

Engineering Mod/Sim Workflow Platform and Shock Physics Exemplar

PRESENTED BY

George Orient and Aubrey Eckert-Gallup
Engineering Sciences Center

WITH WORK FROM

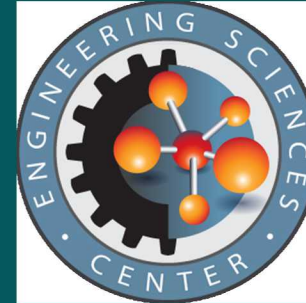
Robert Clay, Ernest Friedman-Hill, and
Edward Hoffman

Engineering Sciences External Review Board
Meeting

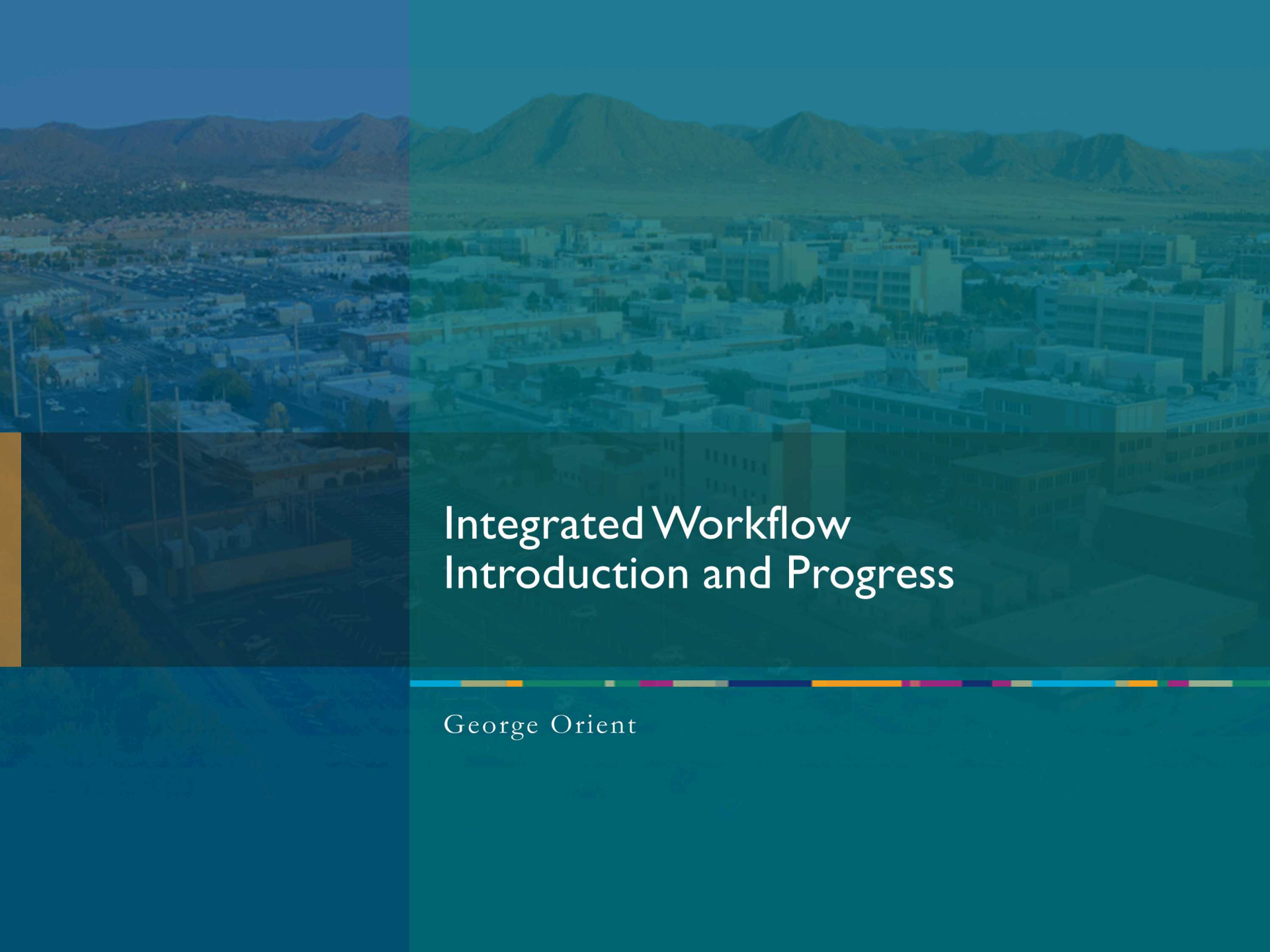
April 8-10, 2019



SAND2019-3818PE



SAND2019-XXXX PE



Integrated Workflow Introduction and Progress

George Orient

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



Model Development Analyst

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

Experimentalist

Experimental Design
Instrumentation Design

Designer

CAD Assembly
Tolerances, Repositories

System Engineer

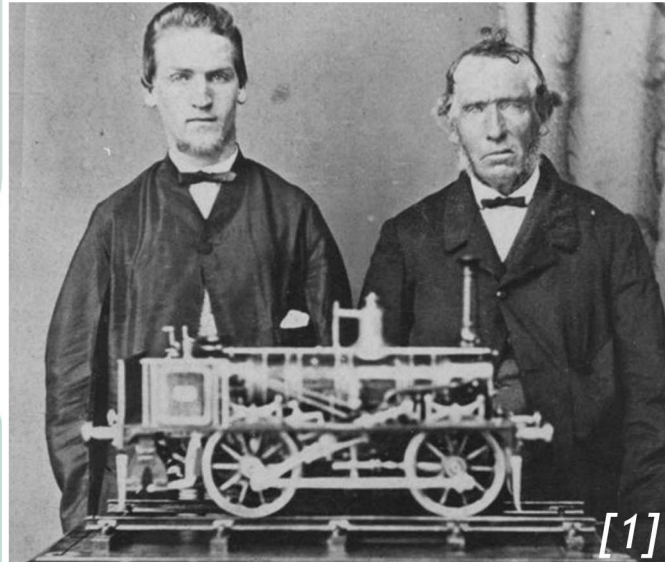
Trade study tool
Requirement Verification

V&V/Credibility Analyst

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

Decision Maker

Credibility Evidence
Decision risk quantification



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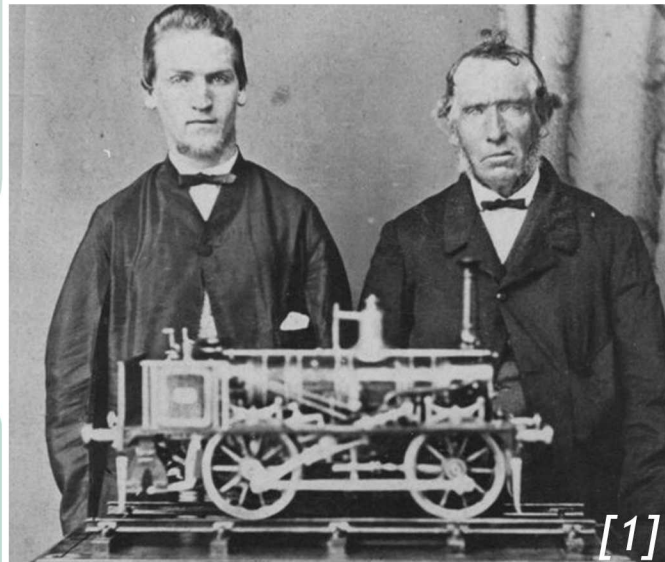
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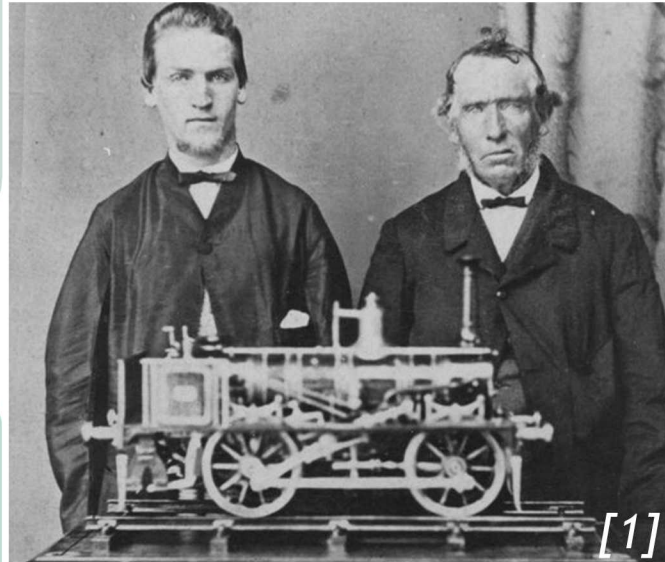
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6 What is an Engineering Model and Who are the Key Stakeholders?



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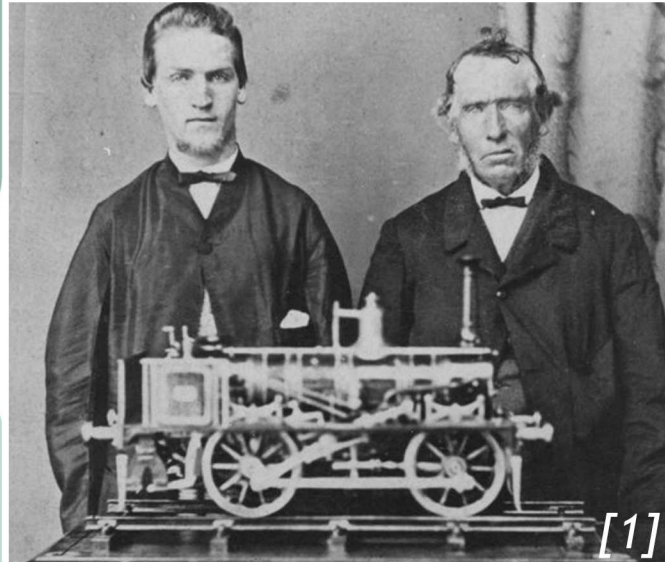
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7 | **What** is an Engineering Model and **Who** are the Key Stakeholders?



