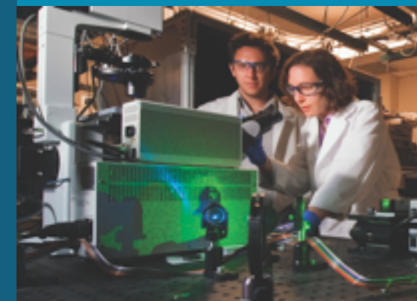

The Role of Workflows in Credible High Consequence Computational Simulation



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WoWoHa (DOE Workflow Workshop and Hackathon) 2020

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- CompSim (Computational Simulation) Models and Credibility
- Enabling Capabilities
- Credible Design through Analysis Exemplar
- Summary

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

Designer

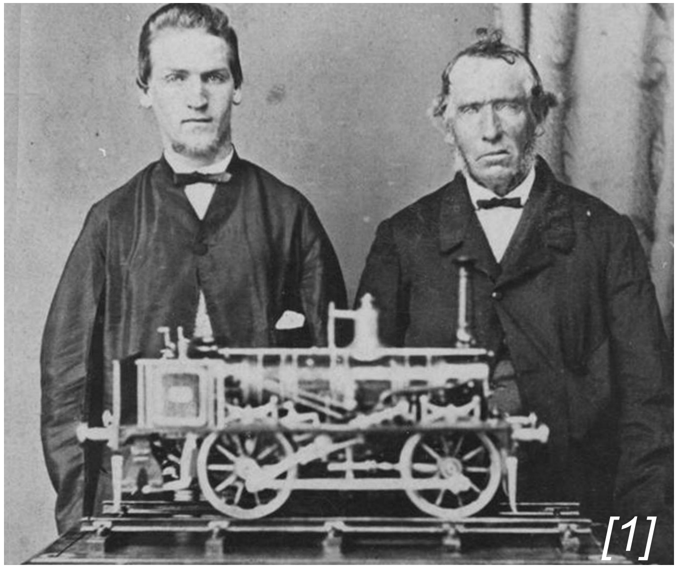
CAD Assembly
Tolerances, Repositories

Model Development Analyst

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

System Engineer

Trade study tool
Requirement Verification



[1]

Experimentalist

Experimental Design
Instrumentation Design

V&V/Credibility Analyst

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

Decision Maker

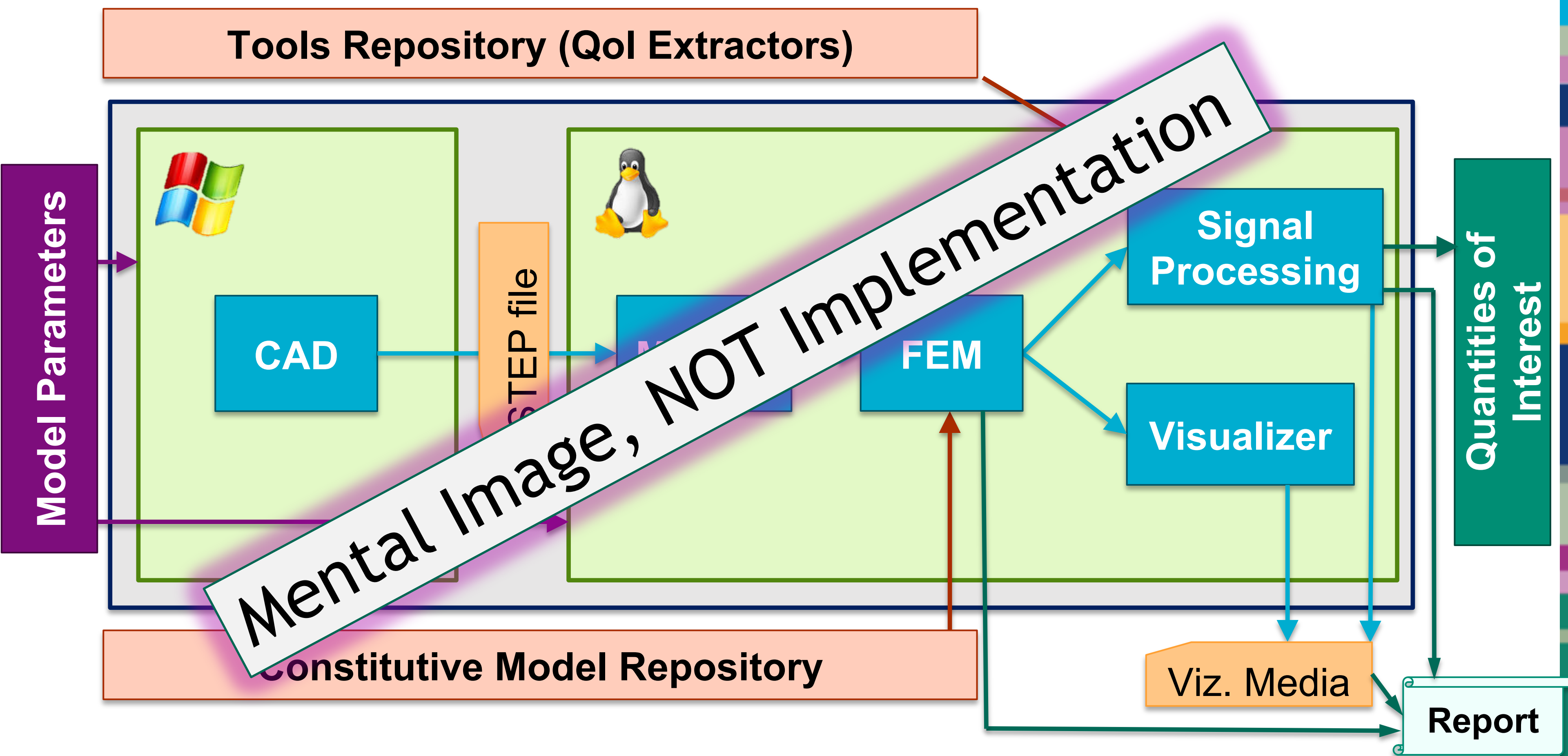
Credibility Evidence
Decision risk quantification

Workflow platform integrates different views of the model needed to communicate among all stakeholders – THE WORKFLOW IS THE MODEL

Notional Analysis Workflow

Analysis workflow is **built** and **iterated upon** to evaluate ensembles of workflow instances
- Maps model parameters to QoIs

Ensembles support product design, qualification and are a vehicle for discovery



Hundreds of instances- need resilience to random HPC hardware and software failures

Grand Challenge of Model Credibility

Qualitative evidence

- SME judgment, tacit organizational knowledge, past history
  - Expected predictiveness of the model for the intended use
- PIRT (Phenomena Identification and Ranking Table) - Defines key physical phenomena ranks their importance, identifies capability gaps
- Analysis governance, peer reviews

Quantitative "flavored" evidence

- PCMM (Predictive Capability Maturity Model) - SME elicitation process designed to characterize and communicate the completeness and rigor of the CompSim process.
  - Quantitative elements such as UQ and Validation but aggregation is difficult

Validation at a handful conditions – mission space is large, response is nonlinear/discontinuous, test data are sparse

Need to combine qualitative and quantitative evidence to support decision making in large untested mission space

