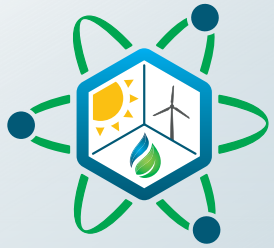

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NEAMS Workbench and IES

Summary

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Purpose of the Work Package

- Context:
  - IES modeling and simulation tools are constantly evolving to support the demonstration of integrated technologies along every step of the technology maturation
  - The problem inputs and workflows are varied and can be complex
  - Modeling and simulation can help scale-up experimental systems, but only if the tools are usable
  - How do we increase usability and deployability?
- Key goals:
  - Improve problem input preparation, execution, and results visualization
  - Simplify problem input and workflow
  - Support an extended user base to increase the toolset's impact

Methodology

- Leverage the **NEAMS Workbench** and its **integrated development environment (IDE)** to streamline user interactions and Framework for Optimization of ResourCes and Economics (FORCE) workflows
- Provide wizards and an active input assistant to accelerate input operations
  - Leverage DOE Nuclear Energy Advanced Modeling and Simulation (NEAMS) campaign development efforts to help automate the creation of more familiar input wizards
  - Use the NEAMS Workbench language processors to provide simplified, case-specific problem input for new users
- Enhance FORCE tools with advanced language capabilities
  - Enable FORCE to communicate, on demand, with the NEAMS Workbench (or other IDEs) information to assist user interaction
  - Important flexibility for increasing adoption of research software

NEAMS Workbench Mission Statement

Provide a cross-platform graphical user interface (GUI) designed to facilitate problem creation, modification, navigation, validation, and visualization, as well as output and data file interaction as needed by new and experienced users.

Latest release available at https://code.ornl.gov/neams-workbench/downloads

For assistance, email nwb-help@ornl.gov

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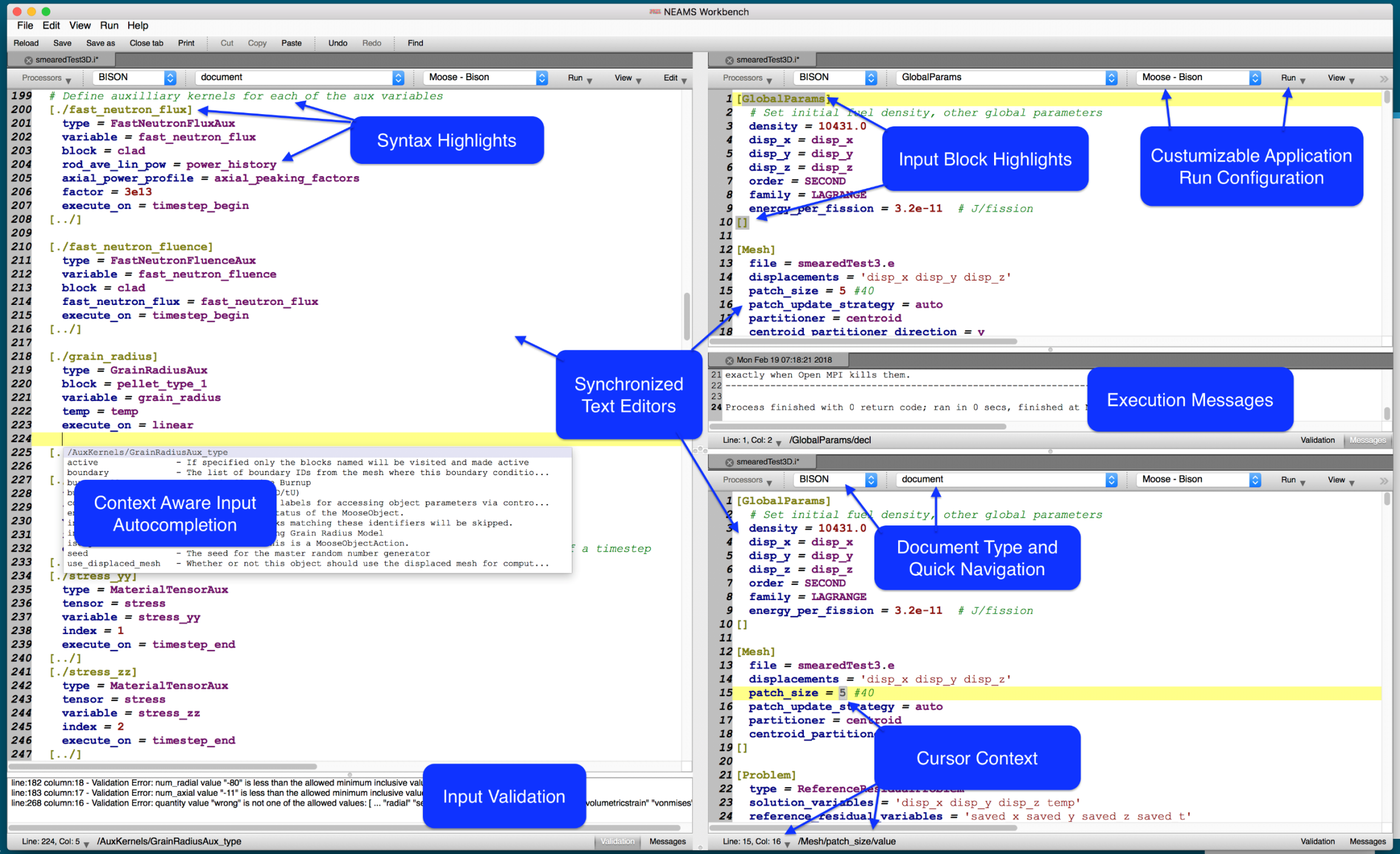
NEAMS Workbench Input Editor



