SAND2016-2976C

ENGINEERING SCIENCES WORKFLOW IN THE SANDIA ANALYSIS WORKBENCH

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Workflow Panel

SOS-20, Asheville, NC

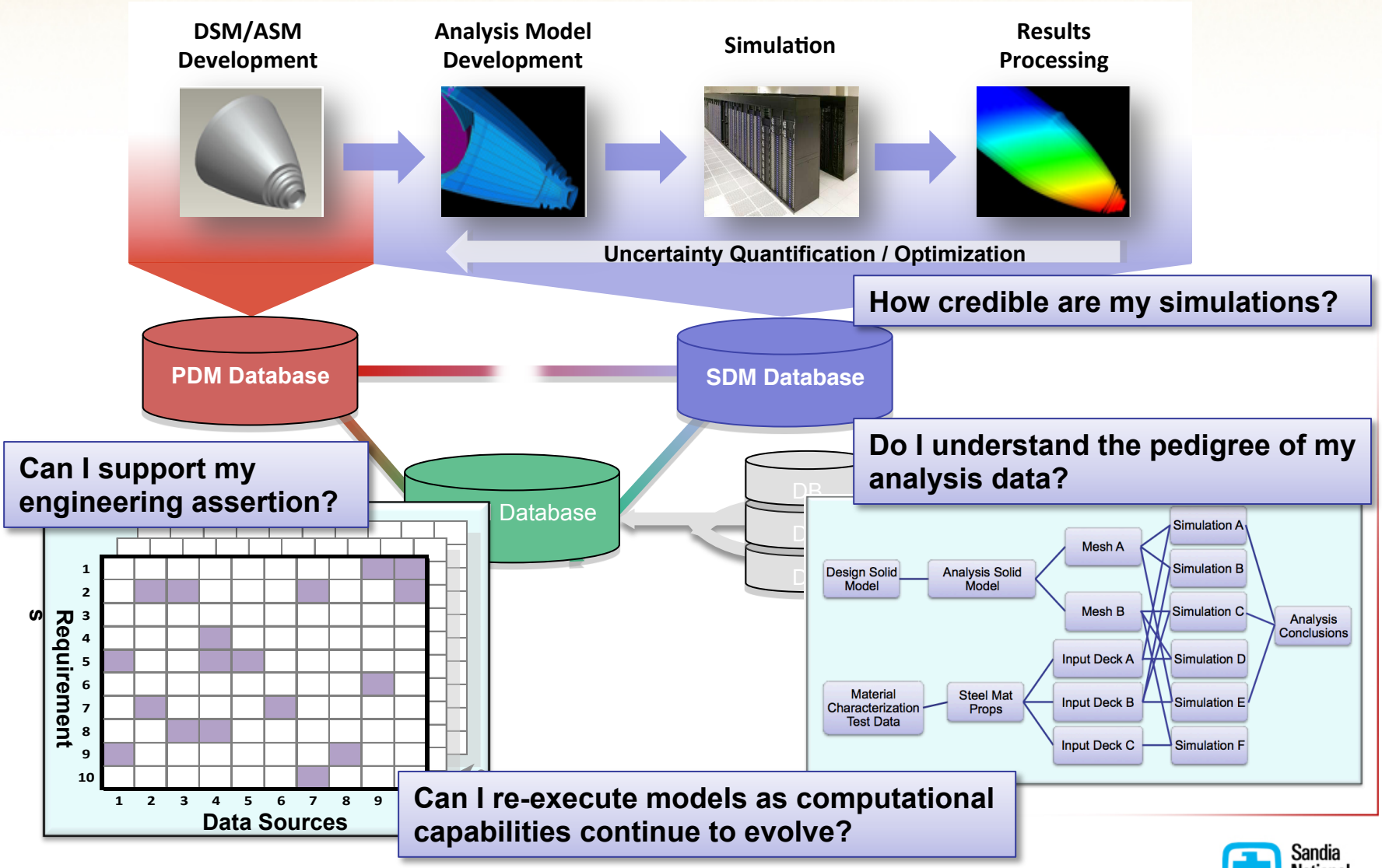
March 23-25, 2016

Workflow for Dummies / Rocket Scientists – Panel Questions

- What applications are driving workflow capability at your lab?
- What is your current workflow capability?
- What level of effort are you investing?
- What is your current focus?
- What does a workflow capability look like in 2025?

