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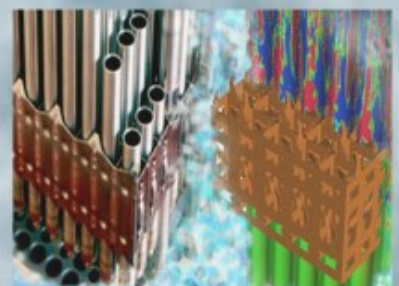
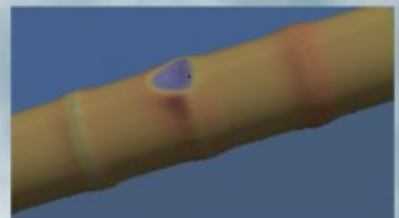
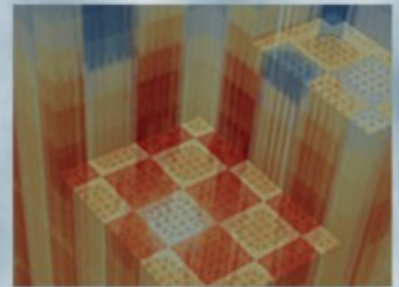
Demonstration of Coupled Tiamat Single Assembly Calculations

Shane Stimpson
Kevin Clarno
Jeffrey Powers
Benjamin Collins
Oak Ridge National Laboratory

Roger Pawlowski
Alex Toth
Sandia National Laboratories

Russell Gardner
Stephen Novascone
Jason Hales
Giovanni Pastore
Idaho National Laboratory

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Requested Distribution:

To: Kevin Clarno, PHI Lead

Copy: Thomas Downar, PHI Deputy

Jeff Banta, CASL Program Manager

EXECUTIVE SUMMARY

This report corresponds to milestone L3:PHI.PCI.P15.03, which was originally intended to investigate the time discretization approaches with the newly developed fully coupled Tiamat capability, targeting single assembly problems. At the time, it was thought that various time discretization approaches would need to be assessed. However, it was decided that this was not necessary as what is currently implemented in the code is adequate to provide consistent and full coupling between MPACT, CTF, ORIGEN, and Bison. As such, the milestone has effectively been repurposed as a stepping stone to the quarter core demonstration milestone slated for completion in August by describing and demonstrating the new fully coupled Tiamat capability on a single assembly case based on VERA Progression Problem 6, but with the addition of depletion throughout a representative cycle.

Additionally, several other contributions that have been critical to this demonstration are also described. These include (1) the 1.5D capability developed by the Bison team, (2) improvements to the burnup representation in Bison through Tiamat, and (3) the additions to MOOSE to allow Bison to resolve the same timestep are also discussed.

Initial simulations have been performed for the Watts Bar Unit 1 Cycle 1 with fully coupled Tiamat. While there are a few things to be improved for the final simulations, the initial results look very promising. The current status and results from this will be presented here, as well as the path forward to resolve the issues observed.

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ACRONYMS

BOC	beginning of cycle
BOL	beginning of life
CASL	Consortium for Advanced Simulation of Light Water Reactors
CMFD	coarse mesh finite difference
EFPD	effective full power days
EOC	end of cycle
IFBA	integral fuel burnable absorber
INF	CASL Infrastructure focus area
INL	Idaho National Laboratory
LHR	linear heat rate
MOC	middle of cycle (or method of characteristics)
ORNL	Oak Ridge National Laboratory
VERA	Virtual Environment for Reactor Analysis
WBN1	Watts Bar Nuclear Unit 1

1. INTRODUCTION

1.1 Motivation

For several years now, the core simulator capabilities provided by coupled MPACT and CTF calculations have been stable and mature. Incorporating additional physics to these simulations is extremely important to the challenge problems set by CASL. For example, coupling MAMBA to simulate the CRUD formation and resulting CRUD-induced power shift have been a focus of recent efforts [1] and has generated a lot of interest from industry partners and potential collaborators. Similarly, coupling Bison to provide fuel performance simulations has been a very important driver for the pellet-clad interaction (PCI) milestones. A few different approaches have been developed for this coupling.

The first, and most basic, is a simple file-based one-way coupling between MPACT/CTF and Bison, where MPACT/CTF coupled simulations are run to completion, and the output from those simulations are 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 are both available through Tiamat, which is a driver package that handles the coupling between MPACT, CTF, and Bison. The first is what is referred to as Tiamat-Inline, which provides the same one-way coupling as the file-based approach, but all of the power and temperature data from MPACT/CTF are passed internally to Bison. The second is Tiamat-Coupled, which couples all three codes, solving each outer iteration. With this approach, MPACT is solved first, 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 it is using a lagged value from CTF from the previous outer iteration. With these approaches, a lot of progress has been made in support of the PCI challenge problem, and hopefully using Tiamat will become more common for typical production level analysis problems.

In the rest of this section, the components of VERA are described for clarity as well as the objectives of the milestone. Then the single assembly and current status of the quarter core demonstrations will be presented in the following sections.

1.2 VERA Description

The Virtual Environment for Reactor Analysis (VERA) is a simulation environment being developed by CASL, which is comprised of codes collectively used for nuclear reactor modeling and simulation. The primary deterministic neutron transport solver is MPACT, and CTF is the subchannel thermal hydraulics solver. Much of the work in this report relates to the Bison fuel performance code. Figure 1.2.1 shows the components of VERA.

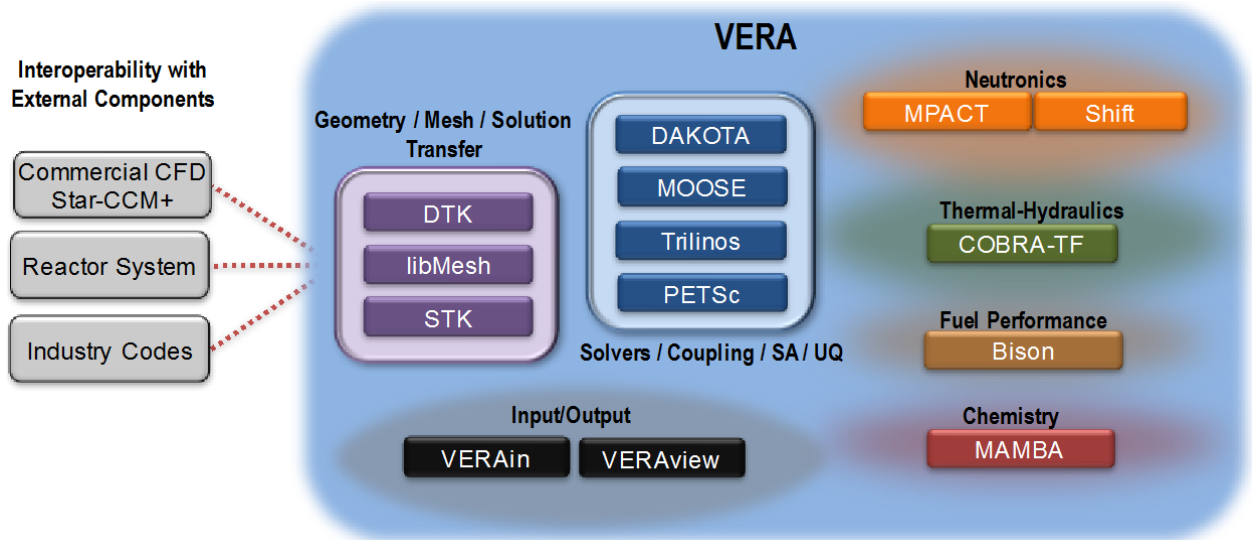


Figure 1.2.1. VERA Components

MPACT

The MPACT neutron transport solver, being developed collaboratively by Oak Ridge National Laboratory (ORNL) and the University of Michigan (UM), provides pin-resolved flux and power distributions [2]. To solve three-dimensional (3D) problems, it employs the 2D/1D method, which decomposes the problem into a 1D axial stack of 2D radial planes [3,4]. Typically, 2D Method of Characteristics (2D MOC) is used to solve each radial plane, and 1D nodal methods are used to solve axially along each rod. While there are a variety of axial solvers available, the nodal expansion method (NEM)-P₃ solver is the default, which wraps a one-node NEM kernel [5]. 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 (CMFD).

CTF

CTF is a subchannel TH code being developed by ORNL and North Carolina State University (NCSU) specifically for light water reactor (LWR) analysis [6]. 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. CTF provides significantly higher resolution and physics detail than the internal thermal hydraulics solver (Simplified TH) in MPACT, thus longer execution times.

Bison

The Bison fuel performance code is being developed by Idaho National Laboratory (INL) to provide single-rod fuel performance modeling capability so that users can assess best-estimate values of design criteria and the impact of plant operation and fuel rod design on thermo-mechanical behavior such as pellet-cladding interaction (PCI) failures in pressurized water reactors (PWRs) [7,8] 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 [9,10] which use the finite element method for geometric representation and a Jacobian Free Newton-Krylov (JFNK) scheme to solve systems of partial differential equations [10]. For this work, Bison uses a 2D azimuthally symmetric (R-Z), smeared-pellet thermomechanical fuel pin model with boundary and heat source data from VERA, which generates the time-dependent power shape/history and moderator temperature inputs needed for Bison.

Tiamat

Tiamat is the driver package between MPACT, CTF, and Bison, handling the necessary data communication through DTK and the general execution of the coupled simulation [11,12]. There are currently two modes of operation: (1) Tiamat-Inline, which provides a one-way data transfer between MPACT/CTF and Bison, where temperatures from Bison are not sent back to MPACT/CTF, and (2) Tiamat-Coupled, in which all three codes execute every outer iteration, which is effectively a residual calculation consisting of a single neutronics, thermal hydraulics, and fuel performance update. In coupled mode, MPACT sends power distribution data to CTF and Bison, CTF provides the clad outer surface to Bison and coolant data to MPACT, and Bison provides the fuel temperature back to MPACT.

1.3 Milestone Objectives

The primary objective of this milestone (L3:PHI.PCI.P15.03) was originally intended to investigate various time discretization approaches. At the time, it was thought that various time discretization approaches would need to be assessed. However, a critical capability was provided within MOOSE to allow the fully-coupled Tiamat to retain a nearly identical iteration scheme as the method implemented in MPACT for VERA-CS, which is adequate to provide consistent and full coupling between MPACT, CTF, ORIGEN, and Bison. As such, the milestone has effectively been repurposed as a stepping stone to the quarter core demonstration milestone slated for completion in August by describing and demonstrating the new fully coupled Tiamat capability on a single assembly case based on VERA Progression Problem 6, but with the addition of depletion throughout a representative cycle.

One of the stretch goals of this milestone was begin testing on quarter core cases with the new capability. Initial simulations have been performed for the Watts Bar Unit 1 Cycle 1 with fully coupled Tiamat. While there are a few things to be improved for the final simulations, the initial results look very promising. The current status and results from this will be presented here, as well as the path forward to resolve the issues observed.

