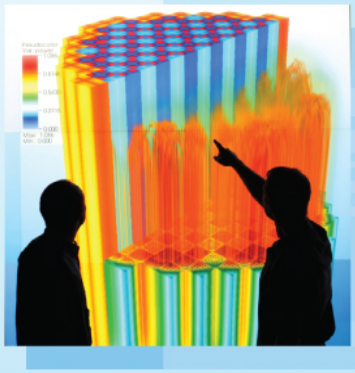
Power uprates
and plant life extension

CASL-U-2014-0054-001

Consortium for Advanced Simulation of LWRs



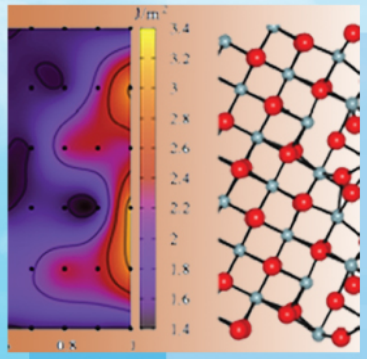
Engineering design
and analysis

VERA Tools and Workflows
Revision 1

Science-enabling
high performance
computing

Prepared by:

Rose Montgomery,
Advanced Modeling Applications



Fundamental science

March 31, 2014

Plant operational data

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Oak Ridge National Laboratory

in partnership with

Electric Power Research Institute
Idaho National Laboratory
Los Alamos National Laboratory
Massachusetts Institute of Technology
North Carolina State University
Sandia National Laboratories
Tennessee Valley Authority
University of Michigan
Westinghouse Electric Company

and individual contributions from

Anatech Corporation
ASCOMP GmbH
CD-adapco, Inc
Core Physics, Inc.
City University of New York
Florida State University
Notre Dame University
Imperial College London
Pacific Northwest National Laboratory
Pennsylvania State University
Rensselaer Polytechnic Institute
Southern States Energy Board
Texas A&M University
University of Florida
University of Tennessee
University of Wisconsin

REVISION LOG

Revision	Date	Affected Pages	Revision Description
0.0	02/28/13	All	Initial draft
1.0	03/20/13	See tracked changes as indicated by lines in the right margin. Note that some minor formatting changes are not tracked.	Revised document as needed to reflect CASL staff and independent reviewer comments and feedback. Added information and reference for Peregrine.
2.0	03/27/14	All	The document is revised to incorporate workflows from the draft Workflow document (CASL-I-2013-0166-000) and refocus the document on the modsim tools. Incorporates information as needed from CPI documents to generally describe the workflows and VERA tools used.

CONTENTS

CONTENTS iii
List of Tables and Figures v
ACRONYMS vi
CHAPTER I Introduction to the Virtual Environment for Reactor Applications 8
I.1 Introduction 8
I.2 CASL's Approach to Developing VERA 9
CHAPTER II The VERA Physics Capabilities 14
II.1 VERA's 3D Radiation Transport codes; Insilico, MPACT and Shift 14
II.1.1.1 VERA's S_N/SP_N Radiation Transport Code 14
II.1.1.2 VERA's MOC Radiation Transport Code 14
II.1.1.3 VERA's Monte Carlo Radiation Transport Code 14
II.1.1.4 VERA Cross-section Processing 14
II.2 VERA's Thermal-Hydraulics Codes, Hydra-TH and COBRA-TF 17
II.2.1 VERA's CFD Code, Hydra-TH 17
II.2.2 VERA's Channel Flow Code, COBRA-TF 19
II.3 VERA's Fuel Performance Code, Peregrine 20
II.4 VERA's Coolant Chemistry Code, Mamba/Mamba-BDM 22
II.5 VERA's Integrated Uncertainty Quantification (IUQ) code, DAKOTA 26
CHAPTER III VERA Supporting Infrastructure 28
III.1 Data Transfer Kit (DTK) 28
III.2 MOAB 30
III.3 LibMesh 30
III.4 STK 31
III.5 MOOSE 31
III.6 Trilinos 32
III.7 PETSc 32
III.8 VERA Common Input (VERAin) for VERA-CS 34
CHAPTER IV VERA Installation and Documentation 35
CHAPTER V Typical Simulations Utilizing the VERA Toolset 36
V.1 Core Cycle Design Simulations 37

V.2 Core Performance Investigative Simulations 39
V.3 Power uprates and Power Escalation-related Applications 40
V.3.1 Power Uprates 40
V.3.2 Power Ramping Study 40
V.3.3 Reactivity-Initiated Accident (RIA) 41
V.4 Fuel System Design 42
V.4.1 Fuel Rod Design 42
V.4.2 Spacer Grid Design 42
V.4.3 Structural Design 43
V.5 System Flow and Coolant Heat Transfer Studies 44
V.5.1 Steady and Unsteady Flow Coolant Flow Path and Velocity Simulations 44
V.5.2 Steady and Unsteady Flow Local Flow Blockage Simulations 44
V.5.3 Departure from Nucleate Boiling (DNB) 44
V.5.4 Loss of Coolant Simulations 45
V.6 Coolant Chemistry Applications 47
V.6.1 CRUD Deposition Calculations 47
V.6.2 CRUD-induced Power Shift Calculations 47
V.6.3 CILC Calculations 48
V.7 Uncertainty and Sensitivity Studies 49
CHAPTER VI References 50

List of Tables and Figures

Table 1 General Needs for Simulation of Commercial PWRs 12

Table 2 Comparison of VERA with Typical Industry Core Simulator Methods [Ref. 3, modified] 13

Table 3 Radiation Transport Computing Requirements for Various Example Calculations..... 15

Table 4 Timescale, Spatial Scale and Physics Coupling by Challenge Problem..... 36

Table 5 Typical Prediction Accuracy for Core Cycle Design Analyses [Ref. 8] 38

Figure 1 Cut view of a PWR without the Fuel..... 8

Figure 2 CASL ModSim Technology (VERA) Layered, Integrated Multi-Physics Developmental Approach..... 11

Figure 3 Multi-phase flow and complex geometry, such as coolant passing through a flow-mixing grid as illustrated here, require CFD simulation for highest fidelity solutions. 17

Figure 4 Illustration of a spacer grid cell and the simulation results for the flow pattern imposed by the mixing vanes 17

Figure 5 Illustration of the flow path (pre-meshing) for full-core PWR CFD simulations 18

Figure 6 Normal wall flow regimes recognized by COBRA-TF..... 19

Figure 7 COBRA-TF Scalar mesh cell and transverse momentum mesh cell configuration 19

Figure 8 Peregrine code workflow..... 20

Figure 9 Peregrine material models code structure..... 21

Figure 10 SEM Image of PWR CRUD Flake (courtesy EPRI) 22

Figure 11 Illustration of Mamba2D Mesh on the Surface of a Fuel Rod 24

Figure 12 Physics Feedback for CIPS ModSim 24

Figure 13 Boundary Conditions for Mamba2D Heat Transfer through the CRUD Layer 25

Figure 14 DAKOTA, Loose Coupling to a Generic Application 27

Figure 15 VERA Subcomponents..... 28

Figure 16 DTK Rendezvous Process 29

Figure 17 PETSc Library Organization 26

Figure 18 Parallel Numerical Libraries in PETSc 33

ACRONYMS

AMA	Advanced Modeling Applications
BWR	boiling water reactor
CASL	Consortium for Advanced Simulation of Light Water Reactors
CILC	CRUD-induced localized corrosion
CIPS	CRUD-induced power shift
CFD	computational fluid dynamics
CRUD	corrosion-related unidentified deposits or Chalk River unidentified deposits
DNB	departure from nucleate boiling
DOE	U.S. Department of Energy
DOE-NE	U.S. Department of Energy Office of Nuclear Energy
EIH	Energy Innovation Hub
EPRI	Electric Power Research Institute
FA	Focus Area
GTRF	grid-to-rod-fretting
HPC	high-performance computing
IC	Industry Council
INL	Idaho National Laboratory
LANL	Los Alamos National Laboratory
LOCA	loss of coolant accident
LWR	light water reactor
M&S	modeling and simulation
MIT	Massachusetts Institute of Technology
MPO	Materials Performance and Optimization
NCSU	North Carolina State University
NRC	Nuclear Regulatory Commission
NSSS	nuclear steam supply system
ORNL	Oak Ridge National Laboratory
PCI	pellet-cladding interaction
PWR	pressurized water reactor
R&D	research and development
RIA	reactivity insertion accident
RSICC	Radiation Safety Information Computational Center
RTM	Radiation Transport Methods
SMR	small modular reactor
SNL	Sandia National Laboratories
T-H	thermal-hydraulics
THM	Thermal Hydraulics Methods
TVA	Tennessee Valley Authority
UM	University of Michigan
V&V	verification and validation
VERA	Virtual Environment for Reactor Applications
VERA-CS	VERA-Core Simulator
VOCC	Virtual Office, Community, and Computing
VRI	Virtual Reactor Integration
VUQ	Validation and Uncertainty Quantification
WEC	Westinghouse Electric Company

CHAPTER I Introduction to the Virtual Environment for Reactor Applications

I.1 Introduction

Commercial nuclear power reactors are easily described: fuel pellets are stacked in thin rods that are maintained in place through a metallic mechanical structure called a fuel assembly; many fuel assemblies are packed together into a pressure vessel; water is pumped through the fuel assemblies to cool them and to collect heat that is transferred to a turbine to make electricity.

Although it is easily described and each of the various aspects of the operation - the fuel pellets producing neutrons, the heating of the metal and water, and the flow of the coolant through the reactor - are routinely simulated individually, we haven't, until recently, had the computing power and coupled, parallelized software to simulate all of the physical phenomenon driving the commercial pressurized water reactor simultaneously.

At most utilities and fuel vendors, the phenomena are broken into the individual physics and are analyzed independently from each other based on simplifications and applied boundary conditions. For example, a nuclear engineer calculates rod power distributions using simplified thermal/hydraulic models to determine the coolant flow, temperature, and density distributions, while the thermal-hydraulics engineer in the next cubicle calculates more detailed coolant flow, temperature, and density distributions based on conservative assumptions for rod power distributions that conservatively bound those calculated by the nuclear engineer. Clearly these phenomena are directly related and a more accurate depiction of the power, coolant temperature and density would be obtained if the calculations were completed in a coupled manner.

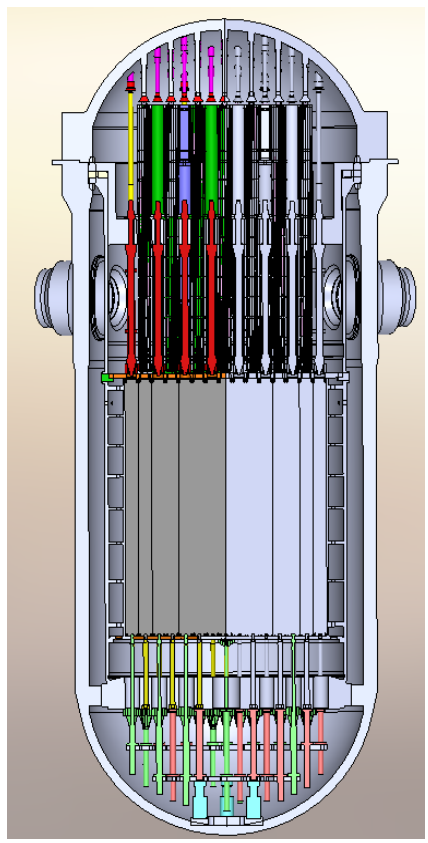


Figure 1 Cut view of a PWR without the Fuel

The Consortium for Advanced Simulation of Light Water Reactors (CASL) is the first DOE Energy Innovation Hub, established in July 2010 for the modeling and simulation (ModSim) of commercial nuclear power reactors. CASL's mission, as established in Ref. 1, is to provide usable coupled, higher-fidelity modeling and simulation capabilities to address light water reactor operational and safety performance-defining phenomena and to transfer the technology to the U.S. nuclear community.[1]

[1] The U.S. nuclear community includes the stakeholders defined by Reference 1: U.S. DOE Office of Nuclear Energy (NE) and the CASL Consortium, U.S. Nuclear Regulatory Commission (NRC), nuclear R&D community (including US Laboratories and Universities), and the nuclear industry.

I.2 CASL's Approach to Developing VERA

CASL's technology represents a step change in the simulation of commercial nuclear power plants and provides new insights on their operation, performance and safety. As mentioned previously, the traditional reactor design and analysis process relies on tools that are not fully integrated and coupled, with the analyses progressing through sequential simulation of different areas of physics, such as radiation transport (neutronics), fluid flow (thermal-hydraulics or T-H), and fuel thermo-mechanics. Structural analyses and coolant chemistry-fuel interaction simulations are usually performed on an as-needed basis.

The primary physics simulating the reactor a included in a Core Simulator functional tool set known as VERA-CS that provides: core depletion, pin powers, peaking factors and margins; control rod movement, detectors and boron search; and fuel shuffles from cycle to cycle. The parameters that have been selected for cross-physics coupling within VERA-CS, based on the sensitivity of the problem to those parameters, are:

- Fuel rod power
- Fuel rod heat flux
- Fuel rod surface temperature
- Moderator density
- Fuel pellet temperature

Since the industry ModSim tools are not fully coupled, multiple conservative assumptions must be made to ensure a conservative simulation, likely resulting in increased energy cost. Additionally, if downstream analyses indicate the necessity of design modifications, the simulation must be repeated from the beginning. CASL's approach allows a more integrated design cycle that can more adequately account for interactions between relevant physical phenomena. The integrated, coupled solutions are expected to reduce the uncertainties intrinsic in sequential analyses and provide a more realistic representation of the reactor behavior. Even more important, it will provide a more rigorous representation of the plant behavior for simulation of accident conditions.

Table 1 provides a summary of the general physics capability needs for simulation of commercial PWRs, and illustrates the mutually dependent relationships among the physical phenomenon. Table 2 provides a comparison between typical industry core simulators and CASL's VERA approach to provide a higher-fidelity, coupled simulation capability for existing LWRs. Note that the current CASL ModSim technologies are focused on quasi-steady state normal operating conditions. Figure 2 illustrates CASL's layered, integrated multi-physics approach: a multi-physics integrator at the hub of a foundational set of applications (VERA) with specialized tool sets interfaced as needed to address specific Challenge Problem requirements.

The foundation of CASL's coupled capabilities lies with the physics encompassed within VERA. CASL's commitment to higher fidelity understanding of reactor phenomenon requires a more rigorous approach to radiation transport, fluid flow and fuel rod performance prediction, and this has spurred investments in 3D discrete ordinates (Sn) radiation transport methods; hybrid finite-volume/finite-element incompressible/low-Mach flow solvers; and 3D finite element solid mechanics utilizing enhanced material modeling techniques.

