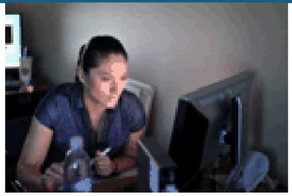
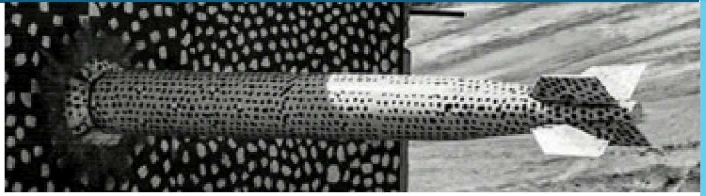
SAND2019-8136PE

V&V and Qualification using Workflow





PRESENTED BY

Ed Hoffman - Scalable Modeling & Analysis (8753)

WITH WORK FROM

George Orient, Robert Clay, and Ernest Friedman-Hill

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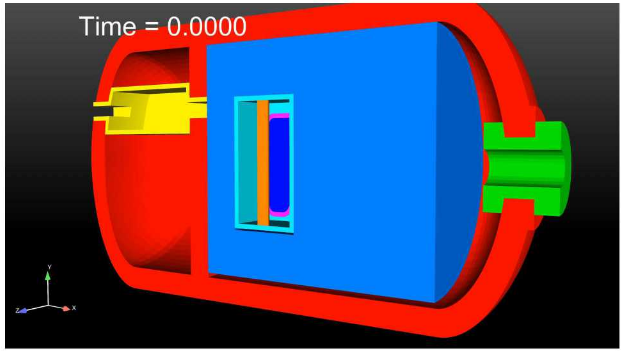
Andrew Rothfuss (SAW dev)

Peter Sholander (Xyce)

Jason Verely (Xyce)

Modeling and Simulation - ModSim

- Physics based mathematical models solved in HPCs to evaluate transient fields (displacement, temperature, velocity, pressure, density)
- QoIs (Quantities of Interest) derived
  - Related to system engineering requirements
  - Measurable in experiments
  - Examples: Gaps and breach, maximum temperature, lift, aerodynamic pressure
- Value proposition:
  - Design the most informative test, reduce number of tests
  - Explore mission space, predict untestable conditions
  - Optimization, sensitivity analysis, uncertainty quantification
  - Reduced manufacturing costs
  - Reduced time to market, by fewer design iterations
  - Improved safety through simulation of multiple accident scenarios to augment full system tests
  - Evidence to present to regulators



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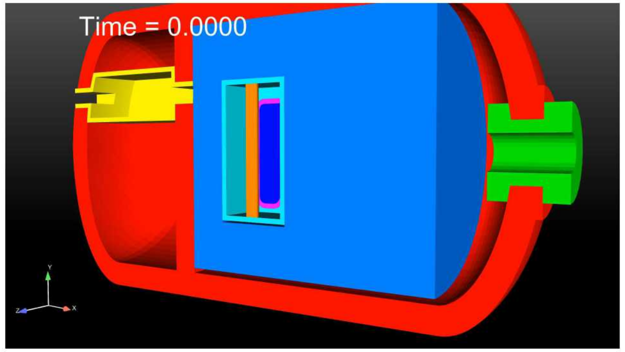

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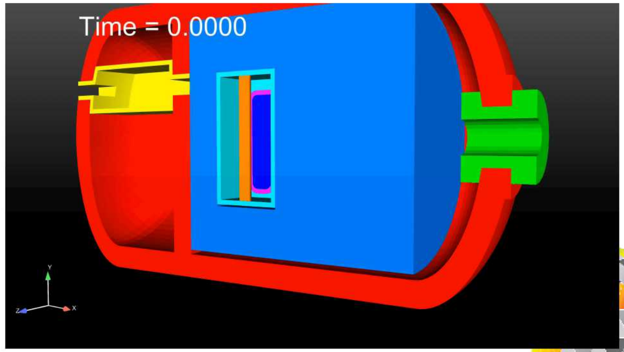


v_3

Accident Predictions

Credibility of ModSim

- Why should the decision maker believe/use model results?

- V&V processes:
  - PIRT (Phenomena Identification and Ranking Table) assess importance and adequacy of basic phenomena modeling capability
  - PCMM (Predictive Capability Maturity Model) collect evidence of trustworthiness
    - Code Verification: Analysis code reproduces closed-form results?
    - Physics and Material Model Fidelity: are “closure models” (constitutive etc.) credible?
    - Representation and Geometric Fidelity: Is the geometric abstraction acceptable?
    - Solution Verification: code solves the equations for the intended use correctly?
    - Uncertainty Quantification: What is the effect of input uncertainties on QoIs?
    - Validation: How well do model predictions match experimental data?
  - Peer reviews; are best practices followed?

COMPSIM

What is an Engineering Model and **Who** are the Key Stakeholders?

Designer

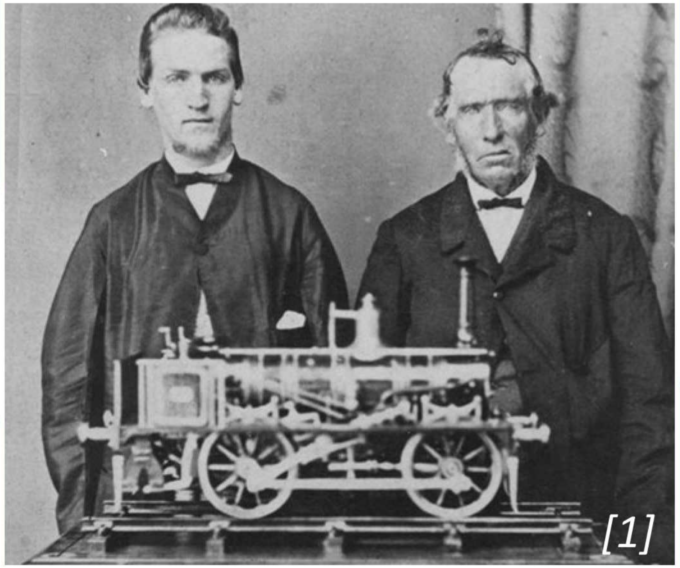
CAD Assembly
Tolerances, Repositories

Model Development Analyst

Map requirements to quantities of interest
Meshing, Finite element model, Post-processing

System Engineer

Trade study tool
Requirement Verification



Experimentalist

Experimental Design
Instrumentation Design

V&V/Credibility Analyst

Qualitative (Expert judgement, peer review)
Quantitative (Sensitivity & uncertainty analysis)

Decision Maker

Credibility Evidence
Decision risk quantification

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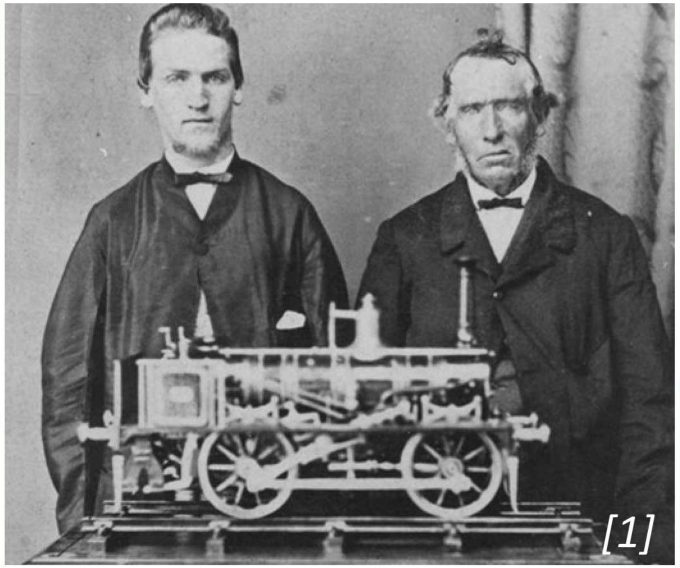

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LIKE IT REALLY HAPPENS

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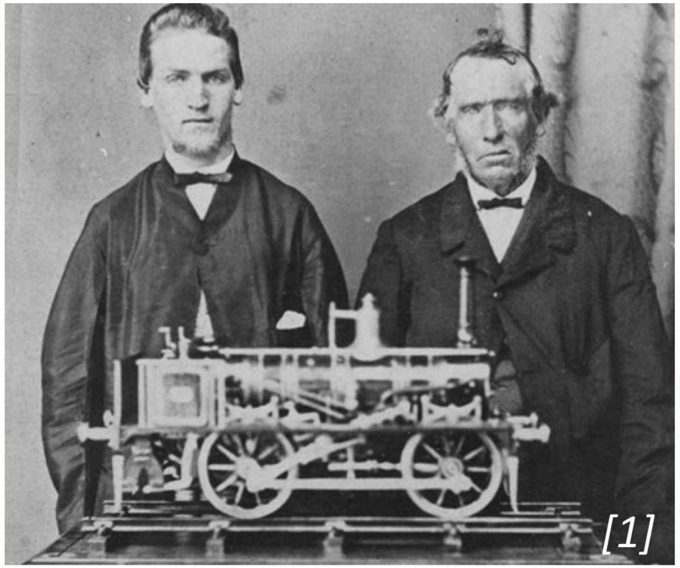

