DEMONSTRATION OF COUPLED FUEL PERFORMANCE CALCULATIONS IN VERA ON WATTS BAR UNIT 1, CYCLE 1

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ABSTRACT

As the core simulator capabilities in the Virtual Environment for Reactor Applications (VERA) have become more mature and stable, increased attention has been given to coupling BISON to provide fuel performance simulations. This technique has been a very important driver for the pellet-clad interaction challenge problem being pursued by the Consortium for Advanced Simulation of Light Water Reactors (CASL).

In this paper, two coupling approaches are demonstrated on quarter core problems based on Watts Bar Nuclear Plant Unit 1, Cycle 1: (1) an Inline approach, in which a one-way coupling is used between MPACT/CTF and BISON, but no fuel temperature information is passed back to MPACT/CTF, and (2) a two-way approach (Coupled) in which the fuel temperature is passed from BISON. In both approaches, power and temperature distributions from MPACT/CTF are used to inform the BISON simulations for each rod in the core.

These demonstrations present the first integrated fuel performance simulations in VERA, which opens many possibilities for future work, including applications to accident-tolerant fuel efforts and transient simulations, which are of critical importance to CASL. They also highlight the potential to move away from the current BISON-informed fuel temperature lookup table approach, which is the default in MPACT/CTF simulations, if performance improvements are made in the near future.

KEYWORDS: VERA, MPACT, CTF, BISON, coupling

1. INTRODUCTION

For several years now, the core simulator capabilities in the Virtual Environment for Reactor Applications (VERA) [1] provided by coupled MPACT and CTF calculations have become more mature and stable. A natural next step is to incorporate additional physics into these simulations. Achieving this next step could lead to extremely important contributions to the challenge problems being tackled by the Consortium for Advanced Simulation of Light Water Reactors (CASL). For example, coupling MAMBA to simulate the CRUD formation, and the resulting CRUD-induced power shift, has been a focus of recent efforts [2]. This has generated significant interest from industry partners and potential collaborators. Similarly, coupling BISON to provide high fidelity, finite-element-based fuel performance simulations has been a very important driver for progress in pellet-clad interaction (PCI) simulations [3,4]. Without this coupling, MPACT/CTF calculations rely on lookup tables to determine the fuel temperature, so important fuel performance characteristics such as thermal expansion, fuel densification, swelling, clad creep, and pellet-clad interaction are only indirectly accounted for. This coupling allows for a much higher fidelity simulation by allowing all of these (and others not listed) to directly impact the fully coupled results through VERA.

A few different approaches have been developed for this coupling. The first and most basic approach is a simple file-based, one-way coupling between MPACT/CTF and BISON in which MPACT/CTF-coupled simulations are run to completion and the output from those simulations is then used to build a separate BISON input for each rod in the core. While this capability has provided a lot of results for larger-scale problems and has been used as a screening tool for PCI analysis, there is no feedback from the BISON rods to the MPACT/CTF simulations.

The next two approaches involve a more direct coupling with BISON using internal data transfers to communicate the power and temperature distributions. The first is referred to as Inline, which provides the same one-way coupling as the file-based approach, but all the power and temperature data from MPACT/CTF are passed internally to BISON, which runs simulations for the rods as the MPACT/CTF calculation is happening. The second is Coupled, which couples all three codes, solving each code every outer iteration. With this approach, MPACT is solved first, and then BISON and CTF both execute concurrently using the power information from MPACT. BISON also uses the clad outer surface temperature as a boundary condition but with a lagged value from CTF from the previous outer iteration.

These approaches have resulted in significant progress on the PCI challenge problem. Ideally, use of these approaches will become more common for typical production-level analysis problems as performance improvements are made in the future. Brief descriptions of the individual codes used in this coupling are given below.

MPACT

The MPACT neutron transport solver being developed collaboratively by Oak Ridge National Laboratory (ORNL) and the University of Michigan provides pin-resolved flux and power distributions [5]. To solve three-dimensional (3D) problems, it employs the two-dimensional/one-dimensional (2D/1D) method, which decomposes the problem into a 1D axial stack of 2D radial planes [6], [7]. Typically, 2D Method of Characteristics is used to solve each radial plane, and 1D nodal methods are used to solve axially along each rod. While a variety of axial solvers are available, the nodal expansion method (NEM)-P_3 solver is the default, wrapping a one-node NEM kernel [8]. These 2D and 1D solvers are coupled together through transverse leakage terms to ensure neutron conservation, and they are accelerated using 3D coarse mesh finite difference.

CTF

CTF is a subchannel thermal hydraulics code being developed by ORNL and North Carolina State University specifically for light water reactor analysis [9]. It simulates two-phase flow with a three-field representation—liquid, droplet, and vapor—assuming that the liquid and droplet fields are in dynamic equilibrium, leaving two energy conservation equations.

