

ANS Annual Meeting 2018

DRIVING THE FUTURE OF NUCLEAR TECHNOLOGY

The NEAMS Workbench and Dakota: Providing an environment for uncertainty analyses

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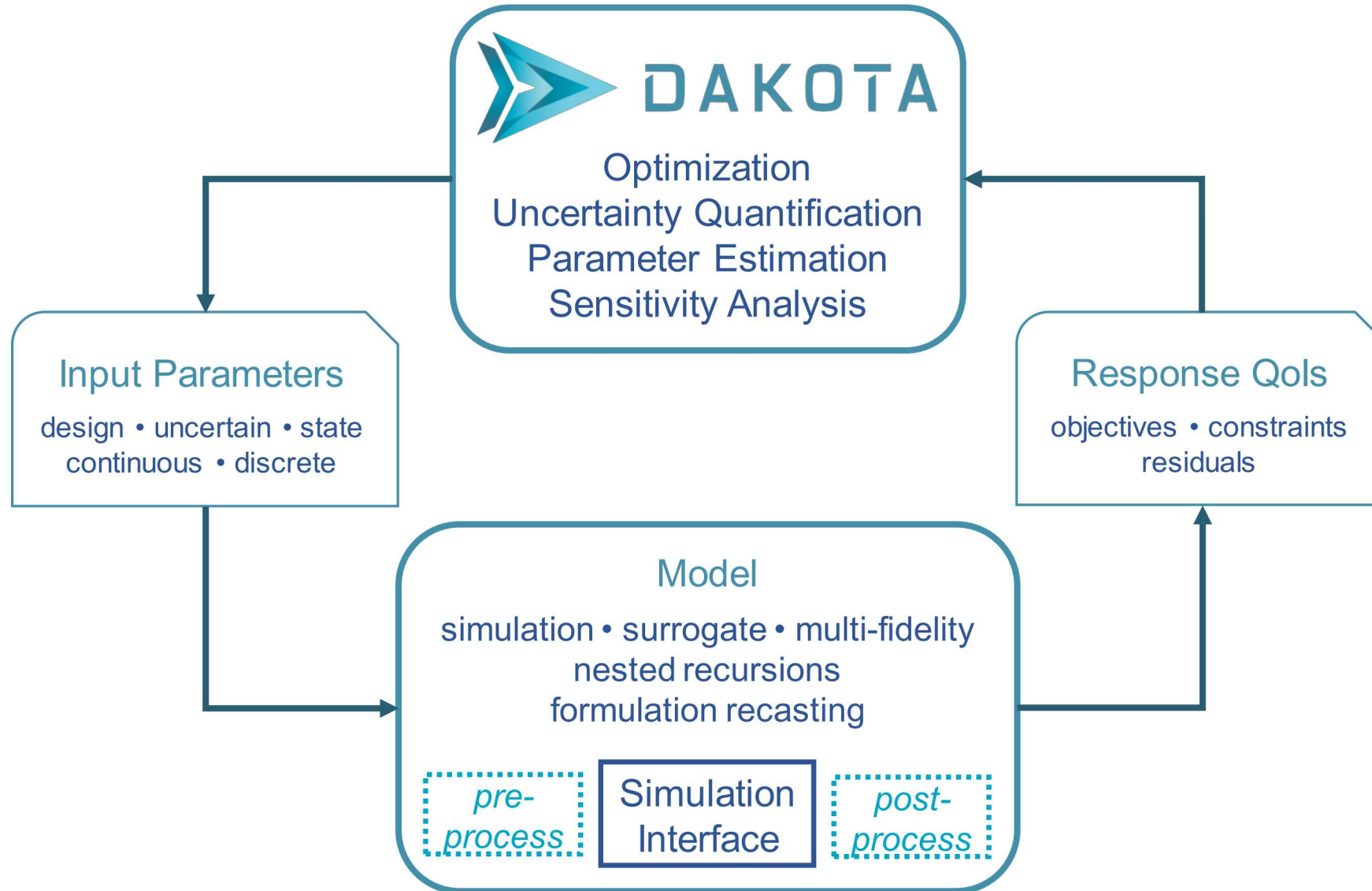
Robert Lefebvre, Brandon Langley, and Adam Thompson, Oak Ridge National Laboratory

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Dakota

Available at <https://dakota.sandia.gov>



Uncertainty Quantification Methods

- Monte Carlo sampling:
 - LHS, Quasi MC, Design of Experiments, Adaptive Sampling
- Local and global reliability
 - Employ optimization to efficiently determine failure probabilities
- Polynomial chaos expansions / stochastic collocation
 - Large research investment, adaptive sparse grids, compressive sensing
- Mixed aleatory-epistemic approaches
 - Regulatory Requirements, “uncertainty on uncertainties”
- Surrogate Models: Gaussian processes, PCE, splines, etc.

We focus on UQ methods that are as efficient and accurate as possible assuming simulations are very costly.

Dakota: Distinguishing Strengths

- Makes **sensitivity analysis, optimization, and uncertainty quantification** practical for costly computational models
- **Flexible interface** to simulation codes: one interface; many methods
- Combined **deterministic/probabilistic** analysis
- Continual **advanced algorithm R&D** to tackle computational challenges
 - Treats non-smooth, discontinuous, multi-modal responses
 - Surrogate-based, multi-fidelity, and hybrid methods, random field modeling, discrepancy modeling, dimension reduction
 - Risk-informed decision-making: epistemic and mixed UQ, rare events, Bayesian inference
- **Scalable parallel computing** from desktop to HPC

