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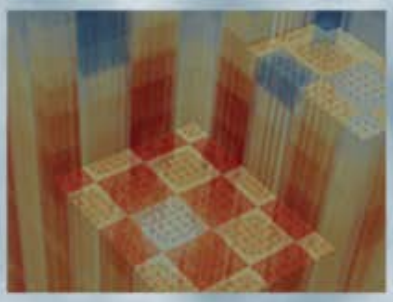
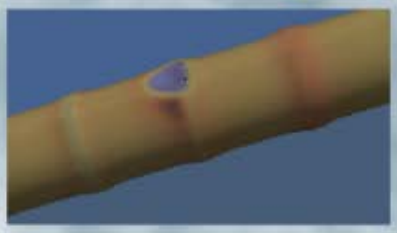
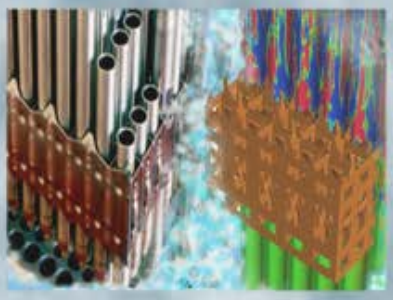
Incorporate MPACT into TIAMAT and Demonstrate Pellet-Clad Interaction (PCI) Calculations







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ABSTRACT

CASL (the Consortium for Advanced Simulation of LWRs) is investing in the development of the multi-dimensional Bison fuel performance code for both transient and nominal peformance analysis. The MPACT whole-core neutronics capability has been integrated with the Cobra-TF sub-channel solver to provide a neutron-transport based core-simulator with substantially improved fidelity over traditional diffusion-based core simulators. The Tiamat code is being developed to provide an integrated tool for predicting pellet-clad interaction and improving the high-fidelity core simulator.

This manuscript documents the completion of the "L3:PHI.CMD.P10.01" CASL milestone to "Incorporate MPACT into Tiamat and demonstrate PCI calculations". [**?**] The MPACT code has replaced Insilico as the primary neutronics component of Tiamat and is currently under nightly testing. The algorithm for incorporating (single-cycle) depletion has been documented and discussed with the lead MPACT developers. Tiamat has been compared with MPACT+CTF for a suite of single-pin analyses and results agree very well. Several large calculations have beeen executed on EOS to model the full 17x17 PWR assembly and a 5x5 cross of PWR assemblies. With the completion of this milestone, Tiamat with Insilico is being placed on idle and continued develoment on Tiamat will focus on the MPACT version.

Key Words: Bison, Peregrine, MPACT, Cobra-TF, Tiamat

1 INTRODUCTION

Pellet-Cladding interaction (PCI) is a local effects cladding failure mechanism that can occur in various fuel rod locations in the reactor core, depending on the core operating strategy, the power maneuvering approach, and the fuel rod design characteristics. The related variables that influence the potential for cladding failure include the rod-average and local burnup, the rod-average power and the power axial distribution both prior to, and during, a power maneuver. An important capability for the assessment of PCI failure is the ability to calculate a key figure of merit as a function of position within the reactor core that identifies a subset of rods that require more detailed 3-D thermo-mechanical simulations of PCI.

The single-rod fuel performance code Bison (previously called Peregrine) can calculate the cladding hoop stress as a function of operating conditions using an 2-D axi-symmetric fuel rod geometric representation. Previous studies have demonstrated that maximum cladding hoop stress can serve as a figure of merit for the potential for PCI failure. Tiamat is being created to couple the Bison fuel performance calculation with a full core representation of the fission density and coolant conditions for each fuel rod within the core. This coupling provides a full core calculation of the maximum cladding hoop stress that can then be used to identify the fuel rods and assemblies of interest for further detailed PCI calculations.

VERA is a suite of simulation capabilities, as shown in Figure 1, which are being developed in order to address the CASL Challenge Problems. VERA-CS (Core Simulator) is an integrated suite of VERA that will provide all of the functionality of a traditional core simulator, but with much higher fidelity. The current version of VERA-CS is integrated within the main MPACT driver and integrates the Cobra-TF (CTF) sub-channel thermal-hydraulics and fuel heat transfer models with the full functionality of the MPACT neutronics capability. Tiamat has been developed for analysis of

PCI and currently integrates a portion of the Bison fuel performance code with the CTF sub-channel thermal-hydraulics and a subset of the MPACT neutronics capability. This report documents the algorithm that will be used by Tiamat to incorporate more of the functionality of MPACT.

