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Integration of Dakota into the NEAMS Workbench

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Abstract

This report summarizes a NEAMS (Nuclear Energy Advanced Modeling and Simulation) project focused on integrating Dakota into the NEAMS Workbench. The NEAMS Workbench, developed at Oak Ridge National Laboratory, is a new software framework that provides a graphical user interface, input file creation, parsing, validation, job execution, workflow management, and output processing for a variety of nuclear codes. Dakota is a tool developed at Sandia National Laboratories that provides a suite of uncertainty quantification and optimization algorithms. Providing Dakota within the NEAMS Workbench allows users of nuclear simulation codes to perform uncertainty and optimization studies on their nuclear codes from within a common, integrated environment. Details of the integration and parsing are provided, along with an example of Dakota running a sampling study on the fuels performance code, BISON, from within the NEAMS Workbench.

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CONTENTS

1. INTRODUCTION

This report summarizes a NEAMS (Nuclear Energy Advanced Modeling and Simulation) project focused integrating Dakota into the NEAMS Workbench. The NEAMS Workbench[1], developed at Oak Ridge National Laboratory, is a new software framework that provides a graphical user interface, input file creation and parsing, input validation, job execution, workflow management, and output processing for a variety of nuclear codes. Dakota [2] is a tool developed at Sandia National Laboratories that provides a suite of uncertainty quantification and optimization algorithms. Providing Dakota within the NEAMS Workbench allows users of nuclear simulation codes to perform uncertainty and optimization studies on their nuclear codes from within a common, integrated environment. Details of the integration and parsing are provided, along with an example of Dakota running a sampling study on the fuels performance code, BISON, from within the NEAMS Workbench.

The outline of this report is as follows: the remainder of this section describes the NEAMS Workbench, Dakota, and BISON in more detail. Section 2 outlines the implementation details, and Section 3 presents results of a Dakota study performed using the NEAMS Workbench.

1.1 NEAMS Workbench

Preparing valid input files is a significant challenge with many nuclear codes. There are several reasons for this: the volume of data required is extensive (e.g., cross section libraries, chemical compositions, nuclide information), the formats of legacy codes are often strict (e.g. a material composition must start on line 7, column 18, and be in scientific notation with 3 significant digits), and the input requirements are often not documented sufficiently or are not easy to find. To address this and provide a common graphical environment from which multiple code inputs can be specified, run, and post-processed, the NEAMS Workbench was developed over the past year.

The NEAMS Workbench is an evolution of the SCALE code system's [3] Fulcrum user interface and provides the capability to create and process input files for various nuclear codes including SCALE [3], ARC [4], and BISON [5], parse the inputs into a parse tree, validate the inputs, run the code with the given input file, and process the output.

In more detail: the input processing involves lexical and syntactical analysis resulting in the generation of a parse tree. The lexical analysis involves the conversion of a sequence of characters to tokens understood by a particular application. The syntactical analysis involves converting the sequence of tokens into a parse tree understood by a particular application. Once the parse tree is generated, it can be interpreted and validated. The validation step involves comparing an input schematic, a.k.a. schema, to the input file created by the user to see if the content (and the structure of the content) is correct. The NEAMS Workbench uses the hierarchical input validation engine (HIVE) to perform this check interactively while the user is making changes. For example, HIVE allows an integrated application to describe the application's input using rules such as "MinOccurs" and "MaxOccurs" which will check that particular input components have a minimum and maximum number of occurrences in an input file, respectively.

The NEAMS Workbench also allows the use of templates, which help users quickly create an input file from scratch or add new blocks of text to existing files. Finally, the NEAMS Workbench has capabilities such as context aware input auto-complete which allows a user to obtain a listing of available input parameters for a given section or context in the input.

Once the steps of parsing, processing, and validating the user input file is complete, the user can then use the NEAMS Workbench capabilities to run the particular input file with the specified nuclear simulation code and analyze the results. The output processing capabilities include plotting capabilities (e.g. bar, line, scatterplots) as well as color maps. The color maps are used to display tabular or matrix information such as covariance or correlation matrices, where the value of the correlation is mapped to a particular color bin.

