SAND2019-0831C

Applying executable, graphical workflows in SAW to electrical simulation-based analysis

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Outline

- Executable, graphical workflows in SAW
- Electrical/EM Applications
  - Wrapping an older, powerful EM code to lower usability barriers
  - Assembling a toolkit for compact model calibration
- Some observations
- Acknowledgements

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SAW: Sandia Analysis Workbench

- Adaptation of open-source integrated software development environment to support analysis via computational simulation

- Developed & refined at SNL over 10 years
- Supports
  - Integrated tools for model composition and configuration
  - HPC job submission and monitoring
  - Management of simulation data via a networked repository
- Value parallels that of software IDE's
  - Integrated, more uniform interface to wide array of capabilities
  - Automation of key functions where possible

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Motivation

- Major steps in CompSim workflows are mediated via a combination of *analyst actions* and *small/informal scripts*
- Hard to scale
  - Analysts are limited resource
  - Scripts suffer from “poor software hygiene”
- Threat to credibility
  - Linkage between steps is obscured or lost, so workflows aren’t traceable, repeatable
- Proposed (SAW) solution
  - *Executable, graphical representation for workflows*

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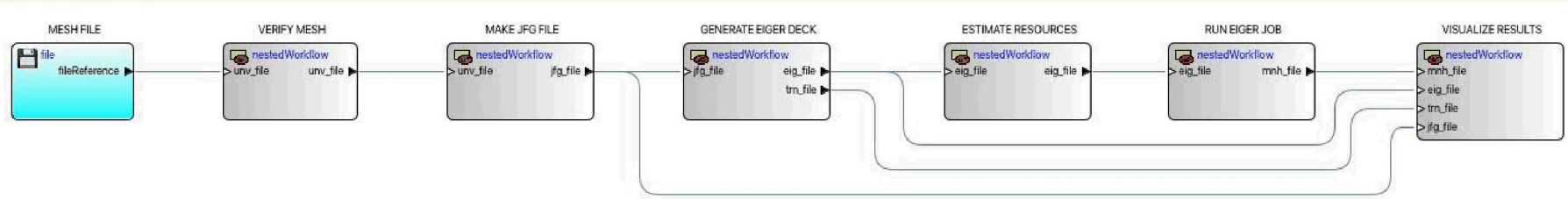
Why graphical workflows?



- Standardized, integrated solution
- Graphical workflows clearly represent linkage between artifacts
- Artifacts identified by *spatial context*, not *names*

- Graphical representation “naturally” constrains complexity

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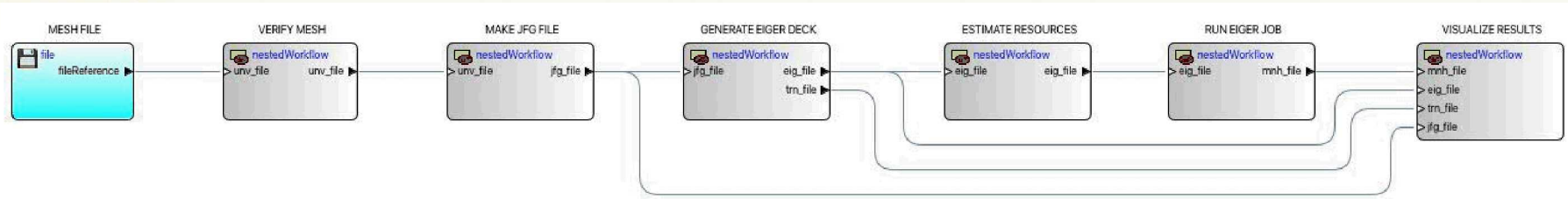

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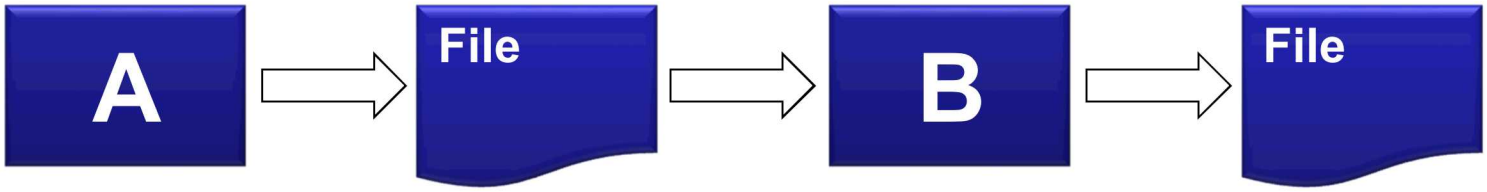

