical relation for turbulence intensity for internal flows shown in equation 16 [20].

$$I = 0.16(Re)^{-1/8} \quad (16)$$

With the Reynolds number given by:

$$Re = \frac{\rho v D_e}{\mu} \quad (17)$$

And D_e is the hydraulic diameter, given by equation 18:

$$D_e = \frac{4 A_e}{W_p} \quad (18)$$

Where A_e is the area of the channel and W_p is the wetted perimeter.

Table 8) Plane wall FLUENT settings.

Inlet Hydraulic Diameter	0.01 [m]
Inlet Tubulence Intensity	3.4 %
Inlet Reynolds Number	2.09e5
Turbulence Model	K- ϵ (Enhanced wall treatment)
Mass Conservation Convergence Criteria	1e-8 [scaled, absolute]
Energy Convergence Criteria	1e-8 [scaled, absolute]
Momentum Flux formulation	2 nd order upwind
Energy Flux formulation	2 nd order upwind
Pressure-Velocity Coupling	SIMPLE

Table 9) Coupling parameters.

Power Under Relaxation Factor	0.38
Maximum Possible Outer Iterations	8
Target eigenvalue tolerance	50 [pcm]
Target Q L2 norm	1e-2

Table 9 provides the multiphysics coupling options used in this case. KCODE histories shown in Table 10 were used in the MCNP computations. The number of particles run per Picard iteration is gradually increased in an attempt to obtain the optimal convergence in minimal compute time. The first 4 outer Picard iterations serve to approach correct result and damp out early numerically induced power oscillations without expending a large computational effort. A factor of 10 increase in the number of particle histories follows, reaching a maximum value after 6 outer iterations.

Table 10) KCODE history for the plane wall case.

Outer Iteration	Particles per Generation	Inactive Generations	Total Generations
1	2e4	200	400
2	2e4	↓	800
3	3e4	↓	800
4	4e4	↓	800
5	5e5	↓	800
6	↓	↓	1200
7	↓	↓	1200
8	↓	↓	1200

A summary of the MCNP and FLUENT mesh statistics is given in Table 11. As discussed in section 3.1.1, the MCNP geometry is coarsely subdivided into bodies inside which unique temperatures and densities are tracked. The fuel region was subdivided into 12 axial 2 equal-sized radial regions; the moderator channel was segregated into 12 axial regions.

Table 11) MCNP and FLUENT mesh statistics for the 2D plane wall case.

Discretization	Number of Elements
Total MCNP UM parts	34
Total MCNP F6 tally cells	488
Total FLUENT cells	43452

4.2.2 2D Plane Wall Results

Eigenvalue results and convergence history of the normalized power distribution are given in Table 12. The target eigenvalue tolerance of 50 [pcm] was easily met. The target L2 Qnorm tolerance of 1e-2 was nearly obtained, but small fluctuations in the

power distribution remained after 8 Picard iterations at which point the simulation was terminated due to a long simulation walltime of 40 hours.

Table 12) Eigenvalue results for plane wall case.

Outer Iteration	Eigenvalue ($\pm 1\sigma$ [pcm])	L2 Q norm
1	1.25504(± 23)	--
2	1.23237(± 16)	0.336
3	1.23229 (± 15)	0.078
4	1.23250 (± 14)	0.039
5	1.23237 (± 11)	0.041
6	1.23229 (± 9)	0.023
7	1.23229 (± 9)	0.013
8	1.23232 (± 8)	0.016

In Figure 19, the energy deposition, temperature, and moderator density scalar fields after 8 Picard iterations are visualized in 2D. The power profile is slightly compressed to the bottom of the geometry where the moderator density is largest. Power peaking is seen at the edge of the fuel moderator boundary.

Figure 19: Left: Energy Deposition [W/m^3]. Center: Temperature [K]. Right: Moderator density [g/cc]. Geometry not to scale.

The velocity field within the moderator channel may be extracted from the CFD results and plotted as velocity profiles as function of axial position. Given a Reynolds number of $\sim 2\text{e}5$, well within the turbulent regime, the entrance length is estimated to be 0.34 [m] by the empirical relationship shown in equation 19 [30].

$$L_e = D_e(4.4Re^{\frac{1}{6}}) \quad (19)$$

Plots of the moderator velocity profiles are shown in Figure 20. Only very small changes in the profile shape are seen past 0.5 [m] indicating a fully developed flow has been achieved. In accordance with mass conservation, the average velocity magnitude across the channel increases slightly as the coolant density falls as it travels up the channel.

Figure 20: Left: Velocity magnitude profiles. Right: Zoom of velocity profiles with viscous sub layer and buffer zones removed. Centerline at 0.005 [m].

Moderator temperature profiles are plotted in Figure 21. Sharp gradients in the temperature field are resolved and can be seen near the fuel moderator boundary. Mesh refinement near the fluid-wall interface was applied such that the viscous sublayer is partially resolved with a maximum y^+ value of 1.2 reported by FLUENT, with an average of 0.65.

Figure 21: Plane wall moderator temperature profiles.

Figure 22: Fuel-Moderator interface axial temperature profile.

A plot of the moderate/fuel interface temperature is given in Figure 22. A maximum moderator temperature of 543[K] is achieved near the axial position of 1.8 [m] at the fuel moderator interface. From this plot it can be seen that energy deposition tally information passed from MCNP to FLUENT is coarsely resolved in the axial direction in relation to the CFD mesh. FLUENT's built in scalar field import functionality maps the

incoming data to the CFD mesh utilizing a piecewise constant formulation. In addition, axial thermal energy diffusion within the fuel is minimal due to the radially thin geometry and small thermal conductivity of the Uranium oxide fuel. Therefore small steps are visible in the axial interface temperature plot.

Figure 23: Plane wall FLUENT convergence behavior. Five outer iterations shown.

Figure 23 displays mass, energy, momentum and turbulence TH balance residuals for five consecutive outer iterations. The convergence rate of the SIMPLE iterative method is rapid in this case: The energy and mass conservation equations were satisfied within the specified tolerance of 10^{-8} in approximately 320 SIMPLE iterations per outer iteration. Outer iterations are visibly delimited in the residual plot as sharp increases in the scaled residuals when the energy deposition scalar field is updated.

Figure 24: Normalized energy deposition rate inside the fuel region.

Figure 25: Left: Volume averaged fuel temperature. Right: Volume averaged moderator temperature in the coolant channel as a function of distance to the bottom of the active fuel.

Radially averaged power density and temperature results are provided in figures Figure 24 and Figure 25 respectively. The power density plot depicts convergence behavior by plotting multiple Picard iterations with the final solution provided as a bold black line. These quantities are conveniently compared to results from other reactor

physics codes since pin-by-pin linear heat rates and channel-average moderator densities are typically available in literature rather than high resolution multi-dimensional data due to code limitations or difficulty in clear, concise portrayal of high fidelity results.

4.2.3 Plane Wall Mesh to Mesh Interpolation Accuracy

Additionally, the results of the mesh to mesh mapping operation were examined for interpolation error. This is done by comparing the volume averaged quantities of a given scalar field in the same region on the source and the destination mesh. Differences that arise in this comparison indicate interpolation error is made consistently in one direction within the domain of interest. Table 13 displays the results of this comparison for both the fuel and moderator regions of the problem. Relative percent difference is computed according to equation (20).

$$\%Relative\ Diff = \frac{100(\bar{X}_{fluent} - \bar{X}_{mcnp})}{\left| \frac{(\bar{X}_{fluent} + \bar{X}_{mcnp})}{2} - X_o \right|} \quad (20)$$

Where X is the volume averaged scalar field quantity of interest. The raw difference is normalized by the difference between the average quantity of interest and a baseline value, X_o defined to be the inlet moderator temperature (500 [K]) and density (0.843 [g/cc]).

