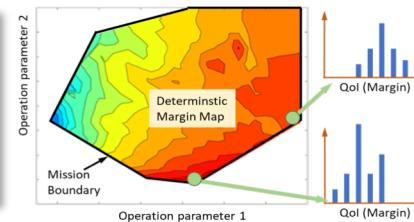
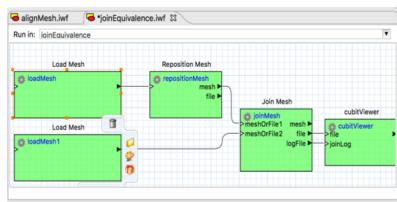
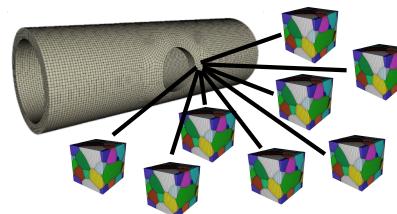




Sandia  
National  
Laboratories

# Integrated Workflow Overview



PRESNTED BY

Robert L Clay

Scalable Modeling & Analysis

Predictive Engineering Science Panel (PESP)

Oct 30, 2019



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# Session Overview



- Integrated Workflow Overview (Clay)
- Credible Design and Qualification Workflows (Orient)
- Next Gen Workflow (Friedman-Hill)
- Workflow Capability Integration (Hoffman)
- Data Movement for Workflow (Oldfield)

# Integrated Workflow at Sandia



- What was the IWF charter?
- Top-level drivers
- Brief history of workflow
- Strategic roadmap
- External engagement

# What was the IWF charter?



- Increase the impact of the ASC tools for ND mission customers
  - Integration of the modsim tool chain via automated workflow.
  - Creation of a cohesive modsim capability for ASC.
  - Focus on improving usability, not new widgets.
- Demonstrate impact on ND mission (W80-4)
- Foster a cultural shift toward integrated solutions

