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VeraShift I/O Optimization for Ex-Core Calculations with VERA

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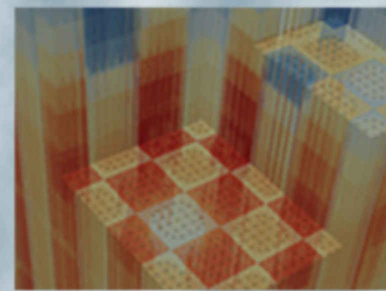

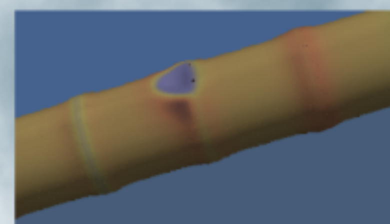

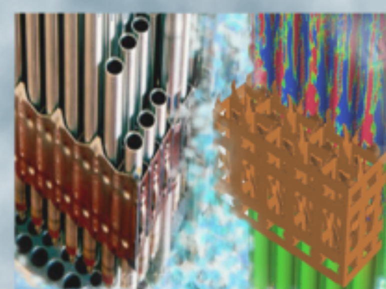

REVISION LOG

Revision	Date	Affected Pages	Revision Description
0	01-15-2020	All	Initial Public Release - Unlimited

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EXECUTIVE SUMMARY

The initial release of Shift in the Virtual Environment for Reactor Applications (VERA) provided users with the ability to perform ex-core calculations. After this release, a task was undertaken to optimize input parameters and output of desired quantities for ex-core calculations. As requested by analysts, this report presents the detailed input and output changes made to VERA to enhance usability. Specifically, some of the major optimizations added were detector and bioshield setup using the VERA common input, updated Shift input defaults, consolidated output, and output of pin importances. Close interaction between developers, analysts, and users enabled these useful optimization updates, which will be included in the release of VERA 4.1, and some are included in VERA 4.0.1. Under these auspices, this work will continue under the VERA Users Group (VUG).

CONTENTS

FIGURES

TABLES

LISTINGS

ACRONYMS

AMA	Advanced Modeling Applications
CASL	Consortium for Advanced Simulation of Light Water Reactors
HDF5	Hierarchical Data Format 5
I/O	input and output
ORNL	Oak Ridge National Laboratory
VERA	Virtual Environment for Reactor Applications
VUG	VERA Users Group
WBN1	Watts Bar Nuclear Plant Unit I

1. INTRODUCTION

The initial implementation of the input/output (I/O) for ex-core calculations with the Virtual Environment for Reactor Applications (VERA) has evolved over the past several years, as it has become more widely used by analysts and industry. The main drivers behind these optimizations are to enhance usability, to incorporate user requests, and to support new ex-core capabilities in future releases of VERA.

Based upon collaboration with VERA developers and users, the following I/O optimizations for ex-core calculations using Shift were implemented as part of this milestone.

- Updated Shift input parameter defaults to be appropriate for ex-core calculations,
- Automated detectors and bioshield setup from the VERA common input,
- Removed/added input parameters,
- Consolidated output of the most relevant ex-core output parameters to the VERA HDF5 output file,
- Updated visualization of output in VERAView, and
- Added output of pin importances to the Shift HDF5 output file.

This report is organized as follows. Section 2 gives the details of the changes made to the various input options for ex-core calculations with VERA. Section 3 provides details on the changes made to the various output files and datasets within these files. Finally, Section 4 summarizes this I/O optimization and presents the current and suggested planned development.

2. INPUT CHANGES

This section provides details on the optimization of the input parameters for ex-core calculations with VERA. As outlined in Section 1, these updates include the following:

- Updated Shift input parameter defaults as appropriate for ex-core calculations,
- Automated detectors and bioshield setup from the VERA common input, and
- Removed/added input parameters.

2.1. DEFAULTS

The default parameters in the SHIFT block of VERA's common input were updated specifically for ex-core calculations. These defaults were determined based upon feedback from Advanced Modeling Applications (AMA) testing. Listing 1 shows these updated default parameters, which are set in the SHIFT.ini file in VERAIn. This listing and a description of each of parameter will be given in the updated VERA ex-core manual [1], so detailed descriptions for all parameters are not given here. Most of the defaults should be left as they are by most users; however, some of them should be updated for the specific ex-core problem being run, as outlined in Table 1. One thing to note from this table is that the number of processors used for the Consistent Adjoint-Driven Importance Sampling (CADIS) calculation is the number of processors used by Shift (**num_blocks_i×num_blocks_j**).