Table 13) Volume averaged mesh to mesh interpolation error for the plane wall case.

	FLUENT mesh	MCNP Mesh	Raw Diff	%rel diff
Average Fuel T [K]	681.135	680.914	0.221	0.12%
Average Moderator Density [g/cc]	0.83131	0.83139	-8E-05	-0.68%

For the plane wall case in which the MCNP and FLUENT meshes are nearly identical due to the geometric simplicity of the problem, only small interpolation error is seen. Interpolation error arises due to non-conformal cells (i.e. cell overlap). Bias in the mapping is introduced if interpolation errors are consistently made in the same direction over the domain. Since the mesh to mesh mapping routine employed in this thesis is not conservative, minor errors are introduced in mapping between two different meshes. Conservative mesh to mesh transfer conserves integral quantities in the solution mapping process. See Data Transfer Kit's documentation for information on conservative mesh to mesh solution transfers [30].

4.2.4 Plane Wall Convergence Rate Study

Two sources of error from the neutronics calculation contribute to coupled solution defects. Non fundamental mode harmonics may persist in the spatial neutron flux distribution as a consequence of the iterative technique used by MCNP to solve the k-eigenvalue problem. See section 2.2.1 for details of the iterative procedure used to solve the k-eigenvalue problem. This source of error is reduced by running a larger number of simulated neutron generations, effectively allowing higher harmonics to decay away. Secondly, Monte Carlo noise is present in the heating tally. Monte Carlo noise in the heating tally can be reduced by either by computing integrals quantities over larger volumes, or by running a larger number of particle histories. Given limited computational resources, a balance between grid fidelity and total number of particle histories should be struck such that the coupled solution is independent of grid spacing. Obtaining the ideal mesh density and number of particle histories run per outer Picard iteration is left as an avenue for future work. The presented results only serve to quantify the benefits of running a larger number of particle histories.

Three KCODE cases are considered in this study. KCODE case information is presented in Table 14 and convergence behavior of the outer Picard iterations for each case is shown in Table 15.

Table 14) KCODE sensitivity study case definitions.

KCODE Case	KCODE History			
I	Outer Picard Iteration Index	Particles per generation	Inactive Generations	Total Neutron Generations
	1	2e4	50	100
	2	2e4	↓	200
	3	3e4	↓	200
	4	4e4	↓	200
	5	5e5	↓	200
	6	↓	↓	300
	7	↓	↓	300
	8	↓	↓	300
II	1	2e4	100	200
	2	2e4	↓	400
	3	3e4	↓	400
	4	4e4	↓	400
	5	5e5	↓	400
	6	↓	↓	600
	7	↓	↓	600
	8	↓	↓	600
	1	2e4	200	400
III	2	2e4	↓	800
	3	3e4	↓	800
	4	4e4	↓	800
	5	5e5	↓	800
	6	↓	↓	1200
	7	↓	↓	1200
	8	↓	↓	1200

The maximum relative local power (Q) difference between Picard iterations provides an estimate of the variability is present in the power distribution and is given by equation 21. The L2 power norm is the root mean squared (RMS) of the power profile differences between outer iterations and is computed by equation 22.

$$\max \Delta Q_i = \max \left[\frac{|P_j^i - P_j^{i-1}|}{P_j^i} \right] \quad (21)$$

$$L2 \ Q \ norm_i = \sqrt{\sum_j \left(\frac{P_j^i - P_j^{i-1}}{P_j^i} \right)^2} \quad (22)$$

Where i is the iteration number, j is the axial position index and P is the normalized linear heat rate. The power normalization is performed such that for the full core, the axial linear power $[W/m]$ profile averages to one.

Case I exhibits good initial convergence rate, obtaining an order of magnitude reduction in the L2 norm after 4 iterations were completed, but stagnates after 5 iterations. Further solution convergence is hampered by Monte Carlo noise present in the heating tally result and numerical oscillations in the neutron fission source distribution. A larger number of simulated particle histories per Picard iteration are required to further reduce the L2 norm of the power distribution. Case II shows moderate improvement in Picard convergence over case I; however local relative power oscillations of $\pm 2.5\%$ remain after 8 outer iterations were performed. Case III, having the largest number of particles simulated per outer iteration, achieves the tightest convergence as indicated by

the L2 norm of the energy deposition, but at great computational cost. Table 16 provides a computation time breakdown for each case.

Table 15) KCODE Convergence sensitivity study results.

Kcode case I				
Iteration	K-eff ($\pm 1\sigma$ [pcm])	K-eff difference between iterations [pcm]	L2 Q Norm	Maximum relative local Q difference between iterations (%)
1	1.25481 (± 45)	--	--	--
2	1.23145 (± 31)	-2336	0.337	21.55%
3	1.23280 (± 29)	135	0.106	7.04%
4	1.23246 (± 29)	-34	0.134	5.46%
5	1.23177 (± 20)	-69	0.043	2.07%
6	1.23236 (± 16)	59	0.104	5.34%
7	1.23209 (± 15)	-27	0.034	2.27%
8	1.23265 (± 15)	56	0.131	8.50%
Kcode case II				
1	1.25428 (± 31)	--	--	--
2	1.23266 (± 24)	-2162	0.322	19.58%
3	1.23216 (± 22)	-50	0.018	1.49%
4	1.23207 (± 20)	-9	0.067	4.40%
5	1.23236 (± 14)	29	0.111	5.41%
6	1.23238 (± 12)	2	0.072	3.62%
7	1.23213 (± 12)	-25	0.018	1.20%
8	1.23250 (± 12)	37	0.053	2.59%
Kcode case III				
1	1.25504(± 23)	--	--	--
2	1.23237(± 16)	-2267	0.336	18.95%
3	1.23229 (± 15)	-8	0.078	3.43%
4	1.23250 (± 14)	21	0.039	2.31%
5	1.23237 (± 11)	-13	0.041	2.23%
6	1.23229 (± 9)	-8	0.023	1.33%
7	1.23229 (± 9)	0	0.013	0.78%
8	1.23232 (± 8)	3	0.016	1.01%

Table 16) KCODE study compute time summary. Wall times summed over all outer iterations. 23 Cores used for FLUENT and MCNP calculations.

KCODE CASE	Total MCNP Wall Time [hr]	Total FLUENT Wall Time [hr]	Total Overhead Wall Time [hr]	Total [hr]
I	10.16	0.17	0.0021	10.34
II	20.19	0.17	0.0021	20.36
III	40.34	0.17	0.0021	40.51

Improving the Picard convergence rate and tolerance is a computationally expensive endeavor for the MCNP-FLUENT coupling method. The majority of the computational expenditure is made in the Monte Carlo calculation. As demonstrated by the runtime results provided Table 6, significant runtime reduction can be made by reducing the number of F6 heating tally cells in MCNP though caution should be observed so that the predicted behavior of the coupled system is not influenced by grid spacing. Averaging the final three L2 power norms for cases I, II, and III yields averaged norms of 0.090, 0.048, and 0.017 respectively. For this particular geometric configuration, a two fold increase in the total number of particles run results in a reduction in the minimal achievable L2 power norm tolerance by a factor of approximately $\frac{1}{2}$. This benefit requires a two-fold increase in computation time.

