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DRIVING THE FUTURE OF NUCLEAR TECHNOLOGY

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

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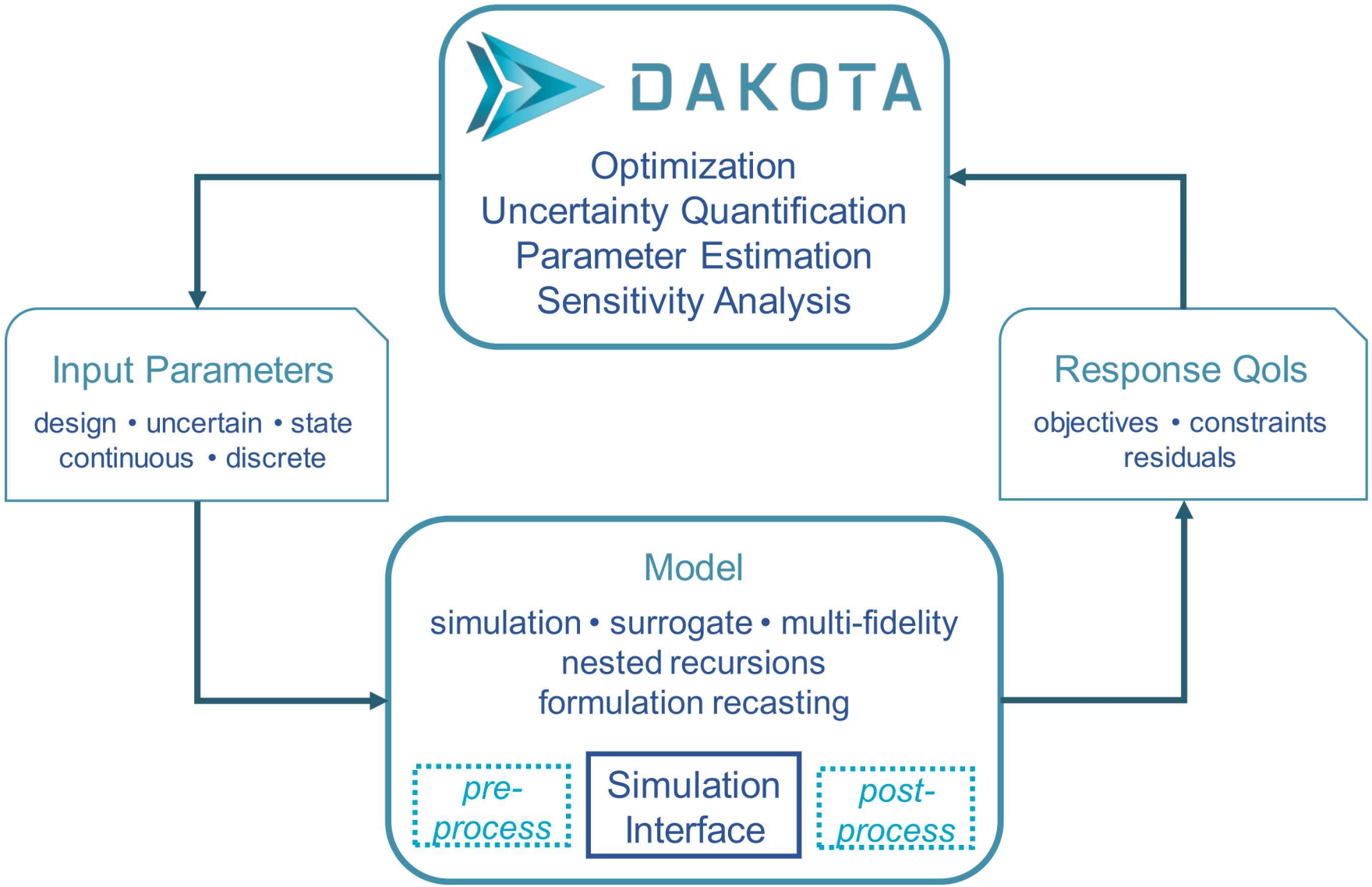
NEAMS

NUCLEAR ENERGY ADVANCED MODELING & SIMULATION PROGRAM

Sandia National Laboratories

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

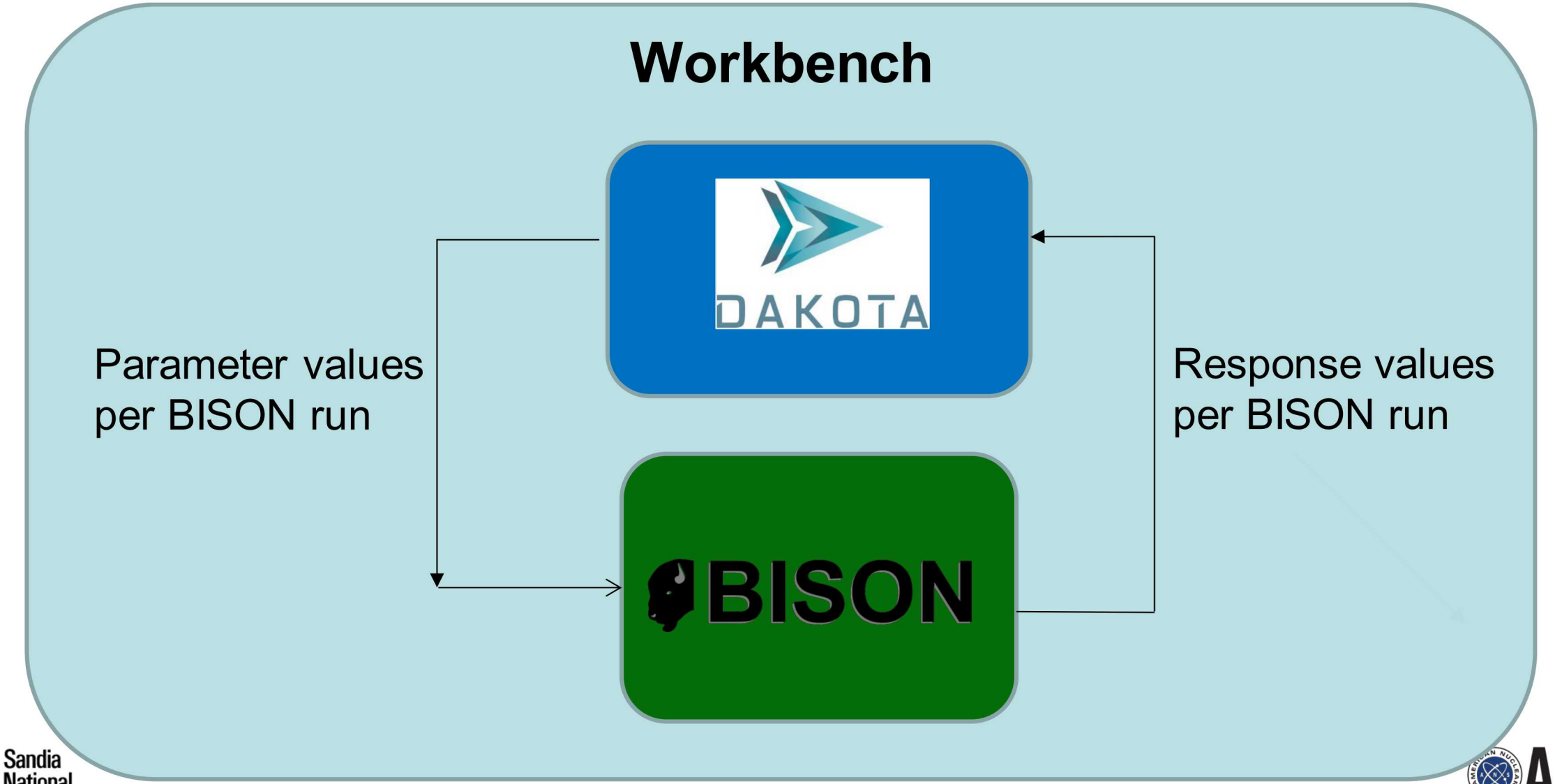
Sensitivity Analysis • Designs: MC/LHS, DACE, sparse grid, one-at-a-time • Analysis: correlations, scatter, Morris effects, Sobol indices	**Uncertainty Quantification** • MC/LHS/Adaptive Sampling • Reliability • Stochastic expansions • Epistemic methods
Optimization • Gradient-based local • Derivative-free local • Global/heuristics • Surrogate-based	**Calibration** • 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.