Simulation-Based Stockpile Stewardship

Moving away from test based certification



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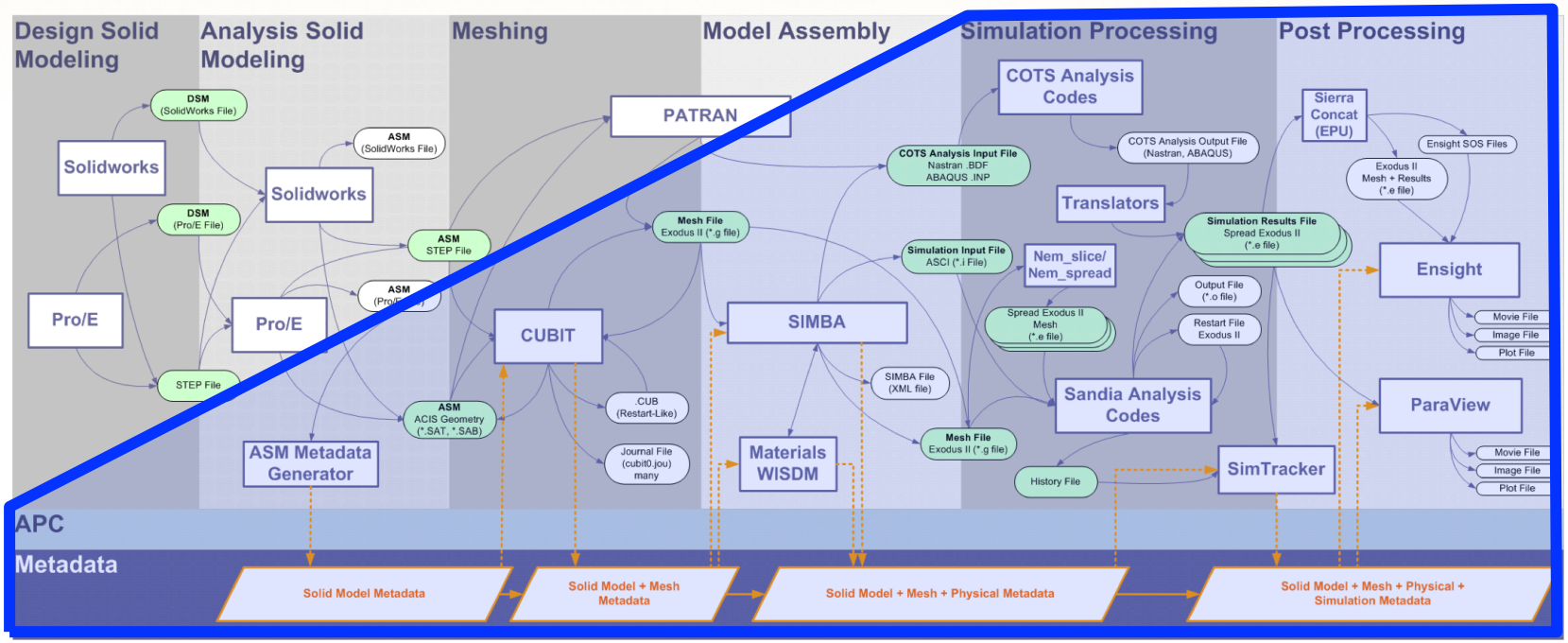
Typical Analysis Workflow – Many tools, many files



Sandia Analysis Workbench

- The analysis process involves many (stove-piped) tools that generate a large number of artifacts, which must be managed by the analyst.
- SAW Vision: an integrated environment for these tools