# Top-level Drivers

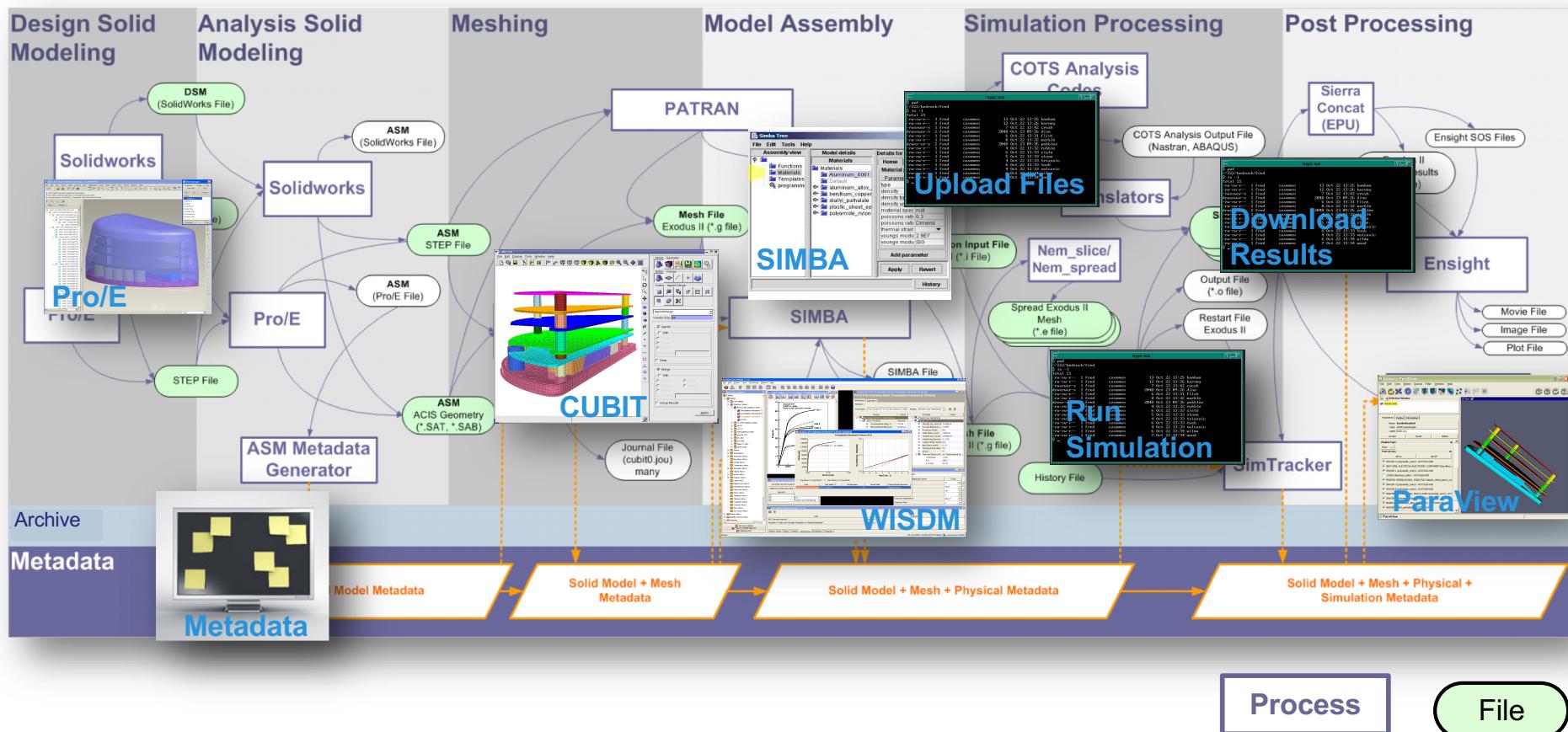


- Increase usability of the modsim tool chain
  - Increase ease of use
  - Lower cognitive load
  - Automate as much as possible (ensembles for V&V)
- Reduce time to solution
  - Factor of 5x or more
  - Get the tools out of the way – focus on the physics
- Increase credibility
  - Save the process with the data (NGW & SDM)
  - Reproducibility (lower A2A variability)
  - Automated reporting (ARG & CF)
  - Simulation governance – who did what when where

# Analysis Process – pre 2005



A collection of tools that were managed on an individual basis utilizing scripts and manual walk through process; making it difficult to trace, share, reproduce, and generally, establish credibility.



Complex, Manual, Disorganized, Steep Learning Curve, No Traceability, Low Reproducibility

# Sandia Analysis Workbench (SAW) – Initial State (2009)



## Integrated tools with archived data

- Eclipse Workbench is the integrating UI platform ([www.eclipse.org](http://www.eclipse.org))
- Capabilities (SDM, Job Submission, Sierra Editor, etc) are modularized as plugins

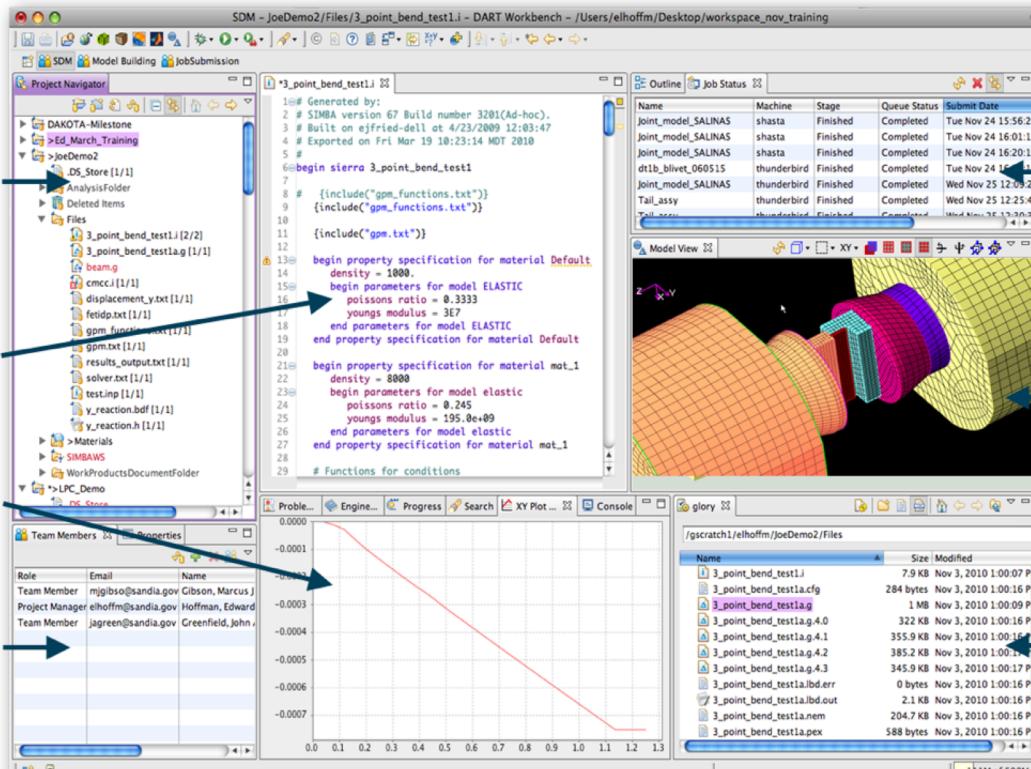
Version control and archive project files