2. VARIOUS IMPROVEMENTS TO TIAMAT

Tiamat development began several years ago, while coupling between MPACT and CTF was still relatively new and VERA-CS did not yet even have depletion. The initial MPACT-CTF coupled capability utilized the DTK transfer tools to pass power (fully-converged in MPACT) to CTF and the temperature and densities (fully-converged in CTF) to MPACT. The initial coupled Tiamat capability was built using the same DTK interfaces with additional transfers for Bison: the power from MPACT to Bison, the fuel temperature (fully-converged in Bison) to MPACT, the clad surface heat flux (fully-converged in Bison) to CTF, and the clad surface temperature (fully converged in CTF) to Bison. Because Bison is always run as a time-dependent execution, this required that Tiamat ensure coordinated time-stepping of every Bison pin in the problem. Because each pin could be at a different state and require a smaller time step for accuracy, the overall computational burden of coordinating time-stepping of thousands of Bison pin was staggering. This constrained progress and created a very awkward algorithm for a single ramp to full power that was going to be difficult to extend to depletion calculations.

Eventually, a new MPACT/CTF coupling was formulated using internal data passing, which allowed MPACT to embed the thermal-hydraulics and fuel temperature solver within each neutron transport outer iteration (instead of fully converging MPACT between CTF updates). This approach has proven to be much more computationally efficient and has been the default for some time. The Tiamat-Inline capability was developed to take advantage of this efficient coupling and robust algorithm by simply transferring, in memory, the Bison source-term and boundary conditions from MPACT and CTF, respectively. This allowed each Bison pin to adaptively time step between each of the user-defined depletion steps communicated from MPACT. With the freedom to converge independently, the computational cost of Bison and management constraints of Tiamat-Inline were dramatically reduced from the original Tiamat. However, the robustness requirements for Bison are extremely high when utilized within an integrated solver executing thousands of fuel performance calculations at once with unpredictable source-term and boundary condition variation: every pin must converge every time or the entire Tiamat-Inline solver would crash.

Two key developments were required to enable the development of a new fully-coupled algorithm: 1) a “perfectly” robust Bison and 2) the ability to “backup” to a previous user-defined time step and re-solve through a series of adaptive time steps.

2.1 MOOSE Backup/Restore Capability

As described in Figure 2.1.1, the new fully coupled mode requires Bison to be repeatedly solved over the same time interval during the course of a coupled solve, with new power and clad surface temperatures being provided each coupled iteration. However, in the manner in which Tiamat uses Bison with timestep subcycling, i.e. allowing the individual Bison apps to choose their own manner of stepping through time to reach the target time provided by MPACT, the state of each app is automatically updated after each solve. This means that any subsequent calls to advance the Bison model evaluator to the same time would have no effect, as the apps have already been solved to that target time. Hence, the fully coupled mode of Tiamat requires the ability to rewind the Bison apps to their states at the beginning of the coupled solve in order to re-solve the time interval. Fortunately, the ability to do this was fairly recently introduced into the MOOSE multiapp framework. This feature works through two interface functions: one which serializes and saves off the current stateful data in all the apps, and another which restores the apps to the previously saved state. In fully coupled Tiamat, this is used by saving the multiapp state at the beginning of a coupled solve, and restoring to the saved state prior to any subsequent attempts to resolve that time interval with new power and clad conditions.

There are still a few outstanding issues related to this capability. Most notably, unexpected behavior is observed when attempting to save off and restore to the initial state. When attempting this, restored Bison solves begin subcycling with the minimum allowable timestep, which is $1.0e-14$ by default. This issue seems to be related to some restartable data being incorrectly being initialized or restored in the MOOSE timestepper. This issue has been reported to the MOOSE team and is being addressed. This is currently dealt with in Tiamat by simply performing the first state solve in uncoupled mode. As the first state typically solves to HZP, this should have little impact on overall accuracy as the feedback between Bison and MPACT/CTF should be fairly minimal under these conditions.

2.2 1.5D Bison

Historically, VERA's usage of Bison has focused on 2D-RZ simulations, but these have been found to be both very slow and not extremely robust. In February 2017, the Bison team delivered an initial 1.5D capability, which effectively solves the fuel rod using an axial stack of 1D-radial problems. All of the 1D-radial problems are coupled together through the gas pressure and an axial pressure applied to the fuel/clad, so axial conduction is ignored. The goal of the 1.5D capability is to resolve computational performance issues (both speed and robustness) that were observed with the 2D-RZ.

To test this capability, one of the regressions tests (`bison_from_vera`) was chosen. It is a simple, single rod problem that starts at nominal power and observes two 10% power increases at ~ 1 and ~ 4.5 GWd/MT. Both a 2D-RZ and a 1.5D version were executed on 12 processors. The 2D-RZ case took 302 seconds and the 1.5D case, 130 seconds, so only about a 2.3x speedup. It is worth noting that both cases used 6 radial mesh in the fuel and 3 in the clad, but the 2D case used 100 axial quadratic finite elements and 1.5D used 49 axial planes in the fuel. Additionally, the figures below show the current status of the solution differences between 2D and 1.5D. Figure 2.2.1 shows the output power that is reported by Bison, which should basically be an echo of the input power (or very close with minor errors due to finite element integration). Both 1.5D and 2D cases do a sufficient job of conserving the input power here.

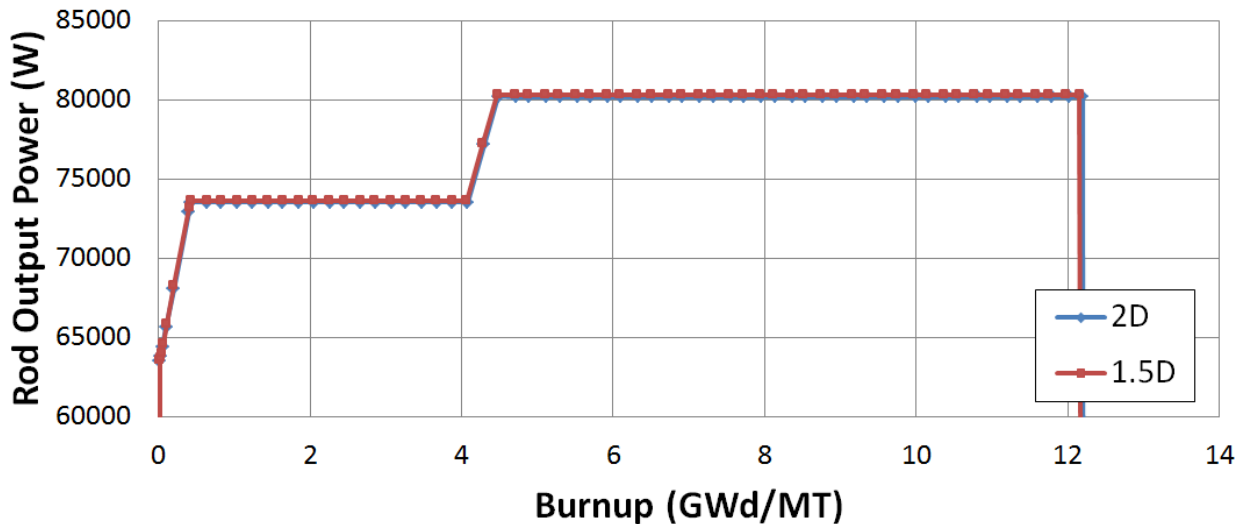


Figure 2.2.1. Rod Output Power [W] Comparison Between 1.5D and 2D-RZ Standalone Bison Cases

Figure 2.2.2 shows the fuel-clad gap thickness. As expected, the gap quickly decreases near BOC as the rod expands from CZP to HFP and gradually continues to decrease with burnup. Unfortunately, larger discrepancies are observed as the 1.5D case achieves contact much quicker than the 2D case. Both cases are using the ZIRLO model in Bison, which does reduce clad creep and contact is generally observed later than with Zirc4 cladding.

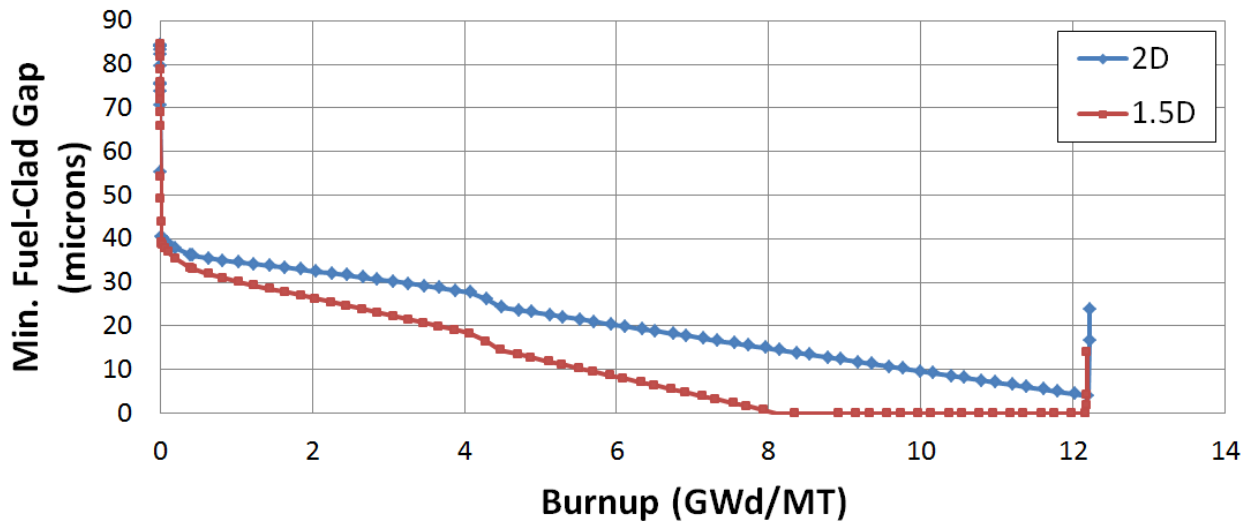


Figure 2.2.2. Minimum Fuel-Clad Gap Thickness [microns] Comparison Between 1.5D and 2D-RZ Standalone Bison Cases

Figures 2.2.3 and 2.2.4 show the average and maximum centerline fuel temperatures. Most of the differences here are driven by the difference in gap thickness and differences of ~50K are observed.