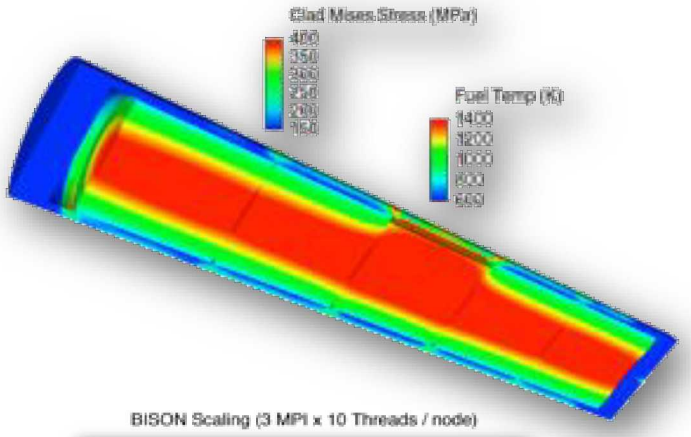
NEAMS Workbench

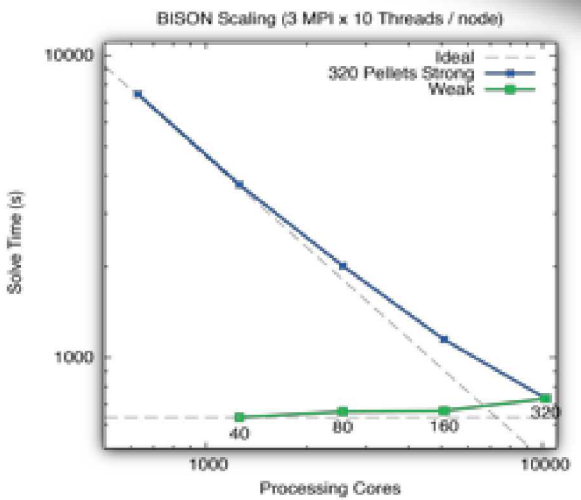


BISON Fuel Performance Code

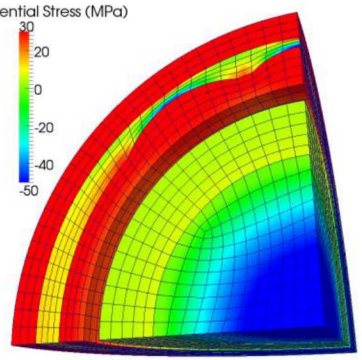
Solution method: Implicit finite element solution of the coupled thermomechanics and species diffusion equations using the MOOSE framework; 1D spherical, 2D axisymmetric or 3D

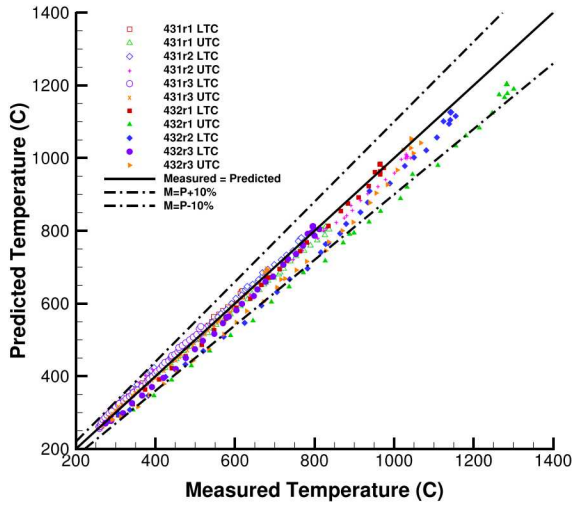
Multiphysics constitutive models: large deformation mechanics (plasticity and creep), cracking, thermal expansion, densification, fission gas release, radiation effects (swelling, thermal conductivity degradation, etc.)

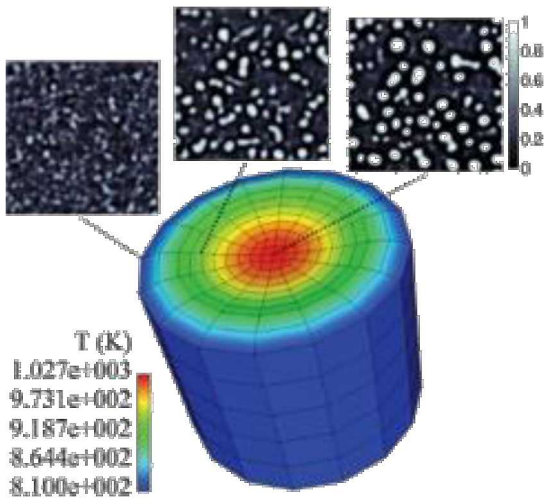




Parallel: has been run on 1 - 12,000 cpus.

