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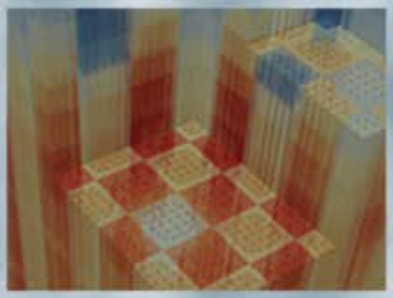
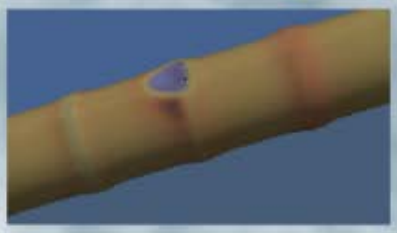
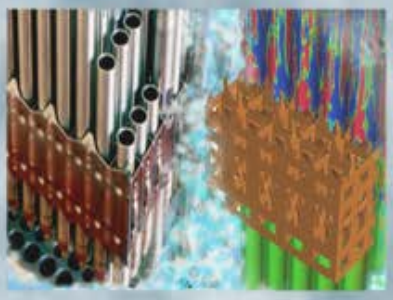
High Fidelity Modeling of Pellet-Clad Interaction using the CASL Virtual Environment for Reactor Applications







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HIGH FIDELITY MODELING OF PELLET-CLAD INTERACTION USING THE CASL VIRTUAL ENVIRONMENT FOR REACTOR APPLICATIONS

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ABSTRACT

The Tiamat code is being developed by CASL (Consortium for Advanced Simulation of Light Water Reactors) as an integrated tool for predicting pellet-clad interaction and improving the high-fidelity core simulator. Tiamat integrates the advanced core simulator capabilities of CASL, VERA-CS, with the multi-dimensional Bison-CASL fuel performance code. VERA-CS provides the coupling of the COBRA-TF sub-channel thermal hydraulics and fuel heat transfer capability with either the Insilico or MPACT neutronics solvers. This report discusses the two neutronics components of VERA and provides a parametric study of the performance of Tiamat using both neutronics codes and a comparison with the VERA-CS version of both. It is demonstrated that Tiamat is robustly capable of modeling pellet-clad interaction and highlights some differences in results due to inclusion of a rigorous fuel performance model rather than simple rod heat transfer.

Key Words: Bison-CASL, Insilico, MPACT, COBRA-TF(CTF), Tiamat

1 INTRODUCTION

VERA (Virtual Environment for Reactor Analysis) is a suite of simulation capabilities (Figure 1) that is being developed to address the Consortium for Advanced Simulation of Light Water Reactors (CASL) challenge problems [1–3]. The VERA-CS (core simulator) is an integration of VERA components to provide all of the functionality of a traditional core simulator (multi-cycle analysis of power, temperature, and flow distributions), but with a much higher fidelity [4, 5]. The primary components of VERA-CS have consisted of either the Insilico or MPACT neutronics capability coupled with COBRA-TF (CTF) for sub-channel thermal hydraulics and fuel heat transfer [6–9]. A suite of progression problems has been developed to guide the development and

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evaluate the progress of the capabilities of the core simulator [3]. Collaboration with Westinghouse, the Tennessee Valley Authority (TVA), and the Jozef Stefan Institute (JSI) has enabled initial validation of VERA-CS based on the the first cycle of the Watts Bar 1 and Krsko nuclear power plants, along with code-to-code comparisons with traditional core simulators and continuous energy Monte Carlo codes [4, 5].

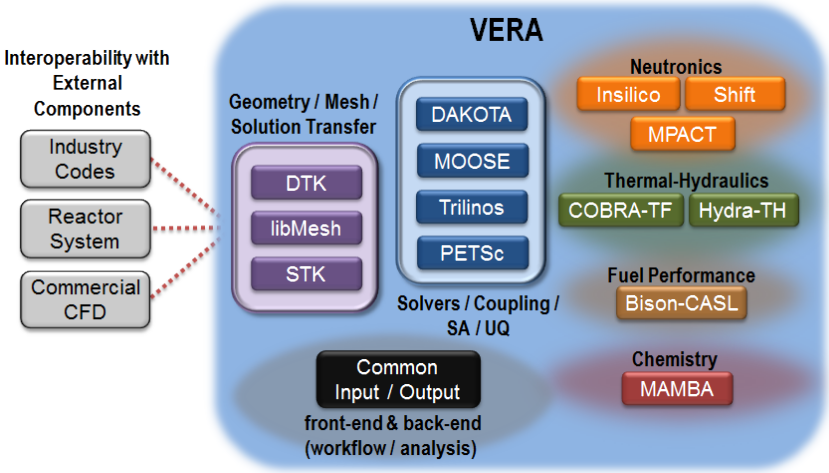

Figure 1. The VERA code suite.

