

VERA Release Notes

Release ID	2013 VERA RSICC Release (VERA 3.2)
Release Date	Sept. 30, 2013
Support Information	Email questions or comments to the VERA development team at casl-support@CASL.gov

1. Introduction

VERA, a “Virtual Environment for Reactor Applications”, is a collection of software being developed under DOE sponsorship by CASL, the Consortium for Advanced Simulation of Light Water Reactors (see <http://www.casl.gov>). The goal of VERA development is to *“predict, with confidence, the performance of nuclear reactors through comprehensive, science-based modeling and simulation technology that is deployed and applied broadly throughout the nuclear energy industry to enhance safety, reliability, and economics.”*

This document contains release notes for the “2013 VERA RSICC Release” version of VERA. This is an early-access release for evaluation and usage by select partners. Feedback is important to and welcomed by the developers, but support for requested changes or fixes cannot be promised.

2. Release Features

VERA consists of two broad categories of software,

- Physics Components: These include standalone, integrated and coupled-code multiphysics applications for modeling problems in nuclear reactor performance.
- Infrastructure Components and TPLs: The computational infrastructure (e.g. code-coupling and VUQ related software, etc.) and software development environment.

Specific components included in this release are listed in the following two tables.

Table 1 Physics Components

Name	Type of Physics	Comments
COBRA-TF	Subchannel-resolved thermal hydraulics coupled to fuel rod heat transfer.	Can be used standalone using VERA Common Input.
Exnihilo	Parallel deterministic and Monte Carlo transport. Includes Denovo and Insilico subpackages. Requires Scale/XSProc for Nuclear data and cross section processing	Both Sn and Spn methods supported. Uses Scale/XSProc. Can be used standalone using VERA Common Input.
Insilico+COBRA-TF	Coupled-code multiphysics application. Neutronics coupled to Thermal Hydraulics	Limited to single assembly. Located in “PSSDrivers” repository. Uses VERA Common Input.
MPACT	Neutron transport and cross section physics.	2D assembly-level lattice physics. No 3D in this standalone version

Table 2 Infrastructure Components and TPLs

Name	Brief Description	Comments
Dakota	Software library for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis	VERA 3.2 includes COBRA-TF examples (VUQDemos)
DataTransferKit	Data transfer utilities for parallel coupled-code applications	
LIME	Lightweight Integrating Multiphysics Environment for coupling codes.	
TriBITS	Enhanced CMake-based build system	In VERA 3.2 TriBITS is delivered as part of Trilinos
Trilinos	Software library for the solution of large-scale, complex multi-physics eng. and scientific problems.	Only a subset of the Trilinos packages are used in VERA 3.2
VERAIn	Common VERA input tools	
Other required TPLs	LAPACK, Boost, Zlib, MOAB, HDF5, PETSC, SILO, QT	To be installed from external sources

3. Installation Notes

3.1 Minimum System Requirements

Hardware and OS:

32 core (or greater) cluster running under Linux OS

System Software:

GNU compilers (for C, C++, and Fortran), Version 4.6.1 or greater

MPI wrapper (e.g. OpenMPI, MPICH, MVPICH, ...)

Git

SVN

X11

CMake

3.2 Installation

A current installation guide is included in the main VERA directory tree, i.e.

VERA/doc/VERAInstallationGuide.pdf

This document describes the structure and setup of the standard VERA development environment and standard TPLs that need to be in place before installing the VERA simulation components. It describes everything from the initial setup on a new machine to the final builds and testing of VERA components.

A smaller less comprehensive “quick reference” guide on how to configure, build, test, and install VERA using the TriBITS CMake build system is also included at

VERA/VERABuildQuickRef.pdf

3.3 Compatibility-Breaking changes:

NA

4. Recent Changes and Bug fixes

NOTE: The unique git repository identifiers for each of the VERA components included in this release are found in the following file:

/VERA/VERARepoVersion.txt

COBRA-TF

Version: No formal versioning system is currently used for COBRA-TF. However, the unique git repository identifier effectively serves this purpose.

All COBRA-TF bug fixes and changes are documented in the git repository commit logs. These can be viewed by typing “git log” in the VERA/COBRA-TF directory.

Significant enhancements to COBRA-TF since being adopted into the VERA code suite include:

- * Creation of a preprocessor tool for simplified creation of COBRA-TF PWR models
- * Implementation of fluid mesh visualization capabilities through introduction of VTK output option
- * Serial optimization performed for significantly reduced memory requirements and problem runtimes
- * Parallelization of the code using MPI and PETSc for significantly reduced runtimes for large-scale, high-resolution models
- * Implementation of the Thom nucleate boiling model as an alternate option to the default Chen model, which has been shown to over-predict rod surface temperatures during sub-cooled nucleate boiling

Exnihilo (contains Insilico and Denovo)

Version: 4.0.0

All Exnihilo bug fixes and changes are documented in the git repository commit logs. These can be viewed by typing “git log” in the VERA/Exnihilo directory.

In VERA 3.2, Exnihilo links to a subset of Scale libraries that provide for nuclear data and cross section processing. All Scale bug fixes and changes are documented in the native mercurial repository and a snapshot is in the git repository commit logs. These can be viewed by typing “git log” in the VERA/Scale directory.

Insilico+COBRA-TF (located in VERA/PSSDrivers)

Version: No formal versioning system is currently used. However, the unique git repository identifier effectively serves this purpose.