SAW is a Collaborative Modeling & Simulation Platform

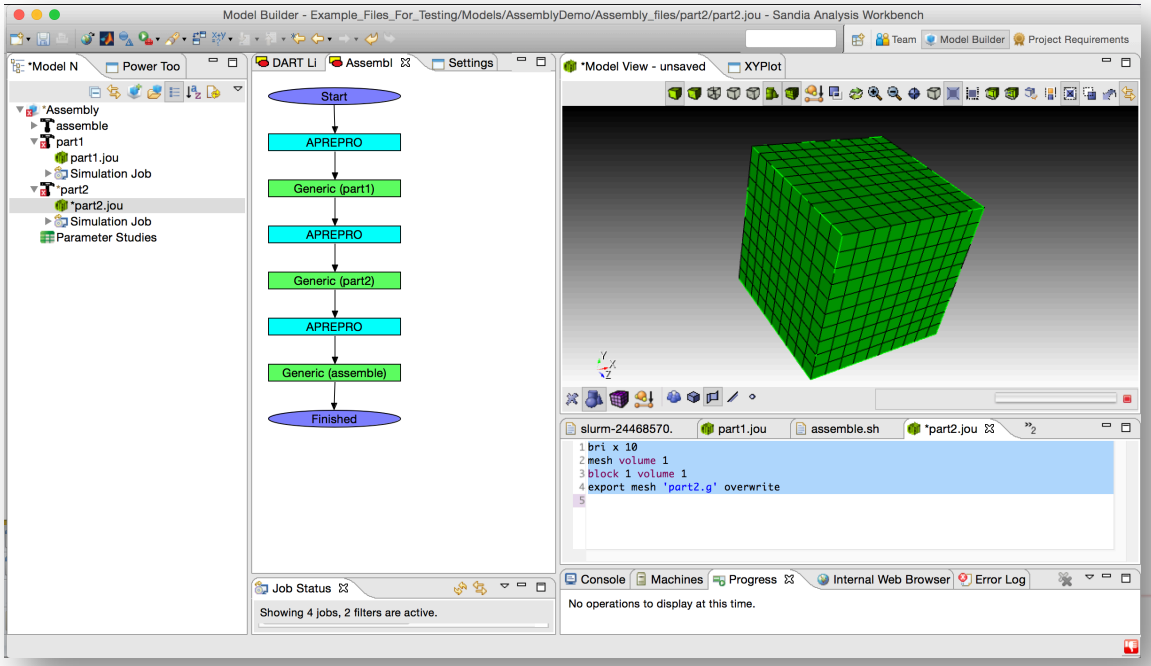
SAW products contain contributions from multiple teams throughout Sandia:

- SAW core framework (org 8900)
- Cubit (org 1500)
- Dakota UI (org 1400)
- V&V Visualization Tools (org 1500)
- Analytics and Visualization Tools (1400)
- PLATO – Topology Optimization (org 1500)
- Electrical Analysis Codes (org 1300)
- Computational Mechanics Codes (org 1500)

