

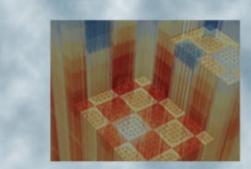
# VERA 4.2 Release Notes

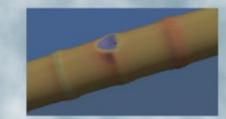
Mark Baird, ORNL Ben Collins, ORNL Will Cramer, ORNL Andrew Godfrey, ORNL Aaron Graham, ORNL Brendan Kochunas, UM Ron Lee, ORNL Robert Lefebvre, ORNL Lori Moore, ORNL Tara Pandya, ORNL Bob Salko, ORNL Erik Walker, ORNL

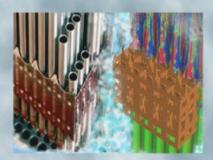
September 1, 2021



CASL-U-2021-1977-000













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# **REVISION LOG**

| Revision | Date     | Affected Pages | <b>Revision Description</b> |
|----------|----------|----------------|-----------------------------|
| 0        | 9/1/2021 | All            | Initial Release             |
|          |          |                |                             |
|          |          |                |                             |
|          |          |                |                             |

#### **Document pages that are:**

| Export Controlled   | None          |      |  |      |
|---------------------|---------------|------|--|------|
| IP/Proprietary/ND   | A Controlled_ | None |  |      |
| Sensitive Controlle | edNone        |      |  | <br> |

# **Requested Distribution:**

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## 1. VERA 4.2 SOFTWARE PRODUCT SUITE

The Virtual Environment for Reactor Applications (VERA) components contained in this distribution include selected computational tools and supporting infrastructure that solve neutronics, thermal-hydraulics (T/H), fuel performance, ex-core radiation transport, and CRUD/chemistry problems for commercial pressurized water reactors (PWRs). In many cases, these tools can be executed standalone or coupled to other VERA components. VERA also provides a simplified common user input and output capability, and the infrastructure components support the physics integration with data transfer and coupled-physics iterative solution algorithms [1].

Neutronics analyses can be performed for 2D lattices, 2D cores, and 3D core problems for PWR geometries that can include reactor criticality and fission rate distributions at the fuel rod level for input fuel compositions. MPACT uses the method of characteristics (MOC) transport approach for 2D problems [2]. For 3D problems, MPACT uses the 2D/1D method, which uses 2D MOC in each radial plane and 1D  $P_n$  in the axial direction. MPACT includes integrated cross section capabilities that provide problem-specific 51 energy group cross sections generated using the subgroup self-shielding methodology. MPACT also includes the isotopic depletion and decay capability in ORIGEN [3] for the simulation of all reactor operating regimes as a function of time or burnup. MPACT also handles the simulation of other aspects of reactor operation, such as control rod movement, fuel shuffling, refueling outage decay, and in-core instrumentation response. The code can solve both 2D and 3D problems on parallel processors to significantly reduce overall run time.

A thermal-hydraulics capability is provided with CTF, an updated version of COBRA-TF [4], that allows T/H sub-channel analyses for single and multiple fuel assemblies using the simplified VERA common input. This distribution also includes coupled neutronics, T/H, and depletion capabilities to allow calculations using MPACT coupled with CTF and ORIGEN, and it includes a fuel rod temperature model in CTF that provides intra-pellet temperature coupling with MPACT for doppler feedback to the neutronics.

The VERA fuel rod performance component BISON [7] calculates—on a 1D, 1.5D, 2D, or 3D basis—fuel rod temperature, fuel rod internal pressure, free gas volume, clad integrity, and fuel rod waterside diameter. These capabilities allow for the simulation of power cycling, fuel conditioning and deconditioning, high burnup performance, power uprate scoping studies, and accident performance. In VERA, BISON is run uncoupled from the other components, but templates and tools are provided to automatically generate and execute BISON input for all fuel rods in a VERA core model (approximately 15,000 parallel BISON executions).

BISON is not included in VERA 4.2 distributions through the Radiation Safety Information Computational Center (RSICC). To obtain BISON, please contact <u>agradmin@inl.gov</u>.

VERA 4.2 is distributed with the Shift Monte Carlo (MC) radiation transport code [8], which can be run standalone using a VERA common input with the vera\_shift executable and directly coupled to MPACT/CTF using the vera\_to\_shift executable. VERAShift uses the SCALE ENDF/B-VII.1 continuous energy (CE) data library and has been used to model a broad set of problems for the Consortium for Advanced Simulation of Light Water Reactors (CASL), including massively parallel eigenvalue problems as reference solutions and a variety of coupled ex-core transport applications. The breadth of commercial reactor applications using VERAShift is partially documented in the verification and validation (V&V) report shown in Section 5. VERAShift has been successfully demonstrated for ex-core detector responses and vessel fluence applications.

VERA 4.2 also includes the MAMBA [9] code for CRUD/chemistry capabilities. MAMBA provides CRUD growth and soluble boron uptake on the fuel rod surfaces based on the surface heat flux from MPACT and subcooled boiling duty from CTF. MAMBA is also capable of system mass



balance of the CRUD sources as well as CRUD removal and shuffling during refueling outages. A computational fluid dynamics (CFD)-informed subchannel methodology implemented in CTF provides the capability of producing very detailed local CRUD deposits with consideration for complex fluid behavior downstream from spacer grids with mixing vanes. MAMBA provides a CRUD-induced power shift (CIPS) and CRUD-induced localized corrosion (CILC) analysis capability, but is still under development and requires more testing, calibration, and validation prior to end user applications.

Input processing capabilities include the VERA Common Input (VERAIn) processor, which provides a simple and user-friendly input interface for all VERA components [10]. VERAIn converts the ASCII common input file to an intermediate XML format and serves as a common geometric database for each of the physics components in VERA. VERA component codes read either the VERA XML format directly or provide a preprocessor that can convert the XML into native input.

VERAView [11] is an interactive graphical interface for the visualization and engineering analyses of output data from VERA. The Python-based software is easy to install and intuitive to use, and it provides instantaneous 2D and 3D images, 1D plots, and alphanumeric data from VERA multiphysics simulations. VERAView is open-source and can be obtained from GitHub at <a href="https://github.com/CASL/VERAview">https://github.com/CASL/VERAview</a> or by contacting <a href="https://github.com/CASL/VERAview">vera-support@ornl.gov</a>.

VERA 4.2 has been extensively tested against a broad series of small-scale, automated tests as part of its continuous integration and build development environment. Full-scale commercial power plant models have also been tested, but the breadth of these tests is limited. Generally, the following commercial power plants have been successfully simulated or analyzed to some degree with VERA 4.2:

- Watts Bar Unit 1
- Catawba Unit 1
- Vogtle Unit 1
- Publicly available B&W plant model
- Holtec SMR-160

VERA 4.2 has also been successfully used to generate solutions to the CASL core physics benchmark progression problems [12], which is a publicly available set of test problems based on Watts Bar Unit 1 that includes plant measurements and high-fidelity reference solutions for software testing and validation. The VERA 4.2 results to these problems can be provided upon request.

The following components of VERA 4.2 are not recommended for use by end users due to the current level of maturity or lack of sufficient testing. These items are not supported software quality level 1 (SQL1) capabilities (see Section 2).

- MAMBA: The MAMBA capabilities in VERA 4.2 are still under active development and should not be used or tested by end users. To access a more capable and tested version of MAMBA, please contact <u>vera-support@ornl.gov</u>.
- VERA-to-BISON scripts and processors: The one-way coupling software that supports the generation of BISON input from VERA output data for all fuel rods over multiple fuel cycles is not included in the VERA quality assurance (QA) program. This software is still under active development and is not recommended for use in VERA 4.2. More recent software is available for testing, if desired. Please contact <u>vera-support@ornl.gov</u>.