https://ies.inl.gov

NEAMS Workbench 2D Plots

- Extensible data processor
- Export plot to image and PDF (supports SVG)

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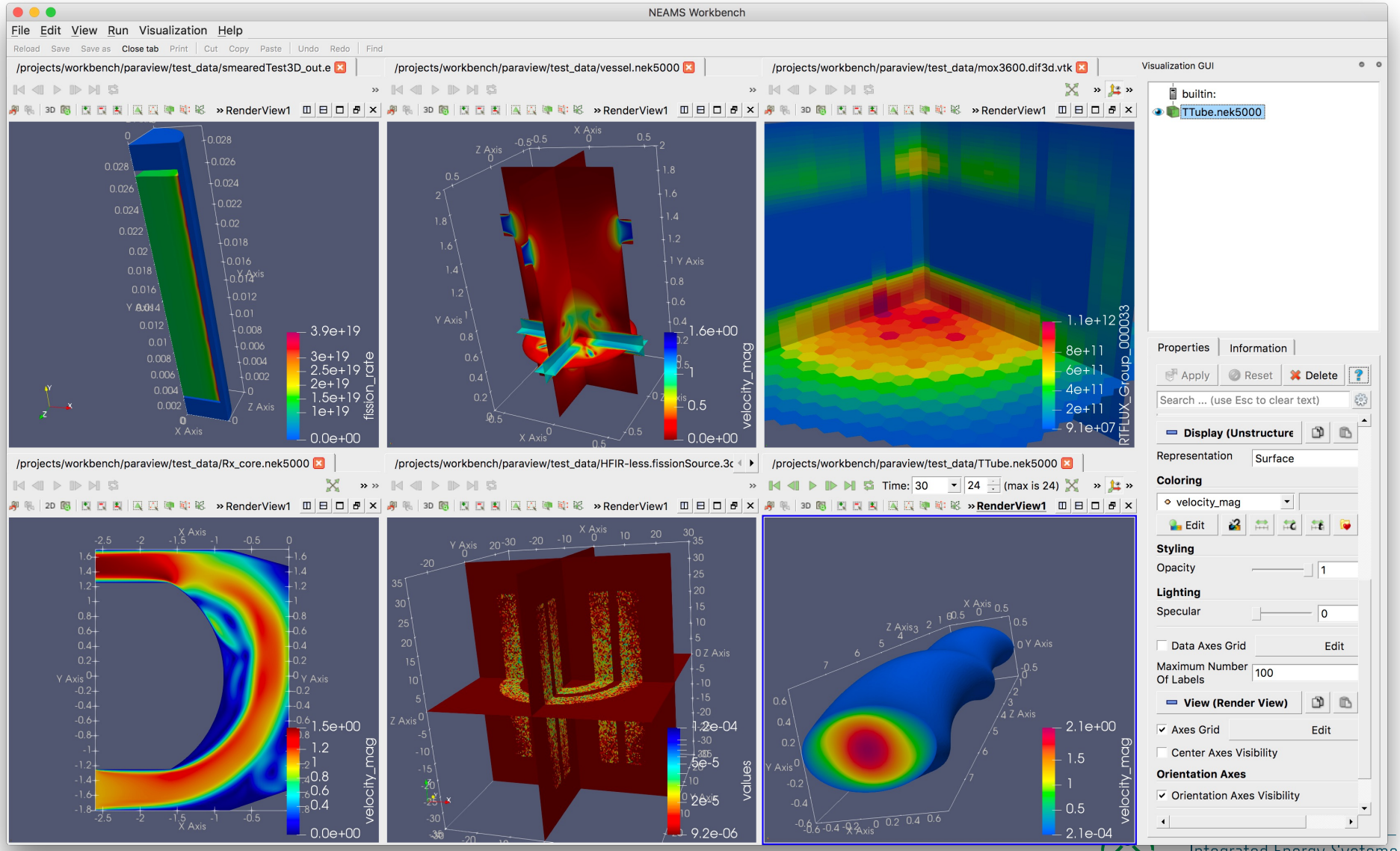
NEAMS Workbench ParaView Visualization