VERA is developed using a continuous integration model, which enables on-going development while ensuring stability through extensive testing. This allows innovation in both physics components and infrastructure (e.g. numerical approaches to coupling). Insilico, discussed in more detail in Section 2.1, has been the workhorse for CASL neutronics and provides a relatively fast, accurate, massively parallel approach to integrated neutronics; however, extending it to handle isotopic depletion would be challenging. MPACT (Section 2.2), the replacement for Insilico, provides a 2-dimensional/1-dimensional (2D/1D) transport solution based on the method of characteristics (MoC) that has been integrated with the ORIGEN depletion code [6–10]. Some VERA applications use the LIME (Lightweight Integrating Multiphysics Environment) interfaces to Trilinos solvers to utilize simple Picard and complex Jacobian-Free Newton-Krylov (JFNK) solvers [11]. However, a study of advanced algorithms for coupling Insilico and conjugate heat transfer using JFNK revealed minimal efficiency benefits compared with a simple Picard iteration scheme [12, 13]. Therefore, MPACT has integrated direct coupling of CTF to eliminate the complexity required by the use of LIME [14].

By modeling in two dimensions (radial and azimuthal) at every axial plane for every fuel rod in the core, the CTF fuel heat transfer model provides a high-resolution solution in comparison with traditional core simulators. However, there are significant limitations in the accuracy of CTF due to inadequate physics (e.g., mechanics, fission gas release) and simplified material models. The Bison-CASL fuel performance code is an extension of the Bison code developed at Idaho National Laboratory (INL) by the NEAMS (Nuclear Energy Advanced Modeling and Simulation) program within the US DOE Office of Nuclear Energy [15, 16]. Bison-CASL provides a modern parallel simulation capability for modeling nominal and transient operation using a 2D axisymmetric or a 3D geometric representation of fuel rods [17, 18]. In addition, CTF with MPACT can only

provide the bounding state for estimating pellet-clad interaction (PCI), which is one of the key challenge problems for CASL [2]. Bison-CASL, with input from CTF and MPACT, can model the time-evolution of PCI to estimate the potential for rod failures, but a key uncertainty of fuel failure estimation is the power distribution. Therefore, the Tiamat code has been developed to integrate the improved fuel heat transfer modeling of Bison-CASL with the high-resolution neutronics and thermal-hydraulics modeling in VERA-CS. Tiamat provides an improved, integrated approach to PCI prediction.

This report documents the benchmarking of the Insilico and MPACT versions of Tiamat with their LIME-based equivalents in VERA-CS. It explores the robustness, computational performance, and consistency through a thorough parametric study. A more comprehensive manuscript of the design of Tiamat and a demonstration for large-scale problems is included in these proceedings [19]. Many of these results are discussed in more detail in a related technical report [20]. Section 2 describes the MPACT and Insilico neutronics components of VERA. Section 3 describes the problem specification for the parametric study.

2 NEUTRONICS COMPONENTS

2.1 Insilico (Denovo/XSProc)

Insilico is one of the neutronics solvers in VERA-CS and is part of the SCALE nuclear analysis code suite that leverages the Exnihilo transport suite, both of which are in active development at Oak Ridge National Laboratory (ORNL) [21]. Insilico includes reactor toolkit modules used for defining and meshing pressurized-water reactor geometries and a variety of cross section processing modules within XSProc. Insilico uses the Denovo deterministic transport code to solve for the flux and eigenvalue solutions for the 3D problem using either the discrete ordinates or the Simplified Legendre (SP_N) angular discretizations [8, 22]. Exnihilo also includes the Shift Monte Carlo transport package, which is also integrated within Insilico [23]. VERA uses the Insilico code to solve for the leading eigenvalue at a single state point, and for the eigenvector, which represents the multigroup, angle-dependent neutron distribution within the system. For all the calculations in this study, the SP_N discretization of the transport problem was used exclusively. XSProc provides problem-dependent, microscopic and/or macroscopic multi-group cross sections that account for the shielding of the resonances. XSProc includes options to process a variety of cross section libraries (from an 8 energy-group test library to a 252 energy-group production library) with a variety of methods, which include the narrow- or intermediate-resonance approximation with full-range Bondarenko factors and near-continuous-energy deterministic transport, in one spatial dimension. The fine energy-group structure of the resonance self-shielding calculation can optionally be spatially homogenized and/or collapsed to a coarse energy-group structure through a 1D discrete ordinates transport calculation. For all of the calculations in this study, the fine energy-group structure leveraged either the spatially homogenized 8-group test library with no energy collapsing, a 56-group library collapsed to 11 groups, or a 252-group library with energy collapsing to 23 groups; all neutron libraries are based on ENDF/B-VII.0 from SCALE-6.2 (β.3), which contains data for 417 nuclides and 19 thermal-scattering moderators. Insilico has been coupled to CTF using LIME and to both CTF and Bison-CASL within Tiamat.