4.2.5 Plane Wall Gamma Transport Sensitivity

Table 17 provides the fraction of energy produced by fission that was absorbed in the moderator channel. A large fraction of the energy deposition in the moderator is due

to neutron collision heating while the remainder heating is due to gamma ray interactions with the moderator. The ability to toggle photon transport and photon heating is trivial in MCNP, requiring modification of the F6 tally card and the transport MODE card. A 0.19% increase in the energy deposited in the moderator channel was observed when photon transport was enabled, an insignificant difference.

Table 17) Fraction of energy deposited in the moderator channel.

Gamma Transport	Average Energy Deposition in fuel [W]	Average Energy Deposition in moderator [W]	Percent energy deposited in moderator
Off	6813.8	245.679	3.48%
On	6806.7	259.145	3.67%

Figure 26: Comparison of the plane wall energy deposition with gamma transport enabled and disabled in MCNP.

Figure 26 shows the predicted power distributions after 8 Picard iterations were performed. The power distribution was not discernibly impacted by enabling gamma transport. As discussed in section 4.2.4, a relative maximum percent difference of 2.2% in the local normalized power is within the expected fluctuations in the solution due to residual numerical oscillations in the solution. The KCODE cycle history for this study was identical to Case II in section 4.2.4. In all remaining cases, gamma rays will not be tracked in the MCNP simulations and assumed to deposit their energy locally when generated by fission events.

4.2.6 Plane Wall Conclusions

The plane wall case provided a test-stand in which all aspects of the MCNP-FLUENT coupling method could be exercised. The axial power profile was shown to be cosine in shape with slight power bias towards the moderator inlet. Plots of the moderator velocity field were provided to demonstrate the level of detail produced by the CFD computations. These detailed velocity and pressure field data are required to tune pressure loss and turbulent mixing coefficients used by lower fidelity nodal TH codes such as CTF. Furthermore, a review of the scaled mass, energy and momentum balance residuals provided by ANSYS FLUENT showed the excellent convergence rate of the SIMPLE pressure-velocity coupling scheme, with only 150 iterations per outer (FLUENT/MCNP) iteration required for this case.

Relatively small runtimes allowed an investigation of eigenvalue and power profile convergence as a function of number of particle histories utilized in each MCNP run. Evidence of improved convergence achieved by increasing the number of particle

histories run in MCNP as measured by the L2 norm of the power profile, maximum relative change in the power profile, and change in the eigenvalue between outer iterations was put forth in Table 15. It was concluded that a reduction in uncertainty in the power profile (*with* TH feedback enabled) by a factor of two required a factor of two increase in compute time.

In cases where the total number of particle histories per KCODE cycle approached 0.6 billion power oscillations persisted with a maximum magnitude of approximately 1%. The key observation is that power oscillations can be reduced but cannot be eliminated by increasing the particle count alone.

Finally, the impact of explicit gamma transport on the axial power profile was shown to alter the results to a degree that lies within the uncertainty inherent in the result due to residual power oscillations. Gamma transport will not be considered in the following cases.

4.3 FULL HEIGHT SINGLE ROD

The purpose of this case is to compare the power, fuel temperature, and moderator temperature distributions computed by MCNP-FLUENT to a solution provided by MPCACT-CTF. The MPACT-CTF solver parameters were set according to the values stated previously in Table 4. This is the first and simplest instance in which a coupled solution may be compared between the two codes. Despite the problem's simplicity, disparate details in the solution method, cross section data, and thermophysical material properties between the two codes can explain some small differences in the predicted solutions. The problem was run at both 100% and 75% of nominal PWR operating

power conditions. Thermophysical material properties used in the FLUENT CFD simulations are provided in Appendix A.

4.3.1 Problem Setup

A top down view of the single quarter symmetric rod is shown in Figure 27. The problem was run in quarter symmetry in MCNP and in FLUENT to reduce computation time. Reflecting boundary conditions were applied on all radial surfaces.

Figure 27: Top view of MCNP single fuel rod geometry in quarter symmetry. Constituent pseudo-cells differentiated by color.

The fuel is zoned into two equal volume radial regions. A single radial cladding region is used. The moderator is zoned by octant. In the figure, material zones are designated by color. Spacer grids were not included in the MCNP or FLUENT models. 30[cm] thick axial moderator reflector regions directly above and below the active fuel region were included into the MCNP model to properly treat neutron leakage. The reflector regions were not modeled in FLUENT. The fuel was subdivided into 2 radial and 22 axial zones. The moderator channel was subdivided into 2 octant zones and 22 axial zones. The problem geometric parameters are given in Table 18.

Table 18) Single Pin problem setup.

Moderator Inlet Temperature	500 [K]
Pressure	2250 [psia]
Full Thermal Power	0.067 [MW]
Moderator Inlet Mass Flux	1721 [kg/m ² s]
Moderator Reflector height	30 [cm]
Boron Concentration	0 [ppm]
Fuel Radius	0.4016 [cm]
Cladding inner radius	0.418 [cm]
Cladding outer radius	0.475 [cm]
Pin Pitch	1.26 [cm]
Fuel Enrichment	2.11%
Fuel Density	10.24 [g/cc]
Active Fuel Height	365.76 [cm]

Table 19) Single full height pin coupling parameters.

Power Under Relaxation Factor	0.38
Maximum Possible Outer Iterations	9
Target eigenvalue tolerance	50 [pcm]
Target Q L2 norm	1e-2

The coupling and FLUENT specific solver parameters for the single pin case are given in Table Table 19 and Table 20 respectively. The inlet turbulence intensity was estimated by equation 16. The second order upwind scheme was used in the computation of surface integral values overall enhancing solution accuracy when compared to a first order flux formulation [Flu. Manual].

Table 20) Single full height pin cell FLUENT parameters.

Inlet Hydraulic Diameter	0.015 [m]
Inlet Turbulence Intensity	3.1 %
Turbulence Model	K- ϵ w/ Enhanced wall treatment
Mass Conservation Convergence Criteria	1e-7 [scaled, absolute]
Energy Convergence Criteria	1e-8 [scaled, absolute]
Momentum Flux formulation	2 nd order upwind
Energy Flux formulation	2 nd order upwind
Pressure-Velocity Coupling	SIMPLE

Table 21) Single pin mesh statistics.

Discretization	Number of Elements
Total MCNP UM parts	92
Total MCNP F6 tally cells	14,776
Total FLUENT cells	1,112,384

The FLUENT mesh was refined at the cladding/moderator interface to achieve a maximum y^+ value of 6.6. This value is within acceptable limits, but indicates that the mesh does not resolve the viscous sub layer. The “enhanced wall treatment” option was utilized in the K- ϵ turbulence model to smoothly blend the log law of the wall at $y^+ \geq 10$ with a linear law of the wall profile at $y^+ < 10$ to improve the calculation accuracy of the interfacial convection coefficient and wall sheer stress [20].

The KCODE cycle history used in both the 100 and 75% power cases is shown in Table 22. Despite a reduction in the total number of particles run per outer iteration in comparison to the plane wall case, computation time remained large for the single fuel rod cases as the number of F6 tally elements expanded by over an order of magnitude relative to the plane wall case. The computation times required to complete the single fuel pin cases are reported in Table 23.

Table 22) 1x1 KCODE history.

