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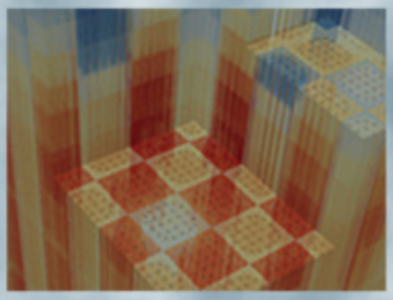

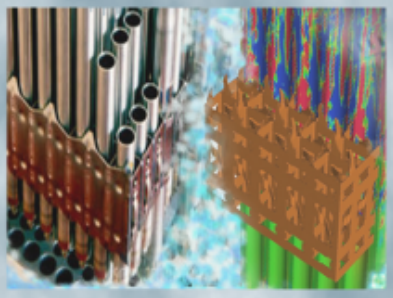

VeraShift Usability Updates for Production Releases of VERA for Ex-core Calculations

Tara Pandya, ORNL
Katherine Royston, ORNL
Tom Evans, ORNL

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EXECUTIVE SUMMARY

The recently developed capability to perform ex-core calculations in the Virtual Environment for Reactor Applications (VERA) with Shift is now available in production releases of VERA. To support these production releases, updates to the VeraShift interface are needed continually. The updates completed under this milestone are documented in this report, including improvements to memory usage and code robustness, as well as the resolution of issues with unexpected behavior that arose during testing.

CONTENTS

TABLES

ACRONYMS

CADIS	Consistent Adjoint-Driven Importance Sampling
CASL	Consortium for Advanced Simulation of Light Water Reactors
CE	continuous energy
HDF5	Hierarchical Data Format 5
ORNL	Oak Ridge National Laboratory
VERA	Virtual Environment for Reactor Applications

1. INTRODUCTION

With the production release of the Virtual Environment for Reactor Applications (VERA) with Shift, several updates were identified to improve the usability of VERA for ex-core calculations. These improvements were driven by close collaboration between developers and analysts and are particularly vital, as the user base of the VERA ex-core capabilities is expanding going forward. Updates implemented for this milestone include:

- Using the Hierarchical Data Format 5 (HDF5) form of the continuous-energy (CE) cross-section data,
- Enabling pole data for on-the-fly Doppler broadening,
- Updating parameters at each statepoint,
- Enabling use of the latest fuel card formats available in VERA,
- Enabling use of non-uniform core pads from the VERA input file,
- Adding more robust testing of features, and
- Resolving defects/issues.

The remainder of this report is organized as follows. Section 2 discusses the improvements made to the code base in support of memory usage and robustness. Section 3 gives details on the issues encountered and resolved during testing of the ex-core capability. Finally, Section 4 summarizes the updates made to VeraShift and gives current and planned updates for this ongoing process.

2. CODE IMPROVEMENTS

2.1. UPDATED DATA

Two improvements to the CE cross section data were made that will reduce memory usage when running Shift:

1. HDF5 formatted CE cross section data
2. HDF5 formatted pole data [1, 2, 3]

Using the HDF5 version of the CE cross section data will save memory for Shift ex-core calculations with VERA. In the SHIFT block of the VERA input file, users can indicate whether they would like to use the pole CE data for on-the-fly Doppler broadening. The pole data can provide considerable memory savings for Shift calculations, but it may increase run times. This pole data option is still experimental and should be used with caution. Its effect on the eigenvalue and other ex-core quantities of interest for light water reactors has not been fully investigated.

2.2. UPDATED TESTING

While unit tests are always added as new capabilities are added to the code, efforts were made to also improve testing capabilities by identifying any missing test cases and expanding the current comparison against fixed reference output files. Previously, only the Shift HDF5 composition files from the first state point were checked against reference output files. Now, reference files are also used to check the fission source, tally results, adjoint flux, and eigenvalue, as well as compositions at every state point. Table 1 shows the full list of unit testing in VeraShift and indicates what each test covers. Although this internal testing does not directly affect the usability as seen from the user, it does affect the usability of VeraShift by decreasing the chances of issues arising and ensuring code coverage.

A set of Jupyter notebooks has also been added to the VeraShift testing. These notebooks are set up to read in and visualize the appropriate outputs for every VeraShift test so that the outputs can easily be reviewed after code changes are made.

Finally, output of memory diagnostics at specific points throughout the VeraShift calculation was added to enhance usability. This output is dumped to the screen and can be used to diagnose issues encountered by users.

2.3. INPUT PROCESSING

Several input processing updates were made in VeraShift to facilitate usability for ex-core calculations.