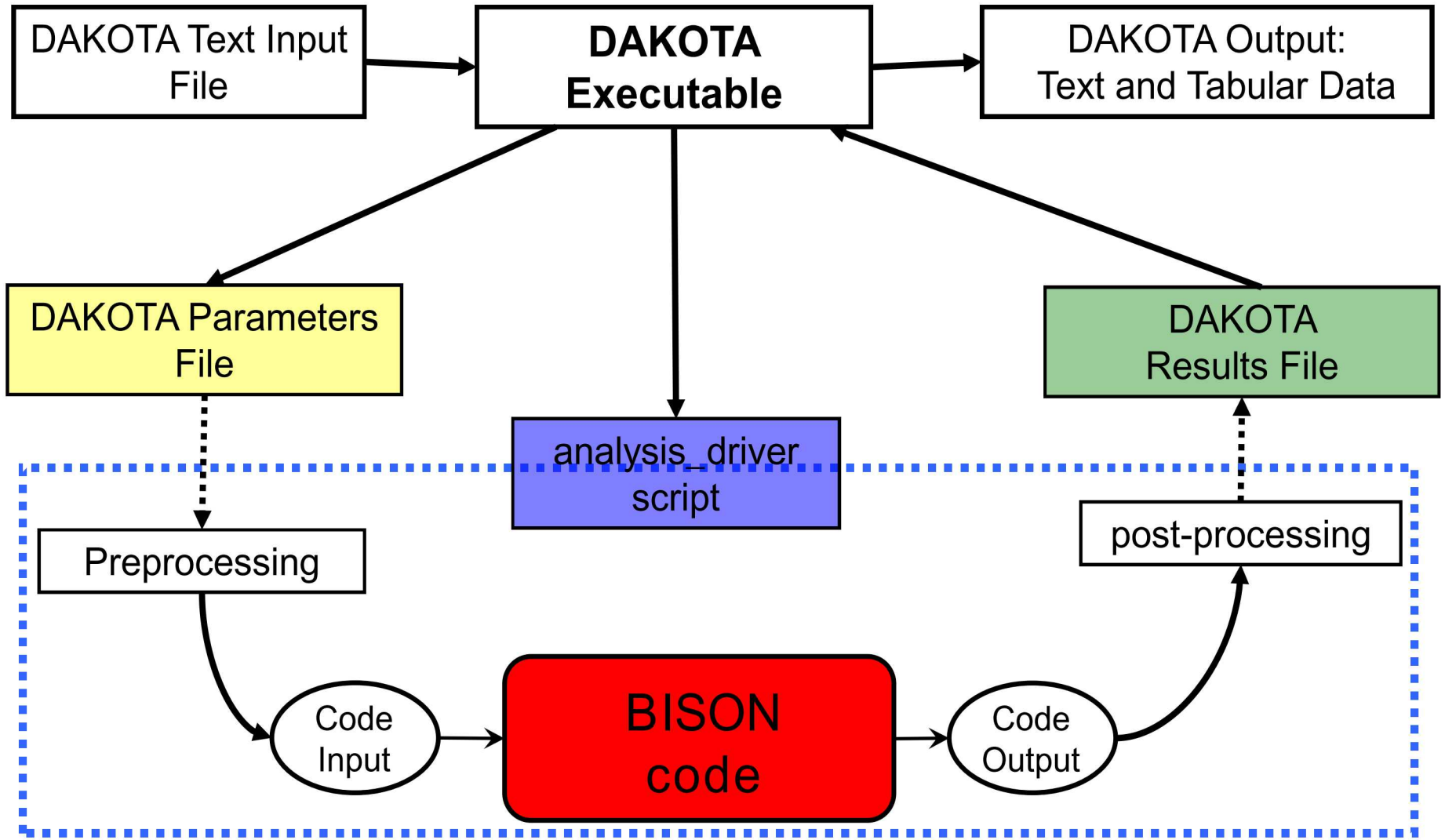




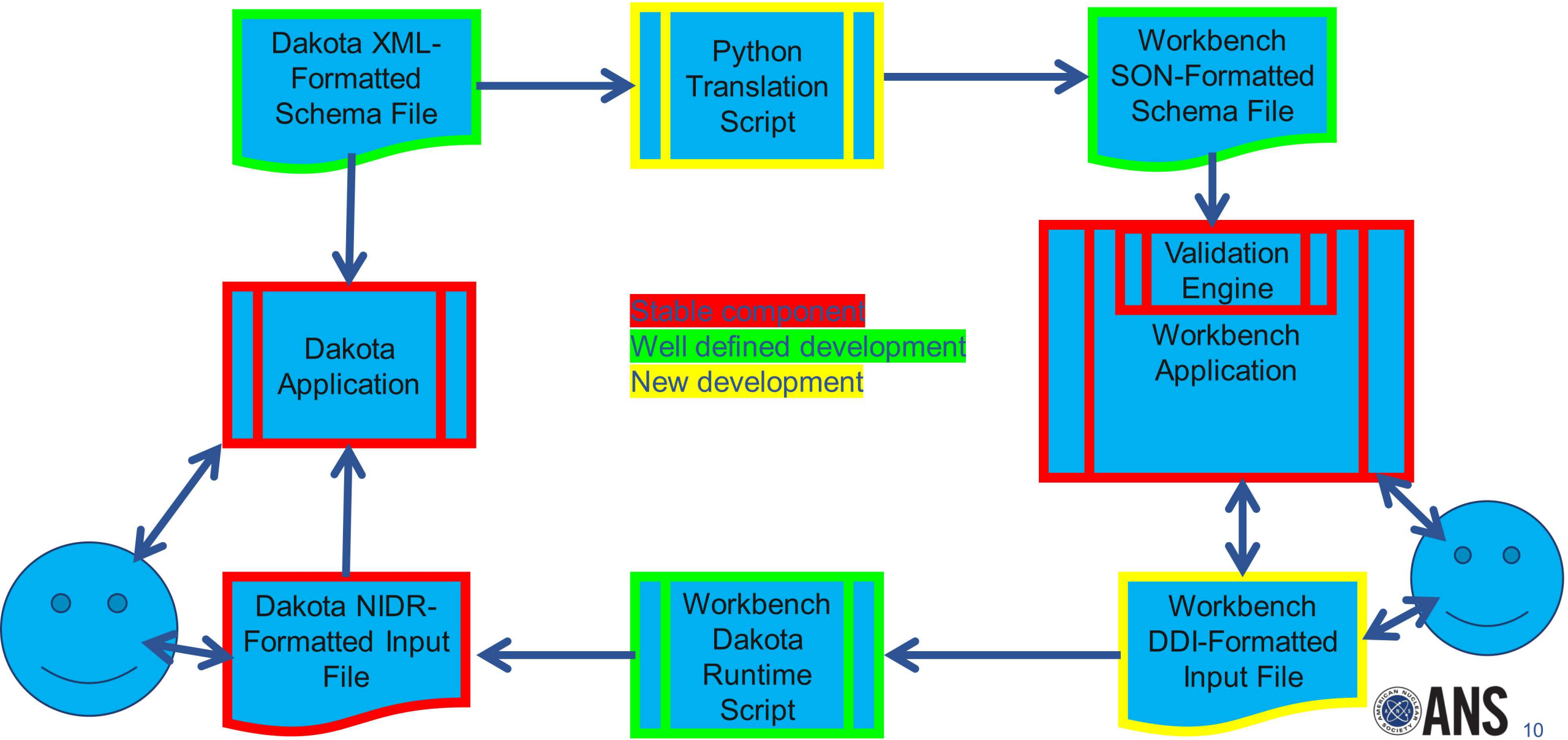


Couples readily to lower length scale models (MARMOT)