Many Methods in One Tool

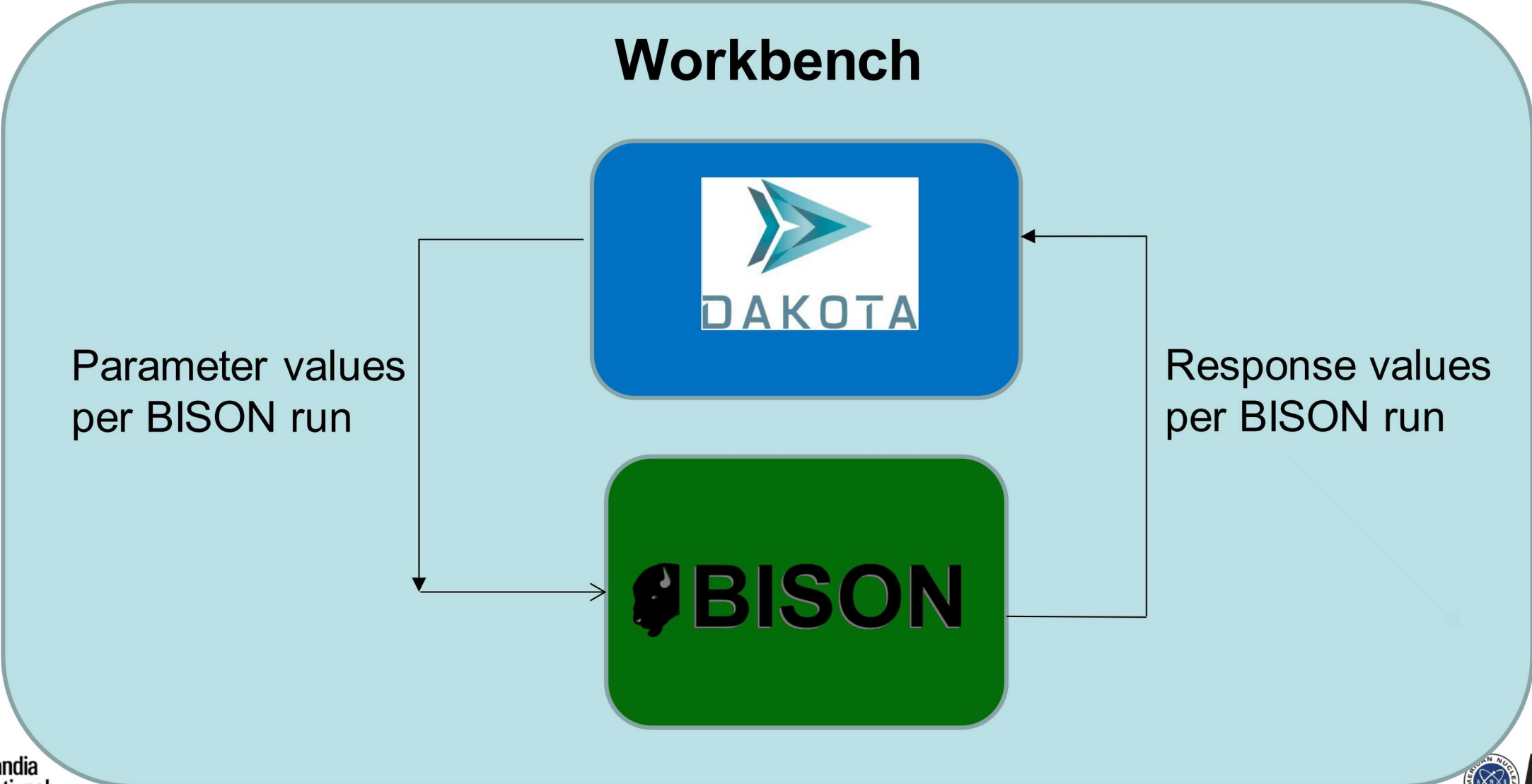
| | |
|--|--|
| <h2>Sensitivity Analysis</h2> <ul style="list-style-type: none">• Designs: MC/LHS, DACE, sparse grid, one-at-a-time• Analysis: correlations, scatter, Morris effects, Sobol indices | <h2>Uncertainty Quantification</h2> <ul style="list-style-type: none">• MC/LHS/Adaptive Sampling• Reliability• Stochastic expansions• Epistemic methods |
| <h2>Optimization</h2> <ul style="list-style-type: none">• Gradient-based local• Derivative-free local• Global/heuristics• Surrogate-based | <h2>Calibration</h2> <ul style="list-style-type: none">• Tailored gradient-based• Use any optimizer• Bayesian inference |

Interface Dakota to your simulation once, then apply various algorithms depending on your goal...

NEAMS Workbench

- Provides the capability to:
 - create and process input files for various nuclear reactor codes including SCALE, ARC, and BISON
 - Parse the inputs into a parse tree
 - Validate the inputs
 - Run the code with the given input file
 - Postprocess the output.
- “One stop” which provides a graphical user interface to perform input file creation and parsing, input validation, job execution, workflow management, and output postprocessing
- Challenge: The Workbench allows a user to create input and run a nuclear code (typically once or a few times). Dakota is another layer in the process.