Listing 1. Default SHIFT block parameters.

```
[SHIFT]
  problem_mode                  cadis
  mode                          n
  verbosity                     low
  do_transport                  true
  transfer                      fiss_src
  output_geometry               true
  output_fission_source         true
  output_external_source        false
  transport                     ce
  thermal_energy_cutoff         10.0
  Np                            1e6
  src_disc_l2_error             1e-3
  src_disc_samples_per_batch    1e7
  src_disc_max_samples          1e9
  fiss_src_spectrum             nuclide_watt
  use_fission_source            true
  use_external_source           false
  use_pole_data                 false
  create_unique_pins            false
  global_log                    info
  eq_set                        sc
```

```
    Pn_order                    0
    mesh                        1
    adjoint                     true
    output_adjoint              false
    num_blocks_i                10
    num_blocks_j                10
    xs_library                  v7-56
    num_groups                  8
    new_grp_bounds              6.0653E+06  3.6788E+06  2.3457E+06
                                1.6530E+06  8.2085E+05  2.4176E+04
                                1.0130E+02  1.0000E-05
    cell_homogenize             true
    max_delta_z                 5.0
    upscatter_verbosity         high
    upscatter_subspace_size     20
    refl_mesh_size              5.0
    extend_axial_mesh_size      5.0
    store_fulcrum_string        false
```

Table 1. Important SHIFT input block defaults that should be updated by the user.

Input Parameter	Description	Typical Options
Np	number of particle histories to simulate	1E+08 (very problem dependent)
problem_mode	ex-core calculation mode to run Shift	*forward* or *cadis*
num_blocks_i	number of processors to decompose the X domain for the adjoint calculation	10 or 20 (only for *cadis*)
num_blocks_j	number of processors to decompose the Y domain for the adjoint calculation	10 or 20 (only for *cadis*)

There are other parameters outside of these defaults that should be set depending on the type of ex-core calculation being performed. These details are outside the scope of this milestone and are covered in the VERA ex-core manual [1].

2.2. AUTOMATED DETECTORS AND BIOSHIELD

One of the significant undertakings regarding Shift I/O for VERA was including the ability to define specific detectors and a bioshield in the VERA common input and to automatically generate the supplemental ex-core model input file. The user can specify a *bioshield* parameter with materials in concentric cylinders beyond the vessel, and different detector types can be defined and placed in locations outside the vessel by using the *det* and *det_locations* parameters in the CORE block. Table 2 gives the detailed descriptions and allowable input options for the detectors and bioshield. If the user would like to include additional ex-core details, the automatically generated supplemental ex-core file can be modified directly. A current limitation of this capability is that the materials used in the generated supplemental ex-core file are taken from a template file and may not be consistent with the corresponding materials in the VERA common input. This discrepancy will be resolved as part of the planned future development of this feature. Full details on this capability are given in the VERA ex-core manual [1].

An example of these parameters for a modified Watts Bar Unit 1 (WBN1) model based on Progression Problem 9 [2] is given in Listing 2. This example defines two ex-core detector types: a power range detector identified as *PWR* and a source range detector identified as *SRC*. Both of these detector types use a wedge-shaped well in the bioshield in this example. Overall, four power range detectors and two source range detectors are placed in specific locations using the *det_locations* parameter. The raytrace generated when running VERA with this input is shown in Fig. 1.

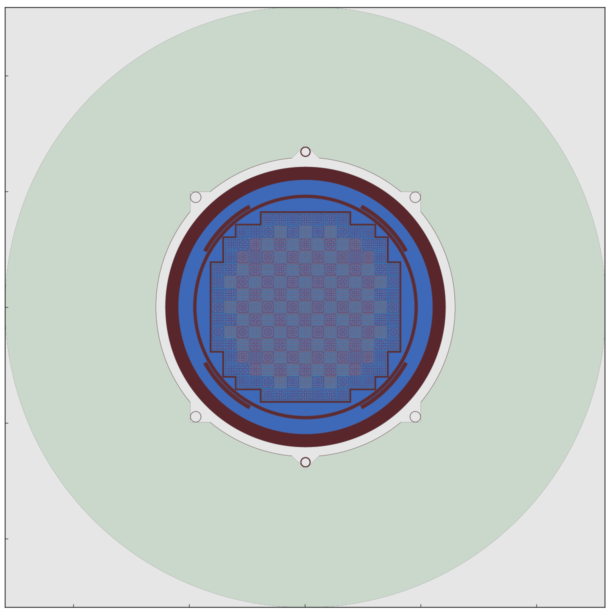


Figure 1. Raytrace through an automatically generated ex-core geometry for Watts Bar Unit 1.