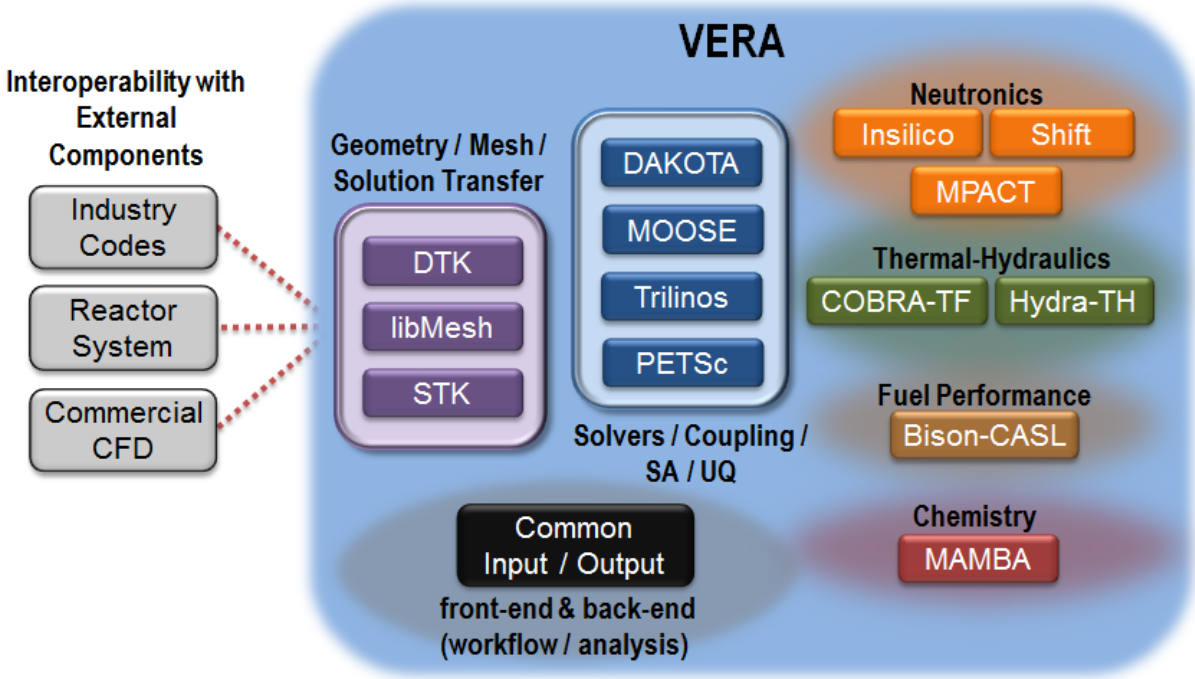

Figure 1. The VERA code suite.

This report documents the completion of CASL Milestone L3:PHI.CMD.P10.01, "Incorporate MPACT into Tiamat and Demonstrate PCI Calculations." [**?**] The goal of this report is to document the incorporation of MPACT into Tiamat as a replacement for Insilico and define the path forward with respect to the addition of depletion. The report documents also provides a discussion about how multi-cycle depletion could be handled in Tiamat. Section 2 describes the overall design of Tiamat, including the sub-components. Section 3 describes the conversion from Insilico to MPACT. Section 4 describes the unit testing and single pin parametric study of Tiamat with MPACT. Section 5 describes the larger problems executed to demonstrate the capabilty for full assembly problems. Section 6 describes the algorithms that could be used for various depletion scenarios. Section 7 describes the unit tests that will be required to test the ability of each of the physics codes to provide the functionality required by Tiamat. Section 8 summarizes the report.

2 DESIGN OF TIAMAT

This section describes the overall design of Tiamat and the individual applications used in the coupling. Tiamat is named for a multi-headed dragon tracing back to Babylonian mythos to reflect that this coupled driver allows for simple extension to additional physics and couplings. A previous version of Tiamat leveraged the Insilico neutronics code, but that is in the process of being deprecated because MPACT is the driver for VERA-CS. Section 2.2 describes the MPACT neutronics code. Section 2.4 describes the Bison nuclear fuel performance code. Section 2.5

describes the data transfers that couple each of the codes. Section 2.6 describes the PIKE numerical analysis kernels that provide the coupled physics solvers, and Section 2.7 describes the Tiamat driver that integrates all of the other pieces.

2.1 COBRA-TF (CTF)

COBRA-TF (CTF) is a thermal-hydraulic simulation code designed for Light Water Reactor (LWR) analysis [3]. CTF has a long lineage that goes back to the original COBRA developed in 1980 by Pacific Northwest Laboratory under sponsorship of the U.S. Nuclear Regulatory Commission (NRC). The original COBRA began as a thermal-hydraulic rod-bundle analysis code, but subsequent versions of the code have been continually updated and expanded over the past several decades to cover almost all of the steady-state and transient analysis of a both PWRs and BWRs. CTF is being developed and maintained by the Reactor Dynamics and Fuel Management Group (RDFMG) at the Pennsylvania State University (PSU). CTF includes a wide range of thermal-hydraulic models important to LWR safety analysis including flow regime dependent two-phase wall heat transfer, inter-phase heat transfer and drag, droplet breakup, and quench-front tracking. CTF also includes several internal models to help facilitate the simulation of actual fuel assemblies. These models include spacer grid models, a pin conduction model, and built-in material properties. CTF uses a two-fluid, three-field representation of the two-phase flow. The equations and fields solved are:

- Continuous vapor (mass, momentum and energy)
- Continuous liquid (mass, momentum and energy)
- Entrained liquid drops (mass and momentum)
- Non-condensable gas mixture (mass)

Some of the reasons for selecting CTF as the primary T/H solver in the VERA core simulator is the modest run-time, as compared to CFD (Computational Fluid Dynamics), the fact that it is being actively developed and supported by PSU, and for the ability to support future applications such as transient safety analysis and BWR (Boiling Water Reactor) and SMR (Small Modular Reactor) applications. CTF is a time-dependent, control volume code that enforces conservation between volumes and is being used within Tiamat in a steady-state mode. Internally CTF uses a pseudo-transient solver to converge towards a steady-state convergence for a particular flow/power state.

2.2 MPACT

The reactor core simulator MPACT has been developed collaboratively by researchers at the University of Michigan (UM) and Oak Ridge National Laboratory (ORNL) to provide an advanced pin-resolved transport capability within VERA. The key characteristics of the MPACT code include

the subgroup method and the embedded self-shielding method (ESSM) for resonance treatment, depletion capability based on the ORIGEN exponential matrix method, and a whole core solver with a 2-D/1-D synthesis method on the frame of 3-D coarse mesh finite difference (CMFD) method for which axial and radial correction factors are obtained from 2-D method of characteristics (MOC) and 1-D nodal expansion method (NEM) or Simplified PN, respectively. Reference [1] contains a detailed description of the methods used in MPACT as a part of the VERA Core Simulator.

In addition, MPACT contains other "Feedback Solvers" to execute code that will effect the cross sections during a multi-cycle core depletion. One of the primary effects is due to changes in the fuel temperature and moderator density. MPACT contains both an internal simplified thermal-hydraulic model and a direct connection to CTF.

2.2.1 MPACTs Internal TH

The thermal-hydraulic model that is internal to MPACT is based on a one-dimensional fuel conduction at a series of axial nodes coupled to a one-dimensional, single-phase flow model that neglects cross flow between the channels. The fuel thermal conductivity models are not dependent upon the burnup, temperature, or porosity of the fuel. The gap heat transfer coefficient is fixed and does not change during a multi-cycle depletion calculation. The clad thermal conductivity models does not depend on the porosity of the fuel either. Because the mechanical changes to the fuel and cladding or not modeled it is incapable of modeling PCI, but can provide an estimate of the fuel temperature and clad coolant density.