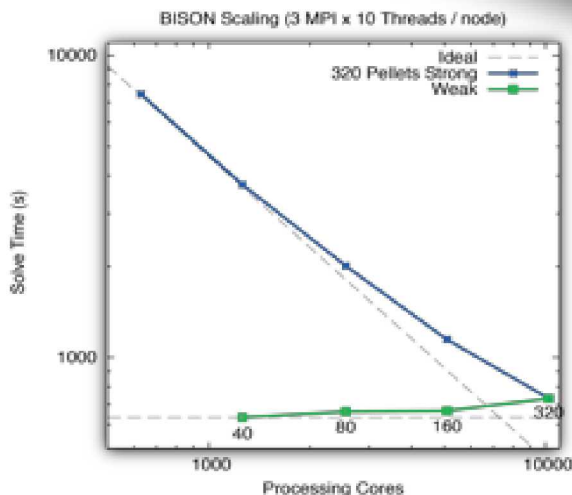
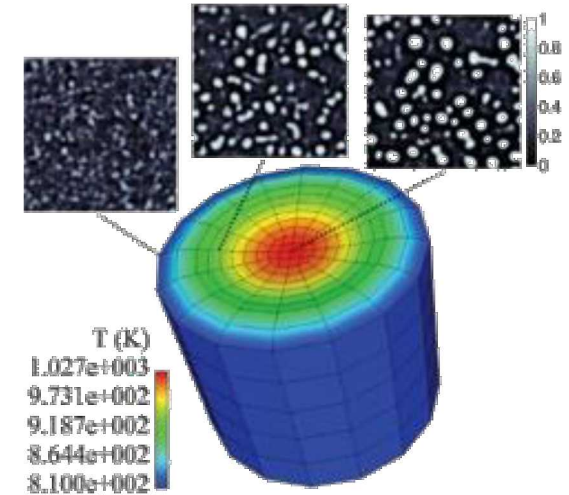
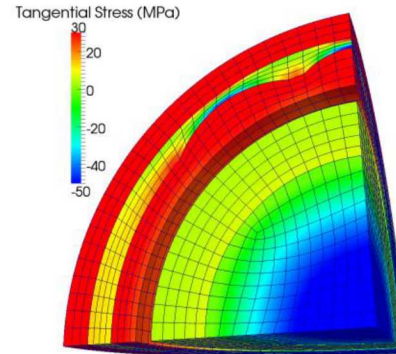
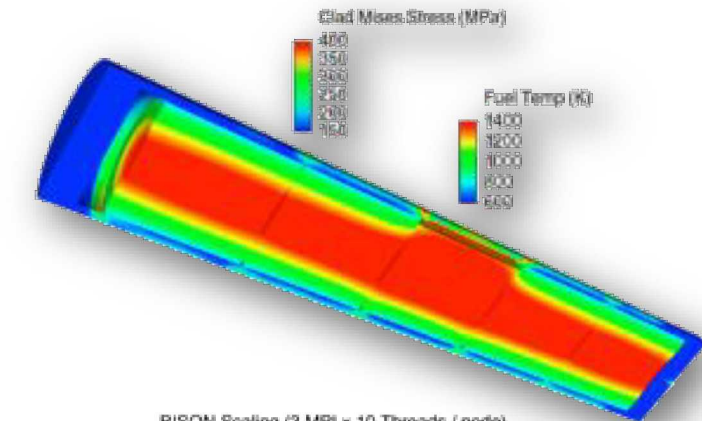
NEAMS Workbench



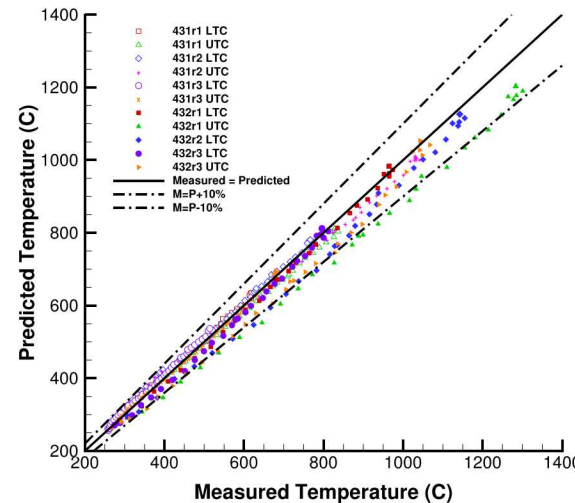
BISON Fuel Performance Code

Solution method: Implicit finite element solution of the coupled thermomechanics and species diffusion equations using the MOOSE framework; 1D spherical, 2D axisymmetric or 3D

Multiphysics constitutive models: large deformation mechanics (plasticity and creep), cracking, thermal expansion, densification, fission gas release, radiation effects (swelling, thermal conductivity degradation, etc.)

