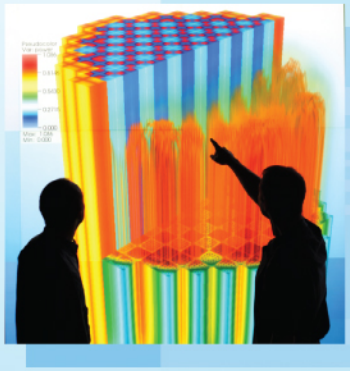
Power uprates
and plant life extension

CASL-U-2014-0041-0000

Consortium for Advanced Simulation of LWRs



Engineering design
and analysis

Milestone L3.VUQ.V&V.P8.04

PERCEPT Capabilities in CASL Dakota

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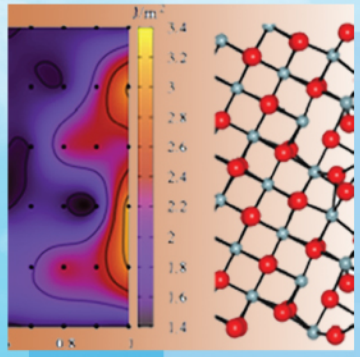
Science-enabling
high performance
computing



Fundamental science

Plant operational data

March 31, 2014

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

L3.VUQ.V&V.P8.04 : PERCEPT Capabilities in CASL Dakota

Russell Hooper

March 28, 2014

This report describes how Validation and Verification (V&V) will be automated inside of VERA. It is motivated by an initial solution verification study of a simplified version of Progression Problem 6 represented by solving only the thermal-hydraulic physics via Cobra-TF (CTF). This is simplification replaces the coupling to Insilico neutronics with a fixed uniform power specified from input. The approach we use and the utilities we develop to perform this study comprise the starting point for building a more general and automated V&V capability in CASL VERA.

1 Approach

We perform a solution verification study of the CTF-only version of Problem 6 by generating a sequence of meshes of various refinements in the axial direction. Initially we employ a manual process of calculating the appropriate axial locations defining a mesh characterized by size Δz and placing this information in the Problem 6 VERA Common Input within the block `EDITS/axial_edit_bounds`. We then use the VERA Common Input toolchain to convert this text file first into a corresponding xml file and then into a CTF input deck. This is accomplished using the following sequence of steps:

```
VERAInExt/verain/scripts/react2xml p6a_sa_1300_vuq_1.0.inp vera.xml

BUILDS/PSSDriversExt/VRIPSS/drivers/cobra_preproc/xml2ctf \
    --xmlfile=vera.xml
```

This produces a native CTF input deck, `deck.inp`, which we then run CTF with by invoking:

```
BUILDS/COBRA-TF/cobra_tf/ctf_src/cobratf
```

We choose as our Quantity of Interest (QoI) the total pressure drop across the assembly, `TotalPressure`. This is the same QoI used in the studies performed in L3.VUQ.V&V.P8.01 and documented in the CASL Dakota User Manual contained therein. Thus, this choice allows for a consistent quantitative relationship of this convergence study to broader VUQ capabilities and studies.

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2 Solution Verification without Spacer Grids

We initially approach our solution verification study by making one additional simplification to the CTF-only version of Problem 6. We choose to neglect the presence of spacer grids within the assembly. We do this for two reasons. First, the way in which CTF treats spacer grids prevents spatial refinement of the spacer grid domains because the associated loss coefficients are based on a particular spacer grid thickness consisting of a single axial mesh element. The second reason has to do with defining a single value for mesh size. The single assembly configuration of Problem 6 has distances between spacer grids and the top and bottom plenum caps different than the distance between the spacer grids themselves. Because an integer number of axial mesh elements are required to fit between the grids and plenums, the same value for Δz cannot be used for all regions in general.

We obtained from the PHI focus area a VERA Common Input file for Problem 6 which after removing the presence of spacer grids consisted of an axial mesh of 44 elements with $\Delta z = 8.225$ cm. We then scaled this element size to produce meshes of different refinements. Table 1 summarizes the meshes considered in this study along with values for the TotalPressure QoI obtained using each. In order to assess

factor f	Δz (cm)	# Axial elems	TotalPressure (bar)
0.5	4.160	87	0.68788
0.75	6.240	58	0.68759
1.0	8.225	44	0.68731
1.5	12.479	29	0.68673
2.0	16.450	22	0.68620

Table 1: Meshes used in solution verification study.

order-of-convergence of the CTF solution we use a simplified model for Robust-Multi-Regression (RMR) given as follows:

$$P = \bar{P} + a\,(\Delta z)^b \tag{1}$$

where $\bar{P}$ is an estimate for the true value of TotalPressure at infinite mesh refinement. A simple regression fit to this expression using the data in Table 1 provides values $(\bar{P}, a, b) = (0.688511, -0.000163315, 0.94627)$. From these, we can define the discretization error as

$$E = P - \bar{P} = a\,(\Delta z)^b \tag{2}$$

which is plotted against Δz in Figure 1. The exponent of the error dependence on Δz of 0.95 agrees very favorably with the expected theoretical value of 1.0 for CTF.