2.2 MPACT

The reactor core simulator MPACT is being developed collaboratively by researchers at the University of Michigan and ORNL to provide an advanced pincell-resolved transport capability within VERA [24]. The key characteristics of the MPACT code include the subgroup method and the embedded self-shielding method for resonance treatment, depletion capability based on the ORIGEN exponential matrix method, and a whole core solver with a 2D/1D synthesis method on the frame of the 3D coarse mesh finite difference method, for which axial and radial correction factors are obtained from the 2D MOC and 1D nodal expansion method or Simplified P_N, respectively. Reference [6] contains a detailed description of the methods used in MPACT as a part of the VERA-CS.

All calculations performed in this report use a 56-group cross section library with 4 subgroups in the resolved-resonance range. The mesh for the base (single-rod) 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 subgroups was used with a transport-corrected P0-scattering approximation and a 2×2 Chebyshev-Gauss quadrature set with a 0.1 cm ray spacing. In all cases, the neutronics solution was converged to 10^{-5} for both the flux and eigenvalue using three inner iterations per group and two 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. A standard coarse mesh finite difference acceleration was used with a maximum of 20 iterations per outer and an eigenvalue shift of 1.5.

MPACT has been coupled to CTF using LIME and to both CTF and Bison-CASL within Tiamat. In addition, MPACT also contains an internal simplified thermal-hydraulic model (without crossflow) and a direct connection to CTF. MPACT, using both the internal thermal hydraulics model and internal coupling to CTF, has been benchmarked against the LIME-coupled MPACT+CTF solver. This report does not include results using the internal thermal hydraulics or direct coupling with CTF.

3 TEST PROBLEM SPECIFICATION

The test problem used in this manuscript is a single fuel rod based on the dimensions and state conditions of Watts Bar Unit 1 Cycle 1, with detailed geometric and material specifications for fuel rods in the CASL "Progression Benchmark 6" or simply "Problem 6" [3]. Problem 6 is at hot full-power, which requires modeling the coupled neutronics, fuel heat transfer, and thermal hydraulics. There are no axial blankets or enrichment zones in the first cycle. The primary geometry specifications of the fuel rod and thermal-hydraulic conditions are given in Table I.

The single-rod benchmark calculation was used to develop a suite of cases to test Tiamat and develop an understanding of the expected performance. While full-scale problems introduce additional challenges, any discrepancies that arise on a single-rod case will be evident in full-scale results as well. Incorporated in this analysis is a comparison of the "base" Bison-CASL model from the CASL fuel performance team and the "base" models used in CTF+Insilico and CTF+MPACT by

Table I. Fuel Rod Description

Parameter	Value	Units
Fuel Pellet Radius	0.4096	cm
Fuel Rod Clad Inner Radius	0.418	cm
Fuel Rod Clad Outer Radius	0.475	cm
Rod Pitch	1.26	cm
Outside Rod Height	385.10	cm
Fuel Stack Height (active fuel)	365.76	cm
Plenum Height	16.00	cm
End Plug Heights ($\times 2$)	1.67	cm
Inlet Temperature	559	degrees F
System Pressure	2250	psia
Single Channel Flow	2600	lb/hr
Linear Power (100% of Rated)	183	W/cm
Pellet Material	UO_2	
Clad & Cap Material	Zircaloy-4	

the CASL VERA-CS team. The only exception to the "base" CTF+Insilico is the use of the 8-group cross section library, which does not provide an accurate solution but is sufficiently representative for testing purposes; MPACT used the production 56-group library. The basic models used in this study include parameters shown in Table II. The Bison-CASL mesh is approximately defined by specifying the number of axial and radial elements for the fuel and cladding desired, but Bison-CASL internally determines the specific mesh, which is why the number of elements (465) does not match the discretization (432).