Modeling and Simulation Credibility Process at Sandia

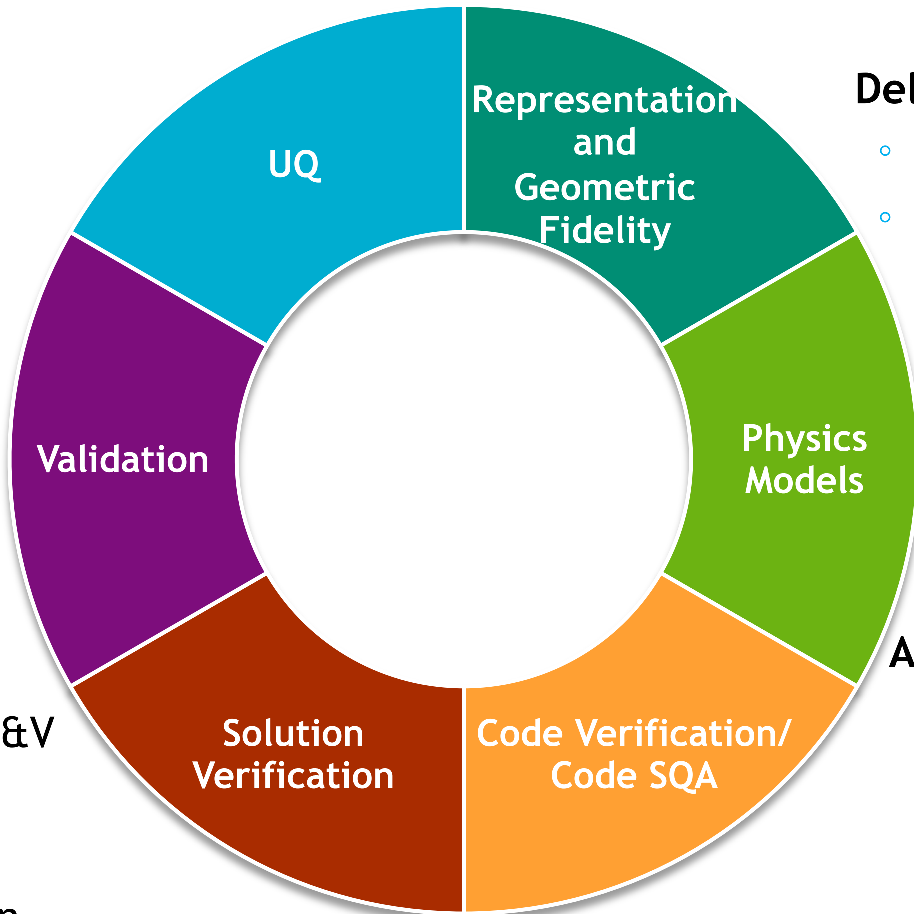
- The process of assembling and documenting **evidence** to ascertain and communicate the **believability** of **predictions** that are produced from computational simulations
- Quality process for CompSim (Computational Simulation)

Application Context

- Application Requirements
- Negotiate Role of CompSim in Decision Making
- Derived CompSim Requirements
- QoIs (Quantities of Interest)
- Test-CompSim Integration

Planning and Execution

- Model development; V&V
- Documentation
- Analysis governance
- Workforce qualification



Deliver Predictions

- Plausible margin bounds
- Credibility evidence

Assess & Communicate

- Customer engagement
- Peer reviews
- Prediction issues
- Gaps and path forward

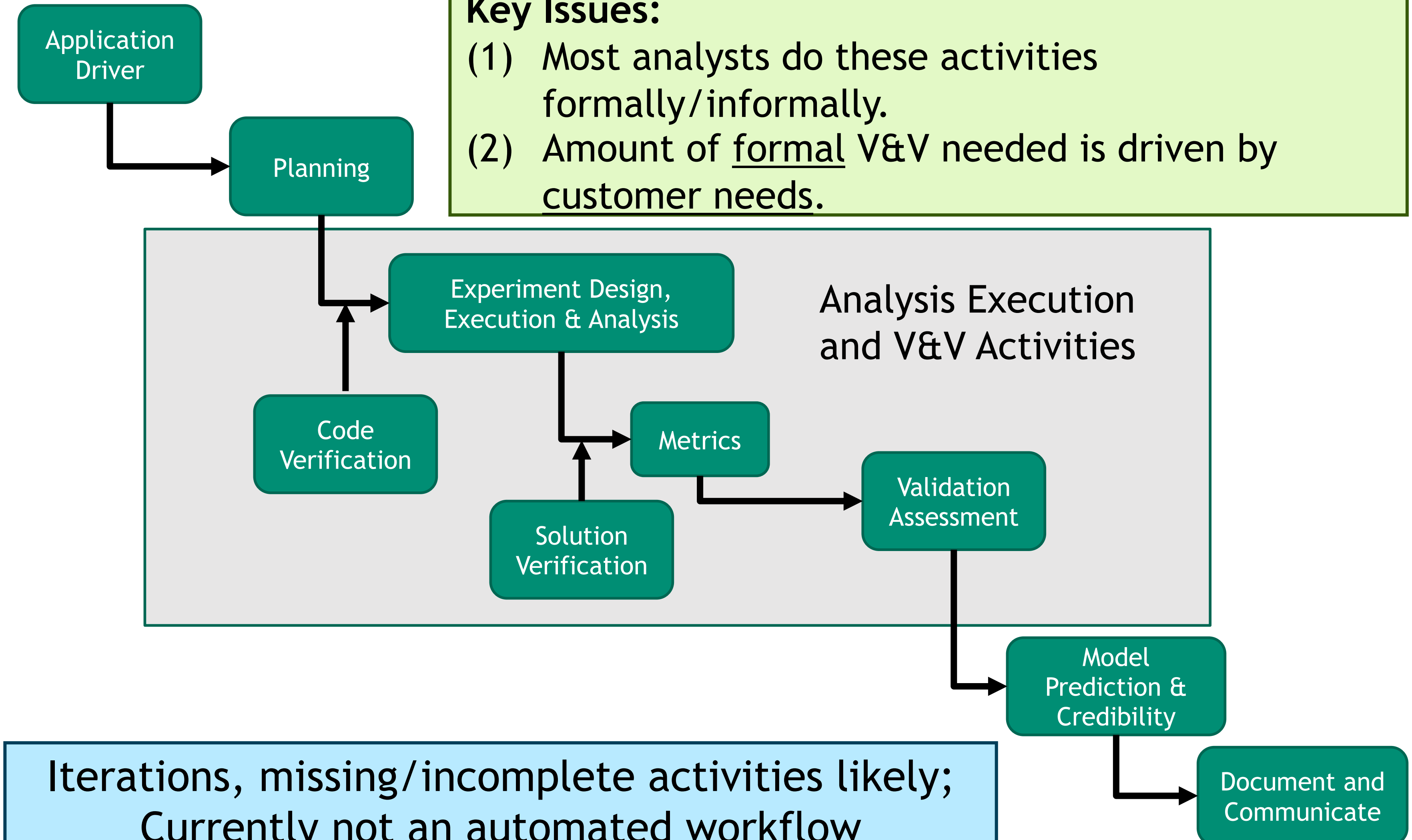
ND mission space: non-monotonic, discontinuous system responses - design and margin assessments under uncertainty REQUIRE agile execution of large model ensembles

Notional V&V Workflow

Key Issues:

(1) Most analysts do these activities formally/informally.

(2) Amount of formal V&V needed is driven by customer needs.