- Supports all ParaView 5.6 default data types
- ParaView is deployed within the NEAMS Workbench



Workbench Analysis Sequence Processor (WASP)

- Provides input editor components to the NEAMS Workbench
- Includes reusable input processors accessible via C++ and Python API
  - Standard Object Notation (SON) used by PyARC and Nek5000 integration
  - Definition Driven Interpreter (DDI) used by Dakota and CTF integration
  - MOOSE Application Input Syntax (HIT)
  - VERA Input Interpreter (EDDI) used by VERA-CS and CTFFuel integration
  - Language Server (LS) and client interface used by MCNP ® integration
    - **Latest efforts involve incorporation of LS into the MOOSE framework to enable native diagnostics in Workbench**
- Utilities (input validation, retrieval, and template engines) and Python
- Open source at https://code.ornl.gov/neams-workbench/wasp

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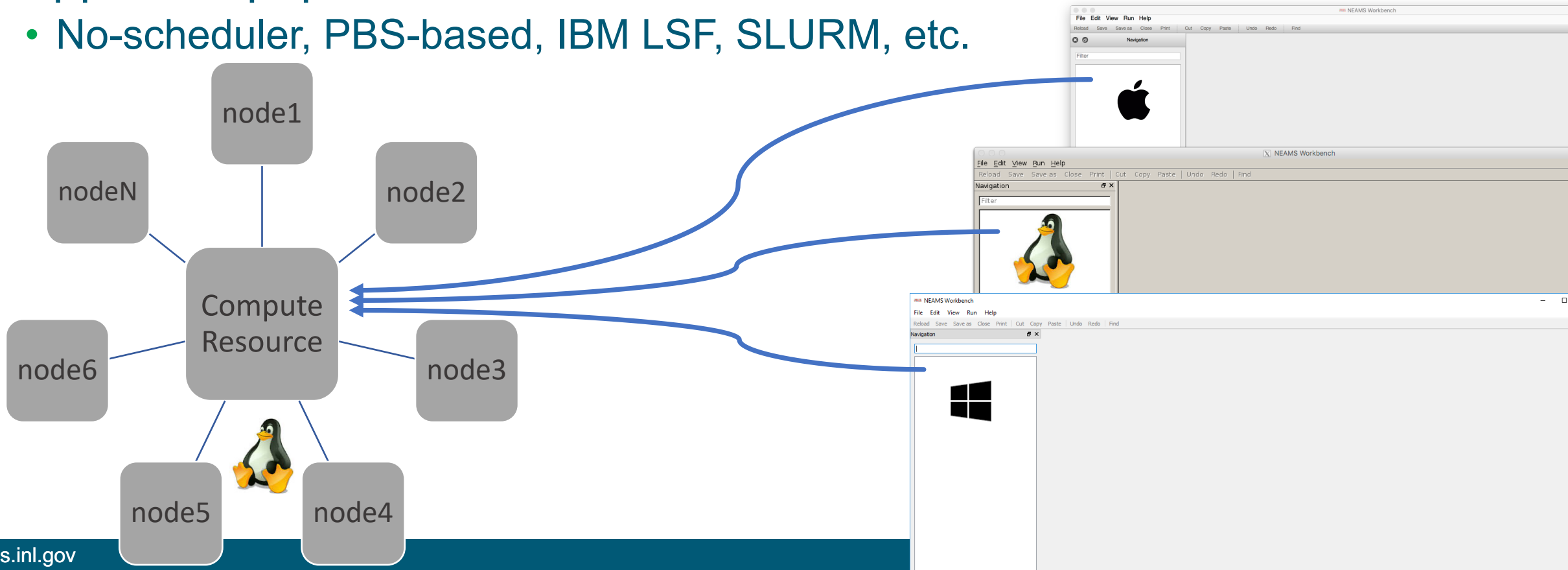
NEAMS Workbench Application Runtime Layer