Table 2. Ex-core Shift-related parameters in the CORE block of the VERA common input.

Parameter	Description	Default	Type	Options
bioshield	bioshield materials and radii	none	strings and doubles	materials: *al*, *concrete*, *cs*, *mod*, *ss*, *void*
det	detector ID, type, radii, materials, heights, response type, well type	none	strings and doubles	type: *power*, *source* response type: *u*235, *b*10 well type: *none*, *wedge*
det_locations	detector ID, radius, degree, elevation	none	string and double	—

Listing 2. WBN1 input example with automated excore detectors.

```
[CORE]
  vessel  mod 187.96        ! barrel IR (cm)
           ss 193.68        ! barrel OR (cm)
          mod 219.15        ! vessel liner IR (cm)
           ss 219.71        ! vessel liner OR / vessel IR (cm)
           cs 241.70        ! vessel OR (cm)

! neutron pad ID,OD arc length (degrees), and angular positions (degrees)
  pad ss  194.64 201.63 32 45 135 225 315

! User defines the outer radii beyond RPV (cm)
  bioshield  void      257.70
             ss        258.20
             concrete  518.16

!      ID   type       radii      / mats    / heights / response_type well_type
! -----------------------------------------------------------------------------
  det  PWR  power   8.75   9.5  / void cs / 152.4 152.4 / u235  wedge
  det  SRC  source  7.0612 8.89 / void cs / 148.0312    / b10   wedge

!                ID,  radius, degree, elevation
! ----------------------------------------------
  det_locations  PWR   267.7  315   42.431
                 PWR   267.7  225   42.431
                 PWR   267.7  135   42.431
                 PWR   267.7   45   42.431
                 SRC   267.7   90  120.8154
                 SRC   267.7  270  120.8154
```

2.3. GENERAL CLEANUP

Finally, a general cleanup was performed of the current input options and the newly added options to govern VERA ex-core calculations with Shift. The following obsolete SHIFT block input parameters were removed:

1. *dimension*,
2. *SPN_matrix_type*,
3. *SPN_order*, and
4. eq_set: *spn_fv*.

The following SHIFT block input parameters were added:

1. *num_threads* (integer),
2. *use_pole_data* (boolean),

3. *fiss_src_spectrum* (‘mpact‘, ‘nuclide_watt‘, ‘u235_watt‘),
4. *seed* (integer), and
5. *rtk_output_format* (‘hdf5‘, ‘xml‘).

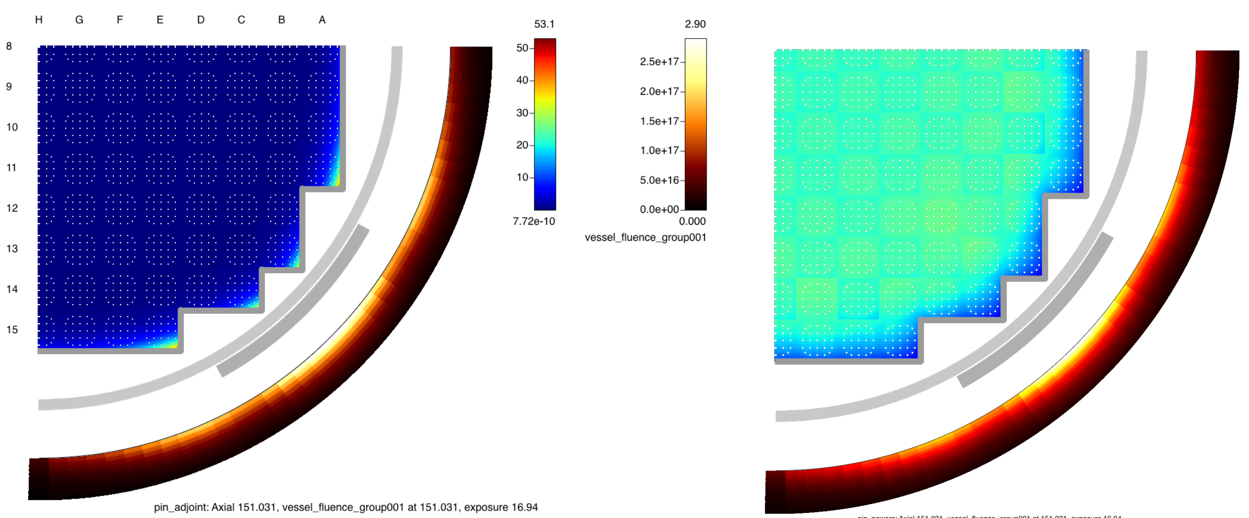
Full details on the definitions and allowable options for these new parameters can be found in the new VERA ex-core manual [1].