Recognizing the need for higher-fidelity simulations on an industry-sized computing platform, CASL has elected to provide additional capabilities using alternative, less computationally intensive methods such as 2D/1D Methods-of-Characteristics (MOC) radiation transport; sub-

channel flow solutions; and 2D (r,z) finite element fuel rod mechanics utilizing enhanced material modeling techniques. These faster running higher-fidelity foundational capabilities are available within the VERA framework. However, it should be noted that even VERA's less computational-intensive methods require a fairly large computing cluster (500 cores and higher) to run larger problems.

Pervasive uncertainty quantification ensures an understanding of the extents of the simulations, and a utilities tool set provides the necessary user interfaces (note that meshing is not within the current CASL development scope but is recognized as a necessary utility). The conditions of the simulation, representing the initial and boundary conditions of the simulations, are derived from the Normal Conditions of operation (current CASL scope) and Hypothetical Accident Conditions of operation (potential future CASL scope).

The selective advancement of the underlying phenomological models and the numerical implementations of those models, the judicious coupling of the physics, and the integrated uncertainty quantification provide the unique capability and higher-fidelity simulations needed to enhance efficiency and power production at the existing nuclear power fleet. In order to ensure that CASL Technologies include the necessary physics capability advancements within the VERA, the CASL project has adopted a "Challenge Problem" approach to focus and motivate specific development and enable R&D, and the Challenge Problems correspond to several of the problem workflows discussed in later sections.

As illustrated in Figure 2, CASL's VERA relies upon a multi-physics integrator infrastructure to couple the CASL physics. This functionality includes two tools: a tool used to couple existing physics applications and a tool to facilitate additional parameter coupling. These infrastructure tools can be used by users to couple additional parameters and to couple in new applications.

To couple different parts of a multi-physics problem using already existing physics applications, VERA contains a well-defined approach (including example templates) with specific interface requirements for participating physics applications to enable the assembly of the applications into a robust and efficient multi-physics simulation capability [Ref. 2, 10, 11]. The tool was developed to minimize the barriers to integrating new physics applications without limiting the sophistication of the applications themselves, and can integrate and couple physics applications written in different languages, leveraging multiple numerical discretization approaches (e.g. Finite Element). The infrastructure can be leveraged to couple user physics applications in place of the CASL physics applications. It is important to note that this capability does not support "plug and play" of applications for coupling; rather a more appropriate description is "adapt and apply." Additionally, in order to provide an alternative to the custom schemes developed for each combination of VERA physics, a set of infrastructure tools for parallel data transfer are included in VERA [Ref. 2]. This infrastructure capability provides a set of interfaces and tools that application developers can use to aid in the parallel transfer of data between physics applications. More information on these capabilities is available in Reference 14.

VERA contains many leveraged subcomponent capabilities, and each subcomponent retains its native input methods and requirements. However, it is desirable to streamline the input requirements such that the user is not required to provide multiple input decks with repetitious information. Therefore, CASL has established a Common Input for VERA in XML format that can be generated in multiple ways (text, script, or GUI) [Ref. 2].

VERA provides an integrated and coupled suite of robust, validated, and usable multiphysics tools within a common virtual environment that can produce higher-fidelity predictive capability, including scalable, robust, modern applications for:

- 3D full-core pin-resolved radiation transport;
- 3D full-core thermal hydraulics;
- 3D full-core pin-resolved fuel performance;
- Physics-based materials models applicable to the fuel system, reactor vessel and internals, with improved constitutive models of the coolant and corrosion chemistry;
- A Core Simulator functional tool set (VERA-CS) that provides: core depletion, pin powers, peaking factors and margins; control rod movement, detectors and boron search; and fuel shuffles from cycle to cycle.
- Integrated uncertainty quantification tools for VERA verification and validation, calibration through data assimilation, sensitivity analysis, discretization error analysis and control, uncertainty quantification, and predictive maturity assessment; The VERA simulation framework that allows other subcomponent physics applications to be utilized in a coupled manner with or without CASL subcomponent physics applications;
- Models and mesh established through Benchmark simulations and Pilot simulations;
- "Challenge Problem" simulations with comparisons against operational data from commercial reactors to demonstrate application performance and to facilitate potential User licensure.

It should be noted that VERA includes applications that scale from industry-class computing clusters to high performance computing (HPC) clusters to provide useful and sustainable VERA products across the VERA user group.

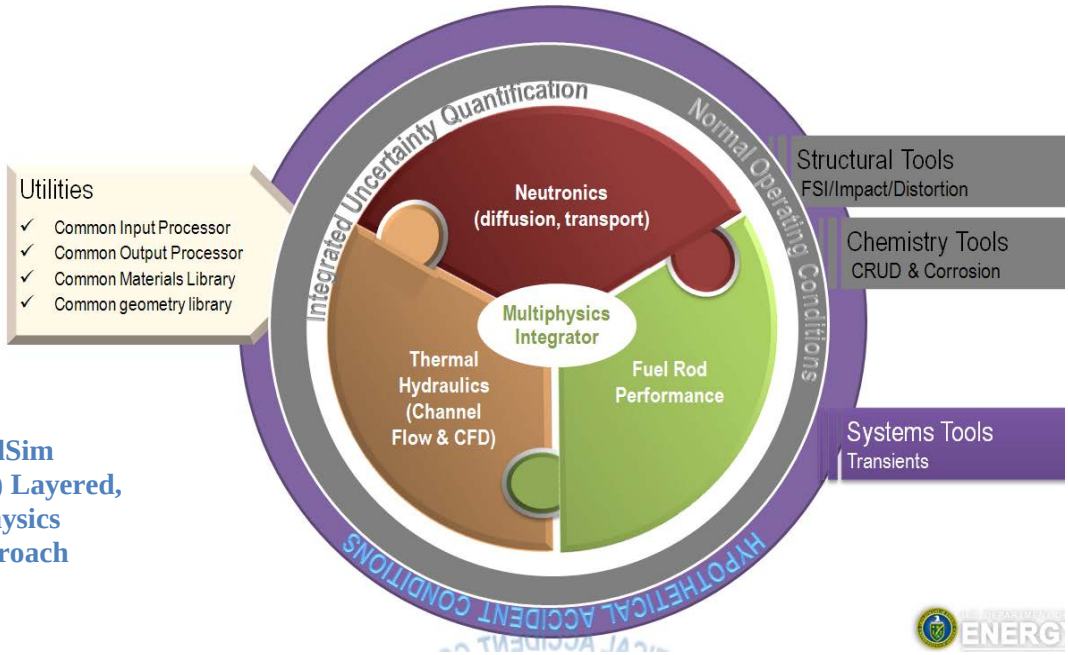


Figure 2 CASL ModSim Technology (VERA) Layered, Integrated Multi-Physics Developmental Approach

Table 1 General Needs for Simulation of Commercial PWRs

	Foundational Physics Needs	Specific Challenge Problem Tool Set Needs	Feedback Effects
Neutron Transport	• Local neutron flux; • Local Rod power; • Fission and depletion cross-sections;	• Depletion tracking; • Ability to model grids discretely; • Azimuthal cladding and pellet temperatures; • Capability to calculate reactor and fuel structure doses; • Local Boron concentration;	• Local coolant temperature & density; • Local Fuel temperature • Rod bow performance; • Assembly bow performance • CRUD deposition feedback;
Thermal-Hydraulics	• Local axial and cross flow; • Local coolant temperature and density; • Coolant pressure drop; • Coolant mixing/turbulence; • Bypass mass flow Local rod surface temperature; • Net hydraulic loads; • Heat transfer coefficients; • Flow friction/continuity descriptors.	• Analytical DNB predictions and DNBR/margin; • Fluid-structure interaction excitation loads; • Ability to accurately calculate pressure drop across components	• Local fuel temperature; • CRUD deposition feedback;
Fuel Rod Performance	• Local fuel temperature; • Pellet densification and swelling; • Fission gas release; • Pellet crack/relocation & rim size; • Pellet thermal conductivity; • Clad oxidation, hydrogen pickup and hydriding; • Clad thermal and irradiation creep; • Fuel rod internal pressure; • Cladding stress/strain; • Pellet/clad interaction status and local stress/strain, pellet relocation effects; • Maneuvering performance	• Coupled ability to analyze missing pellet surfaces and prediction of localized clad stress and strain; • Assembly distortion performance; • Component and assembly vibration frequency & amplitude and wear depths, including grid-to-rod fretting wear; • Clad plasticity models; • Rod bow model; • Irradiation growth and creep;	• Local Rod Power; • Local coolant heat transfer coefficients; • CRUD deposition feedback; • GTRF wear feedback;
Challenge Problem Specific		• Coolant chemistry and CRUD deposition models; • Fluid-structure interaction models; • Clad-grid support gaps; • Reactor CRUD inventory. • Assembly distortion model; • Structure/rod Oxidation and hydriding • Structure/Joint/nozzle stress & strain	• Local boron concentration & depletion; • structure and rod irradiation growth; • Rod waterside diameter;

Table 2 Comparison of VERA with Typical Industry Core Simulator Methods [Ref. 3, modified]

Physics Area	Typical Industry Core Simulator Method	VERA Higher Fidelity Capability	VERA Highest Fidelity Capability
Neutron Transport	3-D diffusion (core) 2 energy groups (core) 2-D transport on single assemblies	2D/1D transport 23+ energy groups	3D transport 23+ energy groups
Thermal-Hydraulics	nodal average (1-D)	subchannel (w/crossflow)	subchannel (w/crossflow) or CFD
Fuel Performance	Bounding empirically-based	pin-by-pin (r,z)	pin-by-pin
Fuel & clad Temperatures	nodal average & peak	pin-by-pin (r,z)	pin-by-pin
Power Distribution	nodal average with pin-power reconstruction	explicit pin-by-pin	explicit pin-by-pin
Xenon/Samarium	nodal average w/correction	pin-by-pin	pin-by-pin
Depletion	infinite-medium cross sections, quadratic burnup correction history corrections, spectral corrections, reconstructed pin exposures	pin-by-pin with actual core conditions	pin-by-pin with actual core conditions
Reflector Models	1-D cross section models	actual 3D geometry	actual 3D geometry
Target Platforms[2]	Workstation (six-core)	1,000 cores and up	10,000 – 300,000 cores
	~110 Gflops[3]	~18 Tflops	~180 Tflops - 20 Pflops
	~16 GB	~3 TB	~30 TB - 700 TB

[2] ORNL Titan performance is more than 20 Pflops, sustaining more than 20,000 trillion calculations per second. the Titan cluster has almost 300 thousand cores and 710 TB of RAM. So, how much faster would this be than a typical workstation PC? First it should be said that operating speed is highly dependent upon the particular processor. However, as an example, in 2010 the fastest six-core PC processor reached 109 gigaFLOPS (Intel Core i7 980 XE)[16]in double precision calculations. Therefore, the Titan is about 18,350 times faster than a workstation with this processor. If you had a 1000-core cluster with this processor, Titan would still be more than 1000 times faster. The typical RAM with this 1000-core workstation would be around 16 TB, about 2% of the Titan's capacity. How much would this typical workstation PC cost? About $275K for hardware and installation, electricity not included.

[3] Flops = cores x clock x flops/cycle.

CHAPTER II The VERA Physics Capabilities

II.1 VERA's 3D Radiation Transport codes; Insilico, MPACT and Shift

The VERA infrastructure includes three options for radiation transport: a deterministic S_N/SP_N solver, a deterministic Method of Characteristics (MOC) solver, and a stochastic Monte Carlo solver.

II.1.1.1 VERA's S_N/SP_N Radiation Transport Code

The S_N/SP_N radiation transport code, Insilico, solves the multigroup discrete ordinates (S_N) form of the Boltzmann transport equation for both fixed-source and k-eigenvalue problems. It uses the well-established S_N discretization and solves the transport equation on Cartesian grids using the Koch-Baker-Alcouffe wavefront parallel algorithm.

II.1.1.2 VERA's MOC Radiation Transport Code

The MOC code, MPACT, is a solution to the transport equation in which rays are drawn across the global geometry in discrete angles and the transport equation is integrated along those rays [Ref. 8].

II.1.1.3 VERA's Monte Carlo Radiation Transport Code

Shift is a radiation transport hybrid code, utilizing the capabilities of both deterministic and Monte Carlo codes. Shift is being developed as a massively parallel code and supports multiple parallel decompositions ranging from full domain replication, full domain decomposition, domain decomposition with overlapping regions, and multiple-set-overlapping domain (MSOD) decomposition. Shift is designed to allow multiple physics and geometric representations in the Monte Carlo transport components without code modification. Thus, for example, multigroup and continuous energy physics can be supported without changing the core transport mechanics; all of the physics-dependent operations are encapsulated in the physics abstraction. Currently, Shift supports KENO and Reactor-Tool-Kit geometry packages and simple multigroup physics. Because Shift is written in the same code base as the Insilico Denovo S_N solver, it can efficiently access the deterministic code mesh generation and solver mechanics to enable integrated hybrid capability [Ref. 1].

II.1.1.4 VERA Cross-section Processing

VERA performs resonance self-shielding with full range Bondarenko factors using either the narrow resonance approximation or the intermediate resonance approximation [Ref. 5]. For uniform fuel lattices, Dancoff factors are automatically generated from the user-input geometry and material descriptions. VERA also allows user-input Dancoff factors to treat non-uniform lattice effects. The fine energy-group structure of the resonance self-shielding calculation can optionally be collapsed to a coarse group structure through a one-dimensional (1D) transport calculation. The module provides the following capabilities:

- Temperature interpolation,
- Problem-dependent resonance self-shielding,
- Macroscopic mixing of multigroup cross-section data,

- Energy collapse of cross-section data,
- Serialize/deserialize unit cells and cross-section data,
- Dancoff factor calculation, and User input Dancoff factors.

VERA's radiation transport codes are capable of performing massive fixed source and eigenvalue problems and can be scaled to 200,000 cores, allowing simulation of very large radiation transport problems. Pin-homogenized quarter core simulations have been performed with VERA, and show excellent results. Typical computing requirements for single-physics and coupled physics calculations with VERA radiation transport codes are listed in Table 3.

Table 3 Radiation Transport Computing Requirements for Various Example Calculations

Calculation description	Number of Cores/FLOPS	Computing time (all times approximate)	Reference
AP-1000 cycle 1 2D lattice, single state point	12	1 min	
AP-1000 cycle 1 2D quarter-core, single state point	144	5 min	
AP-1000 cycle 1 3D single assembly, single state point	64	30 min	
AP-1000 cycle 1 3D 3x3 assembly, single state point	144	40 min	
AP-1000 cycle 1 3D, quarter-core, single state point (eigenvalue)	320	100 min	
Watts Bar cycle 1 3D hot full power, quarter-core VERA-CS (Insilico + Cobra-TF)	18,769	17.5 hr	

References for this section:

1. N.C. Sly, B.T. Mervin, S.W. Mosher, T.M. Evans, J.C. Wagner, and G.I. Maldonado. "Verification of the Shift Monte Carlo Code," *PHYSOR 2012 Advances in Reactor Physics Linking Research, Industry, and Education*, Knoxville, Tennessee, April 15- 20, American Nuclear Society, LaGrange Park, IL, 2012
2. F. Franceschini et. al. Westinghouse Test Stand: Zero Power Physics Test Simulations for the AP1000 PWR. CASL-U-2014-0012-000, March 6, 2014.