- All applications integrated into the NEAMS Workbench have a runtime layer written in Python (3)
  - A configuration-controlled *offline* Python environment is included with Workbench (Workbench/rte/entry.sh or Workbench/rte/entry.bat)
- Enables consistent job launch interactions between all integrated codes
  - Some applications lack any level of runtime (e.g., requiring users always name inputs ‘input’), this layer normalizes application job launches with options available to users in Workbench
- Enables remote job launches across networks

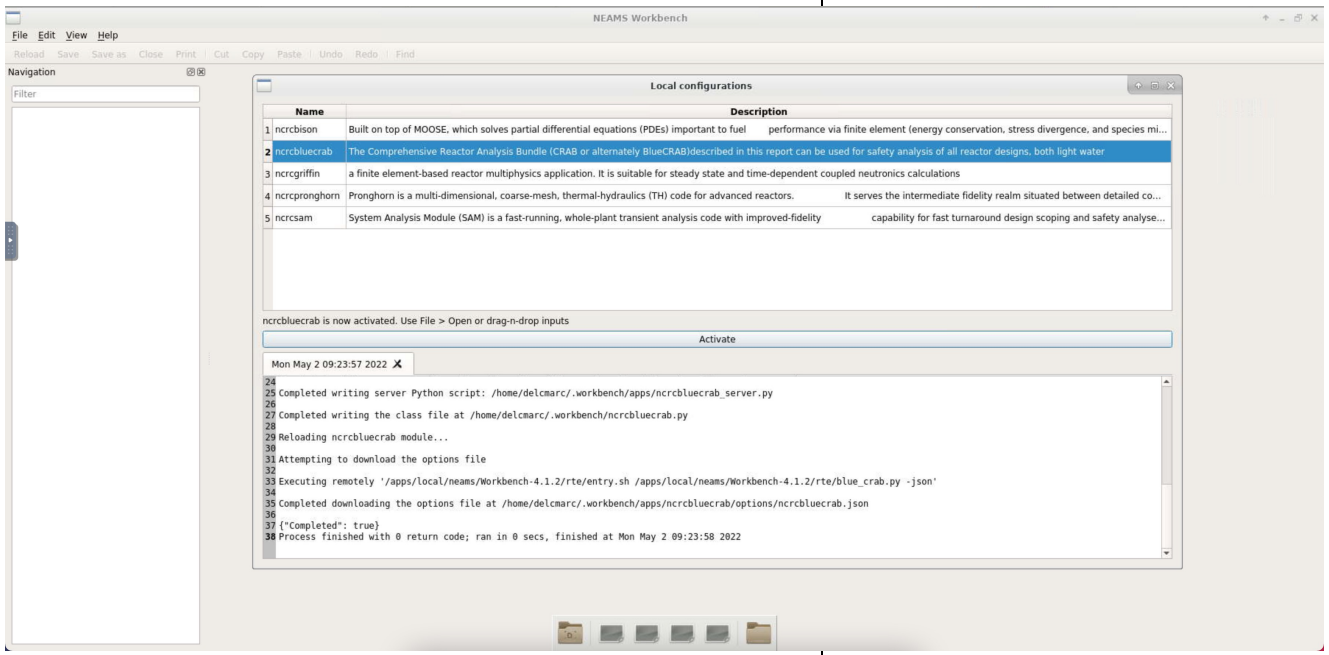
Job Scheduling

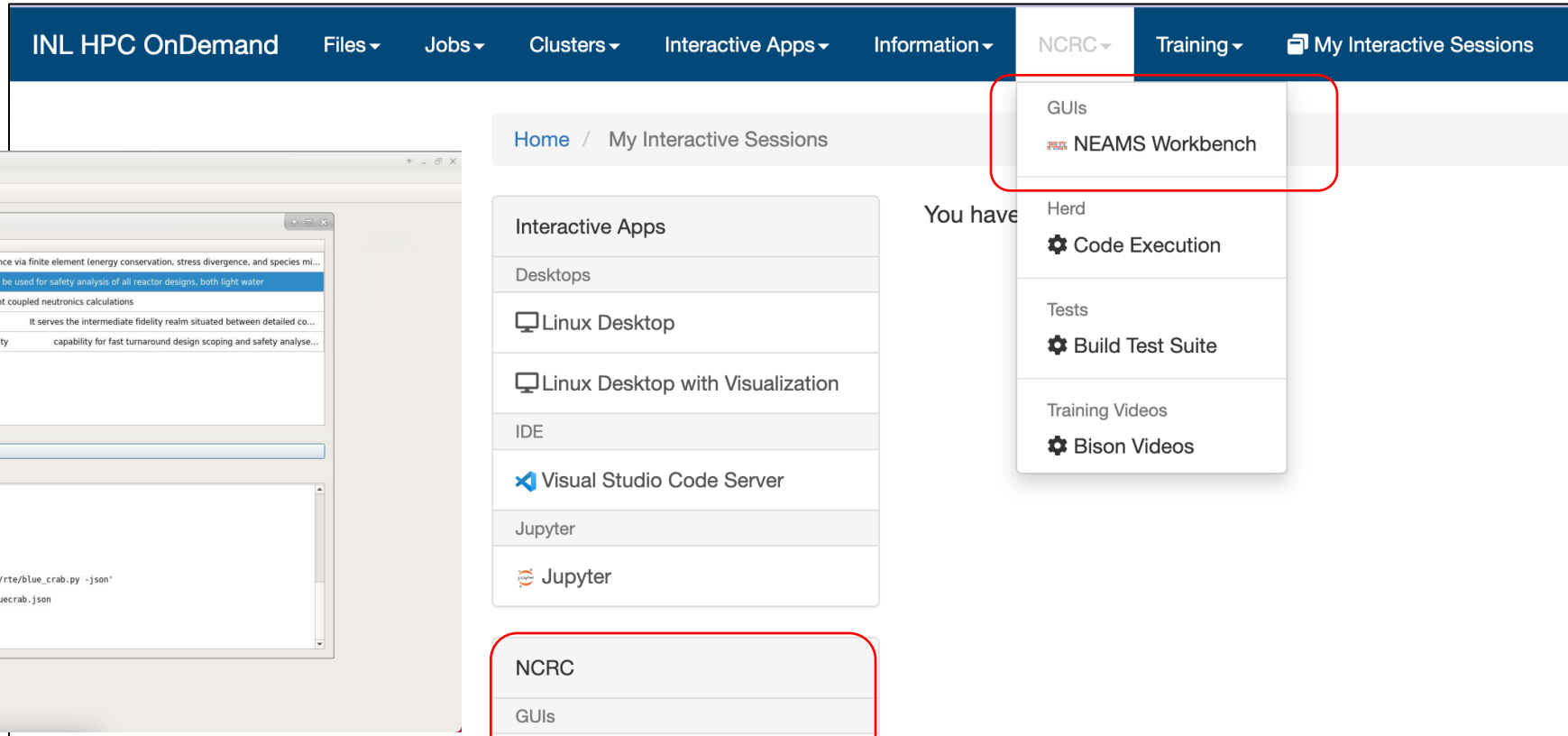
- Under development
  - Support Windows, Mac, Linux, and **Open OnDemand** clients
  - Only supports Linux compute resources
- Support for popular schedulers
  - No-scheduler, PBS-based, IBM LSF, SLURM, etc.