2.2.2 MPACTs direct coupling with Cobra-TF

The direct coupling of MPACT to CTF allows VERA-CS to leverage a higher fidelity fuel heat transfer model (2D in R-Θ) and account for both cross-flow and boiling. However, the fuel thermal conductivity models are not dependent upon the burnup, temperature, or porosity of the fuel. The gap heat transfer coefficient is fixed and does not change during a multi-cycle depletion calculation. The clad thermal conductivity models does not depend on the porosity of the fuel either. Because the mechanical changes to the fuel and cladding or not modeled it is incapable of modeling PCI, but also can provide an estimate of the fuel temperature and clad coolant density.

2.3 Predictor-Corrector Solution Algorithm

The MPACT solution algorithm for single-cycle depletion problems with feedback is as follows:

1. Solve the coupled problem at the first state with the initial isotopics
2. Loop over all state-points in the problem
    (a) Loop over depletion steps of this state point

i. **Isotopic Predictor:** Given the coupled solution at the beginning of the step, solve for the isotopics at the end.
ii. **Prediction Solve:** Given the predicted isotopics at the end of the step, solve the coupled problem at the end.
iii. **Isotopic Corrector:** Given the average coupled solution, solve for the isotopics at the end.
iv. **Coupled Solve:** Given the corrected isotopics at the end of the step, solve the coupled problem at the end.

2.4 Bison

The Bison fuel performance code is being developed to provide a single-rod, fuel performance modeling capability to assess safety margins, and the impact of plant operation and fuel rod design on the thermo-mechanical behavior, including Pellet-Cladding Interaction (PCI) failures in PWRs [11,12]. PCI is controlled by the complex interplay of the mechanical, thermal and chemical behavior of a fuel rod during operation, and therefore modeling PCI requires an integral fuel performance code to simulate the fundamental processes of this behavior. Bison is built upon INL's MOOSE/Fox packages, which are also common to the Bison code [8]. This code architecture uses the finite element method for geometric representation and MOOSE uses a Jacobian-free, Newton-Krylov (JFNK) scheme to solve systems of partial differential equations [9]. While the MOOSE framework can solve either steady state or transient problems, the Bison application is a transient code because the material models are strongly influenced by the time history. The focus of Bison is to establish a modern computational framework based on the finite element method to represent the geometric domains of a single nuclear fuel rod composed of UO_2 ceramic pellets contained within a Zircaloy tube. The Bison framework consists of a numerical representation of the heat conduction and the equilibrium mechanics equations, which are coupled via the temperature and displacement variables. A material property and constitutive model library has been incorporated into the framework that allows for thermal, mechanical, and chemical property models and irradiation effects models, such as fission product-induced swelling or irradiation creep, to be utilized and modified easily. Finally, the framework allows for versatile time-marching algorithms to capture the different temporal regimes associated with fuel performance, such as burnup accumulation over several years followed by a rapid power ramp over several minutes. For this milestone, the fuel rod geometric representation in Bison was a 2D R-Z axially-symmetric, smeared-pellet model. The base mesh is shown in Figure 2, where the red region is fuel and the blue region is cladding; the radial dimension is scaled by a factor of 100.

Because Tiamat simulates thousands of fuel rods in parallel, Bison is accessed using the MOOSE MultiApp capability. A separate instance of Bison is built for each fuel rod and the applications are aggregated and solved via the MOOSE MultiApp object interface and coupled to the other physics application components: CTF and Insilico via the Data Transfer Kit (DTK). Bison computes the thermal expansion and elastic deformation of the cladding and pellet in response to the energy generation (heat) and mechanical forces. The interaction of the temperature solution and

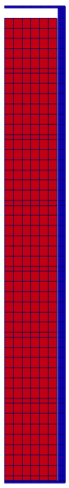

Figure 2. 2-D Axisymmetric Finite Element Mesh (FEM) Representation of a Fuel Rod.

the mechanical solution is non-linear due to the complex dependency of the material properties on temperature, stress, and strain. As a result, Bison must model the heating of a fuel rod from zero power to full power to appropriately account for these non-linearities. While a core-simulator is traditionally uses a quasi-static model, with a series of steady-state calculations, the material models within Bison are inherently time-dependent. Therefore, Bison was used in a way to approximate steady-state conditions, as discussed in the following section of this report. Advancements in this approximation were a significant part of this milestone.

2.5 DATA TRANSFERS

To couple the codes, data must be passed between each code. There are five data transfer objects implemented in Tiamat for this capability. All data transfers have to account for patterns for parallel communication, unit conversions, pin axis orientation, and active fuel offset height. DTK was used for determining the parallel MPI communication mappings and for moving all data between codes. As part of this procedure, DTK performs an intersection search for target coordinate points in source geometry representations. A very valuable benefit was that if a target point was not found in the source geometry, it was recorded and reported. This was critical in tracking down misaligned meshes and coordinate transformation issues between codes. At runtime, if a user makes a mistake in specifying the geometry/mesh information, DTK will help to catch this. All three codes use different unit systems that are to be converted during data transfers: CTF uses English units, Insilico uses a mix of CGS and MKS units, and Bison used MKS units. Pin-axis alignment deals with the direction that the fuel rod axes are oriented. CTF and Insilico align the pin axis in the ‘z’ direction in three-dimensional (3D) Cartesian coordinates, but Bison uses a two-dimensional (2D), axially-symmetric ‘R-Z’ model with the pin axis aligned on the second coordinate index. In the MOOSE MultiApp DTK interface, an internal translation from 2D cylindrical to 3D Cartesian coordinates is provided, but it keeps the pin aligned in the second coordinate direction (‘y’ direction in Cartesian). Therefore, when implementing data transfers involving Bison, the ‘y’ and ‘z’ coordinates of the target coordinate point had to be swapped before

passing to the DTK detection algorithm. In addition, each code models different spatial components of the reactor above and below the active fuel region; Insilico models the upper and lower coolant plenums, Bison models the full fuel pin, and CTF was restricted to coolant adjacent to the active fuel. This results in different origins in the axial dimension for each code. Therefore, each transfer must adjust the coordinates to a common specification when communicating with DTK so that the active fuel regions are aligned between codes during the source/target intersection search.