• VERAShift: A software issue in the development of VERA 4.2 resulted in a substantial memory increase for VERAShift applications. The new memory usage is approximately double that of VERA 4.1. Please contact <u>vera-support@ornl.gov</u> for assistance in executing VERAShift applications in VERA 4.2.

# 2. SOFTWARE QUALITY ASSURANCE

The VERA 4.2 software product suite was developed, validated, and tested under a Nuclear Quality Assurance 1 (NQA-1) QA program established in 2019 [13]. CASL initiated this QA program based on nuclear industry feedback identifying the NQA-1 standard, which is used throughout the US nuclear industry, as a top priority to enable the adoption and commercialization of VERA.

The VERA software components included in this distribution are still under active development and are subject to change. However, all software life cycle work activities are performed, managed, and controlled under the NQA-1 compliance program. Software quality levels (SQLs) are established to define the controls, rigor, and formality applied to software engineering processes, documentation, verification, and validation activities based on the maturity of the code.

- **SQL1**: Mature core software product codes CTF, MPACT, and VERAIO are assigned SQL1 status to reflect the completion of specified product-specific management plans, input requirements and tests, baseline documentation, independent reviews, and other NQA-1 work activities.
- **SQL2:** Third-party libraries (TPLs) and utilities that are used to support the SQL1 codes but do not directly implement the theoretical model are designated as SQL2. Acceptance for their use is documented in core product software management plans, baseline software documentation, and testing protocols.
- **SQL4:** Software in the R&D stage are included under the NQA-1 program as SQL4 to drive toward mature processes, controls, and documentation consistent with SQL1. MAMBA and VERAShift are included in the distribution of VERA 4.2 as SQL4. They have not been fully validated or assessed and should be used primarily for test, evaluation, and research purposes only.

The BISON software quality program is managed by Idaho National Laboratory (INL) separately from the other VERA components. The BISON version used in VERA 4.2 should be considered for test and evaluation purposes only (SQL4). To obtain a more recent version of BISON, please contact agradmin@inl.gov.

Within the SQL1 codes CTF, MPACT, and VERAIO are both mature and research capabilities. The mature capabilities are rigorously implemented and tested before software release. The research capabilities are still under R&D and have not been thoroughly tested, demonstrated, or validated. These R&D capabilities are not supported features of VERA 4.2 but may be more mature in future releases. Examples include the following.

- Examples of supported features: PWR steady-state core follow, depletion, decay, fuel shuffling, xenon transients, PWR standalone T/H analyses, and single phase flow.
- Examples of unsupported R&D features: BWR, fully coupled transients such as reactivity insertion accident (RIA), ex-core neutron transport calculations, CRUD analyses (CIPS and CILC), CFD-informed subchannel applications, and pellet-clad interaction (PCI) risk assessments.



During release testing of VERA 4.2, the code development teams identified and addressed several defects and issues. Some of these were corrected in VERA 4.2, and some will be addressed in later VERA versions. Section 9 contains a comprehensive list of known defects, issues, and workarounds in this release. Please report any additional new defects identified to <u>vera-support@ornl.gov</u>.



## **3. SYSTEM REQUIREMENTS**

Linux platforms with functioning gcc, g++, and gfortran compilers and X11 libraries are supported. For quarter-core simulations of commercial reactor problems of fidelity consistent with CASL analyses, a minimum of approximately 500 compute cores are needed with approximately 4 GB memory available per core. 1,000 cores are recommended for these problems. When running VERA with VERAShift ex-core calculations, another 100–400 cores are recommended, and the memory requirement per process is approximately doubled.

Detailed system software and TPL requirements are specified in the provided VERA Installation Guide.

This distribution has been tested and verified to install and execute on the following OS distributions:

- CentOS 7
- CentOS 7.4
- RedHat 7.4
- SUSE 3.0.101
- SUSE 3.0.76
- CRAY OS
- Ubuntu 16.04.2

#### 4. INSTALLATION

Detailed installation instructions are provided in the VERA Installation Guide located in the distribution tarball under the VERA/doc/installation\_guide folder. Documentation is also delivered with the distribution.



# 5. DOCUMENTATION

The documentation listed in Table 1 is available with the VERA 4.2 release distribution. Other CASL and VERA technical reports and publications are available upon request from <u>vera-</u>support@ornl.gov.

| Document ID                                 | Document Title  |  |
|---|---|--|
| ORNL/TM-2021/1979                           | VERA 4.2 Installation Guide   |  |
| CASL-U-2014-0014-005                        | VERA Common Input User Manual   |  |
| CASL-U-2019-1886-002                        | CTF Theory Manual   |  |
| CASL-U-2019-1885-002                        | CTF User's Manual   |  |
| CASL-U-2019-1887-002                        | CTF Validation and Verification   |  |
| CASL-U-2019-1874-001                        | MPACT Theory Manual   |  |
| CASL-U-2019-1873-002                        | MPACT User's Manual   |  |
| CASL-U-2019-1877-006                        | MPACT Verification and Validation Manual (Revision 6)   |  |
| CASL-U-2017-1445-000<br>/<br>LA-UR-17-29083 | User Guidelines and Best Practices for CASL VUQ Analysis Using Dakota<br>(https://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-17-29083) |  |
| SAND2014-4253                               | DAKOTA 6.6 Theory Manual<br>(https://dakota.sandia.gov/sites/default/files/docs/6.6/Theory-6.6.0.pdf)   |  |
| SAND2014-4633                               | DAKOTA 6.6 User's Manual<br>(https://dakota.sandia.gov/sites/default/files/docs/6.6/Users-6.6.0.pdf)  |  |
| (Online)                                    | DAKOTA Reference Manual ( <u>https://dakota.sandia.gov/content/latest-reference-manual</u> )  |  |
| (Online)                                    | DAKOTA Developer's Manual ( <u>https://dakota.sandia.gov/content/latest-developers-manual</u> )   |  |
| INL/EXT-13-29930                            | BISON Theory Manual ( <u>https://bison.inl.gov/SiteAssets/BISON_Theory_ver_1_3.pdf</u> )  |  |
| INL/MIS-13-30307                            | BISON User's Manual ( <u>https://bison.inl.gov/SiteAssets/BISON_Users_ver_1_3.pdf</u> )   |  |
| CASL-U-2016-1099-001                        | File-Based One-Way BISON Coupling Through VERA: User's Manual   |  |
| CASL-U-2019-1924-001                        | VERAShift Theory Manual   |  |
| CASL-U-2019-1921-001                        | VERAShift User's Manual   |  |
| CASL-U-2019-1925-000                        | VERAShift Verification and Validation   |  |
| CASL-U-2016-1186-000                        | Shift Verification & Validation   |  |
| CASL-U-2019-1836-000                        | MAMBA v.2.0 Theory Manual   |  |
| CASL-U-2016-1058-003                        | VERAView User's Manual  |  |

| Table 1.  | <b>VERA 4.2</b> | component | documentation |
|-----------|-----------------|-----------|---------------|
| I abic I. |                 | component | uocumentation |

# 6. SUPPORT

Questions, issues, bugs, and suggestions should be reported to <u>vera-support@ornl.gov</u>. Some documentation and examples are also available at <u>https://vera.ornl.gov</u>. Software builds and examples are available at /projects/vera-user/vera on INL's Sawtooth high-performance computer and for VERA Users Group (VUG) members at /projects/vera-users-grp.