All bug fixes and changes to the PSSDrivers repository are documented in the git repository commit logs. These can be viewed by typing “git log” in the VERA/PSSDrivers directory.

MPACT

Version: 1.0.0

All MPACT bug fixes and changes are documented in the git repository commit logs. These can be viewed by typing “git log” in the VERA/MPACT directory.

This is a first release. Subsequent releases will note revisions from this reference.

Dakota

Version: 5.3.1+ dated August 8, 2013
Subversion revision of Dakota core: 1674

Dakota specific release notes are available at:

<http://dakota.sandia.gov/distributions/dakota/5.3/release-notes.html>

<http://dakota.sandia.gov/distributions/dakota/5.3.1/release-notes.html>

DataTransferKit

Version: 0.5.0

All DTK bug fixes and changes are documented in the git repository commit logs. These can be viewed by typing “git log” in the VERA/DataTransferKit directory.

LIME

Version: 1.0.31

All LIME bug fixes and changes are documented in the git repository commit logs. These can be viewed by typing “git log” in the VERA/LIMEExt directory.

Notable enhancements since the release of version 1.0.0 (April 12, 2012) concern

- * interfacing DTK (Data Transfer Kit) with LIME
- * minor changes to enable “stacked case” CTF-Mamba coupling

TriBITS

Version: No formal versioning system is currently used for TriBITS. However, the unique git repository identifier effectively serves this purpose.

All TriBITS bug fixes and changes are documented in the git repository commit logs. These can be viewed by typing the following command in the VERA/Trilinos directory.

```
git log --name-status -- cmake/tribits
```

Trilinos

Version: 11.5 (development)

All Trilinos bug fixes and changes are documented in the git repository commit logs. These can be viewed by typing “git log” in the VERA/Trilinos directory.

The most recent Trilinos-specific release notes are available at:
http://trilinos.sandia.gov/release_notes-11.4.html

VERAIn

Version: No formal versioning system is currently used. However, the unique git repository identifier effectively serves this purpose.

All VERAIn bug fixes and changes are documented in the git repository commit logs. These can be viewed by typing “git log” in the VERA/VERAInExt directory.

5. Known Issues and Workarounds

MPACT:

This version is limited to 2D lattice physics.

Exnihilo/Insilico:

This version has modeled VRI benchmark Problem 5 – zero-power, full-core neutronics testing.

Insilico + COBRA-TF:

This version is limited to single assembly physical domains.

6. Documentation

Cobra-TF

Theory	VERA/COBRA-TF/doc/CTF_Theory_Manual.pdf
User	VERA/COBRA-TF/doc/CTF_Users_Manual.doc
Other	VERA/COBRA-TF/doc/CTF_Preprocessor_Users_Manual.pdf VERA/COBRA-TF/doc/CTF_list_of_variables.pdf

Exnihilo

Theory	not available
User	not available
Other	VERA/Exnihilo/doc/design/Exnihilo_Overview.docx (1-page Exnihilo Overview) VERA/Exnihilo/doc/methods/denovo.pdf (Denovo Methods Manual - incomplete draft) J. Gehin, A. Godfrey, F. Franceschini, T. Evans, B. Collins and S. Hamilton “Operational Reactor Model Demonstration with VERA: Watts Bar Unit 1 Cycle 1 Zero Power Physics Tests,” CASL Report for Milestone L1: CASL.P7.01, CASL-U-2013-0105-000, June 7 2013.

Insilico + COBRA-TF

Theory not available
User not available
Other S. Palmtag, “Coupled Single Assembly Solution with VERA (Problem 6),” CASL Report for Milestone L3:AMA.VDT.P6.03, CASL-U-2013-0150-000, July 25, 2013.

MPACT

Theory In preparation by MPACT developers. A draft version may be available by request.
User VERA/MPACT/doc/MPACT_User_Manual.pdf
Other VERA/MPACT/doc/MPACTBuildQuickRef.pdf

Dakota

Theory <http://dakota.sandia.gov/docs/dakota/stable/Theory-stable.pdf>
User <http://dakota.sandia.gov/docs/dakota/stable/Users-stable.pdf>
Other <http://dakota.sandia.gov/docs/dakota/stable/html-ref/index.html> (Reference Manual)
<http://dakota.sandia.gov/docs/dakota/stable/html-dev/index.html> (Developers Manual)

DataTransferKit

Theory VERA/DataTransferKit/doc/domain_model/domain_model.pdf
User not available
Other <http://cnerg.github.io/DataTransferKit>
S.R. Slattery, P.P.H. Wilson and R.P. Pawlowski, “The Data Transfer Kit: A Geometric Rendezvous-Based Tool for MultiPhysics Data Transfer,” M&C 2013 International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Sun Valley Idaho, May 5-9, 2013

LIME

Theory VERA/LIMEExt/LIME/doc/Manuals/Theory_1.0/LIME_TheoryManual.pdf
User VERA/LIMEExt/LIME/doc/Manuals/Theory_1.0/SAND2011-8524_LIME_UsersGuide.pdf

TriBITS

Theory not available
User VERA/VERABuildQuickRef.pdf

Trilinos

Theory See trilinos.sandia.gov and trilinos.sandia.gov/documentation.html
User See trilinos.sandia.gov and trilinos.sandia.gov/documentation.html

VERAIIn

Theory -
User VERA/VERAIInExt/verain/docs/verain_UM.pdf