The capabilities of the NEAMS Workbench have been developed under the NEAMS program this past year. They allow a user to quickly create an input file and start running the nuclear simulation code. The NEAMS Workbench has been designed for interoperability across a range of codes and computing platforms, with goals of lowering the barriers to running these codes (especially legacy codes) in a common framework making for a more consistent user experience across applications accelerating results post-processing making code comparisons easier.

1.2 Dakota

Dakota is a suite of iterative mathematical and statistical methods that interface to computational simulations [1]. Dakota's goal is to make parametric explorations of simulations practical for a computational design-analyze-test cycle. Dakota is an open-source software toolkit (https://dakota.sandia.gov) and has algorithms for optimization, uncertainty quantification, parameter studies, and model calibration.

One of the primary advantages that Dakota has to offer is access to a broad range of iterative capabilities through a single, relatively simple interface between Dakota and a simulator. In this context, we interfaced Dakota to BISON. To perform different types of analyses, it is only necessary to change a few commands in the Dakota input and start a new analysis. The need to learn a completely different style of command syntax and the need to construct a new interface each time you want to use a new algorithm are eliminated. Dakota has been used for various UQ and calibration studies within the NEAMS program [7-9]. For more details on the Dakota-BISON coupling, see [10].

1.3 BISON

BISON is an implicit, parallel, fully-coupled nuclear fuel performance code under development at the Idaho National Laboratory (INL) [5]. BISON is built on the MOOSE computational framework [6] which allows for rapid development of codes involving the solution of partial differential equations using the finite element method. Nuclear fuel operates in an environment with complex multiphysics phenomena, occurring over distances ranging from inter-atomic spacing to meters, and time scales ranging from microseconds to years. This multiphysics behavior is often tightly coupled and many important aspects are inherently multidimensional.

BISON is able to simulate tightly coupled multiphysics and multiscale fuel behavior, for 1D, 2D, and 3D geometries.

2. DAKOTA IMPLEMENTATION INTO THE WORKBENCH

The overall software framework for the integration of both Dakota and BISON into the NEAMS Workbench is shown in Figure 1. As shown in Figure 1, the NEAMS Workbench provides a top layer with various capabilities for user input parsing, processing, and validation. The particular codes available to the user to execute are below that, with the interface depicted by the solid black lines. For Dakota to run the application code, Dakota itself needs an interface with the application code for a particular study (e.g. sampling), the coupling between Dakota and BISON is represented by the dashed line.