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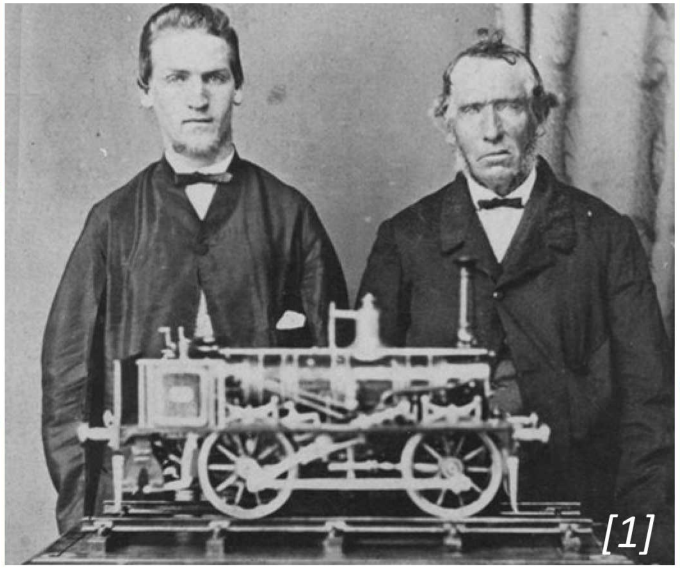

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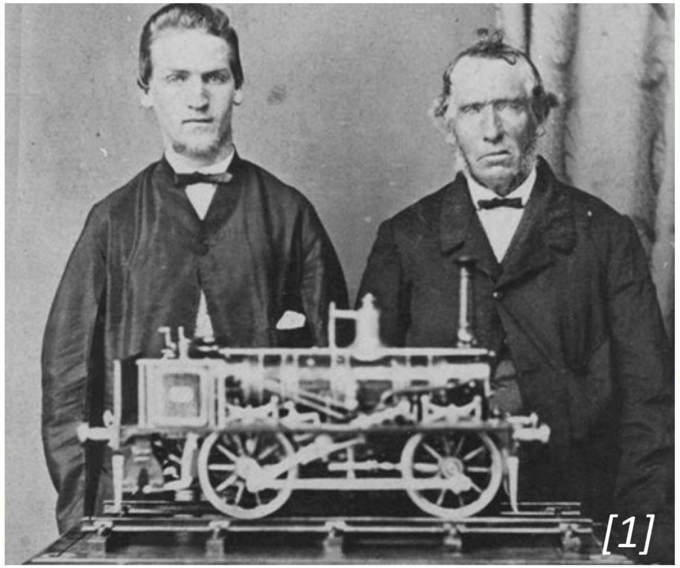

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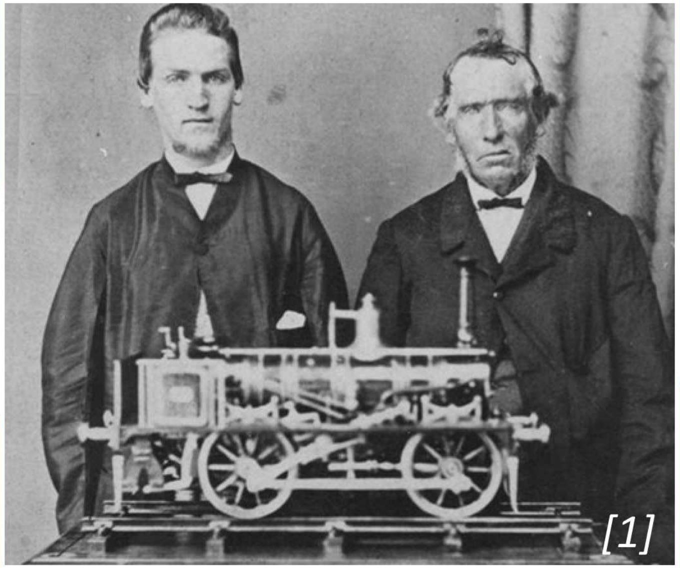

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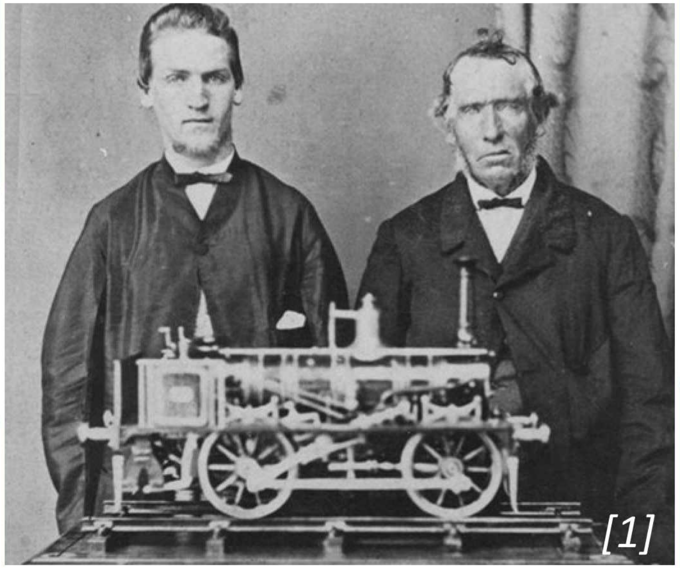

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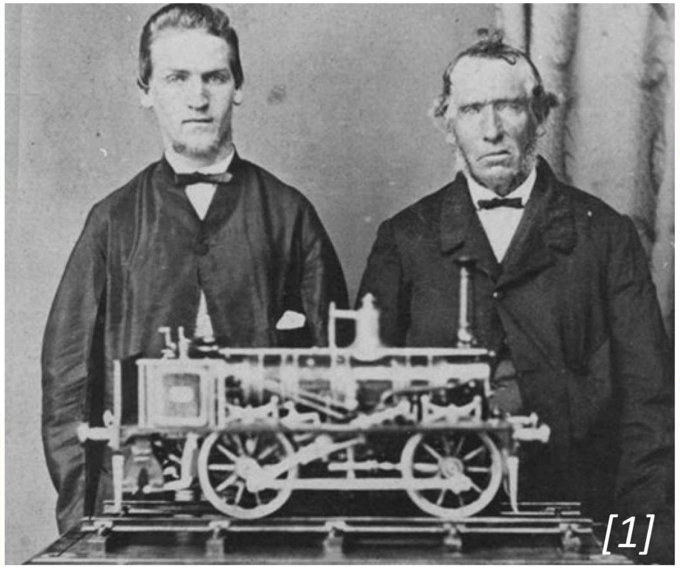

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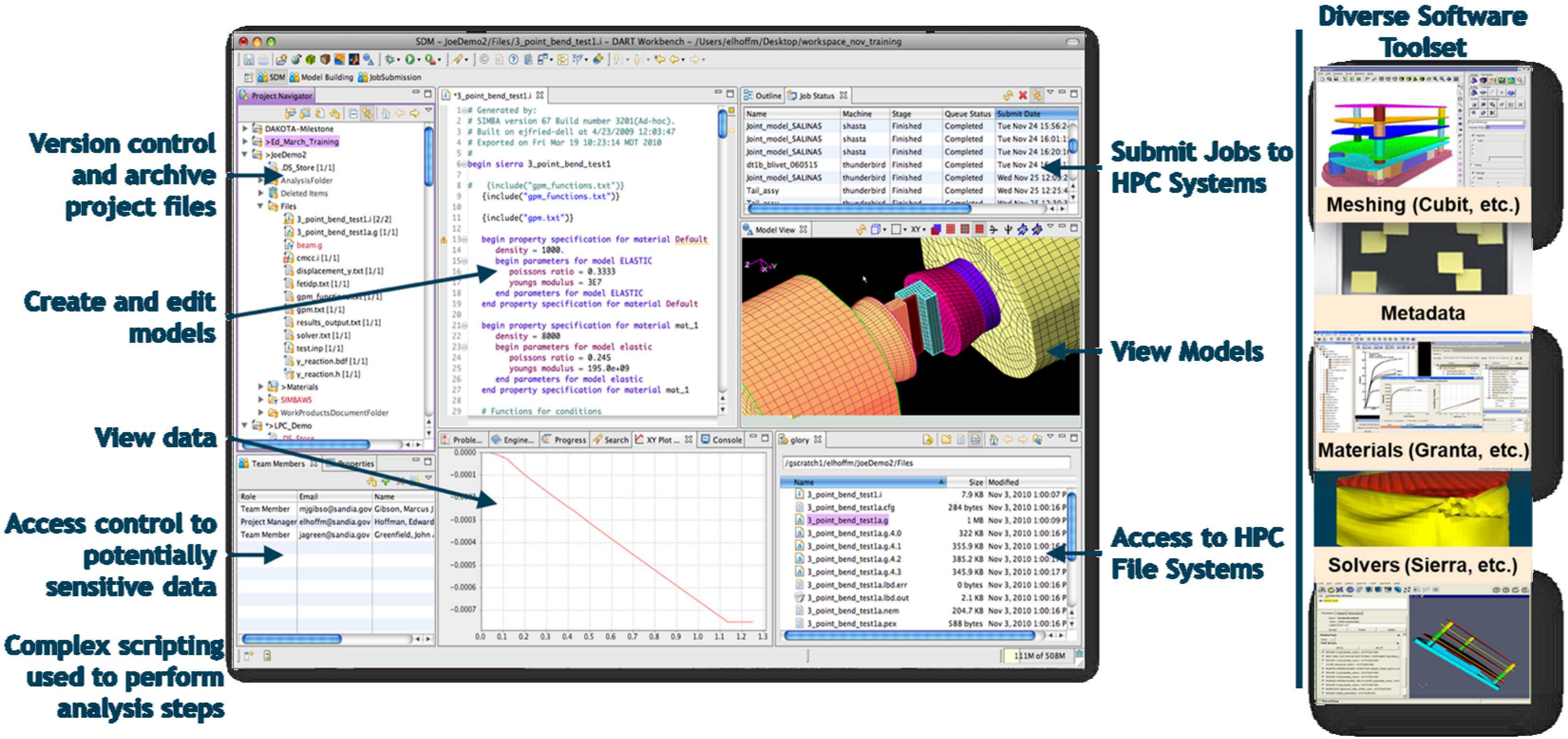
COMPSIM