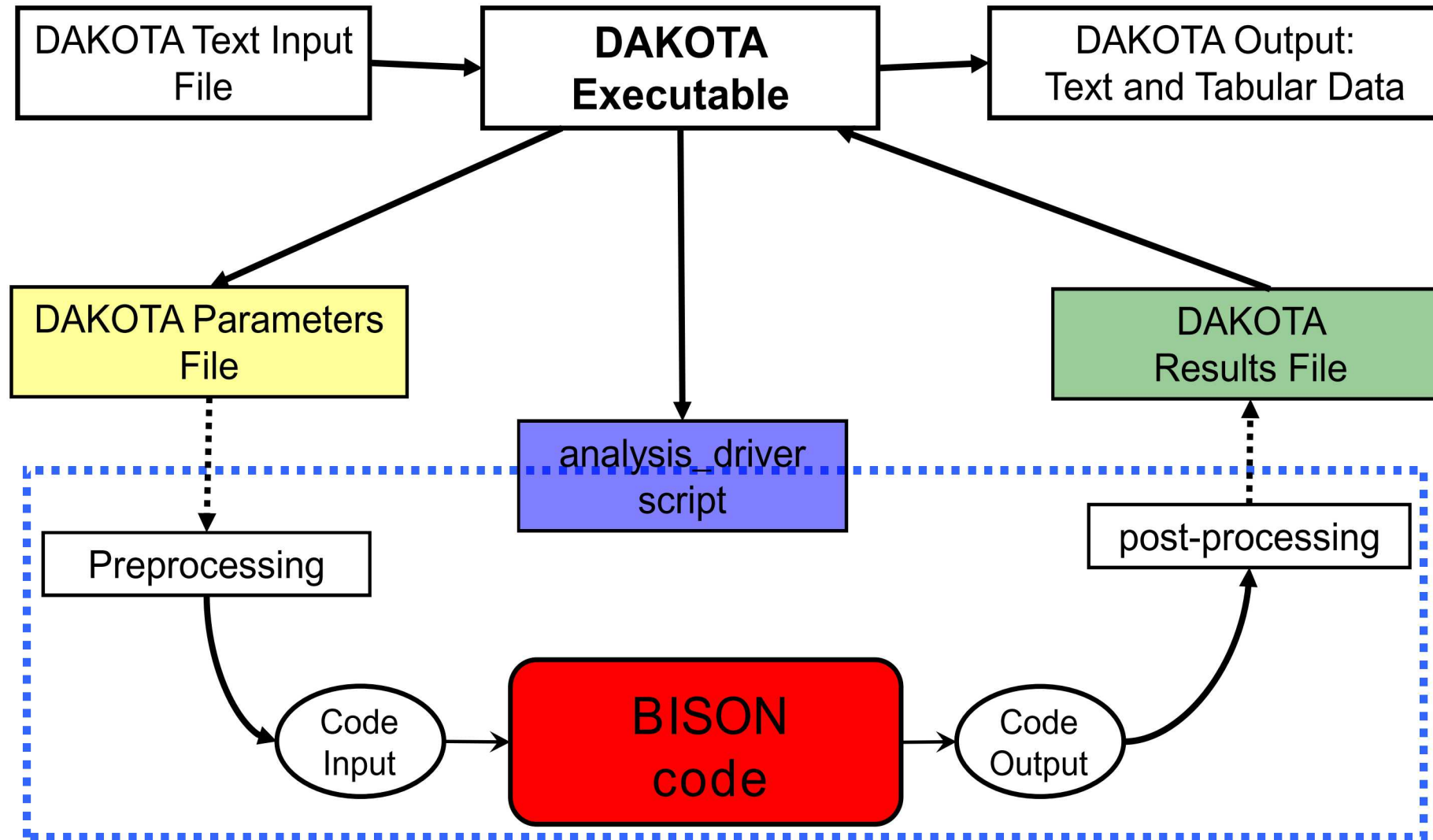


Parallel: has been run on 1 - 12,000 cpus.

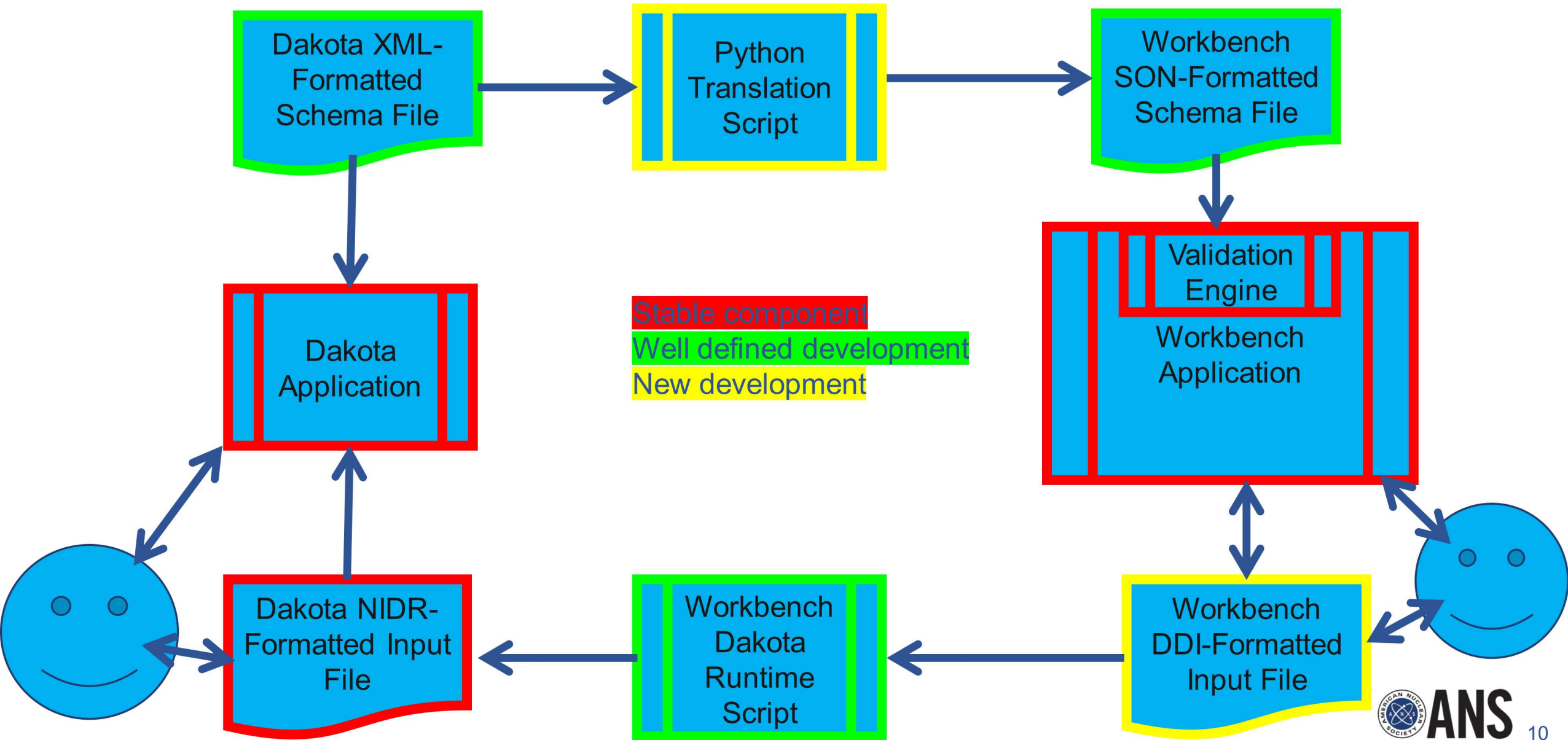


Couples readily to lower length scale models (MARMOT)

Dakota-Bison Coupling



Dakota within the NEAMS Workbench



Dakota within the NEAMS Workbench

Dakota NIDR-
Formatted Input
File

New Input Deck Reader (NIDR)
VS
Definition Driven Interpreter (DDI)

Workbench
DDI-Formatted
Input File

- Same syntax
- Same input fields
- DDI doesn't support
 - shorthand. E.g., 'desc' in place of 'description'
 - 'relaxed' ordering of input

Well ordered: method sampling sample_type lhs

Relaxed order: method sampling lhs sample_type

Dakota within the NEAMS Workbench

The screenshot shows the NEAMS Workbench interface. On the left is a navigation tree for the file 'lhs2-testing.in'. The tree is expanded to show the 'descriptors' folder under the 'method' section. The main editor window displays the Dakota input file 'lhs2-testing.in'. The file content is as follows:

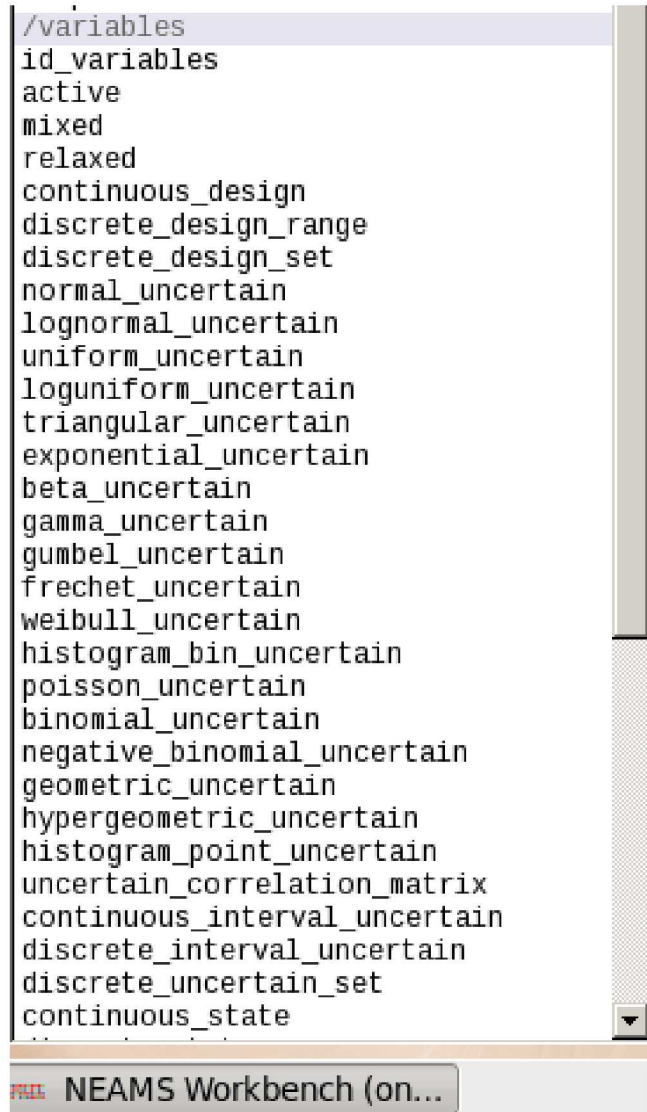
```
1 # DAKOTA INPUT FILE
2
3 environment
4     tabular_data
5
6 method
7     probability_levels = 0.05 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 0.95
8     0.05 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 0.95
9     num_probability_levels = 0 11 11
10
11 sampling
12     sample_type lhs
13     samples = 20
14     seed = 3487
15
16 variable /method/sampling
17     samples
18     seed
19     fixed_seed
20     sample_type GrainRad'
21     refinement_samples
22     d_optimal 0.316
23     variance_based_decomp 0 3.162
24     backfill
25     principal_components ff" 'ResolParam' 'GrainBoundCoeff'
26     wilks
27
28 interface /method
29     ana id_method
30     output ript'
31     final_solutions ms.in'
32     hybrid lts.out'
33     multi_start
34     pareto_set
35     concurrency = 30
36     iterator_servers
37     iterator_scheduling
38     processors_per_iterator
39     branch_and_bound 1' 'Swelling'
40     surrogate_based_local
41     surrogate_based_global
42     dot_freq
43     dot_mmfd
44     dot_bfgs
45     dot_slp
46     dot_sqp
47     dot
48     max iterations
```

Line 14 is highlighted in yellow. An autocomplete menu is open below it, showing a list of options: 'samples', 'seed', 'fixed_seed', 'sample_type', 'refinement_samples', 'd_optimal', 'variance_based_decomp', 'backfill', 'principal_components', 'wilks', 'ana', 'id_method', 'output', 'final_solutions', 'hybrid', 'multi_start', 'pareto_set', 'iterator_servers', 'iterator_scheduling', 'processors_per_iterator', 'branch_and_bound', 'surrogate_based_local', 'surrogate_based_global', 'dot_freq', 'dot_mmfd', 'dot_bfgs', 'dot_slp', 'dot_sqp', 'dot', and 'max iterations'. A blue arrow points from the text 'Autocompletion showing options' to the autocomplete menu.

← Dakota input file

Autocompletion showing options

Dakota within the NEAMS Workbench



Pull down showing options for specifying variable types

Dakota within the NEAMS Workbench

The screenshot displays the NEAMS Workbench interface. The top menu bar includes File, Edit, View, Run, and Help. Below the menu bar, there are tabs for 'textbook_uq_sampling.in', 'lhs.Simple correlation matrix.spf', and '/home02/l7u/lhs.Simple correlation matrix.spf'. The main window is divided into a left-hand navigation pane and a right-hand code editor. The navigation pane shows a tree view with 'lhs.Simple correlation matrix.spf' selected. The code editor contains the following text:

```
1 # Dakota Input File: textbook_uq_sampling.in
2 environment
3   tabular_data
4     tabular_data_file = 'textbook_uq_sampling.dat'
5
6
7 method
8   sampling
9     sample_type lhs
10    samples = 10
11    seed = 98765 rng rnum2
12    response_levels = 0.1 0.2 0.6
13                    0.1 0.2 0.6
14                    0.1 0.2 0.6
15    distribution cumulative
16
17 variables
18   uniform_uncertain = 2
19   lower_bounds = 0. 0.
20   upper_bounds = 1. 1.
21   descriptors = 'x1' 'x2'
22
23 interface
24   id_interface = 'I1'
25   analysis_drivers = 'text_book'
26   direct
27
28 responses
29   response_functions = 3
30   no_gradients
31   no_hessians
32
```