Outer Iteration	Particles per Generation	Inactive Generations	Total Generations
1	3e4	100	400
2	3e4	200	800
3	3e4	200	800
4	3e4	300	1000
5	4e4	↓	1000
6	↓	↓	1200
7	↓	↓	1500
8	↓	↓	1500
9	↓	↓	1500

Table 23) 1x1 Full height pin cell computation time. Sum of all iterations.

	Total MCNP Wall Time (52 cores) [hr]	Total FLUENT Wall Time (12 cores) [hr]	Total Overhead Wall Time (1 core) [hr]	Total [hr]
Total	73.60	0.87	0.051	74.52

4.3.2 1x1, 75% Power Results

The total energy produced by the fuel at 75% of the full power rating is 0.05025 [MW]. An outlet temperature of 534.26[K] is predicted by MCNP-FLUENT, a difference of -0.4[K] compared to the MPACT-CTF result. Excellent agreement for the moderator temperature along the length of the channel is seen in Figure 28. Since the problem is run at steady state it is expected that the outlet moderator temperatures exhibit excellent agreement in order to obey conservation of energy. Small differences in outlet temperature are primarily due to differences in the thermophysical properties of water

between the FLUENT implementation (see Appendix A for details) and the steam tables used in CTF [32, 33].

Figure 28: Coolant channel plots for the full height single pin case operating at 75% power. Left: Moderator temperature profile. Right: Moderator density profile.

Figure 29: MCNP-FLUENT vs. MPACT-CTF Power distribution comparison. Single full height pin operating at 75% power conditions.

The axial power profile shown in Figure 29 yields a root mean squared (RMS) percent difference of 2.6%. The RMS difference is computed by equation 23.

$$\%RMS\ diff = \sqrt{\sum_j \left[\frac{P_{MCNP}^j - P_{MPACT}^j}{\bar{P}} \right]^2} \quad (23)$$

Where $\bar{P}$, the average normalized power, is defined to be unity.

Figure 30: MCNP-FLUENT vs. MPACT-CTF average fuel temperature comparison. Single full height pin operating at 75% power conditions.

Figure 30 depicts the radial-averaged fuel temperatures versus axial height predicted by the two approaches. A maximum average fuel temperature difference of 18[K] occurs at an axial position of 245 [cm].

Eigenvalue results alongside the L2 Q Norm convergence history are given in Table 24. MPACT-CTF reports an eigenvalue of **1.24668** for this case, a difference of **-352 [pcm]** when compared to the final eigenvalue estimate of **1.25021(±13)** after 9 outer iterations of MCNP-FLUENT were performed.

Table 24) Eigenvalue and convergence history for the 1x1 75% power case.

Outer Iteration	Eigenvalue ($\pm 1\sigma$ [pcm])	L2 Q norm	Maximum relative local Q difference between iterations (%)
1	1.25762(± 23)	--	--
2	1.25077(± 21)	0.661	25.1%
3	1.25001 (± 21)	0.076	3.2%
4	1.24983 (± 19)	0.102	3.4%
5	1.25002 (± 16)	0.038	1.4%
6	1.25002 (± 13)	0.069	2.7%
7	1.25021 (± 13)	0.077	2.7%

The 2.61% RMS predicted axial power difference between MCNP-FLUENT and MPACT-CTF is approximately equivalent to the magnitude of local power fluctuations after 9 outer iterations were performed. Therefore, a large portion of the discrepancy seen in the compared codes' power distributions may be attributed to remaining numerical fluctuations in the MCNP-FLUENT predicted power distribution. To further damp the oscillations in the power profile would require implementing and improve under-relaxation method or utilizing more particle histories in MCNP per outer iteration.

Figure 31: 1x1 pin cell CFD convergence behavior.

Figure 31 displays mass, energy, momentum and turbulence TH constitutive equation residuals for three consecutive outer iterations. Similar to the plane wall case, the energy and mass conservation equations were satisfied to within the specified tolerance of $1e-8$ and $1e-7$ respectively in approximately 150 SIMPLE iterations per outer iteration.

4.3.3 1x1, 100% Power Results

In this subsection the power of the rod is increased to 100% and results analogous to those of section 4.3.2 are presented. A moderator outlet temperature of $545.8[K]$ is predicted by MCNP-FLUENT, giving a total $\overline{\Delta T_{mod}}$ of $45.8[K]$.

Figure 32: Coolant channel plots for the full height single pin case operating at 100% power. Left: Moderator temperature profile. Right: Moderator density profile.

In Figure 32 the MCNP-FLUENT moderator temperature and density traces closely tracks the MPACT-CTF result. CTF yields an outlet temperature of 545.7[K] giving an outlet temperature difference of 0.1[K].

Figure 33 displays differences in the predicted power profiles for this case. The RMS axial power percent difference between MCNP-FLUENT and MPACT-CTF is 2.3%. The maximum relative difference is -4.0%.

Figure 33: MCNP-FLUENT vs. MPACT-CTF Power distribution comparison. Single full height pin operating at 100% power conditions.

Seen in Figure 34, a maximum radially-averaged fuel temperature difference of 22[K] occurs at an axial location of 245[cm].

Figure 34: MCNP-FLUENT vs. MPACT-CTF average fuel temperature comparison. Single full height pin operating at 100% power conditions.

Eigenvalue results and convergence history are provided in Table 25. MPACT-CTF reports an eigenvalue of **1.24110** for this case, a difference of **-355 [pcm]** when compared to the final MCNP-FLUENT eigenvalue result.

Table 25) Eigenvalue and convergence history for the 1x1 100% power case.

Outer Iteration	Eigenvalue ($\pm 1\sigma$ [pcm])	L2 Q norm	Maximum relative local Q difference between iterations (%)
1	1.25752 (± 24)	--	--
2	1.24578 (± 21)	0.982	36.1%
3	1.24443 (± 21)	0.140	6.2%
4	1.24487 (± 18)	0.082	3.6%
5	1.24492 (± 16)	0.132	5.1%
6	1.24446 (± 13)	0.072	2.9%
7	1.24491 (± 13)	0.062	2.7%
8	1.24468 (± 12)	0.132	4.6%
9	1.24465 (± 13)	0.118	3.8%

The maximum local power fluctuation in the MCNP-FLUENT coupled solution after 9 outer iterations was approximately 3.8% in magnitude. Since a maximum power differential of -4.0% between the compared codes was observed for this case, a large portion of the discrepancy can be explained by numerical error due to undamped oscillations remaining in the power profile.

4.3.4 1x1 Pin Cell Mesh to Mesh Interpolation Accuracy

Mesh to mesh interpolation error as measured by volume averaged scalar field quantity comparisons between the MCNP and FLUENT meshes remains minimal for the single pin case. The relative error reported in Table 26 is computed by equation (20).

Care was taken to ensure mesh conformality along material boundaries between the MCNP and FLUENT geometric representations to ensure, for instance, that nodes which lie within the cladding region inside the FLUENT mesh do not overlap with the Moderator region in the MCNP mesh. Cell-by-cell parity between the MCNP and FLUENT mesh was not enforced. This does not pose a significant issue to the mesh to mesh interpolation algorithm if the source data is finely sampled when volume integrals are computed on the destination mesh, especially in regions of steep gradients.

Table 26) 1x1 pin cell volume averaged quantity comparison.