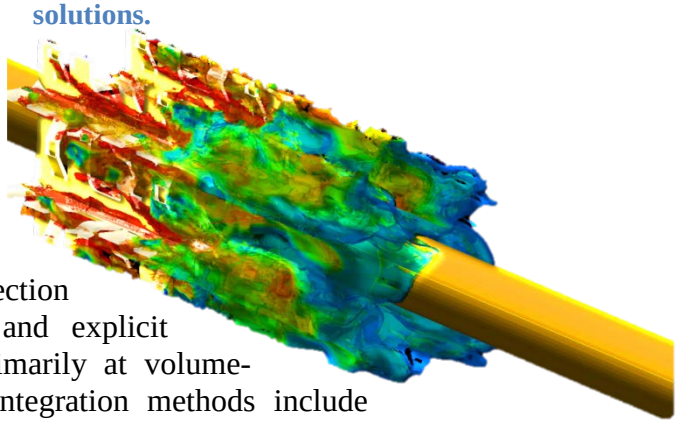
II.2 VERA's Thermal-Hydraulics Codes, Hydra-TH and COBRA-TF

The VERA infrastructure includes two options for thermal-hydraulics: a computational fluid dynamics (CFD) code, and a channel flow code.

II.2.1 VERA's CFD Code, Hydra-TH

VERA includes a computational fluid dynamics capability, Hydra-TH, that utilizes a hybrid finite-element/finite-volume incompressible/low-Mach flow Navier-Stokes equation solver [Ref. 6]. All transport variables are cell-centered and treated with a conservative discretization that includes a high-resolution monotonicity-preserving advection algorithm. The spatial discretization is formally derived using a discontinous-Galerkin framework that, in the limit, reduces to a locally-conservative finite-volume method. The high-resolution advection algorithm is designed to permit both implicit and explicit advection with the explicit advection targeted primarily at volume-tracking with interface reconstruction. The time-integration methods include backward-Euler and the neutrally-dissipative trapezoidal method.

Figure 3 Multi-phase flow and complex geometry, such as coolant passing through a flow-mixing grid as illustrated here, require CFD simulation for highest fidelity solutions.



The solution algorithm used in Hydra-TH is based on a second-order incremental projection algorithm. Projection methods are the most computationally efficient solution method available for solving the time-dependent Navier-Stokes equations. The projection method permits treating the momentum equations in a coupled manner.

In order to address fluid-structure problems, Hydra-TH uses an arbitrary Lagrangian-Eulerian (ALE) formulation and provides a mesh-deformation interface that can support multiple different mesh smoothing algorithms. The added-mass terms are computed for the structural coupling and can be exported for any structural solver. For explicit coupling, Hydra-TH provides a pressure-stabilized algorithm based on Nitche's variational method that circumvents the stability limitations associated with highly flexible structures and near unity fluid/solid density ratios.

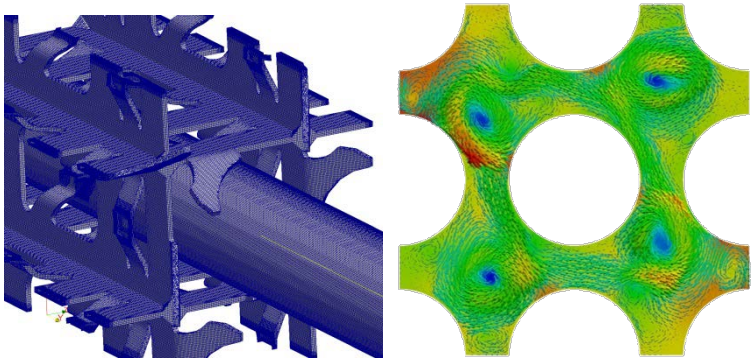


Figure 4 Illustration of a spacer grid cell and the simulation results for the flow pattern imposed by the mixing vanes

Multiple alternatives for conjugate heat transfer are available in Hydra-TH, including explicit coupling with third-party heat conduction solvers, internal coupling using the existing heat conduction solver or direct integration (with continuous meshing). Figures 3 through 5 provide illustrations of flow geometry and mesh utilized in CASL CFD simulations.

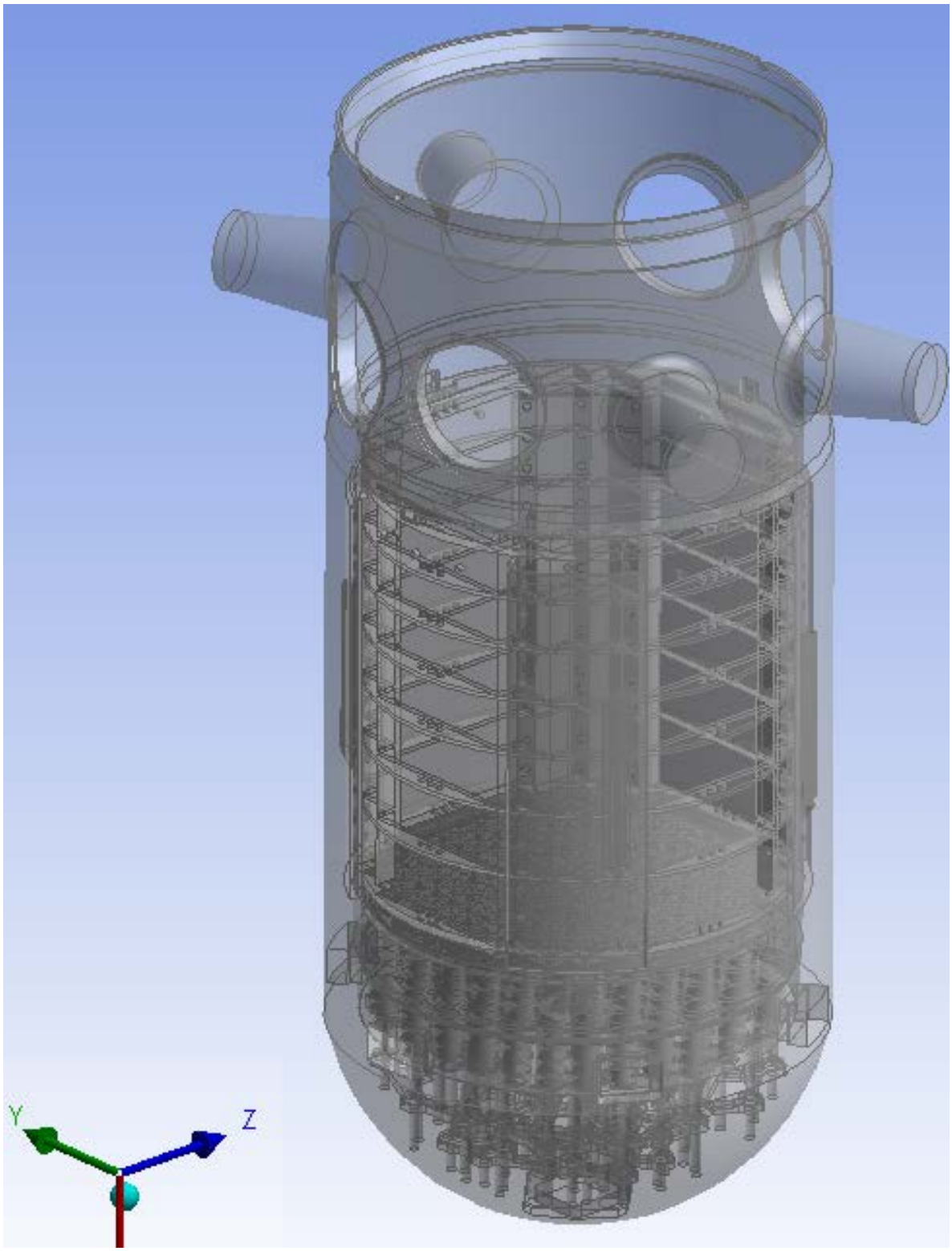


Figure 5 Illustration of the flow path (pre-meshing) for full-core PWR CFD simulations

II.2.2 VERA's Channel Flow Code, COBRA-TF

COBRA-TF includes a rod-bundle subchannel thermal-hydraulics application used to perform transient simulation for the full range of two-phase flow regimes based upon the geometry inherent in current commercial nuclear power reactors [Ref. 2, 9]. The subchannel approach can be thought of as an extremely coarse-mesh approximation, in which the control volume is of a size equivalent to a single fuel rod and its surrounding coolant. It uses a two-fluid, three-field (i.e. liquid film, liquid drops, and vapor) modeling approach. Both sub-channel and 3D Cartesian forms of nine conservation equations are available for LWR modeling.

In COBRA-TF, the conservation equations for each of the three fields and for heat transfer from and within the solid structure in contact with the fluid are solved using a semi-implicit, finite-difference numerical technique on an Eulerian mesh, where time intervals are assumed to be long enough to smooth out the random fluctuations in the multiphase flow, but short enough to preserve any gross flow unsteadiness. The fluid volume is partitioned into a number of computational cells by COBRA-TF. The equations are solved using a staggered difference scheme. The phase velocities are obtained at the cell faces, while the state variables - such as pressure, density, enthalpy, and void fraction - are obtained at the cell center. The momentum equations are solved on staggered cells that are centered on the scalar mesh face.

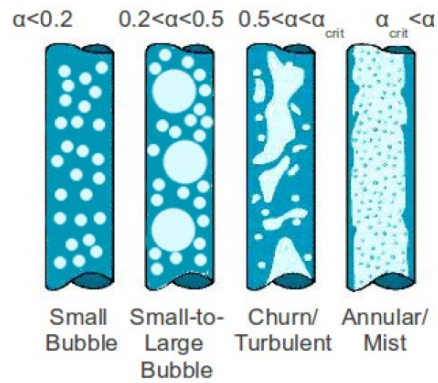


Figure 6 Normal wall flow regimes recognized by COBRA-TF

COBRA-TF is developed for use with either 3D Cartesian or sub-channel coordinates and features flexible noding for both the thermal-hydraulic and the heat-transfer solution. This flexibility allows a fully 3D treatment in geometries amenable to description in a Cartesian coordinate system and the use of the sub-channel approximation for faster calculations when the flow is principally in one direction.

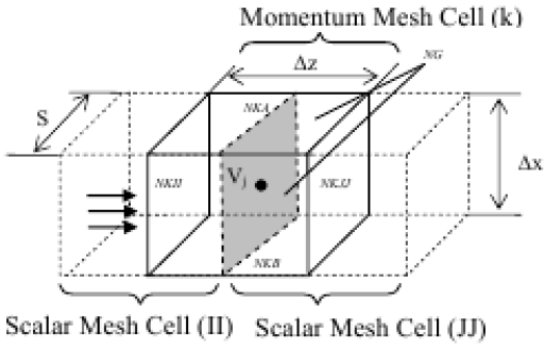


Figure 7 COBRA-TF Scalar mesh cell and transverse momentum mesh cell configuration

The application is able to handle both hot wall and normal flow regimes maps and it is capable of calculating reverse flow, counter flow, and cross-flow situations. COBRA-TF utilizes its own internal methods to calculate the thermo-physical properties of water, and includes simplified conduction models for fuel rod conduction that can be used in place of VERA Peregrine when a lower fidelity solution is acceptable.

COBRA-TF thermal-hydraulics is currently a serial capability, but is planned for parallelization of key routines and algorithms in future.

II.3 VERA's Fuel Performance Code, Peregrine

The VERA infrastructure includes the capability to predict fuel rod performance utilizing 3-D, coupled multi-physics and represents a significant advancement for the modeling/analysis capabilities in LWR fuel rod behavior. Figure 8 provides an illustration of the Peregrine code workflow, as well as an illustration of the typical output format from a Peregrine simulation. The capability is being constructed within a computational framework that supports:

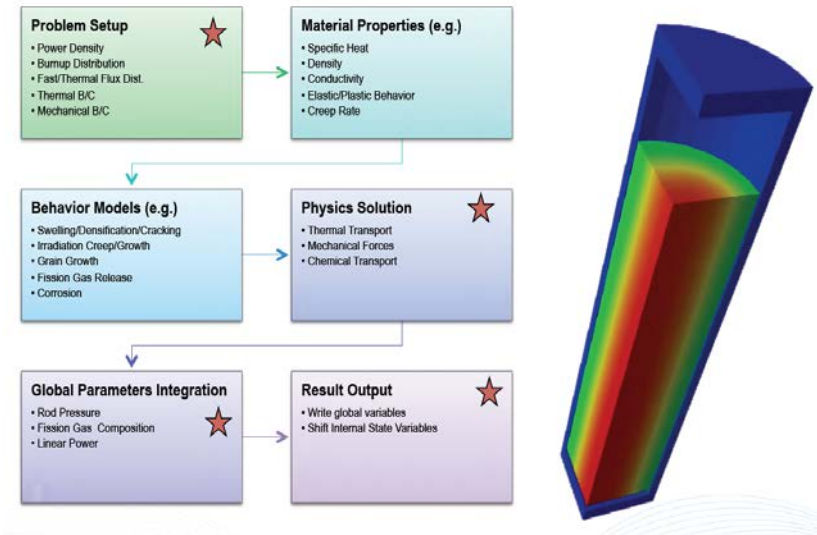


Figure 8 Peregrine code workflow

- Statics with elasticity, plasticity with strain hardening, creep, large strains, large displacements, and smeared plus explicit cracking;
- Unsteady (transient) heat transfer including conduction, convection and radiation with time and spatial (axially, radially and potentially azimuthally in a cylindrical fuel element) dependent internal heat generation;
- 2D axisymmetric, plane strain, and plane stress representations, including contact and friction interactions between pellets and between the pellet and cladding;
- 3D statics and dynamics with contact and friction, and heat transfer;
- Mixed dimensional coupling (via multipoint constraint equations, etc.), e.g., combined 2D and 3D numerical representations for coupled global (2D) and local effects (3D) modeling; and
- Utilizes high performance computing platforms to achieve the massively parallel performance and scalability required to perform coupled multi-physics simulations of full length 3D representations of the fuel rod components.

The full 3D capability can be resolved to a less computationally intensive resolution (fewer solution points) using a (r,z) meshing capability using the identical capabilities described for the 3D capability.