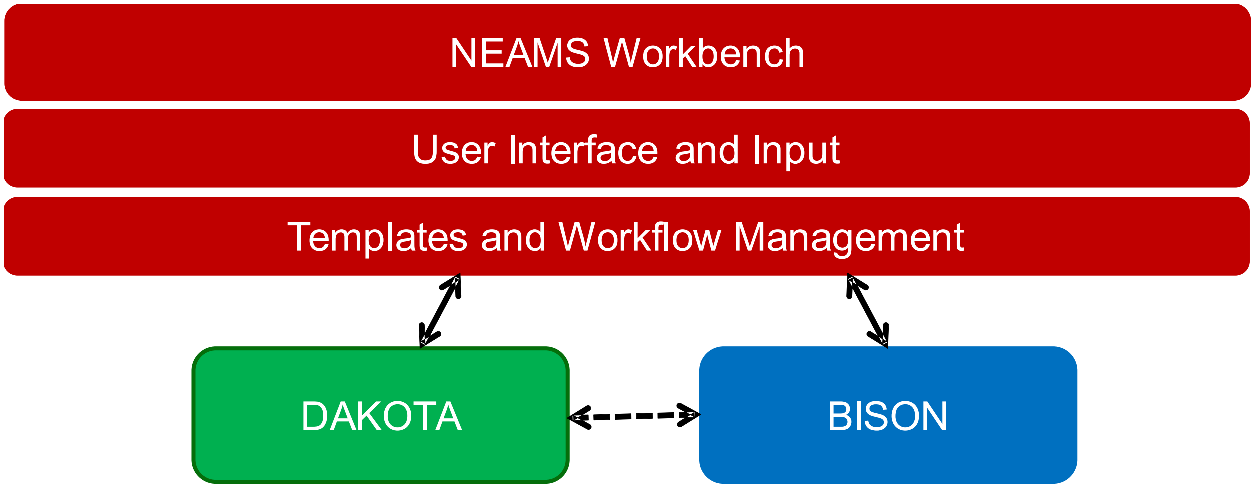


Figure 1. *Overall Structure of NEAMS Workbench, Dakota, and BISON.*

Dakota's input file requirements are specified in an XML-formatted file, dakota.xml. Currently, there are two possible approaches by which the NEAMS Workbench provides user access to Dakota input. Before the Dakota input can be parsed and processed, the input requirements must be known. This is done by translating the input requirements available in dakota.xml into a schema format supported by the NEAMS Workbench. This is currently accomplished with a Python script, as shown in Figure 2, which generates a Standard Object Notation (SON)-formatted schema. This is subsequently used with the Hierarchical Input Validation Engine (HIVE) to validate Dakota input. With the input requirements known, the user input can be processed using two approaches. The first uses the SON-formatted schema with the NEAMS Workbench integrated Definition-Driven Interpreter (DDI) to process all Dakota's NIDR-formatted input as depicted in Figure 2. There are 3 existing exceptions to the Dakota's NIDR input processing using DDI. Specifically, Dakota input alias, short-hand, and relaxed-order are not yet supported. The second approach is using a syntactically unambiguous SON-formatted user input. This SON-formatted input contains the same input data but with clear section delimiters which aid the user and the NEAMS Workbench in interpreting the input. These delimiters are subsequently removed by the NEAMS Workbench Dakota runtime wrapper leaving the regular NIDR-formatted input which Dakota itself processes, as depicted in Figure 2.