	FLUENT mesh	MCNP Mesh	Raw Diff	%rel diff
Average Fuel T [K]	970.97	969.25	1.72	0.37%
Average Moderator Density [g/cc]	0.8189	0.81905	-1.5e-4	-0.63%

4.3.5 1x1 Pin Cell Conclusions

Axial power profile comparisons between MCNP-FLUENT and MPACT-CTF codes revealed a maximum relative error of -4% at both the 100% and 75% power conditions. A greater degree of power peaking was predicted by the MCNP-FLUENT coupling with a slight power shift towards the moderator inlet when compared to the MPACT-CTF result. For these conditions, eigenvalue differences of -355 and -352[pcm] were reported respectively. Excellent moderator density and temperature agreement was seen in at both power levels with a maximum outlet temperature difference of 0.4K.

The to mesh interpolation accuracy was quantified by comparing volume averaged quantities over the domain of interest between the parent and destination meshes. Between meshes the difference in the volume averaged temperature within the

fuel-zone was shown to consistently remain less than 1%. Likewise, the volume averaged moderator density between the two meshes was also less than 1%.

4.4 3x3 FUEL ROD ASSEMBLY

The 3x3 case represents a significant increase in geometric complexity compared to the single pin, quarter symmetric case in the previous section. The 3x3 case affords the opportunity to investigate the interplay of varied enrichments in each pin and empty guide tubes on the axial and radial power distributions. In contrast to previous cases, coolant cross flow plays an important role in the fluid model. Cross flow impacts the moderator density and temperature fields which in turn affects the fuel reactivity. Spacer grids were not included in the MCNP or FLUENT models. As in the previous single pin case, the results of the MCNP-FLUENT calculations are compared against solutions provided by MPACT-CTF.

4.4.1 3x3 Fuel Rod Assembly Problem Setup

The MCNP F6 tally for the 3x3 pin case contains over an order of magnitude more cells than in the single pin, quarter symmetric case. The number of UM parts, or equivalently the number of materials specified in the MCNP input, was increased from 92 to 3170. The total number of F6 tally cells present in the 3x3 problem are given in Table 27.

Table 27) 3x3 Case meshing summary.

Total MCNP UM parts	3,170
Total MCNP F6 Cells	208,928
Total FLUENT Cells	2,148,600

Figure 35 depicts the 3x3 pin layout and enrichments. Pins 6, 8, and 9 are contain 3.1% enriched fuel. Pin 5 is replaced with a moderator filled zircaloy tube with an inner radius of 0.418[cm] and an outer radius of 0.475[cm]. All other fuel pins are 2.11% enriched.

Figure 35: 3x3 case with zoned enrichment and empty central guide tube.

4.4.2 3x3, 100% Power Results

An eigenvalue of $1.29895 \pm 8e-5$ was reported by MCNP for this case after 5 Picard iterations were performed. The simulation was terminated at this point due to excessive CPU time on the cluster. MPACT reported an eigenvalue of 1.29629 for this case, a difference of 266 [pcm]. In this instance, good eigenvalue agreement is attributed to cancelation of errors. On average the moderator density is larger in the MCNP-FLUENT result when compared to MPACT-CTF increasing reactivity. In contrast, the fuel temperatures are much greater in the MCNP-FLUENT model when compared to the MPACT-CTF result, depressing reactivity.

A normalized pin power comparison plot is given in Figure 36 for this case. The MCNP-FLUENT model predicts peak power at a lower axial location than the MPACT-CTF result. A maximum relative difference of 14.5% occurs at pin 4 at a location of 25[cm] from the inlet. Differences can be partially attributed to lower average moderator densities in the immediate vicinity of the active pins at higher axial elevations in the assembly. The lower density near the active pins is a symptom of poor moderator mixing. In figure 37 the impact of poor flow mixing when compared to CTF is seen on the moderator temperature profiles for each pin cell. The central channel is not heated, and thus is contained in relatively high density, low temperature flow which does not substantially migrate to the surrounding channels due to the absence of strong turbulent mixing. The MPACT results suggest that the moderator experiences much more mixing than predicted by the FLUENT model despite the absence of spacer grids.

Figure 36: Normalized pin power plot for 3x3 case. MPACT-CTF result shown as broken black lines.

Figure 37: Average moderator temperature in each pin cell as a function of axial position.

The average outlet temperature reported by MCNP-FLUENT was 540[K]. The average moderator outlet temperature according to the MPACT-CTF result for this case was 545[K]. This discrepancy indicates the thermal power produced inside the fuel is not flowing at the expected rate into the coolant, given the total power produced in the fuel is identical between the two codes. Also, as shown in Figure 38: Average fuel temperature as function of axial position., the fuel temperatures inside the fuel are much higher than anticipated in the MCNP-FLUENT model. Due to the long compute time for this case a second computation addressing issues in the thermal transport model could not be performed.

Figure 38: Average fuel temperature as function of axial position.

Figure 39: Energy deposition rate [W/m^3] in the 3x3 assembly. 3.1% enriched pins are in front.

In Figure 39 the 3.1% enriched pins are rotated to the front of the isometric view to avoid obfuscation of the pin power variability between pin enrichments. The element-averaged energy deposition field is supported at the centroids of the $2.05e5$ elements comprising the unstructured MCNP F6 tally/mesh. The temperature and density fields are likewise supported at the cell centroids of the CFD grid which contains $2.15e6$ elements. The discrepancy in the number of cells between the meshes is due to CFD grid refinement at the fluid-cladding interface. The resolution present in the energy deposition, temperature, and density fields is superior to the MPACT-CTF result.

Figure 40: Moderator density [g/cc] (left) and temperature [K] scalar fields for the 3x3 assembly.

In the moderator temperature plot given in Figure 40 the 3.1% enriched pins are located furthest from the observer. The plot shows depression in the moderator density field surrounding the high power, 3.1% enriched pins.

4.4.3 3x3 Pin Conclusions

The temperature field produced by MPACT-CTF differs significantly from the result produced by the MCNP-FLUENT coupling. This difference is partially attributed to a discrepancy in the degree of moderator mixing predicted between the CTF and FLUENT models. In addition, the average moderator outlet temperature between the two codes differed by 5[K], indicating the FLUENT computation did not obey energy conservation. Addressing these issues in the thermal hydraulics model was not possible due to exceptionally long compute times.

To complete 5 outer iterations for this problem consumed in excess of 19,000 CPU hours on 64 AMD Opteron 2.1GHz cores. This corresponds to a wall time of 12.5 days. In terms of number of F6 tally cells and number of distinct materials tracked by MCNP the 3x3 pin configuration is approaching the limit of problem size tractable to the MCNP-FLUENT coupling on the available computing equipment. The fidelity required in the F6 heating tally in order to reduce aliasing error in the mapping of the volumetric heating field to FLUENT precludes the user from coarsening the heating tally in an effort to reduce runtimes. The FLUENT and mesh to mesh mapping runtimes were negligible when compared to the MCNP runtime. Future improvements to the tally rendezvous and particle tracking routines on unstructured meshes inside MCNP in addition to the the availability of much larger computers could reduce run times.

4.5 SCALABILITY SUMMARY

In this section, CPU time results for MCNP are presented for a variety of cases. CFD and overhead run times are omitted as the MCNP computation comprises >95% of all computation time for all studied cases. Table 28 provides MCNP CPU times in relation to the number of particles run and number of F6 tally elements. CPU time is estimated as the number of cores multiplied by wall clock time. The timing results include the setup and teardown time internal to the MCNP calculation. The setup time includes the time required to build the F6 mesh from an ABAQUS unstructured mesh file input and to setup communication between all MPI processes. Teardown time includes the time to write results to the hard disk.