BISON

The BISON fuel performance code is being developed by Idaho National Laboratory (INL) to provide single-rod fuel performance modeling capability so users can assess best-estimate values of design criteria and the impact of plant operation and fuel rod design on thermomechanical behavior such as PCI failures in pressurized water reactors (PWRs) [10,11]. Because PCI is controlled by a complex relationship of multiple physics, modeling PCI requires an integral fuel performance code to simulate the fundamental processes of these behaviors. BISON is built on INL's Multiphysics Object- Oriented Simulation Environment (MOOSE) package [12,13], which uses the finite element method for geometric representation and a Jacobian Free Newton-Krylov scheme to solve systems of partial differential equations [13]. For this work, BISON uses a 2D azimuthally symmetric (RZ) smeared-pellet thermomechanical fuel pin model, with boundary and heat source data from VERA, to generate the time-dependent power shape/history and moderator temperature inputs needed for BISON.

It should be noted that many of the details in this paper have been adapted from a larger technical report that contains the full details [14].

2. OVERVIEW OF COUPLING APPROACHES

For each user-defined time step, MPACT computes the axial power distribution within each rod at the end time and passes it to both CTF and BISON. Then, the latest solution for the clad surface temperature is passed from CTF to BISON. The coupling then leverages MOOSE MultiApps to (1) restore every rod to the end time of the previous state, (2) adaptively time step each rod to the next user-defined state, and (3) pass the fuel temperature back to MPACT.

It is also important to note that by running BISON and CTF at the same time, the cladding's outer surface temperature boundary condition—used by BISON, which receives the value from CTF—is actually lagged by an outer iteration. At convergence there is no issue, but since the outer surface temperature does not change substantially, it likely has very little impact on the overall convergence. In fact, when comparing the number of iterations to a normal MPACT/CTF calculation, the Coupled calculations seem to consistently take fewer outer iterations. With the boundary condition lagged, the effect is largely relaxed, which could lead to more optimal convergence.

The left panel of Figure 1 shows a flowchart for a Coupled calculation scheme. MPACT and CTF share processors because of the internal coupling between the codes, and the BISON calculations are performed on an entirely different set of processors. The right panel of Figure 1 shows a comparable flowchart for the Inline calculation in which MPACT and CTF are fully converged. In this case, the processors dedicated to BISON solves will run the BISON cases while the MPACT/CTF processors continue with the next state; therefore, the BISON processors lag behind the MPACT/CTF processors by a statepoint. The MPACT/CTF calculation will not proceed past one iteration ahead if the BISON calculation takes longer. This does not typically occur, although select statepoints may take longer than others, particularly during power ramps.