The Peregrine fuel rod performance code architecture uses the finite element method for geometric representation and a Jacobian-free, Newton-Krylov (JFNK) scheme to solve systems of partial differential equations. The CASL fuel performance application will be validated against industry codes.

The fuel rod performance capability includes models for:

- Clad stress, strain, and strain rate;
- Clad oxidation, hydrogen pickup and hydride formation;

- Pellet stress, strain, and strain rate;
- Fission gas release (transient and pseudo-steady-state);
- Pellet densification, swelling and fission product evolution;
- Pellet restructuring and high-burnup rim thickness;
- Pellet cracking and relocation;
- Thermal expansion, including pellet hour-glassing;
- Thermal and irradiation creep;
- Thermal conductivity effects due to clad oxidation and fuel microstructure evolution;
- Material strength and ductility effects due to irradiation, thermal cycling, hydriding, fission product evolution;
- Pellet-cladding gap evolution and local stress due to partial contact;
- Pellet stack growth and fuel rod growth;
- Explicit modeling of duplex and triplex clad designs;

The VERA fuel rod performance subcomponent calculates, on a 3D basis, fuel rod temperature, fuel rod internal pressure, free gas volume, clad integrity and fuel rod waterside diameter. These capabilities allow simulation of power cycling, fuel conditioning and deconditioning, high burnup performance, power uprate scoping studies, and accident performance.

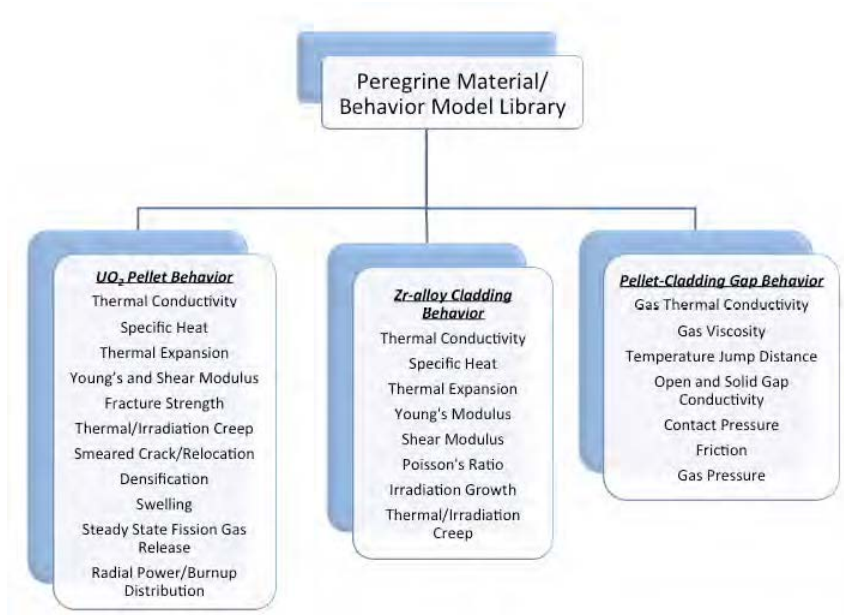


Figure 9 Peregrine material models code structure

It is important to note that these tools are built around the known performance of existing zirconium-based clad with UO_2 fuel and predictions for other fuel types may not be accurate. Estimates for the global effects of minor modifications to the fuel or clad may be possible; for example, chromia-doped pellets may be simulated with user-supplied models for several of the pellet performance characteristics or steel-based clad may be simulated with similar user-supplied models. Materials such as silicon carbides that do not fit the system paradigm can be simulated but are likely to provide inaccurate results.

II.4 VERA's Coolant Chemistry Code, Mamba/Mamba-BDM

As the coolant in light water reactors is circulated through the primary loop, it carries along both soluble and particulate CRUD - nickel and iron corrosion products released by the steel and inconel piping and components. CRUD deposits (an example is shown in Figure 10) are typically porous, and sub-cooled boiling within the porous CRUD layer can result in the concentration of soluble species within the CRUD. In PWRs, thick CRUD deposits (25-50 microns) can result in the concentration and precipitation of boron and lithium components, affecting the local power production and creating CRUD-induced power shifts (CIPS).

CRUD deposition on PWR fuel cladding can be a complicated process to model - it may deposit directly on the fuel cladding, or it may also deposit on non-fuel surfaces. The deposits may precipitate and then re-dissolve into the coolant at some future time due to power changes and refueling shuffles, and the CRUD may also erode over time. The re-dissolved and eroded material can circulate in the coolant and form new deposits on other fuel where sub-cooled boiling occurs. Also, CRUD must be tracked over multiple reactor cycles. Also, some CRUD may be removed by the utility using ultrasonic cleaning. The effect of plant trips is believed to cause some CRUD release, as CRUD is released from control rod drive mechanisms. The quick drop in power can also mechanically remove some of the existing deposits as the CRUD and clad thermally contract.

CRUD also has the potential to produce CRUD-induced localized corrosion (CILC) failures in BWRs and PWRs. Locally thick CRUD produces hot spots on the fuel rods that encourage accelerated cladding corrosion, eventually leading to leaking fuel rods.

CRUD deposits on fuel cladding are made up of various oxides of nickel and iron. Nickel Ferrite ($NiFe_2O_4$) was generally believed to be the predominant form of CRUD deposits in PWRs. However, CRUD scrapes in cores experiencing CIPS often indicated a much higher nickel/iron ratio than would result from nickel ferrite, and industry and CASL studies indicate that NiO is likely mixed in with the Nickel Ferrite, along with some Nickel metal. When thick CRUD is present, bonaccordite may also be present, and this is especially interesting since it contains boron, the neutron absorber causing the power shifts. However, the vast majority of boron deposited in the CRUD is not expected to be part of the CRUD structure; rather it is usually a precipitate that deposits in porosity within the CRUD structure.

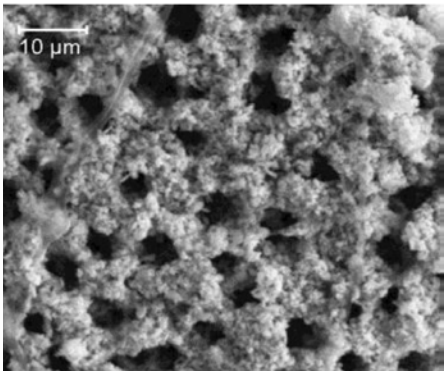


Figure 10 SEM Image of PWR CRUD Flake (courtesy EPRI)

Once CRUD deposits thicken, the sub-cooled boiling process concentrates any additives in the coolant such as lithium hydroxide and boric acid within the CRUD. The boiling process draws these materials into the CRUD, but the formation of vapor then concentrates the additives. Lithium is not particularly volatile, so most of the lithium drawn into the CRUD will not leave with the vapor bubbles. Boric acid has some volatility, but most will still be left behind in the liquid. To leave the vicinity, the CRUD-trapped concentrated species must diffuse back through the porous CRUD deposit. The steady state Lithium hydroxide and boric acid concentration

profile within the CRUD is determined by a balance between the concentration rate from sub-cooled boiling, and the diffusion rate back through the CRUD.

The porosity of CRUD differs from deposit to deposit. Initially PWR CRUD deposits were believed to be very porous and 80% porosity seemed to be the typical expectation. However, plants with CIPS usually have somewhat less porous CRUD, and the porosity can vary throughout the deposit. Porosity is generally expected to decline with overall CRUD thickness, and within the deposit, the porosity at the bottom of the deposit near the cladding is believe to be lower than porosity in the outer portions of the deposit.

The CRUD deposits also affect the sub-cooled boiling process. The CRUD impedes heat transfer and further elevates cladding temperatures, increasing the sub-cooled boiling rate at the clad surface. The CRUD itself also offers additional nucleation sites for bubble formation. Local subcooled boiling rates are expected to increase once CRUD deposits are present.

CASL's coolant chemistry capability models CRUD formation and growth using a general time-dependent 3D heat transport equation to obtain the temperature distribution throughout the CRUD layer on a single pin (or on selected regions of a single pin). The heat transport solution includes the localized heat sinks due to regions of sub-cooled nucleate boiling (SNB) that may occur within the CRUD deposit. The heat flux at the cladding waterside surface and coolant temperature (or flux) at the CRUD waterside surface represent the external boundary conditions and are supplied through coupling with VERA or by the user.

The local CRUD thermal conductivity varies in both space and time due to the changes in porosity. The change in porosity is due to the internal deposition of nickel ferrite ($NiFe_2O_4$) within the pores of the CRUD which slowly fills them. The local porosity can also change more quickly due to the precipitation of lithium-tetraborate ($Li_2B_4O_7$). This is the primary mechanism for boron deposition inside the CRUD.

The deposition of nickel ferrite and lithium-tetraborate within the CRUD are both enhanced by localized SNB which generates significant Darcy flow within the porous CRUD layer. Both the Darcy flow and diffusion within the CRUD layer are modeled and these mass transport mechanisms lead to significant increases in the local concentrations of the various soluble species (Ni, Fe, Li and boric acid) inside the CRUD.

Advanced chemistry/thermodynamic models have also been incorporated into the tools for treating the coolant chemistry (Li, B, H_2, Ni, Fe, $B(OH)_3$, and several ionic species) and for accurately determining the precipitation parameters. These models are based on the mechanisms and equilibrium constant correlations developed by Reference 15. The advanced chemistry/thermodynamic models are applied at both the CRUD/coolant interface as well as each internal volume element inside the CRUD at each time step. The precipitation parameter determines when a given volume element begins to rapidly fill with lithium-tetraborate.

Currently, the industry established values provided by References 14 and 15 are used for several CRUD properties, including porosity, thermal conductivity, chimney density, and chimney radius. An adaptive 3D mesh is used which "grows" the 2D CRUD surface as mass deposits onto the surface elements. The surface particulate deposition rate is governed by two rate parameters: one for non-boiling regions and one for boiling regions. The boiling deposition rate is multiplied by the local mass evaporation (steaming) flux leaving the CRUD surface via the chimneys. Thus, local SNB within the CRUD layer leads to enhanced particulate deposition and CRUD growth.

The basic physics and coupling provided within VERA to simulated CRUD deposition are illustrated in Figure 12. The parameters that have been selected for cross-application coupling, based on the sensitivity of the problem to those parameters, are:

- Fuel rod power
- Fuel rod heat flux
- Fuel rod surface temperature (clad)
- Fuel pellet temperature
- Moderator density
- Coolant boron concentration and depletion
- CRUD thickness, composition, trapped boron concentration, thermal resistance, waterside roughness
- Special user inputs to the application includes: CRUD source term (based on non-CRUD cycle calibration)

Figure 11 illustrates a MAMBA2D mesh. The computational area consists of an axial stack of curved surfaces that extend over a ¼ azimuthal span of only one fuel (or water) rod cladding. Multiple instances of MAMBA2D are evaluated within each simulation, where each instance corresponds to a quadrant of a rod surface, and is bounded by a COBRA-TF sub-channel. The coupled application is run in parallel with each instance of MAMBA2D running simultaneously with all others but coupled to a single instance of COBRA-TF.

Figure 12 illustrates, in simplified form, the coupled physics strategy employed in the calculations. More specific information on the order and resolution of the calculations are provided in Reference 13.

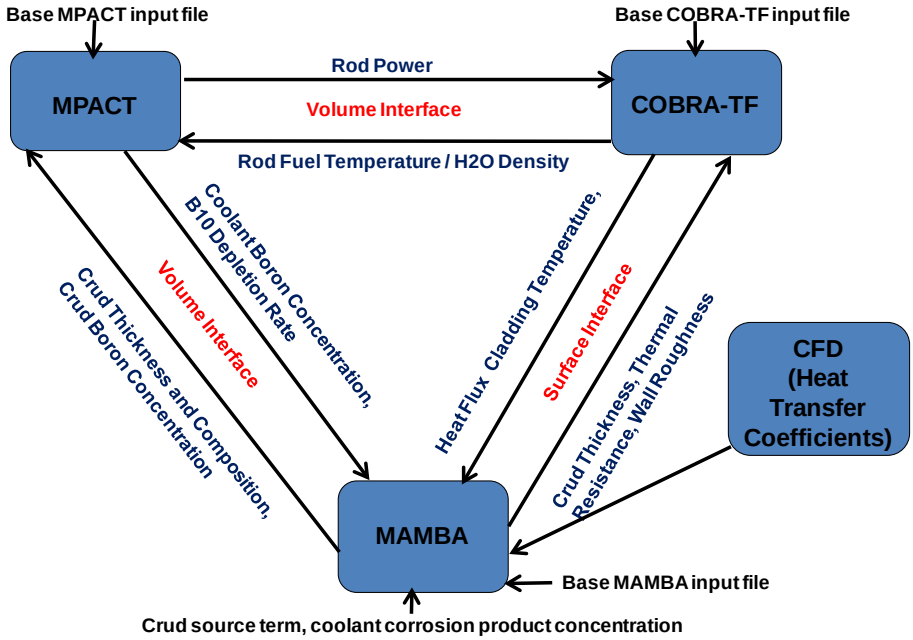


Figure 12 Physics Feedback for CIPS ModSim

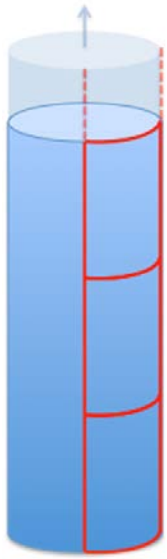


Figure 11 Illustration of Mamba2D Mesh on the Surface of a Fuel Rod

For CIPS and CILC modeling using advanced CASL applications, a two-tiered approach is applied. For CIPS, full core modeling is necessary to accurately determine the distribution of CRUD throughout the core. Early CASL experience suggests that pin-resolved transport linked to CFD, CRUD, and fuel performance models will be too computationally intensive, even on large super-computer clusters, to be practical; thus, sub-channel T-H methods are used. These are augmented with stand-alone CFD models to capture the axial and azimuthal variations in heat transfer components for each fuel rod.

For MAMBA2D to solve its internal heat transfer equations, two boundary conditions must be externally provided: the heat flux at the clad-crud interface, and the surface temperature at the crud-coolant interface Figure 13 illustrates these boundary conditions in the context of a thin crud layer being modeled by MAMBA2D. Of particular importance here is that MAMBA2D has an internal boiling model that computes the rate at which vapor bubbles are formed within the crud layer. A key assumption is that these bubbles immediately condense back into liquid when they are released into the coolant. This physical process is thus an additional mechanism by which energy is transferred from the crud to the coolant, and is denoted q_{boil} in Figure 13. The reason this process is important is that it directly affects the problem of providing a surface temperature at the crud-coolant interface when performing thermal-hydraulic calculations with a sub-channel code like COBRA-TF.