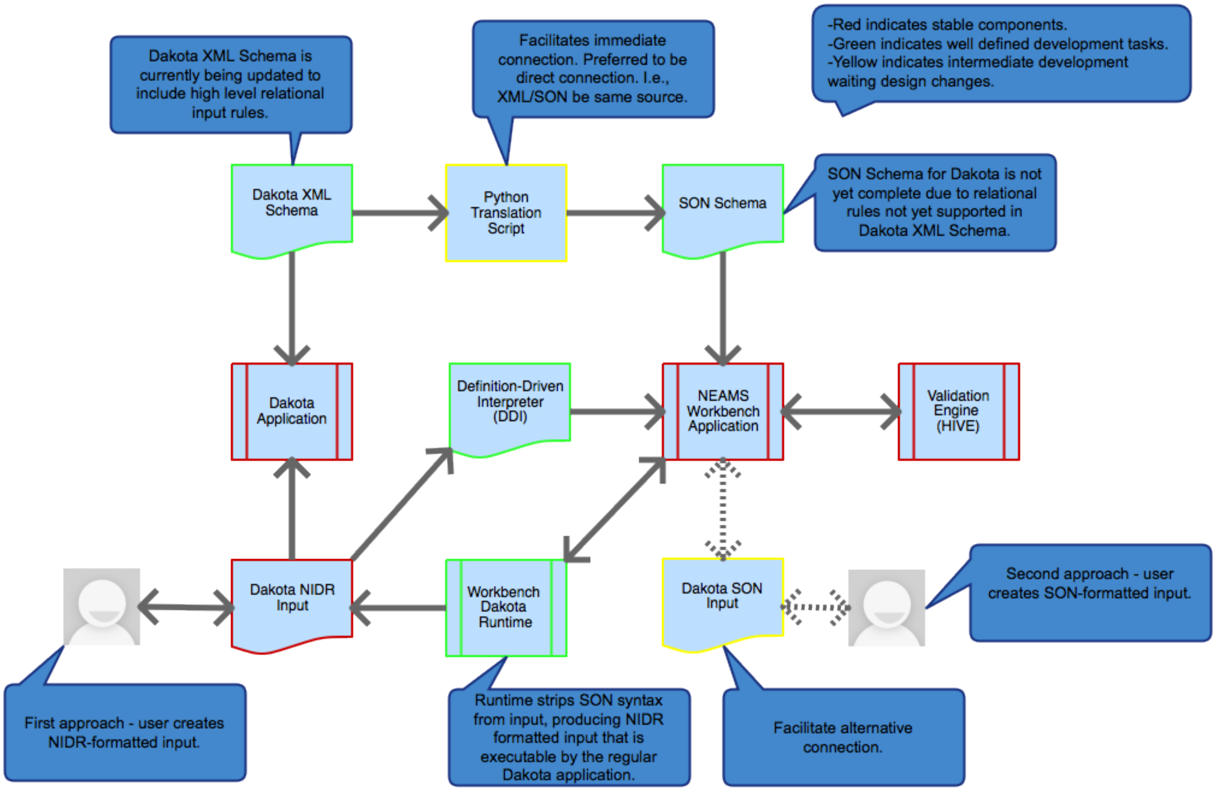
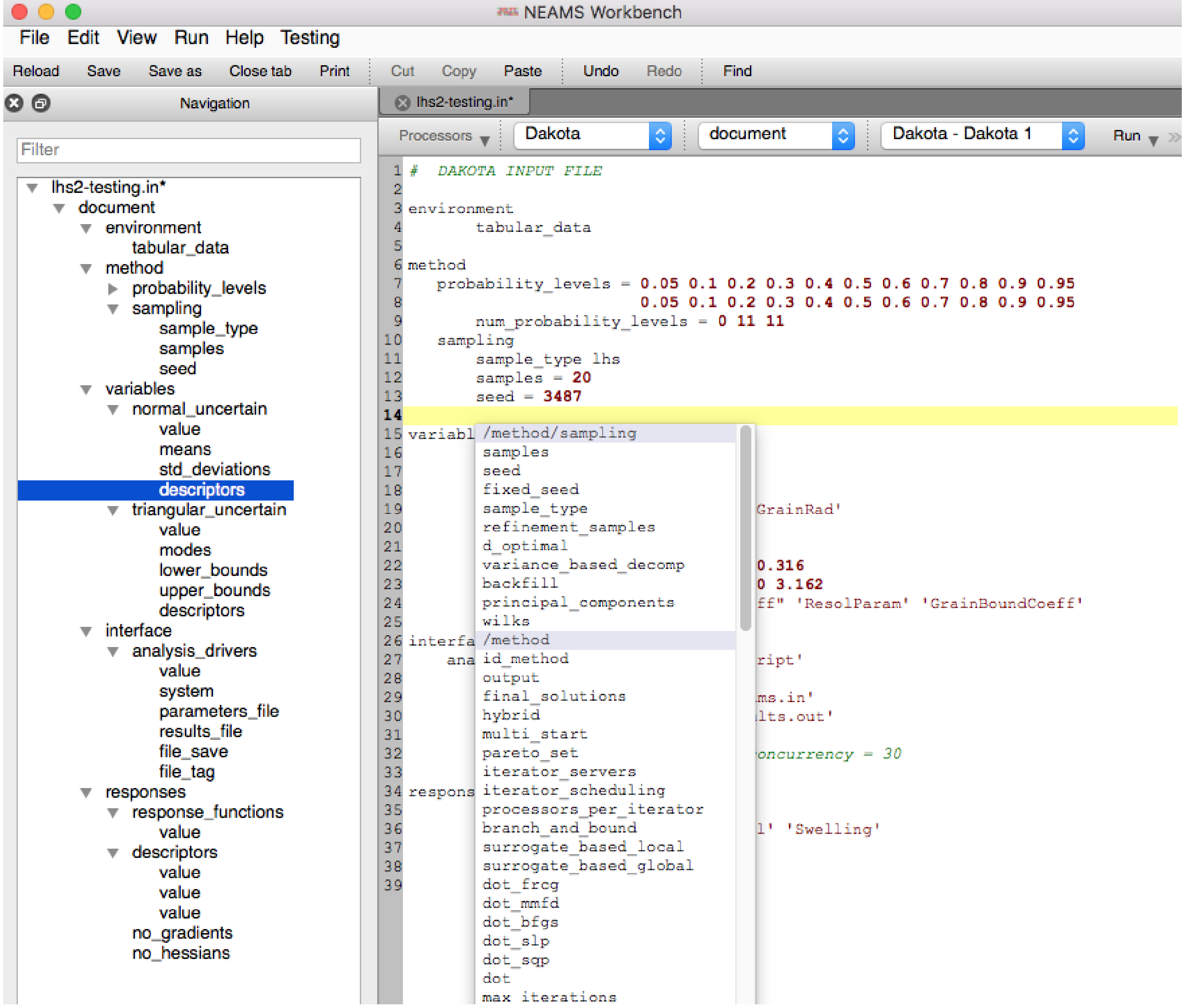