SAW was recently open-sourced

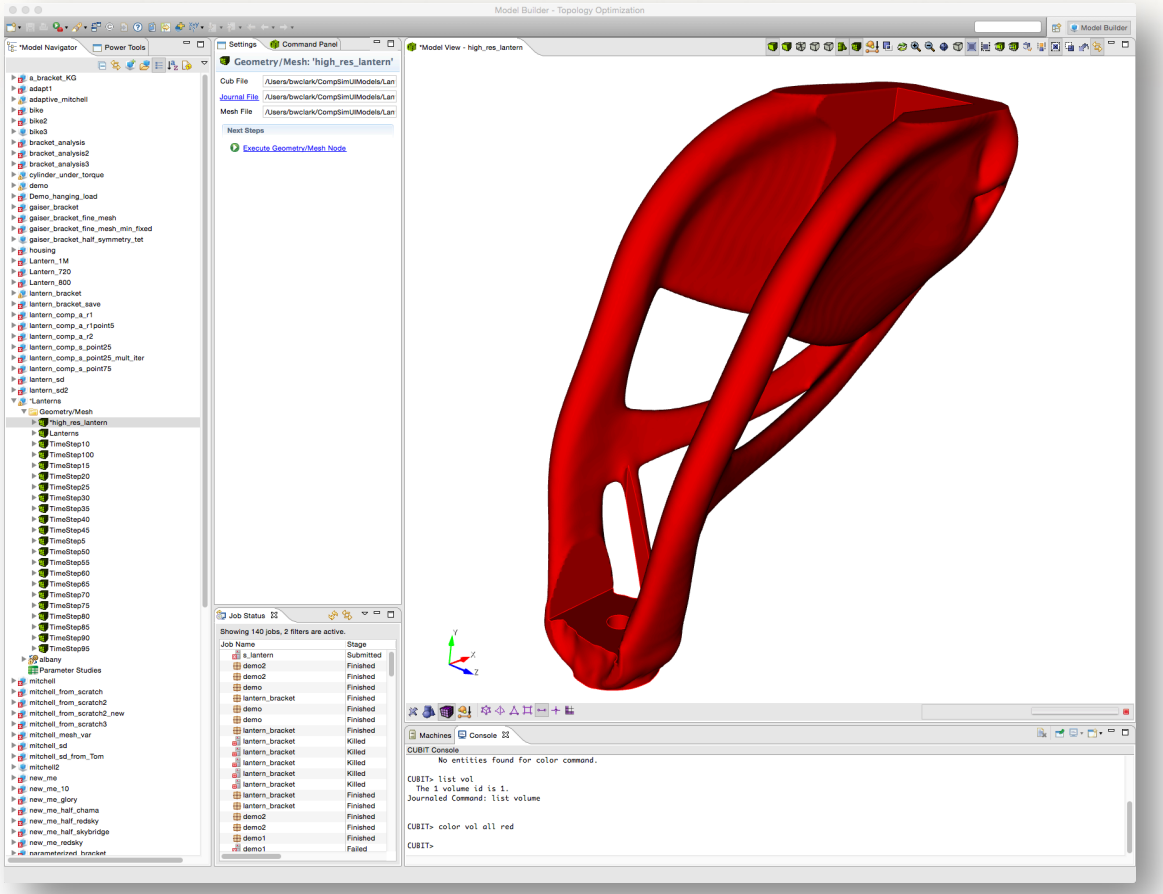
Model Assembly Workflow

- Experimented with using Generic Components to script server-side assembly
  - One generic component for each Cubit part
  - Generic component for assembly script (Gen3d)
  - Run as a linear sequential workflow; Cubits could run in parallel
  - Edit journals for each part locally, experiment with local cubit, then run
  - Next: assembly script generation



PLATO – Topology Optimization

- Powerful topology optimization capabilities in an environment that makes them easy to use
- The PLATO product is built on top of the SAW architecture
- Leverages SAW geometry/meshing, graphical model attribution, HPC job submission and monitoring



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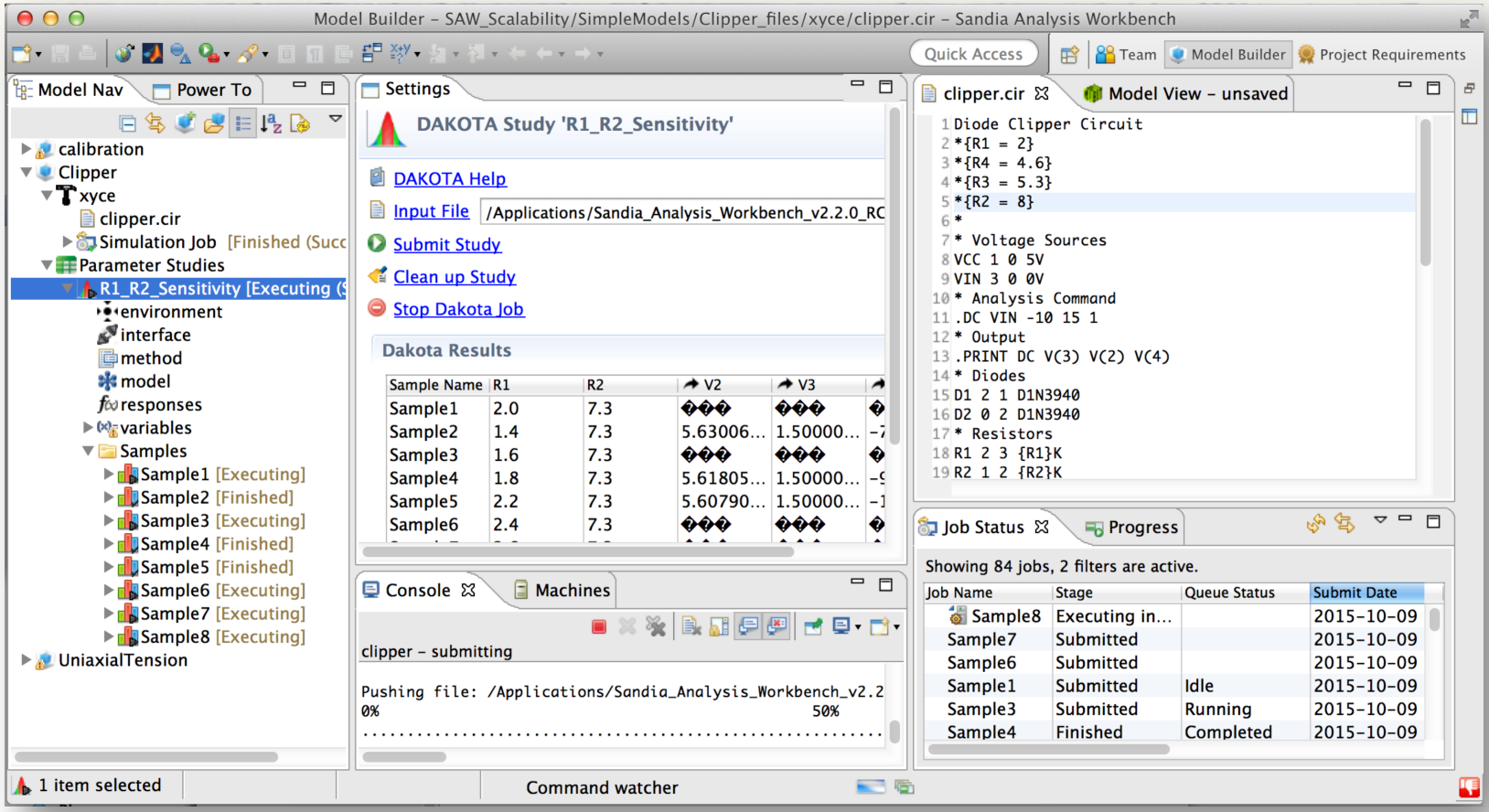
DAKOTA UI: Electrical Workflow (XYCE)