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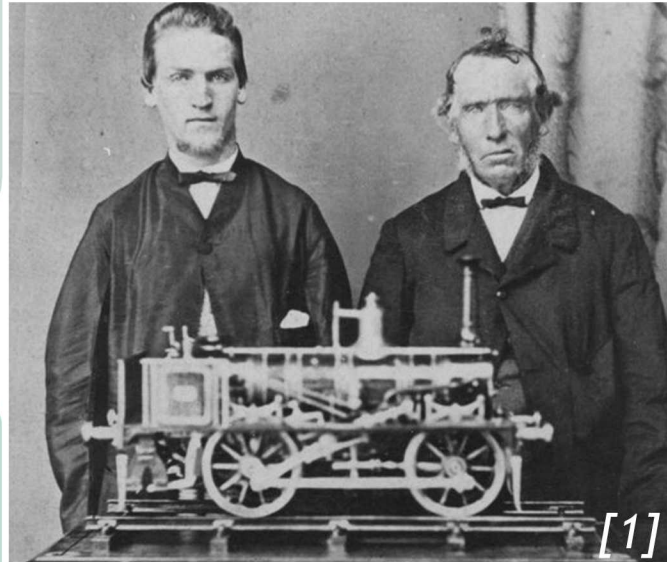
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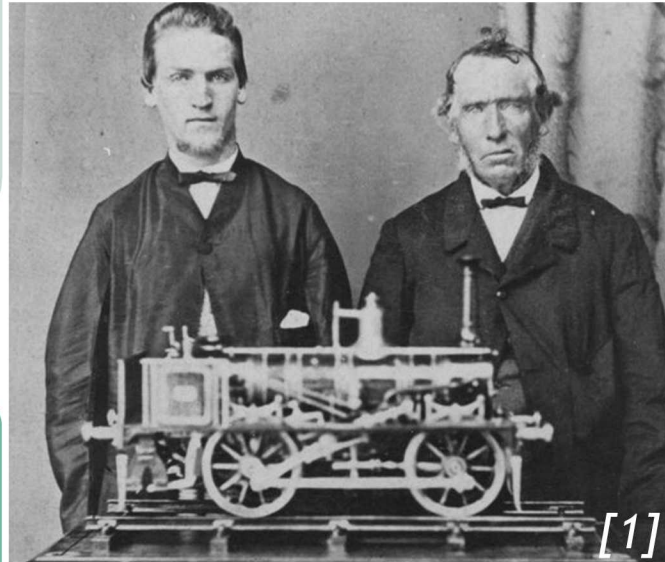
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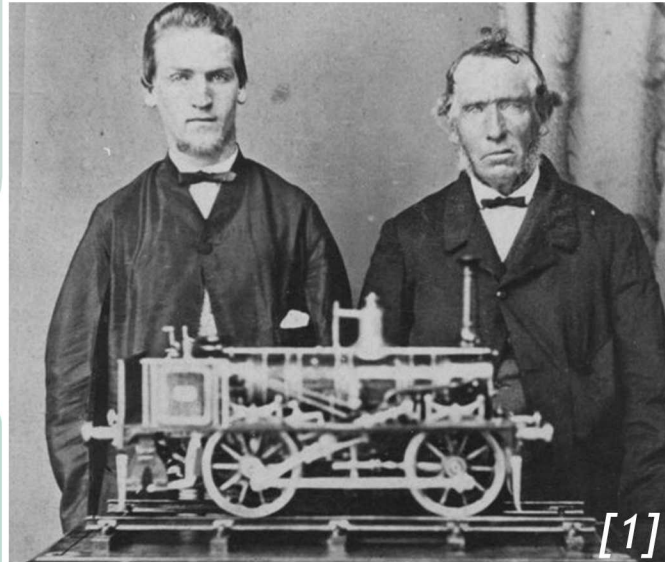
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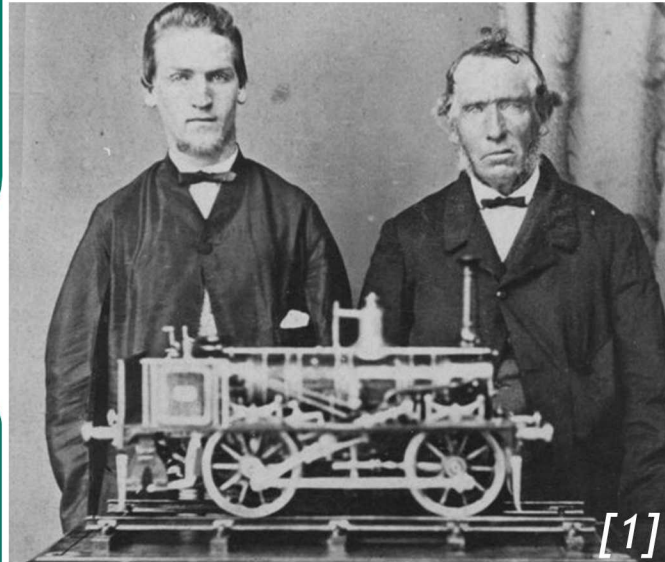
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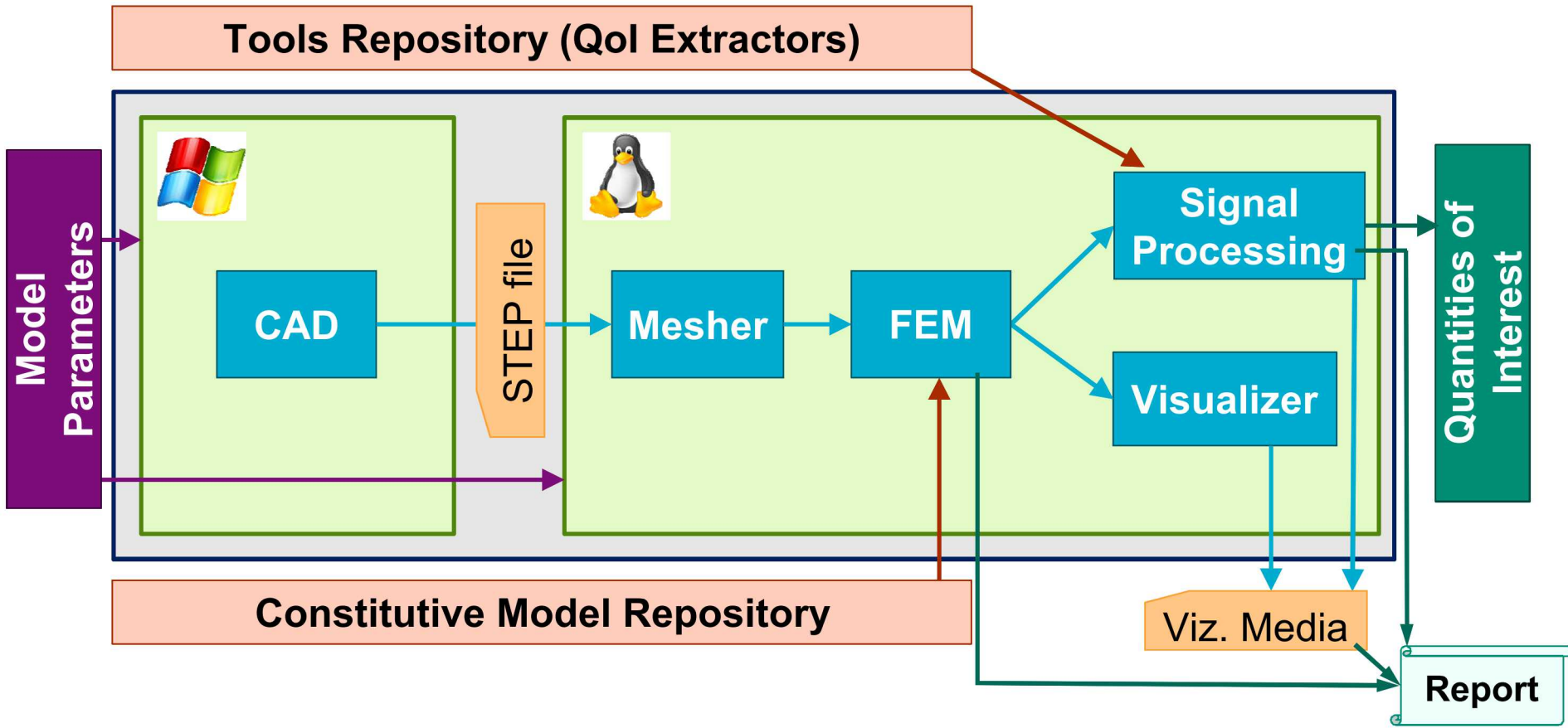
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11 Notional Analysis Workflow

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

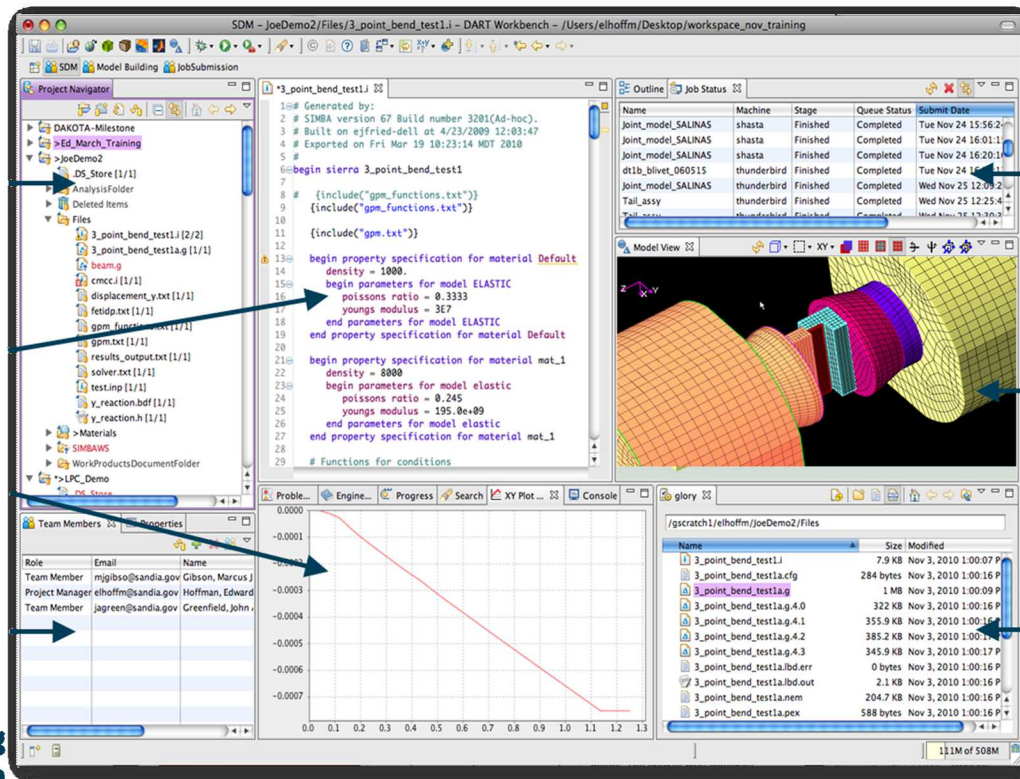
- Electronic product definition/tolerances in CAD/Product Lifecycle Management system
- All other Modeling and Simulation (ModSim) components of the workflow available on Linux HPC



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

SAW Model Builder Current State

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



Version control and archive project files

Create and edit models

View data

Access control to potentially sensitive data

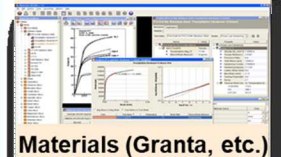
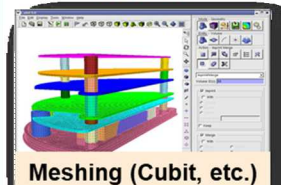
Complex scripting used to perform analysis steps