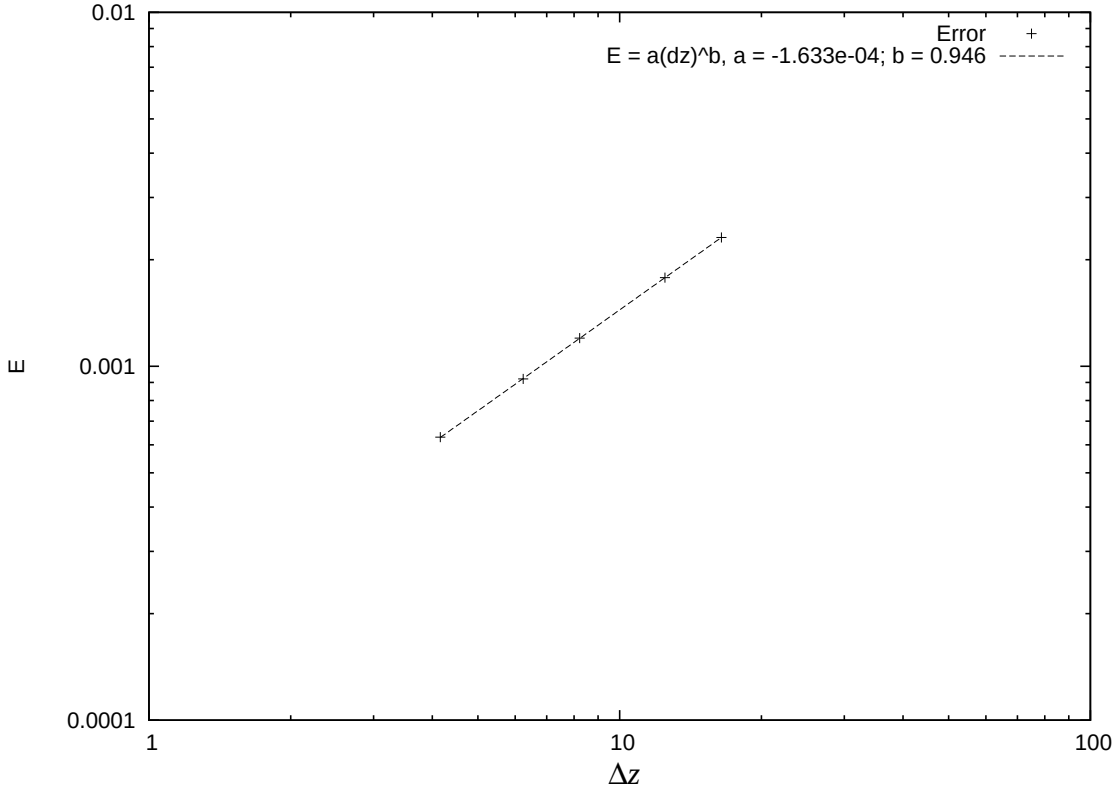

Figure 1: Observed order-of-accuracy for CTF-only Problem 6 without spacer grids. The dashed line is a least-squares fit to the numerical error.

3 Solution Verification with Spacer Grids

This section repeats the solution verification study of the previous section but now includes the presence of the spacer grids. We construct a series of meshes of different refinements again using the scaling parameter applied now to each region outside and between the spacer grids, i.e. the active fuel regions along the assembly axis. Table 2 summarizes the characteristics of these meshes. It is clear from Table 2 that there is no unambiguous way to specify the mesh size with a single parameter. However, we consider two possible choices: $\Delta z \sim f$ and $\Delta z \sim 1/\mathrm{N}_{tot}$. Applying eq.(1 using these values for Δz produces the following fits for the parameters, respectively: Figure 2 shows the best-fit to the error model using the two definitions for Δz. The trend that emerges from this plot is that neither characterization of mesh refinement is adequate for recovering near-theoretical order-of-convergence. In this case, the error model needs to be enriched to include multiple mesh sizes with an upper bound being one for each active fuel region along the assembly axis. Work is underway to expand use of RMR in CASL VUQ to accommodate meshes characterized by multiple characteristic sizes.

factor f	Reg. 1		Reg. 2		Reg. 3		Reg. 4		Reg. 5		Reg. 6		Reg. 7	
	Δz	N_z	Δz	N_z	Δz	N_z	Δz	N_z	Δz	N_z	Δz	N_z	Δz	N_z
0.5	4.106	14	4.033	12	4.033	12	4.033	12	4.033	12	4.033	12	3.961	12
0.75	5.748	10	6.049	8	6.049	8	6.049	8	6.049	8	6.049	8	5.658	8
1.0	8.211	7	8.065	6	8.065	6	8.065	6	8.065	6	8.065	6	7.921	5
1.5	11.50	5	12.10	4	12.10	4	12.10	4	12.10	4	12.10	4	9.902	4
2.0	14.37	4	16.13	3	16.13	3	16.13	3	16.13	3	16.13	3	13.20	3

Table 2: Meshes used in solution verification study with spacer grids.

factor f	$1/N_{tot}$	Total Pressure (bar)
0.5	0.01163	1.16978
0.75	0.01724	1.17115
1.0	0.02381	1.17304
1.5	0.03448	1.17451
2.0	0.04545	1.17722

Table 3: Total Pressure (bar) QoI results for verification study with spacer grids.