Workflow platform integrates different views of the model needed to communicate to all stakeholders

SAW Model Builder – Current State

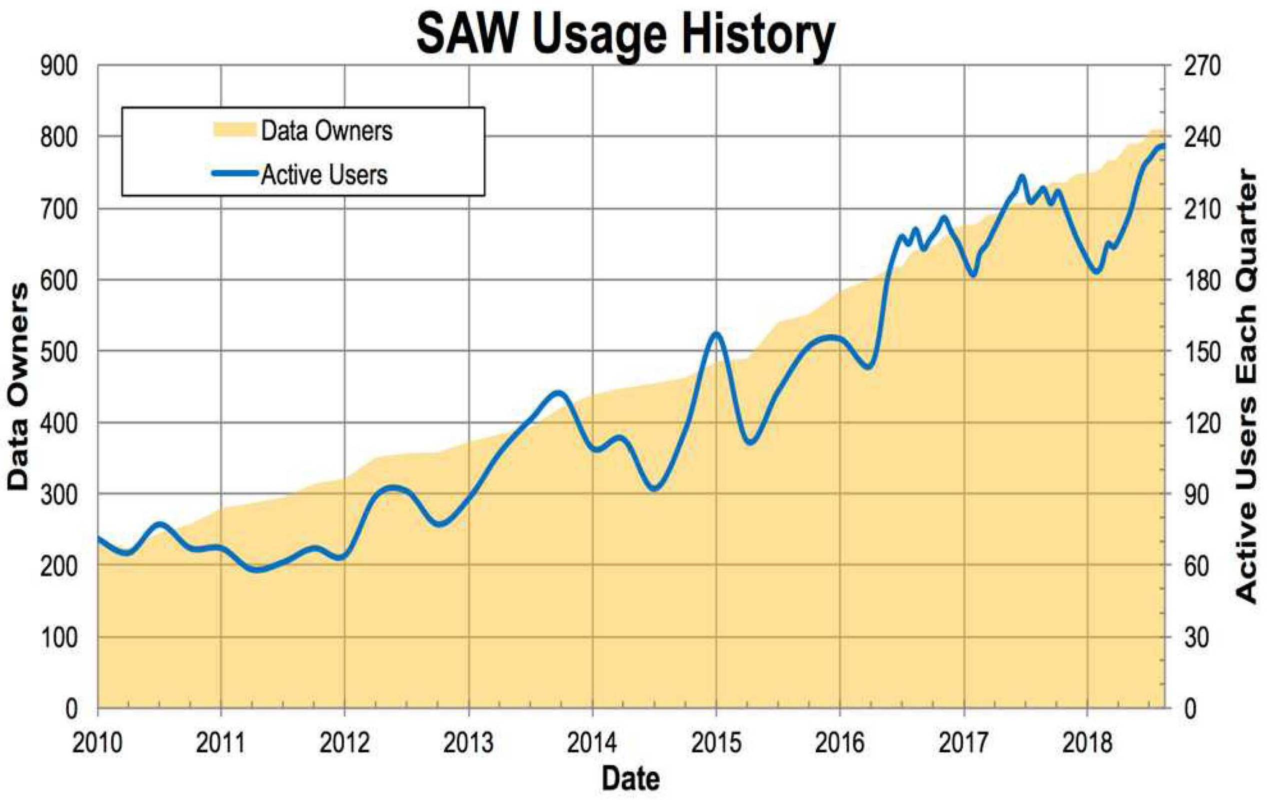
Current analysis workflow is assisted using the Sandia Analysis Workbench (SAW) ASC corporate tool, but remains **highly complex**.



Clear snapshot of current state but no concept of end-to-end workflow

SAW Adoption is Rapidly Increasing

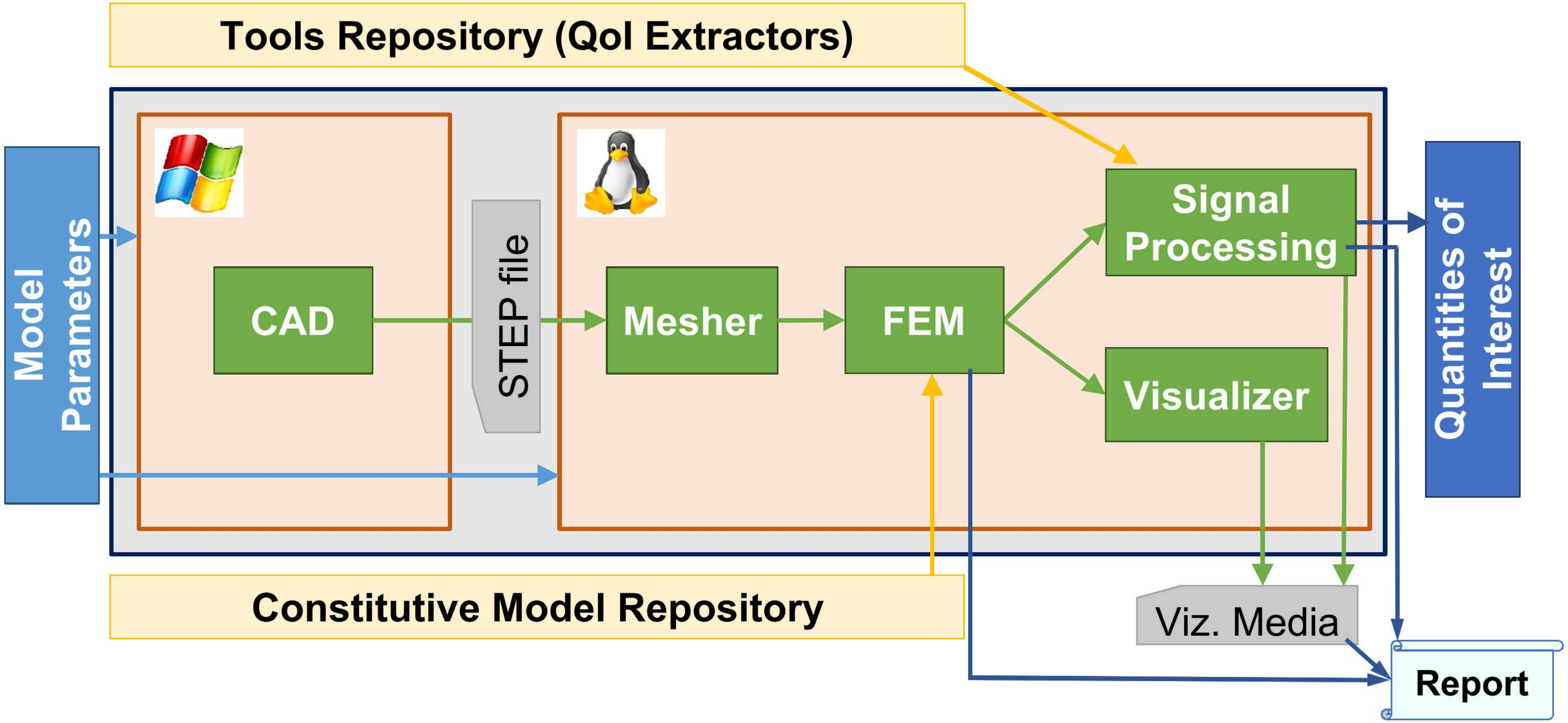
- In production for more than 10 years
- At Sandia: Over 200 active users per quarter & over 800 data owners
  - More than 2 million files stored in the SAW repository
  - Approximately 1000 job submissions per week
- SAW Model Builder: deployed wi used in Sierra training
- Dakota UI built on SAW/Eclipse
  - open source licensed
- Integrated Cubit UI
- PLATO topology optimization toolkit built on SAW Platform
- ASC Investment in SAW ≈ $2M/yr