2.6 SOLVERS

The PIKE (Physics Integration KErnels) solver package, a replacement for LIME 1.0, was recently given DOE copyright approval for release in the Trilinos framework. PIKE contains both a Gauss-Seidel and a Gauss-Jacobi solver for multi-physics applications, along with a time-dependent component that will be utilized for the transition to depletion. PIKE includes simplified model interfaces, explicit separation of global and local convergence criteria, a user defined convergence test hierarchy, local application convergence checks, flexible unified user control via observer design pattern, user extensible factories to allow for solvers to enforce the open-closed principle, and simplified structured parameter and response interfaces.

2.7 TIAMAT

Tiamat couples these physics components using DTK to transfer the data and PIKE to solve the math.

3 CONVERSION FROM INSILICO TO MPACT

To convert the Tiamat code from using Insilico to using MPACT, there were several modifications required. The Insilico-based, LIME-coupling of neutronics with Cobra-TF was designed, developed, tested, and stable before the MPACT interface was required. Therefore, the development of the LIME ModelEvaluator and DTK interface for MPACT leveraged all of the experience from Insilico and was able to replciate the design and many of the unit tests.

The original Tiamat development created a new PIKE-based ModelEvaluator that had a direct connection to the Insilico drivers and by-passed the LIME ModelEvaluator. During FY14, a significant refactoring of the Insilico interfaces was performed to allow for a LIME-free driver, with an extension for both PIKE and LIME, but this refactoring was not done for MPACT. After significant discussion and debate about the future of Insilico and cost of maintaining Tiamat's backwards compatability with it while advancing the MPACT version forward with the addition of depletion, three priorities became clear: (1) keep the Insilico version around and under test, (2) don't let that version impede progress with MPACT, and (3) minimize the cost of incorporating fixes needed for the MPACT version into to Insilico version.

To complete this milestone, there were several modifications required to Tiamat and MPACT:

- Generalization of Insilico to Neutronics
- Creation of a LIME-free MPACT ModelEvaluator
- Separation of Insilico and LIME versions of Tiamat
- Generalization of PETSc Initialize in Cobra-TF

To ensure that the Insilico version is maintained and tested, we have created a separate packages for the MPACT version. To minimize the cost of incorporating fixes into Insilico, we chose to generalize the Insilico version to "Neutronics" before breaking off a copy for the MPACT version. Therefore, all references in Tiamat to Insilico were replaced with Neutronics and the connection of the NeutronicsModelEvaluator (no longer InsilicoModelEvaluator) to Insilico was generalized to use a non-code-specific API. With this change, there are only a few differences in Tiamat between the current versions of MPACT and Insilico that could be eliminated, but don't make sense to because that would likely impede progress with MPACT; the rest of the lines of code in each source directory are identical.

- Trilinos, not Nemesis, initializes and finalizes MPI.
- Insilico requires an explicit call to print the final output.
- Different headers are included in the NeutronicsModelEvaluator.

Because the MPACT model evaluator was hard-wired to work with LIME, we needed to create a general MPACT driver, which had a DTK adapter, and Tiamat could extend with a PIKE-based ModelEvaluator. In Insilico, this involved modifying the LIME-based ModelEvaluator to be a simple extension of both the general driver and the LIME ModelEvaluator. For MPACT we simply made a copy because we don't envision retaining the LIME-based coupling much longer since CTF can be executed within MPACT.

With the creation of two separate TriBITS subpackages for Tiamat-with-Insilico and Tiamat-with-MPACT, we were able to create a suite of tests specific to Tiamat with MPACT. The Insilico-based Tiamat retained all of the original tests and several were ported to the MPACT version. Additionally, the CTF+MPACT tests based on the LIME coupling were ported to work with Tiamat and are tested nightly as well. The specific tests, with a description, are provided in Section 7.

Historically, there have been many challenges when integrating a new component into a VERA package. Examples include: integrated CTF and Insilico took over 1.5 years; integrating CTF and MPACT was over 6 months later than projected; creating Tiamat with MOOSE embedded lead to a massive overhaul of TriBITS to support external codes needing to work with Trilinos, among other things. When we decided to integrate MPACT, there was only a single hurdle - a conflict associated with PETSc initialize.

PETSc has a single global variable to define the PETSC_COMM_WORLD. This is defined by the first call to PETSc initialize; subsequent codes that need to use PETSc should check if PETSc is initialized before trying because a second call to the function will cause PETSc to crash. MPACT and MOOSE were correctly handling the PETSc initialize, but CTF was redefining the PETSC_COMM_WORLD to be the communicator given to COBRA when run in parallel. In LIME, this communicator was MPI_COMM_WORLD, but in Tiamat it was just the communicator used by CTF. The fix was relatively easy (initialize PETSc in Tiamat and replciate MPACTs approach in CTF), but identifying the problem was more difficult because it showed up far from the source of the error with a poor error message. In the end, the conversion took less than one week of effort and was completed in two weeks of real-time.

4 TESTING OF TIAMAT WITH MPACT

This section contains a discussion of the unit tests that are executed nightly to provide regular testing of the Tiamat with MPACT capability as well as a parametric study of single-pin calculations that compare Tiamat with the independently coupled MPACT+CobraTF driver.

4.1 Unit Testing of Tiamat

The unit tests in the tiamat_w_mpact directory include the following suite:

- Tests developed for Tiamat with Insilico and migrated to work with MPACT:
  - *Ser_1x1_asy_1x1_pin_full*: single processor test for a single pin in a single assembly.
  - *Par_1x1_asy_1x1_pin_full*: parallel MPACT for a single pin in a single assembly.
  - *Par_3x3_asy_3x3_pin_full*: parallel CobraTF and MPACT for a 3x3 array of pins in a 3x3 array of assemblies.
- Tests developed for MPACT+CobraTF and migrated to work with Tiamat:
  - *base*: “base case” for single pin results in this document and the L1-milestone report for Tiamat with Insilico.
  - *transfers*: unit testing of data transfers between physics components.
  - *unit_tests*: unit testing of the internal Tiamat componets.
  - *small_mpact_3x3*: unit testing for a single assembly with a 3x3 array of pins.
  - *t_factory_moose*: unit testing of interface to MOOSE applications.