Δz	$\overline{P}$	a	b
f	1.16522	0.00737216	0.682181
$1/N_{tot}$	1.16576	0.119701	0.763406

Table 4: Best-fits for eq.(1) for verification study with spacer grids.

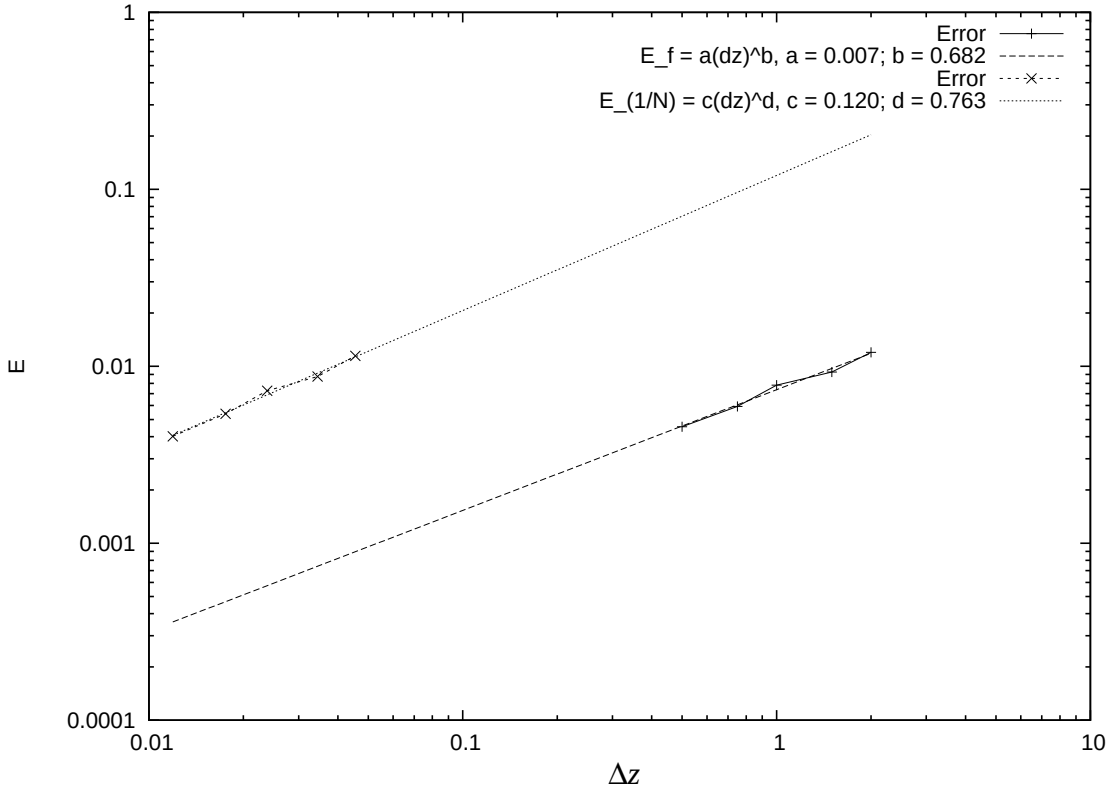

Figure 2: Observed order-of-accuracy for CTF-only Problem 6 without spacer grids. The dashed line is a least-squares fit to the numerical error.

4 Conclusions & Future Work

Because this study represents a first-in-kind capability in CASL VUQ, we learned several things in the course of performing it and identified several items that should be considered for future work. These include the following:

- Much if not all of the generic utilities contained in the C++ xml preprocessor in the VERA Common Input toolchain could be incorporated into the existing collection of python utilities contained in CASL VUQ.
- The RMR utility should be fully unit tested and a representative set of examples provided that demonstrate and provide guidance on how best to use and interpret the rich set of output that RMR provides.
- The solution verification studies contained in this report should be formally added to the automated testing within the VUQDemos product in VERA.

- The ability to extract fields, both scalar and vector, from vtk and hdf5 output should be added to CASL VUQ to enable a broader set of QoI's and for use in norms calculations

- At present CTF does not allow meshes containing more than 100 axial elements. Work is underway to relax this restriction. In spite of this, the behavior exhibited in Figure 1 suggests behavior within the asymptotic regime for theoretical convergence. Finer meshes should be explored when feasible.

- In addition to generalizing use of RMR to accommodate meshes of multiple characteristic sizes, there is also a need to address the contributions to numerical error associated with fixed sources, e.g., numerical errors related to spacer grids which cannot be refined. One idea to address this is to perform a parameter sensitivity study for the loss coefficients and use this value to infer relative contributions to $\bar{P}$ related to the presence of the spacer grids. Contributions from individual spacer grids could likewise be inferred via independent sensitivity calculations for each spacer grid.