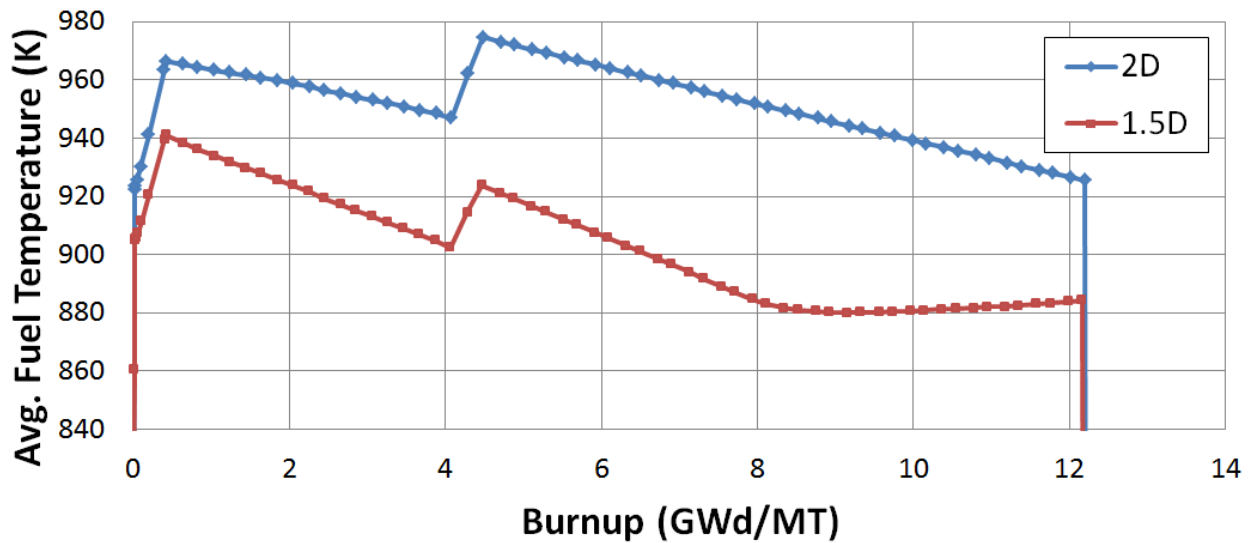


Figure 2.2.3. Average Fuel Temperature [K] Comparison Between 1.5D and 2D-RZ Standalone Bison Cases

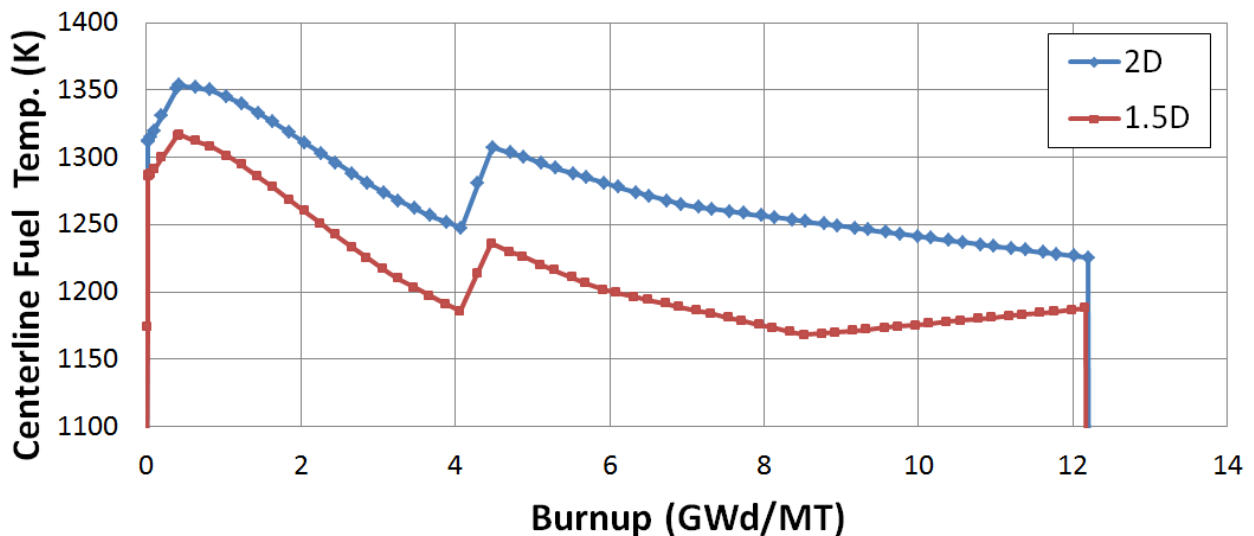


Figure 2.2.4. Maximum Centerline Fuel Temperature [K] Comparison Between 1.5D and 2D-RZ Standalone Bison Cases

2.3 New Fully Coupled Capability

With these new capabilities in MOOSE and Bison, the fully-coupled Tiamat was able to be redesigned to leverage an algorithm that is consistent with VERA-CS. In the new scheme, the MPACT/CTF coupling is the same, but now Tiamat solves each Bison pin concurrently with CTF. 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 and passes the latest solution for the clad surface temperature from CTF to Bison. Tiamat instructs a MOOSE MultiApp to “restore” every rod to the last “backup,” independently adaptively time step each rod to the next user-defined state, and then pass the fuel temperature back to MPACT. When the new fully-coupled capability is used with 2D Bison, the power from MPACT would axially redistribute within the fuel rod so the clad surface heat flux from Bison provide a thermal source for CTF. Because the 1.5D Bison only transfers heat radially, there is no need to lag the power distribution from a given iteration.

It is also important to note that by running Bison and CTF at the same time, the clad outer surface temperature boundary condition used by Bison that comes from CTF is actually lagged by an outer iteration. At convergence there is no issue, but outer surface temperature also does not change very substantially, so 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 Tiamat coupled calculation actually seems to consistently take fewer outer iterations. With the boundary condition lagged, it is effectively relaxing its impact, which could be leading to more optimal convergence. Figure 2.1.1 shows a flowchart of new fully coupled Tiamat calculation scheme. It is also good to keep in mind that MPACT and CTF share processors because of the internal coupling there, but the Bison calculations are performed on a different set of processors entirely.

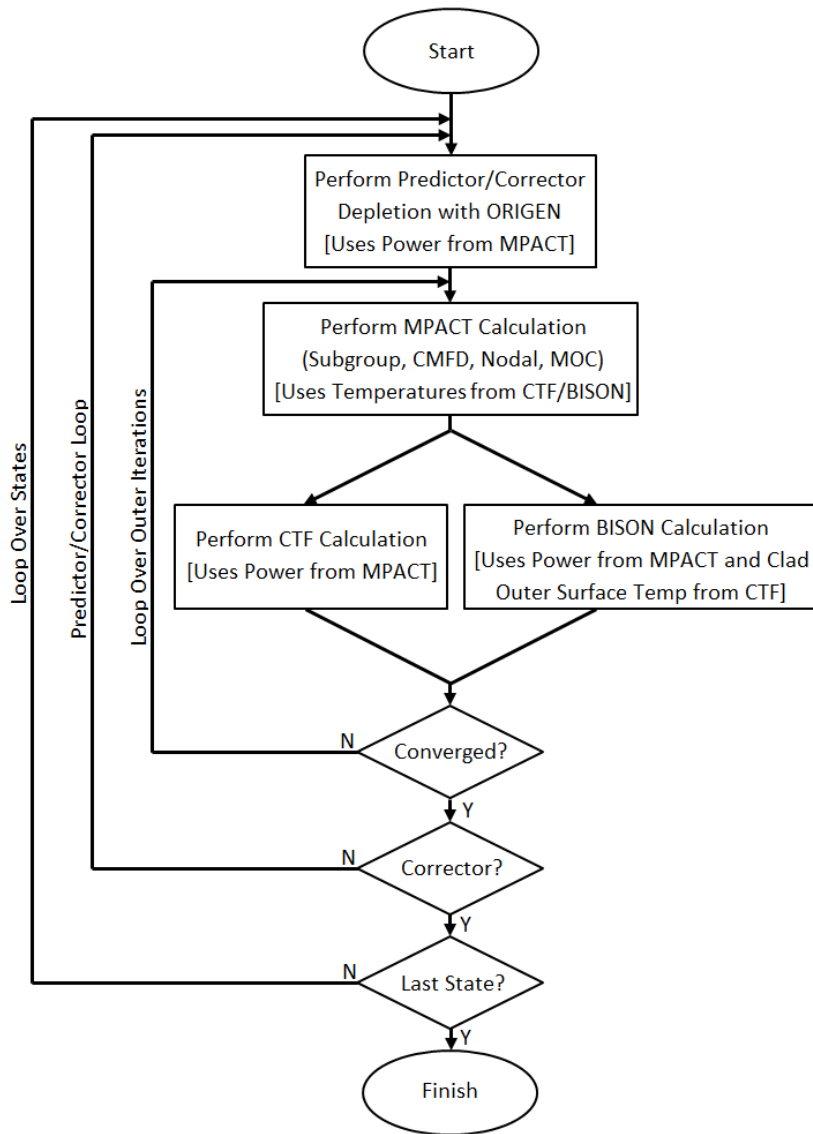


Figure 2.1.1. Flowchart of the Tiamat Fully Coupled Calculation

Figure 2.1.2 shows a similar and comparable flowchart for the Tiamat-Inline calculation. Here MPACT and CTF are fully converged together, then the processors dedicated to Bison solves will run the Bison cases while the MPACT/CTF processors continue with the next state. So 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. In general, this is not usually something that occurs, though select statepoints may take longer than others, particularly during power ramps.

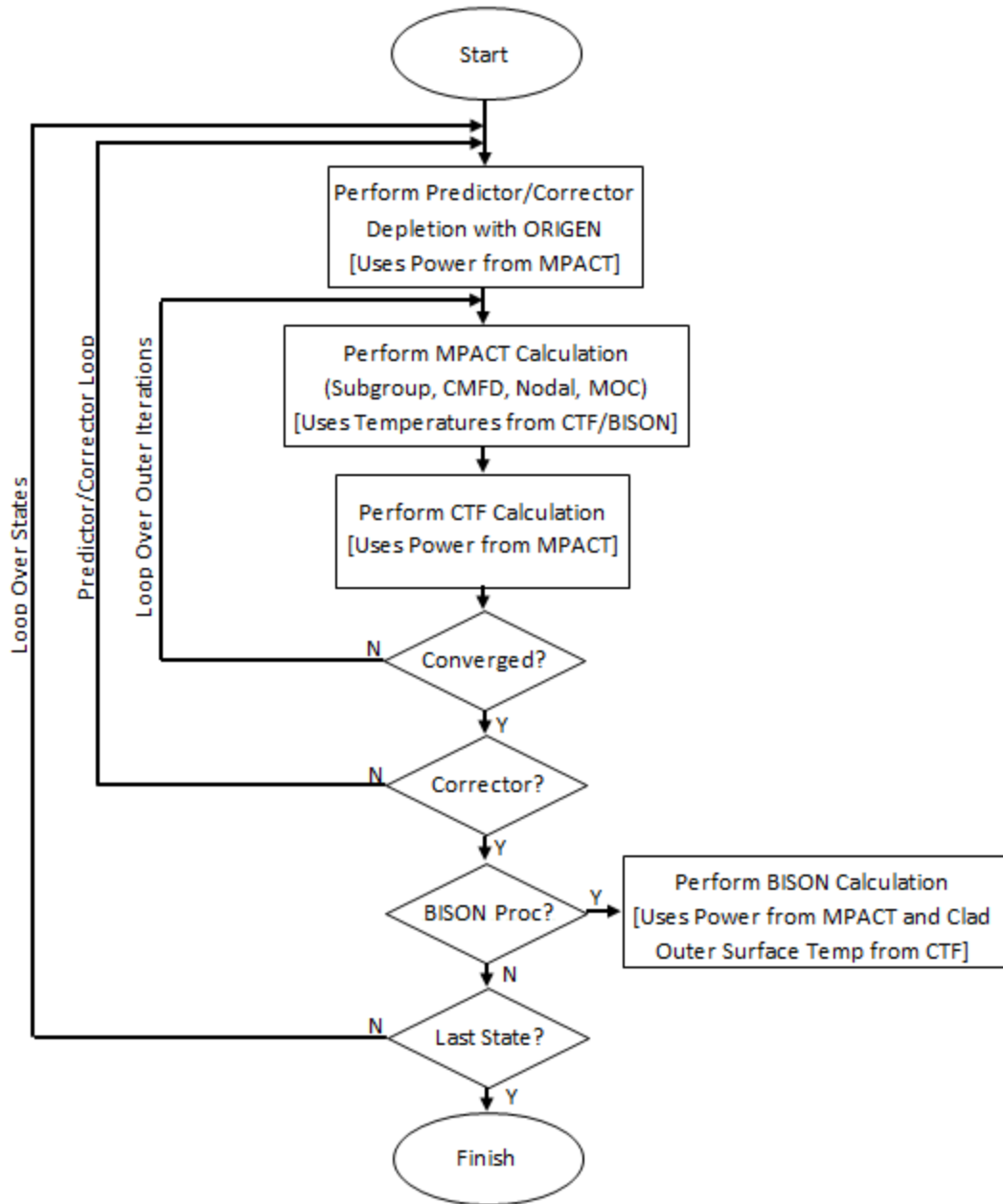


Figure 2.1.2. Flowchart of the Tiamat Inline Calculation

2.3 Burnup Improvements

In addition to the coupling approach changes, modifications were made to the burnup interface to improve the accuracy in Tiamat. The Bison team implemented a new vector postprocessor that effectively evaluates the auxiliary variable manipulated by Tiamat, parsing it as a function, allowing it to be fed into the burnup block. However, Tiamat directly manipulates an axial fission rate auxiliary variable, so an additional function was necessary to convert the axial fission rate into an axial power before being used by the burnup block. Figure 2.3.1 shows these blocks from a sample input. At the bottom, one can see the vector postprocessor (vec_post) that uses a line value sample function to evaluate the casl_fission_rate (from Tiamat) at many points axially. The fission_rate_auxvar_value_function in the Functions block is used to turn the vector postprocessor