4.2 Single Pin Parametric Study

The base problem is described in Reference [1], with details on the Bison, Cobra-TF, and coupled discretizations and iteration schemes.

Table I. Study of MPACT Maximum Outer Iteration Parameter

Max Outer Iterations	100	8	4	2	1	
Coupled Iterations to Converge	8	8	8	8	10	
Time to Solution	193.2	185.8	170.1	160.8	194.5	sec
	Value		Error			
Eigenvalue	1.15604	0	0	-0.0600	-0.7900	pcm
Peak Coolant Temperature	327.799	0	0	-0.0002	-0.0005	C
Peak Clad Temperature	341.704	0	-0.0001	-0.0014	-0.0038	C
Peak Fuel Temperatures	1081.196	0	0.0009	0.0033	-0.1284	C

The MPACT mesh for the base (single pin) problem has 59 axial planes, 8 azimuthal zones, and 6 radial regions (3 fuel, gap, clad, and coolant). The 56-group ORNL cross section library, with 4 sub-groups, was used with the LTCP0 approximation and a 2x2 Chebyshev-Gauss quadrature set with a 0.1 cm ray spacing. In all cases the neutronics solution was converged to 1e-5 for both the flux and eigenvalue using 3 inner iterations per group and 2 upscatter iterations per outer iteration. Unless otherwise noted, a maximum of 100 outers per coupled iteration solve was used to fully-converge the eigenvalue problem for each coupled iteration. The standard "mgnode" CMFD acceleration was used with a maximum of 20 iterations per outer and a shift of 1.5. Because MPACT with both the internal TH and internal coupled to Cobra-TF have been benchmarked against the externally coupled MPACT+CTF solver, we will continue the trend of direct comparison with the LIME-coupled MPACT+CTF.

4.2.1 MPACT Outer Iterations

Table I displays the effect of the maximum number of MPACT outer iterations per coupled-physics solve on a variety of paramters. The number of coupled iterations required to converge the solution does not change until there is but one mpact outer iteration per coupled solve. Because it increases from 8 to 10 copuled iterations, the runtime increases for this option. Similarly, the time to solution is consistently reduced by reducing this parameter until it equals one. In addition, reducing the number of iterations per coupled solve doesn't effect the solution because even a 0.8 pcm change in the eigenvalue and 0.1 C change in the tmperature is insignificant with respect to other uncertainties in the problem.

4.2.2 Gauss-Jacobi Iteration Scheme

Tiamat utilizes two primary solvers for single-statepoint coupled physics solves: Gauss-Seidel (GS) and Gauss-Jacobi (GJ). The GS solver iterates serially through each physics code and provides the downstream codes with the latest estimate of the coupled soluiton. The GJ solver allows each physics code to estimate the solution based on the information from the previous coupled solve. Therefore, the GJ solver makes better use of all three processors, but the algorithm does not converge as quickly as GS.

Table II. Study of Gauss-Jacobi Iteration Scheme

Solver Type	GS	GJ	GS	GJ	GS	GJ
Max Outer Iterations	1	1	2	2	1000	1000
Coupled Iterations to Converge	10	25	8	19	8	19
Time to Solution (sec)	727.3	794.9	564.6	708.7	687.6	1041.0

Table III. Study of MPACT Parallel Efficiency within Tiamat

Total Procs	3	4	6	10	18
MPACT Procs	1	2	4	8	16
Total Solve (sec)	567.4	537.1	470.2	432.2	339.1
MPACT Solve (sec)	261.6	152.7	85.4	46.0	21.8
MPACT Ratio	0.46	0.28	0.18	0.11	0.06
MPACT Efficiency		0.86	0.77	0.71	0.75

Because the optimal maximum number of outer MPACT iterations was shown to be low, this study varies that parameter to determine the effect on each solver. Each of the cases converged to identical (within 1 pcm and 0.1 C) solutions, but Table II shows that the GJ scheme consistently requires more coupled iteration and more execution time than the correspoding GS solver. Therefore, we again recommend the use of the GS solver and place a high priority on allowing Tiamat to execute on a single processor by allowing for the overlap of communication domains.

4.2.3 MPACT Parallel Efficiency

In the original parametric study of Tiamat, using Insilico instead of MPACT, it was clear that there was no benefit to evaluating the parallel performance on this problem. Insilico is based on a spatial domain decomposition in the x-y plane and the XSProc cross section processing is not currently parallelized over the axial domain. Therefore, for this particular problem, Insilico with SPn was effectively a serial component of Tiamat. However, MPACT is naturally decomposed over the axial domain because of the 2D-1D spatial discretizatoin. Therefore, a parametric study was done on the "base" case with increasing processors available to MPACT. Note that this study was performed with the "Max Outer Iterations" of MPACT set to 2, rather than 100.

The MPACT processor count was consistently doubled, while the CobraTF and Bison portions each used a single processor, and the effects on the execution time were compared. In Table III, both the total solve time and the MPACT portion of the solve time were consistently reduced by increasing the processors for neutronics. As the MPACT solution time was reduced, there was a significant reduction in the MPACT portion of the run-time, from 46% with one processor to 6% with 16. MPACT had a significant drop in efficiency from one to two (85%)and two to four processors (71%), but it leveled off as additional cores were made available. As the MPACT solution time was decreased the overall execution time was comparably reduced.

Table IV. Study of Bison Parallel Efficiency within Tiamat

Total Procs	3	4	6	10	18
Bison Procs	1	2	4	8	16
Total Solve (sec)	690.5	702.7	609.0	563.3	517.6
Bison Solve (sec)	299.8	251.3	152.9	106.3	77.2
Bison Ratio	0.43	0.36	0.25	0.19	0.15
Bison Efficiency		0.60	0.49	0.35	0.24

Table V. Benchmarking Tiamat with Boron Variation

Boron (ppm)	Tiamat Eigenvalue	Tiamat pcm/ppm	CTF+MPACT Eigenvalue	CTF+MPACT pcm/ppm
0	1.2909	-10.4	1.2908	-10.4
650	1.2193	-9.7	1.2192	-9.7
1300	1.1560		1.1560	
1950	1.0998	-8.7	1.1039	-8.0

4.2.4 Bison Parallel Efficiency

The Bison, formerly Peregine, parallel efficiency study was performed in Reference [1]. However, that was compared with respect to Insilico with the 8-group cross section library that is only for testing purposes. Because there have been several updates to MOOSE/Bison since that milestone, this study was performed once again.