Notional Analysis Workflow

Workflow can be **organized** and **iterated upon**

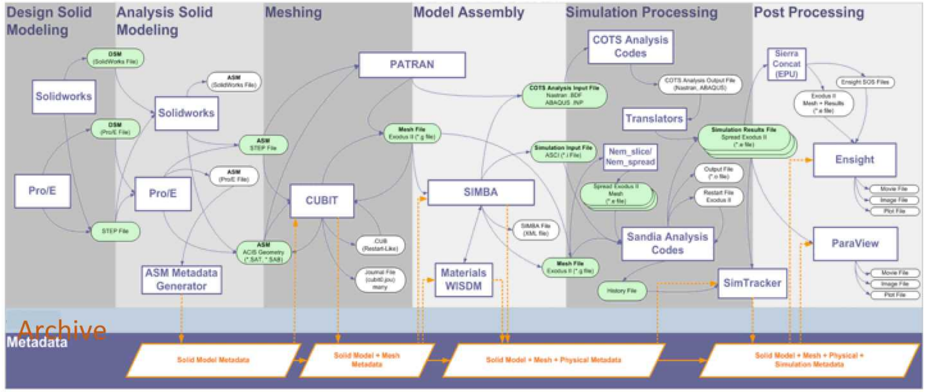
- Electronic product definition/tolerances in CAD/Product Lifecycle Management system
- All other Modeling and Simulation (ModSim) components of the workflow available on Linux HPC



Executed hundreds of times for qualification support - must be robust and resilient

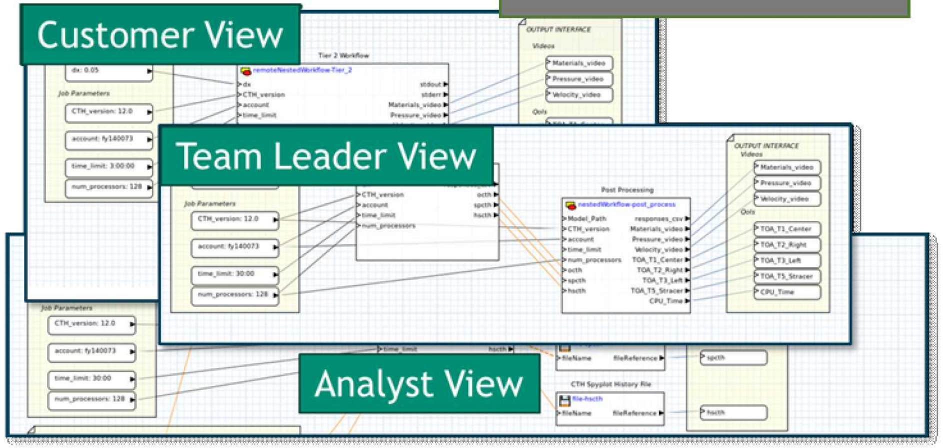
ModSim Process – Current vs. Future States

Current State



- Disconnected analysis components
- Opaque, no communication support
- Not reviewable
- Lack of configuration control
- Specialized non-engineering expertise required
- Effort not reusable
- Long cycle time
- Lack of integration with other tools (CAD, Dakota)

Future State



- Integrated analysis components
- Clear and transparent, easy to communicate
- Fully reviewable by peers and customers
- Intrinsic configuration control
- Minimal training, empowers all analysts
- Reusable workflows shared
- Workflow building cycle time reduction of 10X
- Parametric CAD, Dakota wizard, integration with many tools

Agility

Fundamental shift towards model credibility through clear communication and robust execution

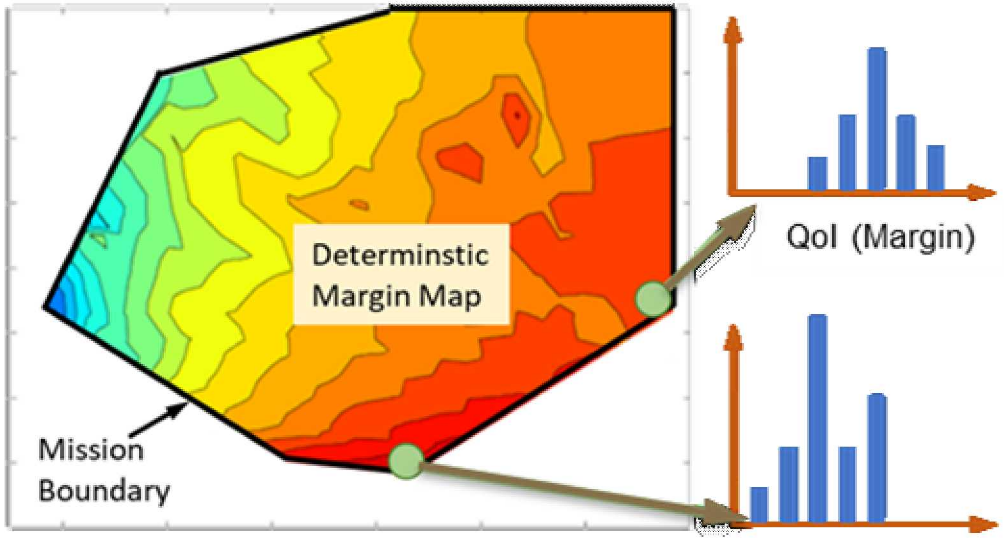
Legacy Case Study – Credible Assessment of Weapon Performance

ModSim supporting System Qualification - **computationally intensive nested workflow** that stresses the computational infrastructure; Goals:

- Identify and characterize impact conditions of interest and quantify uncertainties of margins under low margin operating conditions

Computational Requirements:

- 2000 realizations
- 1 day each
- 1000 Trinity processors
- 100 TB of data



Future work could be completed:

- 3 times faster
- With increased credibility

	Model Development	Analysis Workflow	Sensitivity, Uncertainty, Margins
Current	2.5 years	1 year	0.5 year
Future	0.5 years (NGS)	0.1 year	0.5 year

Difficult problem with intrinsic V&V and real program needs –NOT DELIVERED in time to make real impact

Analysis Workflow Platform

Graphically **define**, **communicate**, and **execute** ModSim process: **the workflow IS the model**.

- Workflow execution engine is driven by Sensitivity Analysis/Optimization/Uncertainty Quantification engine/iterator (Dakota) to execute analysis workflow instances in a manner that is

- Supports analysis credibility evidence/communication and training
  - **Documents all computational steps** from input parameters to responses
  - Committed in repository for **archival** purposes
- Capability delivered in SAW and available to all analysts
- Training, institutional knowledge capture, best practices

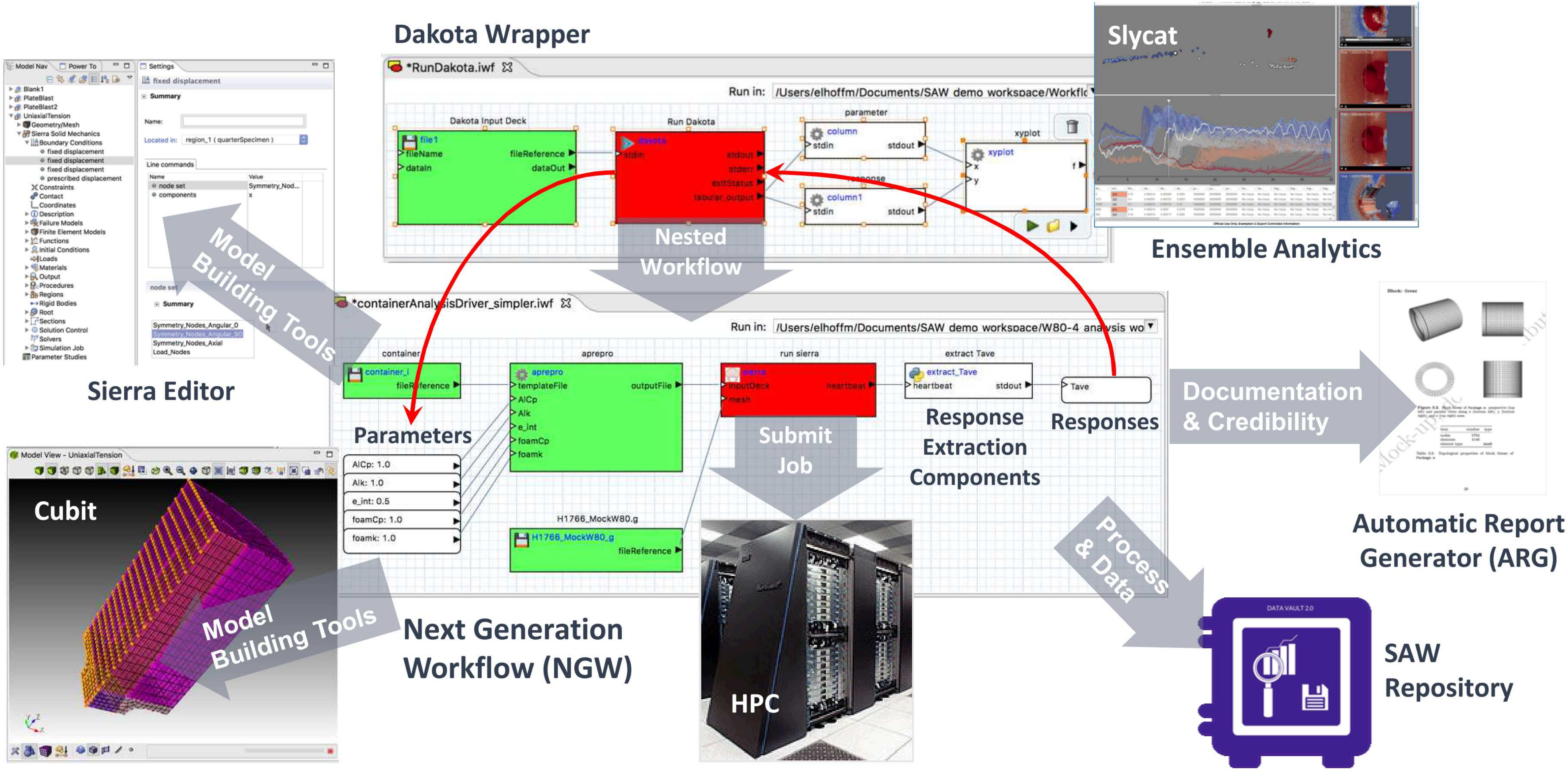
All ModSim activities are accurately documented, communicated, and efficiently executed

Why Workflow?