Submit Jobs to HPC Systems

View Models

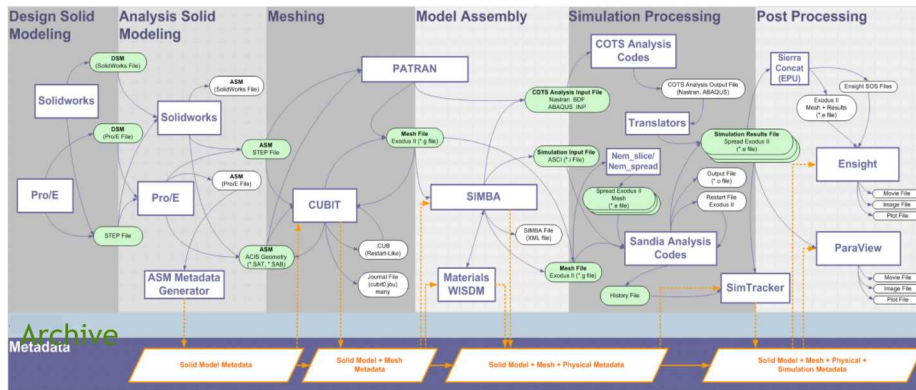
Access to HPC File Systems

Diverse Software Toolset



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

Current State



Disconnected analysis components

Opaque, no communication support

Not reviewable

Lack of configuration control

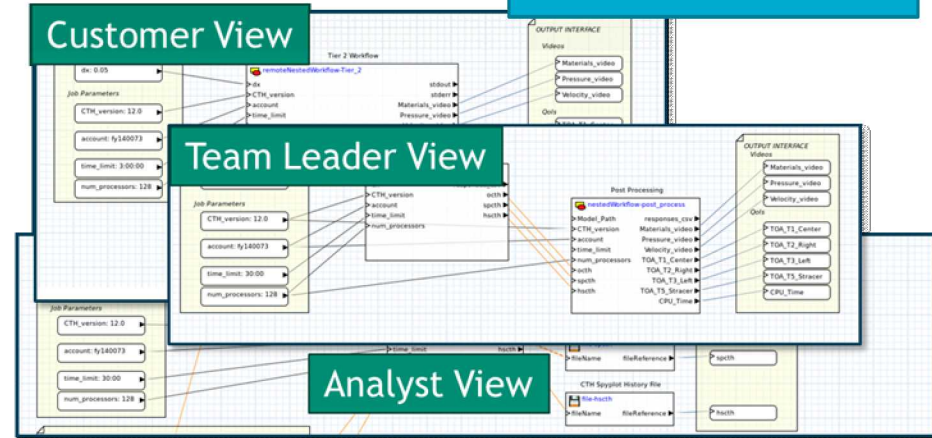
Specialized non-engineering expertise required

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

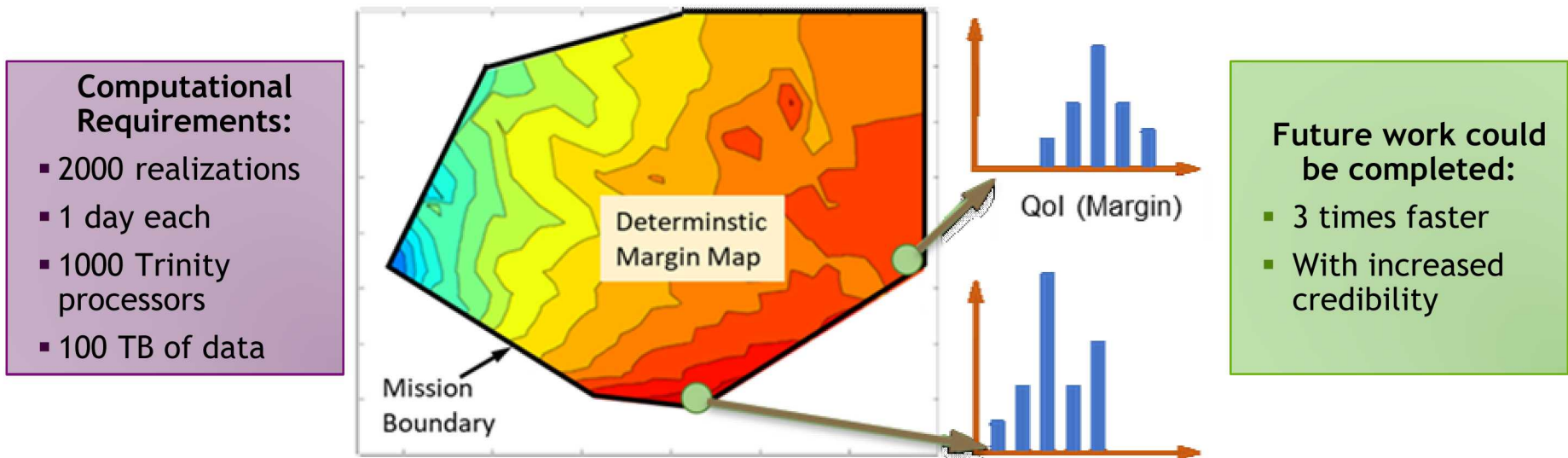
Agility

Fundamental shift towards model credibility through clear communication and robust execution

Legacy Case Study – Credible Assessment of B61-12 Fuzing Performance

ModSim supporting System Qualification - **computationally intensive nested workflow** that stresses the computational infrastructure and has the following goals:

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



	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

Graphically **define**, **communicate**, and **execute** ModSim process: **the workflow becomes 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

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

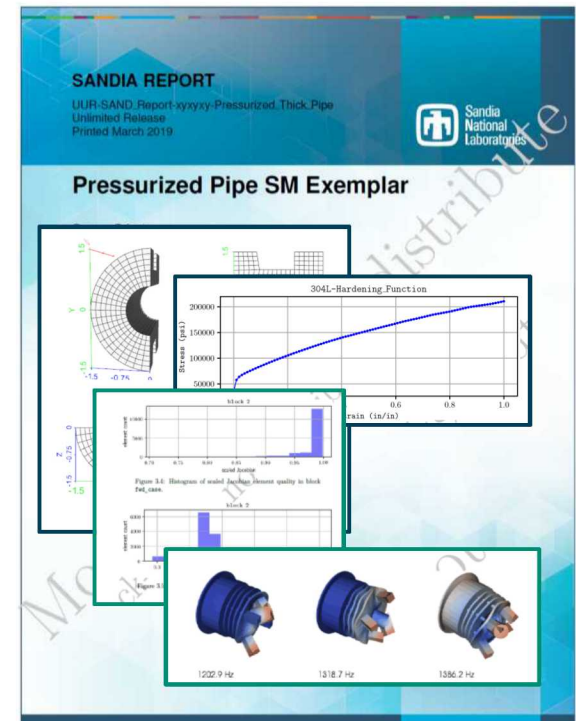
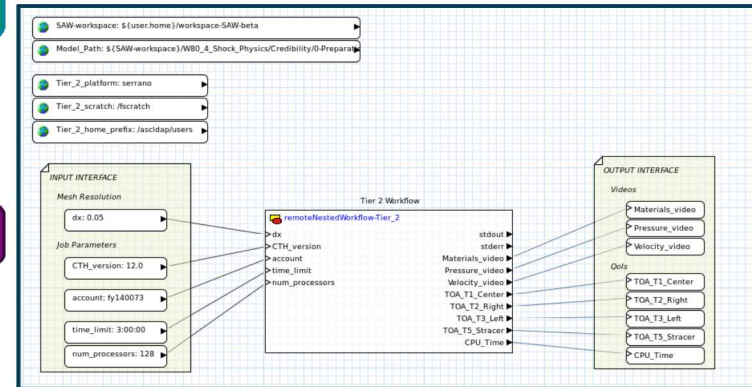
Infrastructure focused on **directly supporting** analysis of the parameter and response space.

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.



Exemplar – Credibility Elements for a Shock Physics Problem

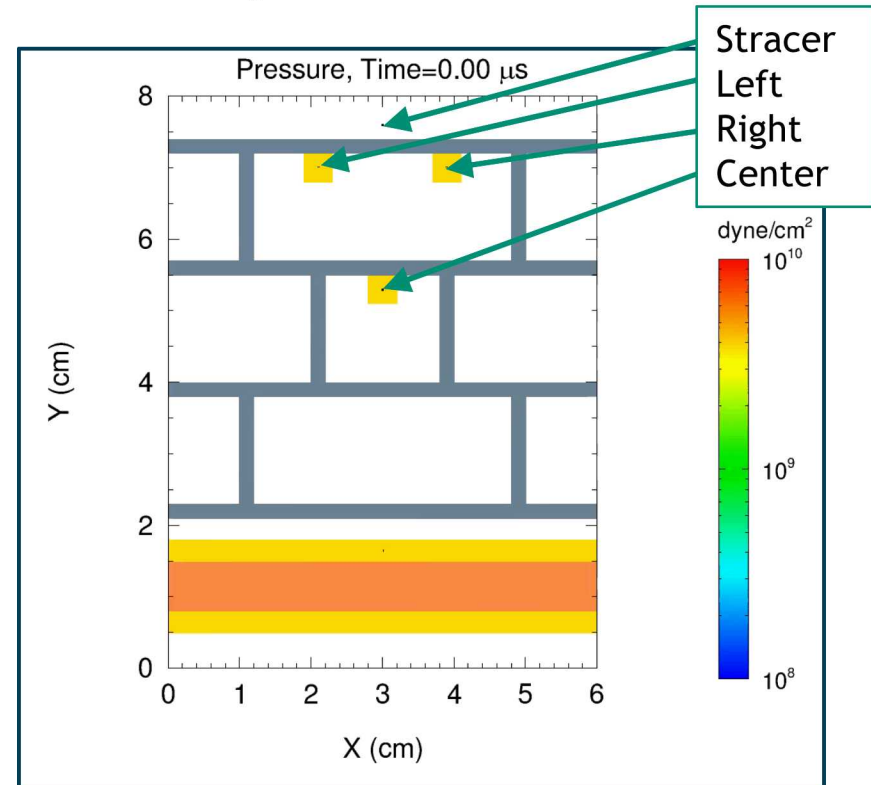
Unclassified exemplar, prototype/test shock physics simulation integration (courtesy N. Peterson)

- 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

Initial Dakota studies before uncertainty quantification to assess:

- Scalability and parallel consistency
- Mesh (cell size) sensitivity

Execution Topology (two-tiered analysis workflow)