Table IV displays the parallel efficiency of Bison for this small problem. There is a significant drop in the parallel efficiecy with every additional processor; adding 16 processors reduces the Bison execution time by only a factor of four. For multi-pin problems, it is still highly-likely that the best use of additonal processors is spent on allowing each Bison pin to have a single core. However, additional processors beyond one per Bison pin would be better spent on MPACT when available.

Note that the Bison scaling study was performed on the “base” problem with the maximum number of MPACT outer iteration set to 100.

4.2.5 Boron and Power Parametric Study

In Reference [1], it was demonstrated that Tiamat with Insilico matched CTF+Insilico for a variety of powers and boron concentrations; we repeat that study here with MPACT.

The sensitivity to the boron concentration is somewhat different for the 56-group MPACT library from the 8-group Insilico library, but the conclusions are the same. As shown in Table V, Tiamat is accurately reproducing the CTF+MPACT sensitivity to boron for a wide range of boron concentrations.

Table VI. Benchmarking Tiamat with Power Variation

Power	Tiamat K-eff	MPACT k-eff	pcm	Tiamat Iters	CTF+MPACT Iters
0	1.1744	1.1744	-1	1	1
1	1.1742	1.1742	3	5	2
10	1.1724	1.1727	32	8	5
25	1.1695	1.1701	62	9	7
50	1.1649	1.1656	72	9	7
75	1.1605	1.1609	49	9	8
100	1.1560	1.1560	-5	10	7
125	1.1517	1.1508	-86	10	7
140	1.1491	1.1476	-149	10	7
150	1.1466	DNC			

Similar to the study with Insilico, the consistency between Tiamat and CTF+MPACT is not perfect as the power in increased from 0 to 150% of the rated hot-full power. While this has not been investigated, it is likely due to differences in the physics; perhaps the axial variation of the gap heat transfer coefficient due to axially-varying thermal expansion.

4.3 Convergence Rate of Damping Factor

As noted in Reference [1], the rate of convergence between Tiamat and LIME-coupled neutronics and CTF differ. In the preceeding subsection (Section 4.2.5), it was shown that CTF+MPACT had a difficult time converging at high power with the default damping factor and that the eigenvalues differed by 149 pcm at 140% of the rated power.

Table VII demonstrates that the damping factor does not significantly effect the eigenvalue but will alter the convergence rate of the code. Tiamat converges for a wider range of damping factors and in fewer iterations than CTF+MPACT. However, the execution times for CTF+MPACT, when it converges, are consistently less than Tiamat.

5 DEMONSTRATION TIAMAT WITH MPACT

Large single- and multi-assembly calculations are in the queue on EOS and will be incorporated into a later revision of this report.

The AMA benchmark progression problem P6a was used to simulate a single assembly for Tiamat-MPACT. This was compared to simulations from the L1 milestone performed with Tiamat-Insilico in Figure 3.

6 DEPLETION ALGORITHM SPECIFICATION

A challenging aspect of this problem is that the different physics associated with these codes are strongly coupled and nonlinear. By strongly-coupled we mean that the quantities calculated in

Table VII. Benchmarking Tiamat with Power Variation

Damping Factor	Tiamat Eigenvalue	Tiamat Iterations	Tiamat Time (sec)	CTF+MPACT Eigenvalue	CTF+MPACT Iterations	CTF+MPACT Time (sec)
25	1.147610	21	845	1.149097	17	1368
30	1.147608	18	725	1.149097	14	1132
35	1.147607	16	645	1.149097	12	1018
40	1.147607	14	586	1.149097	10	890
45	1.147606	13	528	1.149097	9	839
50	1.147606	11	460	1.149097	8	829
55	1.147606	12	487	1.149097	7	754
60	1.147606	18	692	1.149098	6	711
65	1.147606	34	1259	1.149097	8	786
70	DNC	90	3417	1.149097	10	879
75	Diverged	82		1.149097	15	1169

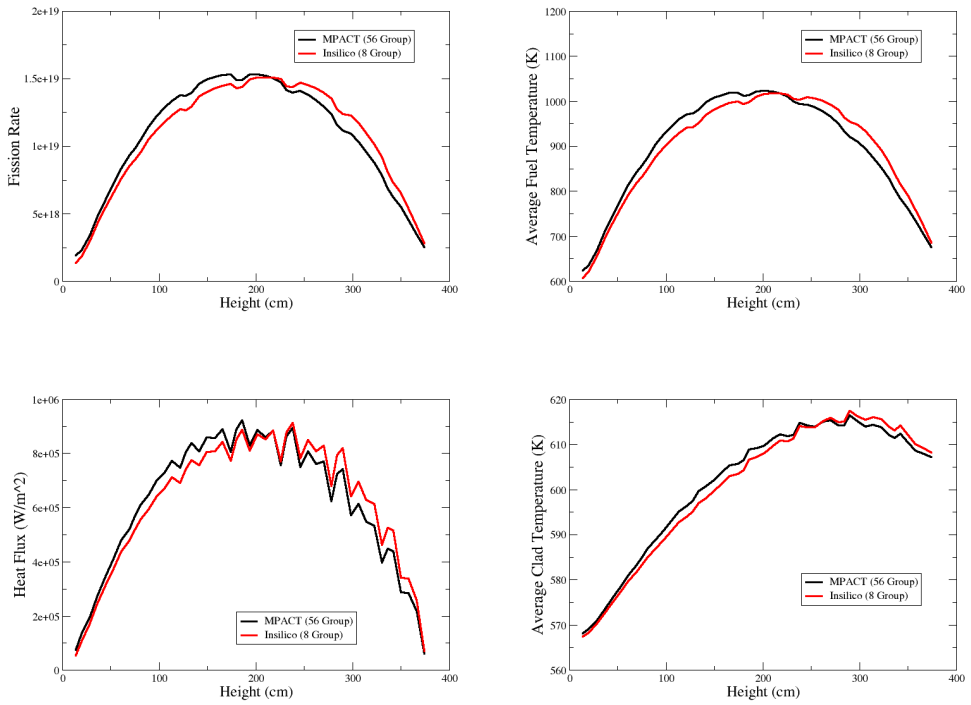

Figure 3. Comparison of 8g Tiamat-Insilico with 56g Tiamat-MPACT for average fuelrod values in p6a single assembly.

each physics component and passed to the other have a significant impact on the physical quantities computed in other physics components. To solve the coupled system, block Jacobi and block Gauss-Seidel fixed-point (FP) iteration strategies are provided through PIKE.