1. The automatic generation of a supplemental ex-core input file with a bioshield and ex-core detectors from the VERA common input has been added. This capability will facilitate detailed ex-core modeling by users; full details can be found in materials by Royston et al. and Pandya et al. [4, 5].
2. Shift can now use and run with values input for each state point in the VERA common input. The following parameters from each STATE block can be used: *boron*, *modden*, *tinlet*, *tfuel*, *bank_labels*, and *bank_pos*.

3. Shift can use and read fuel material definitions in the VERA input defined with enrichments, number densities, or weight fractions. Shift follows the same logic used in MPACT for handling weight fractions.

4. VERA now allows users to define non-uniform core pads, and the building of these in the Shift geometry was added.

Table 1. List of updated unit test coverage in VeraShift

Test Name	Description	Category	Verifies
tstDTK_Adapter_Full_Core	mini full core fission source mapping	Nightly	transfer interface
tstDTK_Adapter_Nonunique	assemblies and small core without unique pins fission source mapping	Nightly	transfer interface
tstDTK_Adapter_Nonunique_Homogen	assemblies and small core without unique pins temp. homogenization	Nightly	transfer interface
tstDTK_Adapter_Unique	small core with unique pins mapping, fission source, temperatures, densities, and isotopics	Nightly	transfer interface
tstDTK_Adapter_Unique_Homogen	small core with unique pins and temp. homogenization mapping, fission source, temperatures, densities, and isotopics	Nightly	transfer interface
tstDTK_Adapter_Unique_Inserts	unique pins and inserts fission source mapping	Nightly	transfer interface
2a	AMA_2a in eigenvalue mode	Nightly	k_{eff}, fission source
2a_cadis_excore	AMA_2a using Consistent Adjoint-Driven Importance Sampling (CADIS) with ex-core file	Nightly	runs successfully
2a_cadis_sn	AMA_2a dummy vessel fluence using CADIS	Nightly	comps, adjoint flux, vessel flux
2a_cadis_sn_nonunique	AMA_2a without unique pins dummy vessel fluence using CADIS	Nightly	comps
2a_cadis_sn_no_transport	multistate AMA_2a using CADIS	Nightly	runs successfully
2a_forward	AMA_2a forward dummy vessel fluence	Nightly	comps, fission source
2a_forward_excore	AMA_2a forward problem with ex-core file	Nightly	runs successfully
2a_forward_nonunique	AMA_2a without unique pins forward dummy vessel fluence	Nightly	comps, fission source

Table 1. Updated unit test coverage in VeraShift (continued)

Test Name	Description	Category	Verifies
2a_isotopes	AMA_2a forward with dummy stainless steel including special nuclides	Nightly	fission source
2a_mpact	AMA_2a in eigenvalue mode and MPACT fiss src spectrum	Nightly	k_{eff}, fission source
2a_mpact_cadis_sn	AMA_2a with dummy vessel and MPACT fiss src spectrum using CADIS	Nightly	vessel flux
2a_ss_nonunique	AMA_2a forward without unique pins with secondary source	Nightly	fission source
2e	AMA_2e eigenvalue	Nightly	k_{eff}, fission source
2e_forward	AMA_2e forward dummy vessel fluence	Nightly	comps, fission source
2e_forward_nonunique	AMA_2e without unique pins forward dummy vessel fluence	Nightly	comps, fission source
2o	AMA_2o eigenvalue with full isotopic tracking and coupling	Nightly	k_{eff}, fission source
2o_forward	AMA_2o forward without *excore_transport* parameter	Nightly	should fail
3_mini	mini version of AMA_3a eigenvalue	Nightly	k_{eff}, fission source
3_mini_forward	mini version of AMA_3a forward vessel fluence	Nightly	comps, fission source, vessel flux
3_mini_forward_nonunique	mini version of AMA_3a without unique pins forward vessel fluence	Nightly	comps, fission source
3a	AMA_3a eigenvalue	Nightly	k_{eff}, fission source
3a_forward	AMA_3a forward vessel fluence	Nightly	fission source
4_mini_forward	mini version of AMA_4 forward vessel fluence	Nightly	fission source
4_mini_forward_nonunique	mini version of AMA_4 without unique pins forward vessel fluence	Nightly	fission source

Table 1. Updated unit test coverage in VeraShift (continued)