Dakota, Tier-1 Analysis Workflow Slycat Input

Tier-2 Analysis Workflow : CTH, SpyPlot, movies

Unclassified

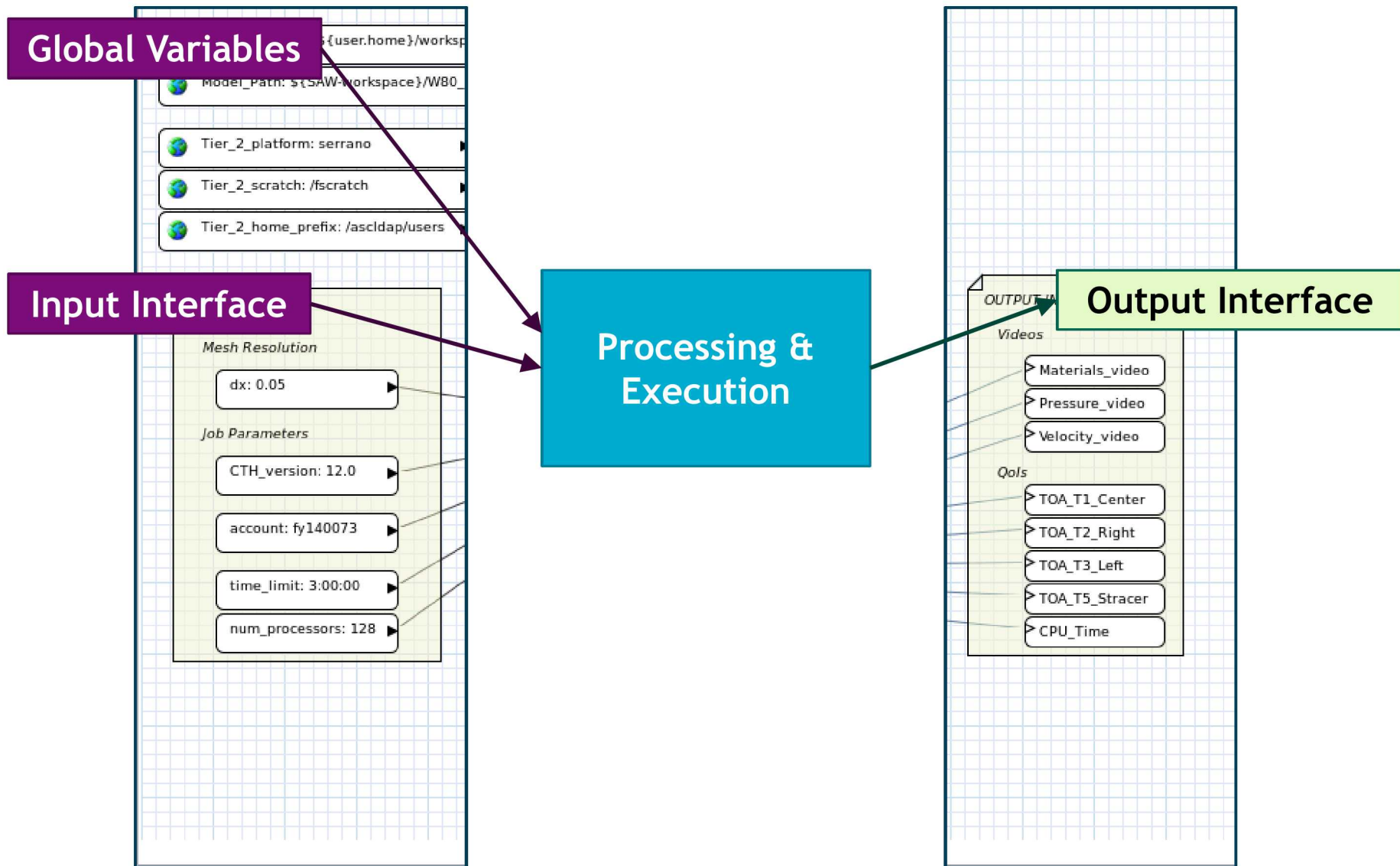
SNL Linux
Workstation

SNL HPC
Serrano

Classified

SNL Linux
Workstation

LANL HPC
Trinity



Global Variables

ome}/workspace-SAW-beta

Tier 1

Model_Path: \${SAW-workspace}/W80_4_Shock_Physics/Credibility/0-Preparation

Tier_2_platform: serrano

Tier_2_scratch: /fscratch

Tier_2_home_prefix: /asclap/users

Input Interface

Mesh Resolution

dx: 0.05

Job Parameters

CTH_version: 12.0

account: fy140073

time_limit: 3:00:00

num_processors: 128

Analysis Workflow

remoteNestedWorkflow-Tier_2

> dx
> CTH_version
> account
> time_limit
> num_processors

Tier 2

stdout
stderr
Materials_video
Pressure_video
Velocity_video
TOA_T1_Center
TOA_T2_Right
TOA_T3_Left
TOA_T5_Stracer
CPU_Time

Output Interface

Videos

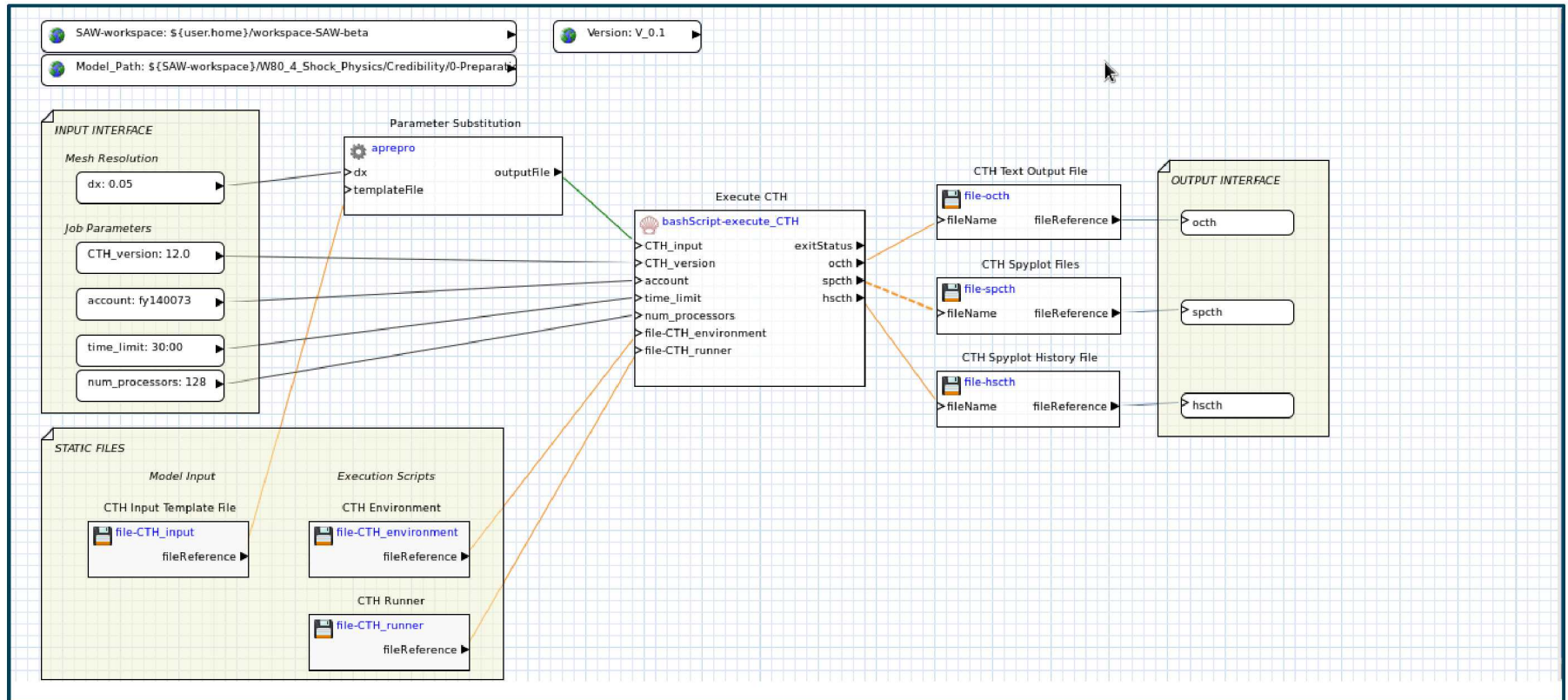
Materials_video
Pressure_video
Velocity_video

QoIs

TOA_T1_Center
TOA_T2_Right
TOA_T3_Left
TOA_T5_Stracer
CPU_Time

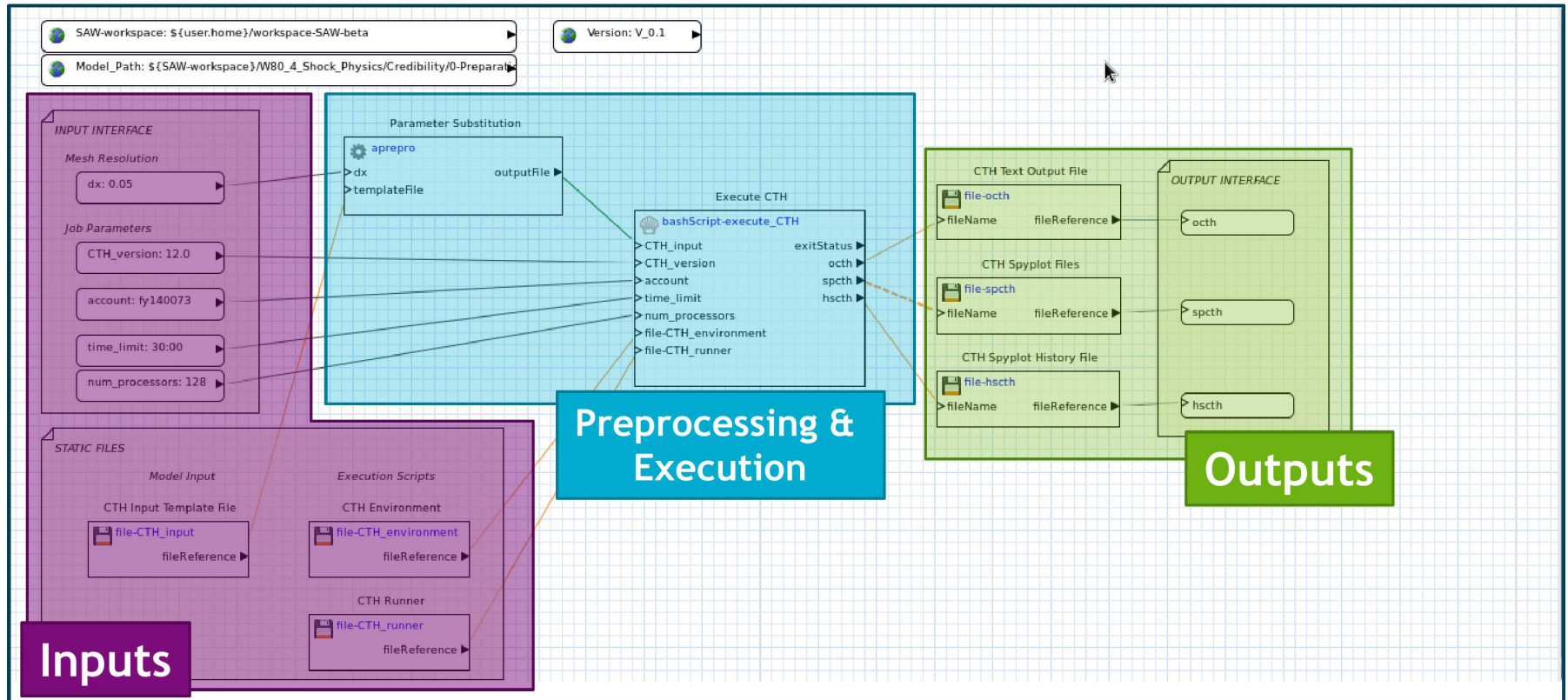
Analysis Execution Workflow Example

Implementation of workflow allows for **ease of communication** and **simplifies modifications**.