The coupled problems were converged to an eigenvalue error of less than 2 percent milli (pcm), a relative power shape error of 10^{-4}, and a maximum temperature (fuel, clad-surface, and coolant) error of 0.1°C. Each physics code was also required to converge to a given tolerance: Insilico used an internal convergence criterion on the L2-norm of the residual of the solution vector (eigenvalue and multi-group flux moments) of 10^{-7}; Bison-CASL used a relative tolerance of 10^{-4} or absolute tolerance of 10^{-10} on the L2-norm of the residual equations; and CTF converged to an approximate steady state using a storage (energy and mass) tolerance of 5×10^{-5} and balance (energy and mass) tolerance of 10^{-6}. The axial discretization in CTF is based on a user-defined discretization (49 cells), which is used for output editing and coupling physics, leading to a direct axial mesh mapping. Unless otherwise noted, Tiamat used a block Gauss-Seidel algorithm with each of the three physics codes onto an independent MPI processor (set of processors when using more then one per code). However, although each physics component can perform its solution in parallel, due to the nature of the Gauss-Seidel algorithm, each physics component is solved sequentially rather than simultaneously.

4 RESULTS

Several key parameters that are used in the convergence checking are shown in Table III, along with a comparison of the execution time. Note that, because of the use of the testing cross section

Table II. Base Parameters In Parametric Study

Bison-CASL Mesh Cells (total)	465
Bison-CASL Discretization (axial, fuel radial, clad radial)	(48, 6, 3)
Insilico [Testing] Cross Sections (groups)	8
MPACT [Production] Cross Sections (groups, subgroups)	(56, 4)
Boron Concentration (ppm)	1300
Relaxation Factor on Linear Power	0.5
MPI Processors (CTF, Neutronics, Bison-CASL)	(1, 1, 1)
Tiamat Solver Algorithm	Gauss-Seidel

Table III. Comparison of Tiamat with CTF+Neutronics

	CTF+MPACT Value	Tiamat Difference	CTF+Insilico Value	Tiamat Difference	Units
Eigenvalue (k-eff)	1.1560	4.9	1.2019	-5.5	pcm
Peak Fuel Temp.	1071.3	9.8	1043.6	16.2	°C
Peak Coolant Temp.	327.4	0.39	327.4	0.40	°C
Linear Power in CTF	183	2.3	183	2.3	W/cm
Time to Solution	463	227	124	262	sec

library for Insilico, the calculated results (e.g., eigenvalue, peak fuel temperature) differ substantially from the MPACT version; the comparison of CTF+Neutronics and Tiamat, for both MPACT and Insilico, using consistent methods and data are the focus of this manuscript. The difference between Tiamat and CTF+Neutronics in the eigenvalue (k-eff) of the system is quite accurate (under 10 pcm) and the increase in run-time is approximately 4 minutes, despite significantly different total execution times. Note that there is no reason to expect the peak fuel temperature from CTF and Bison-CASL to agree exactly, because they include different material models and physics, and yet they are relatively similar. For a single rod model, the peak coolant temperature is the exit coolant temperature and, like the linear power in CTF, is a measure of the conservation of energy in the system. There should be zero difference between Tiamat and CTF+Neutronics; because there is not, it is clear that there is an inconsistency within the system. This conservation of energy error is discussed in more detail in the following section, through refinement of the Bison-CASL mesh.

4.1 Bison-CASL Mesh Refinement

To better understand the performance of Tiamat and issues associated with conservation of energy, the mesh of the fuel and cladding in Bison-CASL was refined by a factor of two ("Tiamat($\times$2)") and four ("Tiamat($\times$4)") in both the radial and axial dimensions. For several key parameters used to check convergence, the "Difference" between Tiamat and the CTF+Neutronics "Value" is shown in Tables IV and V for the MPACT and Insilico versions, respectively. Because Bison-CASL is using linear finite elements, the temperature solution with a fixed power distribution and boundary condition will have second-order convergence with spatial mesh refinement. For reference, the fuel rod model in CTF has 49 axial cells, 4 azimthal cells, and 4 radial cells (3 in the fuel and 1 in the clad), for a total of 784 mesh cells. The peak fuel temperature demonstrates approximately second-order convergence (1.8 and 2.0 for the Insilico and MPACT versions, respectively). This