First demonstration of user-defined workflow components, enabling users to wrap virtually any mod-sim code

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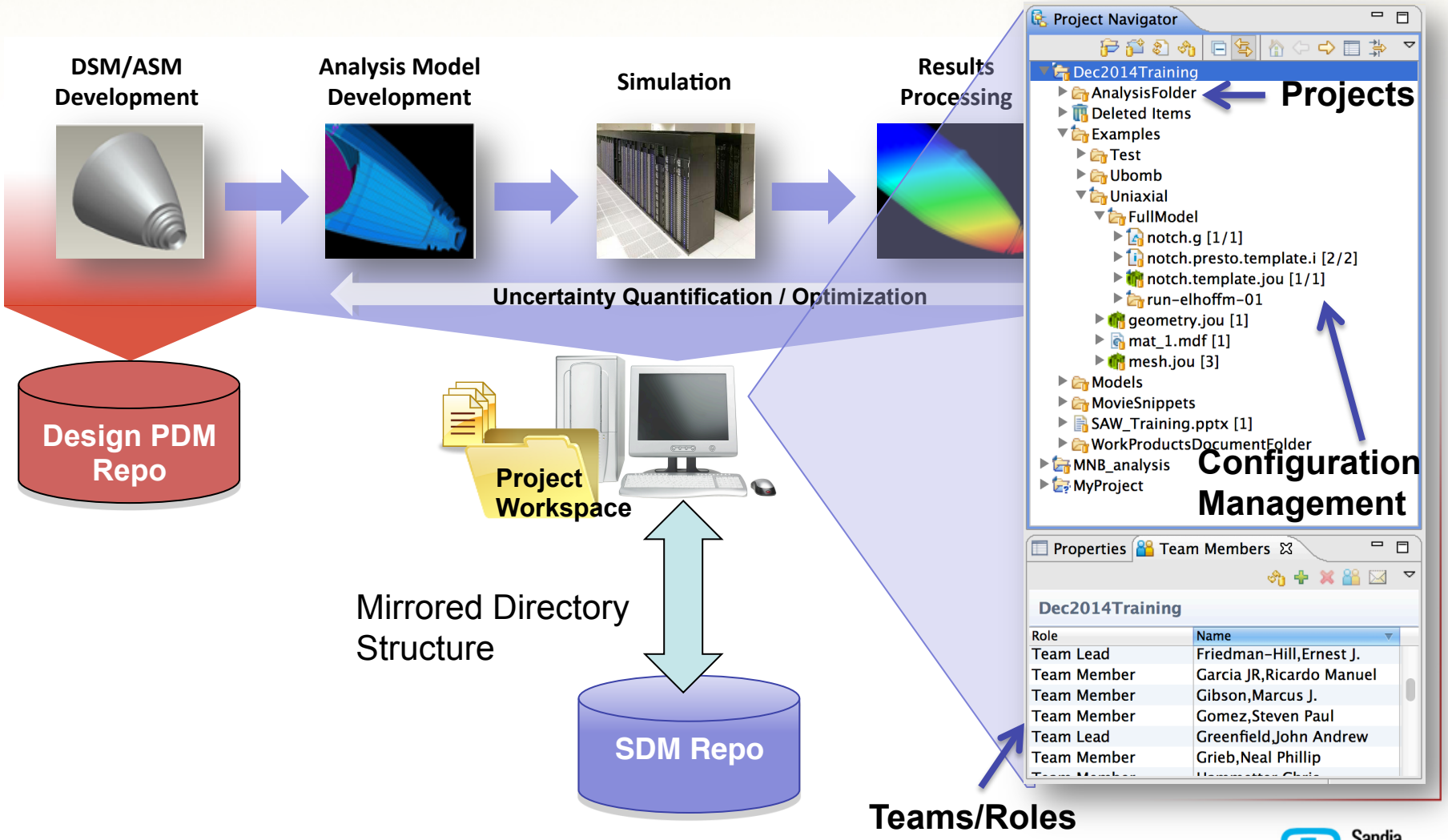
Simulation Data Management

Team-based configuration management and dependency management of analysis data.
Central repository for archiving pedigreed models and simulation-derived knowledge.