Analysis Execution Workflow Example

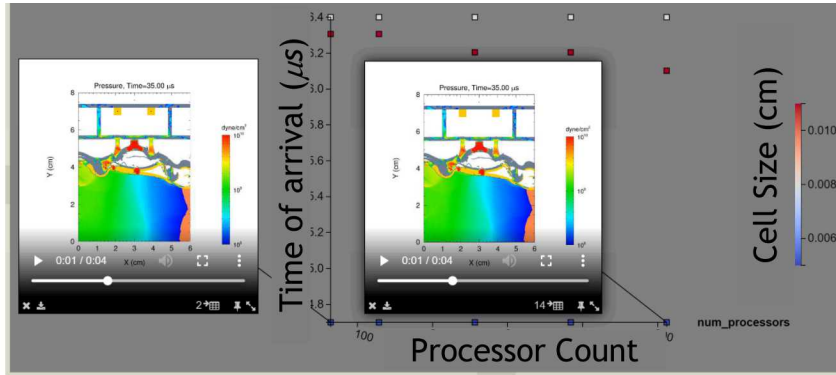
Implementation of workflow allows for **ease of communication** and **simplifies modifications**.



Communication by and with analyst team, ease of collaboration greatly increased

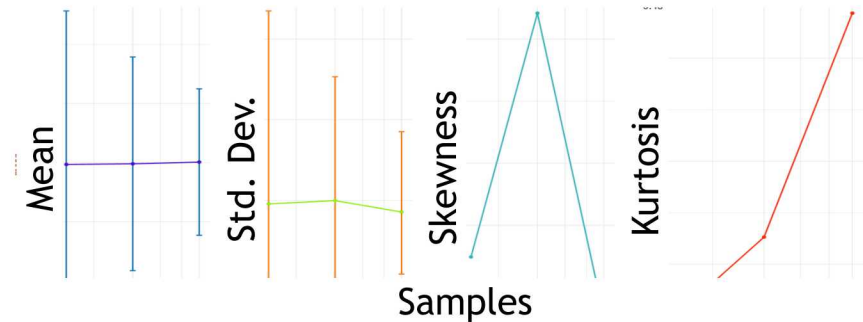
Specialized Workflow Nodes Support Visual Exploration

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



Slycat:

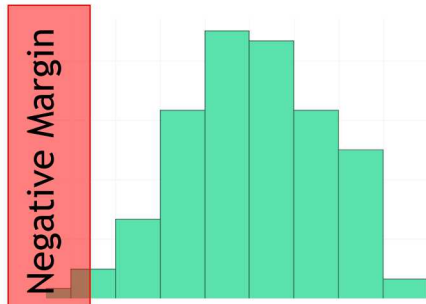
Collect and on-demand display media
Statistical analysis of samples



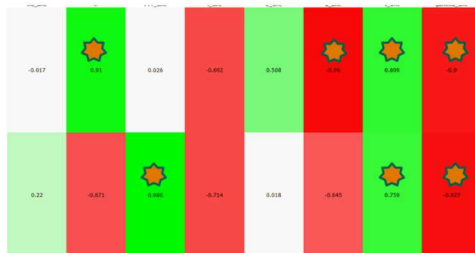
Assess sample size for intended use

Decision alternatives

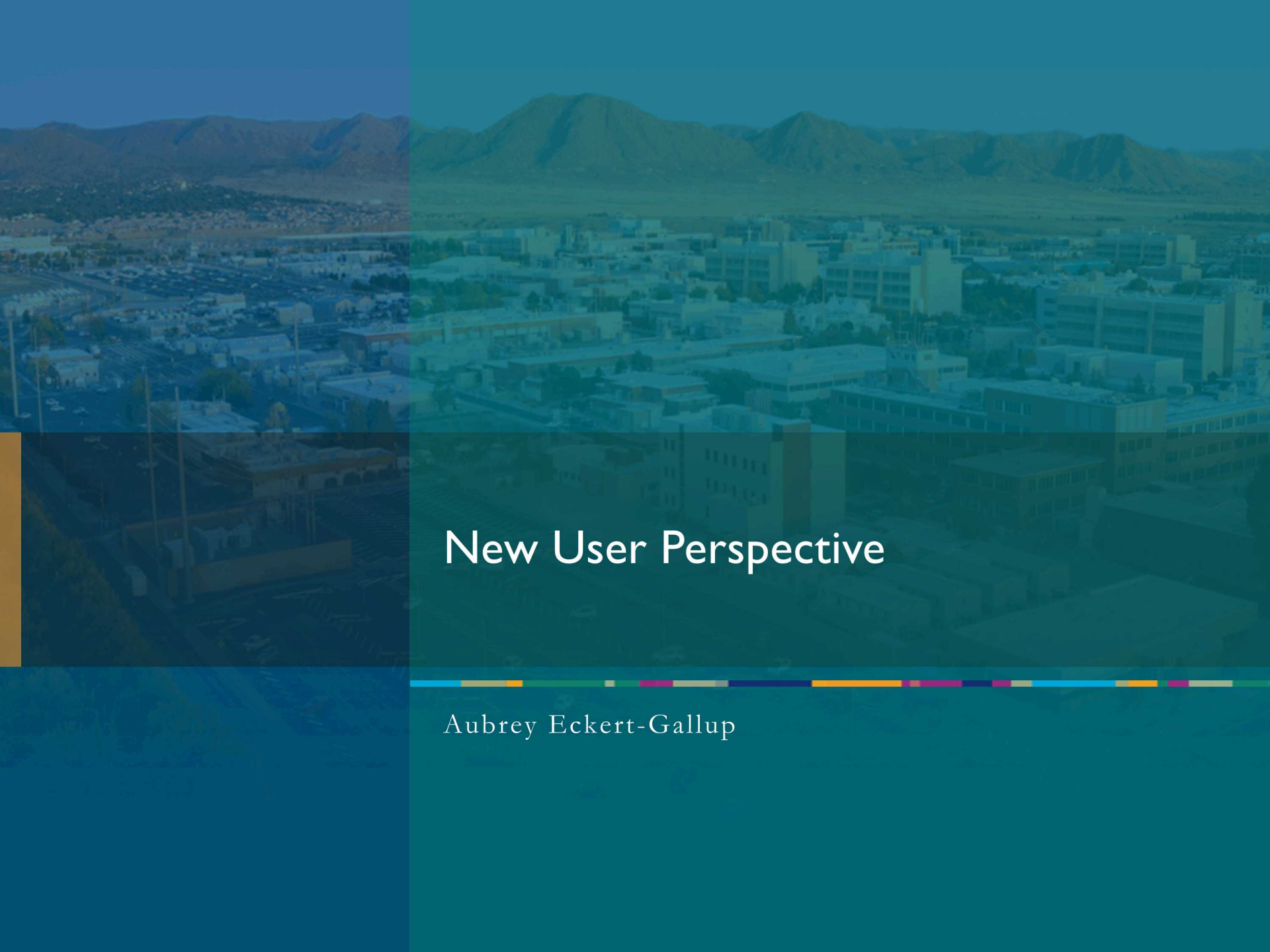
- Live with plausible negative margin
- Quantify $p(\text{margin} < 0)$
- Negotiate criteria
- Use sensitivities to dial design
- Restrict operations



Violating requirement plausible



Most important factors identified



New User Perspective

Aubrey Eckert-Gallup



Relevant Prior Experience

- Newest member of Verification, Validation, and Credibility Processes department
 - Familiarity with engineering analyses, V&V concepts, uncertainty quantification (UQ) methods and software (including Dakota)
- Prior experience with software development for commercial nuclear power applications
- No prior experience with SAW or running Sierra

Project Goals

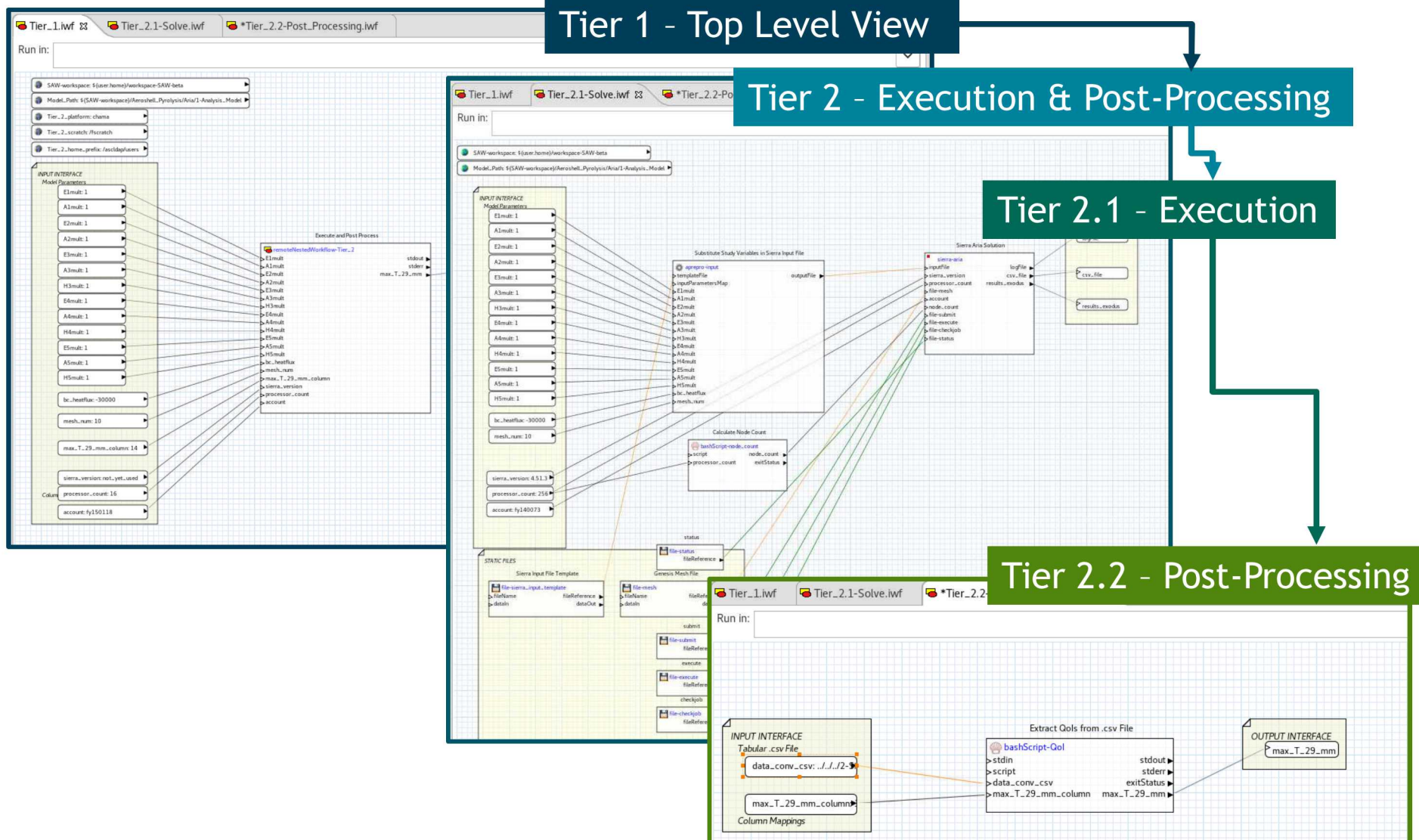
- Implement high-fidelity thermal models for use in modeling abnormal thermal environments
- Quantify and compare uncertainty in model results from various codes and develop design of experiments