#### 7. PHYSICS COMPONENTS INCLUDED IN VERA 4.2

This section describes the new, stable, and experimental features included in this release of VERA. For a full list of known defects and issues, please see Section 9.

The component code versions included with this distribution—and for reference, the previous VERA versions—are listed in Table 2. Cryptographic labels refer to CASL Git repository SHA keys that uniquely identify code versions.

| Componen<br>t | VERA 3.9 Version       | VERA 4.0 Version       | VERA 4.1 Version          | VERA 4.2 Version       |
|---------------|------------------------|------------------------|---------------------------|------------------------|
| MPACT         | 706de3d (Feb 17, 2018) | b5e2cbe (Mar 20, 2019) | 869ab07 (Oct 17, 2019)    | 9fa11cb (Dec 1, 2020)  |
| CTF           | 9105f20 (Feb 13, 2018) | 30aab7c (Mar 25, 2019) | 97514a5 (Nov 14, 2019)    | ee32ff4 (Jan 29, 2021) |
| VERAIO        | N/A                    | N/A                    | ac2e962 (Oct 18, 2019)    | 555ad61 (Dec 2, 2020)  |
| BISON         | f293c4d (Jan 16, 2018) | be31f34 (Feb 26, 2019) | 68913d5 (May 29,<br>2019) | f721711 (Jun 11, 2020) |
| VERAShift     | 911aa80 (Feb 14, 2018) | cc034ad (Mar 19, 2019) | ac561d8 (June 6, 2019)    | e901353 (Dec 21, 2020) |
| MAMBA         | N/A                    | d971461 (Mar 25, 2019) | 6bd9ab2 (May 22,<br>2019) | c9e37e4 (Oct 17, 2020) |
| Dakota        | V6.6                   | V6.6                   | V6.6                      | V6.6                   |

| Table 2. VEF | RA 3 9. 4 0. 4 1 | , and 4.2 com         | ponent versions |
|--------------|------------------|-----------------------|-----------------|
|              | \Л J.J, T.U, T.J | , anu <b>7.</b> 2 com | ponene versions |

Complete version information for all CASL source code repositories associated with this release are documented in CASL-U-2020-1941-000, which is available from CASL records upon request. For VERAIO, the version of VERARun supporting the 4.2 release is Version 1.11. The SQL1 version of VERAView is Version 2.4.3. Any subsequent versions should be considered test or R&D versions until documented in a subsequent release.

For BISON, the compatible commit SHA is 89b676d045cba9018c520afc5885a5778ae42169 (September 20, 2019).

# **7.1 MPACT**

MPACT is an advanced pin-resolved whole-core multi-group deterministic neutron transport capability based on the 2-D/1-D synthesis method, on the frame of a 3-D coarse mesh finite difference method, for which radial and axial correction factors are obtained from 2-D method-ofcharacteristics and 1-D  $P_N$ , respectively [4]. The transport is performed using 51 energy-group cross sections, based on the subgroup method of on-the-fly resonance self-shielding [5]. The discretization of the core is typically three radial and eight azimuthal flat source regions per fuel pellet (See Fig. 3-2) at each of approximately 60 axial planes, explicitly treating such features as spacer grids, fuel and absorber plena, and end plugs. MPACT performs the same neutron transport calculations in the upper, lower, and radial reflector regions of the core, explicitly modeling the baffle, core barrel, neutron pads, nozzles, and core plates, requiring no *a priori* approximations of the core boundary conditions as is needed for nodal diffusion methods. MPACT also controls the functional application features of the VERA core simulator, such as critical boron search, equilibrium xenon calculations, predictor-corrector depletion, in-core detector response calculations, reading and writing restart files, and performing fuel shuffling, decay, and discharge.



New features implemented since the release of VERA 4.1 include the following:

- various bug fixes
- the approximate gamma-smearing energy deposition model
- additions to nodal cross section edits for transient data calculation

New features implemented since the release of VERA 4.0 include the following:

• various bug fixes

New features implemented since the release of VERA 3.9 include the following:

- various bug fixes
- updated documentation
- in-line thermal expansion processing (the ThermalExpandXML.exe preprocessor is no longer needed)
- generation of summary output file
- new input format for "jump-in" cycles
- support for accident-tolerant fuel forms (U<sub>3</sub>Si<sub>2</sub> and UN) and cladding (FeCrAl and SiC/SiC)
- better usability and parallel performance of spatial partitioning via graph partitioning
- linear source method of characteristics solver
- addition of <sup>15</sup>N to cross section library
- nodal cross section edits
- improved ASCII output formats
- consistent check on core height
- explicit delayed energy deposition for transients
- intra-pin edits for VERAView
- coupling of intra-pin power, temperature, and burnup with CTF

The following features are stable:

- support for Linux OS (32 bit and 64 bit)
- parallel spatial decomposition with message passing interface (MPI)
- parallel angular decomposition with MPI
- user-defined macroscopic cross sections
- 51-group macroscopic cross section library data
- subgroup resonance self-shielding
- transport-corrected P<sub>0</sub> scattering treatment
- export of mesh to legacy VTK and VTU file for visualization
- 2D MOC transport kernel
- coarse mesh finite difference (CMFD) acceleration
- 1D nodal kernels based on nodal expansion method (NEM) diffusion and  $SP_N$
- 2D/1D full core solution
- multistate calculation capability
- transient calculation capability



- depletion and decay
- critical boron search
- equilibrium xenon calculation
- direct coupling with COBRA-TF
- simplified internal T/H
- general PWR geometry modeling
  - o Integral Fuel Burnable Absorber
  - o control rods and control rod banks
  - burnable poison inserts
  - o fission chamber detectors
  - o grid spacers, nozzles, plenum, baffle, etc.
  - semi-explicit modeling of grid spacers
- isotopic restart file
- cycle-to-cycle fuel shuffling
- jump-in cycle capability
- radial thermal expansion
- efficient graph-based spatial decomposition
- generation of text summary file
- in-line thermal expansion

The following features are considered to be experimental:

- separate B-10 depletion of soluble boron
- space-dependent Wielandt shift or dynamic Wielandt shifts
- modeling of BWRs
- simplified CRUD modeling
- post-corrector depletion
- 3D MOC solvers
- processing of AMPX working cross section libraries
- processing of ISOTXS cross section libraries
- secondary source calculation
- axial thermal expansion
- multilevel in space and energy diffusion solver for CMFD
- remeshing and fuel rod reconstitution in restart and shuffle
- center assembly homogenization when shuffling fuel
- coupling with MAMBA CRUD chemistry
- coupling with Shift for ex-core detector response calculations
- subplane treatment
- linear source MOC
- nodal cross section edits
- support for accident tolerant fuel (ATF) fuel forms
- explicit delayed energy deposition for transients



- Intrapin edits for VERAView
- coupling of intra-pin power, temperature, and burnup with CTF
- secondary source calculations

# 7.2 CTF

CTF, an updated version of the COBRA-TF code, is a subchannel T/H code that uses a two-fluid, three-field (i.e., fluid film, fluid drops, and vapor) modeling approach for single- and two-phase steady-state and transient conditions [6]. CTF includes a wide range of T/H models important to LWR safety analysis and modeling of normal LWR operating conditions including flow regime-dependent, two-phase wall heat transfer, inter-phase heat transfer and drag, turbulent mixing, two-phase pressure drop, spacer grid effects, and void drift. Because of its 3D capabilities and extensive array of reactor T/H modeling capabilities, CTF has been used extensively in the modeling of LWR, in-core, rod bundle transient analyses.