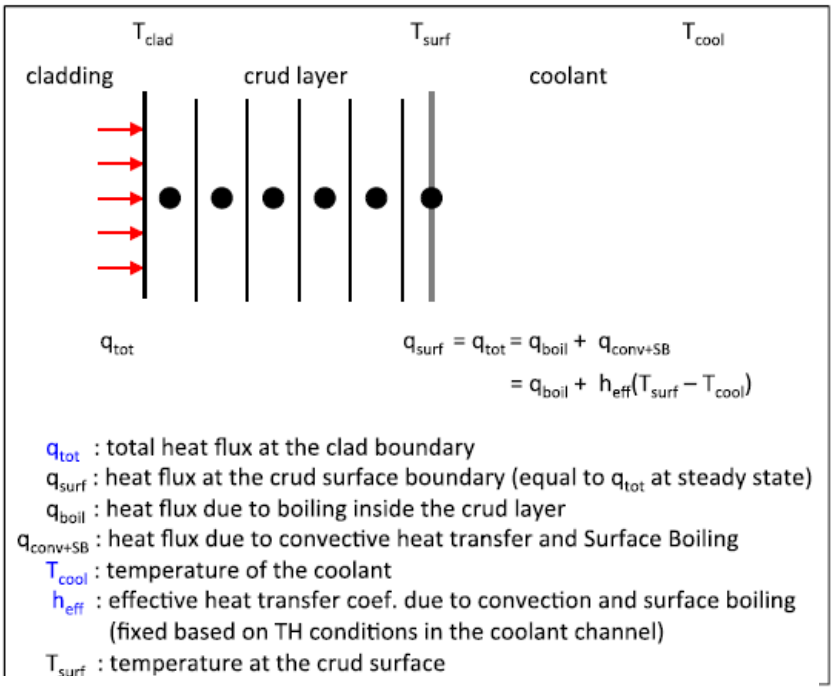


Figure 13 Boundary Conditions for Mamba2D Heat Transfer through the CRUD Layer

Heat transfer is modeled using specially developed correlations that define a heat transfer coefficient (denoted h_{eff} in Figure 13) based on the thermal-hydraulic and thermodynamic conditions in the local sub-channel. For the conditions being considered here, the coolant is modeled as a single phase liquid with the possibility of surface nucleate boiling. The crud surface temperature (T_{surf}) is approximated as the clad surface temperature at this time.

MAMBA-BDM is a sub-code developed to explicitly model small segments of crud with dimensions on the order of 100 microns. BDM explicitly models the porous crud structure, and can be used to investigate localized effects of boron deposition and temperature variations within the small crud segments. MAMBA-BDM can be coupled to the standard MAMBA code to determine average crud and boron deposition parameters for the coarser mesh MAMBA code.

II.5 VERA's Integrated Uncertainty Quantification (IUQ) code, DAKOTA

The VERA IUQ toolkit provides a flexible, extensible interface between analysis applications and iterative systems analysis methods [Ref. 7]. VERA contains algorithms for:

- optimization with gradient and non-gradient-based methods;
- uncertainty quantification with sampling, reliability, stochastic expansion, and epistemic methods;
- parameter estimation with nonlinear least squares methods; and
- sensitivity/variance analysis with design of experiments and parameter study methods.

These capabilities may be used on their own or as components within advanced strategies such as hybrid optimization, surrogate-based optimization, mixed integer nonlinear programming, or optimization under uncertainty.

Given the complex physical systems simulated by VERA, it is essential to quantify the inherent uncertainty contained within the results. Also, it is often desirable to use simulations as virtual prototypes to obtain an acceptable or optimized design for a particular system. DAKOTA enables the use of the VERA tools for design and optimization through a systematic, rapid method of iterative systems analysis, optimization, uncertainty quantification, nonlinear least squares methods, and sensitivity/variance analysis.

As a rule, complex multi-physics applications require an exponentially complex calibration and validation. A potentially higher-fidelity modsim approach and result can be overshadowed by the multiplicative uncertainty of the system. An objective of the CASL toolset is to cross-cut the large, multi-faceted, and evolving body of information related to the available validation database, legacy modeling findings, and VERA ModSim results to provide a systematic method to delineate and rank sensitivity and gaps related to the information. DAKOTA is a freely available, SNL-developed software package for sensitivity analysis, optimization, uncertainty quantification, and calibration with black-box computational models. To perform optimization, uncertainty quantification, or sensitivity analysis in a loose-coupled or "black-box" mode, DAKOTA iteratively writes parameter files, invokes a script to run the computational model, and collects resulting responses from a results file. This overall execution process is depicted in Figure 14. DAKOTA provides a flexible, extensible interface to any analysis code, includes both established and research algorithms designed to handle challenges with science and engineering models and manages parallelism for concurrent simulations. DAKOTA strategies support mixed deterministic/probabilistic analyses and other hybrid algorithms. You can read more about DAKOTA in Reference SAND2001-3796.

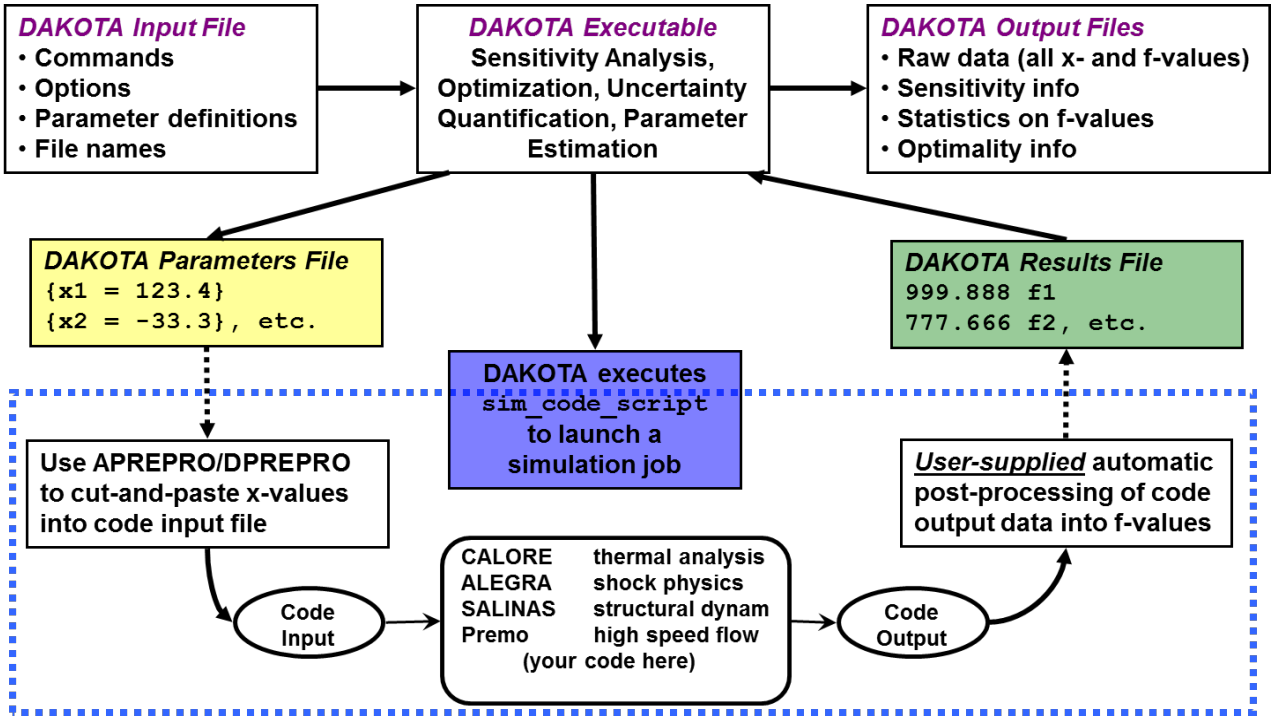


Figure 14 DAKOTA, Loose Coupling to a Generic Application

CHAPTER III VERA Supporting Infrastructure

The VERA physics capabilities are built on a versatile infrastructure that is designed to streamline the exchange of data from code to code and from processor to processor. VERA's infrastructure, as shown in Figure 15, also includes appropriate solvers and a common input and output format.

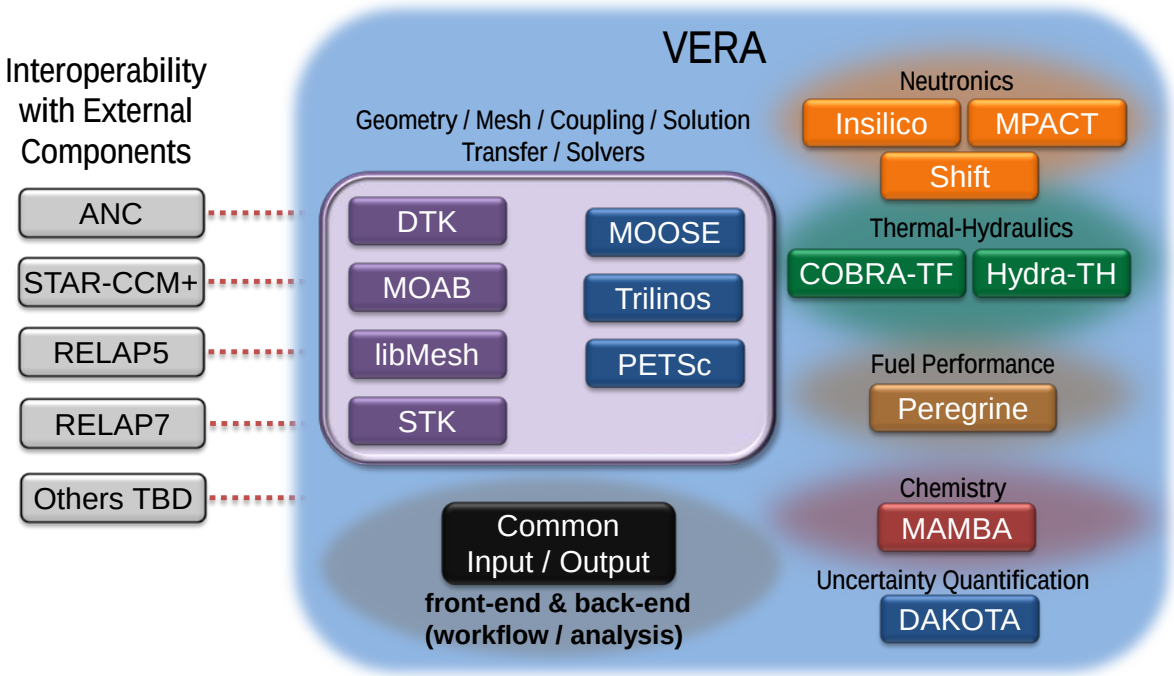


Figure 15 VERA Subcomponents

III.1 Data Transfer Kit (DTK)

In order to provide an infrastructure for data transfer operations between CASL physics codes, VERA includes Data Transfer Kit (DTK). DTK provides a set of interfaces and tools used for parallel transfer of data between physics codes.

Most of VERA's physics components utilize different mesh structures to solve their part of the coupled problem. In a parallel formulation, such as that used by the VERA codes, if these two geometries are arbitrarily decomposed, geometric alignment is not likely. To relate the non-conformal meshes to each other, DTK provides a geometric rendezvous that manipulates the source and target geometries such that all geometric operations and data evaluation operations have a local formulation while data transfer occurs globally.

DTK generates a secondary decomposition of the geometric structures in the problem by imposing a geometry-based repartitioning, as illustrated in Figure 16. To transfer data between these meshes, each partition in the meshes needs to communicate data to each partition in the

other mesh, due to their geometric overlap. The rendezvous decomposition is a geometrically-balanced repartitioning of the source mesh in the transfer problem with the partitioning information shared amongst all meshes. In DTK, the rendezvous algorithm (as illustrated in Figure 16) behaves as a hierarchical parallel and geometric search tree. Using this algorithm, a secondary decomposition of a subset of the source mesh that will participate in data transfer is generated, forming the rendezvous decomposition. It can be viewed as a temporary copy of the source mesh subset that intersects the target geometry.

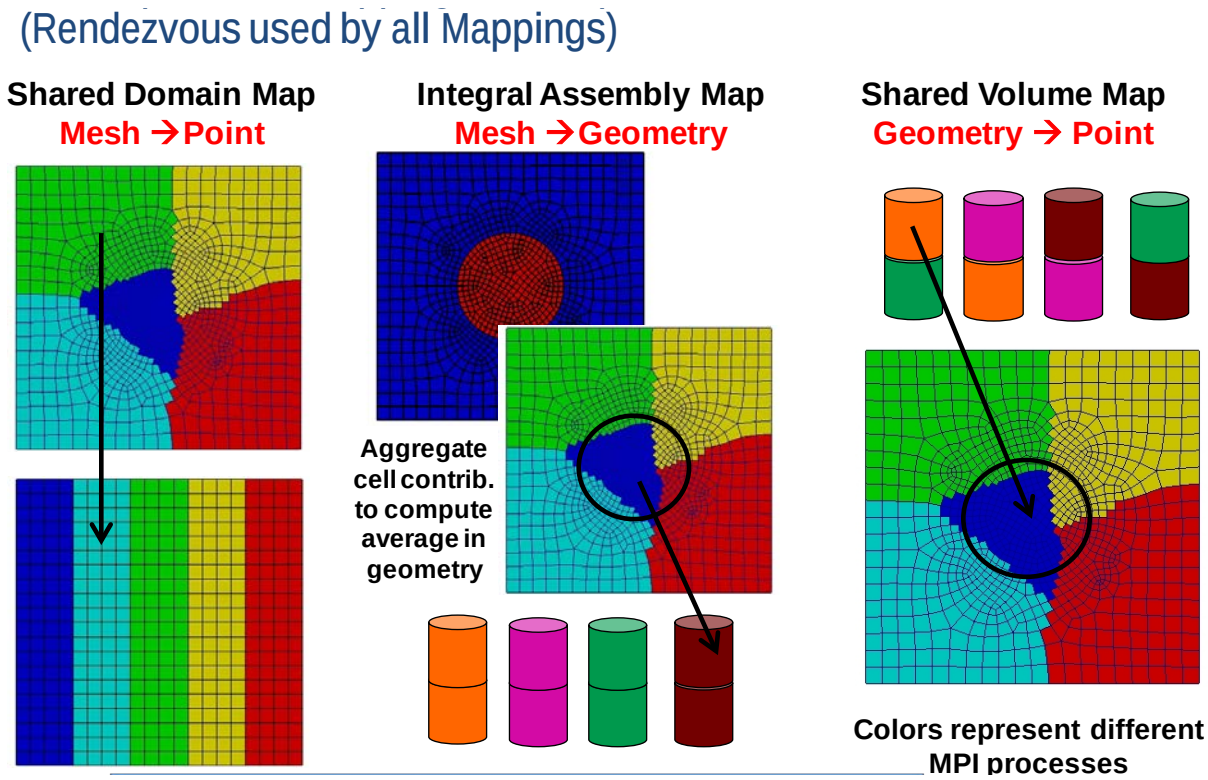


Figure 16 DTK Rendezvous Process

Once points have been accumulated in the rendezvous decomposition, a subset of the mesh that is in the vicinity of each target point is generated. This subset, which is typically much smaller than the mesh owned by a particular rendezvous process, is then searched with a more expensive point-in-element operation that transforms the point into the reference frame of each mesh element in the subset with a Newton iteration strategy. This mapped point is then checked against the canonical reference cell of that mesh element's topology to determine if the point is contained within.