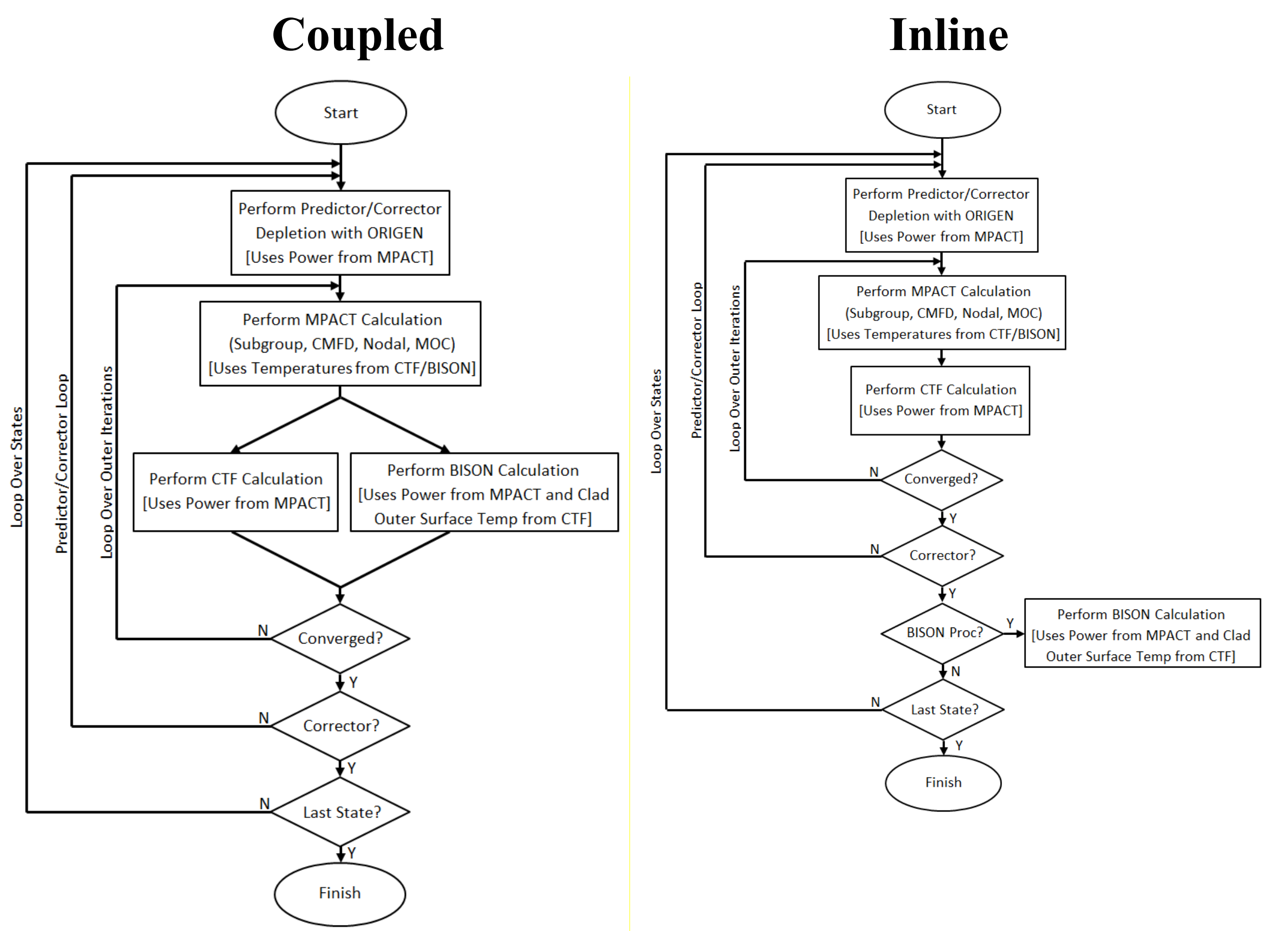

Figure 1. Flowchart of the Coupled (left) and Inline (right) Calculations.

3. BISON 1.5D CAPABILITY

Historically, VERA's usage of BISON has focused on 2D-RZ simulations, but these have been found be both slower and less robust than desired for coupled cases, such as those presented here. In February 2017, the BISON team delivered an initial 1.5D-RZ capability, which effectively solves the fuel rod using an axial stack of layered 1D-radial problems. All the layered 1D-radial problems are coupled together through the gas pressure, and an axial pressure applied to the fuel/clad while axial conduction is ignored. Energy conservation and stress divergence are solved along each plane using finite elements in 1D with thermal and mechanical contact. Axial effects are accounted for by summing displacements in each slice using a generalized plane strain formulation. Figure 2 illustrates the 1.5D capability [15].

The goal of the 1.5D capability is to resolve computational performance issues of speed and robustness that were observed with the 2D-RZ models. The BISON team also released a report documenting the verification and validation efforts of the 1.5D model, comparing it to 2D-RZ calculations [16].

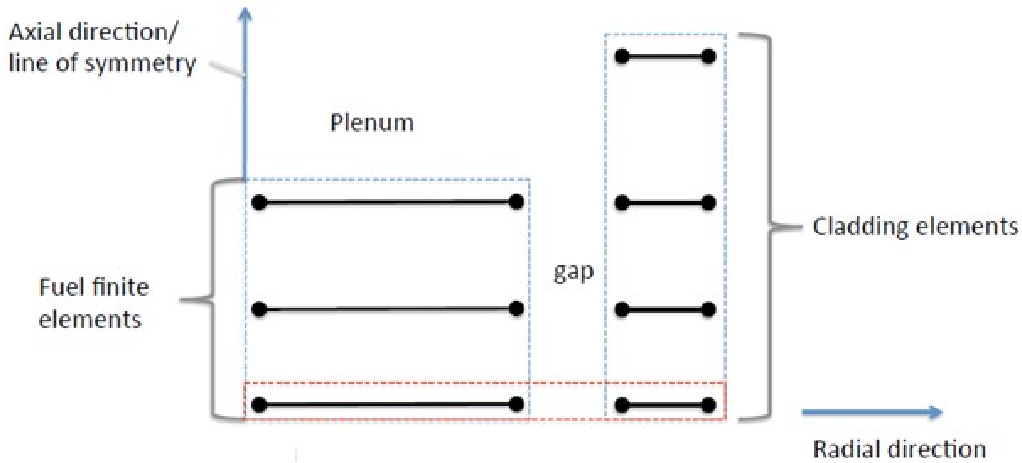

Figure 2. 1.5D Capability Schematic [15].

4. WATTS BAR UNIT 1 DESCRIPTION

All results presented here focus on the Watts Bar Nuclear Plant, a Westinghouse Electric Company four-loop PWR operated by the Tennessee Valley Authority. Online since 1996, it began with a 3,411 MWth power rating and underwent a 1.4% power uprate in 2001. It is currently operating in its 15th cycle, logging over 6,000 effective full power days of operation [17].