Dakota-Bison Coupling



Dakota within the NEAMS Workbench



Dakota within the NEAMS Workbench

Dakota NIDR-Formatted Input File

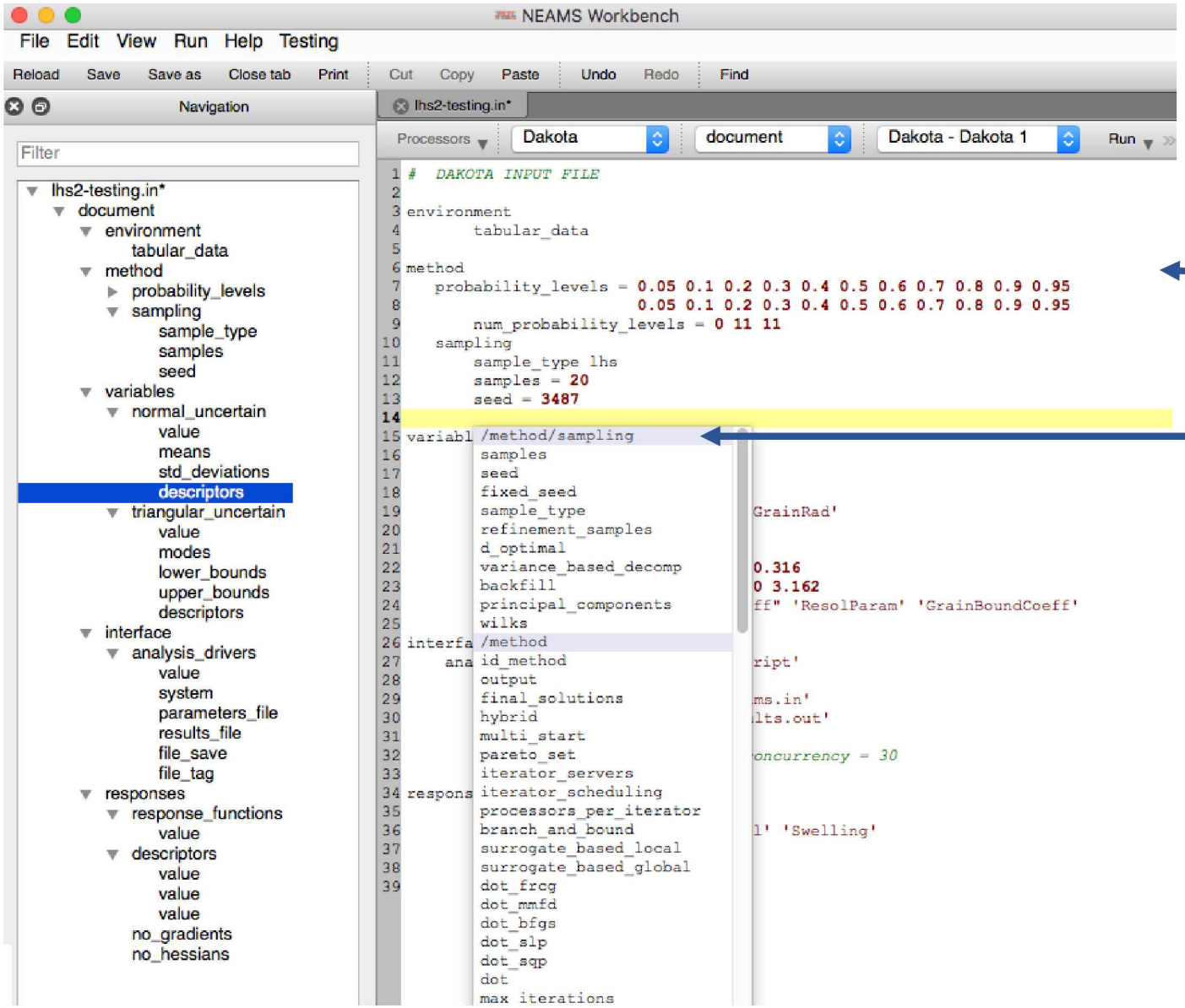
New Input Deck Reader (NIDR)
VS
Definition Driven Interpreter (DDI)