results into a function field. But as this is still the fission rate data, the `fission_rate_convert_to_LHR` function is used to convert it to linear heat rate (W/m). This conversion process happens inside the burnup block as `fission_rate_convert_to_LHR` is passed into the `rod_ave_lin_pow` field and `fission_rate_auxvar_value_function` through the `axial_power_profile` field. These two fields are then multiplied internally to produce the local linear heat rate value at each point axially, and the burnup block is still handling the intrapellet distribution internally.

```
# ===== #
# Time- and Space-Dependent Source and BCs
# ===== #
[Functions]
...
[./fission_rate_convert_to_LHR]
  type = PiecewiseLinear
  x = '-100 0 5000'
  y = '1.68662971E-15 1.68662971E-15 1.68662971E-15'
  scale_factor = 1
[../]
[./fission_rate_auxvar_value_function]
  type = VectorPostprocessorFunction
  component = 1
  argument_column = y
  value_column = casl_fission_rate
  vectorpostprocessor_name = vec_post
[../]
[./q]
  type = CompositeFunction
  functions = 'fission_rate_convert_to_LHR fission_rate_auxvar_value_function'
[../]
[]

# ===== #
# Burnup Equation Set
# ===== #
[Burnup]
[./burnup]
  block = 3
  rod_ave_lin_pow = fission_rate_convert_to_LHR
  axial_power_profile = fission_rate_auxvar_value_function
  num_radial = 80
  num_axial = 100
  fuel_inner_radius = 0.0
  fuel_outer_radius =
  fuel_volume_ratio = 1.0
  i_enrich = '3.100e-02 9.690e-01 0.0000e+00 0.0000e+00 0.0000e+00 0.0000e+00'
  RPF = RPF
[../]
[]
...
[VectorPostprocessors]
[./vec_post]
  type = LineValueSampler
  variable = casl_fission_rate
  start_point = '0 0 0'
  end_point = '0 3.6575 0'
  num_points = 50
  sort_by = y
  execute_on = linear
[../]
[]
```

Figure 2.3.1. Input File Excerpt Showing the Changes Necessary

Figure 2.3.2 shows an example of the burnups that can be extracted from the Tiamat with these changes, showing both axial and radial dependence, as expected.

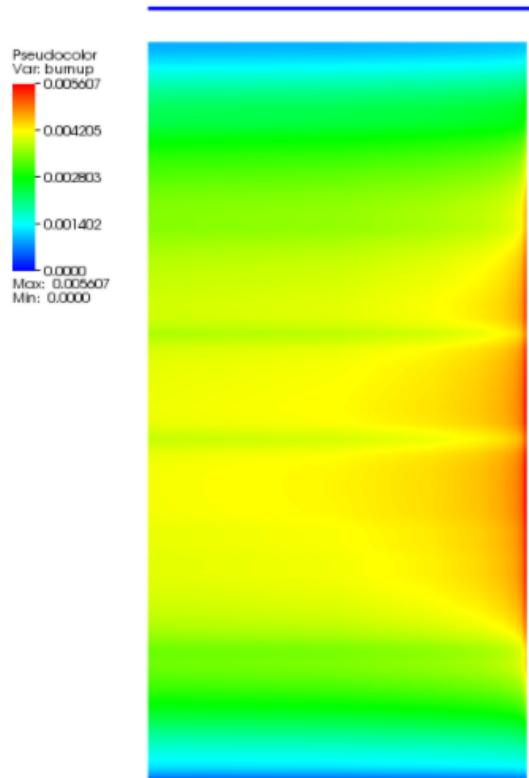


Figure 2.3.2. Improved Burnup [fima] Example with Both Axial and Radial Dependence.

As part of his comparison work, Jeffrey Powers has observed some discrepancies in the burnup between standalone Bison and Tiamat cases. This is still being investigated, but the modifications shown in this section have drastically improved the burnup distributions predicted by Tiamat.

3. SINGLE ASSEMBLY DEMONSTRATION

3.1 Problem Description

The primary problem for the single assembly demonstration is a very familiar VERA Progression Problem 6 case with a simple addition of a power history to extend the case to include a cycle of depletion. Figure 3.1.1 shows the single assembly description along with the state blocks used to define the power history. Essentially, it is a very straight-forward power history with a ramp to power, then maintaining full power for the duration of the cycle. The MPACT model used 58 planes in the axial mesh.

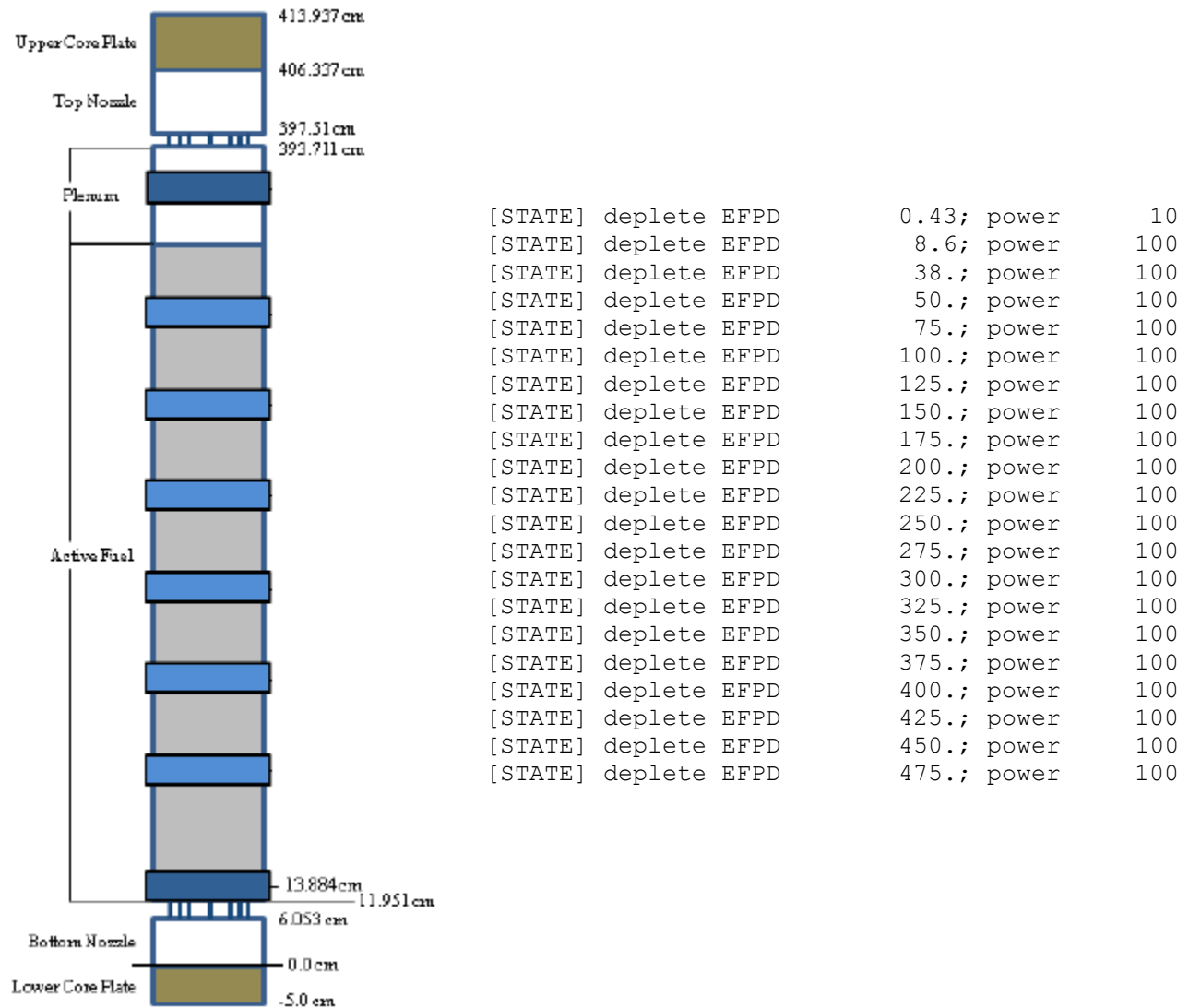


Figure 3.1.1. Single Assembly Axial Geometry and State Blocks in VERA Input [13].

3.2 Results

Three variants were run on the Panacea cluster at ORNL: (1) MPACT/CTF, (2) Tiamat-Inline, and (3) Tiamat-Coupled. The focus here will be on the Tiamat-Coupled results. All cases were run with the current default parameters in MPACT, including the 51-group library. As such, the timing data shown here is a decent representation of what to expect in production level cases (no coarse parameters, no 8-group library, etc.) Table 3.2.1 shows the timing results comparing all three.

The Tiamat-Inline and Tiamat-Coupled cases were run with several different configurations, varying numbers of cores to see the effect of modelling multiple Bison rods per proc. Inline shows a continual decrease in the total core-hours as the number of rods per proc increases (at least up to 9 rods). This means that a lot of the time to solve the Bison cases is hidden while MPACT/CTF are running the next state (i.e. MPACT/CTF calculations take longer than Bison). Coupled, however, would only see the time hidden in a similar manner if the Bison solve is as fast as the CTF solve, so the minimum computation time is observed much earlier. While running 9 rods per proc incurs a substantial penalty, to keep the core counts low on larger problems, it will still be desired to run with

9-12 rods per process, even if it is suboptimal for the time being. Future improvements to the 1.5D capability speed help mitigate this issue, enabling more rods per processor without such a penalty.

Table 3.2.1. Runtime Comparisons for Single Assembly With Depletion

Simulation	BISON Rods Per Proc.	Procs	Iteratons	Walltime (hrs)	core-hours
MPACT/CTF	---	58	220	0.90	52.2
Tiamat-Inline	0.25	382	220	0.91	347.62
	1	139	220	0.91	126.49
	9	67	220	1.19	79.73
Tiamat-Coupled	0.25	382	214	1.18	450.76
	1	139	214	1.92	266.88
	9	67	214	9.83	658.61

Now, it is very important to keep in mind that the all of these cases were fully decomposed and with 4 procs per Bison rod. On larger scale problems, such as the quarter core cases shown in the next section, to keep the number of total cores down, the decomposition has 10-12 Bison rods per proc, not multiple procs per rod. With more rods per proc, one would expect the total walltime to increase significantly.