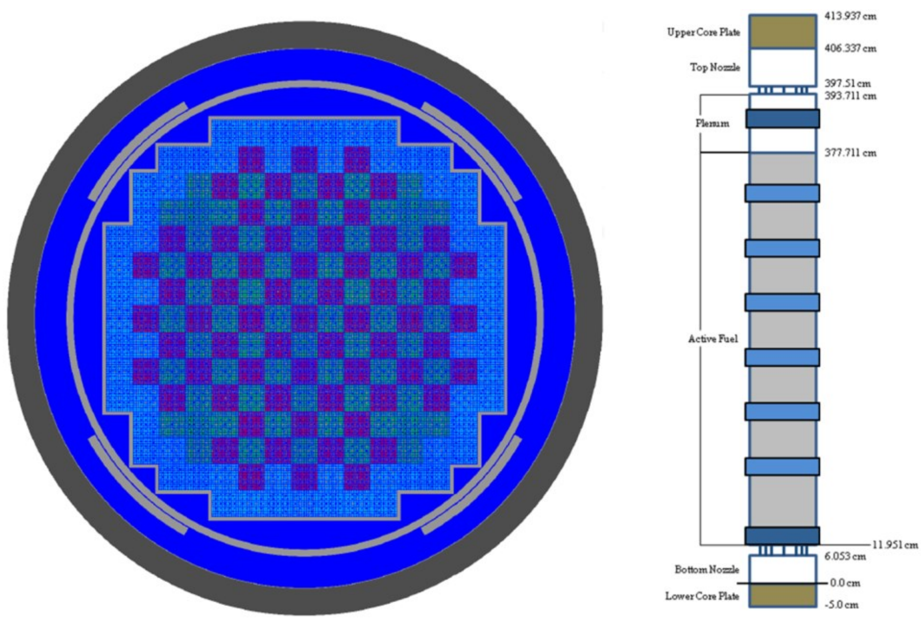

Figure 3. Watts Bar Nuclear Plant Unit 1—radial (left) and axial (right) core layouts.

The left panel of Figure 3 shows a 2D slice of the Watts Bar Nuclear Plant Unit 1, Cycle 1 full core layout. VERA currently does not model the core barrel, pads, or vessel, which are shown in the panel. The unit has 193 Westinghouse 17×17 fuel assemblies, which are 12 ft tall with 264 fuel rods and 25 guide/instrumentation tubes. The right panel of Figure 3 shows a typical axial layout of a fuel assembly used in the nonproprietary model. It includes upper and lower core plates, nozzles, and gaps, with two Inconel and six Zircaloy spacer grids.

Figure 4 shows the idealized power history for Cycle 1 that was used in the VERA simulation. Cycle 1 has a more gradual ramp to power than is seen in subsequent cycles. Shortly after 14 gigawatt-days per metric ton (GWd/MT) in Cycle 1, VERA imposes a step change to 86.9% power. This change can pose a problem for these calculations, so a small burnup increment of 0.05 GWd/MT was added to each point in the step change as an approximation. At all other statepoints, BISON uses a linear interpolation of the power.

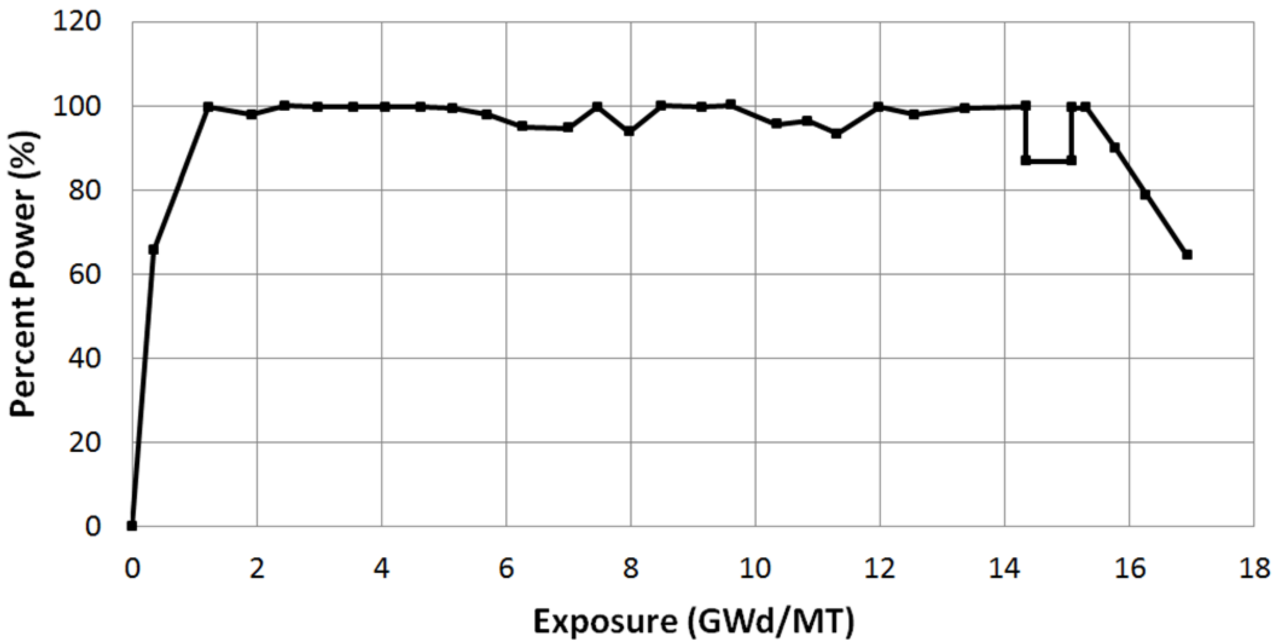

Figure 4. Watts Bar Nuclear Plant Unit 1, Cycle 1—VERA Power History [18,19].