Integrated Workflow Interface

- Hands-on collaborative training with George Orient starting December 2018
- Continued use to develop capabilities to meet project goals

Current Work with Integrated Workflows

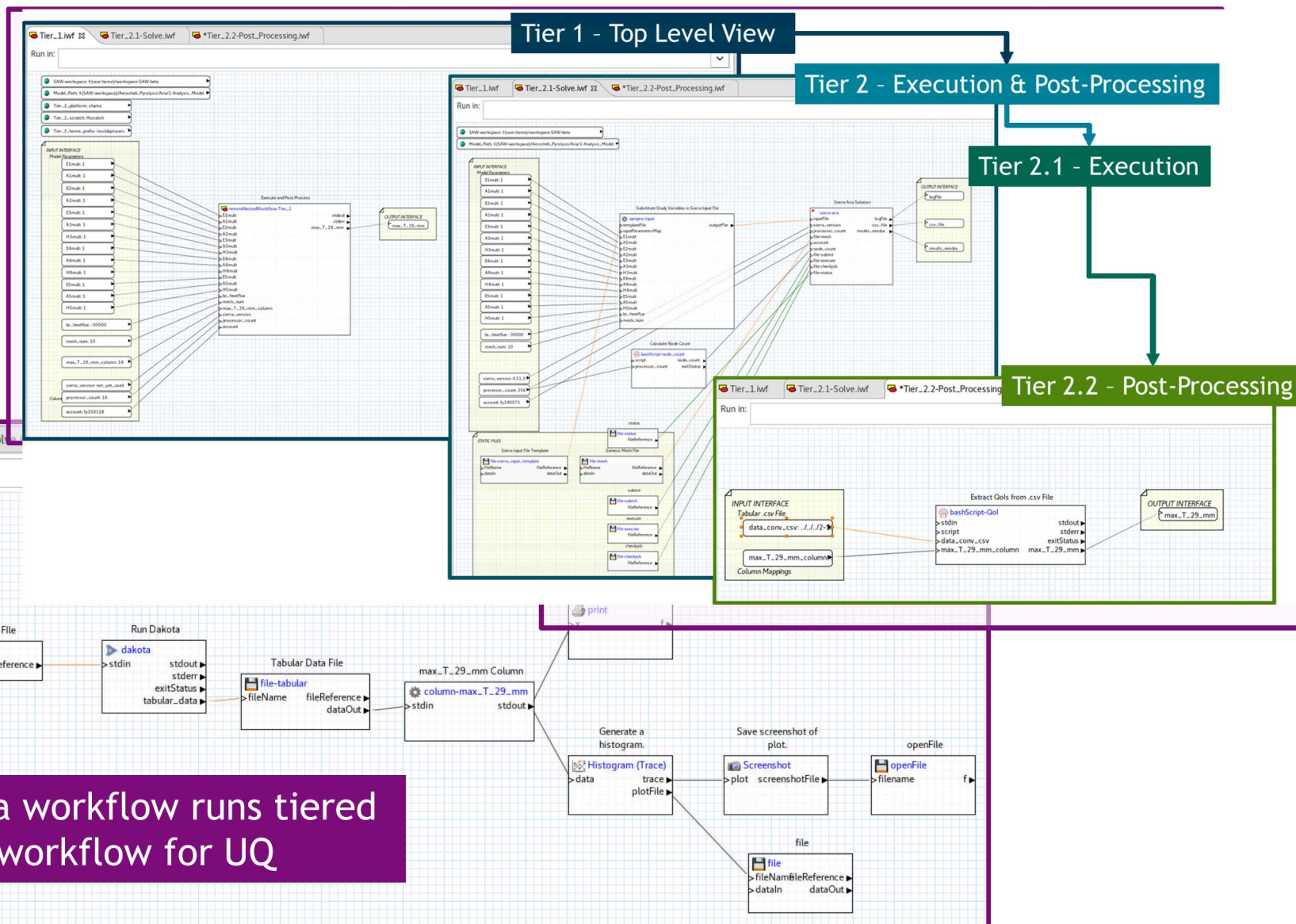
Tiered workflow has been developed to run and post-process simulations.



Analysis can be broken into component parts and tiered hierarchy of complexity

Current Work with Integrated Workflows

Dakota iterator workflow wraps tiered workflow to run uncertainty quantification.



Analyst Training Through Workflow Development

With minimal startup training, development of integrated workflow allowed me to:

Submit jobs to HPCs

Setup and run Sierra

Run Dakota with minimal setup effort

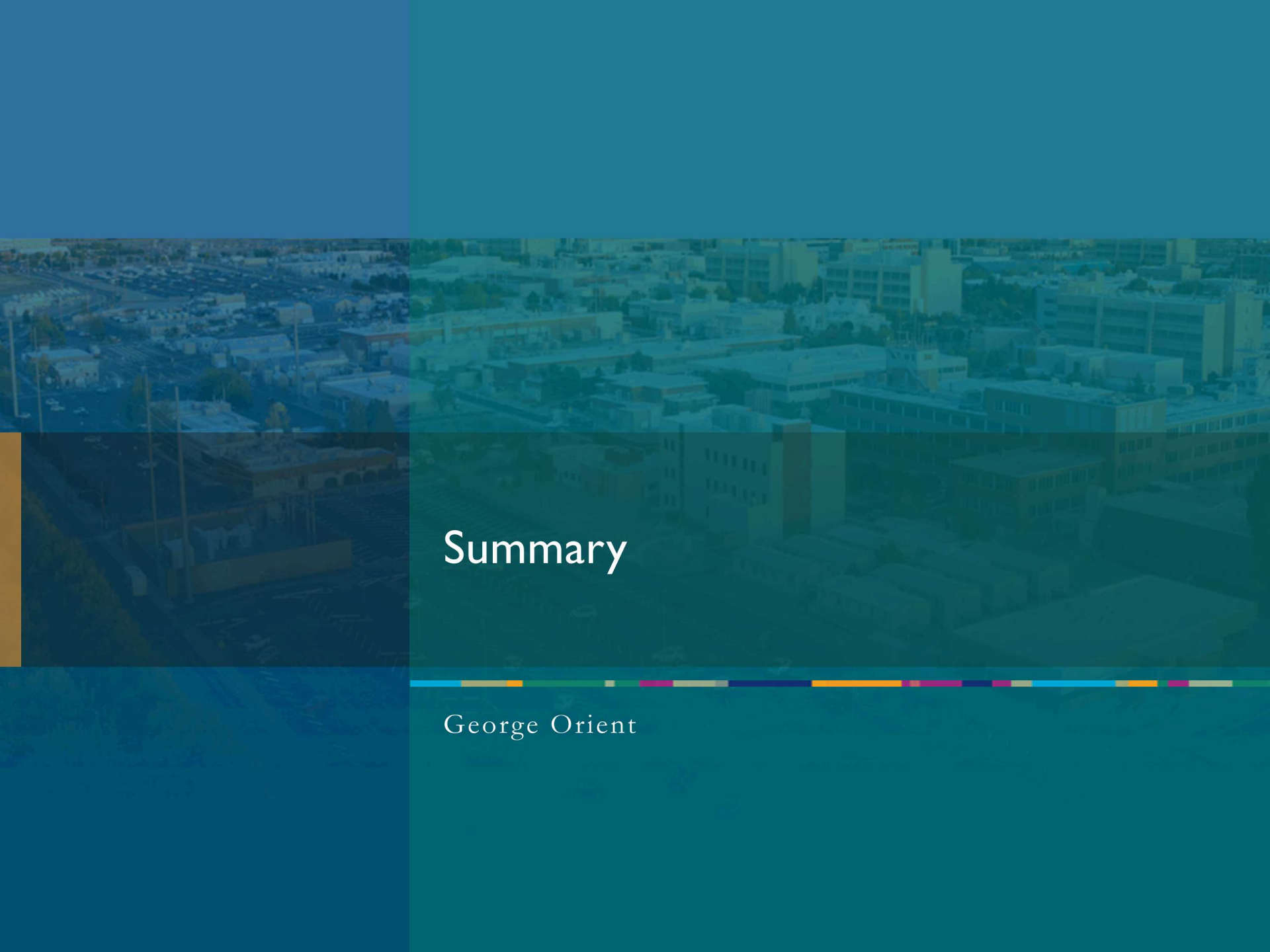
Ensure that simulation setup is repeatable

Work collaboratively to set up simulations and generate results

Dakota workflow runs tiered workflow for UQ

Communicate analysis workflow to customers

New analysts enabled to complete workflows with minimal startup training

An aerial photograph of a city, likely George, British Columbia, showing a mix of residential and commercial buildings, streets, and green spaces. The image is overlaid with a semi-transparent blue filter. The top half of the image is a solid blue gradient. The bottom half is a teal gradient. A horizontal bar with a multi-colored pattern (yellow, green, purple, blue, orange) runs across the middle of the image.