Significant changes implemented since the release of VERA 4.1 include the following:

- added a preliminary bypass modeling capability for core-scale BWR models
- made performance and robustness improvements to pressure balance iteration loop used for core-scale BWR models
- added a preliminary capability for modeling axially varying water rod geometry to the xml2ctf preprocessor
- added inlet orifice map feature for BWR models
- set energy storage printout to zero if it is not being checked to prevent confusion
- added alternative Chisholm and Lockhart-Martinelli two-phase pressure drop models
- added ability to specify which datasets CTF shall print to the HDF5 file through the CTF\_Coupling\_Interface
- switched to solving one pressure matrix per assembly for core-scale BWR models, which allows for using the direct solver without an impact on problem run time
- added basic support for using the Intel 19 compiler for CTF builds
- refactored flow regime map logic to allow for implementing new maps and implemented the Wallis flow regime map
- implemented an outer-iteration loop, which iterates over the mass and energy equation solution to ensure that they are sufficiently converged before advancing to the next timestep
- added preliminary drift-flux model for predicting interfacial drag in bubbly flow regimes
- added support for refining the radial mesh in the fuel rod clad
- implemented a set of common ATF clad and pellet material properties and refactored the material properties section to allow for more easily implementing new properties in the future
- expanded CTF validation matrix to include WALT, Thom, and Rohsenow boiling tests and Bartolomei void measurement tests
- added a validation matrix driver, which allows users to run the entire CTF validation matrix and perform results postprocessing in an automated fashion
- added new subcooled boiling model that uses an onset of nucleate boiling criteria with the Gorenflo heat transfer model and Saha-Zuber critical enthalpy model
- added option to output solver residuals during solution
- added support for modeling quarter symmetry BWR models



- added stopping criteria for species transport non-condensable gas model, allowing users to model steady-state solutions of species transport of noncondensable gas
- added new set of CTF\_Coupling\_Interface procedures that do not expose the cell splitting behavior for fuel rods in CTF, thus simplifying the interface
- added support for modeling of part-length rods in the xml2ctf preprocessor
- modified the external fuel solver coupling interface to support coupling to the FAST fuel performance code

Stable features include the following:

- solid modeling capabilities
  - $\circ$  radial conduction
  - nuclear fuel rod models (e.g., pellet, gap, and clad regions and UO<sub>2</sub> and Zircalloy material properties)
  - dynamic gap conductance model (e.g., pellet relocation and PCI)
- fluid modeling capabilities
  - solid-to-fluid heat transfer
    - single-phase convection
    - subcooled/saturated boiling
  - o critical heat flux (i.e., departure from nucleate boiling)
  - o two-phase flow with droplets
  - o closure models
    - wall drag and form loss modeling
    - turbulent mixing and void drift
    - fluid equation of state
    - droplet entrainment and de-entrainment
  - incorporation of PETSc solvers
  - o variable-size axial meshing
  - grid heat transfer enhancement modeling
  - o multisection modeling with channel splitting and coalescing
  - o general species transport

The following features are experimental:

- solid modeling capabilities
  - o fuel rod axial/azimuthal conduction
  - axial mesh refinement (quench front tracking)
  - o Zircaloy-water thermal reaction
- Fluid modeling capabilities
  - noncondensable gas effects
  - post-CHF heat transfer models (are encountered in validation tests, but no validation of models done)
  - o channel flow area variations (rod ballooning)
  - o grid-directed crossflow modeling



o boron-tracking model with consideration of boron precipitation

## 7.3 BISON

BISON is not included in VERA 4.2 distributions through RSICC. To obtain BISON, please contact <u>agradmin@inl.gov</u>.

VERA includes the capability to predict fuel rod performance by using 2D axisymmetric or 3D coupled multiphysics, and represents a significant advancement for the modeling and analysis capabilities in LWR fuel rod behavior [7]. The capability is being constructed within the MOOSE/BISON computational framework from INL, which supports the following:

- 1.5D-RZ, 2D, and 3D thermo-mechanics, including elasticity, plasticity with strain hardening, creep, large strains, large displacements, and smeared plus explicit cracking
- unsteady (i.e., transient) conduction heat transfer with time and spatial (i.e., axially, radially, and potentially azimuthally in a cylindrical fuel element)-dependent internal heat generation
- gap heat transfer, including conduction, radiation, and enhanced heat transfer from mechanical contact
- 2D axisymmetric, generalized plane strain and plane stress representations, including thermal and mechanical contact interactions between pellets and between the pellet and cladding
- mixed-dimensional coupling (e.g., combined 2D and 3D numerical representations for coupled global [2D] and local effects [3D] modeling)
- the use of high-performance computing platforms to achieve the parallel performance and scalability required to perform coupled multiphysics simulations of full-length 3D representations of the fuel rod components

The BISON fuel rod performance code architecture uses the finite element method for geometric representation and a Jacobian-free, Newton–Krylov (JFNK) scheme to solve systems of partial differential equations. The fuel rod performance capability includes models for the following:

- clad stress, strain, and strain rate
- clad oxidation, hydrogen pickup and hydride formation
- pellet stress, strain, and strain rate
- fission gas release (transient and pseudo-steady-state)
- pellet densification and swelling
- pellet cracking (isotropic and smeared) and relocation
- thermal expansion, including pellet hour-glassing
- thermal and irradiation creep
- thermal conductivity effects due to clad oxidation
- material strength and ductility effects due to irradiation
- pellet cladding gap evolution and local stress due to partial contact
- pellet stack growth and fuel rod growth
- explicit modeling of duplex and triplex clad designs
- reference residual calculations for improved robustness



On a 2D or 3D basis, the VERA fuel rod performance subcomponent calculates fuel rod temperature, fuel rod internal pressure, free gas volume, clad integrity, and fuel rod waterside diameter. These capabilities allow the simulation of power cycling, fuel conditioning and deconditioning, high-burnup performance, power uprate scoping studies, and accident performance.

These tools are principally built around the known performance of existing zirconium-based clad with UO<sub>2</sub> fuel. Estimates for the global effects of minor modifications to the fuel or clad could be possible; for example, chromia-doped pellets could be simulated with user-supplied models for several of the pellet performance characteristics, or steel-based clad could be simulated with similar user-supplied models. Materials such as silicon carbides that do not fit the system paradigm can be simulated but are unlikely to provide accurate results.

#### 7.4 VERAShift

VERAShift is a Monte Carlo radiation transport framework. It was first distributed as part of VERA 3.7, and this release fixes several issues and adds features that build upon VERA 4.1. As before, VERAShift can be run standalone in eigenvalue mode using the VERA common input with the vera\_shift executable. It can also run coupled to the core simulator using the vera\_to\_shift executable, which, as before, runs MPACT/CTF and Shift on different processor domains.

Changes since the release of VERA 4.1 include the following:

- new user manual: CASL-U-2019-1921-001
- general bug fixes
- improved ex-core modeling
- ability to use Forward-Weighted Consistent Adjoint-Driven Importance Sampling (FW-CADIS) for variance reduction of ex-core calculations
- multithreaded Shift Monte Carlo transport solve
- domain-decomposed Shift Monte Carlo transport calculation

Stable features of VERAShift in VERA 4.2 include the following:

- node-based parallelism using domain replication
- multistate calculations
- eigenvalue, forward, and CADIS modes
- fission source coupling between VERA and Shift
- pin cell isotopic coupling between VERA and Shift
- flux tallying in core barrel, core pads, vessel liner, and vessel using VERA common input
- supplemental geometry and tally input for ex-core model features and tallies (extra geometric features that cannot be modeled with VERA common input)

The following features are available but are considered experimental because they have not been tested rigorously:

• transfer of temperatures and densities in fuel, clad, and coolant between VERA and Shift



- FW-CADIS mode
- domain-decomposed Shift calculation

Known limitations include the following:

- Memory usage when using unique pins is very high.
- Memory usage for full-core calculations is high.
- Memory usage when transferring fission source, isotopics, temperatures, and densities from VERA is very high, which requires unique pins.
- When running in CADIS or FW-CADIS modes, the parallel decomposition used for the deterministic adjoint calculation dictates the number of processors the VERAShift calculation must use.