Table 28) MCNP timing results derived from unit cell, plane wall and full height single fuel pin cases.

Picard Iteration	# Mat Cards	F6 Cells	Particles/gen	Total Generations	Total Particles Run	CPU Time [hrs]
Unit Cell						
1	20	2000	5e4	220	1.1e7	133
1	20	3200	5e4	220	1.1e7	154
1	20	4400	5e4	220	1.1e7	172
Plane Wall						
1	32	448	2e4	400	8.0e6	6
2	↓	↓	2e4	800	1.6e7	12
3	↓	↓	3e4	800	2.4e7	18
4	↓	↓	4e4	800	3.2e7	25
5	↓	↓	5e5	800	4.0e8	31
6	↓	↓	5e5	1200	6.0e8	46
7	↓	↓	5e5	1200	6.0e8	46
8	↓	↓	5e5	1200	6.0e8	46
Full Height Pin Cell (quarter symmetry)						
1	92	14776	3e4	400	1.2e7	145
2	↓	↓	3e4	800	2.4e7	285
3	↓	↓	3e4	800	2.4e7	287
4	↓	↓	3e4	1000	3.0e7	358
5	↓	↓	4e4	1000	4.0e7	358
6	↓	↓	4e4	1200	4.8e7	430
7	↓	↓	4e4	1500	6.0e7	712
8	↓	↓	4e4	1500	6.0e7	712
9	↓	↓	4e4	1500	6.0e7	712
3x3 Pin Assembly (full symmetry)						
1	3170	208928	5e4	150	7.5e6	950
2	↓	↓	7e4	300	2.1e7	2850
3	↓	↓	8e4	500	4.0e7	2900
4	↓	↓	1e5	500	5.0e7	5400
5	↓	↓	2e5	500	1.0e8	6800

In addition to the number of F6 tally cells and total number of particles simulated, the number of materials specified in the problem also increases the run time. A larger number of materials demands a larger library of ACE cross sections be loaded into memory. Given these three factors, the available timing data set is not large enough to enable regression analyses to extrapolate run times outside of the investigated material, F6 cell, and particle count range.

CHAPTER 5

Conclusion

The multiphysics coupling methods employed in this work successfully brought together MCNP v.6.1 and ANSYS FLUENT v.14.0. The methodology allowed field data to be passed between the two codes in an automated fashion. An under relaxed Picard iteration scheme provided the multiphysics framework that guided the construction and implementation of coupling routines. NJOY was employed to generate ACE formatted Doppler broadened cross sections at specified 50K intervals which were utilized in a pseudo material mixture routine. As discussed in section 3.1.4 Doppler Feedback, the pseudo material mixing approach allowed the coupling methodology to account for the effects of Doppler broadening on reactivity.

Excellent geometric and F6 tally generation flexibility was provided by leveraging MCNP v6's unstructured meshing capability. In principle, any geometry that can be drawn in a Computer Aided Design (CAD) software can be incorporated into the MCNP and ANSYS FLUENT model. Geometry construction was performed by stacking together individually meshed "parts" to create a complete problem assembly. The number of individual parts corresponded to the number of distinct MCNP material regions in the problem. Control of the size and type of mesh elements used in the F6 heating tally was made possible by harnessing the unstructured meshing capabilities of MCNP and by adopting a highly flexible mesh generation program, in this instance GMSH. This approach to problem construction enables the methods put forth in this thesis to be applied in cases where voxelization of organic, complicated geometries is required. Examples include advanced reactor fuel geometries, and dose computations involving organic geometry.

The single pin case conducted with no thermal hydraulic feedback and no axially dependence exercised MCNP's unstructured mesh tally and geometry construction capabilities. Eigenvalue agreement between MCNP-FLUENT and MPACT-CTF was within 150 [pcm]. The influence of using a linear finite element representation of the curved fuel pin geometry was quantified. Artificially expanding the fuel and moderator regions in the finite element geometry such that fuel and moderator volumes were preserved corrected reactivity differences.

The 2D plane wall configuration with thermal hydraulic feedbacks enabled provided a test-bed for the coupling methodology. The number of particle histories simulated per Picard iteration performed was shown to have a substantial impact on the heating tally tolerance. A factor of two decrease in the magnitude of local power fluctuations was shown to require a factor of two increase in the total number of particle histories run.

Comparisons with MPACT-CTF for the single pin case with thermal hydraulic feedbacks yielded maximum power profile discrepancies of 4.0% at both the 75% and 100% power conditions. Eigenvalue agreements of 355[pcm] were achieved. In the 3x3 assembly, a lack of turbulent mixing and issues with energy conservation lead to large discrepancies between the MCNP-FLUENT and MPACT-CTF solutions. A compute time of 12.5 days for this case precluded additional coupled runs from being performed for this case. Qualitatively correct trends in the power profiles due to varied enrichments were predicted by MCNP-FLUENT, however. With this case, the ability to produce results on a 2e6 element CFD mesh and a 2e5 element F6 tally was demonstrated on modest computer hardware.

Challenges remain to be overcome as development of MCNP-FLUENT's coupling capabilities continues. The outer loop convergence rate in MCNP-FLUENT is

diminished by Monte Carlo noise; however under-relaxation was shown to dampen statistical jitter and to facilitate convergence of Picard iterations. In future work, an optimal under relaxation strategy similar to the method outlined in section 3.1.6, akin to Anderson acceleration, could be implemented to further improve the convergence rate. However, such an implementation of an optimal relaxation scheme is not straightforward due to the presence of Monte Carlo noise introduced in the solution vector by MCNP. It is not expected that Anderson acceleration could be used directly in the case of Monte Carlo radiation transport - CFD coupling applications. Previous work on Anderson acceleration can be used as a starting point for the development of a generalized strategy for optimally choosing weighting coefficients in order to dampen power oscillations.

Improvements in the mesh to mesh solution mapping techniques are possible. Utilizing a higher order interpolation scheme would reduce the aliasing error incurred when mapping the F6 heating tally to the CFD grid. Data Transfer Kit (DTK) can provide the necessary tools to reduce this aliasing error. DTK is a C++ library designed to perform solution mapping between computational grids. DTK offers locally conservative interpolation schemes for point cloud (mesh-free) data representations by leveraging compactly supported radial basis functions [31]. In order to utilize DTK in the current implementation, DTK interfaces must be developed for MCNP and ANSYS FLUENT. The custom interfaces would then be wrapped in Python.

Appendix A

A-1: THERMOPHYSICAL PROPERTIES

The thermophysical properties of water at 2250[psia] utilized in all FLUENT calculations are provided in figures Figure 41 through Figure 43. Steam table data was extracted from the NIST REFPROP program [33]. The data was interpolated by piecewise continuous polynomial functions. All material properties were implemented by User Defined Functions (UDFs) in FLUENT. The UDFs and all Python coupling scripts are available online at bitbucket.org/mcoveri/mcnp-th. The functions and ranges of validity are specified in section Appendix A-2.

Figure 41: Viscosity of water at 2250[psia].

Figure 42: Density of water at 2250[psia].

Figure 43: Isobaric specific heat of water at 2250[psia].

Thermophysical properties of Uranium oxide and Helium fill gas were obtained from [34]. The UDF code is provided in section A-2. In addition to material properties, the UDF code contains the subroutine DEFINE_SOURCE which is required to allocate a

user defined scalar (UDS) field inside FLUENT so that a custom volumetric heat source may be read, interpolated, and stored as a solution variable.