A set of mapping algorithms based on geometric rendezvous are also implemented within DTK and are applied specifically to shared domain problems (the geometric domains of the source and target intersect over all dimensions of the problem). The purpose of the mapping algorithm is to efficiently generate a parallel topology map and the associated parallel communication plan that can carry out the data transfer repeatedly with the minimum required number of parallel messages and data. These maps are generated by creating source/target pairs found by searching the rendezvous decomposition.

Once the field evaluations are complete, the communication sequence moves that data from the source geometry decomposition to the target geometry decomposition to complete the data transfer operations.

References for this Section:

1. S.R. Slattery, P.P.H.Wilson, and R.P. Pawlowski. The Data Transfer Kit: A Geometric Rendezvous-Based Tool for Multiphysics Data Transfer, International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering (M&C 2013), Sun Valley, Idaho, USA, May 5-9, 2013, LaGrange Park, IL (2013).
2. Level 3 Milestone Deliverable Report VRI.PSS.P4.02
3. Data Transfer Kit Error Handling Policy, Revision 0 (Attached to TRAC ticket #2542)

III.2 MOAB

MOAB is a component for representing and evaluating mesh data. MOAB can store structured and unstructured mesh. The MOAB data model consists of the following four fundamental types: mesh interface instance, mesh entities (vertex, edge, tri, etc.), sets, and tags. Entities are addressed through handles rather than pointers, to allow the underlying representation of an entity to change without changing the handle to that entity. Sets are arbitrary groupings of mesh entities and other sets. Sets also support parent/child relationships as a relation distinct from sets containing other sets. The directed graph provided by set parent/child relationships is useful for embedding graphs whose nodes include collections of mesh entities; this approach has been used to represent a wide variety of application-specific data, including geometric model topology, processor partitions, and various types of search trees. Tags are named data which can be assigned to the mesh as a whole, individual entities, or sets. Tags are a mechanism for attaching data to individual entities, and sets are a mechanism for describing relations between entities; the combination of these two mechanisms is a powerful yet simple interface for representing metadata or application-specific data.

References for this Section:

1. MOAB website, www.mcs.anl.gov/~fathom/moab-docs/html/index.html (accessed 03/29/2014).
2. MOAB User's Guide (4.6), located at www.mcs.anl.gov/~fathom/moab-docs/html/userguide.html (accessed 03/29/2014).

III.3 LibMesh

LibMesh provides a research platform for parallel adaptive algorithms designed to reduce the effort required to support parallel and adaptive unstructured mesh-based simulations. The simulation methodology in libMesh employs a standard cell-based discretization using adaptive mesh refinement to produce efficient meshes to resolve small solution features. The adaptive technology utilizes element subdivision to locally refine the mesh and thereby resolve different scales such as boundary layers and interior shock layers. Different finite element formulations may be applied including Galerkin, Petrov–Galerkin, and discontinuous Galerkin methods.

Parallelism is achieved using domain decomposition through mesh partitioning, in which each processor contains the global mesh but in general computes only on a particular subset. Parallel implicit linear systems are supported via an interface with the PETSc library.

References for this Section:

1. B. S. Kirk, J. W. Peterson, R. H. Stogner, and G. F. Carey. `libMesh`: A C++ Library for Parallel Adaptive Mesh Refinement/Coarsening Simulations. CFDLab at the University of Texas in Austin, *Engineering with Computers*, 22(3-4):237-254, 2006. http://dx.doi.org/10.1007/s00366-006-0049-3.

III.4 STK

The SIERRA Toolkit is a collection of software libraries that provide physics-independent capabilities needed by computational mechanics simulations. The intended domain of computational simulations are those requiring massively parallel computations, multiple coupled models with varied physics and scales, unstructured meshes with multiple types of discretization cells, and solution strategies that dynamically modify the unstructured mesh. A fundamental concept of these simulations is of a computational mesh comprised of both the spatial discretization (e.g., the elements, nodes, and connectivity) and field variables discretized over the spatial discretization.

References for this Section:

1. H. Carter Edwards, Alan B. Williams, Gregory D. Sjaardema, David G. Baur, William K. Cochran. SIERRA Toolkit Computational Mesh, Conceptual Model. SANDIA REPORT SAND2010-1192, March 2010.

III.5 MOOSE

The VERA fuel performance code, Peregrine, is built on the BISON application utilizing the MOOSE architecture. The Multiphysics Object Oriented Simulation Environment (MOOSE) is a computational framework created at the Idaho National Laboratory. MOOSE's solution algorithm utilizes the preconditioned Jacobian-free Newton Krylov method (JFNK) and typically provides rapid nonlinear convergence for a fully coupled set of partial-differential equations. MOOSE is a fully object-oriented library. MOOSE incorporates multiple parallel solution capabilities including both Message Passing Interface (MPI) and threading using the Intel Threading Building Blocks (TBB). MOOSE provides a modular, structured interface to significant parallel computational capability.

MOOSE uses several open-source libraries, including the LibMesh finite-element framework which provides parallel finite-element capability. PETSc and Trilinos provide linear and nonlinear solvers. MOOSE utilizes a semi-discrete method where the problem is discretized spatially using the finite element method and temporally using traditional finite difference methods. Element types consist of the standard geometric types: triangles, quadrilaterals, tetrahedrals, hexahedrals, prisms and pyramids. Time integration methods include implicit Euler, Crank-Nicolson and second order backward difference.

BISON is a macro-scale nuclear reactor fuel performance code developed using MOOSE. It is designed for fully-coupled multidimensional steady and transient analysis based upon a thermo-mechanical physics core. The BISON governing relations consist of fully-coupled partial differential equations for energy, species, and momentum conservation.

References for this Section:

1. http://www.inl.gov/research/moose-applications/
2. D. Gaston, C. Newman, G. Hansen, and D. Lebrun-Grandie´. MOOSE: A parallel computational framework for coupled systems of nonlinear equations. Nucl. Eng. Design, 239, p. 1768–1778, 2009.
3. R. Pawlowski, J. Turner, S. Palmtag, and R. Montgomery, "Initial Demonstration of Peregrine in VERA-CS," L2.VRI.P7.02, CASL-I-2013-0165-000, July 31, 2013.

III.6 Trilinos

A core requirement for VERA is the capability to solve linear and non-linear systems of equations, eigen-systems and other related problems while taking advantage of parallel computing capabilites. Trilinos provides robust algorithms using modern object-oriented software design, while leveraging the PETSc (and other) libraries. Trilinos provides robust parallel numerical algorithms for:

- Automatic differentiation
- Data partitioning for load balance and robustness
- Multi-level preconditioners
- Block iterative methods (linear and eigen solvers)
- Incomplete factorizations
- Solution of linear systems with successive and simultaneous right-hand-sides
- Nonlinear methods including continuation
- Large-scale optimization, e.g., SAND
- Time integration methods

References for this Section: http://trilinos.sandia.gov/about.html

III.7 PETSc

The Portable, Extensible Toolkit for Scientific Computation (PETSc) provides the solvers for VERA's CFD code, Hydra-TH. PETSc provides a set of tools for the numerical solution of partial differential equations and related problems on high-performance computers. PETSc consists of a variety of libraries and each library manipulates a particular family of objects (for instance, vectors) and the operations one would like to perform on the objects. Figure X provides an illustration of the modules within PETSc, and Figure Y presents several of the individual parts of PETSc in more detail.

References for this Section: http://www-unix.mcs.anl.gov/petsc/petsc-2

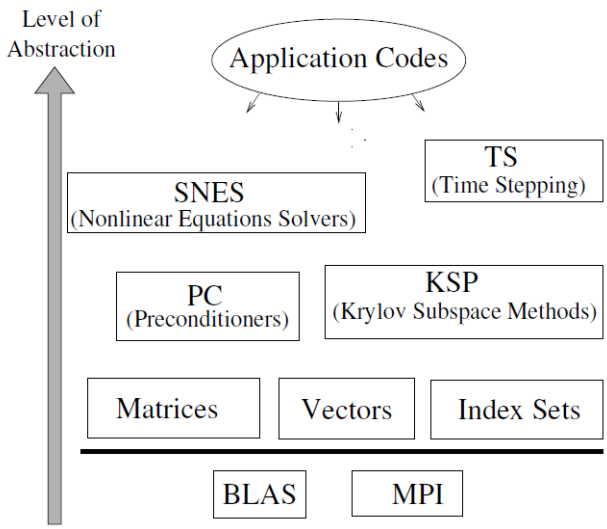


Figure 17 PETSc Library Organization

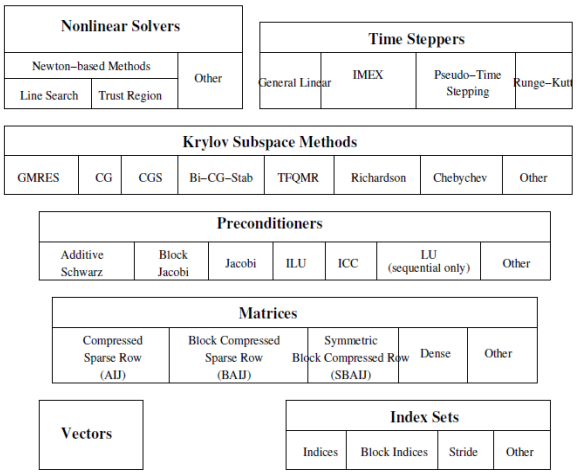


Figure 18 Parallel Numerical Libraries in PETSc

III.8 VERA Common Input (VERAin) for VERA-CS

The VERA Common Input (VERAIn) is a single common input used to drive all of the physics codes in the VERA Core Simulator (VERA-CS); including the radiation transport codes (Insilico, MPACT and Shift), the thermal-hydralics channel flow code (Cobra-TF), the fuel performance code (Peregrine), and the coolant chemistry code (Mamba2D). It is not currently used to provide input for the thermal-hydraulics CFD code (Hydra-TH).

VERAIn generates input decks for the VERA-CS physics codes, as necessary. In addition to the ease-of-use aspects, it is critical in multi-physics applications that all of the different code systems have consistent input. Having a single common input simplifies the user experience and helps ensure that all of the physics applications are solving a consistent geometry.

VERAIn provides several advantages to the users:

- Allows users to easily transfer input and output between different computer systems.
- Allows users ability to easily edit the file on remote computers.
- Provides a format that users can readily read and understand.
- ASCII input files are an approved archive format recognized by the NRC (ASCII, PDF, or TIFF).
- Allows users to “diff” input files on a variety of remote computers
- Allows users to archive inputs in standard source code repositories and/or directories with read-only permissions.

VERAIn utilizes a single ASCII input file with a free-form input format. The input file contains a description of the physical reactor geometry, including: fuel assemblies, removable poison assemblies, control rods, non-fuel structures, detectors, baffle, etc. The input file also contains a description of the current reactor statepoint including: power, flow, depletion, search options, etc.

VERAIn’s input parser reads the text input file and converts it into an XML file. Some physics components, such as Insilico and MPACT, can read the XML file directly. Other components, such as Cobra-TF and Peregrine, require an intermediate step that converts the XML file into the native code input.

The VERAIn User’s Guide is available at www.casl.gov/docs/CASL-U-2014-0014-000.pdf.

References for this Section:

1. S. Palmtag. User Manual for the VERA Input Processor. CASL-U-2014-0014-000, Oak Ridge National Laboratory, November 2013.

CHAPTER IV VERA Installation and Documentation

Using the VERA Installation Guide, build the VERA codes on your system. VERA release 2014 includes[4]:

Component	Included	Not Included	Comments
Physics Components			
COBRA-TF	X		Standalone with VERAIn input.
Insilico	X		Sn/Spn with Scale/XSProc and VERAIn input
Coupled Insilico + COBRA-TF	X		Single assembly
Hydra-TH	X		
MPACT	X		Lattice physics, no 3D
MAMBA-2D	X		
Peregrine/MOOSE/Bison	X		
Tiamat (CTF + Insilico + Peregrine)	X		
Coupled COBRA-TF + MAMBA-2D	X		
Shift	X		
Infrastructure Components and TPLs			
Trilinos	X		
TriBITS	X		
VERAIn	X		Common VERA input parser
Dakota	X		
LIME	X		
DataTransferKit	X		
MOOSE	X		
Other Required TPLs	X		As defined in the VERA Installation Guide.

The release includes the VERA physics codes included in the release. At present, the documentation includes[5]:

Component	Theory Manual	User Manual	V&V Manual	Other Documentation
COBRA-TF	Theory Manual	Users Manual Preprocessor Users Manual		List of Variables
DAKOTA	Theory Manual	Users Manual		Code Reference Manual Developers Manual
DTK	Theory Manual This is a "domain model" document		NA	
Hydra-TH	Theory Manual (Requires password)	Users Manual (Requires password)	V&V Manual (Requires password)	
Insilico	methods.pdf	(Due Mar 2014)		
LIME 1.0	Theory Manual	Users Manual	NA	
Mamba-2D				
Mamba-3D				
MPACT	(Draft in hand, restricted access) 60% compete	Users Manual 80% complete		
Peregrine				
TriBITS			NA	
VERAIn	NA	VERA Input Manual 90% complete	NA	VERA Input Parameter List

[4] https://casl-dev.ornl.gov/wiki/index.php/VERA_2014_RSICC_Release#Targeted_technical_capabilities
[5] https://casl-dev.ornl.gov/wiki/index.php/VERA_Documentation

CHAPTER V Typical Simulations Utilizing the VERA Toolset

VERA is a general purpose, versatile toolset that provides capabilities to address most steady-state normal condition problems. This section provides general guidance on the VERA tools used for typical simulations. Table 4 provides a summary of the range of the typical simulations with respect to time scale, spatial scale and physics coupling needed. Several problems have been highlighted by CASL as Challenge Problems, and can be used as example problems by the User. Links to these problems are provided within the appropriate section.