5. RESULTS

The quarter core cases demonstrated here were executed on the Panacea cluster at ORNL. The Coupled case was executed on 1,984 cores (900 MPACT/CTF and 1040 BISON). This yields 12–13 BISON rods per process and an overall runtime of roughly 67 hours (~133,000 core-hours). The Inline case took roughly 36 hours on 1,504 cores (~54,000 core-hours). For comparison, a similar case using only MPACT/CTF recently took around 36,000 core-hours. Therefore, for Inline, roughly one and a half times the resources of MPACT/CTF alone are required, and for Coupled roughly three to four times the resources are needed.

Figures 5–9 showcase the quarter core Coupled results for (1) normalized pin power, (2) average fuel temperature, (3) fuel–clad gap, (4) maximum clad hoop stress, and (5) burnup. All figures show results near beginning of cycle (BOC) (left panel) and near end of cycle (EOC) (right panel) with the radial distributions at ~200 cm axially (about mid-core), and the axial profiles near the north boundary. The full set of results for all statepoints is shown in [14].

To set the stage for the fuel performance related results from BISON, consider Figure 5 which shows the normalized pin power distribution from MPACT, as this will help explain some of the trends observed in later figures. At BOC, the largest peaking is observed because of both the enrichment variation throughout the core (with assemblies ranging from 2.1% to 3.1% enriched) and various configurations of Pyrex burnable absorber rods. As the core experiences depletion throughout the cycle the power distribution flattens out as the higher enriched assemblies and Pyrex burnable absorber rods have depleted. While the distribution is not perfectly flat, it is substantially flatter than at EOC. It is also worth noting that higher peaking values, particularly at BOC are experienced in 2D slices other than the one around mid-core.

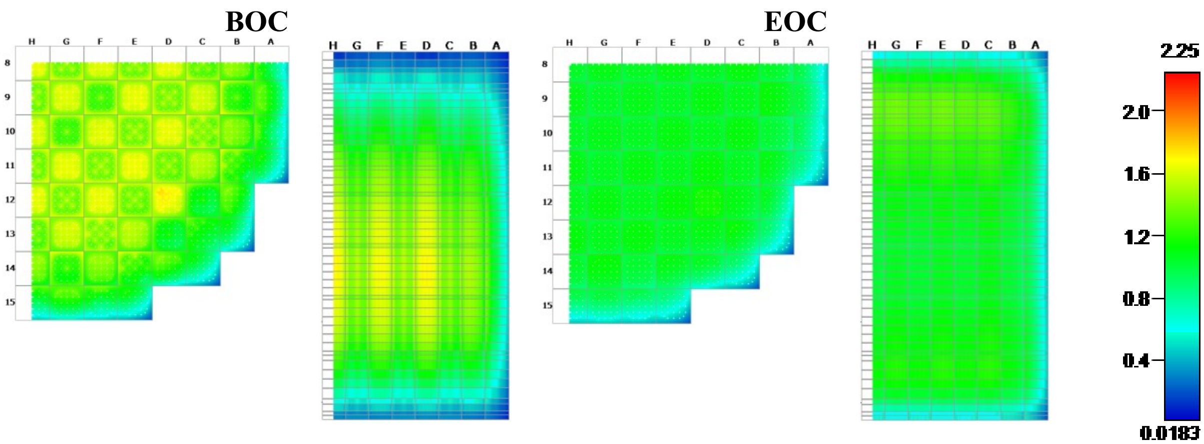

Figure 5. Watts Bar Nuclear Plant Unit 1, Cycle 1—Normalized Pin Power Distributions.

In Figure 6, the fuel temperature is seen to peak near BOC at the first hot full power statepoint. The fuel has essentially experienced only thermal expansion, with negligible depletion/irradiation effects (i.e., densification, swelling, creep). For this reason, the fuel temperatures are highest because the fuel–clad gap is still large (as can be seen in Figure 7). As the cycle progresses, the fuel–clad gap closes for most of the rods by EOC, and the fuel temperature distribution flattens out considerably. It may be difficult to tell from the color scheme, but there is a non-flat distribution of fuel temperature radially, but the variation throughout the core is much less severe than at BOC. Additionally, negative values in Figure 7 indicate an overlap of the fuel and clad elements when assessing penetration. It is a numerical artifact and should be considered simply as being in contact.