Summary

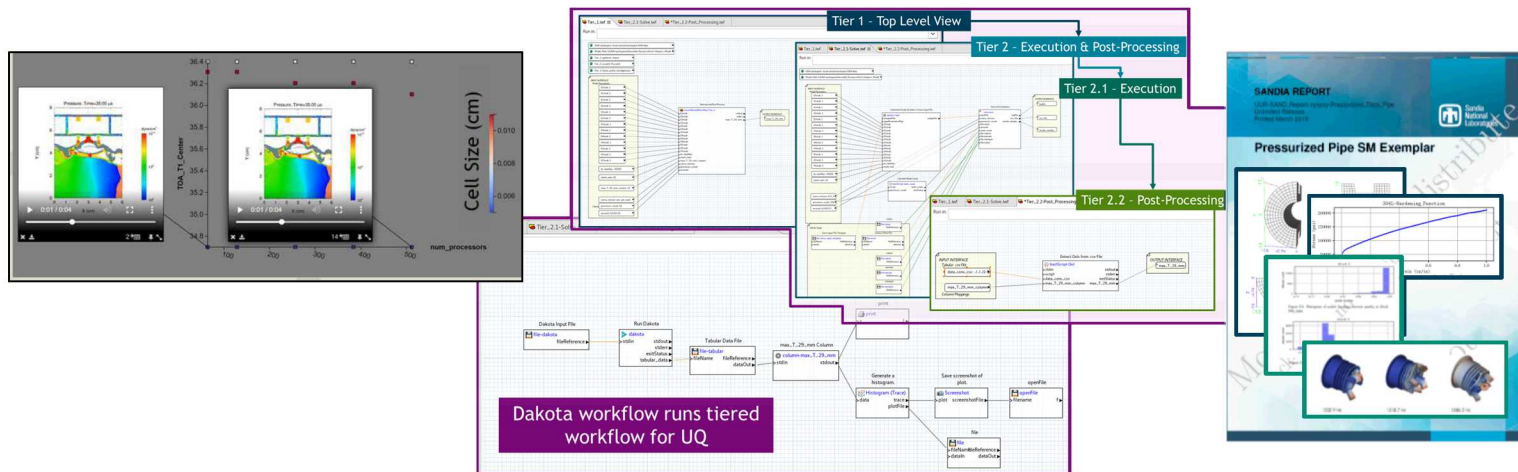
George Orient

Summary

Integrated workflows enable agile and robust model development and execution:

- 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.





Additional Slides

References

Case Study

References

1. [https://upload.wikimedia.org/wikipedia/en/d/d5/Model locomotive by John Satchell Vict Australia 1866 MoV.jpg](https://upload.wikimedia.org/wikipedia/en/d/d5/Model_locomotive_by_John_Satchell_Vict_Australia_1866_MoV.jpg)

Development Process for Workflow Platform

What: Productionizing of workflow platform to **define**, **execute**, and **document** ensembles of high consequence ModSim to support communication and decision making, funded by ASC Integrated Codes.

Current state: Scripted integration of disparate engineering tools takes ~1 year to develop. **Not tractable** by ModSim lead, not reviewable by stakeholders.

Future state: **Reviewable**, **tightly-linked** analysis process definition and execution evidence package, **agile** model development project management.

Stakeholders: High consequence programs (weapons system qualification) need **defensible credibility** communication.

Approach:

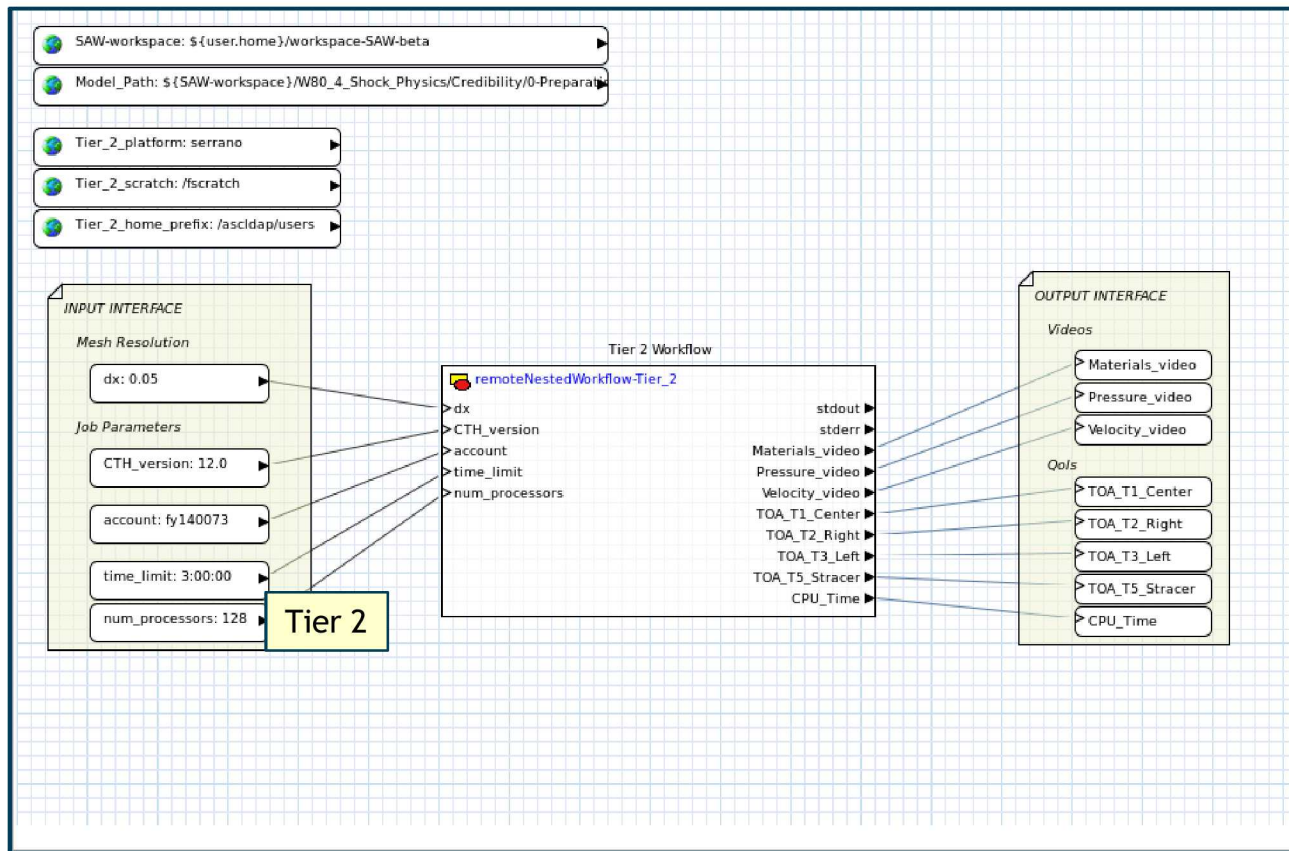


Risks management: Detailed management process focused on capability and reliability risks, scrum/sprint cycle utilized for development.