Dakota XML Schema is currently being updated to include high level relational input rules.
Facilitates immediate connection. Preferred to be direct connection. I.e., XML/SON be same source.
-Red indicates stable components.
-Green indicates well defined development tasks.
-Yellow indicates intermediate development waiting design changes.
Dakota XML Schema
Python Translation Script
SON Schema
SON Schema for Dakota is not yet complete due to relational rules not yet supported in Dakota XML Schema.
Dakota Application
Definition-Driven Interpreter (DDI)
NEAMS Workbench Application
Validation Engine (HIVE)
Dakota NIDR Input
Workbench Dakota Runtime
Dakota SON Input
Second approach - user creates SON-formatted input.
First approach - user creates NIDR-formatted input.
Runtime strips SON syntax from input, producing NIDR formatted input that is executable by the regular Dakota application.
Facilitate alternative connection.

Figure 2. *Input flow, parsing, and schema handling for Dakota within the Workbench.*

3. NEAMS WORKBENCH DEMONSTRATION WITH DAKOTA

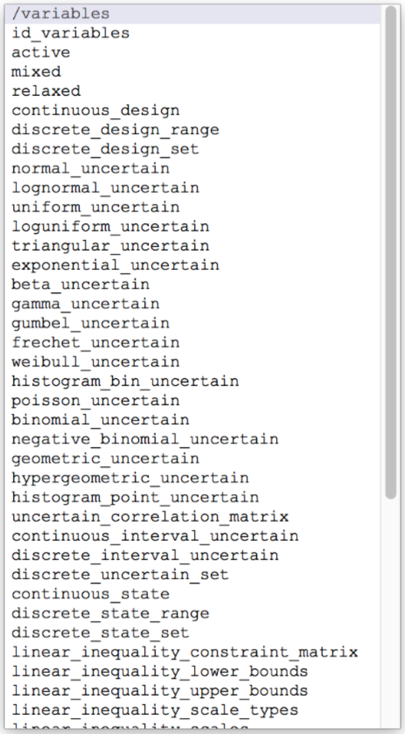
We present the use of the NEAMS Workbench to create a BISON input file and a Dakota input file, and then to run a UQ study with Dakota on BISON within the NEAMS Workbench. Figure 3 shows a Dakota input file displayed in the NEAMS Workbench. This particular file is running a Latin Hypercube Sampling study on various fuel performance parameters for BISON.

Figure 4 shows some of the context dependent help that the NEAMS Workbench can provide once the schema for a particular code is provided. For this example, the user may want to decide amongst several types of random variables to choose the most appropriate one to represent a particular input. This is a way for the user to quickly and easily see what options are available and how to specify them in the input to Dakota.



```
#   DAKOTA INPUT FILE

environment
        tabular_data

method
    probability_levels = 0.05 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 0.95
                         0.05 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 0.95
        num_probability_levels = 0 11 11
    sampling
        sample_type lhs
        samples = 20
        seed = 3487

variabl



                                    GrainRad'


                                    0.316
                                    0 3.162
                                    ff" 'ResolParam' 'GrainBoundCoeff'

interfa
     ana                            ript'

                                    ms.in'
                                    lts.out'

                                    oncurrency = 30

respons

                                    l' 'Swelling'
```

Figure 3. *Dakota Input file created in the NEAMS Workbench, showing some of the Dakota options in the dropdown menu.*



```
/variables
id_variables
active
mixed
relaxed
continuous_design
discrete_design_range
discrete_design_set
normal_uncertain
lognormal_uncertain
uniform_uncertain
loguniform_uncertain
triangular_uncertain
exponential_uncertain
beta_uncertain
gamma_uncertain
gumbel_uncertain
frechet_uncertain
weibull_uncertain
histogram_bin_uncertain
poisson_uncertain
binomial_uncertain
negative_binomial_uncertain
geometric_uncertain
hypergeometric_uncertain
histogram_point_uncertain
uncertain_correlation_matrix
continuous_interval_uncertain
discrete_interval_uncertain
discrete_uncertain_set
continuous_state
discrete_state_range
discrete_state_set
linear_inequality_constraint_matrix
linear_inequality_lower_bounds
linear_inequality_upper_bounds
linear_inequality_scale_types
linear_inequality_scales
```