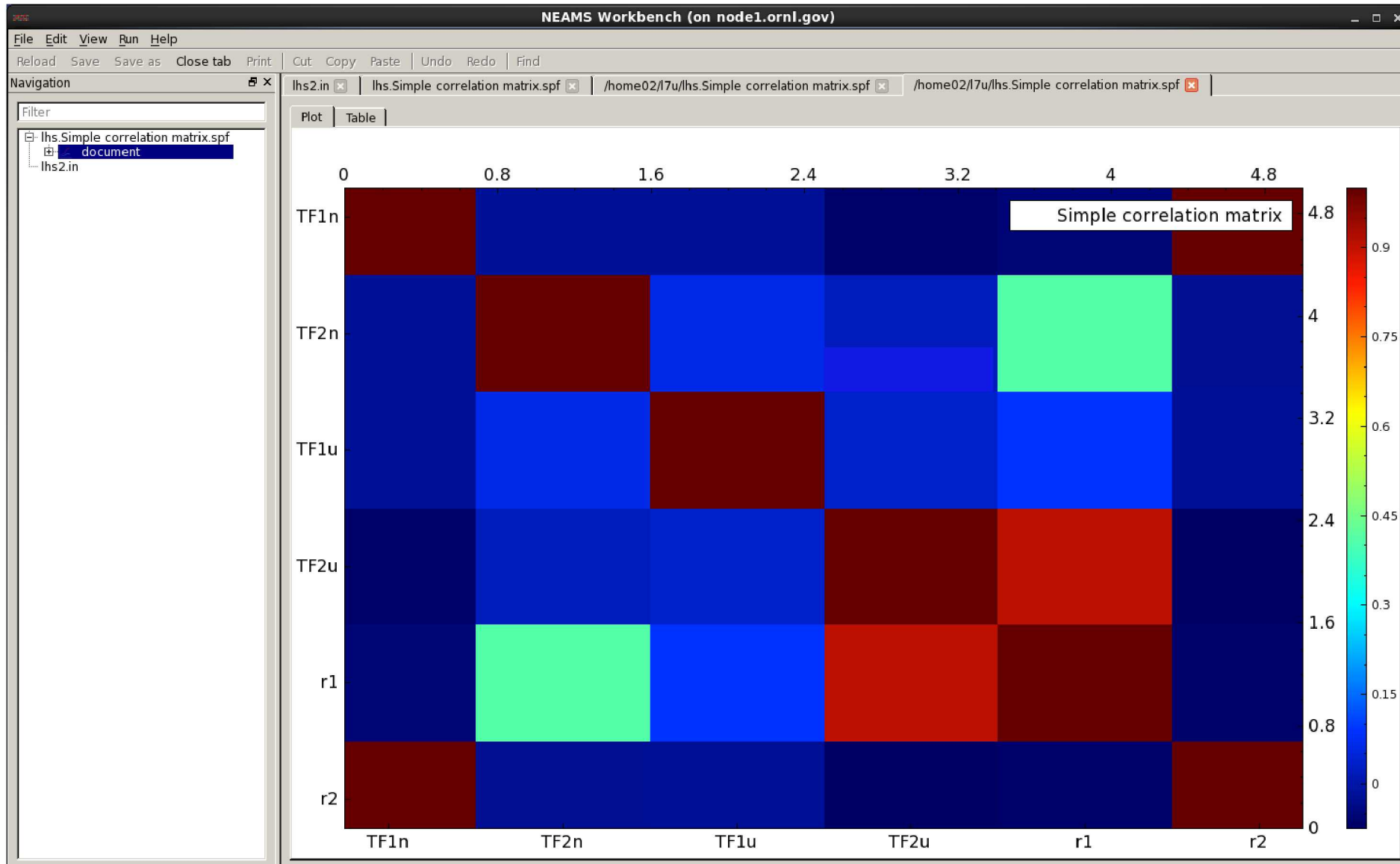
At the bottom of the interface, there is a results panel with the following output:

```
192 -----
193 Begin      I1 Evaluation    9
194 -----
195 Parameters for evaluation 9:
196           6.8346679844e-01 x1
197           6.6215521550e-01 x2
198 -----
199 Direct interface: invoking text_book
200 -----
201 Active response data for I1 evaluation 9:
202 Active set vector = { 1 1 1 }
203           2.3066424677e-02 response_fn_1
204           1.3604925681e-01 response_fn_2
205           9.6716130197e-02 response_fn_3
206 -----
207 -----
208 -----
209 -----
210 -----
```

Dakota input file

Results panel showing function evaluations

Dakota within the NEAMS Workbench



Description of BISON Case Study

- The Bison fuel performance code was coupled to Dakota to analyze rod 1 from the IFA-432 **experimental assembly irradiated at the Halden reactor in Norway.**¹
- Kyle Gamble (Idaho National Laboratory) provided the Bison input and example power history, axial peaking factors, etc.
- Input uncertainties were assumed in manufacturing parameters (e.g., cladding thickness), and model parameters (e.g., fuel thermal conductivity).
- Outputs of interest include fuel centerline temperature and fission gas release.
- Related work in reference 2 and 3.

1. Hann, C.R., et al. "Data Report for the NRC/PNL Halden Assembly IFA-432," NUREG/CR-0560, PNL-2673, 1978.

2. Swiler, L., Gamble, K., Schmidt, R. and R. Williamson. SAND Report 2015-8088 "Sensitivity Analysis of OECD Benchmark Tests in BISON."

3. Gamble, K. and L. Swiler. "Uncertainty Quantification and Sensitivity Analysis Applications to Fuel Performance Modeling." *TOPFUEL American Nuclear Society Conference*, Sept. 2016.