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

Infrastructure

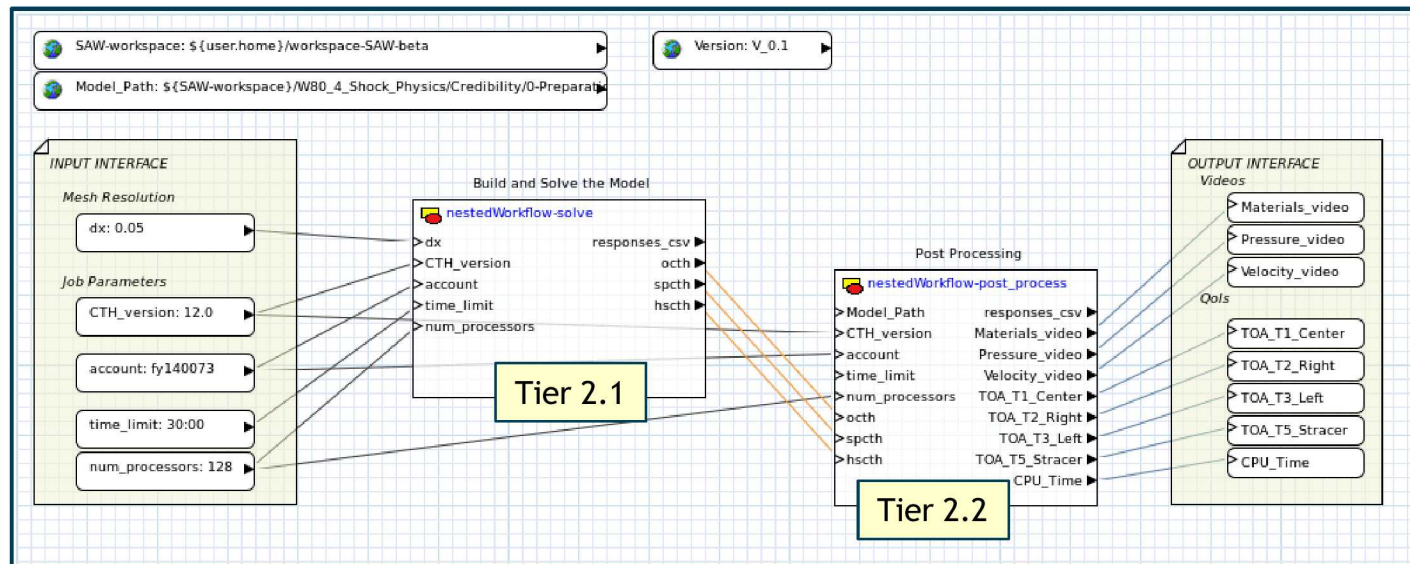
Exemplar



Tier-2 Analysis Workflow - Container for Execution, Post Processing

Infrastructure

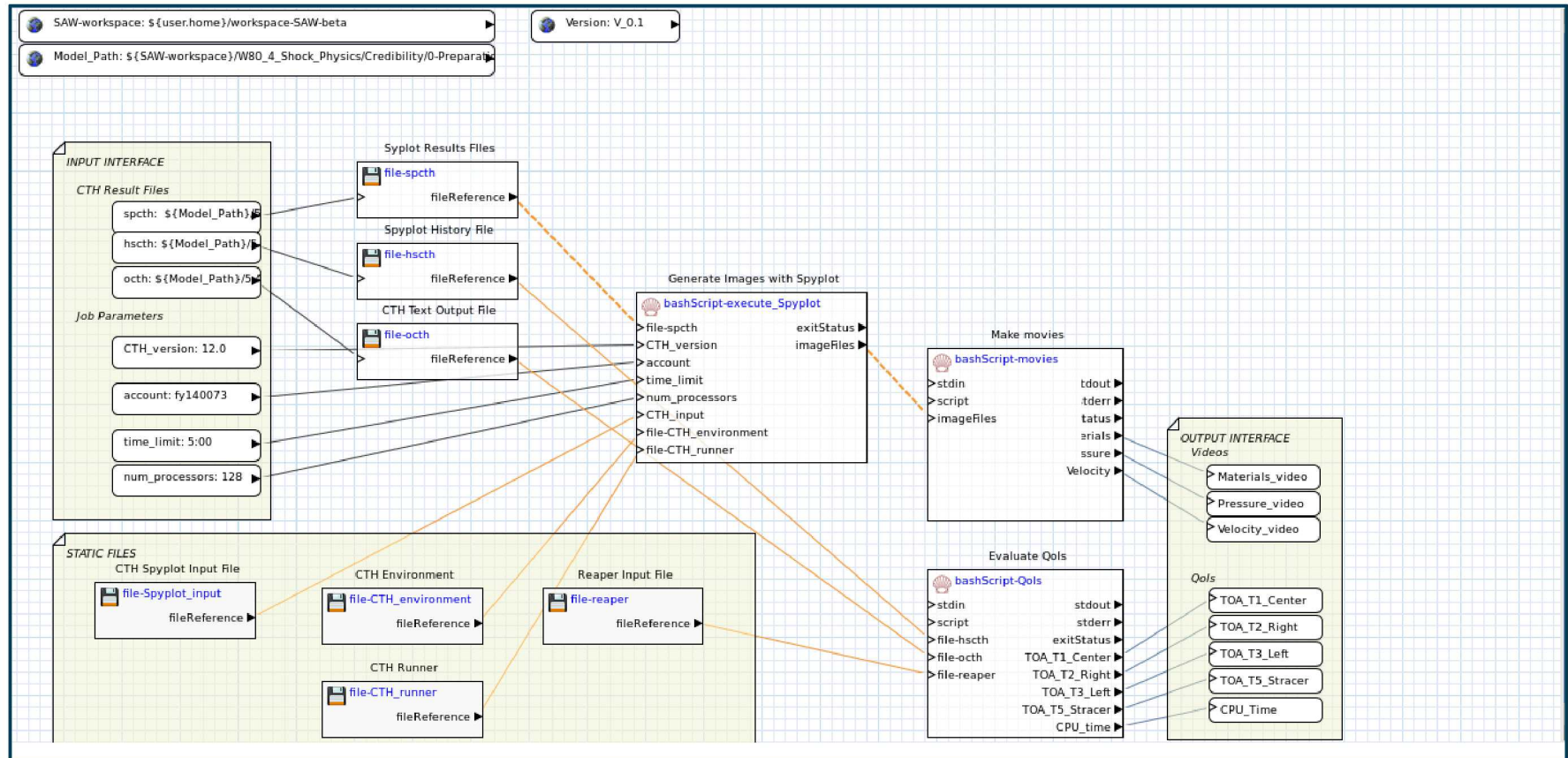
Exemplar



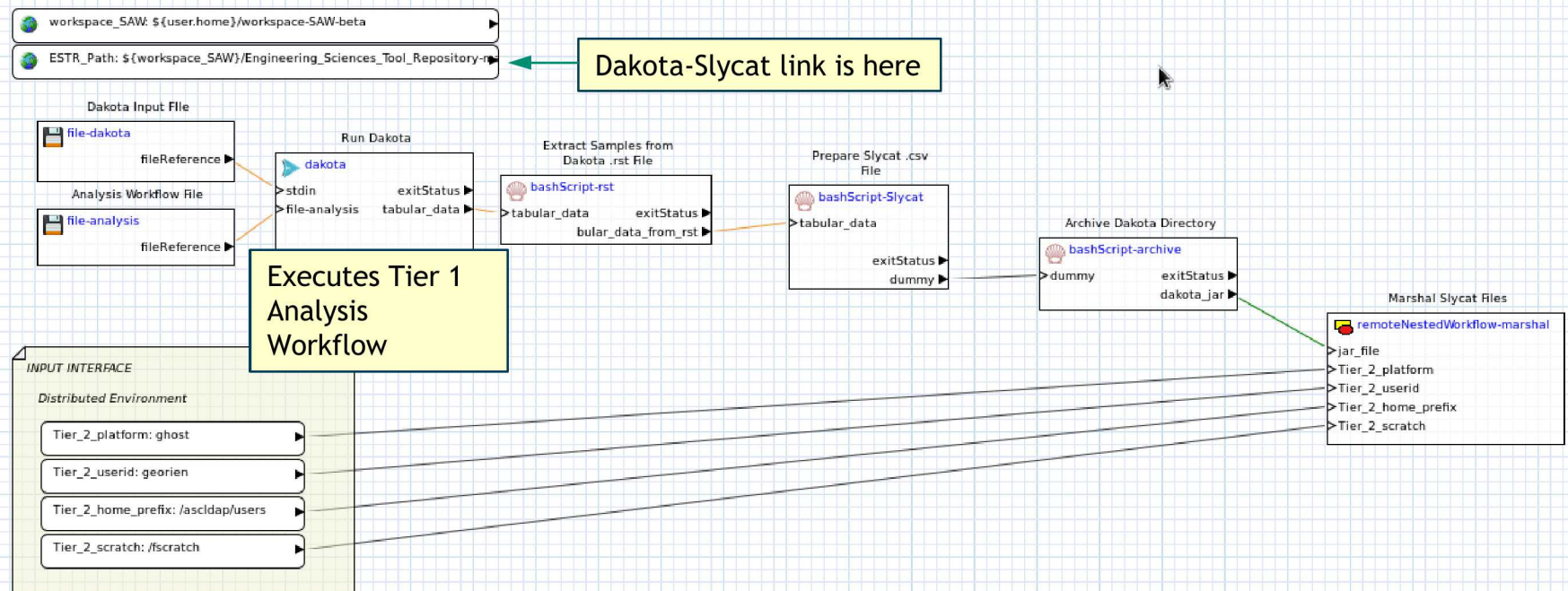
Tier-2.2 Analysis Workflow - Post Processing

Infrastructure

Exemplar



Dakota-Slycat Workflow



Reusable patterns emerge; need library mechanism

Scalability Results in Slycat

Infrastructure
Dakota
Exemplar

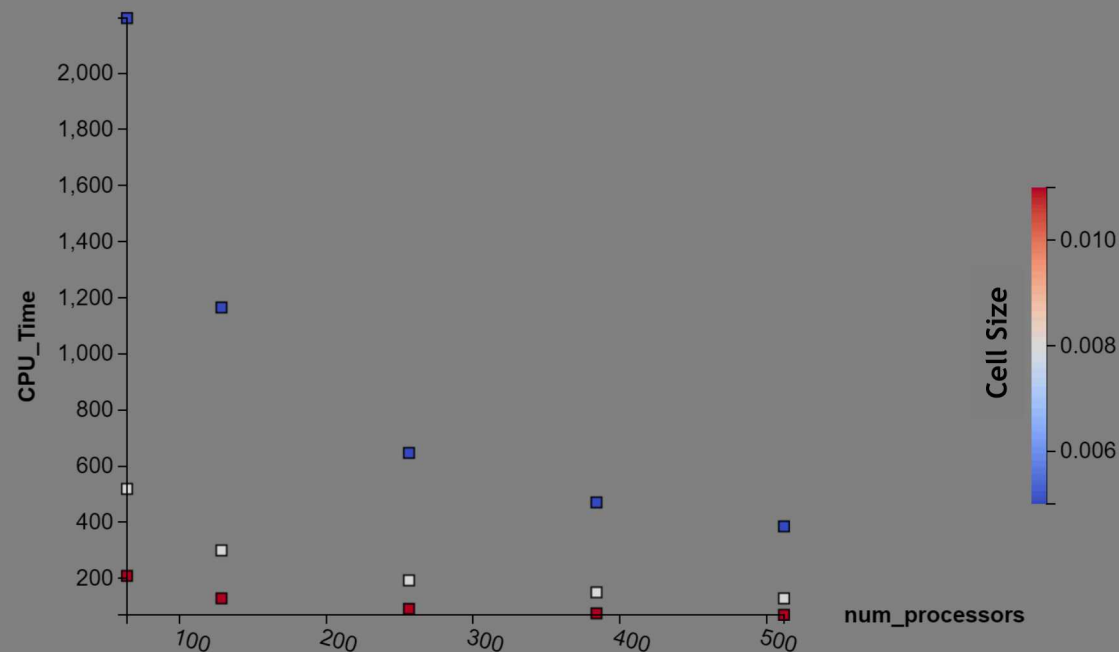


Lattice Crush / Scalability

Create Edit Info Bookmarks Delete



Filter X Axis Y Axis Point Color Media Set Selection Action Show All Close All Pins Color



Irrespective of cell size (dx) the optimum processor count is ~500; SVR and UQ will be submitted to 500 processors

Mesh Sensitivity, ToA at Center

Infrastructure

Dakota

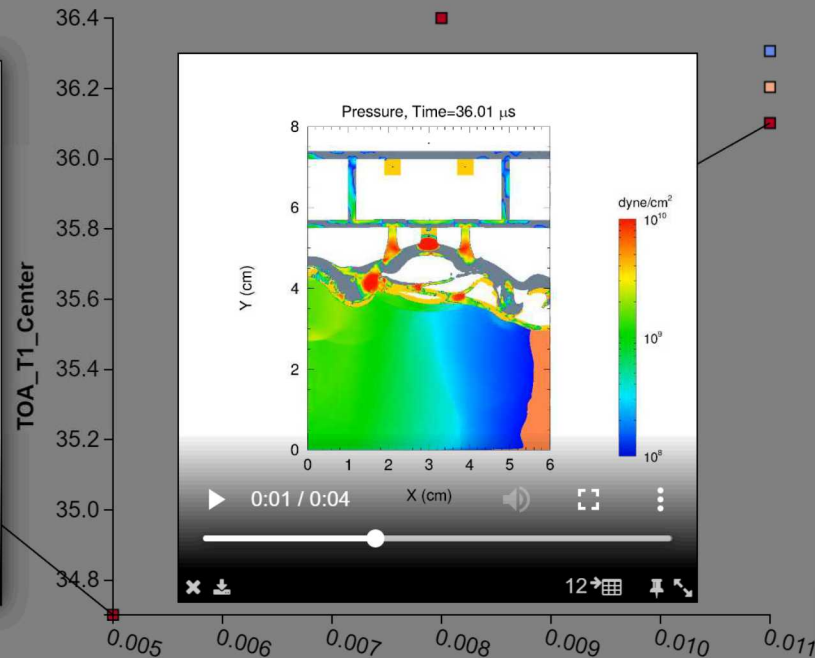
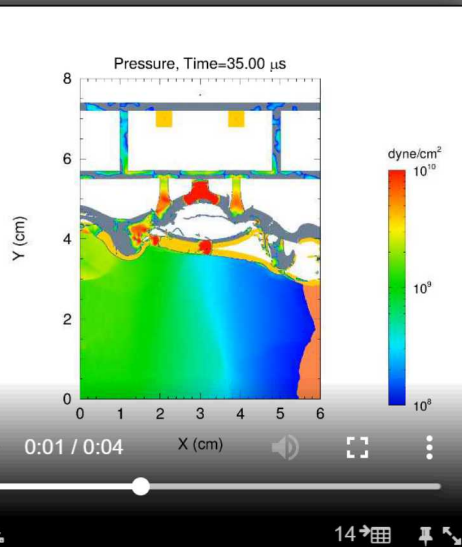
Exemplar



Lattice Crush / Scalability

Create Edit Info Bookmarks Delete

Filter X Axis Y Axis Point Color Media Set Selection Action Show All Close All Pins 1.403154



num_processors

500

400

300

200

100

No convergence at the limit of refinement feasibility for production 3D model; Estimation approach needed