Create and edit models

View data

Access control to potentially sensitive data

Complex scripting used to perform analysis steps

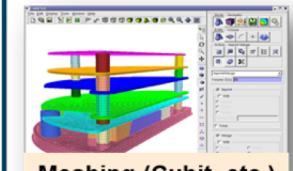


Submit Jobs to HPC Systems

View Models

Access to HPC File Systems

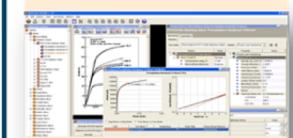
Diverse Software Toolset



Meshing (Cubit, etc.)



Metadata



Materials (Granta, etc.)



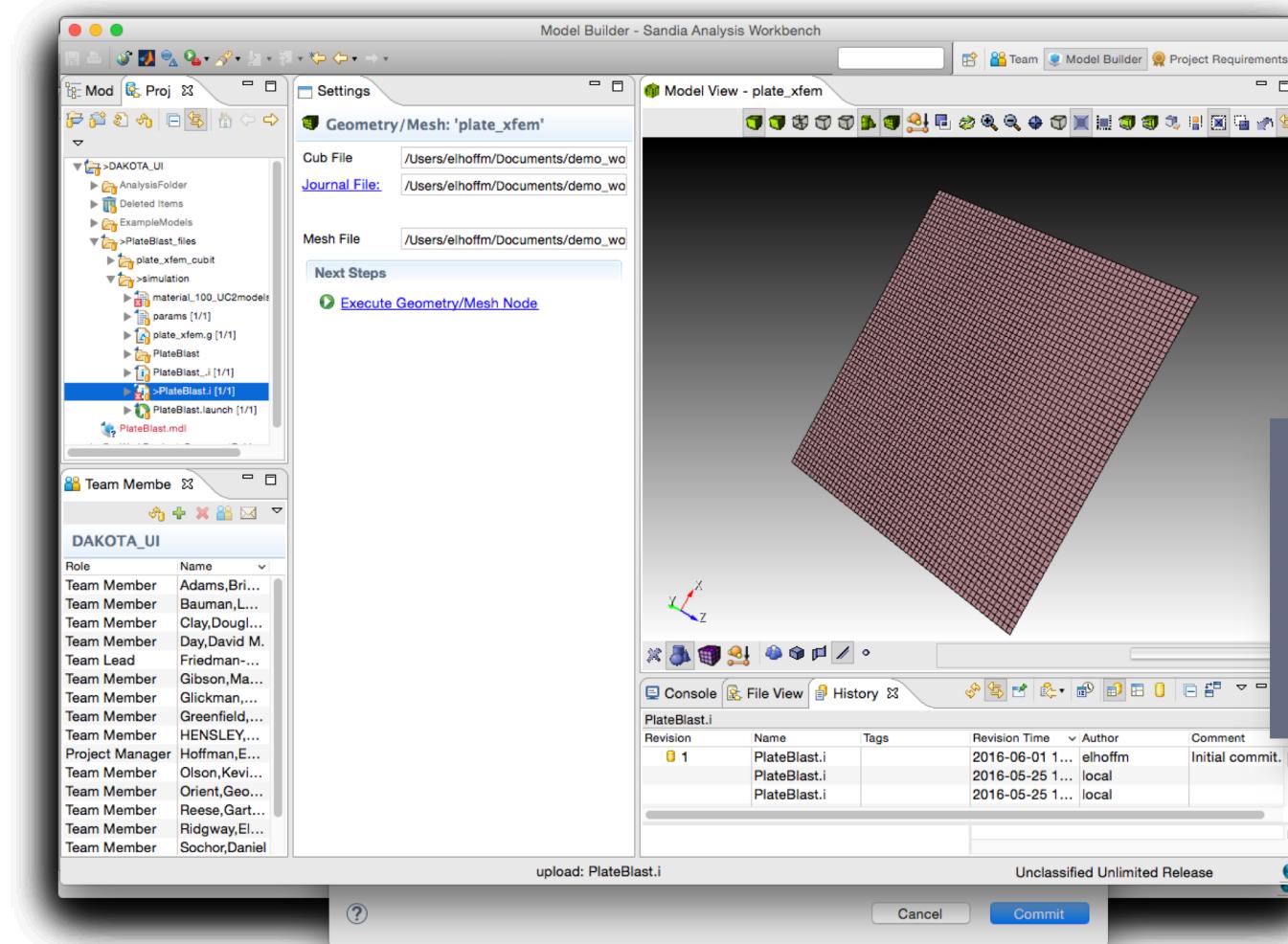
Solvers (Sierra, etc.)