Table IV. Comparison of CTF+MPACT and Tiamat with Bison-CASL Mesh Refinement

	CTF+MPACT Value	Tiamat	Tiamat(×2)	Tiamat(×4)	Order	Units
		Difference				
Mesh Cells	784	465	1686	6648		
Eigenvalue (k-eff)	1.1560	4.9	6.2	6.7	1.3	pcm
Peak Fuel Temp.	1071.3	9.8	-1.4	-4.3	2.0	°C
Peak Coolant Temp.	327.4	0.39	0.12	-0.01	1.0	°C
Linear Power in CTF	183	2.3	0.70	-0.08	1.0	W/cm
Time to Solution	463	227	545	1038	-	sec

Table V. Comparison of CTF+Insilico and Tiamat with Bison-CASL Mesh Refinement

	CTF+Insilico Value	Tiamat	Tiamat(×2)	Tiamat(×4)	Order	Units
		Difference				
Mesh Cells	784	465	1686	6648		
Eigenvalue (k-eff)	1.2019	-5.5	-4.1	-3.6	1.4	pcm
Peak Fuel Temp.	1043.6	16.2	5.7	2.7	1.8	°C
Peak Coolant Temp.	327.4	0.40	0.13	-0.004	1.0	°C
Linear Power in CTF	183	2.3	0.75	-0.02	1.0	W/cm
Time to Solution	124	262	464	1608	-	sec

suggests that refinement of the Bison mesh improves the accuracy of the temperature solution but affects the CTF and neutronics calculations in such a way that there is minimal change to the source and boundary conditions of Bison-CASL on the coupled mesh. The eigenvalue converges at a super-linear rate (1.3 and 1.4 for the Insilico and MPACT versions, respectively), but the magnitude of the change (<2 pcm) is very small. Therefore, the Bison-CASL mesh does not need to be refined to provide an accurate estimate of the eigenvalue. The measures of conservation for both MPACT and Insilico effectively converge to the correct solution in two levels of refinement; we explore the separate refinements of the axial and radial components separately in more detail with the Insilico versions.

In Figure 2, the linear power is plotted for each case as a function of the height above the bottom of the fuel. Note that the coupling mesh provides piecewise constant power values for each edit bound region. The Tiamat simulations show a small difference, primarily near the spacer grids, that is significantly reduced with mesh refinement. It is clear that the power in the fuel adjacent to a spacer grid is overestimated and the power in the mesh cell directly above the grid spacer is underestimated; this is the numerical artifact associated with transferring power to the Bison-CASL nodal basis instead of quadrature points. Because Bison-CASL is requesting power values at finite element basis nodes, which can lie on the interface of two Insilico control volumes, DTK returns the first control volume value found in the list. Insilico created that list from bottom to top, so the grid spacer gets some power from the lower region and the region above gets some power from the spacer grid. This affects the accuracy of the data transfer, but that effect can be controlled with mesh refinement. More details can be found in these proceedings in [19]. In the future, we will modify Bison-CASL to evaluate the external fields (such as the power distribution) at the quadrature points or cell centroids instead of at the nodal locations.