Figure 3.1.2 shows the results at BOC, MOC, and EOC for the average fuel temperature (left) and fuel-clad gap (right). Similar behavior to what has been observed in other reports [14,15,16] is seen, where the temperature is highest at BOC, and eventually decreases and flattens off by EOC. The gap thickness near BOC is mostly driven by thermal expansion, but swelling effects as the fuel is burned eventually drives gap closure by EOC.

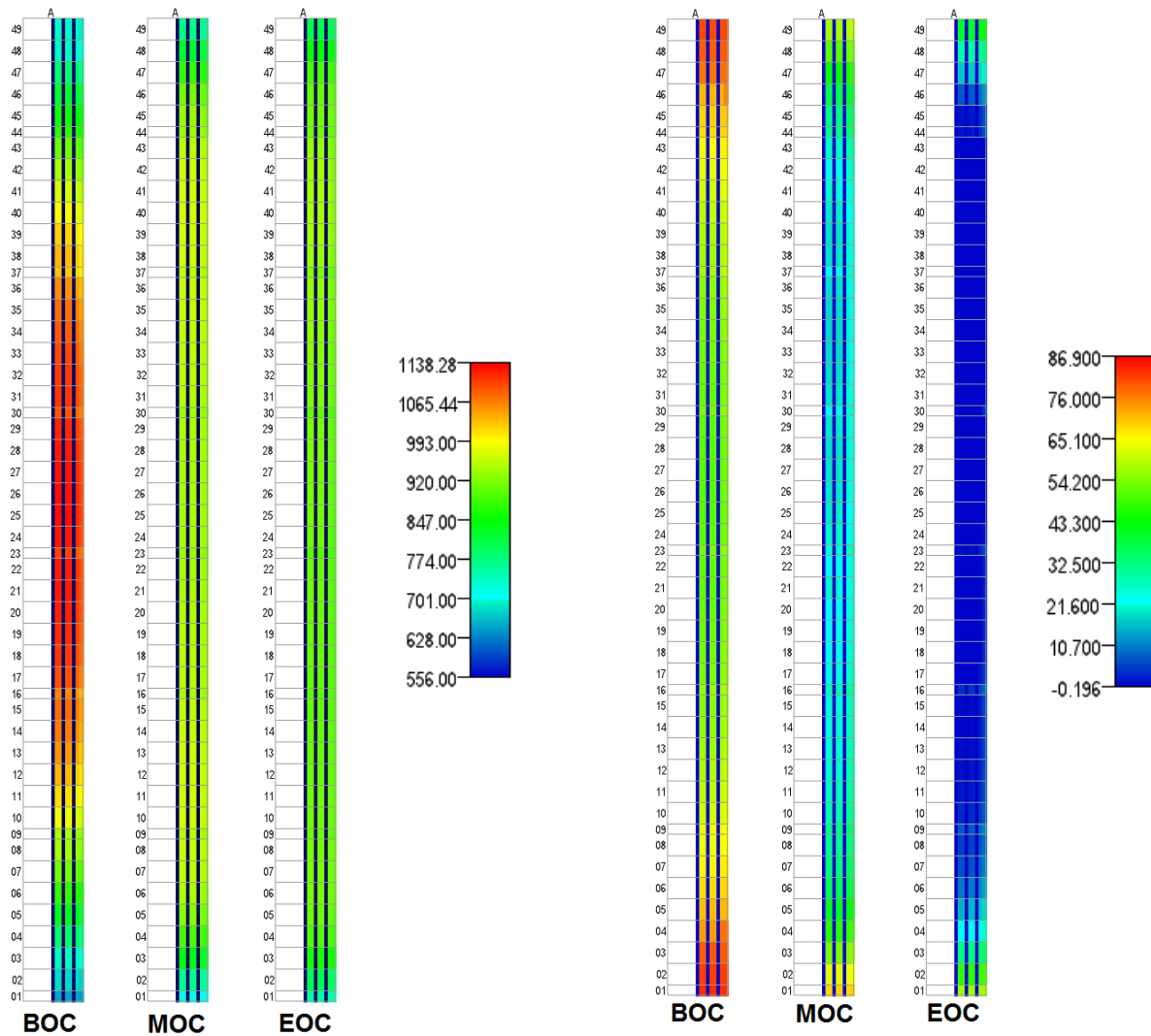


Figure 3.1.2. Single Assembly Results for Average Fuel Temperature [K] (left) and Fuel-Clad Gap Thickness [microns] (right)

Figure 3.1.3 shows the burnup and clad hoop stress distributions. As expected, since the case is using a very simple power history, the burnup is basically a linear function in time. The clad hoop stresses are initially negative because, without contact, the stress is really just driven by the difference between the rod internal pressure (~2 MPa) and the system pressure (~15 MPa). However, by EOC, contact has been made, and some positive hoop stress values are observed.

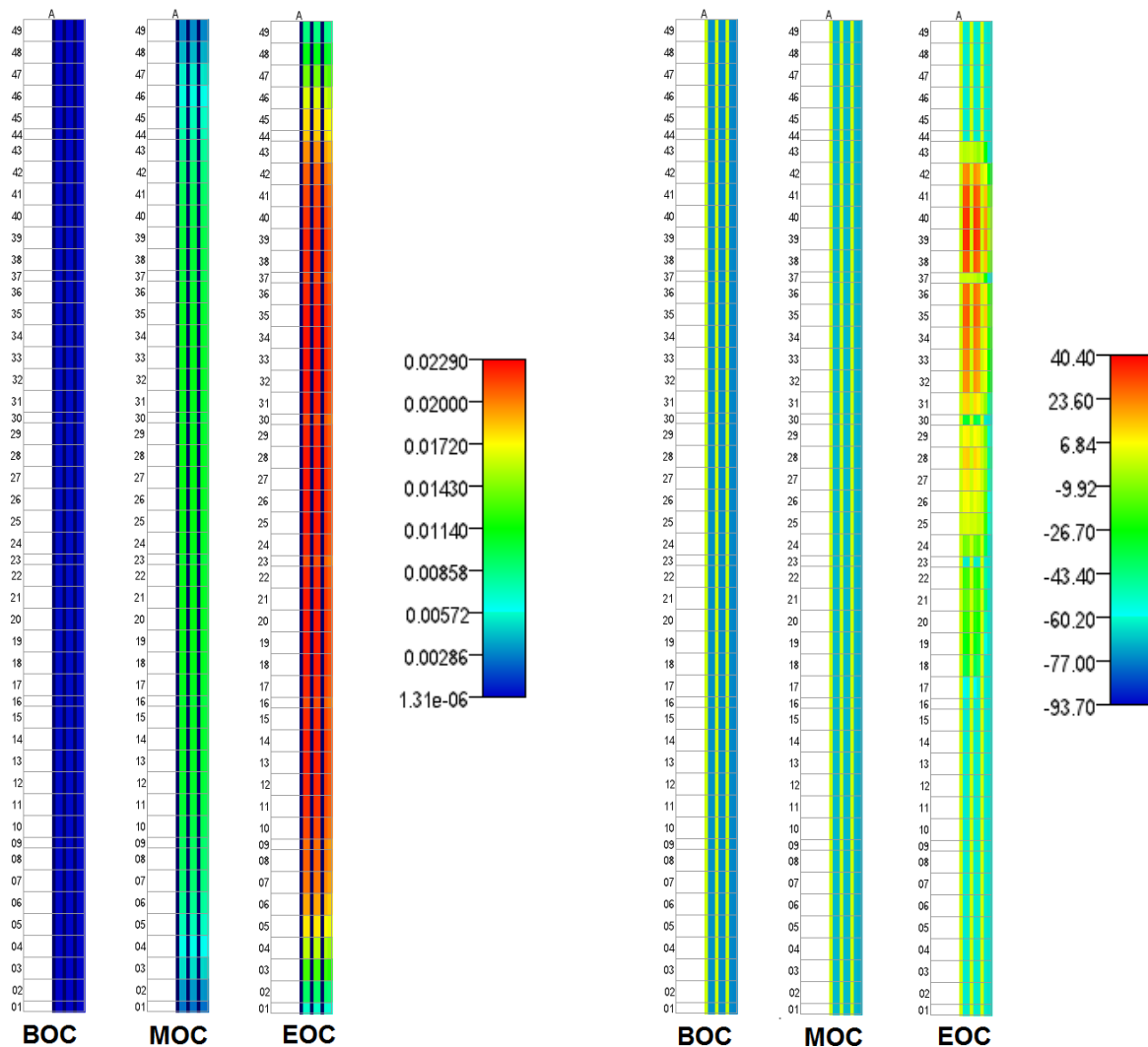


Figure 3.1.3. Single Assembly Results for Burnup [fima] (left) and Maximum Clad Hoop Stress [MPa] (right)

Overall, the results observed demonstrate consistent trends to those seen in previous analyses.

4. STATUS OF QUARTER CORE DEMONSTRATION

4.1 Watts Bar Unit 1, Cycle 1 Description

The Watts Bar Nuclear Plant is a Westinghouse four-loop PWR operated by the Tennessee Valley Authority (TVA) and has been online since 1996. It began with a 3,411 MWth power rating, but it had a 1.4% power uprate in 2001. It is currently operating in its fifteenth cycle, logging over 6,000 effective full power days (EFPD) of operation [17].

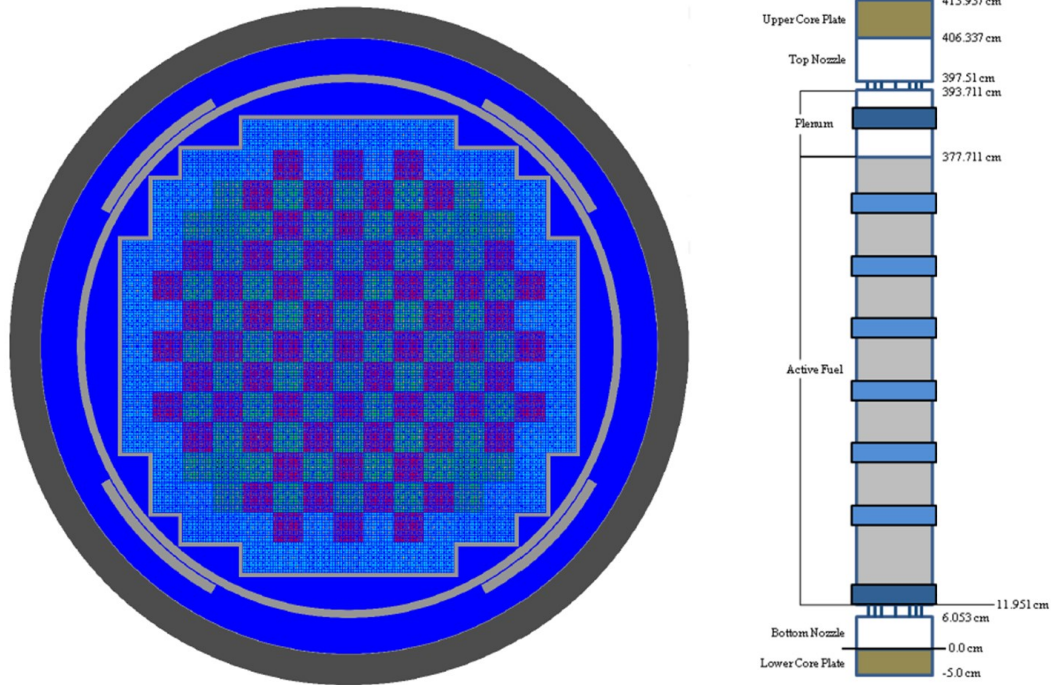


Figure 4.1.1. Watts Bar Unit 1 – Core Geometry

The left component of Figure 4.1.1 shows a 2D slice of the WBN1 Cycle 1 full core layout. It is important to note that VERA currently does not model the core barrel, pads, or vessel, as are shown in the diagram. The unit has 193 Westinghouse 17×17 fuel assemblies which are 12 feet tall with 264 fuel rods and 25 guide/instrumentation tubes. On the right side of Fig. 4.1.1 is a typical axial layout of a fuel assembly used in the nonproprietary model. It includes upper/lower core plate, nozzles, and gaps, with two Inconel and six Zircaloy spacer grids. Figure 4.1.2 shows the core layout in Cycle 1; each assembly is color-coded based on enrichment and select assemblies include the number of pyrex rods in the assembly.