Analysis workflow is assisted by SAW, but process remains highly complex and extremely limited automated workflow capability. The analyst is still the integrator.

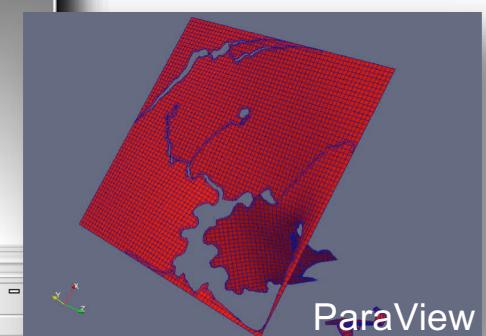
# SAW Model Builder – Recent State (2014)



- Core set of tools becoming integrated in SAW framework.
- Integrated, Graphical, Interactive, Archived Data



- Model Building
- Process Management
- Data & Metadata Management



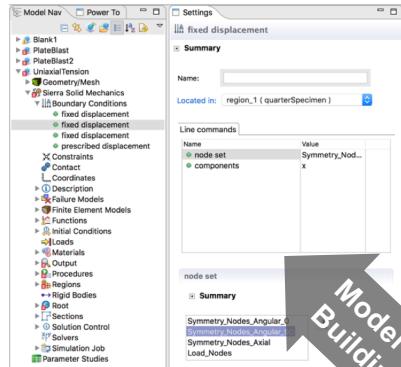
Geometry > Meshing > Loads & Boundary Conditions > Job Submission > Archive > Viz

Helps analysts build models faster but still no end-to-end automated workflow.

