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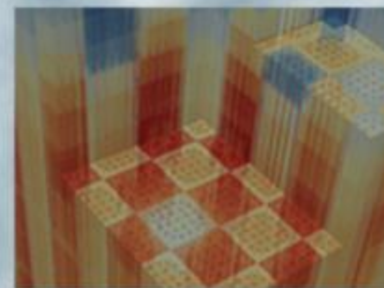
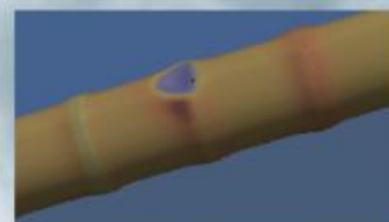


VERAShift Theory Manual



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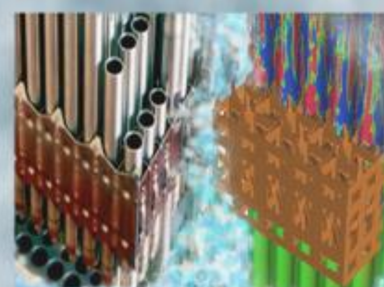

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VERAShift Theory Manual

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Executive Summary

This document describes the basic theory behind the VERAShift software package. Since VERAShift is an application programming interface (API) to Shift for running Monte Carlo (MC) eigenvalue calculations and coupled ex-core calculations, this document presents the theory behind the coupling used in this API and a very high overview of the MC solution methods that are called from VERAShift. The full details on these MC methods is outside the scope of this document as they apply only to Shift and not the VERAShift API.

As mentioned in the VERAShift User Manual (CASL-U-2019-1921-000), VERAShift couples MPACT (which includes COBRA-TF (CTF)) to Shift. This coupling is performed internally and relies on Data Transfer Kit (DTK) to perform the transfer of different quantities. This document gives the details on the theory of the basic solve process in VERAShift and the communication performed between MPACT and Shift.

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Acronyms

API application programming interface

CTF COBRA-TF

DTK Data Transfer Kit

MC Monte Carlo

MPI message passing interface

MSOD multiple-set overlapping domains

VERA Virtual Environment for Reactor Applications

1. Introduction

The motivation for developing VERAShift was to be able to use the converged fission source and other quantities from the core simulator as part of a Shift Monte Carlo (MC) transport solution [1] and to be able to run Shift for validation purposes through Virtual Environment for Reactor Applications (VERA). Since Shift is developed outside of VERA for many different purposes, an application programming interface (API) was developed to be able to run Shift calculations by utilizing the VERA frontend and executables.

VERAShift serves as the driver for running standalone and coupled Shift calculations in VERA. As such, there are no solvers or any theory driving the solution processes used in this API. There are, however, defaults and solve procedures based on practical experience about how to perform and handle the main solution driver, internal code coupling, and communication patterns that comprise VERAShift. These are not based on theory in the traditional sense, but these topics are outlined in the following sections based on practical application.

All of the communication in VERAShift uses message passing interface (MPI) and the transfers are setup and performed using Data Transfer Kit (DTK) [2]. Section 2 discusses how VERAShift uses DTK to do the transfers between the processors running MPACT and those running Shift. This section also discusses the quantities used from the core simulator in the Shift MC solve.

The theory behind the methods used in MPACT and COBRA-TF (CTF) can be found in their respective theory manuals [3] [4]. Some of the theory behind the MC and hybrid deterministic-MC methods in Shift can be found in the Shift user manual [5] as well as the VERAShift user manual [6]. There is no formal Shift theory manual but the Shift MC and hybrid methods are based upon basic MC radiation transport theory and hybrid method theory [7] [8].

1.0.1 Theory or no theory?

As mentioned in the introduction above, there is no traditional theory in VERAShift since it is an API. This code package does not solve any mathematical or numerical models, those solves are done in MPACT, CTF, and Shift. Since VERAShift does not solve any mathematical models, there are no physical approximations or governing equations in it. As such, there are also no direct discretization techniques in VERAShift; discretization of the solution is done in MPACT and Shift. The next section presents the basic solve methodology that VERAShift follows for calling the solvers in MPACT and Shift. Section 2 gives detail about the coupling procedure between these two codes that occurs in VERAShift.