Open OnDemand and INL's NCRC Instance

- NEAMS Workbench is available on INL's Nuclear Computation Resource Center (NCRC)
- 3-click app activation





Main Results and Desired Outcomes

- Accelerate user adoption and onboarding by easing problem definitions – let users focus on data not syntax
- Streamline, improve, and standardize presentation of results
- Improve workflow – especially for multi-level parallel analysis

Conclusions and Next Steps

- Integration has just started
- Initial focus is on improving native capabilities toward a stable foundation in FORCE leading to enhanced usability, advanced areas of research, and successful adoption of the GUI
- Extent of programmatically available metadata can be improved to enable re-use (do not want to recreate software)

- Next steps:
  - Demonstrate lightweight user input syntax (more natural than XML)
  - Increase programmatic accessibility of Holistic Energy Resource Optimization Network (HERON)'s native input
  - Identify highest priority items to aid production analysis

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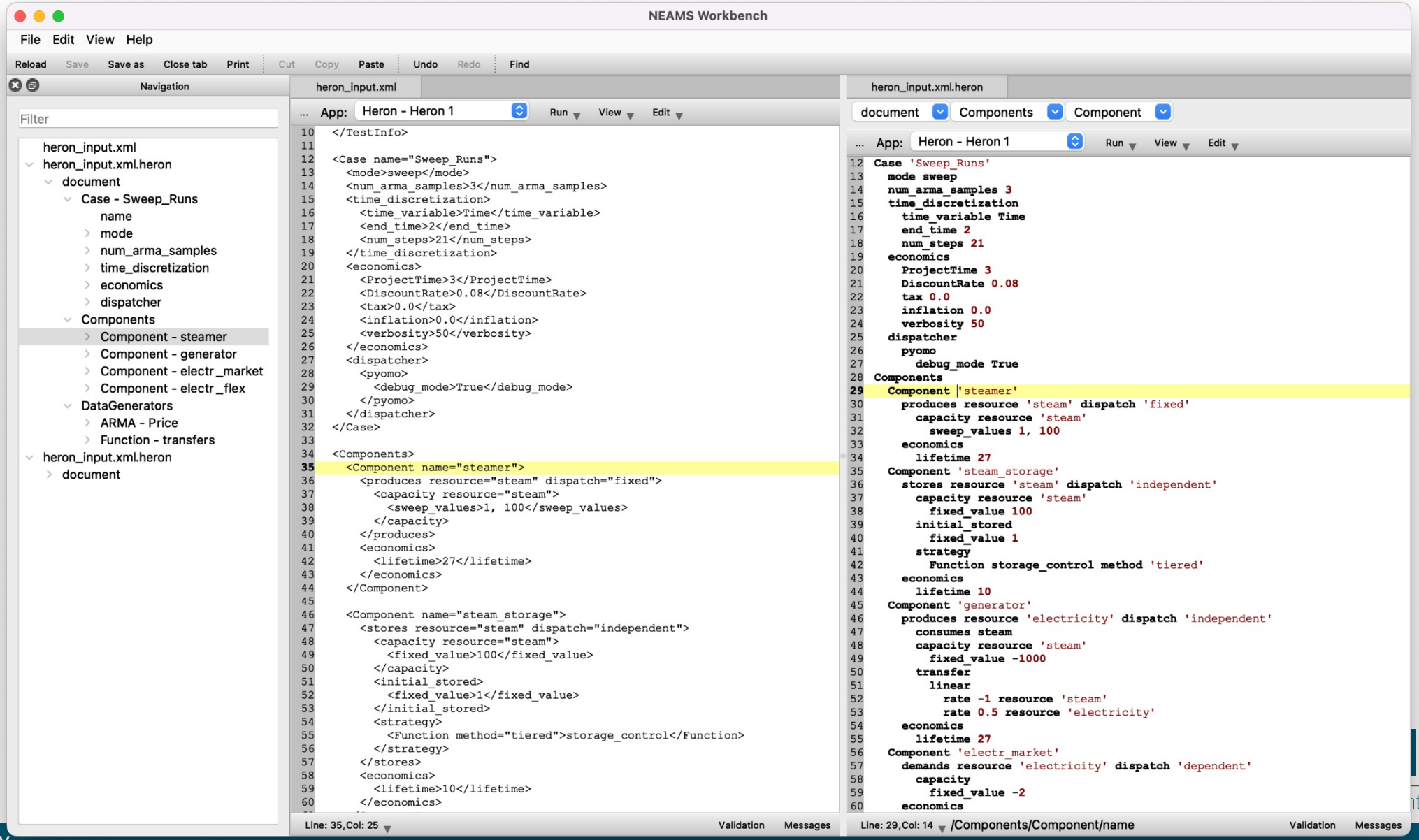
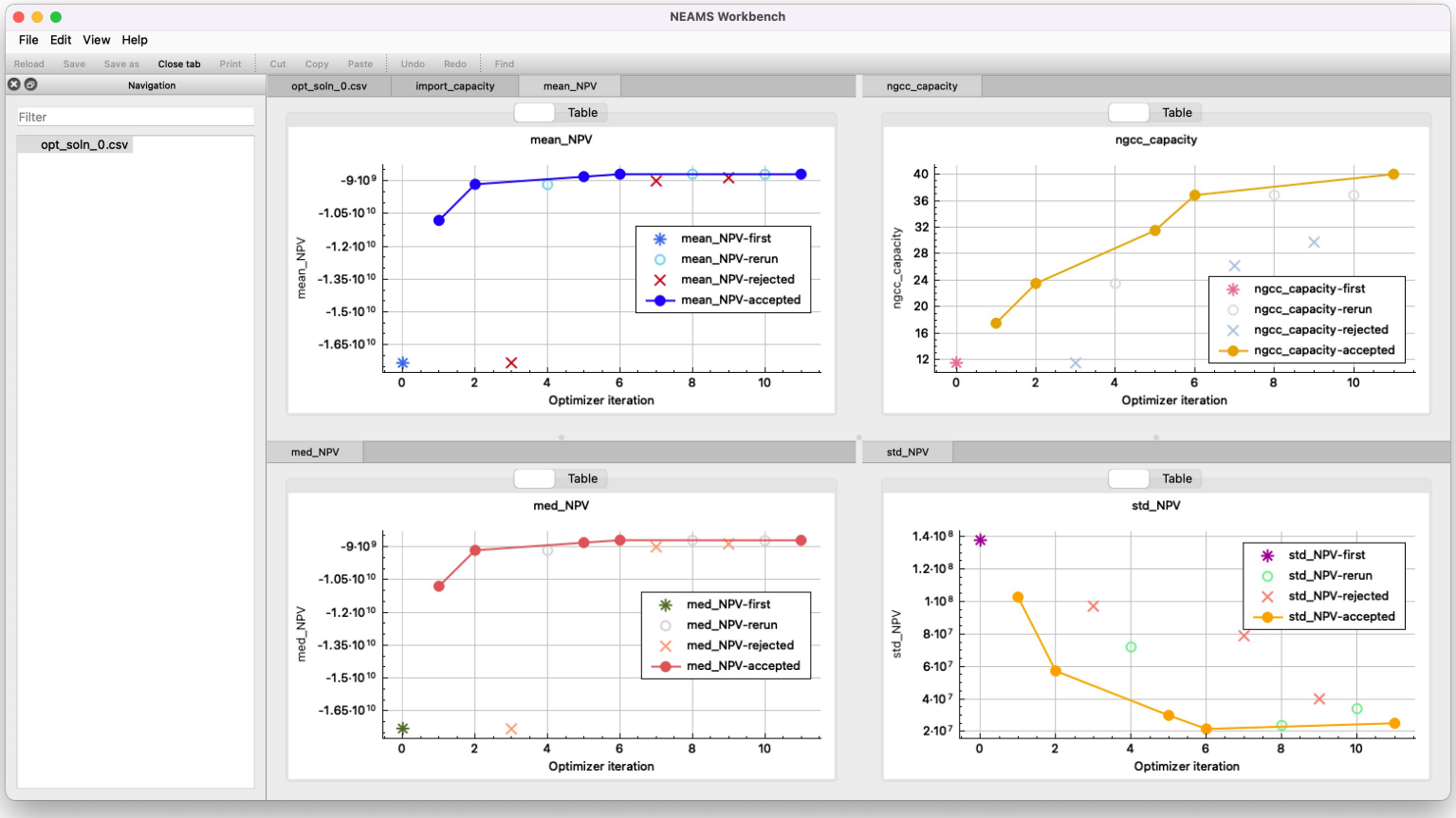
Preview | Lightweight UI



Questions?

- Working lunch session will provide demonstration and hands on opportunity



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