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An approach for coupled-code multiphysics core simulations from a common input

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ABSTRACT

This paper describes an approach for coupled-code multiphysics reactor core simulations that is being developed by the Virtual Environment for Reactor Applications (VERA) project in the Consortium for Advanced Simulation of Light-Water Reactors (CASL). In this approach a user creates a single problem description, called the "VERAIn" common input file, to define and setup the desired coupled-code reactor core simulation. A preprocessing step accepts the VERAIn file and generates a set of fully consistent input files for the different physics codes being coupled. The problem is then solved using a single-executable coupled-code simulation tool applicable to the problem, which is built using VERA infrastructure software tools and the set of physics codes required for the problem of interest.

The approach is demonstrated by performing an eigenvalue and power distribution calculation of a typical three-dimensional 17 × 17 assembly with thermal–hydraulic and fuel temperature feedback. All neutronics aspects of the problem (cross-section calculation, neutron transport, power release) are solved using the Insilico code suite and are fully coupled to a thermal–hydraulic analysis calculated by the Cobra-TF (CTF) code. The single-executable coupled-code (Insilico-CTF) simulation tool is created using several VERA tools, including LIME (Lightweight Integrating Multiphysics Environment for coupling codes), DTK (Data Transfer Kit), Trilinos, and TriBITS. Parallel calculations are performed on the Titan supercomputer at Oak Ridge National Laboratory using 1156 cores, and a synopsis of the solution results and code performance is presented. Ongoing development of this approach is also briefly described.

1. Introduction

VERA, a "Virtual Environment for Reactor Applications", is a collection of software being developed under DOE sponsorship by CASL, the Consortium for Advanced Simulation of Light Water Reactors (U.S. DOE, 2011). A central goal of VERA development is to "*predict, with confidence, the performance of nuclear reactors through comprehensive, science-based modeling and simulation technology that is deployed and applied broadly throughout the nuclear energy industry to enhance safety, reliability, and economics.*"

As part of the CASL project an approach has been developed to enable coupled-code multiphysics simulations of various reactor core problems of interest. This approach is embodied within an analysis capability called VERA-CS that utilizes a subset of VERA components. The objective is for a user to have the ability to define, set-up, and solve a variety of different challenging reactor-core multiphysics problems by following a simple workflow:

Abbreviations: ASCII, American Standard Code for Information Interchange; BWR, boiling water reactor; CASL, Consortium for Advanced Simulation of Light Water Reactors; CFD, computational fluid dynamics; CRUD, corrosion related unidentified deposit, a term used to describe radioactive scaling that builds up on internal reactor components; CTF, COBRA-TF, coolant-boiling in rod arrays – two fluids; GUI, graphical user interface; JFNK, Jacobian-free Newton–Krylov nonlinear solver; ORNL, Oak Ridge National Laboratory; PWR, pressurized water reactor; T/H, thermal–hydraulic; TPLs, third-party libraries, e.g. BLAS; TriBITS, tribal build, integrate, and test system; VERAIn, VERA common input file; VERA, Virtual Environment for Reactor Applications; VERA-CS, Virtual Environment for Reactor Applications – Core Simulator; VUQ, verification and uncertainty quantification; XML, extensible markup language; XSLT, extensible style sheet language transformation.

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1. Choose from a collection of single or coupled-code physics codes as appropriate for the problem of interest,
2. Create a single common input file description for the problem of interest, and
3. Perform a complete simulation, start to finish, with essentially no manual intervention on serial or parallel computing platforms appropriate for the problem size.

There are several important elements that are required to accomplish the objective. They include:

- The availability of a suite of standalone or coupled physics codes that can efficiently solve the various problems of interest.
- An approach and associated software tools to couple different physics codes together (as needed) to solve the multiphysics problems of interest.
- The definition of a common input file that can accommodate the information needed by all participating codes.
- Input adapters to process the common input file and generate all code-specific input files that will be required by the participating physics codes.
- The ability to easily submit a problem for execution on a desired computational platform.

In subsequent sections of this paper each element in this approach is described in greater detail.

Current capabilities are demonstrated by performing an eigenvalue and power distribution calculation of a representative three-dimensional 17 × 17 PWR assembly with thermal–hydraulic and fuel temperature feedback.