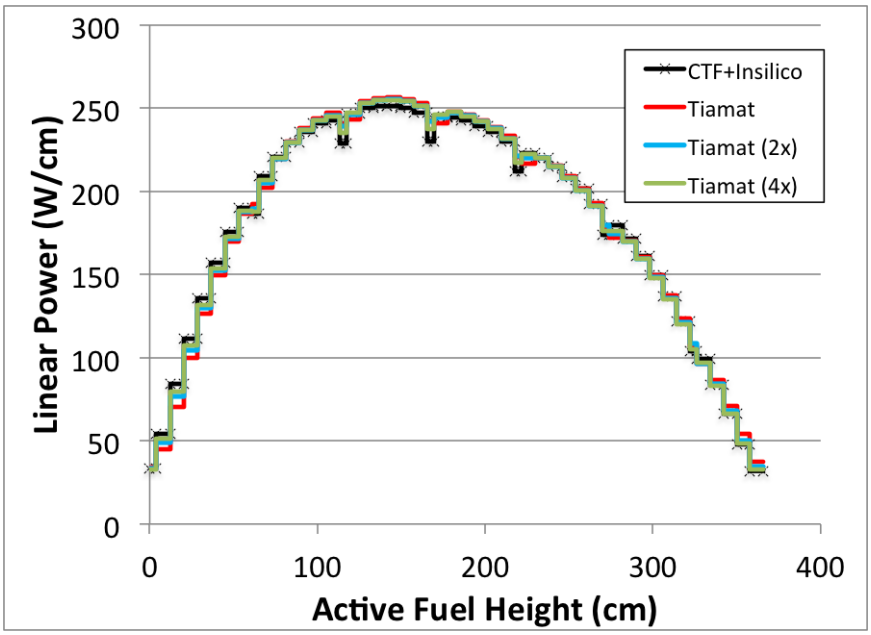

Figure 2. Axial Power Shape of CTF+Insilico and Tiamat with Mesh Refinement

Reference [20] provides a detailed discussion and demonstration of the rod-averaged conservation of energy among all three codes, but the accuracy of the surface heat flux estimate from Bison-CASL depends on the radial derivative of the temperature. In computing the heat flux using the temperature gradients on the clad outer surface, there is a significant loss of accuracy, since finite-element basis gradient values are used. We can assess the error in the heat flux evaluation by converting the transferred heat flux into an equivalent power in each axial edit bound region. The differences in these powers, with respect to the CTF+Insilico case, are shown in Figure 3 and are labeled as "Heat Flux Equivalent." This shows that while the transfer is conservative in each axial edit bound region, the base case heat flux equivalent power is very inaccurate with local oscillations. One level of refinement ($\times 2$) eliminates the large local oscillations, so that only the errors at grid-spacer interfaces persist; it is clear that the base case mesh is too coarse. We also observe that the error in the heat-flux-derived power is larger than the actual power ("Direct Power") used by Bison-CASL. Note that there is no expectation that the error in power between CTF+Insilico and Tiamat will ever go to zero under more levels of refinement, since the codes use fundamentally different fuel rod models.

As shown in Table VI, refinement of the radial mesh strongly influences the total heat transferred from the cladding to the coolant. The discontinuities in the cladding outer surface temperature calculated by CTF may create numerical errors in the Bison-CASL linear finite elements that are minimized with radial refinement. With some modifications, the DTK adapter in Bison-CASL could be adjusted to allow the use of quadratic finite elements, which will provide a much more accurate surface heat flux and will not require additional radial refinement.

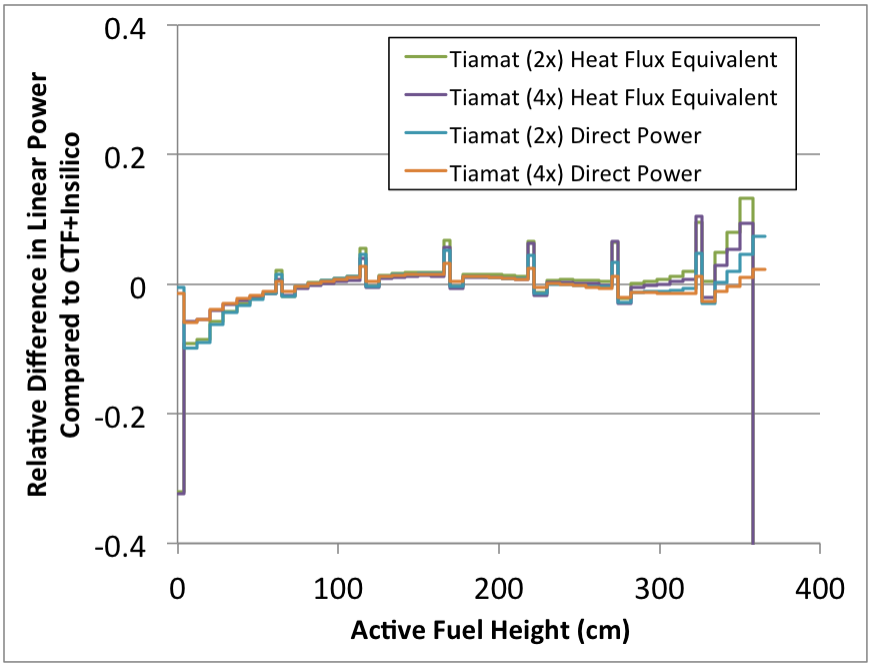

Figure 3. Power shape of CTF+Insilico and Tiamat for mesh refinement with CTF heat flux equivalent power.