## **7.5 MAMBA**

The MAMBA package [9] simulates the growth of CRUD, which refers to metal oxide corrosion products—primarily nickel ferrite (NiFe<sub>2</sub>O<sub>4</sub>)—on fuel cladding and accumulation of boron in the porous CRUD. The precipitation of boron compounds, such as lithium tetraborate (Li<sub>2</sub>B<sub>4</sub>O<sub>7</sub>), can lead to a CIPS in the nuclear fuel. Additionally, the CRUD itself can lead to CILC due to reduced thermal transport and thus increased temperatures, which can cause mechanical failure of the fuel.

The role of MAMBA is to simulate the buildup of CRUD and the precipitation of boron-rich compounds within the porous CRUD layer. Because the formation of CRUD is a fundamentally multiphysics problem, MAMBA is coupled to neutronic and T/H solvers present in VERA to predict CIPS. MAMBA requires T/H conditions as input, namely the cladding surface heat flux, turbulent kinetic energy, and the coolant temperature. Within VERA, CTF provides T/H conditions. Additionally, the CRUD source term is modeled in MAMBA, which originates from corrosion of steam generators and primary loop piping.

MAMBA is available in VERA 4.2, but all features are considered experimental at this time. It is not recommended for use. A more recent version can be obtained by contacting <u>vera-support@ornl.gov</u>.

#### 7.6 Dakota

The Dakota 6.6 package [14] manages and analyzes ensembles of simulations to provide a broader and deeper perspective for analysts and decisionmakers. In its simplest mode, Dakota can automate typical parameter variation studies through a generic interface to a physics-based computational model. This can lend efficiency and rigor to manual parameter perturbation studies already being conducted by analysts. Dakota also delivers advanced parametric analysis techniques that enable design exploration, optimization, model calibration, risk analysis, and quantification of margins and uncertainty with such models. It directly supports V&V activities. Dakota algorithms enrich complex science and engineering models, enabling analysts to answer the following crucial questions about sensitivity, uncertainty, optimization, and calibration.

- Sensitivity: Which are the most important input factors or parameters entering the simulation, and how do they influence key outputs?
- Uncertainty: What is the uncertainty or variability in simulation output, given uncertainties in input parameters? How safe, reliable, robust, or variable is the system? (Quantification of margins and uncertainty [QMU].)



- Optimization: What parameter values yield the best performing design or operating conditions, given constraints?
- Calibration: What models and/or parameters best match experimental data?

A CASL technical report that provides user guidelines and best practices for CASL validation/uncertainty quantification analysis using Dakota (CASL-U-2016-1233-000/SANDIA Report SAND2016-1161) is available at:

https://dakota.sandia.gov//sites/default/files/documents/SAND-CaslDakotaManual-2016.pdf.

The following features are considered mature and robust:

- parameter studies: list, vector, centered, multidimensional
- uncertainty quantification (UQ): Monte Carlo and Latin hypercube sampling, local reliability (probability of failure) methods, stochastic expansions (polynomial chaos and stochastic collocation)
- optimization/calibration: gradient-based local, derivative-free local (pattern search), global (e.g., genetic algorithms, direct), local least squares, surrogate-based local methods
- surrogate models: polynomials, Gaussian/kriging process, neural network
- parameter types: all are mature except discrete string and categorical types
- interfaces: system, fork, and direct
- responses: objective functions; calibration terms, including experimental data; and response functions

The following features are stable:

- design and analysis of computer experiments: DDACE grid, random, orthogonal array, OA-LHS; FSU quasi-Monte Carlo (Halton, Hammersley, centroidal Voronoi tessellation), PSUADE Morris one-at-a-time
- UQ: global reliability (probability of failure) methods, adaptive stochastic expansions, importance sampling (including adaptive, and surrogate-based), Probability of Failure Darts, epistemic interval uncertainty, Dempster–Shafer, Bayesian inference (QUESO, DREAM), incremental LHS
- optimization: NOMAD directional search, surrogate-based global including EGO, hybrid, and pareto optimization
- surrogate models: MARS, Taylor/TANA, hierarchical and multifidelity
- interfaces: Python interfaces; work directory and parallel interface scheduling features refactored recently

The following features are experimental:

- design and analysis of computer experiments: DDACE Box–Behnken, central composite designs
- UQ: D-optimal sampling, multilevel and multifidelity Monte Carlo methods, topology-based adaptive sampling, Bayesian inference (GPMSA)



- optimization: Genie Opt-Darts, Genie Direct
- surrogate models: moving least squares, radial basis functions, active subspace methods for dimension reduction
- variables: string/categorical variable support is limited
- interfaces: Matlab, Scilab, and grid
- responses: field data for both simulations and experiments, including interpolation capability

Release notes for Dakota 6.6 (and previous versions the capabilities of which are also included in Dakota 6.6) are available at <u>https://dakota.sandia.gov/content/release-notes</u>. Known limitations of Dakota 6.6 are listed in Section 9.



# 8. VERA INPUT/OUTPUT TOOLS

#### 8.1 VERAIn

The VERA Common Input (VERAIn) [10] provides a simple and user-friendly input interface for the VERA components. It is a PERL script that converts the ASCII common input file to the intermediate XML format used as an input and geometric database for the physics codes in VERA. VERA component codes either read the VERA XML format directly or provide a preprocessor that can convert the XML into native input (such as CTF and BISON). When processing the ASCII common input file, VERAIn performs basic error checking to ensure that common input errors are caught before running a simulation. Additionally, VERAIn performs geometry processing by expanding symmetric geometry inputs to their full geometry.

## 8.2 VERAView

VERAView is an interactive graphical interface for the visualization and engineering analyses of output data from VERA [11]. The Python-based software is easy to install and intuitive to use, and it provides instantaneous 2D and 3D images, 1D plots, and alphanumeric data from VERA multiphysics simulations. It reads files in HDF5 format that meet the VERAOut specification [15]. A user manual is provided that provides a brief overview of the software and descriptions of the major features of the application, including examples of each of the encapsulated "widgets" that have been implemented thus far.

| Table 3. VERAView required Python packages. |                 |  |
|---|-----------------|--|
| Package                                     | Minimum version |  |
| h5py  | 2.9.0           |  |
| hdf5  | 1.10.4          |  |
| matplotlib                                  | 1.5.1           |  |
| mayavi                                      | 4.5.0           |  |
| numpy                                       | 1.11.3          |  |
| pillow                                      | 3.0.0           |  |
| pyparsing                                   | 2.4.2           |  |
| scipy                                       | 1.2.1           |  |
| wxpython                                    | 3.0             |  |

VERAView currently requires Python 2.7 and the packages listed in Table 3.

VERAView is packaged in a prebuilt Python environment based on Miniconda (<u>https://docs.conda.io/en/latest/miniconda.html</u>) and includes all required packages. Single-click GUI installers are provided for Windows and Mac OSX, and an installation script is provided for Linux based on RedHat Enterprise Linux / CentOS version 6.