- **Complexity** → multi-physics simulation processes, involving many mod/sim codes and post-processing tools to build, execute and analyze models
  - Require manual execution/intervention
  - Error prone
- **Process automation**
  - Faster turn-around needed to support design.
- **Knowledge preservation**
  - Processes that could only performed by specialists can now be performed by many.
  - Processes are documented and archived with data
- **Repeatable**
  - Enables regression testing of large system models to ensure the same behavior as mod/sim technologies evolve
- **Large ensemble simulations**
  - Automated, parameterized workflows are required for UQ
- **Simulation governance**
  - Versioned workflows can be used to enforce rules, best practices, and quality control of the simulation product.

Integrated Workflow – Transforming Engineering Science Analysis

Integrated, Graphical, Automated, Self-Documented, Archived Process and Data



FY19 Milestone Deliverables and Products

Infrastructure to Implement Graphical Programming Paradigm for Workflows

Define and execute complex multi-platform engineering workflows in a **user-friendly**, **robust**, and **responsible** manner.

Library for Reusable Tools with Known Provenance

Author and distribute **configuration-controlled tools** (workflow components) generated by analysts.

Dakota Usability through GUI, Integration

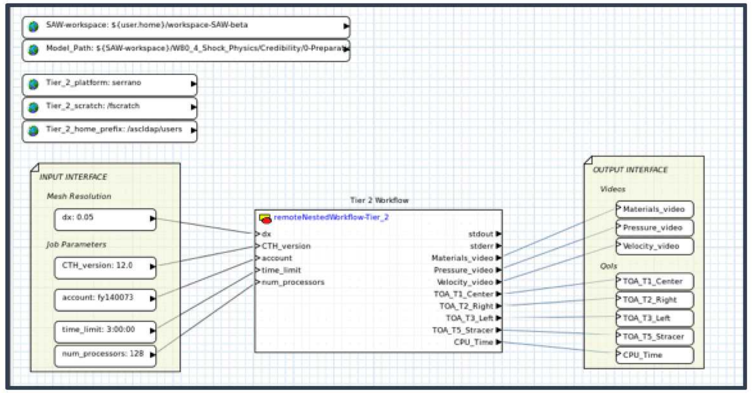
Infrastructure focused on **directly supporting** analysis of the parameter and response space.

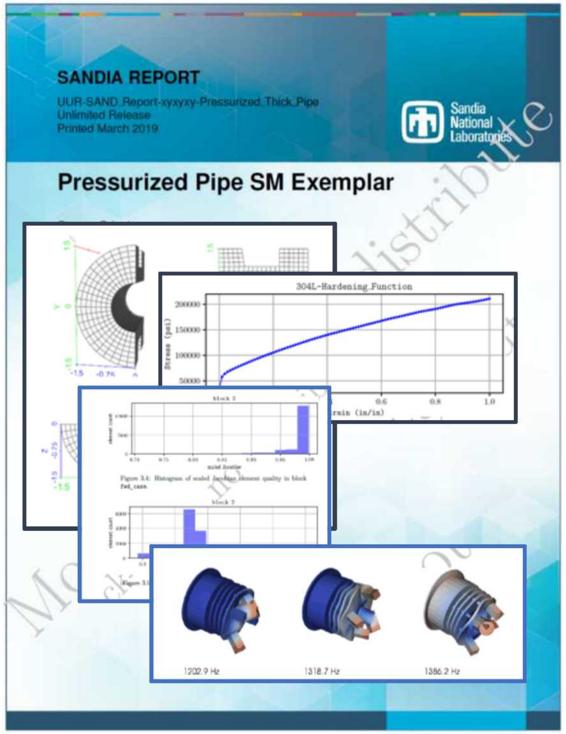
Automatic Report Generation

Model becomes **self-documenting** through automatic report generation.

Exemplars, Training, User Engagement

Documented end-to-end exemplar for solid mechanics **supporting training** and **reducing analyst-to-analyst variation** by encapsulating best practices.



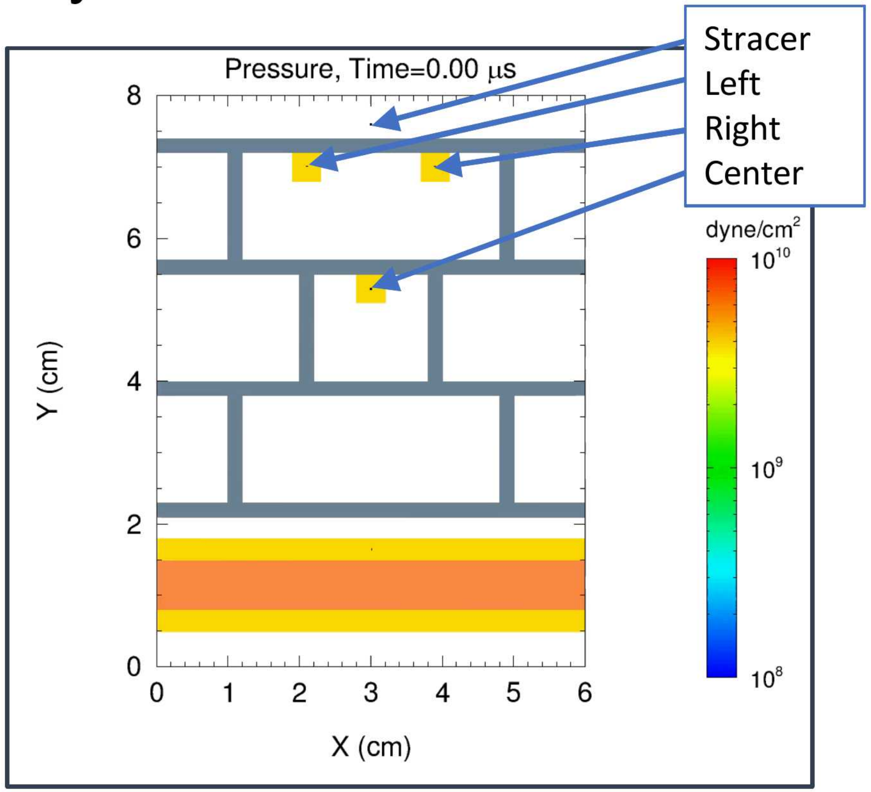


Sub-projects target elements of agility, credibility, continuity

Exemplar – Credibility Elements for a Shock Physics Problem

Exemplar, prototype/test shock physics simulation integration

- Uniform grid, no adaptive mesh refinement
- Material models from CTH material library
- Quantity of Interest: Time of arrival of shock event at different observation points



Dakota studies

- Scalability, platform and parallel consistency
- Mesh (cell size) sensitivity, solution verification
- Uncertainty informed sensitivity, uncertainty quantificaiton

Execution Topology (two-tiered analysis workflow)

	Unclassified	Classified
 akota, Tier-1 Analysis Workflow Slycat Input	SNL Linux Workstation	SNL Linux Workstation
Tier-2 Analysis Workflow : CTH, SpyPlot, movies	SNL HPC Serrano	LANL HPC Trinity