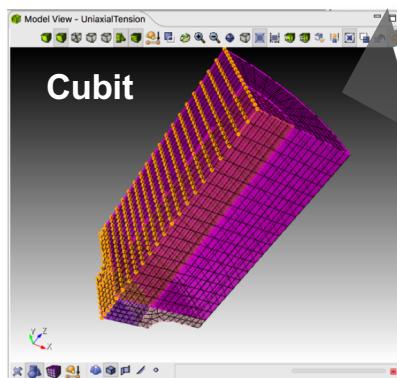
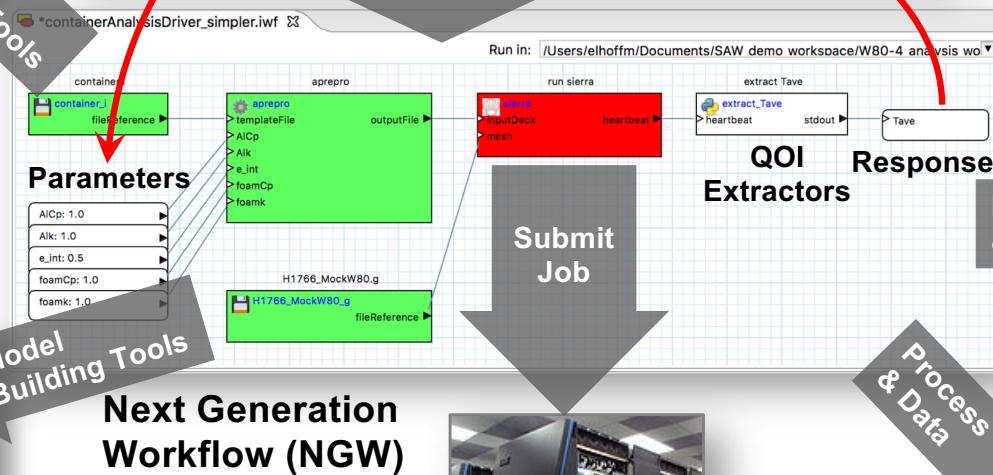
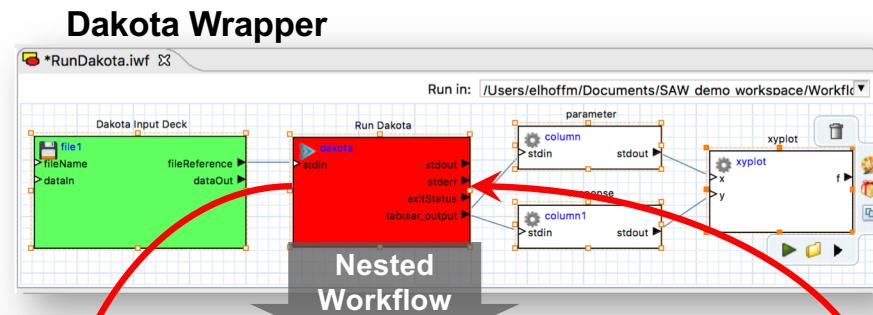
# IWF – Transforming Engineering Science Analysis (today)



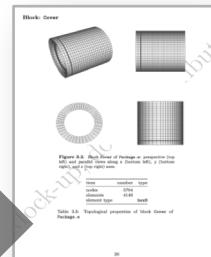
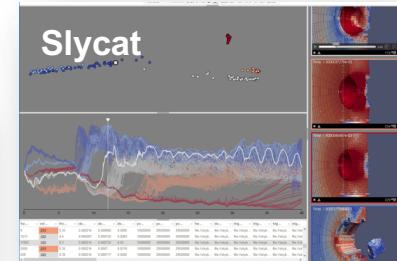
Integrated, Graphical, Automated, Self-Documented, Archived Process and Data



Sierra Editor



Model Building Tools  
Next Generation Workflow (NGW)



Documentation & Credibility

Process & Data

IWF is a project and an approach, more than a product.