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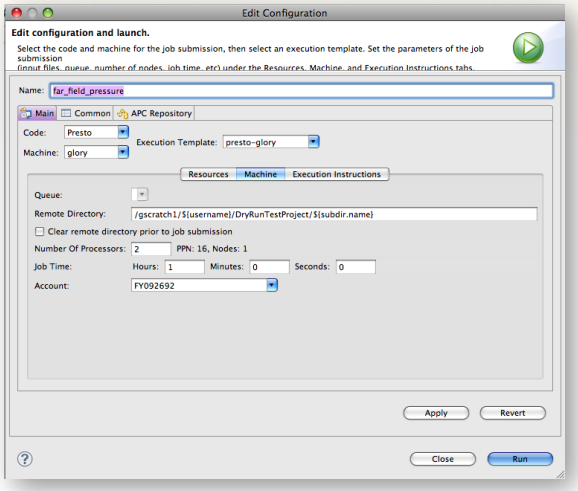
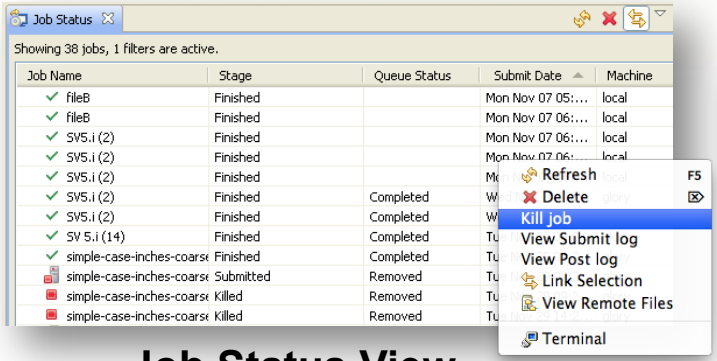
Job Submission Tools

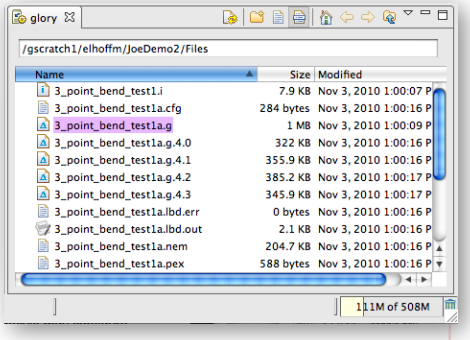
Simplifies the process of running simulations in a diverse computing environment.
Remote simulation jobs and data are managed as if they were on the analysts desktop