Figure 4. *Dropdown menu showing the syntax of variable input specification in Dakota.*

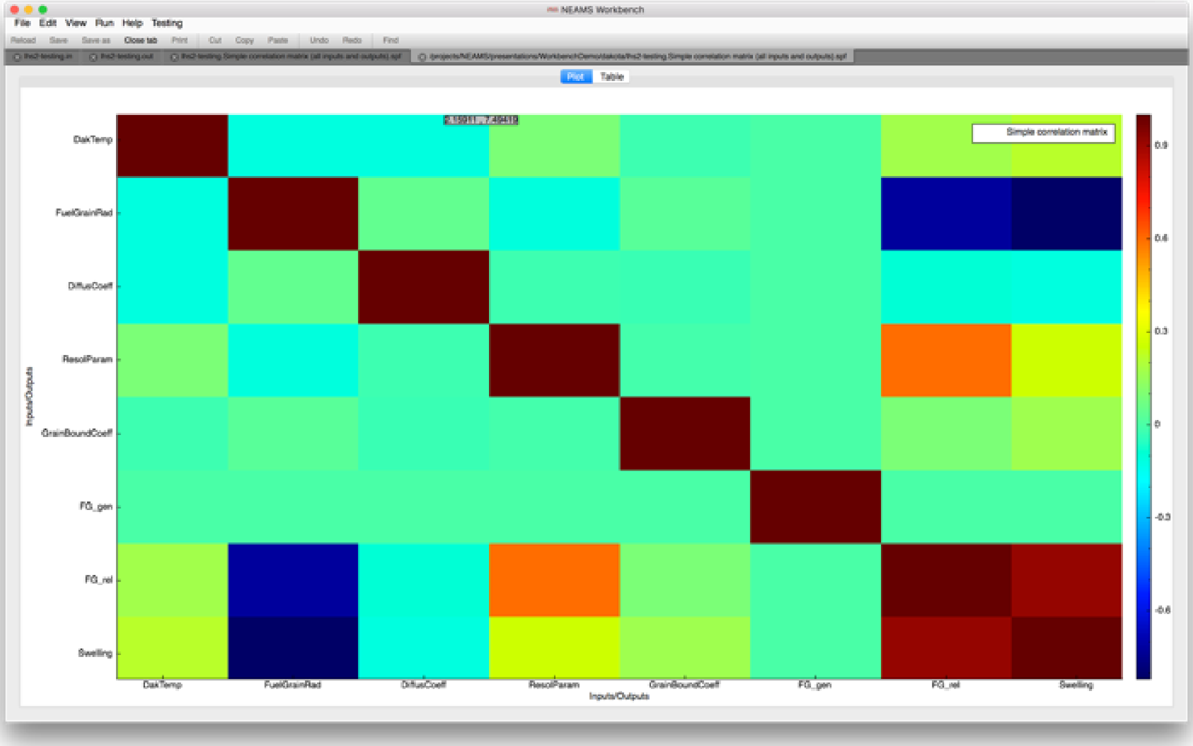


Figure 5: *Colormap showing Dakota results of the correlations between BISON inputs and outputs based on the sampling study.*

Figure 5 shows a resulting colormap from a correlation result from the Dakota study. The colormap shows the correlation between the five inputs (including temperature and fuel grain radius) and the 3 responses (fission gas generated, fission gas released, and swelling).

The NEAMS Workbench is a new initiative which will facilitate the transition from conventional tools to high-fidelity tools by providing a common user interface and common user input. This paper demonstrates the use of an analysis code, Dakota, to a fuels performance code, BISON, to perform uncertainty quantification within the NEAMS Workbench environment. These types of studies are greatly enabled by the NEAMS Workbench capabilities, including input processing and validation, autocomplete and context-specific menu dropdowns, helpful error messages, access to a runtime environment, and output processing. The integration of multiple nuclear codes under the Workbench will broaden the NEAMS tools user community and will facilitate system analysis and design.

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