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`

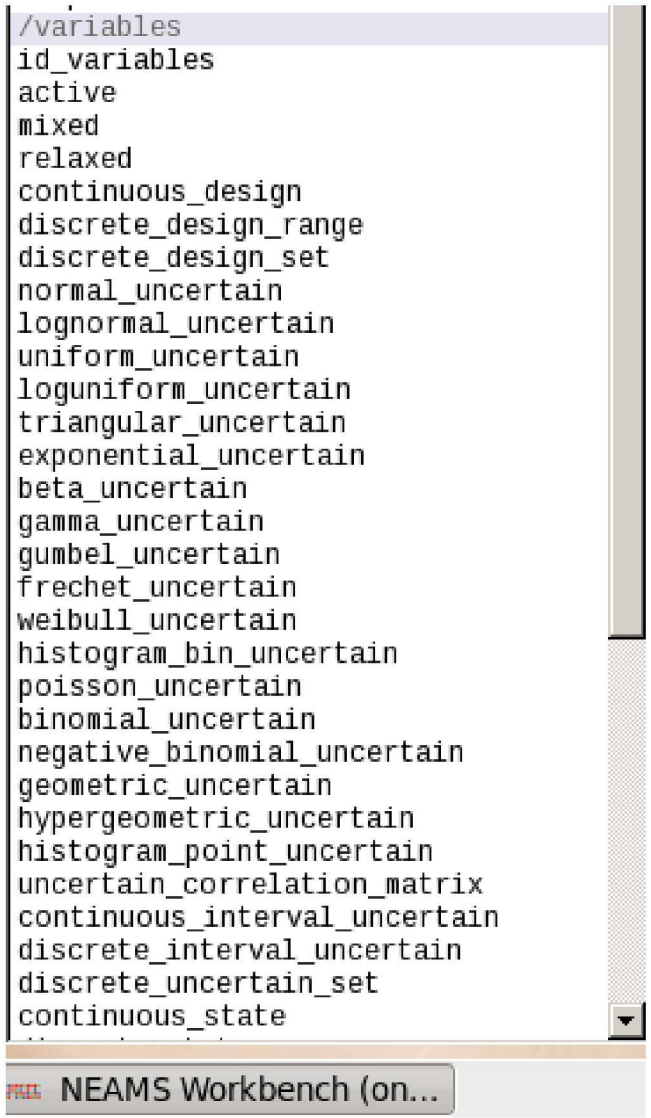
Dakota within the NEAMS Workbench



Dakota input file

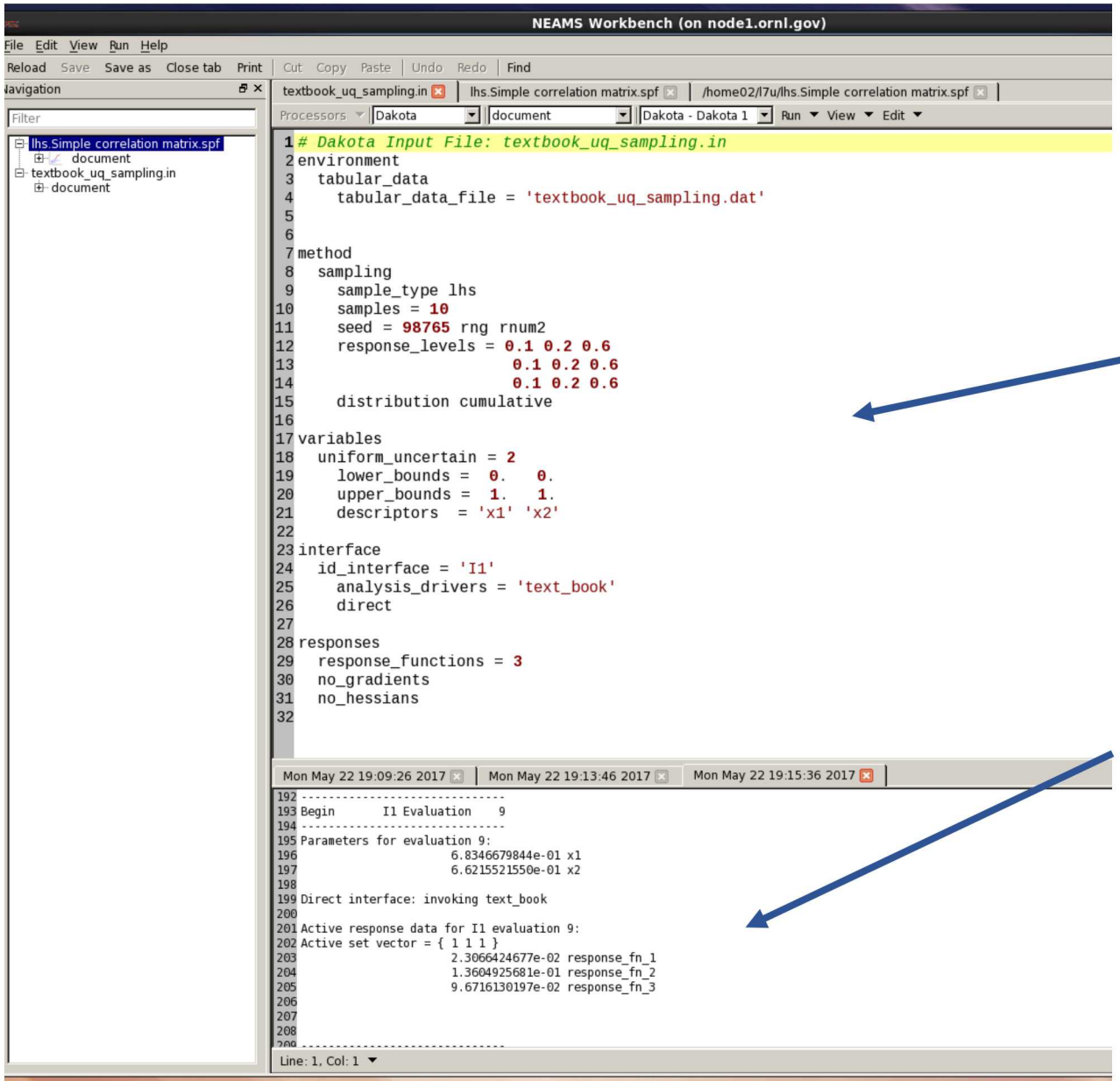
Autocompletion showing options

Dakota within the NEAMS Workbench



Pull down showing options for specifying variable types

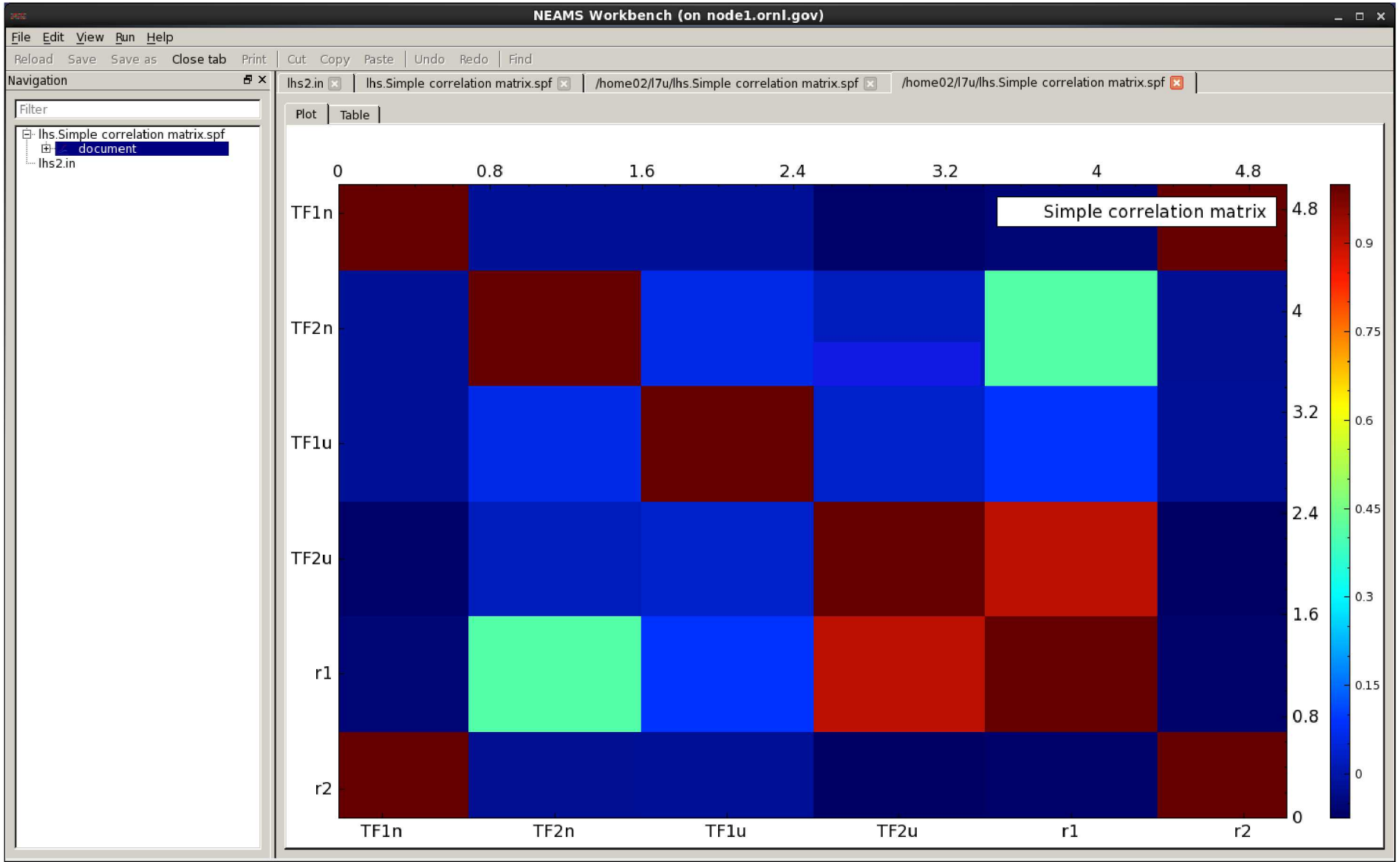
Dakota within the NEAMS Workbench



Dakota input file

Results panel showing function evaluations

Dakota within the NEAMS Workbench



Description of BISON Case Study