VERAView interprets the category or type of datasets in the VERAOut based on their shape and size, and the type determines which widgets can be used to display the data. The following dimensions are determined from the datasets:

- NASS: number of fuel assemblies in the calculated geometry (quarter or full core)
- NAX: number of axial planes in the core region (assumes same for all data except detectors)
- NPIN: number of fuel rods across a fuel assembly (assumes equal X and Y dimensions)



- NCHAN: number of coolant channels across an assembly (assumes equal X and Y dimensions)
- NDET: number of in-core instrument strings
- NDETAX: number of detector axial planes
- NFDETAX: number of fixed-detector axial planes
- NR: number of fluence radial bins
- NT/HETA: number of fluence angle bins
- NZ: number of fluence axial planes

Datasets for individual statepoints are stored in the HDF5 file in groups with name /STATE\_nnnn, where nnnn starts at 0001 and increments thereafter. Dataset types that are recognized are summarized in Tables 4–7.

| Table 4. Frimary VERAvlew dataset types. |                               |  |  |  |
|--|-------------------------------|--|--|--|
| Туре                                     | Shape                         | Description  |  |  |
| channel                                  | (npiny+1, npinx+1, nax, nass) | 3D coolant channel data                            |  |  |
| detector                                 | (ndetax, ndet)                | 3D detector signals                                |  |  |
| fixed_detector                           | (nfdetax, ndet)               | 3D fixed detector signals                          |  |  |
| fluence                                  | (nz, ntheta, nr)              | 3D fluence data                                    |  |  |
| node                                     | (4, nax, nass)                | Nodal data   |  |  |
| pin                                      | (npiny, npinx, nax, nass)     | 3D fuel rod data                                   |  |  |
| radial_detector                          | (ndet)                        | Axially integrated (radial) detector distributions |  |  |
| scalar                                   | 0                             | Scalar quantity                                    |  |  |

#### Table 4. Primary VERAView dataset types.

|                  |                          | <i>v</i> 1  |
|------------------|--------------------------|---|
| Туре             | Shape                    | Description   |
| :assembly        | (nax, nass)              | Axially integrated (radial) assembly-wise distributions |
| :axial           | (nax)                    | Radially integrated (axial) distributions               |
| :chan_radial     | (npiny+1, npinx+1, nass) | Axially integrated coolant channel data                 |
| :core            | 0                        | Core-wise values  |
| :radial          | (npiny, npinx, nass)     | Axially integrated distributions                        |
| :radial_assembly | (nass)                   | Axially and radially integrated distributions           |

#### Table 5. Derived VERAView dataset types.

| Table 6 VERAView ba | sic capability widgets. |
|---------------------|-------------------------|
|---------------------|-------------------------|

| Widget             | Display                                   | Datasets Supported   |
|--------------------|---|--|
| Core 2D view       | Assemblies in the current geometry        | channel, pin, :assembly, :chan_radial, :node,<br>:radial, :radial_assembly   |
| Core Axial 2D view | Vertical cut along assembly column or row | channel, pin, :assembly, :node   |
| Assembly 2D view   | Lattice view of selected assembly         | channel, pin, :chan_radial, :radial  |
| Axial plots        | Plots with axial level as the y-axis      | any with an axial dimension  |
| Time plots         | Plots with time as the <i>x</i> -axis     | channel, detector, fixed_detector, fluence, pin,<br>radial_detector, scalar, :assembly, :axial,<br>:chan_radial, :core, :node, :radial, :radial_assembly |



| Widget                       | Display  | Datasets supported  |
|------------------------------|--|---|
| Detector multi view          | Plots and numerical display of detector values       | detector, fixed_detector, radial_detector   |
| Table view                   | Tabular view of dataset values at current selections | channel, detector, fixed_detector, fluence, pin,<br>radial_detector, scalar, :assembly, :axial,<br>:chan_radial, :core, :node, :radial,<br>:radial_assembly |
| Vessel core 2D view          | Vessel fluence horizontal slice                      | fluence   |
| Vessel core axial 2D<br>view | Vessel fluence vertical slice                        | fluence   |
| Volume slicer 3D view        | Cuts across the three dimensions                     | pin, :assembly, :radial   |
| Volume 3D view               | Volumetric view with cuts                            | pin   |

#### Table 7 VERAView experimental widgets.

Derived datasets representing the average, root mean square, standard deviation, and sum across data axes are shown in Table 5. VERAView can calculate these datasets if they are not already in the VERAOut file.

Multiple files may be opened and viewed simultaneously provided that they have congruent core geometries.

VERAView provides several "basic capability" and "extended capability", or experimental, widgets. The former are covered in the VERAView software test plan requirement and test report, whereas experimental widgets are lightly tested. Additionally, VERAView is designed to be extensible, supporting addition of custom widgets. Refer to the *VERAView API and Programmer's Guide* [16].

VERAView is no longer included in the VERA distribution package. It is available on GitHub at <u>https://github.com/CASL/VERAview</u>. The latest development version is also available for use and can be obtained by contacting <u>vera-support@ornl.gov</u>, or at

/projects/vera-user/vera/veraview/veraview3 on INL's Sawtooth.



# 8.3 VERARun

VERARun is a driver utility designed to automate job submission on a particular computing platform. VERARun evaluates the user input and is configured for each machine specifically so that it can automatically create the scripts needed by a queuing system and easily submit the job for a user with only one simple command-line execution. It is provided as a Python package source distribution that must be extracted and installed using VERA's Python 2.7 environment.

After installing, two executable scripts will be installed in the Python environment: verarun and verastat. The former script submits jobs, and the latter displays a history of submitted jobs. All command-line options and processing features are described by requesting usage help from the command line:

```
verarun -help
```

In its simplest form, VERARun can be executed with the name of the VERAIn input file, for example:

```
verarun 5a_2d.inp
```

VERARun is available on INL's Sawtooth by sourcing the file /projects/verauser/vera/setenv.sh. More information is also available in /projects/verauser/vera/README.

For more information on VERARun, please contact vera-support@ornl.gov.



# 9. CAVEATS AND KNOWN ISSUES

The VERA software components provided in this release are still under active development and might be subject to rapid change. As described in Section 2, the CASL QA program has established software quality levels to represent the stages of maturity exhibited by each code. SQL1 codes MPACT, CTF, and VERAIO are rigorously developed and tested using a successfully audited NQA-1 compliant QA program. However, SQL4 codes VERAShift and MAMBA are less developed, less tested, and still under significant active research. They should be used for test, evaluation, and research purposes only.

Issues that have been identified during development and testing of this release package are listed below. Some of these issues are software errors (reported as part of the software problem reporting process), and some are minor issues or nuances that were encountered in the past and have not been resolved. New issues that are identified that are not listed here should be reported to <u>vera-support@ornl.gov</u> as soon as possible. Software problem reports for defects found in VERA are posted online for VUG members at <u>https://vera.ornl.gov/vera-members-only</u>.