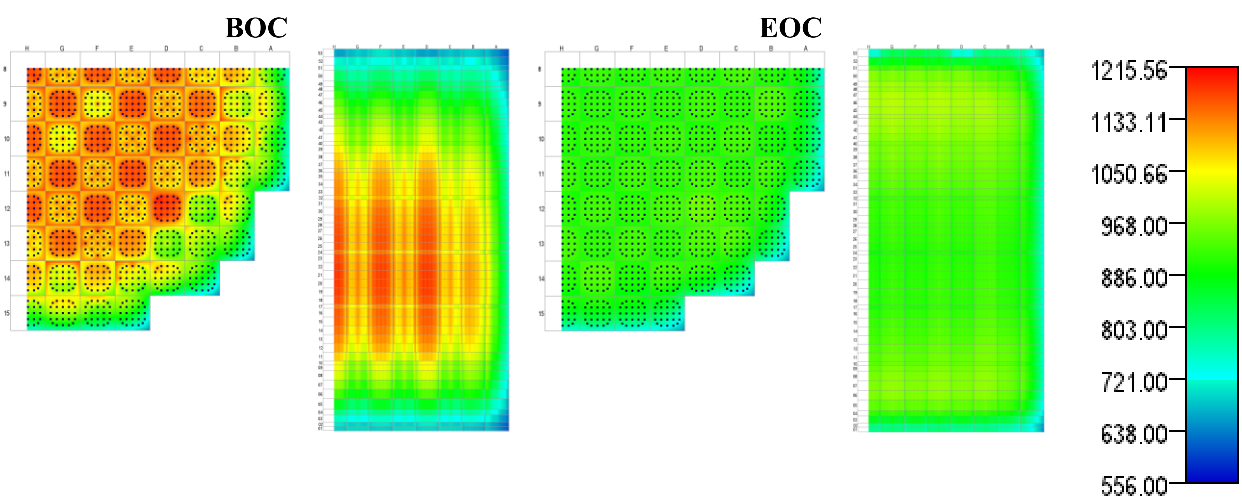

Figure 6. Watts Bar Nuclear Plant Unit 1, Cycle 1—Average Fuel Temperature (K) Distributions.

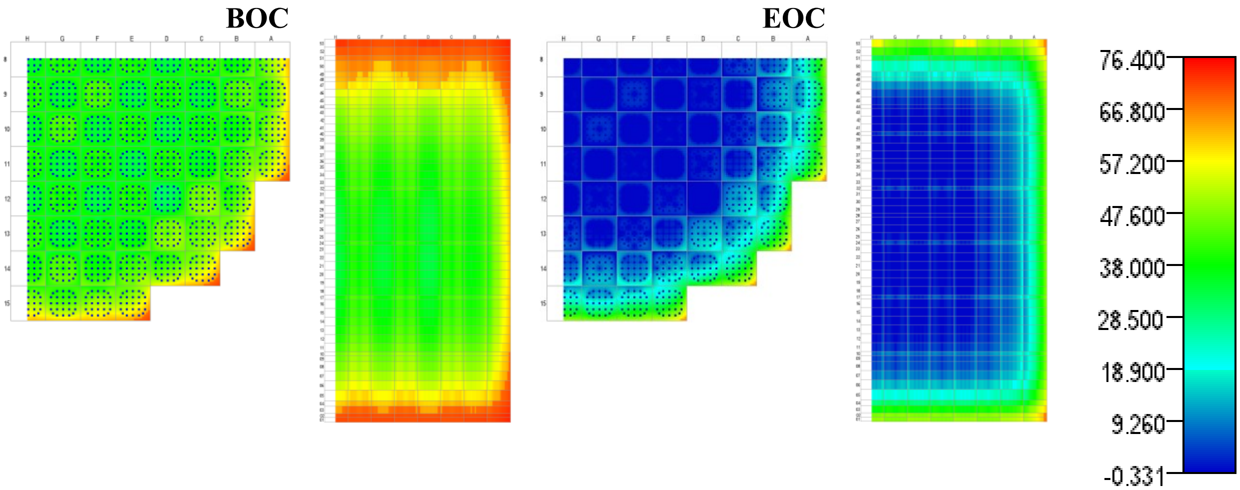

Figure 7. Watts Bar Nuclear Plant Unit 1, Cycle 1—Fuel-Clad Gap (microns) Distributions.

For much of the cycle, the clad hoop stress values (Figure 8) are negative; they are driven by the difference between the rod's internal pressure (initially around 1–2 MPa) and the coolant pressure (~15 MPa). With a higher external pressure, a compressive force is applied to the cladding. About two-thirds of the way through the cycle, fuel–clad contact begins to occur, and the hoop stress values begin to increase and become tensile as the fuel applies force to the clad. The peak hoop stress value of ~27 MPa is very similar to results obtained with a standalone one-way coupling using 2D-RZ rods at roughly 30 MPa [20].