# Acknowledgements

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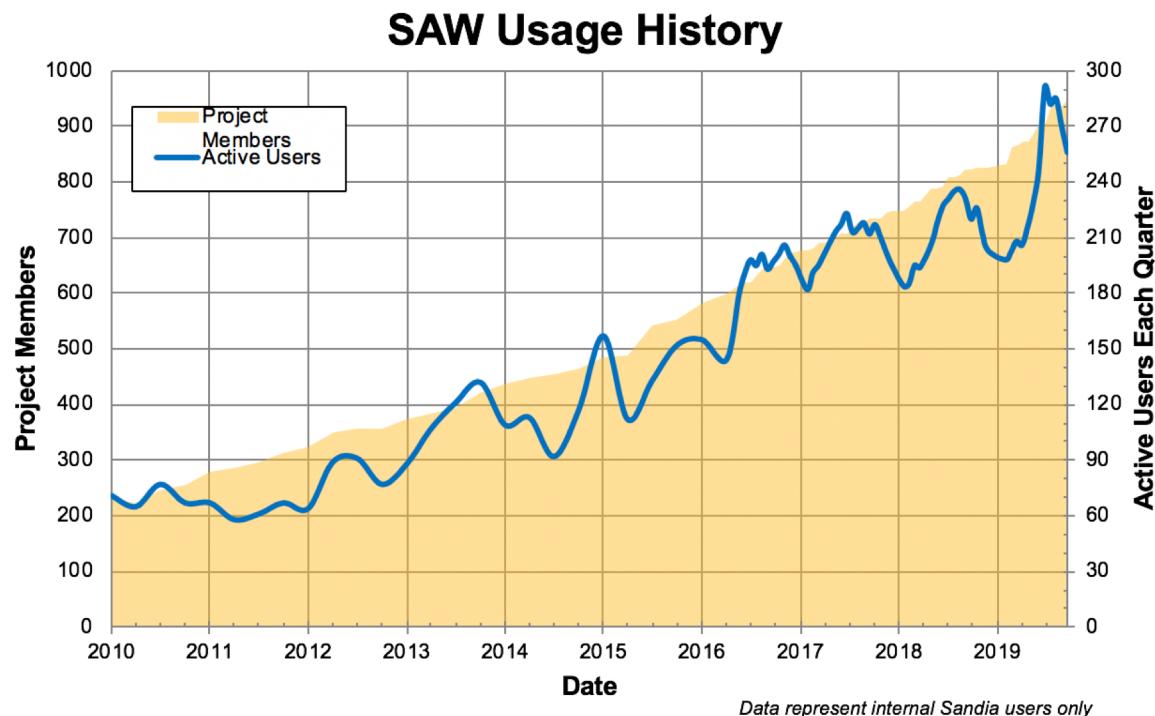
- Brian Adams (Dakota)
- Anthony Agelastos (FOUS)
- Robert Clay (IWF PI & SAW PM)
- Ernest Friedman-Hill (SAW PI)
- John Greenfield (FOUS)
- Marcus Gibson (SAW dev)
- Mike Glass (Sierra)
- Matt Glickman (IWF PO,  
Electrical)
- Trevor Hensley (FOUS)
- Martin Heinstein (NGS)
- Ed Hoffman (IWF PO)
- Patty Hough (User Engagement)
- Warren Hunt (Viz)
- Joe Kotulski (Electromagnetics)
- Jay Lofstead (IOSS)
- Kevin Olson (SAW dev, FOUS)
- George Orient (IWF PO, V&V)
- Roshan Quadros (Cubit PI)
- Elliot Ridgway (Dakota UI)
- Andrew Rothfuss (SAW dev)
- Jason Verley (Xyce)
- ... and many others

Lot of moving parts; lot of teams involved.

# Adoption is Steadily Increasing

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- In production for more than 10 years
- At Sandia: Over 250 active users per quarter & over 900 data owners
  - More than 2 million files stored in the SAW repository
  - Approximately 1000 job submissions per week
- SAW Model Builder: deployed with Sierra and used in Sierra training
- Dakota UI built on SAW/Eclipse
  - open source licensed
- Integrated Cubit UI
- PLATO topology optimization toolkit built on SAW
- ASC Investment in workflow  $\approx$  5 FTE/yr