A-2: UDF CODE

```

/***** FLUENT UDF *****/

#include "udf.h"

// H2O PROPS at 2250 psia
DEFINE_PROPERTY(H2O_density, cell, thread)
{
    real t, rho;
    t = C_T(cell, thread);
    // w / m K
    if (t < 300.)
    {
        rho = 1003.4;
    }
    else if (t < 618.01)
    {
        rho = -6.95709e-8*pow(t,4.)+1.17907e-4*pow(t,3.)-7.61556e-2*pow(t,2.)+21.2884*t-1151.26;
    }
    else
    {
        rho = 594.13;
    }
    return rho;
}

DEFINE_PROPERTY(H2O_solid_density, cell, thread)
{
    real t, rho;
    t = C_T(cell, thread);
    // w / m K
    if (t < 300.)
    {
        rho = 1003.4;
    }
    else if (t < 618.01)
    {
        rho = -6.95709e-8*pow(t,4.)+1.17907e-4*pow(t,3.)-7.61556e-2*pow(t,2.)+21.2884*t-1151.26;
    }
    else
    {
        rho = 594.13;
    }
    return rho;
}

DEFINE_PROPERTY(H2O_viscosity, cell, thread)
{
    real t, mu;
    t = C_T(cell, thread);
    // w / m K
    if (t < 380.)
    {
        mu = -9.09487e-10*pow(t, 3.)+1.01182e-6*pow(t, 2.)-3.78494e-4*t+0.0478904;
    }
    else
    {
        mu = 6.66161e-14*pow(t, 4.)-1.53465e-10*pow(t, 3.)+1.32487e-7*pow(t, 2.)-5.12276e-5*t+7.63282e-3;
    }
    return mu;
}

DEFINE_SPECIFIC_HEAT(H2O_cp, t, Tref, h, yi)
{

```

```

real cp;
// real hRef;
// hRef = 0.0; // enthalpy at ref T of 298.15K
// j / mol K -> j / kg K
if (t < 460.)
{
    cp = 6.7314e-8*pow(t, 4.)-5.94628e-5*pow(t, 3.)+0.0191488*pow(t, 2.)-2.40736*t+4198.27;
    *h = (1./5.)*6.7314e-8*pow(t, 5.)-(1./4.)*5.94628e-5*pow(t, 4.)+(1./3.)*0.0191488*pow(t, 3.)
        -(1./2.)*2.40736*pow(t, 2.)+4198.27*t
        - ((1./5.)*6.7314e-8*pow(Tref, 5.)-(1./4.)*5.94628e-5*pow(Tref,
4.)+(1./3.)*0.0191488*pow(Tref, 3.)
        -(1./2.)*2.40736*pow(Tref, 2.)+4198.27*Tref);
}
else if (t < 618.01)
{
    cp = 7.29113e-6*pow(t, 4.)-1.43767e-2*pow(t, 3.)+10.6559*pow(t, 2.)-3512.65*t+438300;
    *h = (1./5.)*7.29113e-6*pow(t, 5.)-(1./4.)*1.43767e-2*pow(t, 4.)
        +(1./3.)*10.6559*pow(t, 3.)-(1./2.)*3512.65*pow(t, 2.)+438300*t
        - ((1./5.)*7.29113e-6*pow(Tref, 5.)-(1./4.)*1.43767e-2*pow(Tref, 4.)
        +(1./3.)*10.6559*pow(Tref, 3.)-(1./2.)*3512.65*pow(Tref, 2.)+438300*Tref);
}
else
{
    cp = 7.29113e-6*pow(618.01, 4.)-1.43767e-2*pow(618.01, 3.)+10.6559*pow(618.01, 2.)-
3512.65*618.01+438300;
    *h = (1./5.)*7.29113e-6*pow(618.01, 5.)-(1./4.)*1.43767e-2*pow(618.01, 4.)
        +(1./3.)*10.6559*pow(618.01, 3.)-(1./2.)*3512.65*pow(618.01, 2.)+438300*618.01
        - ((1./5.)*7.29113e-6*pow(Tref, 5.)-(1./4.)*1.43767e-2*pow(Tref, 4.)
        +(1./3.)*10.6559*pow(Tref, 3.)-(1./2.)*3512.65*pow(Tref, 2.)+438300*Tref);
}
return cp;
}

// UO2 PROPS
DEFINE_PROPERTY(UO2_conductivity, cell, thread)
{
    real t, k1;
    t = C_T(cell, thread) / 1000.;
    // w / m K
    k1 = 100. / (7.5408 + 17.692*t + 3.6142*pow(t, 2.)) + 6400. / pow(t, 5./2.) * exp(-16.35/t);
    return k1;
}

DEFINE_SPECIFIC_HEAT(UO2_cp, t, Tref, h, yi)
{
    real cp;
    real m;
    real TT;
    real TTref;
    // real hRef;
    // hRef = 0.0; // enthalpy at ref T of 298.15K
    m = 270.0e-3; // kg / mol
    TT = t/1000.;
    TTref = Tref/1000.;
    // j / mol K -> j / kg K
    cp = (1./m) * (52.1743 + 87.951*(TT) - 84.2411*pow((TT), 2.) + 31.542*pow((TT), 3.) -
2.6334*pow((TT), 4.) - 0.71391*pow((TT), -2.));
    *h = (1./m) * (
        -21.1762 + 52.1743*TT + 43.9753*pow(TT, 2.) - 28.0804*pow(TT, 3.) + 7.88552*pow(TT, 4.)
        - 0.52668*pow(TT, 5.) + 0.71391*pow(TT, -1.)
        - (-21.1762 + 52.1743*TTref + 43.9753*pow(TTref, 2.) - 28.0804*pow(TTref, 3.) +
7.88552*pow(TTref, 4.)
        - 0.52668*pow(TTref, 5.) + 0.71391*pow(TTref, -1.))
    );
    return cp;
}

// ZIRC-2 PROPS
DEFINE_PROPERTY(zirc_conductivity, cell, thread)
{
    real t, k1;
    t = C_T(cell, thread);
    // w / m K
    k1 = 12.767 - 5.4348e-4*t + 8.9818e-6*pow(t, 2.);
    return k1;
}

```

```

}

DEFINE_SPECIFIC_HEAT(zirc_cp, t, Tref, h, yi)
{
    real cp;
    // real hRef;
    // hRef = 0.0; // enthalpy at ref T of 298.15K
    // j / kg K
    cp = 255.66 + 0.1024*t;
    *h = 255.66*t + (1./2.)*0.1024*pow(t, 2.)
        - (255.66*Tref + (1./2.)*0.1024*pow(Tref, 2.));
    // *h = cp*(t-Tref);
    return cp;
}

// He PROPS
DEFINE_PROPERTY(he_conductivity, cell, thread)
{
    real t, k1;
    t = C_T(cell, thread);
    // w / m K
    // k1 = -5.84419e-8*pow(t, 2.) + 3.66895e-4*t + 5.38251e-2; // He Prop
    k1 = 0.4769772; // assuming gap of 0.0084 cm and h of 5678.3 W / m k
    return k1;
}

DEFINE_PROPERTY(he_density, cell, thread)
{
    real t, rho;
    t = C_T(cell, thread);
    // kg/m3
    rho = 1.27027e-7*pow(t, 2.) - 3.15058e-4*t + 0.230879;
    return rho;
}

DEFINE_SOURCE(vol_heat_source, cell, thread, dS, eqn)
{
    real source;
    source = C_UDSI(cell, thread, 0);
    return source;
} /***** END FLUENT UDF *****/