Input / Outputs for Sampling Study

- Inputs

- Fill Pressure
- Fuel conductivity
- Clad conductivity
- Fuel thermal expansion
- Gas conductivity factor
- Gap thickness

- Outputs

- Clad Temperature
- Fuel Centerline Temperature
- Fission Gas Release
- Clad Diameter

Dakota within the NEAMS Workbench

The screenshot shows the NEAMS Workbench interface with a Dakota input file open. The interface includes a menu bar (File, Edit, View, Run, Help), a toolbar (Reload, Save, Save as, Close tab, Print, Cut, Copy, Paste, Undo, Redo, Find), and a navigation pane on the left. The main editor displays the Dakota input file with the following content:

```
1 environment
2     tabular_graphics_data
3     method_pointer = 'UQ'
4
5 method,
6     id_method = 'UQ'
7     sampling
8     sample_type lhs
9     samples = 10
10    seed = 50923
11
12 variable /method
13     n id_method
14     m output
15     s final_solutions
16     d sampling
17     c 'lad_thick' 'fp_out_rad' 'fuel_density' 'fuel_rough' 'clad_rough' 'fill_pressure' 'clad_cond' 'fuel_therm_exp' 'gap_thick'
18 interface
19     /method/sampling
20     a tion_concurrency = 6
21     'python dakota_driver.py'
22     ctory named = "work"
23     s = "IFA-432_test.tmpl" "dakota_driver.py"
24         "lhs.drive"
25         "powerhistory.csv" "peakingfactors.csv"
26     _tag directory_save
27
28
29
30 response
31     resp model_pointer
32     descriptors = 'avg_clad_temp' 'centerline_temp_bottom' 'fission_gas_gen' 'fission_gas_release'
33     no_gradients
34     no_hessians
35
```

Annotations in the image include:

- A yellow highlight underlines lines 11-12.
- A blue arrow points from the text "Autocompletion showing options" to the dropdown menu for the 'variable' entry on line 12.
- The text "Dakota input file" is centered over the main editor area.
- The text "Document Navigation" is positioned on the left side of the image.

Document
Navigation

Dakota input file

Autocompletion
showing options

Line: 11, Col: 9

Validation Messages

Dakota within the NEAMS Workbench

Document Navigation

Dakota input file

```
1 environment
2 /variables
3 id_variables
4 active
5 meth mixed
6 relaxed
7 continuous_design
8 discrete_design_range
9 discrete_design_set
10 normal_uncertain
11 lognormal_uncertain
12 vari loguniform_uncertain
13 triangular_uncertain
14 exponential_uncertain
15 beta_uncertain
16 gamma_uncertain
17 gumbel_uncertain
18 inte frechet_uncertain
19 weibull_uncertain
20 histogram_bin_uncertain
21 poisson_uncertain
22 binomial_uncertain
23 negative_binomial_uncertain
24 geometric_uncertain
25 hypergeometric_uncertain
26 histogram_point_uncertain
27 uncertain_correlation_matrix
28 continuous_interval_uncertain
29 discrete_interval_uncertain
30 resp continuous_state
31 discrete_state_range
32 discrete_state_set
33 linear_inequality_constraint_matrix
34 linear_inequality_lower_bounds
35 linear_inequality_upper_bounds
linear_inequality_scale_types
linear_inequality_scales
linear_equality_constraint_matrix
linear_equality_targets
linear_equality_scale_types
linear_equality_scales
```

Pull down showing options for specifying variable types

```
1.1E-03 10421.5 2.2E-06 6.4E-7 1.1E+5 16. 1.00E-05 1.15E-4
1.1E-04 1042.15 2.2E-07 6.4E-8 1.1E+4 1.6 1.00E-06 1.15E-5
out_rad' 'fuel_density' 'fuel_rough' 'clad_rough' 'fill_pressure' 'clad_cond' 'fuel_therm_exp' 'gap_thick'
```

...
ncy = 6
_driver.py'
"work"
st.templ" "dakota_driver.py"
"
ory.csv" "peakingfactors.csv"
save

...
line_temp_bottom' 'fission_gas_gen' 'fission_gas_release'

Dakota within the NEAMS Workbench

The screenshot displays the NEAMS Workbench interface with two input files open. The top window shows the Dakota input file (`IFA-432_test.tmpl`) with the following content:

```
1 environment
2   tabular_graphics_data
3   method_pointer = 'UQ'
4
5 method,
6   id_method = 'UQ'
7   sampling
8   sample_type lhs
9   samples = 10
10  seed = 50923
11
12 variables,
13   normal_uncertain = 9
14   means = 0.94E-03 5.335E-03 10421.5 2.2E-0
15   std_deviations = 0.94E-04 5.335E-04 1042.15 2.2E-0
16   descriptors = 'clad_thick' 'fp_out_rad' 'fuel_density' 'fuel_
17
18 interface,
19   id_interface = 'I1'
20   asynchronous_evaluation_concurrency = 6
21   analysis_drivers = 'python dakota_driver.py'
22   fork_work_directory named = "work"
23
24 [Mesh]
25 type = SmearedPelletMesh
26 clad_mesh_density = customize
27 pellet_mesh_density = customize
28 nx_p = 17
29 nx_c = 4
30 ny_p = 175
31 ny_c = 296
32 ny_cl = 3
33 pellet_outer_radius = <fp_out_rad> # Varying parameter
34 pellet_height = 12.842222222222222e-3
35 pellet_quantity = 45
36 clad_thickness = <clad_thick> # Varying parameter
37 clad_gap_width = <gap_thick> # Varying parameter
38 clad_bot_gap_height = 1e-3
39 plenum_fuel_ratio = 0.04395224 # Dependent upon varying parameters
40 top_bot_clad_height = 2.7e-3
41 elem_type = QUAD8
42 displacements = 'disp_x disp_y'
43 patch_size = 10 # For contact algorithm
44 patch_update_strategy = auto
```

The bottom window shows the Bison input file (`IFA-432_test.tmpl`) with the following content:

```
545
546 [./TimeStepper]
547 type = IterationAdaptiveDT
548 dt = 2.0e2
549 optimal_iterations = 10
550 iteration_window = 2
551 growth_factor = 10
552 linear_iteration_ratio = 100
553 force_step_every_function_point = true
554 timestep_limiting_function = power_history
555 max_function_change = 3e20
556 [./]
557
558 [./Quadrature]
559 order = FIFTH
560 side_order = SEVENTH
561 [./]
562 []
563
```

Annotations on the image include:

- Dakota input file**: A yellow highlight over the Dakota input file content.
- Bison input file**: A yellow highlight over the Bison input file content.
- Document Navigation**: A blue label pointing to the left-hand navigation pane.
- Bison transient options**: A blue label pointing to the Bison input file content.
- Bison input file**: A blue label pointing to the Bison input file content.