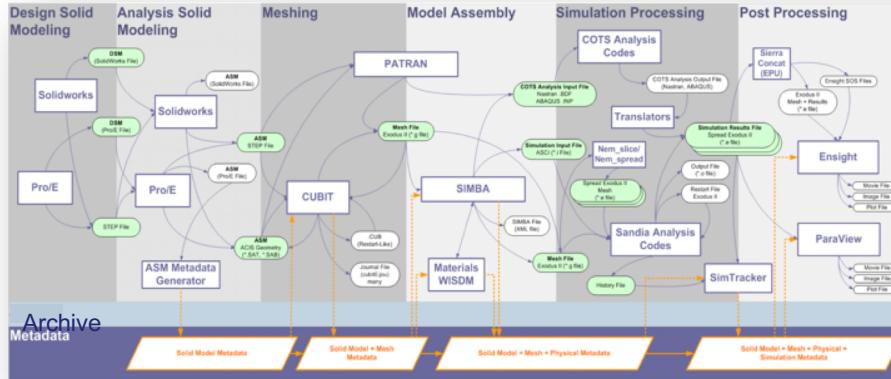


# ModSim Process – Past vs. Current States

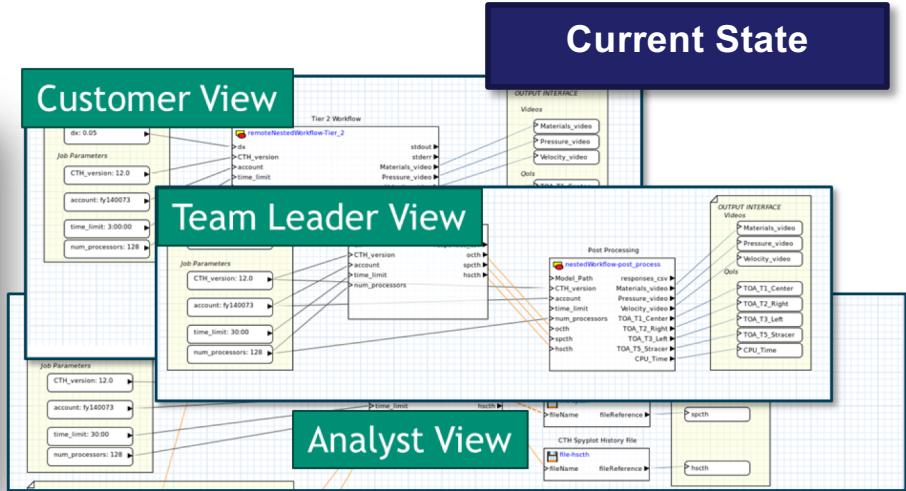
12



## Past State



## 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)

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

# Implementation Strategy

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- Maintain focus on original goals
  - Focus on ND analysts needs
  - Focus on usability: “From hero to hundreds”
- Move toward an open source software stack
- Move toward open, stand-alone services model
- Continue strategic partnership with NGS
- Continue collaborations with labs – NNSA, OS, CEA, ...
- Continue non-lab external collaborations
- Contribute to the Sandia ND data architecture/solution

# Strategic Roadmap – near term (FY20-21)



- FY20
  - Hardening the system and broad internal rollout (training, tutorials, GitLab, etc.)
  - Model Builder 2.0 based on new architecture driven by NGW
  - Automatic Report Generator (ARG) internal rollout
  - Vertical integration with experimental workflows
- FY21
  - Open SDM deployment
  - UX/UI alignment with Next Generation Simulation (NGS)
  - Support common model framework
  - Support [full] simulation governance
  - Credibility Framework (CF) internal rollout
  - Library of reusable workflow components
  - Integration with engineering data systems (e.g., GRANTA)
  - PLATO (AM) workflow support

# Strategic Roadmap – mid term (FY22-23)

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- FY22
  - Integration with ND data management infrastructure
  - Full integration with NGS UX/UI
  - Full XML (or similar) support for Sierra and RAMSES
  - Full integration with CAD metadata
  - Multi-lab standards (SDM, workflow components, ...)
  - Infrastructure to support a broad external rollout
  - Automated updates
- FY23
  - In-memory data transfer in workflows
  - Support for non-ND applications
  - Workflow management on any device anywhere
  - Smart workflows – [partially] self-assembling
  - Real-time design-through-analysis workflows

# Strategic Roadmap – long term (FY24 on)



- NNSA cross-lab interoperability
- Broad external interoperability
- AI-driven workflow – workflow-driven AI (scary?)
- Deep data analytics built on SDM
- [Really] smart workflows
- Easy-to-configure ARG and CF [for new domains]
- Analyst onboarding in days, not months
- Siri 10.0 (?) interface
- ... the list is potentially endless.

# External Engagements

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- NNSA Workflow WG
- NNSA/CEA WG (NNSA/CEA-DAM)
- NNSA/AWE (JOWOG-34, HOWOG)
- KCNSC (user community)
- NAFEMS SPDM Working Group
- CRADA partners
- Conferences and Workshops
  - NAFEMS World Congress & SPDM
  - Workflow Workshop & Hackathon (WoWoHa)
  - Others (SC, SOS, Salishan, ...)

# Glossary

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- A2A – Analyst-to-Analyst (variability)
- AM – Additive Manufacturing
- ARG – Automatic Report Generator toolkit
- CF – Credibility Framework
- ND – Nuclear Deterrence
- IWF – Integrated WorkFlow project
- NGW – Next Gen Workflow manager
- NGS – Next Gen Simulation project
- SAW – Sandia Analysis Workbench
- SDM – Simulation Data Manager capability
- UX – Usability
- UI – User Interface
- V&V – Verification and Validation

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