	H	G	F	E	D	C	B	A
8		20		20		20		12
9	20		24		20		24	
10		24		20		16		8
11	20		20		20		16	
12		20		20		24		
13	20		16		24	12		
14		24		16				
15	12		8					

Number of Pyrex Rods

Figure 4.1.2. Watts Bar Unit 1 – Cycle 1 Core Layout [13]

Figure 4.1.3 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 was reflected in the Bison inputs, allowing a one-day transition to and from 86.9% power (an instantaneous power change would be problematic for Bison). At all other statepoints, Bison uses a linear interpolation of the power.

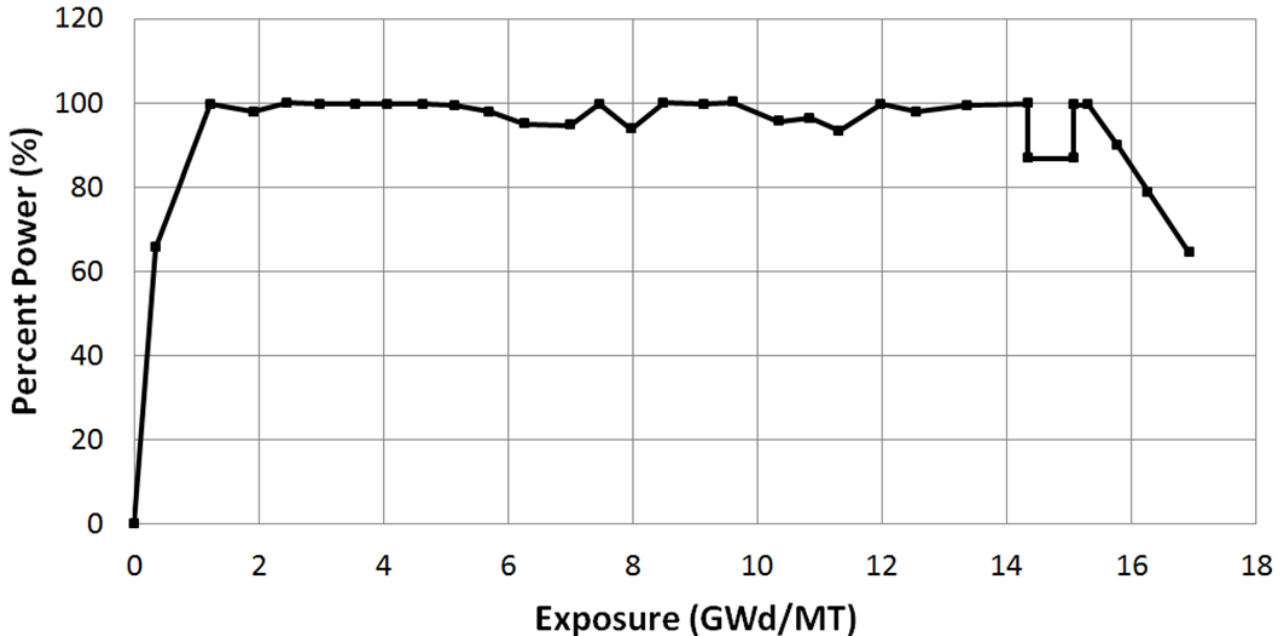


Figure 4.1.3. Watts Bar Unit 1 – Cycle 1 VERA Power History [15]

4.2 Current Status

The quarter core cases were also executed on the Panacea cluster. Both Tiamat-Inline and Tiamat-Coupled were executed on 2240 cores (900 MPACT/CTF and 1340 Bison). This yields 10-11 Bison rods per process. Both cases eventually hit the walltime limit on the jobs, 48 hours for Tiamat-Inline and 96 hours for Tiamat-Coupled, but both were nearly complete. The inline case completed 26 out of 32 states and coupled, 29 out of 32. If one were to estimate the final remaining states of each of these cases, the final numbers would be ~130,000 core-hours for inline and ~240,000 core-hours for fully coupled. A comparable MPACT case was run on 1920 core and took 16.86 hours (~32,400 core-hours).

For the remainder of this section, focus will be given to the fully coupled results, particular the performance. Figure 4.2.1 shows the timing per outer iteration for the fully coupled case for all states. The timing components are broken down into two categories: (1) MPACT+ORIGEN and (2) CTF+Bison. This was done because of how the timing data is reported to the log file. Since CTF and Bison are run concurrently, it is difficult to distinguish the runtime of each from the log file, but Bison is likely a vast majority of it based on comparisons to outer iterations in MPACT/CTF calculations.

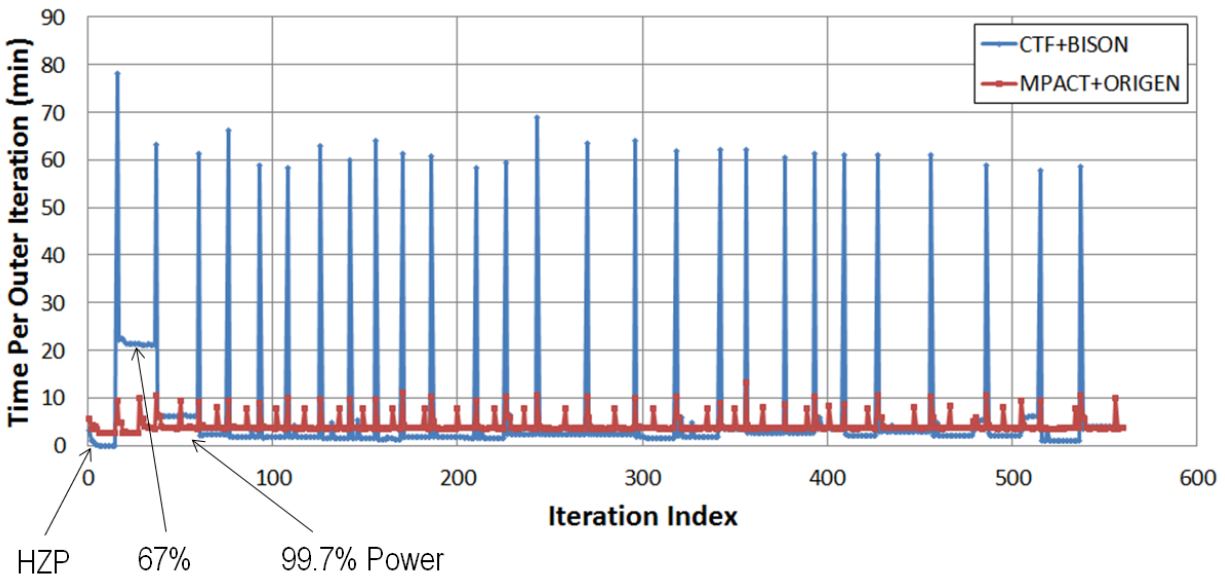


Figure 4.2.1. Watts Bar Unit 1 – Cycle 1, Fully Coupled Tiamat Timing Per Outer Iteration

To get a better visual of what is happening early in the calculation, Figure 4.2.2 shows the same timing data, but for only the first 4 statepoints. From this, it is much easier to pick out some of the noteworthy characteristics. For example, the predictor and corrector steps, which are the only contribution of ORIGEN to the runtime, can easily be identified from the spike in MPACT+ORIGEN data. Additionally, it can be seen that the Bison runtime increases dramatically during the second state, which is the 67% power statepoint in the ramp to HFP. Because of this increase State 2 took a total of 10 hours to complete, compared to the rough average of 3 hours for the rest of the statepoints. The Bison runtime is still elevated during the third state, which is nearly full power, but eventually the Bison time per outer iteration becomes comparable to the MPACT runtime for the rest of the calculation. That is, however, with the exception of the first outer iteration in each statepoint, which is where the HDF5 data is collected from Bison and written to the file. Initial investigations suggest that the HDF5 time is only about 30 minutes of the ~60 increase, but continue investigations are underway to identify all sources of the issue.

The last remaining feature to discuss of Figure 4.2.2 is the MPACT timing in that it does not look like the logic to stop running the subgroup self-shielding calculation is working properly for coupled calculations. This can be seen from the log directly, as subgroup runs nearly every outer iteration, even once the TH solution is nearly converged, but also from the timing data as there is no drop in the MPACT time as the state continues to converge. In normal MPACT/CTF and Tiamat-Inline cases, the subgroup calculation typically only runs 3-6 times in a predictor/corrector step in each statepoint. Initial debugging has identified this to be an issue with the two-way coupling, as both Bison and CTF are modifying the fuel temperature data field in MPACT, so the assessment of a converged TH solution is not correct. This is also actively being pursued. Since the self-shielding time is actually a significant portion of the MPACT time per outer iteration, it would be possible to reduce the total runtime by 1.25-2x by fixing this defect in the logic. This would help close some of the gap in the Tiamat-Inline and Tiamat-Coupled timing data.