```

Bibliography

- [1] J.R. Haines, et. al. Spallation neutron source target station design, development, and commissioning. Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment. Volume 764, 11 November 2014, Pages 94–115
- [2] Cold Neutron Source. ANSTO. Web. 23 Nov. 2015. <http://www.ansto.gov.au/>
- [3] S.I., WU, and KIM Y.K. INSTALLATION OF COLD NEUTRON SOURCE AT HANARO. Korea Atomic Energy Research Institute (KAERI). http://www-pub.iaea.org/MTCD/Publications/PDF/P1575_CD_web/datasets/papers/A25%20Wu.pdf
- [4] Technische Univ. Muenchen (Germany); Framatome ANP GmbH, Erlangen (Germany). Intense positron source at the Munich research reactor FRM-II. Meeting of the International Group on Research Reactors (IGORR). Munich (Germany). 17-20 Apr 2001.
- [5] B. Kochunas. D. Jabayy. T. Downar. VERA Problem 10: Restart and Shuffling in MPACT. CASL-U-2014-0231-001. February 2015. www.casl.gov/docs/CASL-U-2014-0231-001.pdf
- [6] T. S. Blyth. Improvement of COBRA-TF Subchannel Thermal-Hydraulics Code (CTF) using CFD. CASL-U-2015-0020-000. December 2014. www.casl.gov/docs/CASL-U-2015-0020-000.pdf
- [7] B. Collins, et. al. Demonstration of Full Core Reactor Depletion with MPACT. CASL-U-2014-0140-000. 2014. www.casl.gov/docs/CASL-U-2014-0140-000.pdf
- [8] S. Palmtag, A. Godfrey. User Manual for the VERA Input Processor. CASL-U-2014-0014-002. 2015. www.casl.gov/docs/CASL-U-2014-0014-002.pdf
- [9] Neutronics and CFD Analysis: MCNPX-ANSYS Fluent Coupling. Idom Nuclear Services. April 2013.
- [10] C. Hughes, K. Jordan, D. Schubring. Coupled Computational Heat Transfer and Reactor Physics for SCWR. Proceedings from the ASME Heat Transfer Summer Conference. 2013.

- [11] J.L. Collins. et al. Pseudo Material Construct for Coupled Neutronic-Thermal-Hydraulic Analysis of VHTGR. Transactions of the American Nuclear Society. 2005.
- [12] Jianwei, Hu, and Rizwan-uddin. "Coupled Neutronics and Thermal-Hydraulics Simulations Using MCNP and FLUENT." Advancements in Multi-Physics Reactor Simulation, 2008.
- [13] Cardoni, Jeffery. Thesis: NUCLEAR REACTOR MULTI-PHYSICS SIMULATIONS WITH COUPLED MCNP5 AND STAR-CCM+. U of Illinois at Urbana-Champaign, 2011.
- [14] J. Yan, B. Kochunas, M. Hursin, T. Downar, Z. Karoutas. Coupled Computational Fluid Dynamics and MOC Neutronic Simulations of Westinghouse PWR Fuel Assemblies with Grid Spaces. 14th International Topical Meeting on Nuclear Reactor Thermalhydraulics, NURETH14-254. 2011.
- [15] V. Seker, J.W. Thomas, T. Downar. Reactor Physics Simulation with Coupled Monte Carlo Calculations and Computational Fluid Dynamics. International Conference on Emerging Nuclear Energy Systems (ICENES). 2007.
- [16] Lewis, E. E., and W. F. Miller. Computational Methods of Neutron Transport. La Grange Park, IL, USA: American Nuclear Society, 1993.
- [17] Yun, Sunghwan, and Nam Zin Cho. "Acceleration of Source Convergence in Monte Carlo K-eigenvalue Problems via Anchoring with a P-CMFD Deterministic Method." Annals of Nuclear Energy 37.12, 2010: 1649-658.
- [18] MCNP6 Users Manual - Code Version 6.1.1beta, LA-CP-14-00745. June 2014.
- [19] R.L. Martz. The MCNP6 Book on Unstructured Mesh Geometry: User's Guide. [LA-UR-11-05668-rev8](#). 2014.
- [20] ANSYS INC. "Fluent 14 Theory Guide." 2009.
- [21] S. Patankar. Numerical Heat Transfer and Fluid Flow. CRC Press, 1980.

- [22] C. Geuzaine and J.-F. Remacle. [Gmsh: a three-dimensional finite element mesh generator with built-in pre- and post-processing facilities](#). International Journal for Numerical Methods in Engineering 79(11), pp. 1309-1331. 2009.
- [23] SciPy Reference guide v 0.14.0. The Scipy Community. <http://www.scipy.org>
- [24] Macfarle et al. The NJOY Nuclear Data Processing System: User's Manual. Los Alamos USA. 1993.
- [25] R. Stammler and M. Abbate, Methods of Steady-State Reactor Physics in Nuclear Design, Academic Press 1983.
- [26] R. Pawlowski, R. Bartlett, N. Belcourt, N. Hooper. R. Schmidt. A Theory Manual for Multi-Physics Code Coupling in LIME. Sandia National Laboratory. SAND2011-2195. 2011.
- [27] Kelley, C.T., and A.R. Toth. Convergence Analysis for Anderson Acceleration. Society for Industrial and Applied Mathematics (SIAM) Journal on Numerical Analysis (SINUM), November 13, 2014.
- [28] Toth, A.R., C.T. Kelley, S.R. Slattery, S.P. Hamilton and K.T. Clarno, "Analysis of Anderson Acceleration on a Simplified Neutronics/Thermal Hydraulics System," Proceedings of the ANS MC2015 - Joint International Conference on Mathematics and Computation (M&C), Supercomputing in Nuclear Applications (SNA) and the Monte Carlo (MC) Method, Volume ANS MC2015 CD, April 19, 2015, Nashville, Tennessee, 2015.
- [29] Godfrey, A., VERA Core Physics Benchmark Progression Problem Specifications, Revision 4, CASL Technical Report: CASL-U-2012-0131-004, August 29, 2014.
- [30] Munson, Bruce Roy, T. H. Okiishi, and Wade W. Huebsch. Fundamentals of Fluid Mechanics. Wiley & Sons, 2009.
- [31] S. R. Slattery. Mesh-Free Data Transfer Algorithms for Partitioned Multiphysics Problems: Conservation, Accuracy and Parallelism. CASL-U-2014-0128-000. 2014. [http://www.casl.gov/docs/ CASL-U-2014-0128-000.pdf](http://www.casl.gov/docs/CASL-U-2014-0128-000.pdf)
- [32] R. Salko, M. Avramova. COBRA-TF Subchannel Thermal Hydraulics Code (CTF) Manual. CASL-U-2015-0054-000. 2015.

- [33] Eric. W. Lemmon, Marica L. Huber, Mark O. McLinden. REFPROP User Guide. NIST, 2007. <http://www.nist.gov/srd/upload/REFPROP8.PDF>
- [34] Thermophysical Properties Database for Light Water Reactors and Heavy Water Reactors. IAEA-TECDOC-1496. 2006.
- [35] Jin, M., and M. Short, Two-Phase Fluid Flow Modeling in CRUD using MAMBA-BDM, CASL Technical Report CASL-U-2014-0143-000, February 17, 2014.