Table VI. Tiamat Difference from CTF+Insilico with Bison-CASL Mesh Refinement

Mesh		Exit Coolant Temperature	Linear Power in CTF	Power Shape Differences
Tiamat		0.399	2.3	0.87
Tiamat(×2)	Axial	0.411	2.37	0.51
	Radial	0.118	0.68	0.83
	Both	0.13	0.75	0.45
Tiamat(×4)	Axial	0.415	2.39	0.48
	Radial	-0.02	-0.12	0.82
	Both	-0.004	-0.02	0.40

4.2 Tiamat Timing

The “base” case in Tiamat with Insilico, using the 8-group cross section library, completed in 386 seconds; Tiamat with MPACT, using the 56/4 group library, required 691 seconds. The codes used a single step for estimating the hot full-power conditions, 12 time steps in Peregrine to ramp the fuel model to hot full power, and then 7–8 iterations to converge the coupled solution. Tables VII–VIII show the timing breakdown by component for MPACT and Insilico, respectively.

4.3 Sensitivity to Soluble Boron

To ensure that the effects of the soluble boron concentration have been incorporated correctly, Tiamat is compared with both CTF+Insilico and CTF+MPACT for a variety of boron concentration

Table VII. Timing Breakdown in Tiamat with Insilico

8-Group Insilico	Time (s)	Bison-CASL	Insilico	CTF	DTK	Steps
Setup	10					
HFP Estimation	12	0%	76%	24%	~0.0%	1
Ramp to HFP	135	100%	0%	0%	~0.0%	12
Coupled Solve	228	68%	27%	5%	~0.0%	7
Total Solve	376	77%	19%	4%	~0.0%	
Total	386					

Table VIII. Timing Breakdown in Tiamat with MPACT

56/4-Group MPACT	Time (s)	Bison-CASL	MPACT	CTF	DTK	Steps
Setup	3					
HFP Estimation	66	0%	96%	4%	~0.0%	1
Ramp to HFP	127	99%	0%	0%	0.7%	12
Coupled Solve	495	35%	63%	2%	0.2%	8
Total Solve	688	44%	54%	2%	0.4%	
Total	691					

levels. As shown in Tables IX and X, the boron concentration is varied from 0 to 1950 ppm and the eigenvalue trend for Tiamat follows the trend of the LIME equivalent, as demonstrated by equivalent ratios of the change in eigenvalue (pcm) per change in boron (ppm).

4.4 Sensitivity to Power Magnitude

Similar to the study of boron in the preceding section (4.3), a parametric study was performed on the magnitude of the power to determine the consistency between Tiamat and both CTF+MPACT and CTF+Insilico. As shown in Tables XI and XII, when the power is varied from zero to 125% of the rated power, there is an interesting trend in the variation of the eigenvalue.

Although the eigenvalues of the "base" case at 0% and 100% power agree very well, the difference grows to over 70 pcm between them. Bison-CASL models the gap closure due to densification, swelling, thermal expansion of the fuel, and thermal expansion and creep in the cladding. Although CASL is not yet using it, CTF does include an effective gap conductance model that accounts for thermal expansion, but it does not yet account for burnup in either thermal conductivity or gap closure. The use of this model for the CTF+MPACT and CTF+Insilico

Table IX. Benchmarking Tiamat-Insilico with Boron Variation

8-Group Boron (ppm)	**Tiamat** Eigenvalue	Worth (pcm/ppm)	**CTF+Insilico** Eigenvalue	Worth (pcm/ppm)
0	1.3294	-9.8	1.3295	-9.8
650	1.2621	-9.3	1.2621	-9.3
1300	1.2018		1.2019	
1950	1.1475	-8.4	1.1476	-8.4

Table X. Benchmarking Tiamat-MPACT with Boron Variation

56/4-Group Boron (ppm)	**Tiamat** Eigenvalue	Worth (pcm/ppm)	**CTF+MPACT** Eigenvalue	Worth (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

Table XI. Benchmarking Tiamat-Insilico with Power Variation

Power (% Rated)	Tiamat Eigenvalue	CTF+Insilico (pcm)	Tiamat Iterations	CTF+Insilico Iterations
0	1.2188	0	2	2
1	1.2187	4	4	6
25	1.2141	-59	8	9
50	1.2099	-71	8	10
75	1.2058	-51	8	10
100	1.2018	-5	8	11
125	1.1980	69	8	25

simulations could improve agreement. Additionally, the Tiamat simulation could be used to tune the CTF gap conductance models in the future. Further study is required to evaluate and understand these differences as the power level changes.