Iterations, missing/incomplete activities likely; Currently not an automated workflow

Evidence based application focused credibility process and communication needed

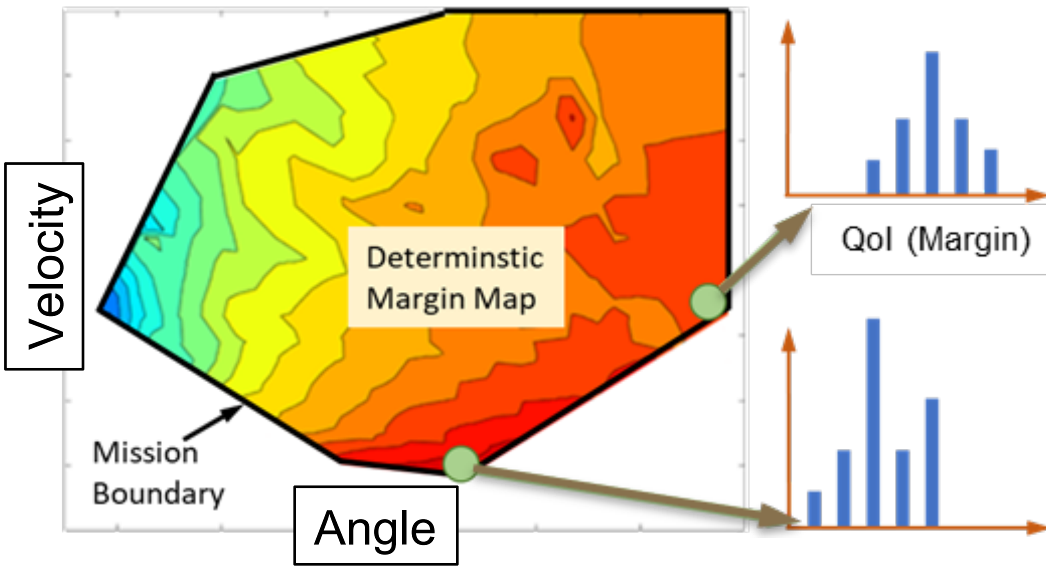
Legacy Case Study – Motivation for NGW (Next Generation Workflow) Platform Development

Solid Mechanics ModSim supporting System Qualification - **computationally intensive nested workflows** that stress computational infrastructure

- 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:

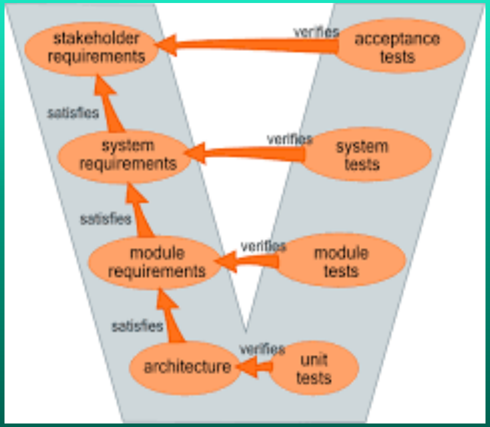
- 3-4 times faster
- With increased credibility

	Model Development	Analysis Workflow	Sensitivity, Uncertainty, Margins
Current	2.5 years (meshing, attribution)	1 year (fragile, unreviewable)	0.5 year
Future	0.5 years	0.1 year (robust, graphically expressive)	0.5 year

Difficult problem with intrinsic V&V and real program needs – Required significant competence overhead beyond engineering analysis; NOT DONE ROUTINELY

CF - Credibility Framework and the CompSim Ecosystem

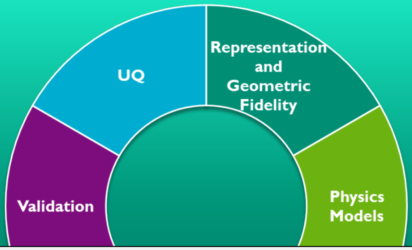
Requirements



PIRT

Math. Model Formulation	Code Implementation
H	H
H	H
M	H
H	H
H	H
M	H
L	H
L	N
M	H
H	N/A
H	H
L	M

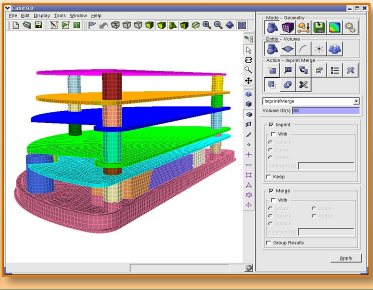
PCMM/Risks

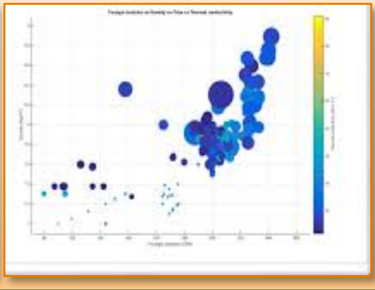


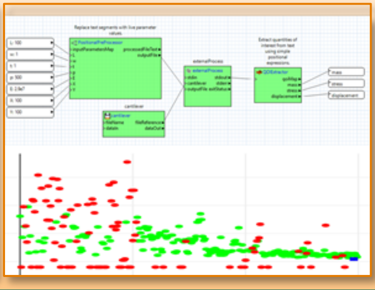
Risk Assessment Matrix					
		Consequence			
		High	Medium	Low	N/A
Probability	High				
	Medium				
	Low				
Completed					

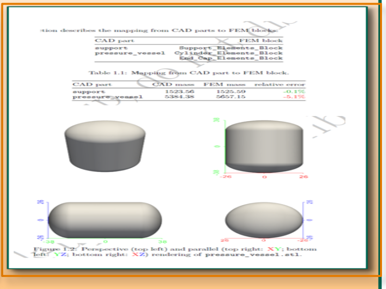
Reviews

Simulation Data Management	CAD and Model Building	Materials (Granta)	Ensemble Workflows	Report Generation









Aspirational effort to answer: Why should the customer believe predictions? What is the risk of making decisions based on CompSim?