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Graphical workflow for EIGER

- EIGER: powerful, frequency-domain EM modeling code with unique capabilities
- Designed for “developers = users” use-paradigm
  - Heavy emphasis on computation (not usability)
  - Complicated, unforgiving toolchain, cryptic error messages
- Desired benefits from graphical workflow:
  - ability to generate flexible workflow schema allowing *non-developer analysts* to set up, run, and post-process EIGER jobs, including integration with Dakota
- Workflow highlights:
  - input deck preparation
  - HPC job submission
  - overall integration

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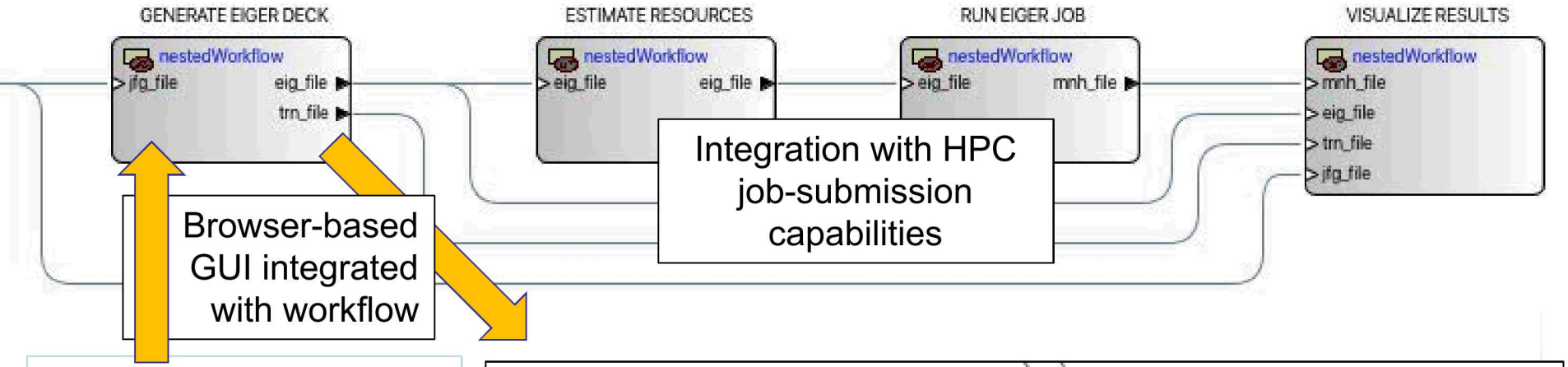
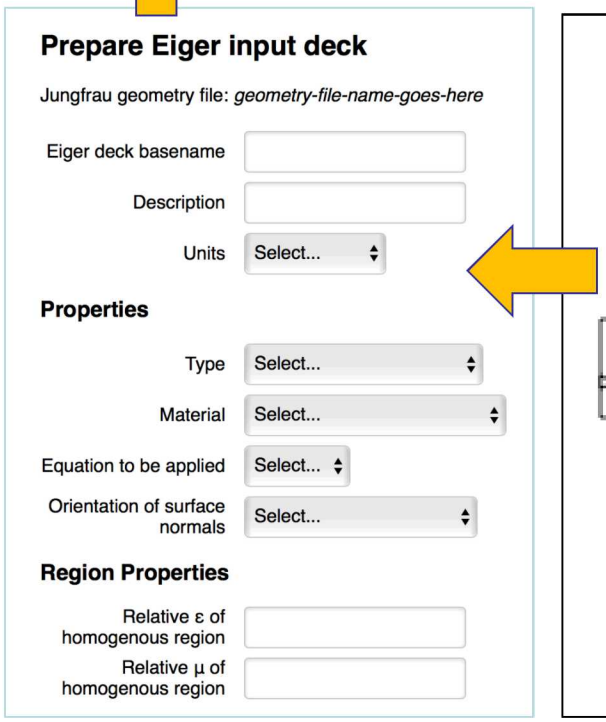
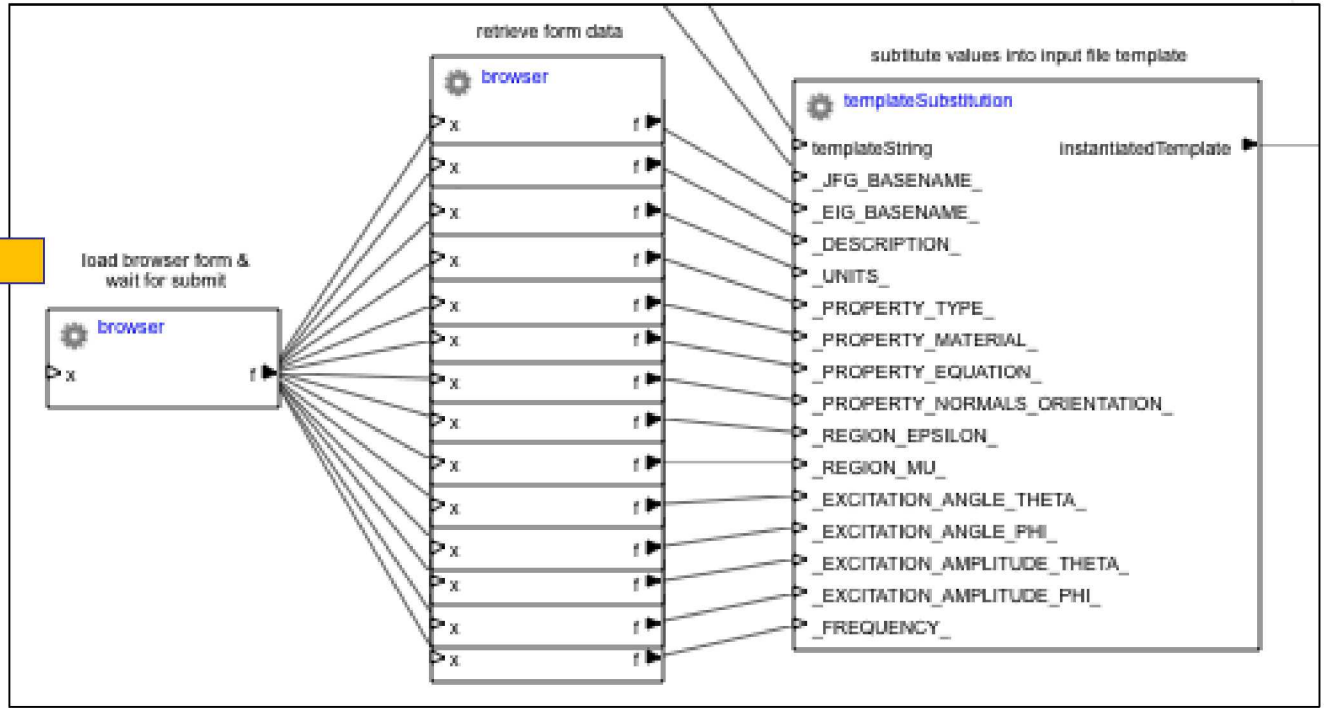
End-to-end EIGER workflow







Compact model calibration framework

- Currently carried out via commercial tools
  - Workflow hard to capture, difficult to integrate
- Goal: a “toolkit” from which calibration workflows may be *constructed*, *saved* and *shared*
  - "Jailbreak for model calibration”
- Benefits
  - Customization/flexibility
  - Share, reuse, traceability
  - Ability to integrate with new capabilities as developed