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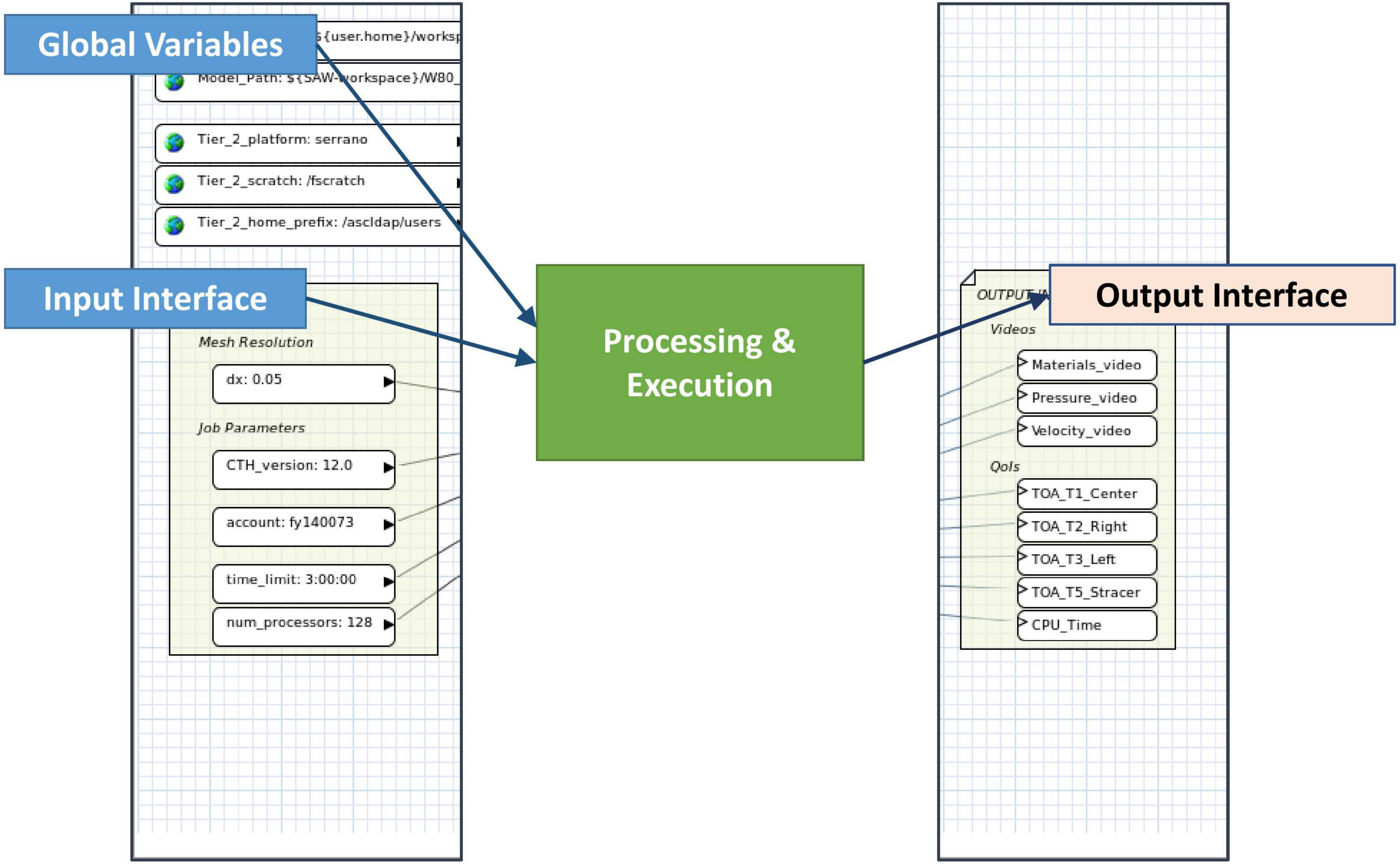
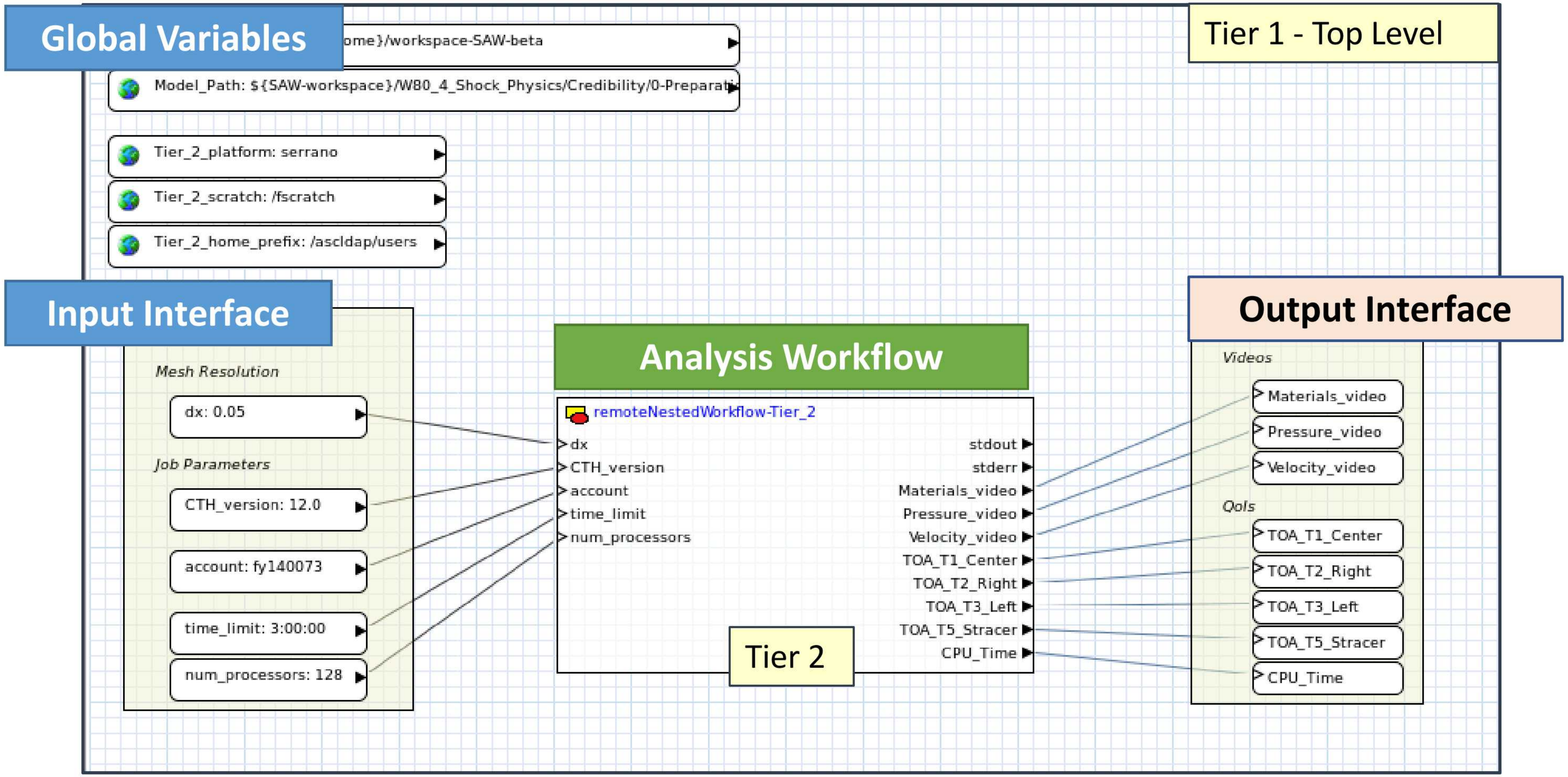
Non-trivial model from NW program ModSim suitable to stress test the workflow infrastructure

Tier-1 Analysis Workflow - Contract with Customer



Customer and ModSim team negotiate data interface

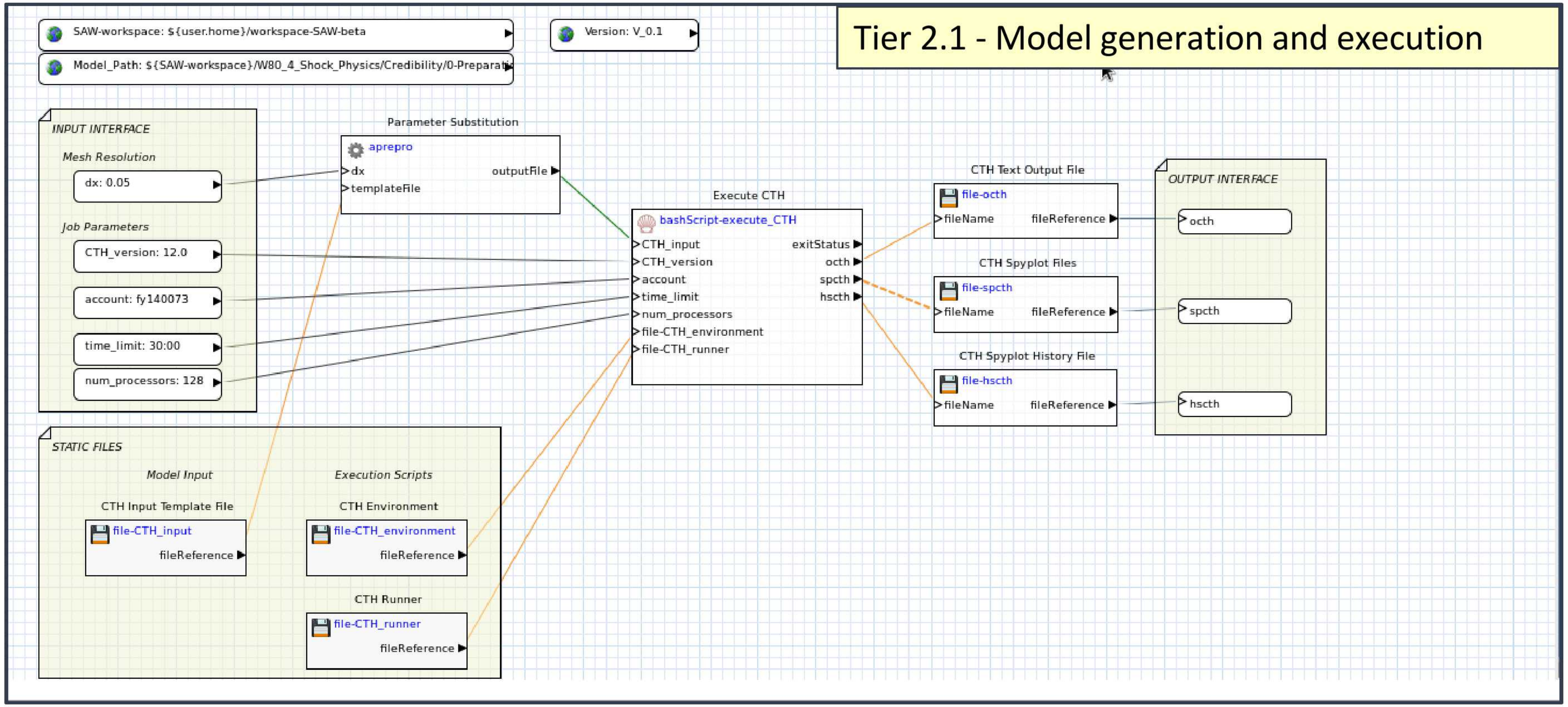
Tier-1 Analysis Workflow - Top Level View of the ModSim Problem



Communication with ModSim lead, customer

Analysis Execution Workflow Example

Hierarchical of workflow design enables **communication** and **agility**.