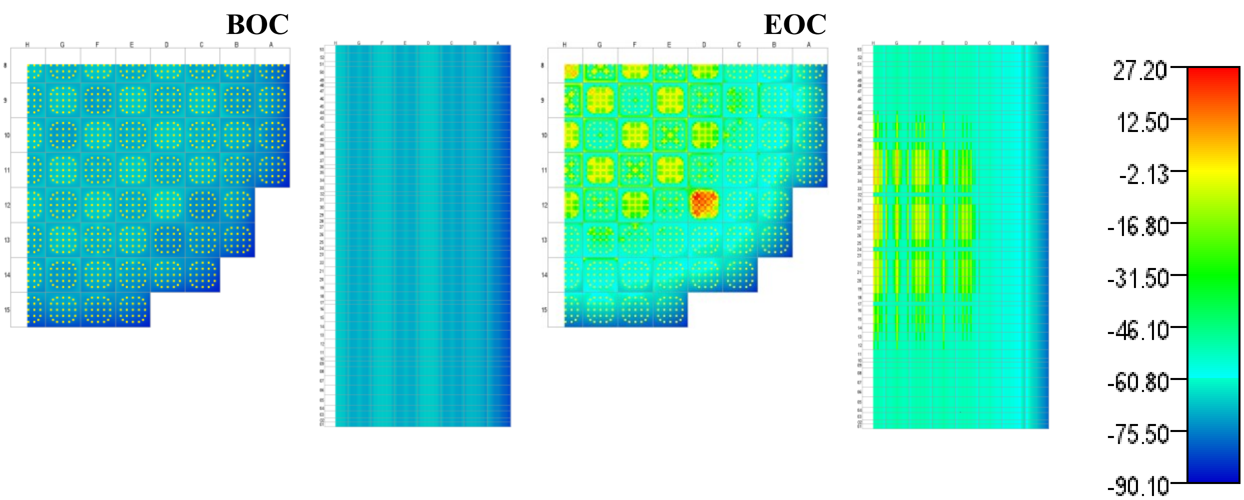

Figure 8. Watts Bar Nuclear Plant Unit 1, Cycle 1, Maximum Clad Hoop Stress (MPa) Distributions.

Figure 9 shows the burnup distribution. At BOC, burnup is zero, so nothing interesting is shown there. By EOC, some locations have upwards of roughly 26 GWd/MT, with a pretty large range, which is not surprising.

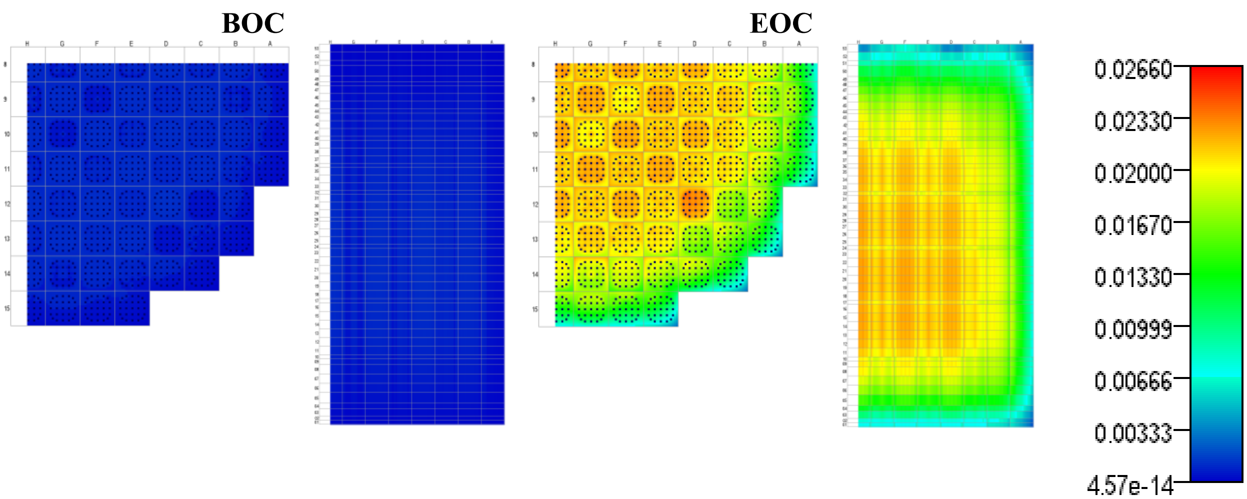

Figure 9. Watts Bar Nuclear Plant Unit 1, Cycle 1, Burnup (fima) Distributions.

6. TIMING DISCUSSION

Because the Coupled calculation is performed so that both CTF and BISON are run concurrently, the research team does not currently have the timer information separating CTF from BISON. However, aggregate timing information is reported at the end of the simulation, which allows for greater insight into the runtime of various components (Figure 10).

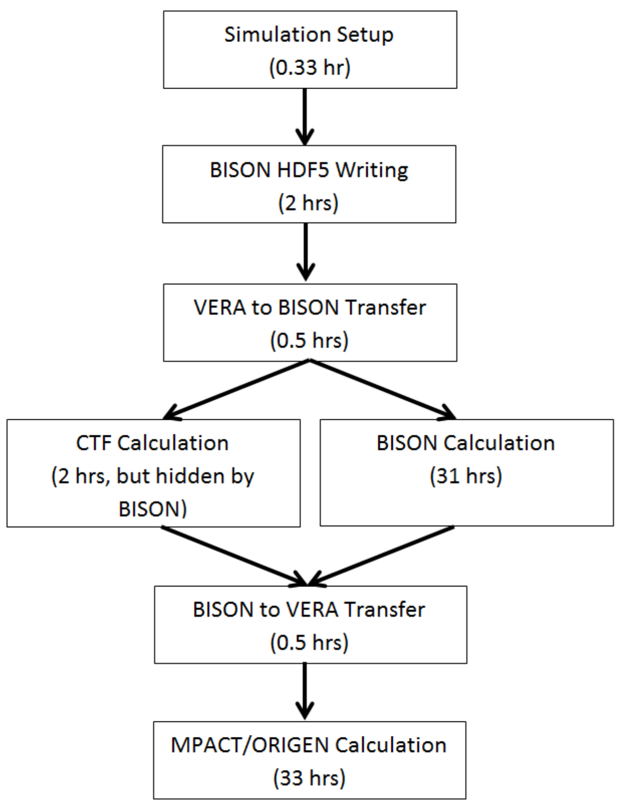

Figure 10. Estimated Timing Breakdown of Calculation Components.