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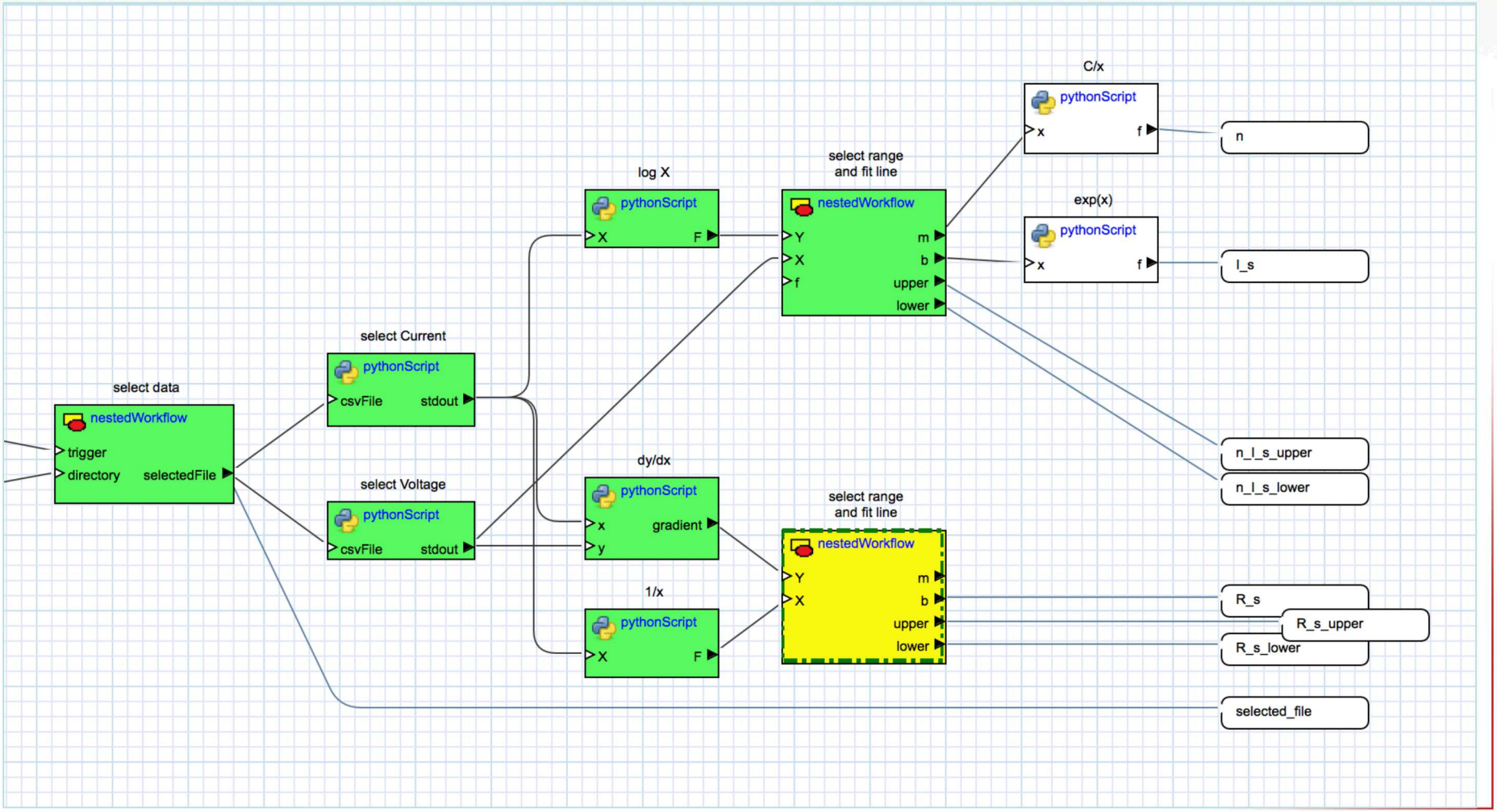
Zener Diode Forward Parameter Extraction



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Observations

- Crafting the highest-utility subcomponents is likely a long, iterative process.
- Rich GUI elements seem highly valuable, but so far require “classical” programming.
- Building end-to-end workflows is alluring, but risks over-constraining analysts
  - *Better: rapid iterations with smaller prototypes*
- Intrinsic benefits, appeal of graphical representation continue to appear very real.

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Acknowledgements

- SAW
  - Ernest Friedman-Hill *(principal architect of SAW workflow capability)*
  - Ed Hoffman
  - Marcus Gibson
  - Kevin Olson
  - George Orient
  - Robert Clay
- EIGER
  - Joe Kotulski
- Compact model calibration
  - Shahed Reza
  - Tom Buchheit
  - Ian Wilcox
  - Jason Verley

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