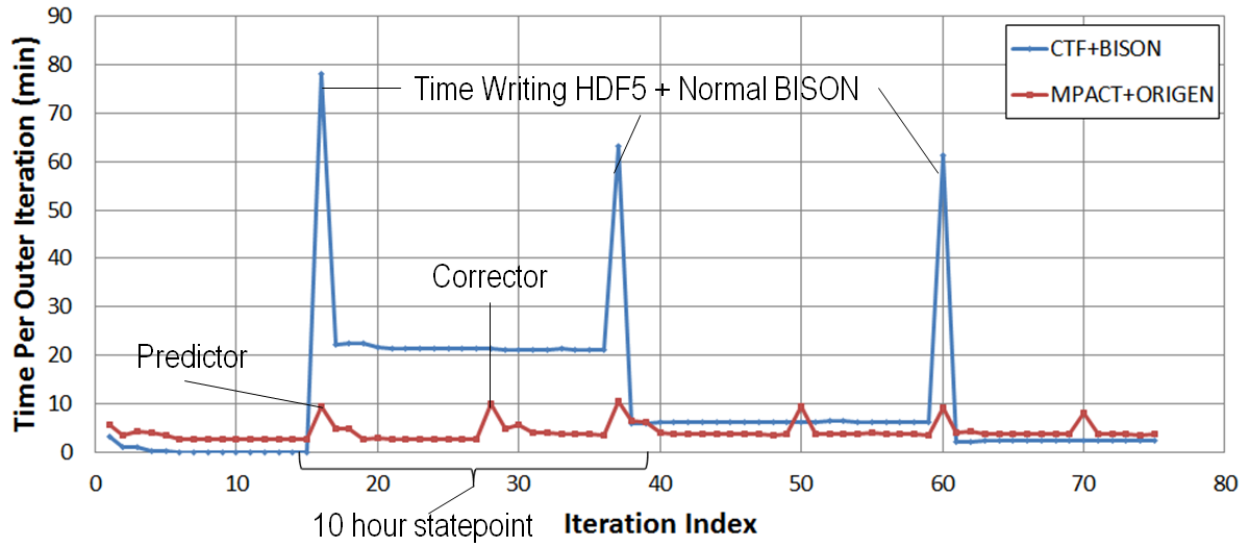


Figure 4.2.2. Watts Bar Unit 1 – Cycle 1, Fully Coupled Tiamat Timing Per Outer Iteration (first 4 statepoints)

Figure 4.2.3 shows a comparison of the Bison average fuel temperature reported by Tiamat-Inline and Tiamat-Coupled for the first 15 states of each case. The differences increase during the ramp to HFP, but stay relatively constant once the core is at power, with an RMS of ~ 1 K and a MAX ~ 5 K.

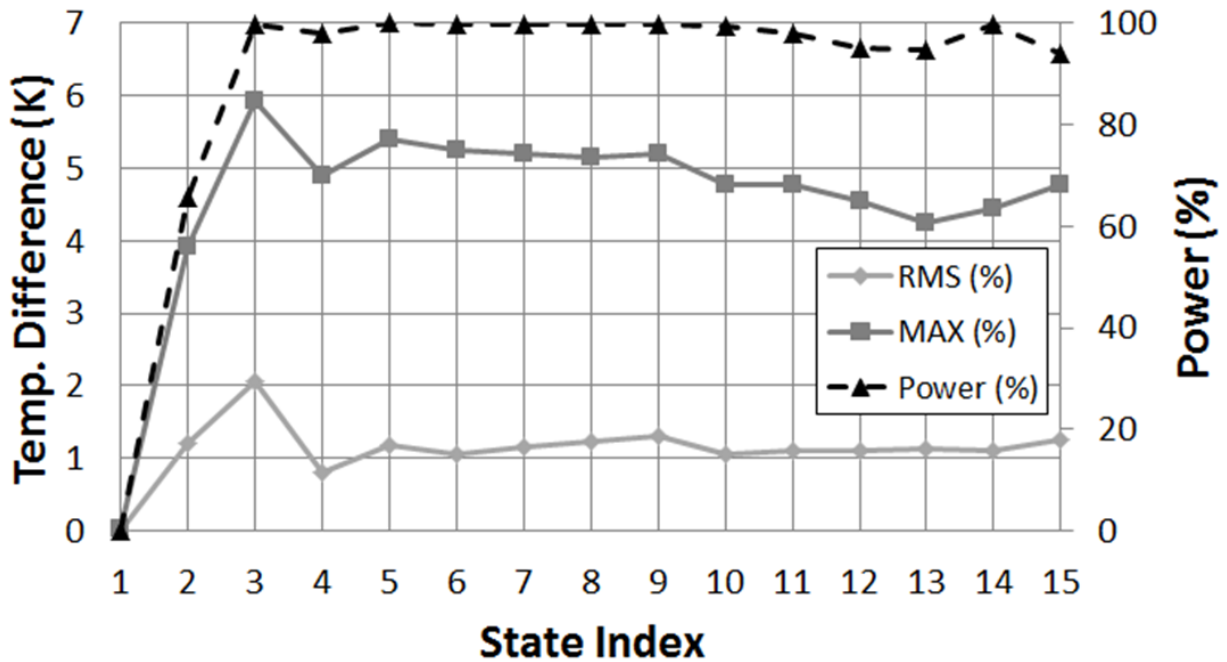


Figure 4.2.3. Watts Bar Unit 1 – Cycle 1, Average Temperature Comparison Between Fully Coupled and Inline Tiamat.

Figures 4.2.4-4.2.7 showcase the quarter core Tiamat-Coupled results for (1) average fuel temperature, (2) fuel-clad gap, (3) maximum clad hoop stress, and (4) burnup. All figures show the results for BOC (left) and EOC (right) with the radial distributions at ~ 200 cm axially shown on the top and the axial profiles near the north boundary shown on the bottom.

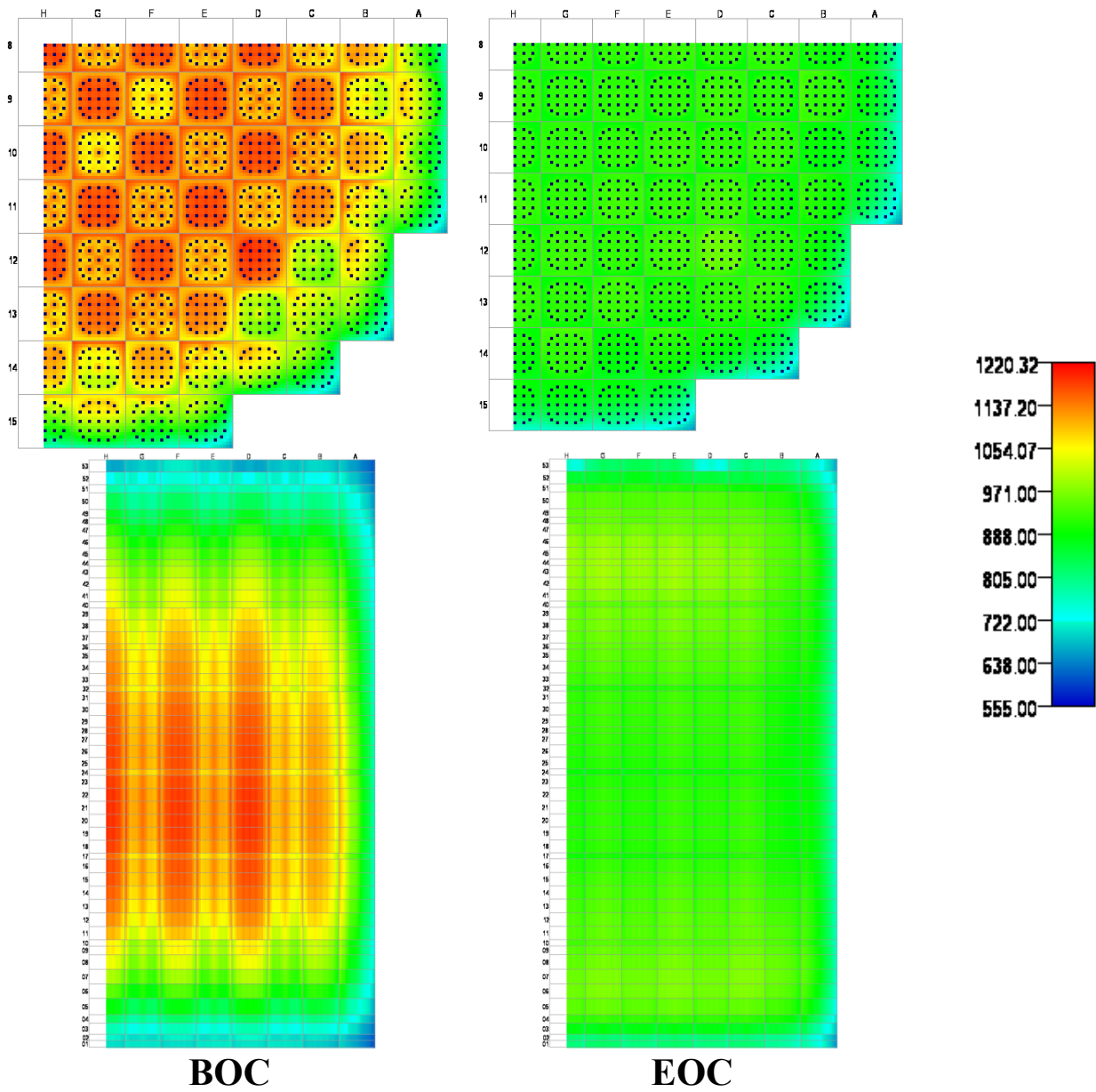
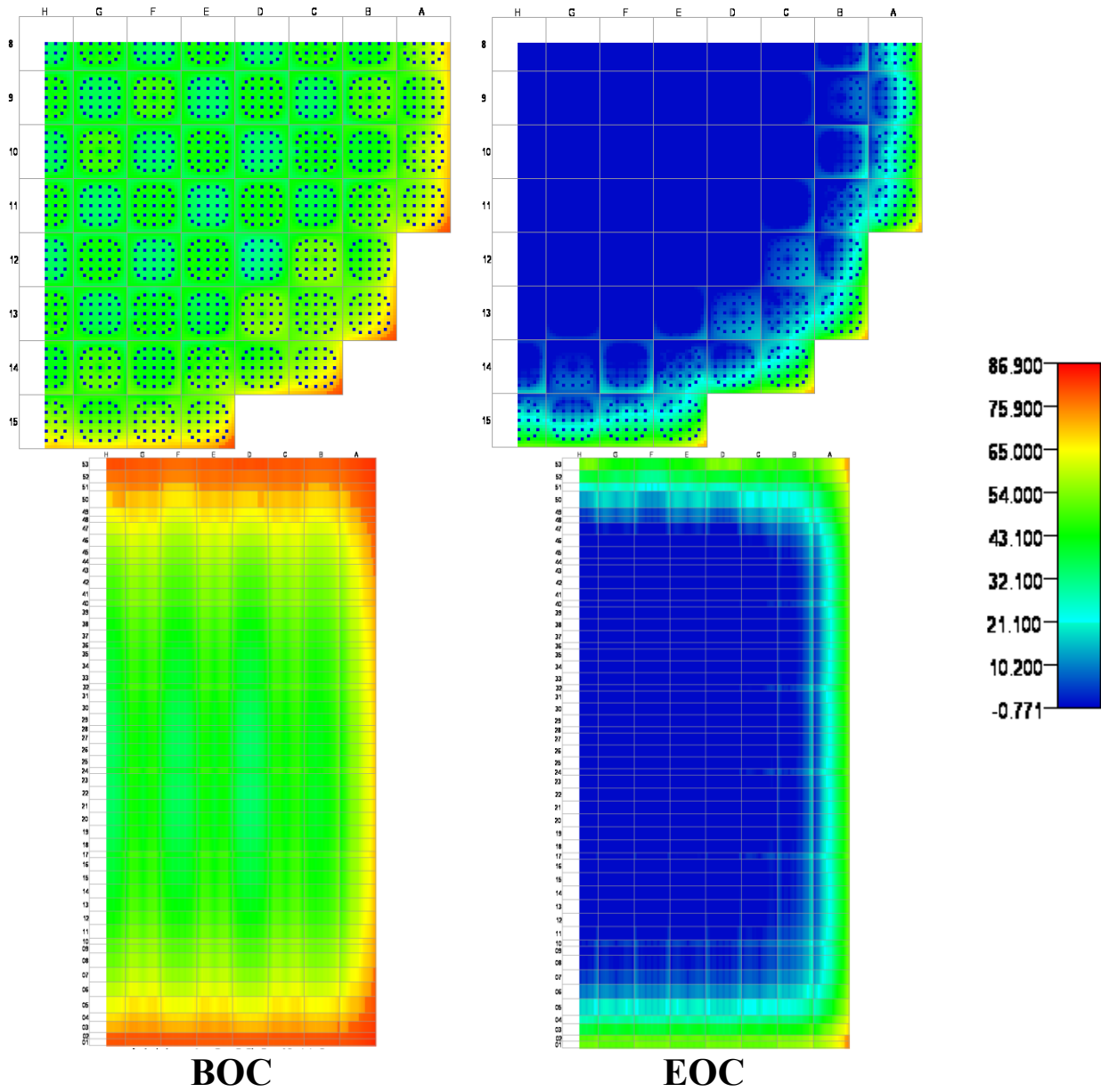