Job Submission Dialog

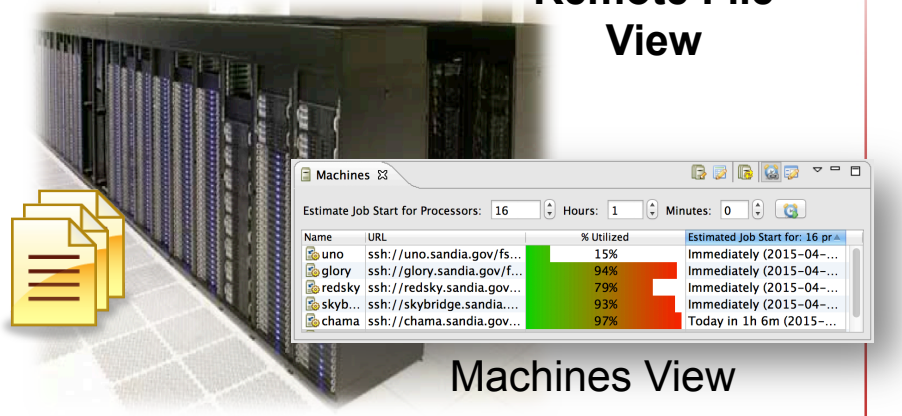


Job Status View



Remote File View

Local Project Files



Machines View

HPC Distributed Data

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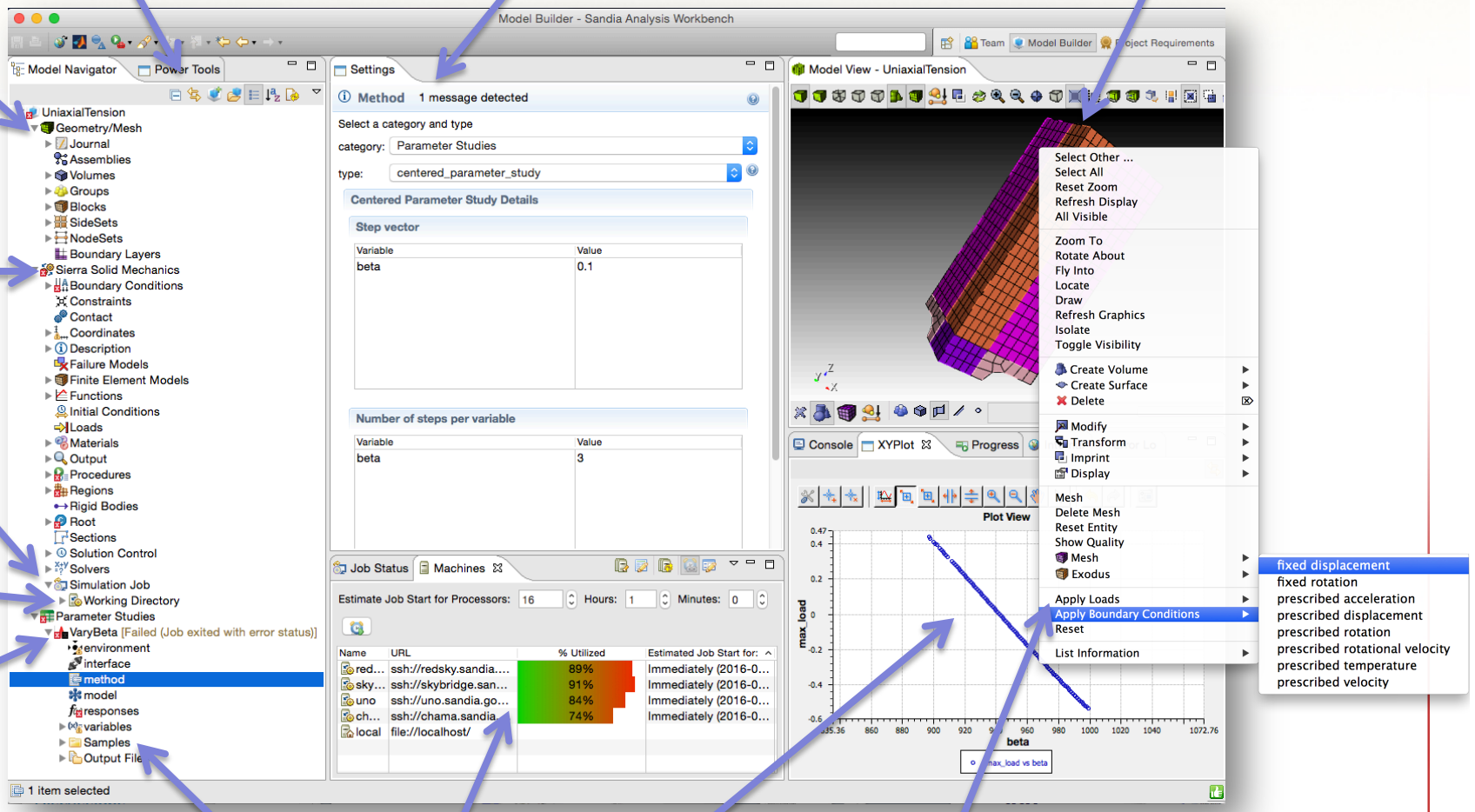
SAW Model Builder