2. Elements of the approach

2.1. VERA physics codes

As a whole, VERA consists of a large collection of different computer codes, utilities and software components that address a range of computational needs for reactor modeling and simulation. Conceptually indicated in Fig. 1, VERA can be divided into two broad categories:

- Infrastructure Components and Third Party Libraries (TPLs): The computational infrastructure (e.g. code-coupling and VUQ related software, etc.) and software development environment including compilers and TPLs.

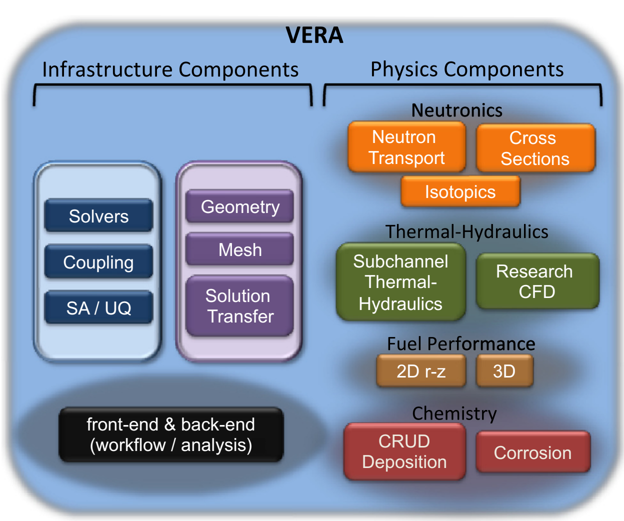

Fig. 1. VERA consists of a collection of application codes and software components.

- Physics Components: These include standalone, integrated and coupled-code multiphysics applications representing component models which together model nuclear reactor performance.

Physics-related VERA application codes can themselves be grouped into several modeling sub-categories; neutronics, thermal–hydraulics, fuel performance, and chemistry:

- Neutronics includes neutron transport modeling (of various degrees of fidelity and cost), cross section calculations, isotopic decay and depletion calculations, fission-based energy release and so forth. Neutronics-related physics codes in VERA include Insilico (see Mervin, 2013), Scale (Bowman, 2011; Oak Ridge National Laboratory, 2011) and MPACT (Kochunas et al., 2013).
- Thermal-hydraulics spans the topics of single and two-phase turbulent flow modeling, conduction, convective and boiling heat transfer, pressure drop modeling, high-fidelity CFD codes as well as engineering-type subchannel codes. Thermal–hydraulics related codes in VERA include the Cobra-TF (CTF) (Avramova, 2009; Salko and Avramova, 2012; Salko et al., this issue) subchannel code and the Hydra-TH (Nourgaliev et al., 2013) CFD code.
- Fuel Performance concerns the thermal–mechanical response of reactor fuel rod materials as well as the time-dependent changes in material properties and morphology that occur to the fuel during the operation of a reactor. The Peregrine fuel performance code (a variation of Bison (Hales et al., 2013), is currently being developed and incorporated into VERA.
- Chemistry issues of particular importance to VERA include the chemical mechanisms causing corrosion and CRUD buildup that contribute to clad failures and/or affect power shape changes. The MAMBA (Kendrick and Barber, 2012) code is currently being developed and incorporated into VERA to address these chemistry issues.

2.2. Multiphysics coupling

To computationally simulate a reactor problem, relevant physical processes are described by models and equation sets that define how the important state variables (e.g. temperature, density, velocity, neutron flux, etc.) behave over the spatial and temporal domain of relevance. When these physical processes interact with one another we say they are "coupled", and the equations must be solved so that changes in any state variable are properly reflected in all equation sets that are affected by that variable. If the effect of changes in variable "X" on the evolution of variable "Y" is small, then the coupling is said to be weak. Conversely, if the effect is large, then the coupling is said to be strong. Another important aspect of coupling is whether the effect is a linear effect, or a nonlinear effect. The most challenging problems to model accurately are those where the coupling is both strong and nonlinear. Another potential challenge is that the degree of weak versus strong coupling can vary over time in a transient simulation.

Note that when describing multiphysics simulations, we use the word "coupled" in two related but different contexts; one with respect to physics, and one with respect to computer codes. One computer code might be written to solve only one set of physics, but another might be designed to internally solve several coupled physical processes (i.e. a single physics code is not restricted to a single physics). The reactor core problems being targeted for solution with VERA-CS involve a range of physics including thermal–hydraulics, fuel performance, and various aspects of neutronics. For some problems a single physics code is capable of modeling the applicable phenomenon. However, for other problems of interest the important phenomena will span a range of physics