CompSim (Computational Simulation) Models and Credibility

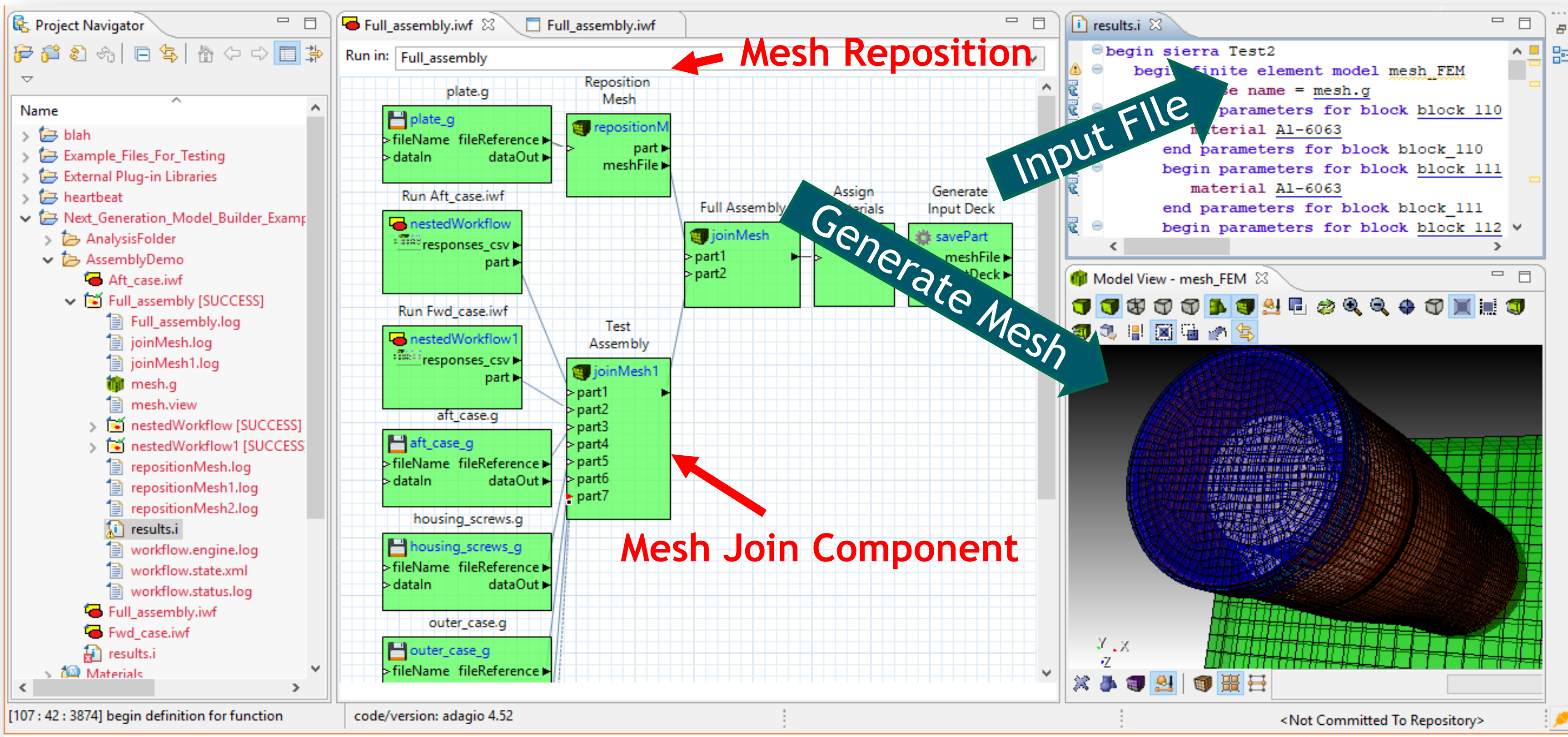
Enabling Capabilities

Credible Design through Analysis Exemplar

Summary

FEM Model Building and Assembly as Workflow

- Mesh assembly (legacy): mesh parts separately, assemble later
  - Advantages: simplifies hex meshing, enables team collaboration
  - Disadvantages: mesh overlap uncontrollable, significant experience required for hex meshing, difficult for complex geometry, mesh refinement to geometry requires planning; “dumb unrefinable meshes”
- Direct geometry meshing with tet elements (emerging)
  - Advantages: fast turnaround, design intent driven abstractions/simplifications, refinement to geometry
  - Disadvantages: not all disciplines have credible tets, large model sizes, custom mesh patterns difficult



Workflow Definition and Execution Functional Requirements

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

Must be **intuitive** and graphical
- Training, institutional knowledge capture, **share** best practices

Must be composable to accurately express **hierarchical** workflow through nesting
- Enables **agile model development** by multiple analysts

Must support analysis **credibility evidence**/communication and training
- **Documents** all computational steps from input parameters to responses
- Committed in repository for **archival** purposes

Must be delivered in **SAW** (Sandia Analysis Workbench) and in **open source**
- Integrated with Sandia model development tools (meshing, solution postprocessing, etc.)
- Can be **executed** by iterators (Dakota, for example)
- Available to all analysts without license burden; supporting Trilab and beyond

All CompSim activities comprising a model are repeatable, documented, efficiently communicated and executed

Credibility Framework Functional Requirements

Tailor credibility process to match consequence of the CompSim predictions

- Trade studies in design support
  - Quick turn-around, V&V trained analyst, input data starved, comparative
- CompSim based qualification
  - Significant effort, dedicated V&V budget, up-front constitutive and subsystem tests, predictive
- Configurable by non-programmers through simple spreadsheets

Be flexible to adapt to organizational differences (PCMM, TRL, etc.)

- Credibility process elements and subelements vary
- If the organization/program requires then support gap analysis through assessment
  - Acceptability of assessment while acknowledging metrics are not precise

Flexible configuration of business logic (sequencing, decision gates, etc.)

Record different states throughout the lifecycle of the program

Support queries to identify important capability gaps

Integration with diverse data sources (SPDM, PLM, etc.) used for storing evidence

Auto-generating human readable credibility report distilled from vast data repositories

Open source effort aims to serve and be developed by diverse technical community

CompSim (Computational Simulation) Models and Credibility

Enabling Capabilities

Credible Design through Analysis Exemplar

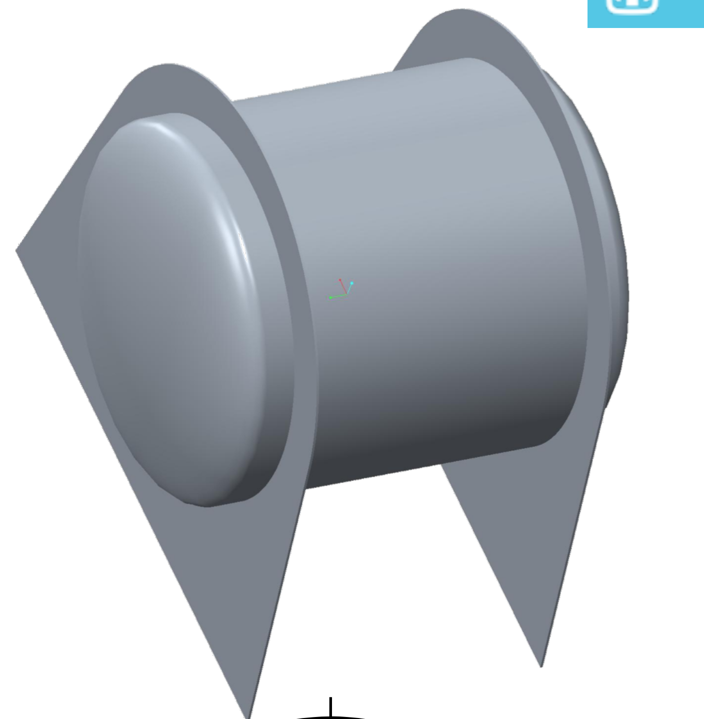
Summary

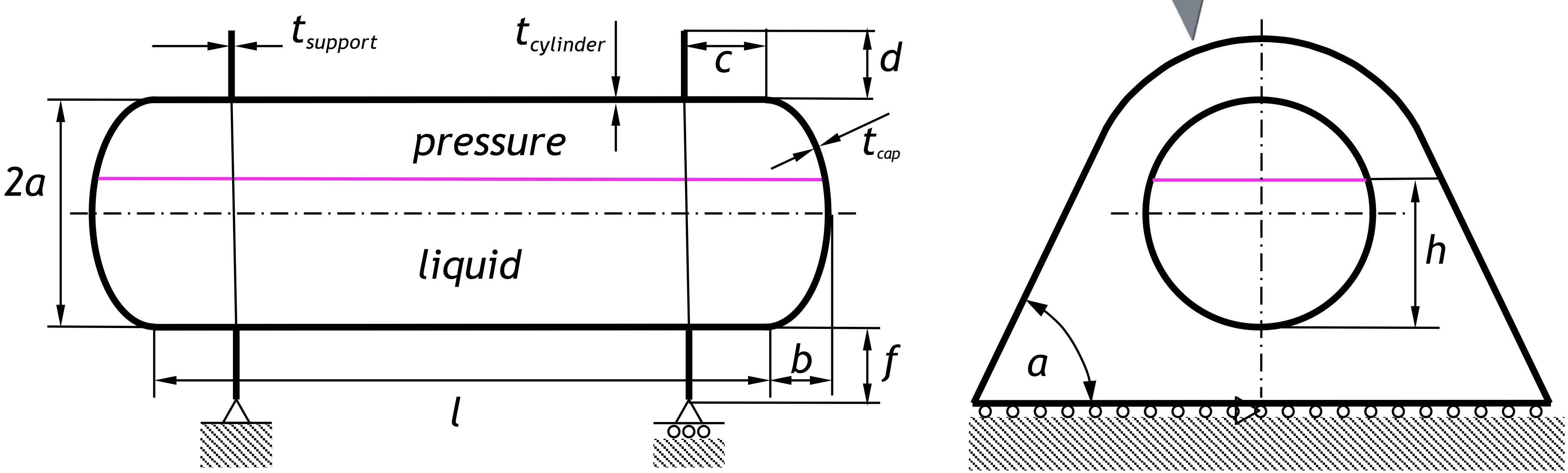
Exemplar: Tank Assembly Partially Filled with Liquid (Solid Mechanics)