| Ticket       | Component | Issue   |
|--------------|-----------|---|
| 3262         | MPACT     | For some MPI distributions, the communication routines for the MG MOC kernels<br>experience an error in MPI.<br>* WORKAROUND: Use the shield_moc_kernel 1g or moc_kernel 1g option.   |
| 1284         | MPACT     | On some platforms, depletion cases run with spatial and angular decomposition fail.<br>* WORKAROUND: Use threading instead of angle decomposition.  |
| 1301         | MPACT     | When using TCP0, in some cases can drive the solution negative, and this can lead to cases diverging. This is more likely to happen in 3D problems with large reflectors.<br>* WORKAROUND: Use the moc_kernel mg option. Using P2 scattering is also an option at the expense of longer run times.              |
| N/A          | MPACT     | The number of azimuthal divisions in the flat source region mesh of a fuel pin or guide<br>tube in the visualization file is not representative of the computational mesh. The<br>visualization contains extra divisions to approximate a curved surface as a series of line<br>segments.                       |
| 3262         | MPACT     | For some MPI distributions, the communication routines for the 1G MOC kernels<br>experience a memory leak in MPI.<br>* WORKAROUND: Use moc_kernel mg and moc_mg_data_passing true.  |
| N/A          | MPACT     | Support for the depletion of absorbing materials in control rods is not yet implemented.<br>The absorber material in a control rod should be defined in the CONTROL block to<br>ensure that rod materials are not depleted. If the materials are placed elsewhere, then they<br>might be flagged as depletable. |
| 3742         | MPACT     | Entries in the shuffle_label and assm_map must be consistent geometrically between fuel cycles. Shuffling by assembly serial number is not implemented. Shuffling errors do not produce useful messages.  |
| 3995         | MPACT     | Assemblies with stainless-steel rods must have the same thermal expansion temperatures with performing core shuffles.   |
| 3837         | MPACT     | MPACT geometry error if many digits are specified on the axial_edit_bounds  |
| 3855         | MPACT     | Segmentation fault when BISON/shuffle_xml is empty.   |
| 4082<br>4637 | MPACT     | Extended coupling mesh T/H passed back from CTF not placed in MPACT properly.   |
| 3863         | MPACT     | Axial mesh boundaries must align with spacer grid boundaries in the active fuel region.   |
| 3865         | MPACT     | Smaller timesteps are required for depletion of fuel bearing the Gadolinia neutron absorber.  |
| 3795         | MPACT     | Subplane calculations give inconsistent results when using graph partitioning.  |

#### Table 8. Known issues and defects in VERA 4.2.



| Ticket | Component | Issue  |
|--------|-----------|--|
| 3897   | MPACT     | Extended coupling mesh does not work when smearing axial reflector regions together.   |
| 4065   | MPACT     | Use of "edits" option across multiple STATE blocks results in some default edits not<br>being included in HDF5 output.<br>* WORKAROUND: When specifying the "edits" option in multiple state blocks, also list<br>default edits such as "pin powers."  |
| 4206   | MPACT     | If the number of depletable regions changes while using higher order depletion, MPACT will segfault.   |
| 4226   | MPACT     | MPACT automeshing does not capture spacer grids in axial reflector regions.  |
| 4294   | МРАСТ     | Code segfaults instead of throwing an error if the user inputs mismatched pins on the $x$ and $y$ symmetry lines while using rotational symmetry.  |
| 4315   | MPACT     | Custom radial meshing for fuel cells performs incorrectly  |
| 4338   | МРАСТ     | Using a nonconstant Wielandt shift method in the "cmfd_shift_method" option can result<br>in an incorrect eigenvalue for adjoint flux calculations.<br>* WORKAROUND: Use the default "cmfd_shift_method" input if adjoint flux<br>calculations will be performed.  |
| 4343   | MPACT     | Intrapin_volume edit is incorrect for pins that are split across modules.  |
| 4404   | MPACT     | Intrapin edits crash if too many are specified due to excessive memory consumption.  |
| 4587   | MPACT     | BWR core_map and detector_map are not properly unfolded in quarter symmetry.   |
| 4593   | MPACT     | In very rare cases, the same calculation can take a different number of iterations to converge. The reason for this is unknown. When this occurs, the solution is the same, regardless of the number of iterations taken.  |
| 4613   | MPACT     | Homogenized spacer grid volume fractions are underestimated.<br>* WORKAROUND: Use explicit spacer grids, if possible.  |
| 4614   | MPACT     | Axial void card boundaries are applied incorrectly when axial reflector regions are present.   |
| 4645   | MPACT     | Baffle is not modeled properly if the (baffle gap + baffle thickness) is less than the (assembly gap + pin pitch).   |
| 4673   | MPACT     | Negative void shown at spacer grid locations in BWR summary files.   |
| 4693   | MPACT     | VTU edits might place data in the incorrect regions if the "pin_cell_mod_mesh" is used.<br>The same issue can also occur if the "mesh" option is used to specify different numbers of<br>azimuthal divisions for different radial regions.<br>* WORKAROUND: Do not use these options when visualizations are needed. |
| 4704   | МРАСТ     | The code attempts to run with invalid baffle gap values (less than the assembly gap) instead of throwing a useful error. Only occurs for invalid baffle inputs.  |
| 4729   | MPACT     | The MPACT .out file has incorrect values for "Minimum Axial Mesh" and "Maximum Axial Mesh."<br>* WORKAROUND: Use the "axial_mesh" dataset on the HDF5 file for postprocessing.   |
| 4798   | МРАСТ     | MPACT simplified T/H incorrectly calculates flow area for PWR models with guide tubes.   |
| 4799   | МРАСТ     | MPACT simplified T/H incorrectly calculates heat transfer coefficient for assemblies split by symmetry line.   |
| 4809   | MPACT     | MPACT simplified T/H assumes equal volume rings when performing the conduction solve, even if the fuel is meshed differently.<br>* WORKAROUND: Use equal volume rings or use CTF coupling.   |
| 4828   | MPACT     | MPACT sometimes encounters a race condition when automatically deleting an old restart file and writing a new file of the same name.<br>* WORKAROUND: Rerun the case, and it should succeed on the second try.   |
| 4846   | МРАСТ     | Heavy reflectors for SMR models sometimes have patches of water in the MPACT model<br>that should not be there.<br>* WORKAROUND: Most issues are resolved by ensuring that the baffle gap + baffle<br>thickness = assembly gap + pin pitch.  |



| Ticket | Component | Issue  |
|--------|-----------|--|
| 4849   | МРАСТ     | MPACT crashes if a control bank contains control rods with different numbers of axial levels.  |
| 4876   | MPACT     | VTK edits do not work in parallel<br>* WORKAROUND: Use VTU edits instead   |
| 4877   | МРАСТ     | Restart cases sometimes crash when restarting in full symmetry from a quarter core<br>symmetric calculation<br>* WORKAROUND: Generate the restart file in full symmetry or run the restarted<br>calculation in quarter symmetry  |
| 4879   | MPACT     | MPACT .h5 output has wrong units for pin_isotopes_* edits  |
| 4880   | MPACT     | Isotope Edits Wrong in First Statepoint after Restart until a depletion step is taken<br>* WORKAROUND: Use isotopics from the final state point of the original calculation<br>instead of the first statepoint of the restarted calculation  |
| 4905   | MPACT     | Inlet flow distribution is not passed from MPACT to CTF for full symmetry calculations<br>* WORKAROUND: Use quarter symmetry; there is no workaround for full symmetry   |
| 4951   | MPACT     | Semi-PC Calculates Wrong Burnup<br>* WORKAROUND: Use PC depletion (default)  |
| 4959   | MPACT     | Incorrect Core Exposure in summary file for high order depletion<br>* WORKAROUND: Do not use high order depletion (experimental)   |
| 4967   | MPACT     | MPACT crashes with too many decimal places on axial_edit_bounds<br>* WORKAROUND: Round the values of axial_edit_bounds to four decimal places or<br>less, and ensure exact consistency with fuel and grid spacer elevations.   |
| 1591   | CTF       | The channel splitting feature of CTF enables users to split a large channel into several small channels in the axial direction or, vice versa, condense several small channels into one large channel. This can be done only in multiaxial section models. It has been observed that the code could create mass in the system when using this feature for transient simulations. |
| 1157   | CTF       | The grid droplet breakup model is used to divide the droplet field into large and small<br>drops due to impacting with spacer grids in loss-of-coolant accident conditions. An<br>uninitialized variable has been detected in this model that leads to unpredictable results.<br>This is an experimental feature and is minimally tested, so its use is cautioned.               |
| 1636   | CTF       | There is a bug in the way that the calculated critical heat flux is being time-relaxed for cases that use the W-3 correlation. This bug only affects models using the W-3 correlation and only transient simulations. Steady-state cases will still arrive at the same answer as that obtained if this bug did not exist.  |
| 1171   | CTF       | The CTF legacy restart feature is not currently working.   |
| 1579   | CTF       | The droplet de-entrainment model for annular mist flows that travel into top quench fronts is not working correctly. The wetted perimeter that is used as input to this model is not calculated correctly. This model would only be encountered in accident condition simulations (loss-of-coolant accident).  |
| 1611   | CTF       | For cases with reversed flow at the outlet, when using the outlet pressure boundary condition, and with outlet voids greater than 0.2, the outlet void boundary condition could become inconsistent and lead to the code crashing.   |
| 1780   | CTF       | Using an inlet pressure/outlet pressure boundary condition has been observed to lead to discontinuous mass flow rates in the inlet momentum cell.  |
| 1826   | CTF       | Form losses specified for the inlet plane of the model will not be captured in the pressure losses when using an inlet mass flow rate boundary condition.  |
| 1819   | CTF       | Pressure distribution is discontinuous at the inlet boundary when modeling cases with reversed flow.   |
| 1786   | CTF       | CTF-predicted axial temperature distribution is nonlinear for cases with a uniform axial power distribution when using a nonuniform axial mesh.  |
| 2079   | CTF       | The fine mesh renoding capability used for quench front tracking on fuel rod surfaces does not work.   |