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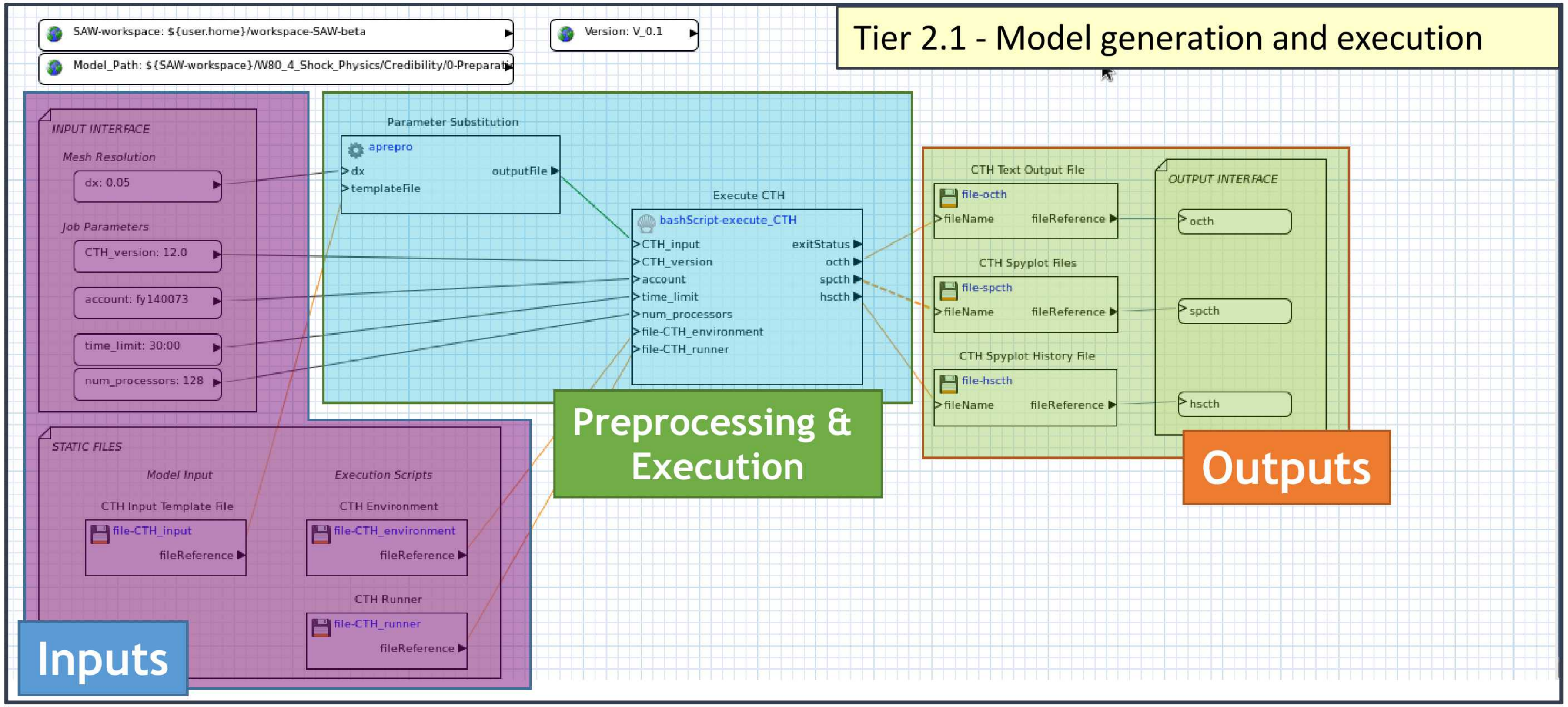
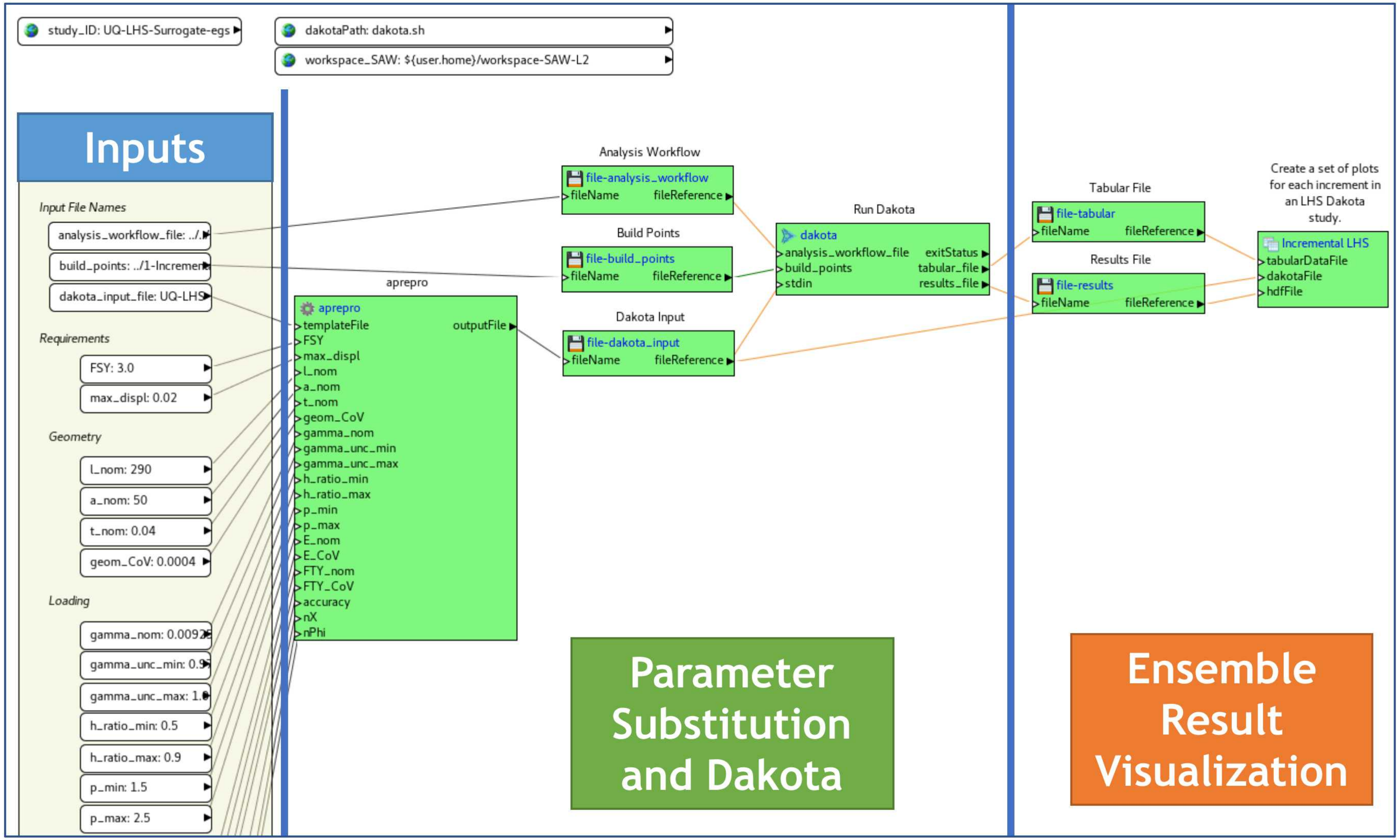
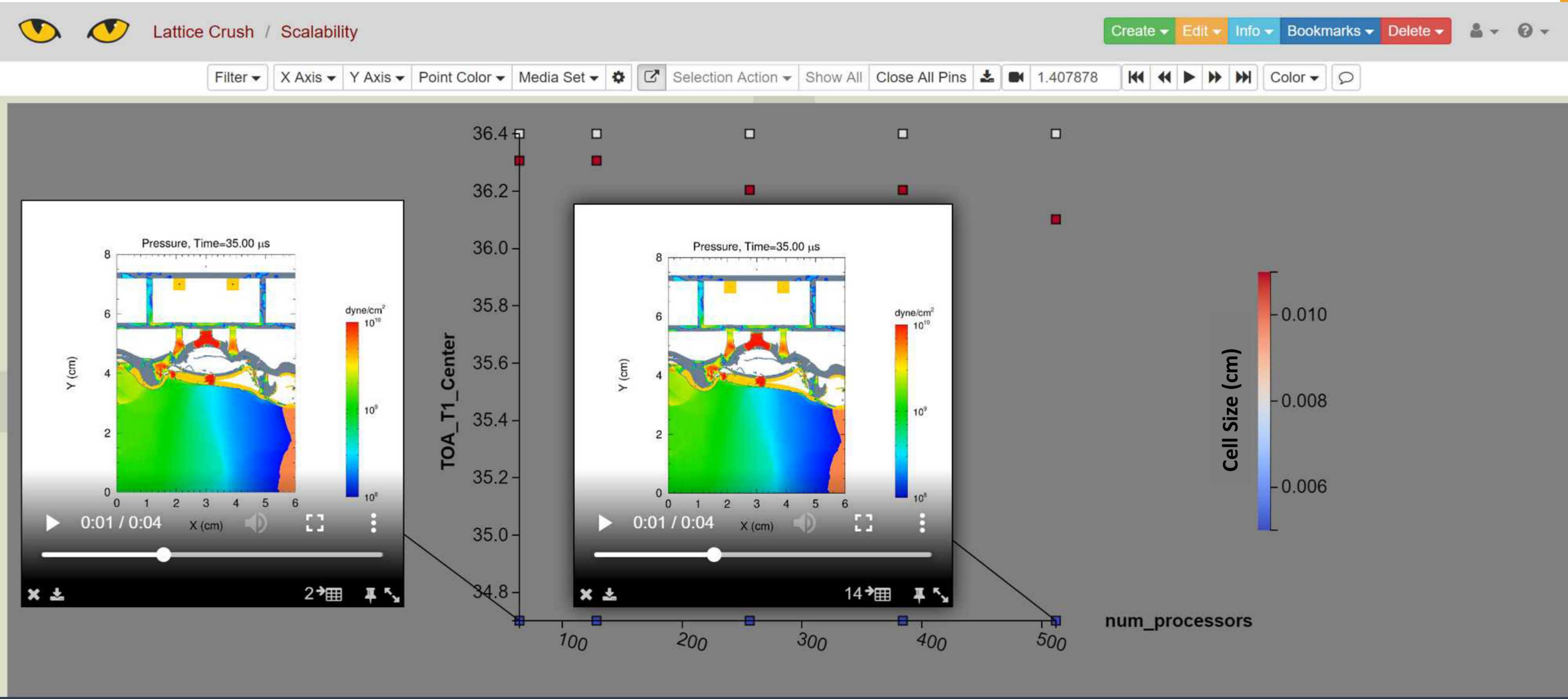


