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VERA Release Notes ID: 2013 VERA RSICC Release (VERA 3.2)

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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

<table>
<thead>
<tr>
<th>Name</th>
<th>Type of Physics</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>COBRA-TF</td>
<td>Subchannel-resolved Thermal Hydraulics coupled to fuel rod heat transfer</td>
<td>Standalone with VERAIn input</td>
</tr>
<tr>
<td>Scale</td>
<td>Nuclear data and cross section processing (XSProc) to support Insilico</td>
<td>VERA contains a subset of the full Scale suite of software.</td>
</tr>
<tr>
<td>Denovo</td>
<td>Neutron transport; within the Exnihilo repository</td>
<td>Sn and Spn transport</td>
</tr>
<tr>
<td>Insilico</td>
<td>Integration of Denovo and Scale; within the Exnihilo repository</td>
<td>Sn/Spn. Uses Scale/XSProc and VERAIn input</td>
</tr>
<tr>
<td>Insilico+COBRA-TF</td>
<td>Coupled-code multiphysics application. Neutronics coupled to TH.</td>
<td>Limited to single assembly. This capability is part of the “PSSDrivers” repository.</td>
</tr>
<tr>
<td>MPACT</td>
<td>Neutron transport and cross section physics</td>
<td>Lattice physics, no 3D in this standalone version</td>
</tr>
</tbody>
</table>
Table 2 Infrastructure Components and TPLs

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

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

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:

TriBITS
   Version: No formal versioning system is currently used for TriBITS

   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

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

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.

VERAIn
   Version: No formal versioning system is currently used for VERAIn
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.

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/5.3.1/release-notes.html

COBRA-TF

Version:  No formal versioning system is currently used for COBRA-TF

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.

Scale

NOTE: VERA 3.2 only includes a subset of the full Scale suite of software that is a development version of Scale (Version 6.2) and that includes some components not found in Scale 6.1 (including XSProc).

Version: 6.2 (development)

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.
Notable additions to Scale 6.2 not included in Scale 6.1 include:
* XSProc (cross section processing)

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.

PSSDrivers (Contains drivers for coupled Insilico+COBRA-TF)
Version: No formal versioning system is currently used for PSSDrivers

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.

5. Known Issues and Workarounds

MPACT:
This version is limited to 2D lattice physics.

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.

Scale:
see http://scale.ornl.gov/known_issues.shtml