| Ticket | Component | Issue   |
|--------|-----------|---|
| 2220   | CTF       | The code crashes when attempting to include a heated plate geometry in the model.   |
| 2290   | CTF       | Radiative heat transfer model input does not work.  |
| 3133   | CTF       | The code is very susceptible to roundoff error for long-running transients. It has been   |
|        |           | observed that some tests will fail in different builds or on different machines due to  |
|        |           | roundoff error.   |
| 4575   | CTF       | HDF5 dataset core_avg_linear_heatrate is incorrect for some multistate models with power changes  |
| 4623   | CTF       | The pin bounding box used for transferring data between CTF and VERAShift will be   |
| 1023   |           | wrong for large water rods in BWR models  |
| 4698   | CTF       | The flow and bypass cards will not impact the initial flow rate in the CTF input deck for   |
| 1697   | CTF       | BWR models. Flow will always be at the nominal rated flow.  |
| 4687   | CIF       | The inlet orifice map input in the CTF input will not allow users to enter form losses that have a value of 100 or larger due to a formatting issue.                      |
| 4699   | CTF       | CTF is not correctly averaging the boron/lithium passed into MAMBA. The first value   |
| +099   | CII       | passed in at the beginning of the state is used for all following iterations in that state.   |
|        |           | Furthermore, if the source term values are being explicitly set, then CTF will not use the  |
|        |           | average of the two statepoints for the depletion step as it should.   |
| 3363   | CTF       | CTF does not write data correctly to the VERA HDF5 file for multiassembly BWR   |
|        |           | models. Data are not mapped correctly based on their core locations.  |
| 4624   | CTF       | Bounding box, which is used for data transfers between CTF and VERAShift, is not being placed correctly for large water rods in CE-style fuel.                            |
| 3973   | CTF       | Upwind differencing is not being calculated correctly for the calculation of vapor mass   |
|        |           | flux used in the calculation of wall shear.   |
| 4347   | CTF       | Nodal models that include a model map will crash due to an out of bounds error if bounds  |
|        |           | checking is enabled during the build  |
| 4601   | CTF       | Multistate_cobra will not correctly read an input file if it has a custom name (not named   |
|        |           | deck.mstate.inp or deck.inp).   |
| 4407   | CTF       | The axial-variation table is not being set up correctly for channels that are adjacent to more than one part-length rod when those rods end at different axial locations. |
| N/A    | VERAIO    | Canopy might not run on some of the most recent Linux distributions. This is based on   |
| 1011   | . 210 110 | feedback from various users. (VERAView)   |
| 4053   | VERAIO    | User errors with multiline input cards can lead to unexpected behavior or errors.   |
| N/A    | VERAShift | Out of memory errors will occur if using unique pins for various quarter- and full-core   |
|        |           | problems.   |
|        |           | *WORKAROUND: Do not use unique pins (only transfer the fission source).   |
| 4736   | VERAShift | VERAShift might segfault when a <i>restart_write</i> is present in the first STATE block.   |
| 4069   | VERAShift | VERAShift dies ungracefully when specifying tally outside reflecting boundary for   |
| 4120   |           | quarter core problems.  |
| 4120   | VERAShift | Pin adjoint in VERAShift output is incorrect for 2-loop B&W plants.   |
| 4737   | VERAShift | VERAShift multistate p9 FW-CADIS vessel fluence calculation runs out of memory.   |
| 4738   | VERAShift | VERAShift might segfault when running a detector response calculation.  |
| 4760   | VERAShift | Neutron pad locations between MPACT and Shift are inconsistent for full-core problems.  |
| 4756   | VERAShift | Neutron core pads are missing in Shift geometry without a barrel present.   |
| 3861   | MAMBA     | Axial remeshing is not supported for CRUD shuffling.  |
| N/A    | BISON     | The number of processors used by the libresh build process within MOOSE is controlled   |
|        |           | by the environment variables MOOSE_JOBS and LIBMESH_JOBS. If building on less than eight cores, then it is advisable to set these environment variables equal to the      |
|        |           | number of available processors.   |
| N/A    | BISON     | The standalone BISON test suite is experiencing EXODIFF failures. The root cause has  |
|        |           | been traced to an issue with test output files missing a $t = 0$ time step point in the exodus  |
|        |           | file compared with reference "gold" files. This issue is related to the tests themselves and  |
|        |           | is not believed to be reflective of a code failure.   |



| Ticket | Component | Issue   |
|--------|-----------|---|
| N/A    | Dakota    | Some methods that write intermediate files (e.g., LHS.err) cannot be run as concurrent iterators.   |
| N/A    | Dakota    | dprepro does not support the full range of permitted variable descriptors or string variable values.<br>*WORKAROUND: Use variables names currently accepted: \w, which is [a-zA-Z_]). |
| N/A    | Dakota    | Support for categorical variables missing from several methods.   |
| N/A    | Dakota    | Importing tabular files into Matlab no longer works straightforwardly due to the presence of interface ID.  |
| N/A    | Dakota    | Separate work directories are not created for concurrent iterators.   |
| N/A    | Dakota    | D-optimal sampling designs do not work reliably.  |
| N/A    | Dakota    | Coliny COBYLA methods might not return optimal solution.  |
| N/A    | Dakota    | The sequential hybrid method might only propagate solutions with explicit model specification.<br>*WORKAROUND: Use model_pointer.   |
| N/A    | Dakota    | Initial points are ignored by surrogates built from imported data.  |
| N/A    | Dakota    | Efficient global method might not produce tabular output.   |
| N/A    | Dakota    | PCE methods do not produce statistics when used with design variables; use uncertain instead.   |
| N/A    | Dakota    | User interrupt might not reliably terminate Dakota when running moga/soga methods.  |
| N/A    | Dakota    | Discrete to continuous variable mapping does not work in nested studies.  |
| N/A    | Dakota    | Global Reliability's input spec has invalid keywords.   |



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