Figure 4.2.4. Watts Bar Unit 1 – Cycle 1, Average Fuel Temperature [K] Distributions



BOC **EOC**
Figure 4.2.5. Watts Bar Unit 1 – Cycle 1, Fuel-Clad Gap [microns] Distributions

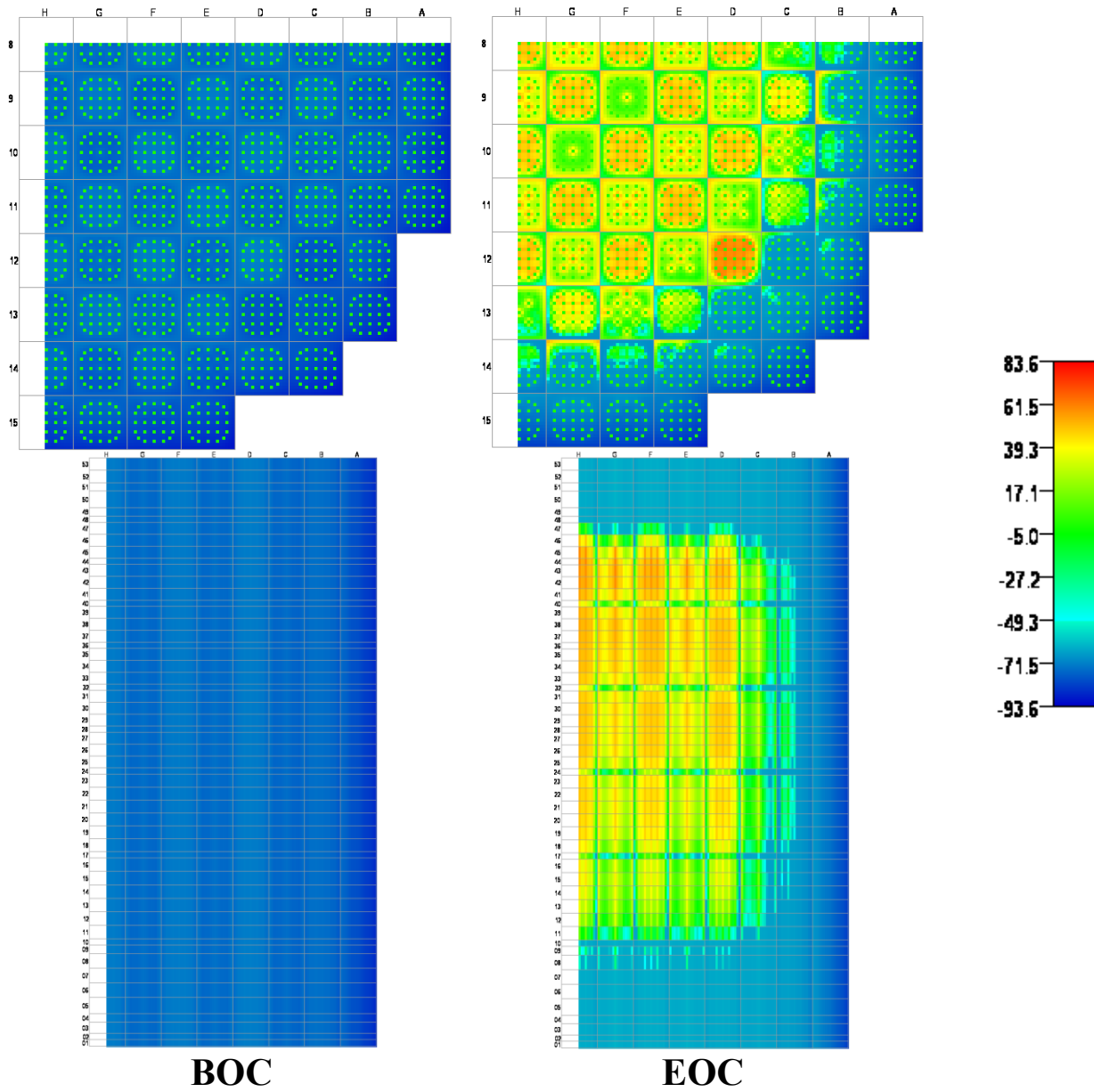


Figure 4.2.6. Watts Bar Unit 1 – Cycle 1, Maximum Clad Hoop Stress [MPa] Distributions

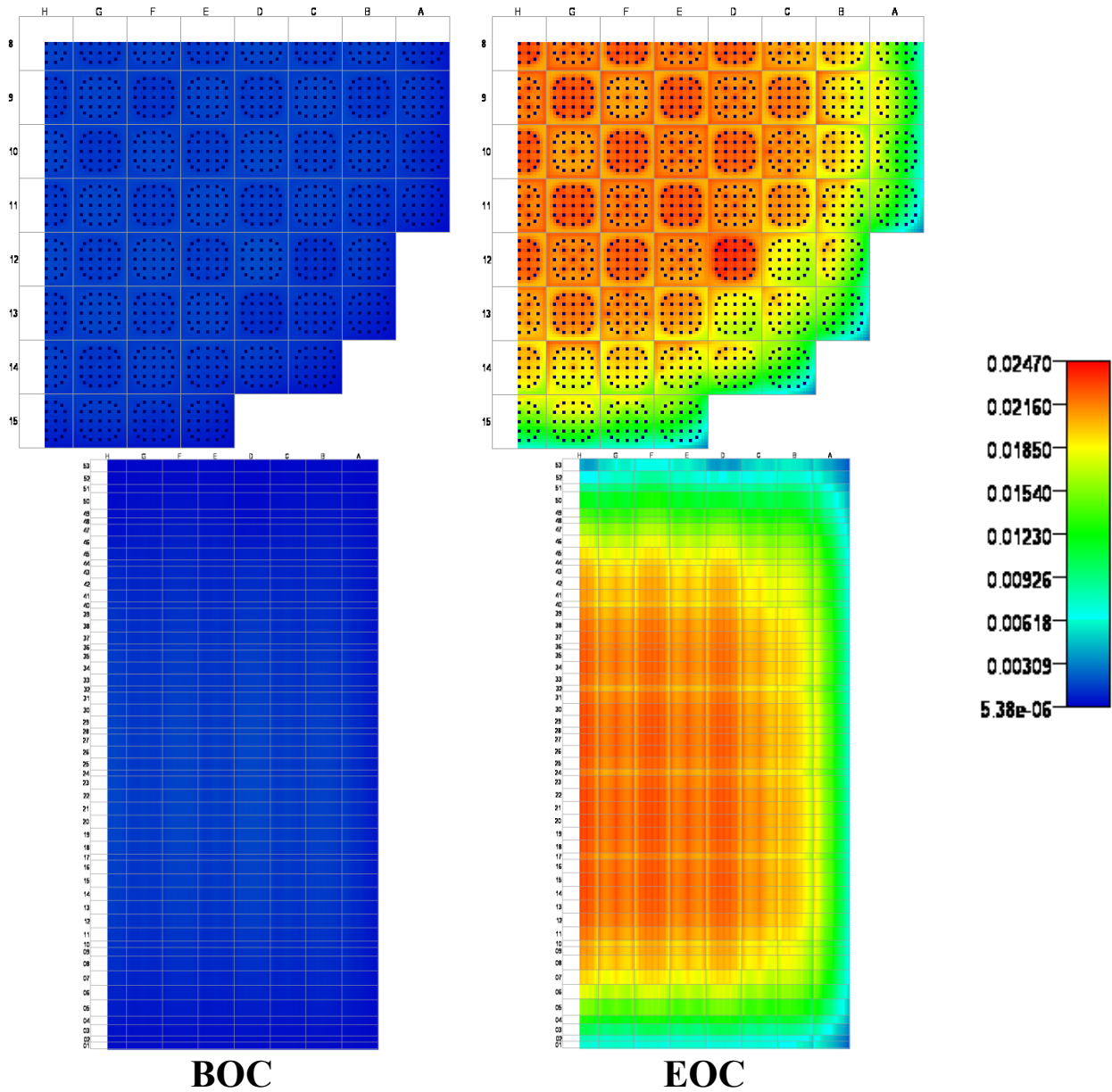


Figure 4.2.7. Watts Bar Unit 1 – Cycle 1, Burnup [fima] Distributions

4.3 Path Forward

The good news is that the Tiamat coupling seems to be working well, and the 1.5D Bison capability appears to be robust. Most of the remaining issues to be sorted out relate to computational performance. The first goal will be to resolve the subgroup self-shielding logic so it is only performed when necessary (in a consistent manner to current MPACT/CTF calculations). This alone will provide a significant speedup. Second, the HDF5 writing times and other operations happening the first iteration of each statepoint need to be resolved. This could potentially cut ~30 walltime hours out of the simulation, closing much of the gap between Tiamat-Coupled and MPACT/CTF calculations. Lastly, any performance improvements that can be made to the 1.5D capability will go a long way to improve the overall Tiamat runtime. As was observed, the second state took around 10 hours because the power ramp required more Bison timesteps than in the rest of the states.

5. CONCLUSIONS

In this report, the recent development efforts that have gone into Tiamat were presented. This included improvements to the overall algorithm, better burnup representation, the 1.5D capability that the Bison team has produced, and the incorporation of the ability in MOOSE to resolve the same timestep repeatedly in Bison. From there, the demonstration for the single assembly was presented. VERA Progression Problem 6 was used for this, adding depletion for a representative cycle. Runtime comparisons for MPACT/CTF, Tiamat-Inline, and Tiamat-Coupled were shown, where Tiamat-Inline required roughly 7x more core-hours than MPACT/CTF; Tiamat-Coupled was around 9x.

With the optimistic results from the single assembly cases, the current status of the quarter-core cases were presented. While both Tiamat-Inline and Tiamat-Coupled ran into walltime limitations on the Panacea cluster, both jobs nearly completed without any signs of convergence issues in Bison. Part of this may be attributable to the robustness of the 1.5D capability, but Bison is generally more stable early in the rod history, such as during Cycle 1.

Overall, things are looking very positive for the quarter core demonstration milestone due in August. There are several performance issues that are currently under investigation and being addressed. With the fixes to Tiamat, a cycle depletion target of 96,000 core-hours (~2000 cores for 2 days) seems reasonable. If additional gains are realized in the 1.5D capability in Bison, an even lower target runtime may be achievable.

6. ACKNOWLEDGMENTS

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Many of the figures shown here were generated using the VERAView software package [18].

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