Model: Creo -> Cubit -> Sierra -> Python -> ARG

General intended use of the model

- Credible design definition (*where did the design come from?*)
- Pre-test predictions (*is a test program based on model predictions going to yield useful data?*)
- QMU (*what is the probability of not meeting margin requirements?*)
- Support risk informed decision





Simple but comprehensive exemplar supports training in credible CompSim workflow

Model Parameters and Responses

Input	
Description	**Symbol**
FSY	Factor of safety on yield
max_displ	Maximum allowed sagging
t	Vessel thickness
a	Vessel radius
l	Vessel length
p	Pressure
rho	Liquid density
h	Liquid height
E	Elastic modulus
nu	Poisson's ratio
FTY	Tensile yield stress
accuracy	Model accuracy

Output, Quantities of Interest (QoIs)	
Description	**Symbol**
g_yield	Yield constraint
g_displ	Displacement constraint
struct_vol	Structural volume

Design Constraints

$$\text{g\_yield}= \frac{\frac{FTY}{FSY}-\sigma_{eff}}{\frac{FTY}{FSY}} > 0$$

$$\text{g\_displ}= \frac{\max\_displ-displ}{\max\_displ} > 0$$

Requirements conceptually defined, design space and quantitative details needed

Design Space and Requirement Definition

p	[150, 250] psi	FSY	3
rho	0.03179	max_displ	0.02 in
h_ratio	[0.5, 0.9]	vessel_t	[1, 3] in
E	30.0e6 psi	vessel_a	[25,55] in
nu	0.3	vessel_l	[40,90] in
FTY	80 e3 psi	vessel_b	[15,56] in

Intervals signify operating condition ranges or design space NOT uncertainty

PIRT, Phenomena Identification and Ranking Table

A Phenomena Identification and Ranking Table, or PIRT, provides a structured approach to identify and prioritize the important physical phenomena in an engineering application.

- Define **key physical phenomena** and rank their importance
- Importance is relative to **quantity of interest** in the application scenario
- Assess **adequacy** and **gaps** in simulation capabilities and available data
- Adequacy of capabilities is relative to **intended use**
- **Gaps** are identified when adequacy scoring is below importance ranking

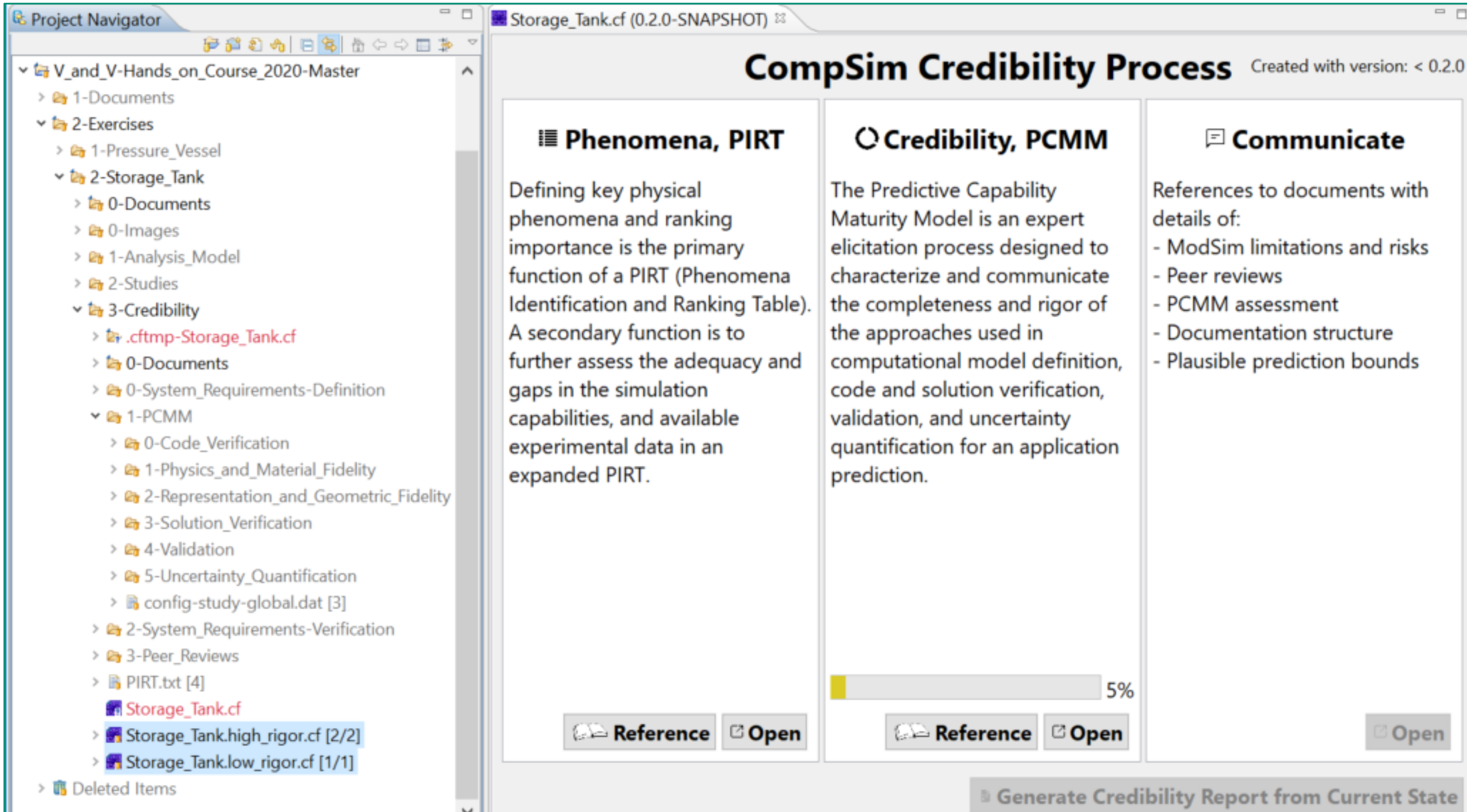
A PIRT is developed through expert judgment for a particular intended use.