1.0.2 Solve procedure methodology

VERAShift serves as the driver code for running the *vera_shift* and *vera_to_shift* executables. The code implementation details based on the general procedure outlined in this section are given in the VERAShift Programmer Manual [9]. The procedure detailed in this section applies to the *vera_to_shift* sequence.

VERAShift was designed to be able to run MPACT and Shift simultaneously by solving lagged state points and using different sets of processors for each code. For single state point calculations, Shift must wait on MPACT to complete and transfer the needed coupled information before starting the state point solve. For subsequent state points after the first (when considering multistate calculations) the MPACT solve continues to the next state point calculation while the Shift processors calculate a solution for the previous state point.

2. Coupling

VERAShift controls the in-memory code coupling of data between MPACT (including CTF) and Shift. The following quantities are coupled for each state point:

- pin-averaged fission source,
- pin-averaged depleted isotopic compositions,
- pincell region temperatures,
- pincell moderator densities, and
- boron concentration.

The purpose of using these calculated quantities in the Shift MC calculation is to investigate the effects of each on the calculation of ex-core quantities and to produce higher-fidelity MC results. Also, the fission source serves as the forward source for any forward or hybrid calculations. As mentioned previously, DTK handles the setup, communication, and transfer of these coupled quantities.

2.0.1 Communication

All of the communication in VERAShift uses MPI. There are several different communicators needed and used in VERAShift. First, MPACT and Shift run on their own sets of processors so each of these codes have a respective communicator. Second, a transfer communicator is used to facilitate the coupling done through DTK which includes all of the MPACT processors and all of the Shift processors on the first set (see details about multiple-set overlapping domains (MSOD) [10]). Finally, there is a communicator to handle sending output quantities from Shift to MPACT consisting of the master Shift processor and the master MPACT processor.

Bibliography

[1] T. M. Pandya, S. R. Johnson, T. M. Evans, G. G. Davidson, S. P. Hamilton, A. T. Godfrey, Implementation, Capabilities, and Benchmarking of Shift, a Massively Parallel Monte Carlo Radiation Transport Code, J. Comp. Phys. 308 (2016) 239–272.

[2] S. R. Slattery, P. P. H. Wilson, R. P. Pawlowski, The Data Transfer Kit: A Geometric Rendezvous-Based Tool for Multiphysics Data Transfer, in: M&C 2013, American Nuclear Society, 2013.

[3] E. Larsen, B. Collins, B. Kochunas, S. Stimpson, MPACT Theory Manual, Tech. Rep. CASL-U-2019-1874-001, CASL (July 2019).

[4] R. Salko, M. Avramova, A. Wysocki, A. Toptan, J. Hu, N. Porter, T. Blyth, C. Dances, A. Gomez, C. Jernigan, J. Kelly, A. Abarca, CTF Theory Manual, Tech. Rep. CASL-U-2019-1886-001, CASL (November 2019).

[5] S. Johnson, T. Evans, G. Davidson, S. Hamilton, T. Pandya, K. Royston, E. Biondo, Omnibus User Manual, Tech. Rep. ORNL/TM-2018/1073, ORNL (TBD 2020).

[6] T. Pandya, T. Evans, K. Royston, K. Clarno, B. Collins, S. Stimpson, S. Henderson, VERAShift User's Manual, Tech. Rep. CASL-U-2019-1921-000, CASL (January 2020).

[7] J. C. Wagner, A. Haghighat, Automated variance reduction of Monte Carlo shielding calculations using the discrete ordinates adjoint function, Nuclear Science and Engineering 128 (2) (1998) 186–208.

[8] J. Wagner, D. Peplow, S. Mosher, FW-CADIS Method For Global And Regional Variance Reduction Of Monte Carlo Radiation Transport Calculations, Nuclear Science and Engineering 176 (1). doi:10.13182/NSE12-33.
URL http://www.ans.org/pubs/journals/nse/a_35437

[9] T. Pandya, K. Royston, VERAShift Programmer Manual, Tech. Rep. CASL-U-2019-1923-000, CASL (April 2020).

[10] J. C. Wagner, S. W. Mosher, T. M. Evans, D. E. Peplow, J. A. Turner, Hybrid and Parallel Domain-Decomposition Methods Development to Enable Monte Carlo for Reactor Analyses, Prog. Nucl. Sci. Technol. 2 (1) (2011) 815–820.