In traditional PCI analyses, the power distributions, ramping rates, and coolant (or clad) boundary conditions are defined in the input to the fuel-performance code. For ?nominal operation? PCI analyses (as with FRAPCON), the boundary conditions are based on independently executed multi-cycle, quasi-static, core simulator results. For ?transient? PCI analyses, the fuel performance code boundary conditions are based on results from a transient core simulator analysis, which used an initial state that was based on the results from a quasi-static core-simulator solution. This section is not intended to define, or even propose, the approach that CASL will take in determining the methodology used for nominal or transient PCI analyses, but simply to begin a discussion of potential use-cases for Tiamat. We first review the algorithm that was used for the initial ramp to full power (Section 6.1) and then propose an algorithm (Section 6.2) for nominal operation PCI analysis of a first cycle core. In Section 6.3, we discuss the challenges and potential of extending this to multi-cycle analyses using either Tiamat alone or in conjunction with the core simulator.

6.1 SINGLE-RAMP

The overall execution is to perform an initialization phase to bring all codes to hot full power (HFP) conditions and then perform the fixed-point coupled iterations between the codes at HFP until convergence for one or more time steps. In order to apply a linear power ramping to BisonCASL, an estimate of HFP conditions are needed. There are currently three choices to obtain this estimate. The first is to perform several iterations of CTF+MPACT (not coupled to BisonCASL) at HFP conditions. The second choice is to restart from a converged run using restart data saved on the coupling mesh. The third choice is to use a combination of the first two choices ? restart close to the solution and perform a few iterations of CTF+MPACT. The following describes the startup procedure.

1. **Model transition from cold, zero-power (CZP) to hot, zero-power (HZP) in BisonCASL.**
   - BisonCASL transient for 100 seconds
   - Linear ramp of clad surface temperature from 20 to 293 C
   - Power in every pin is zero.
2. **Estimate the final (HFP) state clad surface temperature and power.**
   - Read restart file and/or perform several iterations of CTF+MPACT to estimate HFP conditions.
   - Estimate of clad surface temperature for each pin at each axial node
   - Estimate of power distribution for each pin and axial node.

3. **Model the thermo-mechanical changes in the fuel from HZP to the estimated HFP**
    - BisonCASL transient for 48 hours.
    - Linear ramp of clad surface temperature from 293 C to estimated HFP value (Step 1).
    - Linear ramp of power distribution from zero to estimated HFP value (Step 1).
4. **Model the final (HFP) state with CTF+MPACT+BisonCASL**
    - Subcycle all three codes using a fixed-point iteration scheme for each time step.
    - Converge MPACT with pin temperatures from BisonCASL and coolant conditions from CTF
    - Converge CTF to steady-state with a BisonCASL heat flux using a series of time-steps
    - Model a single time-step in BisonCASL at each coupled iteration using power from MPACT and clad surface temperature from CTF

The numerical coupling of all three codes for the HFP conditions leverage the algorithms within PIKE and include parallel, block Jacobi and parallel, block Seidel iterations schemes. The algorithms are discussed in [6]. There are nuances within this general approach that were enhanced as part of this milestone and are discussed in more detail in Section 3.

6.2 FIRST-CYCLE, QUASI-STATIC

For freshly-fueled core, such as Cycle 1 of Watts Bar 1, the as-manufactured initial state of the fuel can be well-defined with a VERA input file. For nominal operation of a single cycle with no rapid transients, the core simulator, with the CTF fuel model, can provide an estimated representation of the smooth temporal variations in the power and clad surface temperature using large, quasi-static time steps. Using the traditional approach, this could provide the input to BisonCASL to model the spatial and temporal variation of the power, coolant pressure, and coolant (or clad surface) temperature to estimate PCI. However, differences in the fuel modeling between CTF and BisonCASL will account in some loss of accuracy. If Tiamat were capable of modeling the first cycle, the error in the traditional approach could be estimated and minimized.

In stand-alone BisonCASL, there are generally many small, logarithmicly-increasing, time-steps are used to accurately model the transition due to changes in the power or coolant conditions. Similarly, MPACT models isotopic depletion between quasi-static states with many small, logarithmicly-increasing, time steps. As noted in Section 2.2, Tiamat could solve the coupled problem for each of the small time steps that are required by BisonCASL and isotopic depletion. However, experience with core-simulators has shown that this is generally not required for the accuracy needed from a core simulator. Therefore, as a first step, we propose an algorithm that is consistent with the traditional core-simulator algorithm (coupled physics solutions at a set of pre-defined, large, time steps) that preserves the accuracy required by both depletion and fuel performance using many, logarithmicly-increasing, time steps. The single ramp to HFP described in

Section 2.2.2 contains three steps (2-4) required for modeling a single large-time step. To model depletion, this would be expanded to five-steps and used for each large, quasi-static time step:

1. **Predict the the final isotopic distribution.**
   - MPACT isotopic predictor step, with many subcycles, for the large time step.
   - Based on initial power distribution.
2. **Estimate the final clad surface temperature and power.**
   - MPACT coupled solve at the final state using the internal TH model.
   - For each pin at each axial node.
3. **Model the thermo-mechanical changes in the fuel between steps.**
   - BisonCASL transient for the large time-step using adaptive time steps.
   - Linear ramp of clad surface temperature from initial to estimated value (Step 2).
   - Linear ramp of power distribution from initial to estimated value (Step 2).
4. **Predict the final state [3 options]**
   - **Internal TH:** do nothing, this step has already been done (Step 2).
   - **CTF TH:** Improve the fidelity with a MPACT+CTF solve.
   - **Coupled Solve:** Model the final state with CTF+MPACT+Bison (Step 6).
5. **Correct the final isotopic distribution.**
   - MPACT isotopic corrector step, with many subcycles, for the large time step.
   - Based on average power distribution.
6. **Model the final state with CTF+MPACT+Bison**
   - Subcycle all three codes using a fixed-point iteration scheme for each time step.
   - Converge MPACT with pin temperatures from Bison and coolant conditions from CTF
   - Converge CTF to steady-state with a BisonCASL heat flux using a series of time-steps
   - Model a single time-step in BisonCASL at each coupled iteration using power from MPACT and clad surface temperature from CTF