Tiamat consistently converged to the same tolerance with fewer iterations, which was especially apparent at high power. In the high-power (>130%) cases, the coupled codes consistently had difficulty in converging with the default damping parameter. In these cases, numerical oscillations caused the solution to diverge until physical limits were exceeded in the material models of Bison-CASL or CTF. Tiamat was consistently more robust than the CTF+Neutronics version, probably because of a very small difference in the iteration scheme: the Bison-CASL clad surface temperature is lagged in Tiamat between coupled iterations, but CTF solves for the full conjugate heat transfer solution. (More details of the iteration scheme can be found in these proceedings in [19].) The result is additional damping of the solution that results in a more robust simulation. In all cases, reducing the damping factor consistently eliminated the oscillations in all the coupled codes but drove the number of global iterations up. Further study is required to fully understand why the algorithm is consistently converging faster in Tiamat than in CTF+Neutronics.

4.5 Convergence Rate Evaluation of Tiamat with MPACT

In the Tiamat iteration scheme, which uses a Picard iteration scheme between physics codes, approximately solving each physics code during the early iterations can reduce the overall solution time if it does not (significantly) increase the total number of coupled iterations required. One method of implementing this simplification is to limit the maximum number of eigenvalue iterations that MPACT performs during each coupled solve. However, this has the potential to lead to false convergence, because MPACT may not be fully converging internally when the coupled solve

Table XII. Benchmarking Tiamat-MPACT with Power Variation

Power (% Rated)	Tiamat Eigenvalue	CTF+MPACT (pcm)	Tiamat Iterations	CTF+MPACT Iterations
0	1.1744	-1	2	2
1	1.1742	-3	3	6
25	1.1695	-62	8	10
50	1.1649	-72	8	10
75	1.1605	-49	9	10
100	1.1560	5	8	11
125	1.1517	86	8	11

Table XIII. Study of MPACT Maximum Outer Iteration Parameter

Maximum # Outer Iterations	100	4	2	1	
	Value	Error			Units
Eigenvalue	1.1560	0	-0.06	-0.79	pcm
Peak Coolant Temperature	327.8	0	-2	-5	$\times 10^{-4}$ °C
Peak Clad Temperature	341.7	-1	-14	-38	$\times 10^{-4}$ °C
Peak Fuel Temperatures	1081.2	9	33	-1300	$\times 10^{-4}$ °C
Total Solve Time	688	639	565	727	sec
Coupled Iterations to Converge	8	8	8	10	

appears converged.

Table XIII displays the effect of the maximum number of MPACT outer iterations per coupled-physics solve on a variety of parameters. 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 eight to ten coupled iterations, the run time 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 affect the solution because even a 0.8 pcm change in the eigenvalue and a 0.1°C change in the temperature is insignificant with respect to other uncertainties in the problem.

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

Because the optimal maximum number of outer MPACT iterations was shown to be low, this study varied 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 XIV shows that the Jacobi scheme consistently requires more coupled iterations and more execution time than the corresponding GS solver. Therefore, we recommend the use of the GS solver when possible and place a high priority

Table XIV. Study of Gauss-Seidel (GS) and -Jacobi (J) Iteration Schemes

Solver Type	GS	J	GS	J	GS	J
Maximum # Outer Iterations	1	1	2	2	100	100
Coupled Iterations to Converge	10	25	8	19	8	19
Total Solve Time (sec)	727	795	565	709	688	1041

on allowing Tiamat to execute on a single processor by allowing for the overlap of communication domains. Note that memory constraints may prevent the overlapping of applications on the same MPI processes and will be explored in the future.

5 CONCLUSIONS

Through comparison of the Tiamat code with independently developed and benchmarked versions of VERA-CS, we have evaluated the single-rod performance of Tiamat using both Insilico and MPACT neutronics. It has been shown that Tiamat is capable of robustly solving single-rod problems, and a related paper (Reference [19]) has demonstrated that this capability extends to large, multi-assembly problems as well. It has been shown that the "base" mesh used for fuel performance analysis in CASL is too coarse to use within Tiamat, and quadratic finite elements will be required to improve the accuracy of the quantities transferred from Bison-CASL to CTF. The execution times for single-rod analysis were described, including details for the different components of the Tiamat solve. Although Bison-CASL dominates computational requirements when using a few-group cross section library, Bison-CASL and neutronics exhibit similar computational requirements when a 56-group production cross section library is used. Because both MPACT and Bison-CASL have the ability to leverage significantly more cores, the relative distribution of work between the codes will likely change significantly for full and multi-assembly problems. Tiamat behaves exactly like VERA-CS with changes in boron concentration, but there is an interesting trend in the changes due to the power level. Because of the different material models and physics in Bison-CASL, compared with CTF, there are clear differences in the eigenvalue as a function of the power curve; this is likely due to the axially varying gap-conductance model in Bison-CASL.

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