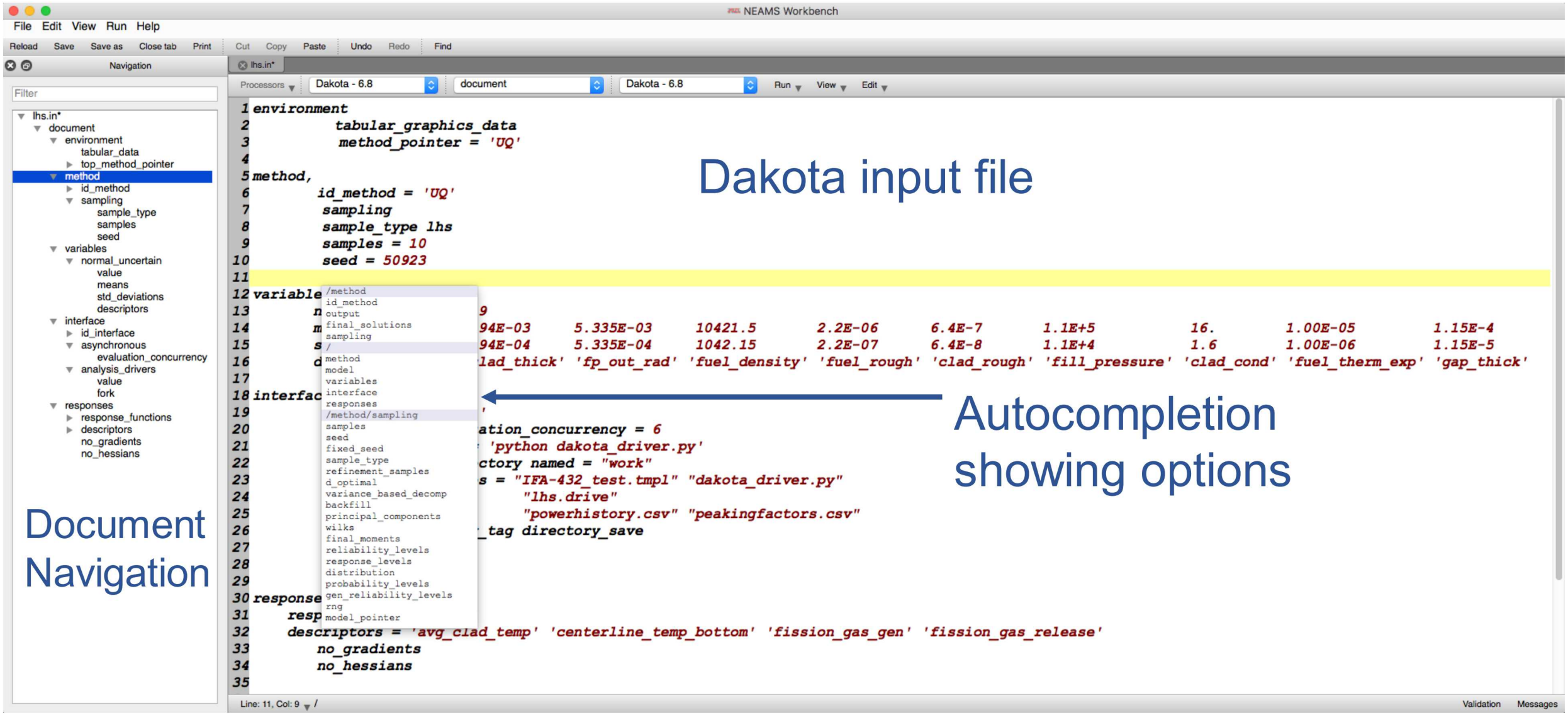
- The Bison fuel performance code was coupled to Dakota to analyze rod 1 from the IFA-432 **experimental assembly irradiated at the Halden reactor in Norway.**[1]
- Kyle Gamble (Idaho National Laboratory) provided the Bison input and example power history, axial peaking factors, etc.
- Input uncertainties 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



Dakota input file

Autocompletion showing options

Document Navigation

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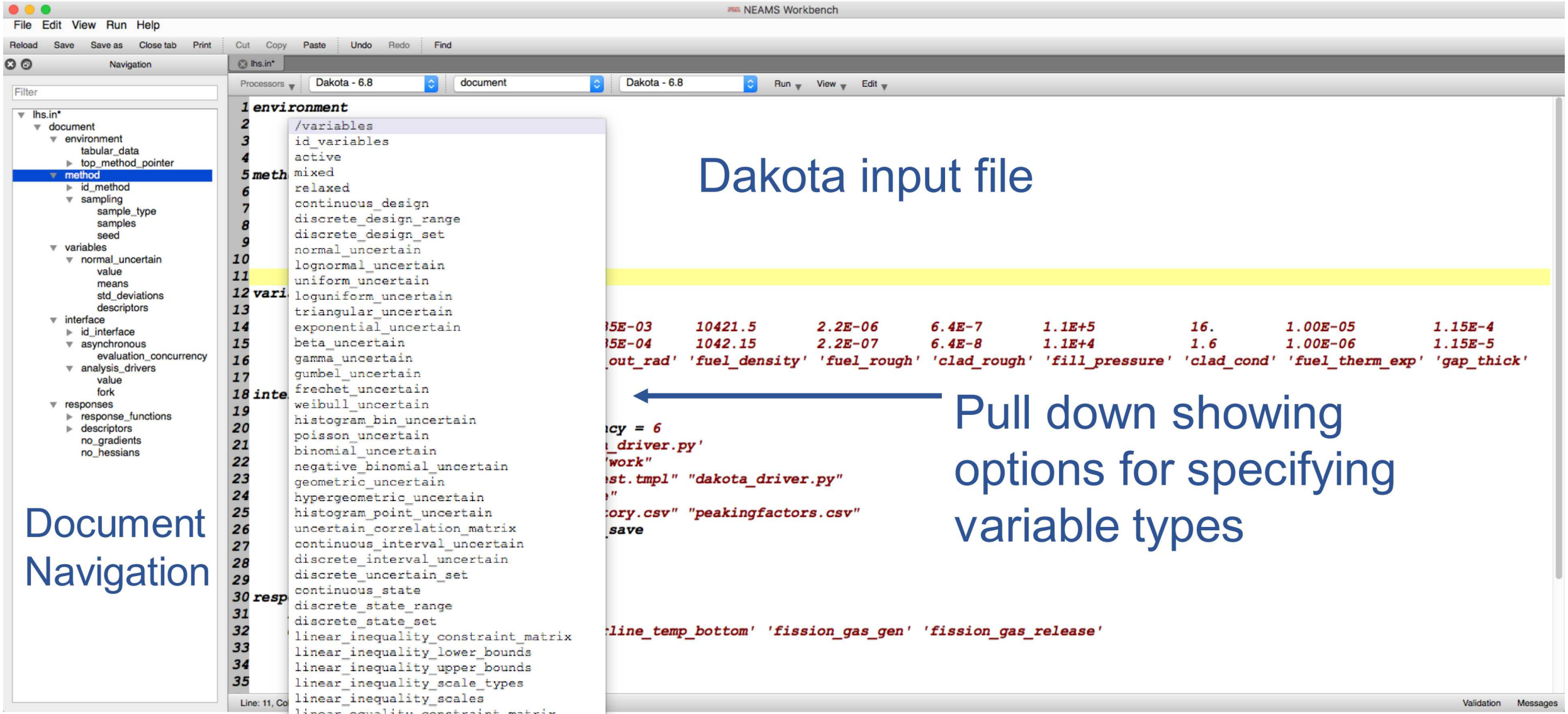