Table 4 Timescale, Spatial Scale and Physics Coupling by Challenge Problem

Simulation Topic	Time Scale (Seconds, Minutes, Hours, Days, Years)	Spatial Scale of Phenomena	Code Coupling Required
Core Performance Investigative Simulations	Y	Core to assembly	MPACT-COBRA-Peregrine
Power Uprates	Y + M to H	Core, assembly, pin	MPACT-COBRA-Peregrine
Power Ramping Study	Y + M to H	Core, assembly, pin	MPACT-COBRA-Peregrine
Reactivity-Initiated Accident (RIA)	Y + S	Core, pin	MPACT – Hydra – Peregrine
Fuel Rod Design	Y + M to H	Core, assembly, pin	MPACT/Insilico - Hydra - Peregrine
Spacer Grid Design (flow)	Y + S	System, Core, assembly, pin	Hydra/COBRA
Spacer Grid Design (neutronics)	Y	core, assembly	MPACT-COBRA-Peregrine
Structural Design	Y	assembly, pin	N/A
Normal Condition Coolant Flow Path and Velocity Simulations	Steady/Unsteady	System, core	Hydra/COBRA
Local Flow Blockage Simulations	Steady/Unsteady	System, core	Hydra/COBRA
Departure from Nucleate Boiling (DNB)	Y + S to M	System, assembly	MPACT – COBRA/Hydra – Peregrine - RELAP
Loss of Coolant Simulations	Y + S to M	System, core, pin	MPACT-COBRA-Peregrine
CRUD Deposition Calculations	Y	pin	Hydra/COBRA - MAMBA/Mamba-BDM
CRUD-induced Power Shift Calculations	Y	Core	MPACT- COBRA - MAMBA (light)
CILC Calculations	Y	Few pin-wide	MPACT/Insilico – Hydra – Peregrine – MAMBA

V.1 Core Cycle Design Simulations

The objective of a typical core performance simulation to design a core that can achieve the utility-specified energy requirements with the inventory of partially used fuel and fresh fuel while maintaining the technical specification (tech spec) limits for reactivity and safe shutdown with a low peaking and a balanced core power distribution.

Typical workflow for core cycle designs includes the use of a fast-running core simulator with a relatively coarsely meshed model to optimize the utilization of fresh and burned fuel available for the cycle. The fuel vendor typically runs hundreds of cases to optimize fuel utilization; the utility performs independent analysis with other coarser tools to verify the conclusion.

It is notable that the popular approach to PWR core cycle design is to "bound" the performance aspects of the fuel with a challenging power history and ensure that all fuel operates under the challenging power history to avoid doing extensive rod mechanics and thermal hydraulics simulations every cycle. This approach reduces the scope of a core cycle design to a neutronics-only task (usually including minimal thermal hydraulics modeling to calculate the coolant temperature and density), although there are still a few PWR units that have automated the analysis to allow explicit performance evaluations of every assembly and fuel pin for every cycle. Ref. 5 provides further discussion on the core cycle design workflow.

The analyst typically runs eighth-, quarter-, or full-core simulations to determine the combination of fuel and fuel locations that provide the cycle power and length require while maintaining necessary operating limits.

The VERA Core Simulator (VERA-CS) is used to address the majority of the core performance applications. VERA-CS is used to run standalone neutronics or coupled thermal-hydraulics channel flow and neutronics. Currently supported codes and code combinations include:

- Insilico
- MPACT
- Shift
- Coupled Insilico + Cobra-TF
- Coupled Insilico + Cobra-TF + Peregrine

Each of these codes and code combinations are set up and executed using the common input, VERAIn. The VERAIn User's Guide is available at www.casl.gov/docs/CASL-U-2014-0014-000.pdf. The User should consult the individual physic's User Guide and Theory Manual as needed to achieve an understanding of the VERAIn input parameters.

Several examples of VERA-CS applications using standalone neutronics and neutronics coupled with thermal-hydraulics are available at:

www.casl.gov/docs/VERA_Benchmarks_1-5_r2_disclaimer.pdf

www.casl.gov/docs/CASL-U-2012-0131-000.pdf

www.casl.gov/docs/CASL-U-2013-0273-000.pdf

http://www.casl.gov/docs/CASL-U-2013-0150-000.pdf

Table 5 Typical Prediction Accuracy for Core Cycle Design Analyses [Ref. 8]

Parameter	Typical Prediction Accuracy for Industry Codes	Typical Prediction Accuracy for VERA
Transient FQ Margin (%)	±5	
Maximum steady state FQ (relative difference, measured versus predicted, %)	±5	
Maximum steady state FDH (relative difference, measured versus predicted, %)	±5	
In core axial offset (%)	±3	
Relative Assembly Power (%)	±15	
Boron (ppm)	±50	
Estimated critical condition (pcm)	±500	
Control rod worth (pcm)	±10	
Control bank worth (pcm)	±100	
End of full power capability (EFPD)	±7	

V.2 Core Performance Investigative Simulations

For fuel failures that do not fit into the known issue descriptions, the utility owner-operator and the fuel vendor will initiate an Apparent Cause or Root Cause investigation. These investigations typically survey the operating history of the failed component, with increased fidelity simulations where parameters are flagged as potential causal factors. Often the investigations begin with a team review of the operating condition summary. When requested by the review team, analytical investigations typically begin with a coarse simulation to identify parameters of interest, with finer simulations initiated as identified by the coarse simulation.

For fuel failures that do not fit into the known issue descriptions, the utility owner-operator and the fuel vendor will initiate an Apparent Cause or Root Cause investigation. These investigations typically survey the operating history of the failed component, with increased fidelity simulations where parameters are flagged as potential causal factors. Often the investigations are begun with a team review of the operating condition summary. When requested by the review team, analytical investigations typically begin with a coarse simulation to identify parameters of interest, with finer simulations initiated as identified by the coarse simulation.

a. Create a coarse mesh comprehensive reactor core model utilizing coupled neutronics, thermal-hydraulics and fuel performance and simulate the operating history where the failures occurred.
b. Survey the simulation results for atypical performance predictions.
c. Survey the simulation results at the component failure location.
d. Shuffle the fuel to capture multi-cycle effects.
e. Impose power transients as desired to observe effects.
f. Impose CRUD, FSI, accelerated corrosion, manufacturing variations or defects, material property variations, or other effects as desired.
g. Identify areas for finer scale simulations and create as needed to further evaluate apparent/root cause.

VERA-CS can support a more rigorous investigation through the higher fidelity coupled capability:

- Coupled Insilico + Cobra-TF + Peregrine

It should be noted that capabilities for fast transients aren't currently available in the VERA neutronics toolset.

V.3 Power uprates and Power Escalation-related Applications

V.3.1 Power Uprates

It is desirable to operate commercial power reactors at a higher power to derive the largest return on investment. It the past, nearly all U.S. commercial power reactors have been uprated based on measurement uncertainty recapture (MUR). Many plants have also re-evaluated their design calculations and re-licensed to achieve as much as 7% higher power density. Others have replaced hardware in addition to re-evaluating and re-licensing in order to achieve uprates greater than 7%. It is possible that further uprates can be facilitated through the use of coupled physics simulation capabilities and through the implementation of science-based models that identify previously unrecognized operating margin. Note that this section does not consider hardware modifications to the plant.

The objective of the power uprate simulation is to re-evaluate plant and core performance given a proposed higher power production, to the CASL evaluation boundary (pressure vessel). Thus, a comprehensive evaluation of the potential for uprating the rated power of a nuclear unit includes many simulations. As an example, these may include:

- Anticipated typical core cycle design at the higher power density (see Section V.1),
- Evaluation of the fuel rod performance given the higher power density, including steady state normal condition performance and AOO performance (see Section V.4),
- Evaluation of the bulk coolant response to the increased power density and the feedback to the core cycle design and mechanical features such as required assembly holddown load (see Section V.6),
- Evaluation of the capability of the materials and structure to support the higher power density, including the effects of irradiation growth, irradiation creep, and thermal creep (see Section V.4, V.7),
- Evaluation of normal operating conditions and identified operating issues (pellet thermal conductivity degradation, CRUD, GTRF, distortion, etc) to determine if higher power can be supported (see Section V.2, V.7, V.8),
- Evaluation of bounding licensing conditions (RIA, LOCA, DNB, long term cooling) using a multi-physics tool to evaluate the higher power density (see Sections V.3.3, V.6.4, V.6.3)

V.3.2 Power Ramping Study

During plant start up, and as the plant is operated, movements in the control rods control the power in the core. As the control rods are moved, the local fuel rod power is influenced directly by the control rods, with large power differentials occurring near the tips of the rods. As the power is increased, the fuel pellets swell. Once the pellet-cladding gap is closed (or when the gap is small enough to allow power-related pellet swelling to contact the cladding), changes in the pellet geometry stress the fuel rod cladding. In order to avoid over-stressing the cladding during power ramping, the power is increased slowly, allowing time for the cladding to become “conditioned” to the power level. Simulations are completed using VERA-CS:

- Coupled Insilico + Cobra-TF + Peregrine

Examples using VERA-CS are available at:

R. O. Montgomery, "Peregrine: Advanced Modeling of Pellet-Cladding Interaction (PCI) Failure in LWRs," *Proceedings of the TopFuel 2012 Reactor Fuel Performance Meeting*, Manchester, U.K., Sep. 2-6, (2012).

CASL-U-2013-0165-000, Initial Demonstration of Peregrine in VERA-CS, 7/31/2013.

https://portal12.ornl.gov/sites/casl/Shared%20Documents/Workshops,%20Meetings,%20Telecons/FY13/2013-08-13%20DOE%20Annual%20Review%20(ORNL)/Documents/Milestones/2-19b%20L2_VRI.P7.02%20Report.pdf

It should be noted that capabilities for fast transients aren't currently available in the VERA neutronics toolset.

V.3.3 Reactivity-Initiated Accident (RIA)

A reactivity-initiated accident is a scenario of events that inadvertently results in the addition, or insertion, of power to the reactor. RIA events are divided into four main topics: control system failures, control rod ejections, events caused by coolant temperature and void effects, and events caused by dilution or removal of coolant poison. Of these events, the PWR control rod ejection accident (REA) is considered the limiting event in the RIA class of design basis events [Ref. 6]. A REA begins when a control rod drive mechanism housing fails, resulting in the rapid ejection of a control rod due to the pressure difference. The ejection of the control rod results in a boost of reactivity in the reactor core, causing a power excursion that must be controlled through the automatic insertion of other control rods.

To simulate the REA, the event is modeled explicitly to better understand the progression of the event and points of component failures for margin management. Using a coupled neutronics, thermal-hydraulics, and fuel performance engineering scale model, simulate power excursions and calculate the percentage of fuel rods exceeding the DNB threshold and the fuel enthalpy.

Using a fine mesh fuel performance model, determine the cladding balloon and burst performance for the rod and calculate the core-wide coolability based on the engineering scale core-wide results. Calculate fuel dispersal and fuel-coolant interaction as necessary for prediction validation and/or new fuel design studies

Simulations are completed using VERA-CS:

- Coupled Insilico + Cobra-TF + Peregrine

It should be noted that capabilities for fast transients aren't currently available in the VERA neutronics toolset.

References for this Section:

1. Nuclear Energy Agency. Nuclear Fuel Behavior Under Reactivity-initiated Accident (RIA) Conditions, State of the Art Report. ISBN 978-92-64-99113-2, NEA No. 6847, 2010.

V.4 Fuel System Design

V.4.1 Fuel Rod Design

Each U.S. fuel vendor markets several fuel designs. Fuel designs are approved for use using NRC-licensed methods, showing positive margin under a battery of regulatory-postulated normal conditions of operation, postulated accident conditions, and anticipated operational occurrences (AOOs). These evaluations address the thermal, mechanical, and materials design of the fuel system, including the control components, to provide assurance that (1) the fuel system is not damaged as a result of normal operation and AOOs, (2) fuel system damage is never so severe as to prevent control rod insertion when it is required, (3) the number of fuel rod failures is not underestimated for postulated accidents, and (4) fuel coolability is always maintained.

Calculations performed typically include cladding stress and strain (including expected pellet interaction effects), fatigue, irradiation growth, thermal creep, irradiation creep, rod internal pressure, and cladding oxidation. The objective of the calculation is to verify the integrity of the fuel rod over the range of expected normal operation and AOOs, and predict the performance for postulated accident conditions.

Standalone Peregrine and the VERA Core Simulator (VERA-CS) are used to address the majority of the fuel system design changes.

Currently supported codes and code combinations include:

- Peregrine
- Coupled Insilico + Cobra-TF + Peregrine

For a bounding calculation, the range of operating conditions, or bounding conditions, can be imposed on a single 3D or r,z fuel rod in a standalone Peregrine calculation. Alternatively, a full core simulation can be completed with coupled Insilico + Cobra-TF + Peregrine to obtain a best estimate performance for the rods.

Several examples of VERA-CS applications using standalone neutronics and neutronics coupled with thermal-hydraulics are available at:

CASL-I-2013-0122-000 and CASL-I-2013-0165-000

V.4.2 Spacer Grid Design

Most fuel assembly designs include at least 2 different spacer grids, and several designs incorporate 3 or more different spacer grids. The primary function of the spacer grid, depending on its type and location in the assembly, may include:

- maintenance of the fuel rod location in the array;
- prevention of fuel rod movement/vibration/rotation;
- providing assembly structural stability (resistance to distortion/buckling, lateral impact absorption);
- thermal hydraulic efficiency in mixing/turbulence/heat transfer;
- debris filtering.

The spacer grid design can make or break a fuel design, and optimization of the grid design can lead to better heat transfer, which can lead to many benefits ranging from enhanced safety margins to a power uprate.

Likewise, any modification to an existing spacer grid geometry can constitute a major change to the fuel design. Almost all dimensional changes to the spacer grids require re-evaluation of the assembly performance over the range of expected operation and for AOOs and HAC.

If the spacer grid is a new design, or if the modification is expected to substantially affect flow mixing, the designer is likely to perform additional analytical studies utilizing CFD. The CFD simulation can be as small as a single grid cell, or may include an entire fuel assembly. An array of assemblies may be simulated to investigate mixed core effects. A full core can be simulated to investigate the performance of the design on the periphery of the core. As the size of the problem is increased, the computing requirements are increased.

Currently supported codes and code combinations include:

- Hydra-TH

Results from explicit CFD simulations or flow testing may be used as inputs to channel flow simulations to represent the full core response. The VERA codes and code combinations used are:

- Cobra-TF
- Coupled Insilico + Cobra-TF

For new grids or grid modifications that have a potential to affect neutronics performance, the designer is likely to perform sensitivity studies to determine the effect on power and cost in enrichment. This is completed using VERA-CS as described in the Core Cycle Design section.

Currently supported codes and code combinations include:

- Insilico
- MPACT
- Shift
- Coupled Insilico + Cobra-TF

V.4.3 Structural Design

Changes to the fuel assembly structural components could include modifications to the assembly guide thimbles, top and bottom nozzles, holddown springs, structural joints, or other components that support the fuel assembly structural and coolable geometry. For these applications, the User models the elastic and plastic strain, impacts, buckling, material properties as a function of fluence/burnup.