Ensemble Execution Workflow Example

Dakota followed by ensemble visualization.



Ensemble **Member** Visualization with Slycat

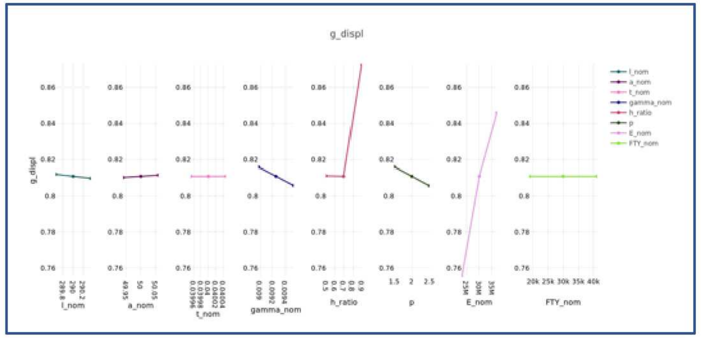


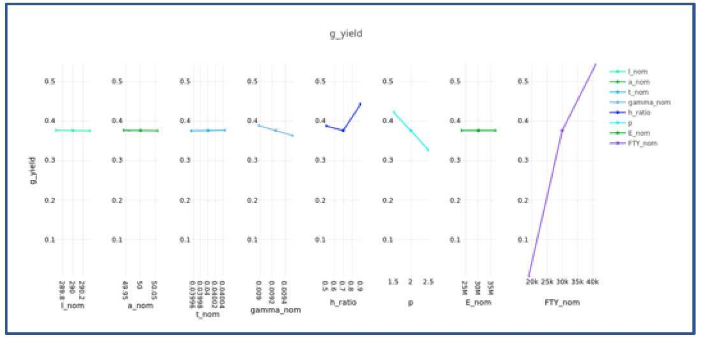
Excellent parallel consistency with fine model (both QoI and spatial)

Specialized Workflow Nodes for Ensemble **Result** Visualization

Workflow **enables** analysts to gather and present **credibility evidence**.

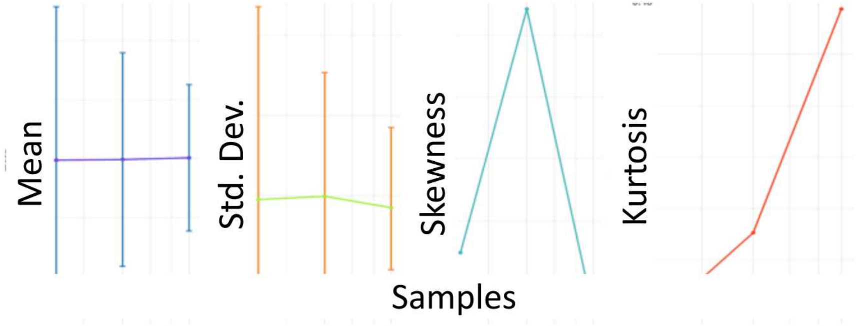
Main effect plots





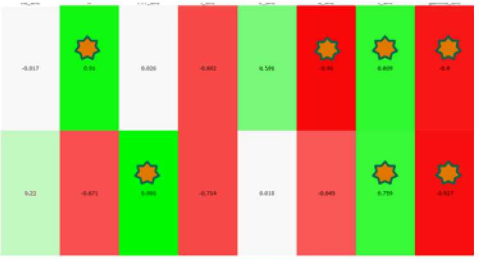
Sampling plots

Violating requirement plausible



Assess sample size for intended use

Correlation plots



Most important factors identified

Decision alternatives

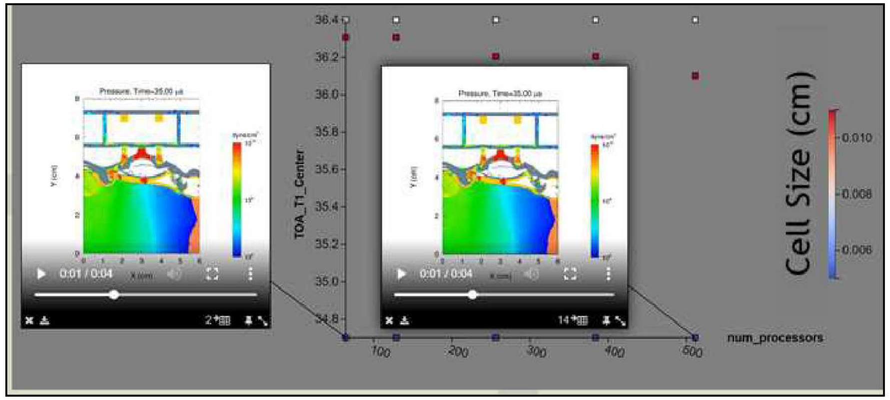
- Live with plausible negative margin
- Quantify p(margin<0)
- Negotiate criteria
- Use sensitivities to dial design
- Restrict operations

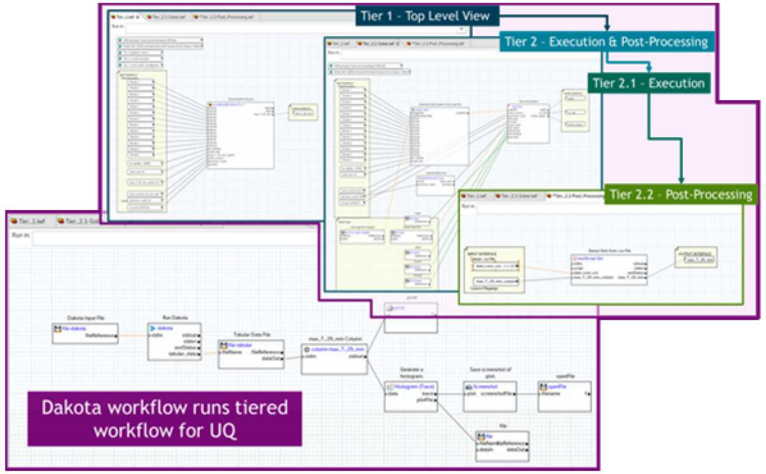
Present customers, ModSim team information, NOT just data

Workflow is Foundational to Credibility

- Clear inter-team **communication**, peer reviews and knowledge capture
- Analysis **repeatability** and **traceability** is important for **V&V** and **credibility** and is enabled by workflow platform
- Collaboration on analysis workflow will **streamline** model development and analysis process
- Use of graphical environment and existing templates helps with **on-boarding** new analysts
- **Repository** of analysis process to make them available for later use
- **Efficient** and **reliable** resource management and **platform independence** enables **agility** and **credibility**
- Developing credible models through ubiquitous **sensitivity** and **UQ**

Integrated workflow project **leverages** partner products, teams, and funding (Dakota, Cubit, Sierra, Slycat, small business) and **develops** new products to deliver a **coherent**, **agile** platform.





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