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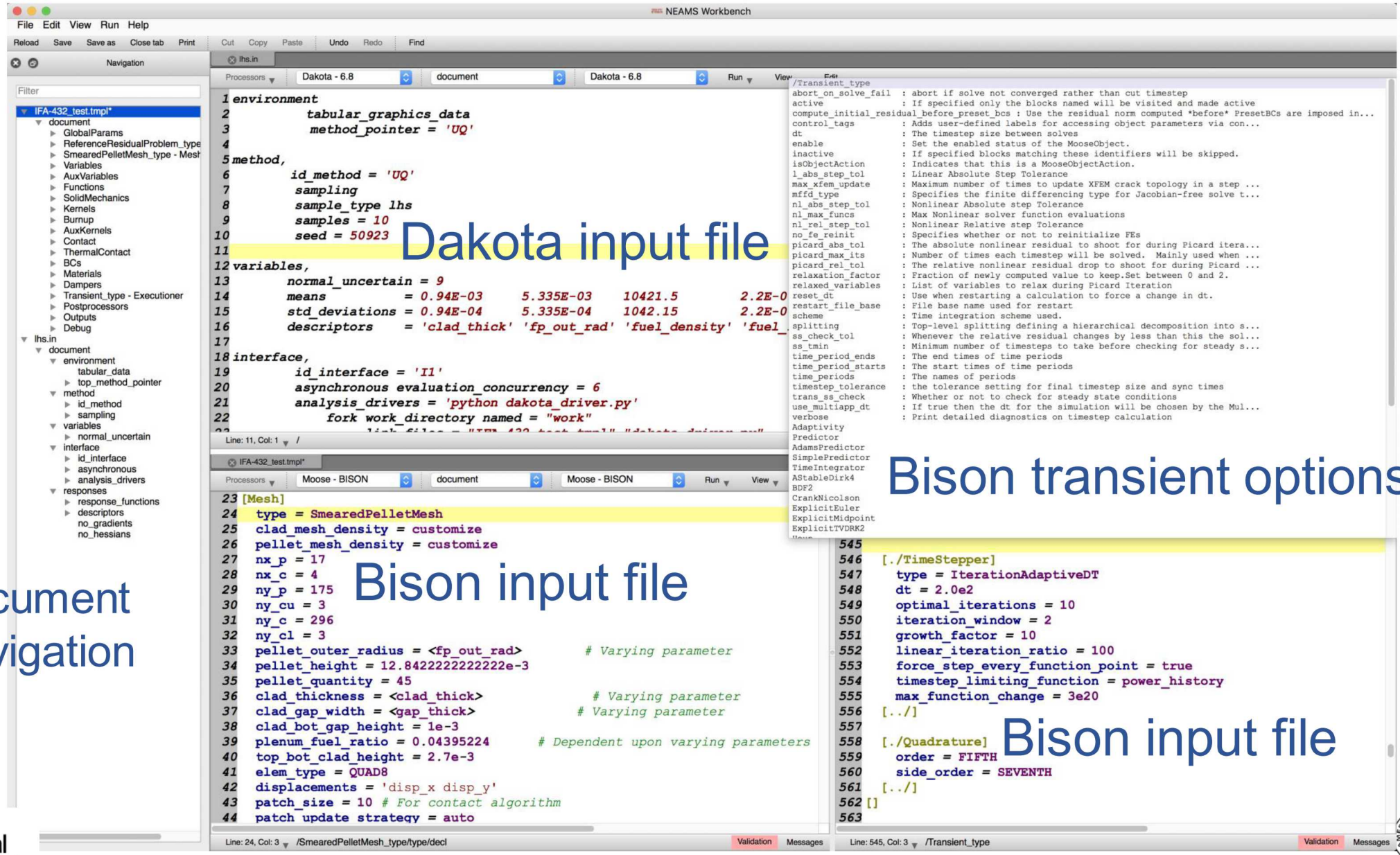

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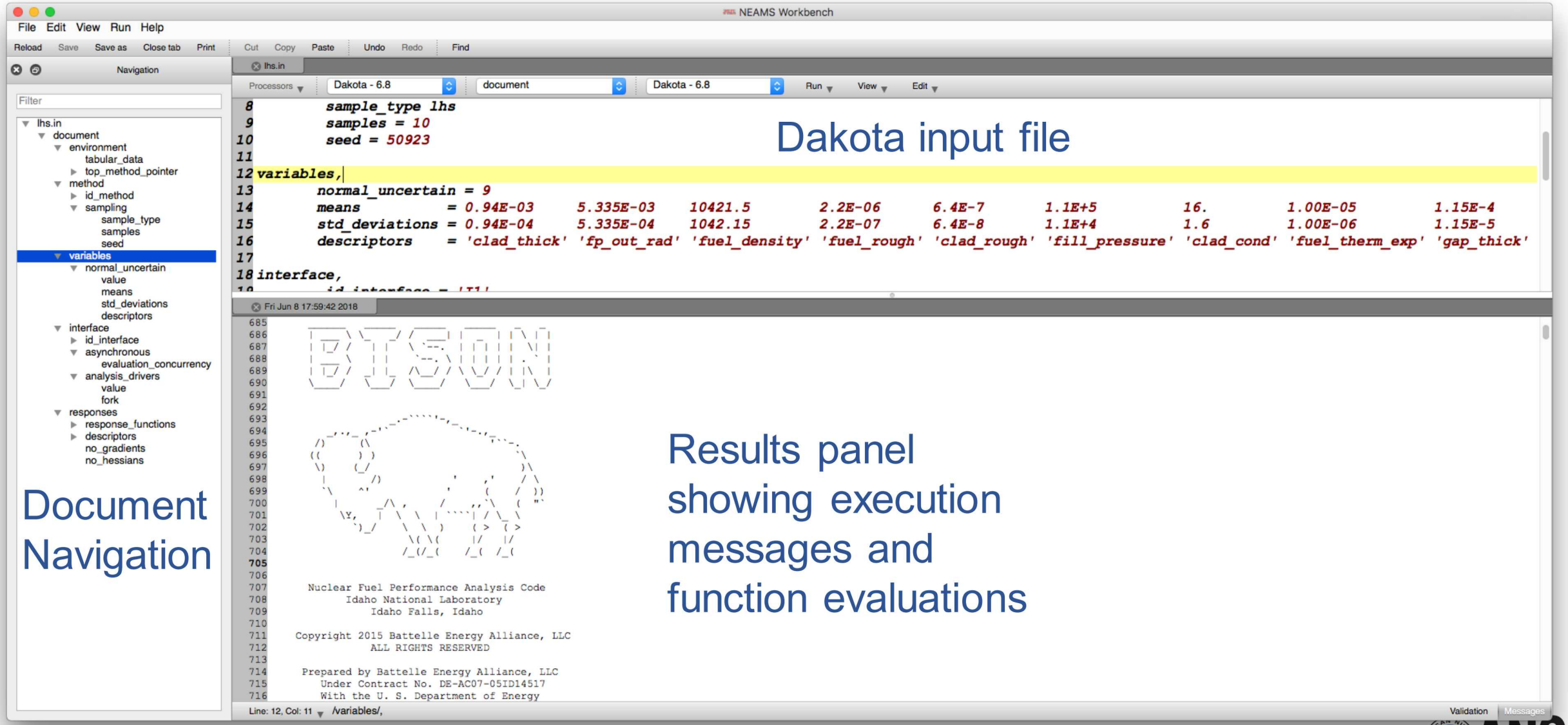