Step 4 will leverage the existing numerical coupling of all three codes for the HFP conditions leverage the algorithms within PIKE and include parallel, block Jacobi and parallel, block Seidel iterations schemes. Step 3 accesses code that is internal to Bison without need for duplication of any logic. Similarly, steps 1, 2, and 5 should be able to access code that is internal to MPACT without duplication of logic. With this infrastructure in place, steps 3 and 4 could be replaced with MPACT+CTF to determine the loss of accuracy in the core simulator due to the approximate fuel

model. In the initial implementation, Bison and MPACT will have some inconsistent data because they both perform isotopic depletion internally. MPACT computes the power and Tiamat converts that to a fission rate, which is used by Bison for limited isotopic depletion and fission gas generation. In the future, DTK can be used to transfer isotopic data between Bison and MPACT. However, substantial clarification will be required because of nuances such as the mesh resolution needs of Bison and expectations on MPACT to consistently accounting for fission gas released from the fuel.

6.3 MULTI-CYCLE, QUASI-STATIC

For multi-cycle analyses with Tiamat, there are several approaches that could be considered. At this point, we document these for discussion purposes alone. The traditional approach would be to model the multiple cycles using VERA-CS to provide boundary conditions for the full lifetime of the single *fuel pin of interest*, which would be modeled with a stand-alone Bison calculation. Note that the *fuel pin of interest* would have a PCI during a particular *cycle of interest*; the *fuel pin of interest* is part of a *fuel assembly of interest* that was first introduced to the reactor in the *first cycle of the assembly of interest*.

The challenge for multi-cycle modeling with BisonCASL is associated with the book-keeping related to the history of the fuel rods. Modeling fuel shuffling is relatively straight forward when using the CTF or internal TH models of MPACT if the assemblies are all identical because the fuel material models in both codes are independent of the prior operating history. Therefore, when assemblies are shuffled the entire infrastructure remains and no changes are required to track which pin moved to which location. However, BisonCASL has many components that are tightly correlated with the previous operation of the fuel; of particular importance are the structural mechanics and fission gas release history. Therefore, the driving code (either MPACT or Tiamat) would need to keep track of the location of each pin and each assembly. Because Tiamat leverages DTK for the coupling, this changes is very easy based on a simple adjustment of the centerline of each pin. Within MPACT, this may require substantial work, but it hasn't been investigated significantly.

More integrated approaches that may be considered include:

- Model the entire reactor for the entire history, including the *cycle of interest*, with Tiamat. (prohibitively expensive)
- Model the entire reactor for all cycles up to the *first cycle of the assembly of interest* with MPACT; model the entire reactor for all remaining cycles with Tiamat. For every pin in the *first cycle of the assembly of interest*, model the full history of all fuel pins using stand-alone BisonCASL to define the initial conditions for Tiamat. (very expensive with challenging BisonCASL restart file management)
- Model the entire reactor for all cycles up to the *cycle of interest* with MPACT; model the entire reactor for the *cycle of interest* using Tiamat. For every pin in the *cycle of interest*, model the full history of all fuel pins using stand-alone Bison to define the initial conditions for Tiamat. (less expensive, but still very challenging bookkeeping)

- Model only the *fuel pin of interest* with a standard BisonCASL input and model the rest of the pins using a simplified fuel model. The simplified model could be BisonCASL with only linear heat transfer enabled, the CTF fuel model, or the MPACT internal TH model.

The final bullet is likely the long-term solution to managing multi-cycle PCI analysis of nominal operating conditions for CASL.

For Phase 2 of CASL, Tiamat will not be modeling transients. The PCI aspects of transients will be modeled with BisonCASL with input from VERA-CS.

7 TESTING REQUIRED FOR THE DEPLETION SPECIFICATION

During PoR-10, we will begin to implement the first-cycle depletion capability. At this point, we recognize that additional interfaces in MPACT will be required to interface with it in this format.

MPACT currently has no multi-state, depletion, or shuffling tests using the VERA input.

The existing accessors/functions include:

initialize - initialize

setup - create data structures

finalize - clean data structures

shield - sub-group cross section shielding

computeXS - recompute cross sections

solve - solve the eigenvalue problem with fixed cross sections

init - initialize the data structures for coupling

clear - clear the data structures for coupling

setTH - set TH data for use in cross sections

We would need the following additional functions for execution:

runPredictorStep - isotopic depletion predictor step

runCoupledSolve - single solve with all internal feedbacks

runCorrectorStep - isotopic depletion corrector step

If this is working correctly, then a single predictor-corrector step with MPACT should be simply four calls: runPredictorStep, runCoupledSolve, run CorrectorStep, runCoupledSolve. Tiamat will also need to process the input, or get from MPACT, regarding the number of states, state values, and depletion steps per state. Tiamat will need to communicate the state values to CTF, or at least tell it to advance to the next state and check that they are consistent. Tiamat will need some ability to check that the state/depletion step it is solving is consistent with the state/depletion step that MPACT is currently on.

The current accessors available include:

getKeff - get eigenvalue for coupled convergence checking

printState - print current state parameters

getPinGeomData - get geometric info for DTK

getPinPower - get power distribution for DTK

getTinlet - get temperature of the current state

getPressure - get pressure of the current state

getFlowRate - get the flow rate of the current state

We would need the following additional accessors for testing purposes:

getNumStates - number of states in the problem

getCurrentState - current state number

getNumSteps - number of depletion steps for this state

getCurrentStep - current step number within this depletion block.

8 CONCLUSIONS

The Tiamat code has been benchmarked to peform comparably to an externally coupled version of Cobra-TF within MPACT. The depletion algorithm has been described and preliminary results will be presented in the full paper.

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