From this flowchart, it can be seen that roughly 49% of the approximately 67-hour walltime is spent performing MPACT and ORIGEN calculations, 46% is spent running BISON, 3% is spent gathering data and writing to the HDF5 file, approximately 1.5% is spent performing transfers between VERA and BISON, and 0.5% is spent performing initialization. It is worth noting that nearly 2 hours is spent performing CTF calculations, but most (if not all) of this is hidden by the BISON runtime.

Table 1 shows a timing comparison between the two modes of operation (i.e., Coupled and Inline) and MPACT/CTF calculations without BISON. For clarity, while Coupled solves MPACT, CTF, and BISON, every outer iteration feeds BISON fuel temperature back to MPACT/CTF. Inline performs a one-way coupling between MPACT/CTF and BISON, feeding no information back from BISON. With the Inline approach, much of the BISON runtime can be hidden to limit the impact on walltime, as BISON calculations lag a statepoint and run concurrently with MPACT/CTF. In each of the three cases, MPACT uses 900 cores, of which 193 are active during the CTF solve and 707 are idle. For the cases using BISON, Inline uses an additional 604 cores, and Coupled uses an additional 1,084 cores for a total of 1,504 and 1,984 cores, respectively.

Table 1. Timing breakdown comparison between Coupled, Inline, and MPACT/CTF

	Time (hrs)			
Calculation Step	**Coupled**	**Inline**	**MPACT/CTF**	**Comments**
Simulation Setup	0.33	0.33	0.33	
BISON HDF5 Writing	2.00	1.00	---	Reduced in Inline because lower number of BISON cores
VERA to BISON Transfer	0.50	0.02	---	Reduced in Inline as it is only called once per statepoint
CTF Calculation	*2.00*	2.00	2.00	Same, but not masked in Inline by BISON runtime
BISON Calculation	31.00*	*2.70*†	---	Once per statepoint in Inline; mostly masked by MPACT/CTF time
BISON to VERA Transfer	0.50	---	---	Not called in Inline
MPACT/ORIGEN Calculation	33.00	33.00	33.00	

Italics indicate that most or all of the time has no impact on overall walltime as it is hidden by other components

* Coupled was executed with 1,084 cores for BISON over a total of 780 outer iterations

† Inline was executed 604 cores for BISON with a total of 32 BISON calculations (once per statepoint)

7. CONCLUSIONS AND FUTURE WORK

This paper presents the latest efforts in developing and demonstrating a coupled BISON capability within VERA, highlighting the results gathered from quarter core calculations of Watts Bar Nuclear Plant Unit 1, Cycle 1. Comparisons are also presented between the Coupled and Inline modes of operation. In total, the coupled calculation required ~133,000 core-hours (67 hours on 1,984 cores). For comparison, the Inline case took ~54,000 core-hours (36 hours on 1,504 cores), and MPACT/CTF alone took ~36,000 core-hours. Much of the additional time spent performing the Coupled calculation is spent in BISON, so future efforts to improve the runtime of the 1.5D capability will likely be effective in reducing the calculation's overall runtime. Many of the results looked very similar to those obtained from the standalone capability, which used the 2D-RZ models. Specifically, the Coupled approach predicts a peak hoop stress of 27.2 MPa, which can be directly compared to the 31.6 MPa estimated in standalone. In general, the fuel temperatures are higher than in the current default temperature table used in MPACT/CTF, but this difference is expected due to some default parameter changes that have occurred since the temperature table was generated.

While this work has been successful in demonstrating the capability, there is room for future extensions and improvements. In particular, MPACT currently passes a radially averaged power profile over each axial slice, and BISON approximates the intrapellet radial power profile using an internal model. Passing the radial power distribution from MPACT—potentially in the form of a radial shape function—would improve the consistency between MPACT and BISON. Additionally, recent analyses were performed to assess the impact of passing the clad fast flux from MPACT into BISON [21] instead of using a fast flux factor, which is the current default. Similar changes should be made in these coupling approaches to allow for a more explicit representation of the clad fast flux distribution, which can impact clad creep and growth.

Another improvement would involve overlapping the MPACT and BISON cores. At present, separate cores are used for MPACT and BISON, but in the coupled algorithm, MPACT and BISON are never run concurrently, so the calculations for these can be performed on the same processors. One concern with this is memory, as MPACT typically requires 2.0–2.5 GB per process for 3D quarter core problems when run on ~1,000 cores. Each BISON rod requires ~100 MB of memory, and 14–18 rods would need to be shared by each processor. On machines with 4 GB per core, this memory load could be a tight fit, but the procedure has a large payoff in guaranteeing a more efficient use of each processor.

Future work should also focus on extending the application space of the capabilities presented here to include both multicycle cases, leveraging the existing restart capability, and transient cases in support of other challenge problems, such as reactivity insertion accident scenarios. In transient cases, it is more likely that having a coupled methodology that utilizes MPACT, CTF, and BISON will have the largest impact on accuracy and fidelity.

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Many of the figures included here were generated using VERAView software package [22].

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