3. OUTPUT CHANGES

To facilitate post processing, Shift now returns important ex-core outputs to VERA for inclusion in the VERA HDF5 output file. In previous VERA releases, these outputs were available only in the separate Shift HDF5 output file. For vessel fluence calculations with no external ex-core geometry file, Shift will automatically send the vessel flux tally result back to VERA at every statepoint to accumulate the vessel fluence. VERA writes both the vessel flux and fluence at each statepoint to the HDF5 output file and requested restart files, along with the corresponding statistical uncertainties. For calculations with an external ex-core geometry file, all cell tallies are passed to VERA to be included in the VERA output after being calculated by Shift at each statepoint.

Several changes were also made to the separate Shift HDF5 output file. The outputs sent to VERA for writing are still located in the separate Shift HDF5 output file, but all tally results have been moved to a *tally* group for each statepoint to consolidate the various tallies and to simplify post-processing. The adjoint function calculated for variance reduction was already provided in the Shift output, but now the normalized pin importances obtained from the adjoint function are also written. These are located in the first statepoint group only, because Shift only calculates the adjoint at the first statepoint of each fuel cycle.

Improvements were also made to enable viewing new output data in VERAView. Previously, VERAView calculated and plotted the vessel fluence by reading in the tallied vessel flux from each statepoint in the separate Shift HDF5 output. Now VERAView can display the fluence and vessel flux directly from the VERA output file. While the pin importances are only written to the Shift output at this time, VERAView can also display them through the use of an external script. For example, Fig. 2 shows the pin importances, vessel fluence, and pin powers from a WBN1 calculation visualized using VERAView.



(a) Pin importances in-core and vessel fluence ex-core

(b) Normalized pin power in-core and vessel fluence ex-core

Figure 2. Example of visualizing the results of a VERA ex-core simulation of WBN1 with VERAView.

4. SUMMARY

Under this milestone, the VERA I/O for ex-core calculations was optimized from its initial implementation. The main updates included the following:

- Updated Shift input parameter defaults to be appropriate for ex-core calculations,
- Automated detectors and bioshield setup from the VERA common input,
- Removed/added input parameters,
- Consolidated output of the most relevant ex-core output parameters to the VERA HDF5 output file,
- Updated visualization of output in VERAView, and
- Output pin importances to the Shift HDF5 output file.

As mentioned previously, the optimization of the ex-core I/O for VERA calculations is a planned, ongoing process for future production releases. Starting in fiscal year 2020 and hopefully beyond, this work will be supported by the VERA Users Group (VUG) to accommodate specific user requests. The following activities are underway or are currently planned:

1. Updating vessel fluence error output to relative fractional uncertainty, and including tally discretization attributes in VERA HDF5 file.
2. Updating the pin importances output to be more physically meaningful.
3. Moving Shift HDF5 output quantities to VERA HDF5 file (fission source).
4. Cleaning and consolidating input parameters for upcoming code releases.
5. Allowing for materials defined in the VERA common input to be used in the automated detector and bioshield definitions.
6. Allowing for materials defined in the VERA common input to be used in the supplemental ex-core model input.
7. Adding new detector types and geometric features in the VERA common input to be used in the automated detector definitions.

5. ACKNOWLEDGMENT

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- Ron Lee
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- Herschel Smith
- Shane Stimpson

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[1] Tara Pandya, Thomas Evans, Katherine Royston, Kevin Clarno, Ben Collins, Shane Stimpson, and Shane Henderson. Ex-Core Radiation Transport Modeling with VERA User Manual. Technical Report CASL-U-2019-1556-002, CASL, Forthcoming 2019.

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