Dakota within the NEAMS Workbench

The screenshot displays the NEAMS Workbench interface. On the left is a 'Document Navigation' tree for the file 'lhs.in', with 'variables' selected. The main window shows the 'Dakota input file' with the following content:

```
8 sample_type lhs
9 samples = 10
10 seed = 50923
11
12 variables,
13 normal_uncertain = 9
14 means = 0.94E-03 5.335E-03 10421.5 2.2E-06 6.4E-7 1.1E+5 16. 1.00E-05 1.15E-4
15 std_deviations = 0.94E-04 5.335E-04 1042.15 2.2E-07 6.4E-8 1.1E+4 1.6 1.00E-06 1.15E-5
16 descriptors = 'clad_thick' 'fp_out_rad' 'fuel_density' 'fuel_rough' 'clad_rough' 'fill_pressure' 'clad_cond' 'fuel_therm_exp' 'gap_thick'
17
18 interface,
19 id_interface = 'IT1'
```

The results panel below shows execution messages and function evaluations, including a large 'BOSSON' logo and a map of the United States. The text in the results panel reads:

```
685
686 BOSSON
687
688
689
690
691
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696
697
698
699
700
701
702
703
704
705
706
707 Nuclear Fuel Performance Analysis Code
708 Idaho National Laboratory
709 Idaho Falls, Idaho
710
711 Copyright 2015 Battelle Energy Alliance, LLC
712 ALL RIGHTS RESERVED
713
714 Prepared by Battelle Energy Alliance, LLC
715 Under Contract No. DE-AC07-05ID14517
716 With the U. S. Department of Energy
```

At the bottom of the interface, the status bar indicates 'Line: 12, Col: 11 /variables/'.

Document
Navigation

Dakota input file

Results panel
showing execution
messages and
function evaluations

Dakota within the NEAMS Workbench

NEAMS Workbench

File Edit View Run Help

Reload Save Save as Close tab Print Cut Copy Paste Undo Redo Find

NEAMS/presentations/WorkbenchDemo/bison/OECD_Benchmark/lhs.Partial correlation matrix between input and output.spf

/projects/NEAMS/presentations/WorkbenchDemo/bison/OECD_Benchmark/lhs.Partial correlation matrix between input and output.spf

Plot Table

| | 3 | 2 | 1 | 0 |
|---|-----------|------------|-----------|-----------|
| 0 | 0.518236 | 0.458274 | 0.834432 | 0.211862 |
| 1 | -0.149007 | -0.0204923 | -0.391797 | -0.039074 |
| 2 | -0.272583 | -0.112252 | -0.282182 | -0.97387 |
| 3 | 0.370904 | 0.327105 | 0.270096 | 0.3716 |
| 4 | 0.0919053 | 0.125938 | 0.142922 | 0.0699791 |
| 5 | -0.273972 | -0.225958 | -0.263899 | -0.221873 |
| 6 | 0.157616 | 0.181101 | 0.14931 | 0.0252665 |
| 7 | 0.719268 | 0.99752 | 0.972551 | 0.983806 |
| 8 | 0.0817386 | -0.0159561 | 0.150233 | 0.964718 |

Plot Table

Partial correlation matrix between input and output

Inputs

- clad_thick
- fp_out_rad
- fuel_density
- fuel_rough
- clad_rough
- fill_pressure
- clad_cond
- fuel_therm_exp
- gap_thick

Outputs

- avg_clad_temp
- centerline_temp_bottom
- fission_gas_gen
- fission_gas_release

Processors: -None- Arc - Arc 1

```

1139
1140
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1163
1164
1165
1166
1167
1168
  
```

BISON

Nuclear Fuel Performance Analysis Code
Idaho National Laboratory
Idaho Falls, Idaho

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dakota_tabular.dat lhs.Partial correlation matrix between input and output.spf

Processors: -None- Arc - Arc 1 Run View Edit

| l%eval_id | interface | clad_thick | fp_out_rad | fuel_density | fuel_rough | clad_rough | fill_pressure |
|-----------|-----------|-----------------|----------------|--------------|-----------------|-----------------|---------------|
| 21 | I1 | 0.000876362519 | 0.005906675363 | 11896.37328 | 2.101993361e-06 | 5.835703118e-07 | 107766.981 |
| 32 | I1 | 0.001095850459 | 0.005679652229 | 9128.978954 | 2.130701325e-06 | 6.076470445e-07 | 121082.611 |
| 43 | I1 | 0.001046062392 | 0.004349743376 | 9927.34438 | 2.066228507e-06 | 6.276306736e-07 | 126527.111 |
| 54 | I1 | 0.0008644713407 | 0.004942739957 | 10595.44973 | 2.282010289e-06 | 5.173950732e-07 | 112647.311 |
| 65 | I1 | 0.0008174079671 | 0.005603384878 | 10018.84026 | 2.216009658e-06 | 6.688544823e-07 | 107041.711 |
| 76 | I1 | 0.001006405768 | 0.005182181158 | 9397.881387 | 2.481656536e-06 | 6.368859374e-07 | 90241.4281 |
| 87 | I1 | 0.001061901031 | 0.005561252232 | 11508.20676 | 2.013002582e-06 | 5.676313276e-07 | 102689.711 |
| 98 | I1 | 0.000767641117 | 0.005121220600 | 12572.52824 | 2.311614681e-06 | 6.878442187e-07 | 122607.211 |

Line: 8, Col: 7

Validation Messages

Line: 1, Col: 21

Validation Messages

Summary

- Dakota is a SNL tool that performs uncertainty quantification, optimization, and sensitivity analysis of simulation models.
- NEAMS Workbench is an ORNL tool to allow the user to create, validate, parse, and process input files for various codes including SCALE, ARC, and Bison.
- Bison is an INL tool to model performance of nuclear fuels.
- We demonstrated the integration of all three: both Dakota and Bison are integrated within Workbench. In one study, we can define the Dakota input and the corresponding Bison input.
- Demonstrated post-processing of sample results with visual display of correlation matrices.