- The intended use is specific to the application driver, scenario, and analysis objective

Each QoI (Quantity of Interest) has its own PIRT

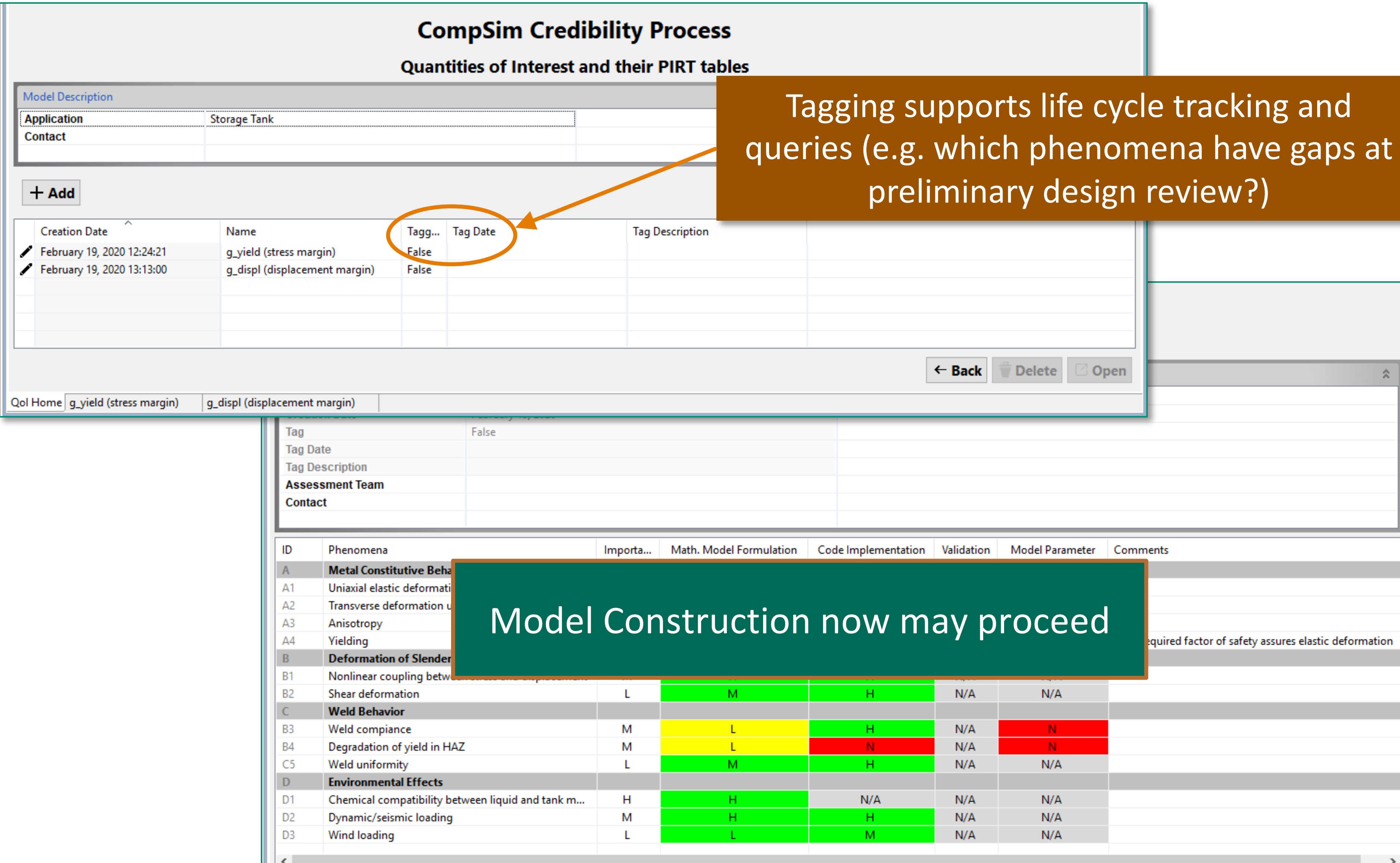
Planning and capability gap analysis tool; must precede model development

CF Opening Page



Shown docked in Sandia Analysis Workbench; also works with plain Eclipse

CF QoI Management and PIRT Tool



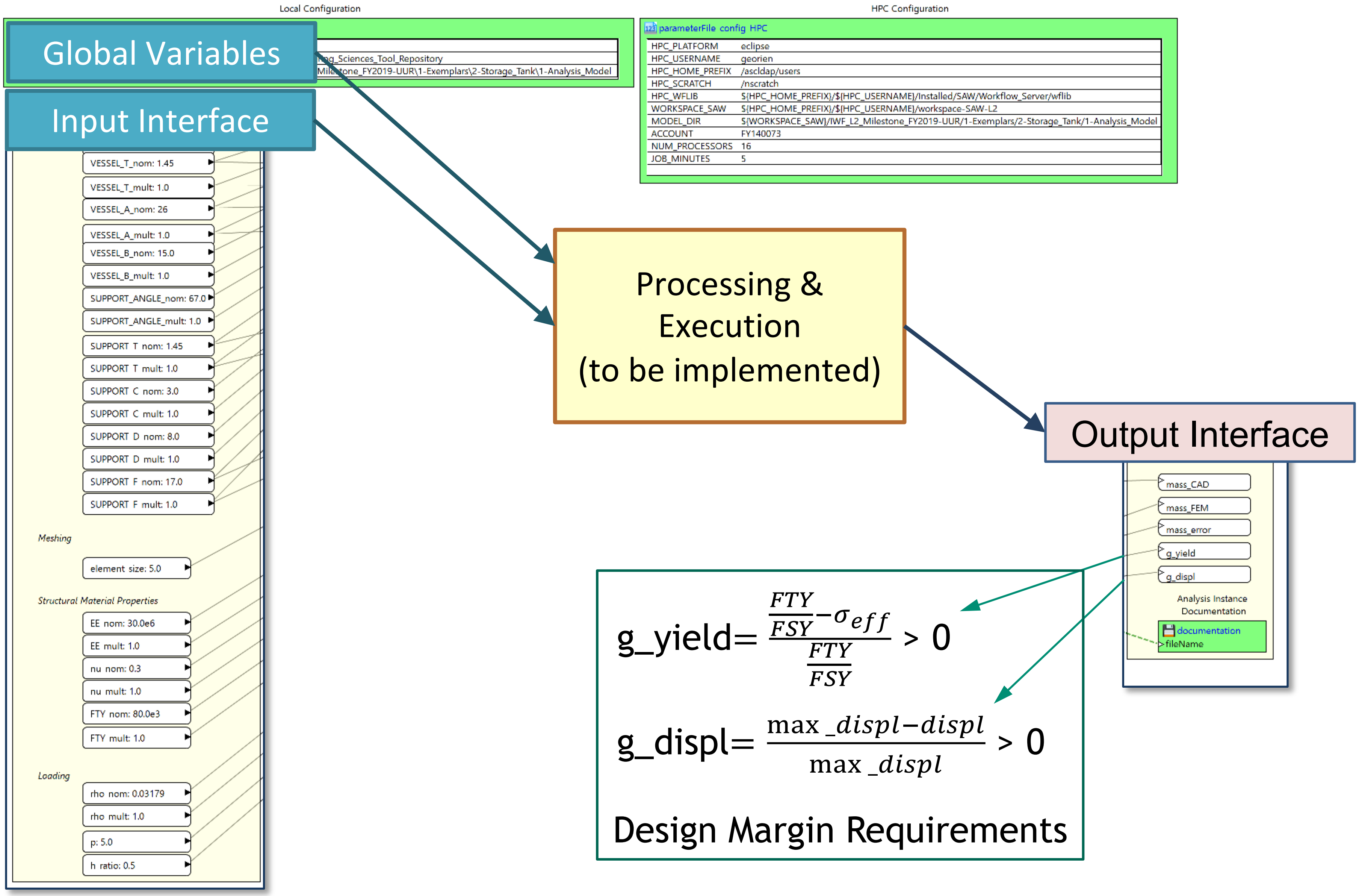
ID	Phenomena	Importa...	Math. Model Formulation	Code Implementation	Validation	Model Parameter	Comments
A	Metal Constitutive Beha						
A1	Uniaxial elastic deformati						
A2	Transverse deformation u						
A3	Anisotropy						
A4	Yielding						equired factor of safety assures elastic deformation
B	Deformation of Slender						
B1	Nonlinear coupling betw						
B2	Shear deformation	L	M	H	N/A	N/A	
C	Weld Behavior						
B3	Weld compiance	M	L	H	N/A	N	
B4	Degradation of yield in HAZ	M	L	N	N/A	N	
C5	Weld uniformity	L	M	H	N/A	N/A	
D	Environmental Effects						
D1	Chemical compatibility between liquid and tank m...	H	H	N/A	N/A	N/A	
D2	Dynamic/seismic loading	M	H	H	N/A	N/A	
D3	Wind loading	L	L	M	N/A	N/A	