Because the CASL tools are currently limited to PWR applications, auxiliary components such as fuel channels are not discussed at this time.

At present time, VERA does not include a physics capability to simulate these parameters for these components. Rather, VERA will in future include the capability to interface with the various commercial structural codes.

V.5 System Flow and Coolant Heat Transfer Studies

One of the key performance parameters of the commercial power reactor is the coolant flow and its ability to maintain the fuel rods below the specified temperature limits at all locations in all normal conditions and AOO. Many of the fuel assembly features are aimed at enhancing the heat transfer of the fuel rod array. Also, the flow paths and velocities of the coolant under postulated transient conditions is of interest. Many of the technical specifications and operating limits are related to coolant flow and heat transfer capability.

V.5.1 Steady and Unsteady Flow Coolant Flow Path and Velocity Simulations

The VERA toolset includes two primary thermal-hydraulic tools to simulate normal condition flow:

- Cobra-TF
- Hydra-TH

Both can address small-scale to full core simulations and cover the range of PWR normal operating conditions.

Several examples of VERA flow simulation and heat transfer applications using standalone thermal-hydraulics are available at:

http://www.casl.gov/docs/NURETH14-254.pdf

http://www.casl.gov/docs/CASL-U-2013-0198-000.pdf

http://www.casl.gov/docs/Comparison_between_CFD_Analysis_and_Experimental_Data.pdf

V.5.2 Steady and Unsteady Flow Local Flow Blockage Simulations

The VERA toolset includes two primary thermal-hydraulic tools to simulate normal condition flow:

- Cobra-TF
- Hydra-TH

Both can address small-scale to full core simulations and cover the range of PWR normal operating conditions. Cobra-TF allows for input of local pressure drop coefficients; Hydra-TH includes a porous media option that can simulate locally higher flow pressure drop, or the blockage can be simulated explicitly at a higher computational cost.

Several examples of VERA flow simulation and heat transfer applications using standalone thermal-hydraulics are available at:

http://www.casl.gov/docs/Pilot_Project_on_Fibrous_Debris_Effects.pdf

V.5.3 Departure from Nucleate Boiling (DNB)

In PWRs, the most efficient heat transfer regime occurs during nucleate boiling, and the rod and coolant are designed to operate below the critical heat flux (CHF). As the heat flux exceeds the CHF the heat transfer regimes moves from nucleate boiling to film boiling, a transition known as departure from nucleate boiling (DNB). At the onset of DNB, steam bubbles remain trapped on the surface of the rod and form a local vapor layer that dramatically increases the temperature of

the fuel rod, leading to fuel cladding failure. DNB is the limiting event in several design basis events. Currently, DNB is predicted through proprietary empirical correlations specific to each fuel design.

One of CASL's objectives is to provide demonstrations validating CASL's Hydra-TH CFD tool's predictions of DNB. This work is currently in progress. Examples of the work to date can be found at:

CASL-X-2014-0032-000, L3.AMA.CP.P8.01, Assessment of Multi-Scale Thermal-Hydraulic Codes and Models for DNB Challenge Problem Applications.

https://portal12.ornl.gov/sites/casl/Shared%20Documents/Program%20Management/Program%20Tracking/Milestone%20Tracking/FY14/PoR8/Milestone%20Evidence/L3s/AMA.CP.P8.01/L3-AMA-CP-P8-01.docx

V.5.4 Loss of Coolant Simulations

The loss-of-coolant accident (LOCA) is the basis of many of the design considerations in a nuclear power plant. For PWRs, there are two categories of LOCA: a large-break and small-break. The design basis large-break LOCA in a PWR is a double-ended guillotine break in a cold leg between the reactor coolant pump and the reactor vessel. Small break LOCAs are defined as coolant system breaks with flow areas less than 1-ft^2 in pipes with a diameter greater than 3/8"; a small break is large enough to depressurize the primary system and initiate the High-Pressure Safety Injection (HPSI) system.

The sequence of events occurring during a large break LOCA include blowdown (rapid ejection of the coolant), core voiding and shutdown, departure from nucleate boiling, stored energy redistribution and fuel heatup, HPSI cooling initiation, low-pressure injection (when system pressure is low enough), and reflood of the core. During the event some fuel rods are expected to burst, and may cause blockage of some of the flow channels during reflooding. Also, the fuel rod cladding may undergo rapid oxidation. If the core cooling is not sufficient, some of the fuel, control components, and reactor components may melt and relocate.

A small break LOCA generally does not lead to core uncovery, and is considered less severe than the large break event.

Give the sequence of events, it is clear that a very detailed simulation is required. VERA's capabilities are focused on the performance of the fuel rods during the LOCA. CASL is currently developing higher fidelity approaches to modeling fuel rod clad and fuel pellet degradation mechanisms, including fuel fragmentation, axial relocation and dispersal, cladding oxidation, cladding ballooning and rupture, breakaway oxidation, and nodular corrosion. These models will be available in the Peregrine fuel performance code, and are expected to be available in later VERA releases.

Additionally, VERA will provide interoperability with the safety analysis code RELAP to provide boundary condition inputs to the analysis. The intended coupled capability is:

- MPACT + Cobra-TF + Peregrine + RELAP

References for this Section:

2. Nuclear Energy Agency. Nuclear Fuel Behavior in Loss-of-coolant Accident (LOCA) Conditions, State of the Art Report. ISBN 978-92-64-99091-3, NEA No. 6846, 2009.

V.6 Coolant Chemistry Applications

Currently the crud is assumed to be nickel ferrite ($NiFe_2O_4$). Additional species such as NiO, Ni, Ni_2FeB0_5 will be included in later VERA releases, as well as potential zinc constituents. The boron deposited in the crud is currently assumed to be $Li_2B_4O_7$. $LiBO_2$ will be added in later VERA releases. B-10 depletion within the crud is not currently modeled and that feature is also expected to be included in later releases. In addition, more advanced thermodynamic models, thermal conductivity models, crud microstructure, crud erosion models and boiling models are under development for inclusion in MAMBA.

The User should also note that the present version does not include a method to determine the corrosion source term (currently in input to the code). Plant measurements are not adequate to establish the concentration input to BOA.

V.6.1 CRUD Deposition Calculations

CRUD deposition calculations utilize:

- Coupled Cobra-TF + Mamba2D

The VERA run is set up and executed using the common input, VERAIn. The User should consult the individual physic's User Guide and Theory Manual as needed to achieve an understanding of the VERAIn input parameters. The parameter of interest for the calculation is the local CRUD thickness as a function of time (single or multi-cycle).

The current application requires that the User calculate the power distribution of the fuel rods/fuel assemblies of interest in advance of the CRUD calculation. Future VERA releases may include additional coupled capability to eliminate this step.

An example problem calculating the local CRUD thickness is provided in:

www.casl.gov/docs/CASL-U-2013-0224-000.pdf

Deshon, J., Hussey, D., Kendrick, B., et al., "PWR Fuel CRUD and Corrosion Modeling", Advanced Fuel Performance: Modeling and Simulation, JOM Vol. 63 No. 8, 2011.

V.6.2 CRUD-induced Power Shift Calculations

The objective of the CIPS calculation Determine if CRUD deposits predicted for the proposed core cycle design will result in unacceptable CIPS. CIPS is caused by boron captured in CRUD deposits on the fuel. Therefore CIPS predictions depend on CRUD-deposition predictions, and the parameters of interested include the local power distribution as a function of time (may require multi-cycle simulations).

The VERA tool suggested for this calculation is:

- Coupled MPACT + Cobra-TF + Mamba3D

For higher fidelity, Peregrine3D is added to provide higher fidelity rod surface temperature calculations. This release of VERA does not include this capability.

An example problem calculating the local CRUD thickness is provided in:

ANC-Vipre-W-BOA:
Secker, J. R. et. al, "CASL Multi-physics PWR modeling including Crud Induced Power

CASL-U-2014-0054-001

Shift (CIPS) and Crud Induced Localized Corrosion (CILC)," Proceedings of the TopFuel 2012 Reactor Fuel Performance Meeting, Manchester, Manchester, U.K., Sep. 2-6,

(2012). http://www.euronuclear.org/events/topfuel/topfuel2012/transactions/Transactions-oral.pdf

V.6.3 CILC Calculations

CRUD deposits on the fuel in high powered locations, where the fuel temperature is already hot. The CRUD insulates the cladding and may prevent the coolant from reaching the surface of the cladding (called "dryout"). The higher temperatures induce a rapid oxidation that can produce a through-wall leak. Therefore CILC predictions depend on CRUD-deposition predictions.

The objective of the calculation is to determine if CRUD deposits predicted for the proposed core cycle design will result in CILC, with parameter of interest including the fuel rod oxidation thickness as a function of time.

The VERA tool suggested for this calculation is:

- Coupled MPACT + Cobra-TF + Peregrine3D + Mamba3D

For higher fidelity, Hydra-TH CFD is substituted for Cobra-TF to provide higher fidelity flow predictions. Optionally, Hydra-TH could be run standalone and the flow channel flow coefficients modified within Cobra-TF. This release of VERA does not include this capability.

V.7 Uncertainty and Sensitivity Studies

As the industry implements best estimate tools, it is important to understand the uncertainties inherent in the reported results. Often when a good understanding of the uncertainty is not available, a large bounding uncertainty must be applied. An important application with each of the studies mentioned in previous sections is a study of the various uncertainties related to the solution technique.

Example problems using Dakota with VERA are provided in:

CIPS with Vipre-W and BOA: http://prod.sandia.gov/techlib/access-control.cgi/2011/119445.pdf

CASL-U-2013-0184-000, Uncertainty Quantification and Data Assimilation (UQ/DA) Study on a VERA Core Simulator Component for CRUD Analysis (H. Abdel-Khalik, NCSU), 8/30/2013.

https://portal12.ornl.gov/sites/casl/Shared%20Documents/Program%20Management/Program%20Tracking/Milestone%20Tracking/FY13/PoR7/Milestone%20Evidence/L2s/VUQ.P7.02/CASL_008_L2_VUQ_P7_02.pdf

CASL-U-2013-0048-000, Apply VUQ Practices with Dakota to COBRA-TF for AMA-Relevant Problems (V. Mousseau et. al., Sandia National Lab), 4/2013.

https://portal12.ornl.gov/sites/casl/Shared%20Documents/Workshops,%20Meetings,%20Telecons/FY13/2013-08-13%20DOE%20Annual%20Review%20(ORNL)/Documents/Milestones/2-12%20L3_VUQ.SAUQ.P6.02.pdf

References for this section:

1. Brian Adams et. al. *User Guidelines and Best Practices for CASL VUQ Analysis Using Dakota* . CASL-U-2014-0038-000, March 28, 2014.

CHAPTER VI References

1. D. Kothe et. al., *CASL Program Plan, Revision 4.0*, Consortium for Advanced Simulation of LWRs, Oak Ridge National Laboratory, 9/20/12.
2. J.A.Turner, *VERA 2.3 Snapshot Report, L2:VRI.P6.01* 12/19/2012, Consortium for Advanced Simulation of LWRs, Oak Ridge National Laboratory, 01/31/2013.
3. J.A. Turner et. al., *ASCR Leadership Computing Challenge (ALCC) Request*, Consortium for Advanced Simulation of LWRs, Oak Ridge National Laboratory, 01/31/2013.
4. *Not used*.
5. SCALE: A Comprehensive Modeling and Simulation Suite for Nuclear Safety Analysis and Design, ORNL/TM-2005/39, Version 6.1, Oak Ridge National Laboratory, Oak Ridge, TN (June 2011). Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-785.
6. M. Christon, *Hydra-TH Theory Manual*, Los Alamos National Laboratory, 2011.
7. The Dakota project, Sandia National Laboratory, retrieved 2/2013, from http://dakota.sandia.gov/.
8. B. Collins, *MPACT User Manual v1.0.0*, University of Michigan, Ann Arbor, January 18, 2013.
9. Cobra-TF Users Manual, Pennsylvania State University, 2012.
10. *Not used*.
11. *Not used*.
12. *Not used*.
13. J. Secker and P. Turinsky, *CASL CRUD CP Implementation Plan (draft)*, Consortium for Advanced Simulation of LWRs, Oak Ridge National Laboratory, 1/2013.
14. Wang, G.; Byers, W.A.; Karoutas, Z.E.; Young, M.Y.; Jacko, R.J. [WEC]; Hochreiter, L.E. [Penn. State Univ.], "Single Rod Heat Transfer Tests to Study the Effects of Crud Deposition," 14th Intl. conf. on nuclear engineering (ICONE 14), 17-20 Jul 2006.
15. G. Wang, W. A. Byers, M. Y. Young, and Z. E. Karoutas, "Westinghouse Advanced Loop Tester (WALT) Update," ASME Conf. Proc. 2008, 469 (2008), DOI:10.1115/ICONE16-48480.
16. Z. Karoutas, *CFD Turbulence Force Calculations and Grid-to-Rod Fretting Simulation (*CASL-I-2012-0135-000) , Consortium for Advanced Simulation of LWRs, Oak Ridge National Laboratory, 12/15/2012.
17. L2:MPO.P5.03, R.O. Montgomery et. al., *Peregrine: Initial Verification and Benchmark Evaluations against Halden Fuel Rod Data and Falcon*, August 2012.
18. R. Williamson, J. Hales, S. Novascone, M. Tonks, D. Gaston, C. Permann, D. Andrs, and R. Martineau, "Multidimensional multiphysics simulation of nuclear fuel behavior," Journal of Nuclear Materials 423(2012) 149-163.

19. D. Gaston, C. Newman, G. Hansen, and D. Lebrun-Grandie´. MOOSE: A parallel computational framework for coupled systems of nonlinear equations. Nucl. Eng. Design, 239, p. 1768–1778, 2009.
20. Fuel Analysis and Licensing Code: Falcon MOD01: Volume 1: Theoretical and Numerical Bases, EPRI, Palo Alto, CA: 2004. 1011307.
21. S. Hess, *VERA Requirements Document (VRD) - Revision 1*, CASL-2011-0074-000-CI.
22. NRC, Standard Review Plan for the Review of Safety Analysis Reports for Nuclear Power Plants: LWR Edition (NUREG-0800, Formerly issued as NUREG-75/087).
23. 10 Code of Federal Regulations 50.59, *Changes, tests and experiments*.
24. G. Swindlehurst, *Challenge Problem Implementation Plan: RIA*, CASL-I-2013-0060-000 (draft for comment), 6/9/2013.
25. J. Secker, *Challenge Problem Charter:Crud Challenge Problem*, CASL-I-2013-xxxx-000, 1/2013.