Test Name	Description	Category	Verifies
5_mini_forward	mini version of AMA_5 forward vessel fluence	Heavy	fission source, vessel flux
5_mini_forward_nonunique	mini version of AMA_5 without unique pins forward vessel fluence	Heavy	fission source, vessel flux
5_mini_mpact_forward	mini version of AMA_5 forward vessel fluence using MPACT source spectrum	Heavy	fission source, vessel flux
5_mini_ss_excore_cadis	mini version of AMA_5 with secondary source using CADIS and ex-core file	Heavy	fission source, ex-core tallies
7_mini_forward	mini version of AMA_p7 forward without enough processors	Nightly	should fail
single_pin_nonunique	pincell with feedback in forward mode	Nightly	runs successfully
multistate_noTH	multistate pincell eigenvalue without feedback	Nightly	k_{eff}, fission source
multistate_mpact_noTH	multistate pincell eigenvalue without feedback using MPACT source spectrum	Nightly	k_{eff}, fission source
multistate_internalCTF	multistate pincell eigenvalue with feedback	Nightly	k_{eff}, fission source
multistate_ctf_fulliso	multistate pincell with feedback forward with full isotopic coupling	Heavy	fission source
small_core_cadis_sn	small core CADIS vessel fluence	Heavy	vessel flux
small_core_excore	small core forward with ex-core file	Nightly	fission source, ex-core tally
small_core_excore_cadis	small core with ex-core file using CADIS	Nightly	fission source, ex-core tally
small_core_excore_cadis_pv	small core with ex-core file pulling in outer vessel using CADIS	Nightly	fission source, ex-core tally

Table 1. Updated unit test coverage in VeraShift (continued)

Test Name	Description	Category	Verifies
small_core_excore_cadis_notrans	multistate small core with ex-core file using CADIS without Shift transport	Nightly	runs successfully
small_core_mpact_excore_pv	small core forward with ex-core file pulling in outer vessel using MPACT src spectrum	Nightly	fission source, ex-core tally
small_core_nuclide_watt_excore_pv	small core forward with ex-core file pulling in outer vessel forward using nuclide watt src spectrum	Nightly	fission source, ex-core tally

3. RESOLUTION OF ISSUES

As the new ex-core features in VERA became more widely used, issues were identified and improvements were made to ensure expected behavior. This section briefly summarizes issues that were identified and resolved as part of this milestone.

1. While running a new test model, a material mapping error was discovered for the case of a vessel defined in the VERA common input with the same material used for multiple shells (i.e., the barrel, the vessel liner, and the vessel). This error was traced back to indexing of material assignments, and once it was resolved in the code, a test was modified to replicate this case.

2. While MPACT solves quarter core symmetric problems on the southeast quadrant of the model, Shift solves the quarter core symmetric problem on the northeast quadrant. The underlying geometric model is the same in MPACT and Shift (just reflected over the x-axis). Along the same lines, rotations in MPACT are clockwise, while rotations in native Shift are counter-clockwise. This discrepancy led to an error when building the pad geometry in which the given angle in the VERA common input was interpreted as a counter-clockwise rotation in Shift; this has now been resolved. This issue was not discovered sooner because all previous models run with VeraShift used symmetric core pad locations of 45°. Tests in Shift and VeraShift have now been updated to include asymmetric pads in the geometry.

3. During testing, it was realized that Shift was not properly updating the boron concentration when a boron search was used (i.e., the boron concentration passed from MPACT was not used). Resolving this issue also provided the opportunity to enable Shift to update a number of state parameters at each statepoint, as described in Section 2.3.

4. SUMMARY

Several updates to VeraShift were made to support production releases of VERA. These updates include:

- Using the HDF5 form of the CE cross section data,
- Enabling pole data for on-the-fly Doppler broadening,
- Updating material properties and control rod positions at each statepoint,
- Enabling use of the latest fuel card formats available in VERA,
- Enabling use of non-uniform core pads from the VERA input file,
- Adding more robust testing of features, and
- Resolving defects/issues.

Work is ongoing to support the next release of VERA. Updates related to ex-core calculations in VERA are currently underway, and the planned updates are as follows:

- Resolve a current case in which Shift "hangs" at various points in the calculation (Trac #6506).
- Resolve a current case using Progression Problem 9 with a supplemental ex-core geometry file, including a *restart_write* that dies with a segmentation fault (Trac #6057).
- Ensure that the moderator density is defined in the VERA common input, as it is needed by Shift: kill the run if it does not exist for the first state (Trac #6063).
- Update the moderator material properties in the downcomer and above the active fuel in Shift based on data from CTF (Trac #5444).
- Enable the ability to run fully coupled (isotopics, temperatures, densities) ex-core calculations by using domain decomposition and threading (delayed milestone L2:RTM.MCH.P19.01).
- Fix the memory issues associated with full core subcritical multiplication ex-core calculations (delayed milestone L3:RTM.MCH.P19.01).
- Enable VeraShift to receive decay and external sources, in addition to the fission source.
- Address defects and issues as they arise.

5. ACKNOWLEDGMENT

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