Tagging supports life cycle tracking and queries (e.g. which phenomena have gaps at preliminary design review?)

Model Construction now may proceed

Application focused capability gap analysis; tracking history over project life cycle

"Contract" - Model Parameters and Responses Abstraction



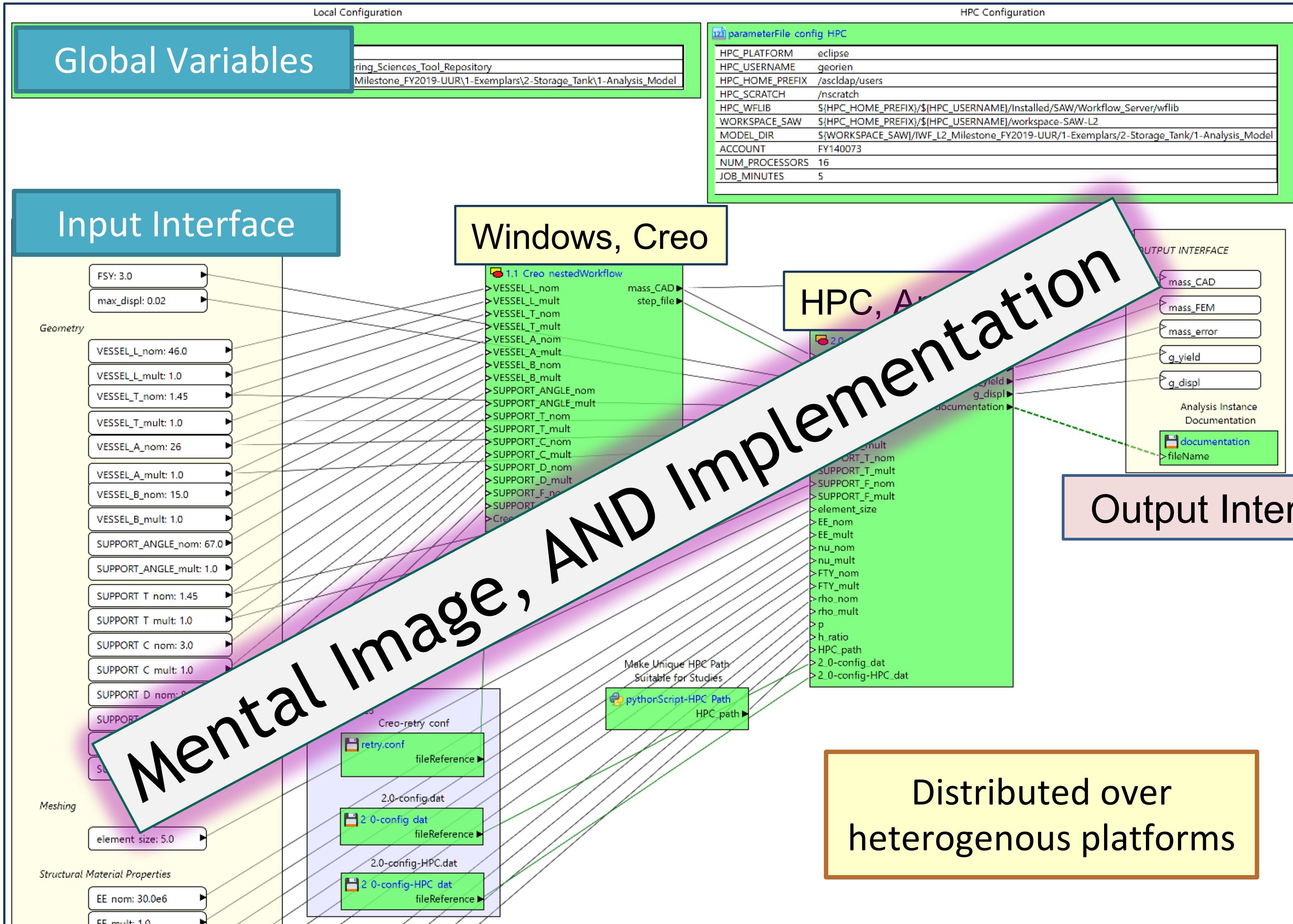
$$g\_yield = \frac{\frac{FTY}{FSY} - \sigma_{eff}}{\frac{FTY}{FSY}} > 0$$