Integrated Graphical Model Building Environment



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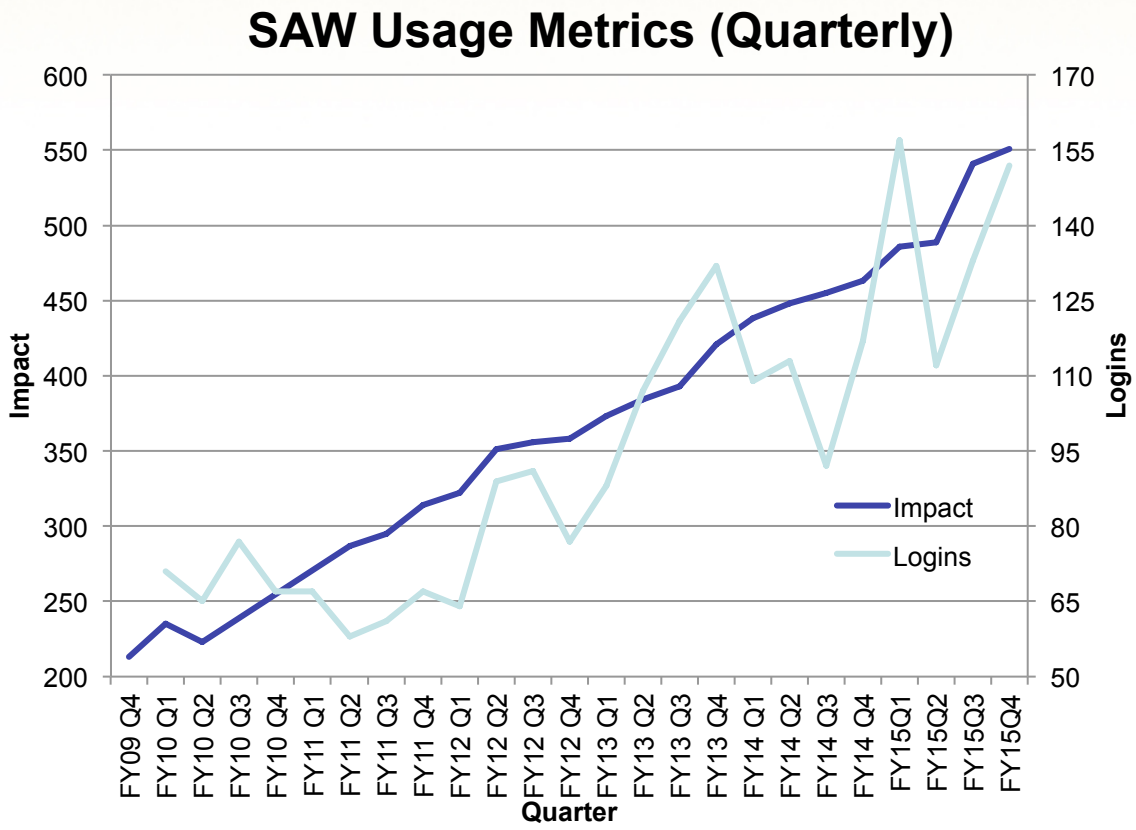
Metrics show widespread adoption of SAW



"Impact" represents staff who own data in our repositories
"Logins" are unique users of our data management service

Scale of Sandia's Effort

- SAW (core workflow integration capability) is about $2M/yr (~ 5 FTEs)
- Integrated Workflow (IWF) Project includes SAW, plus about $2M/yr (~ 5 FTEs) collaborative effort – hence, ~$4M/yr (~10 FTEs)
- Plus, there are other investments that provide enabling capability (e.g., Data Warehouse, Scalable I/O, electrical visualization capability, …)

Sandia's Current Workflow Focus

- Integrated Workflow (IWF) Project is the brand new umbrella project effort (RLC PI)
- Core focus for that effort is enabling analysts for NW mission
  - Faster model building
  - Faster problem setup
  - Faster problem execution
  - Faster/better post processing / analysis
- Bottom line: we want to get the tools out of the way and have analysts spend their time on physics and engineering, not mastering the tools.

Current Workflow Focus (cont)

- Extending computational mechanics workflow capability (V&V/QMU workflows)
- Enabling electrical analysis workflow to full production state (FY17 L2 – calibration workflow)
- Continue to advance our Dakota / V&V capabilities – applies to all physics domains
- Continue to advance scalability of workflows (Trinity workflows, …)
- Community engagement (SDM with LLNL, …)

Workflow in 2025?

Guiding Principles

- Everything is a workflow
- V&V everywhere
- Component architecture
- Federation and cooperation
- Data-driven, not hand-coded
- Small-, meso-, large-scale

Workflow in 2025?

Analysts are 100x More Effective

- Model-building becomes simple
  - Virtual “Parts Library / Warehouse”
  - Anything that can be automated is automated
  - “Smart” components
- Workflow execution becomes effortless
  - Express what you need, not how to do it
  - System finds and manages resources to get the job done
- Analysts only need to think in their domain (not struggle with the mechanics of running simulation and analysis workflows)

Workflow in 2025?

"Smart" Workflows

- Tools understand models and suggest what is possible
- Suggest next steps while building models and workflows
- Suggest missing components
- Suggest missing data
- Can automate routine connectivity
- Can run themselves once built
- Automated lookups (e.g., material properties data)
- Incorporating metadata automatically

Acknowledgements

- Ernest Friedman-Hill (PI)
- Ed Hoffman
- Marcus Gibson
- Kevin Olson
- Mike Glass (Sierra)
- George Orient (V&V apps)
- Brian Adams (Dakota)
- Randy Lober (Xyce)