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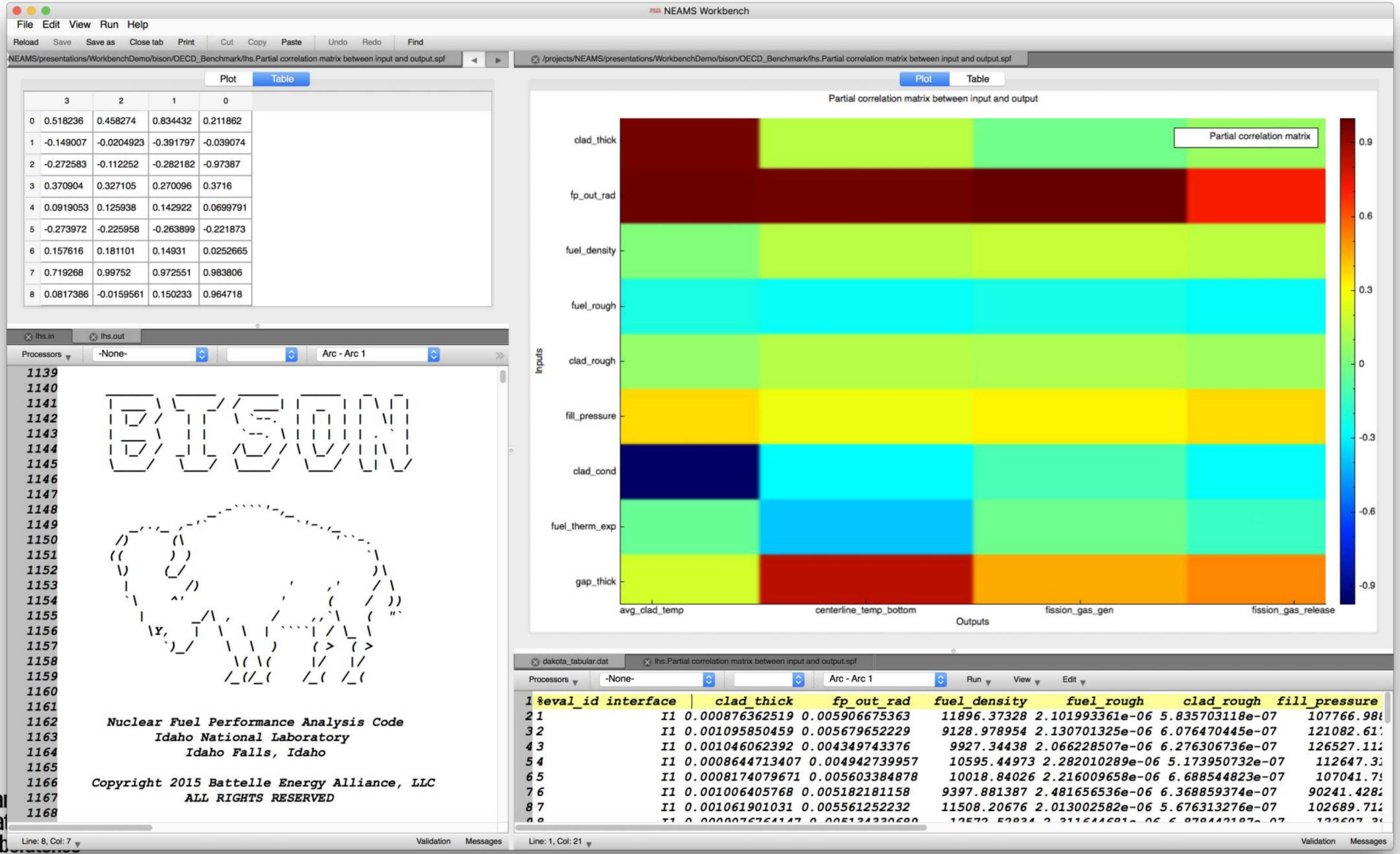

	3	2	1	0
0	0.518236	0.458274	0.834432	0.211862
1	-0.149007	-0.0204923	-0.391797	-0.039074
2	-0.272583	-0.112252	-0.282182	-0.97387
3	0.370904	0.327105	0.270096	0.3716
4	0.0919053	0.125938	0.142922	0.0699791
5	-0.273972	-0.225958	-0.263899	-0.221873
6	0.157616	0.181101	0.14931	0.0252665
7	0.719268	0.99752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

%eval_id	interface	clad_thick	fp_out_rad	fuel_density	fuel_rough	clad_rough	fill_pressure
1	I1	0.000876362519	0.005906675363	11896.37328	2.101993361e-06	5.835703118e-07	107766.98
2	I1	0.001095850459	0.005679652229	9128.978954	2.130701325e-06	6.076470445e-07	121082.61
3	I1	0.001046062392	0.004349743376	9927.34438	2.066228507e-06	6.276306736e-07	126527.11
4	I1	0.0008644713407	0.004942739957	10595.44973	2.282010289e-06	5.173950732e-07	112647.3
5	I1	0.0008174079671	0.005603384878	10018.84026	2.216009658e-06	6.688544823e-07	107041.7
6	I1	0.001006405768	0.005182181158	9397.881387	2.481656536e-06	6.368859374e-07	90241.428
7	I1	0.001061901031	0.005561252232	11508.20676	2.013002582e-06	5.676313276e-07	102689.71

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.