$$g\_displ = \frac{\max\_displ - displ}{\max\_displ} > 0$$

Design Margin Requirements

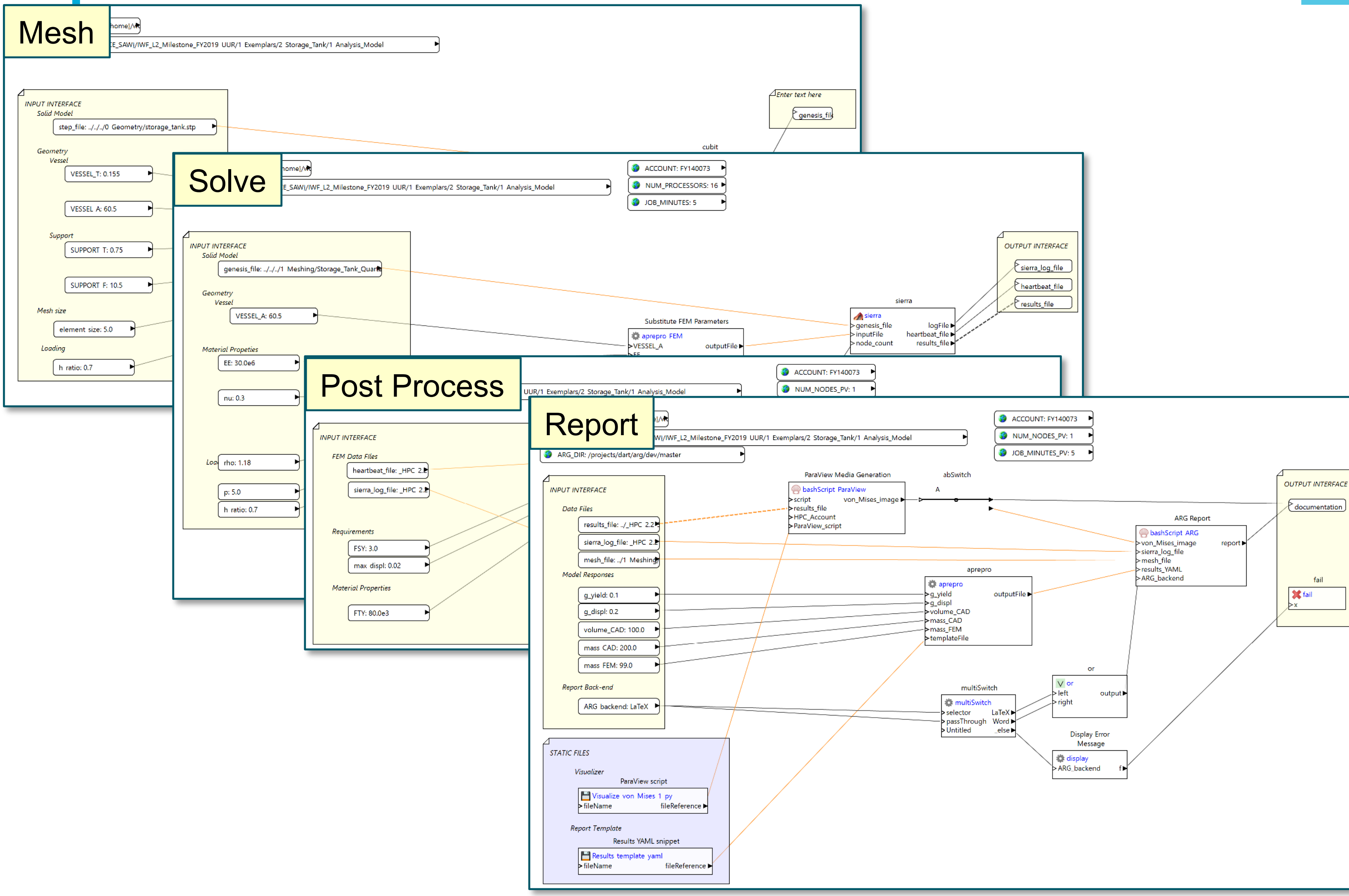
Customer and CompSim team negotiate data interface - communication

"Dashboard" Workflow - Top Level View of the Model



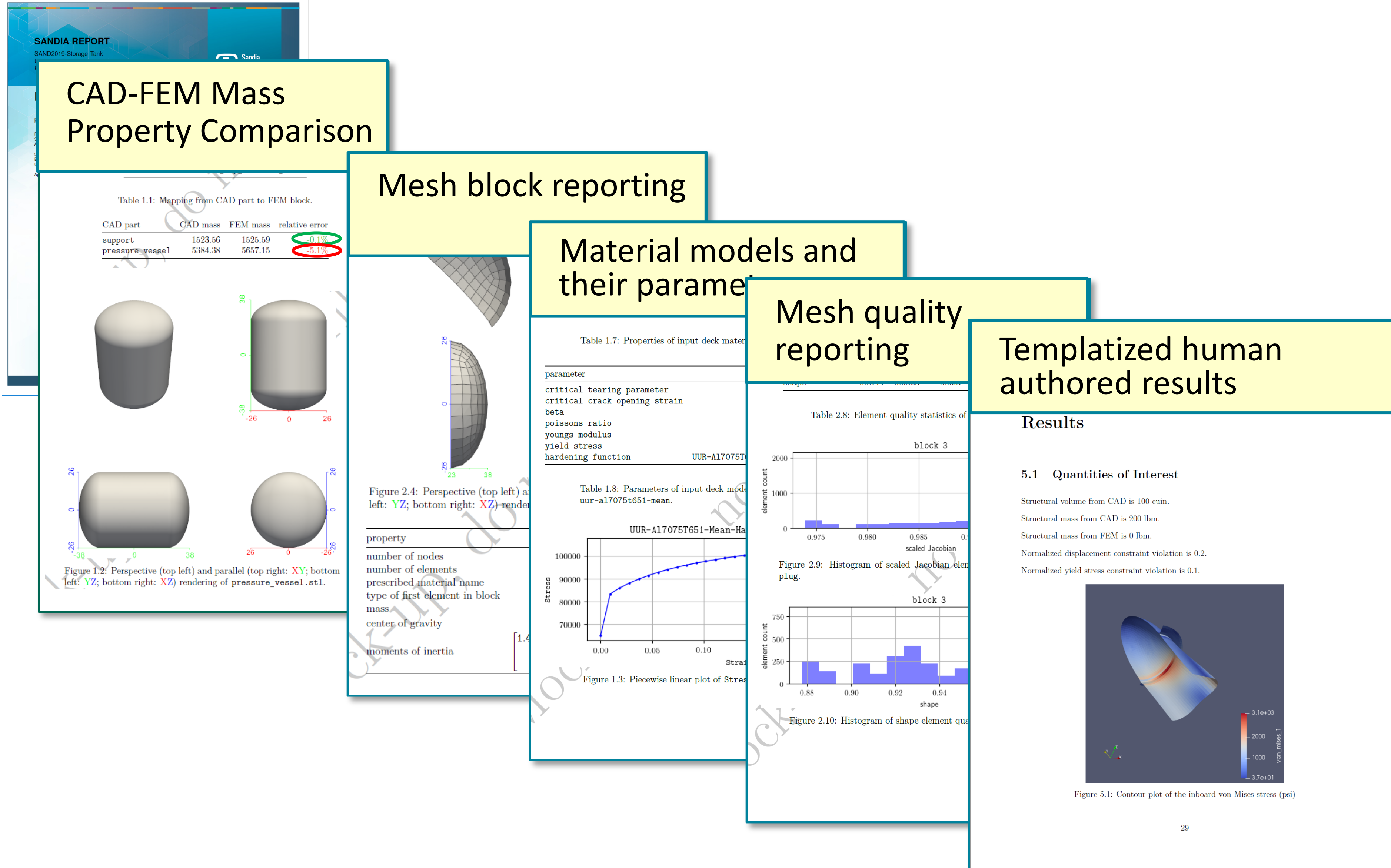
Model architecture - executable, repeatable; THE WORKFLOW IS THE MODEL

"Worker" Workflows Implement Details on HPC



Atomic activities; developed in parallel if data interfaces defined a priori - agility

ARG - Automatic Report Generation: Current Status



Agile and credible documentation process - always in sync with model instance

PCMM – A Quality Process for CompSim

The Predictive Capability Maturity Model (PCMM) is a multi-dimensional qualitative metric to facilitate discussion and communication of credibility evidence

- Primary purposes:
  - Determine readiness of modeling capabilities and simulation products for use in various applications and decisions (e.g., design, environment specification, qualification)
  - Identify gaps in the current credibility evidence for an application and prioritize additional activities
  - Measure progress of an integrated simulation effort over the lifetime of an analysis

- PCMM components:
  - Elements – the dimensions of the credibility evidence
  - Maturity levels – a relative measure of the state of the evidence and level of effort around each element
  - Element criteria – major features of the evidence to consider for each element
  - Roles – who provided evidence and/or assessments? Customer, code developer, analyst, experimentalist, etc.

PCMM Elements

CVER

Code Verification

Analysis code reproduces closed-form results

PMMF

Physics and Material Model Fidelity

Are “closure models” (constitutive etc.) credible?

E. g. MLEP (Multi-Linear Elastic-Plastic) WHY? Model form error?

RGF

Representation and Geometric Fidelity

Is the geometric abstraction acceptable?

SVER

Solution Verification

Code solves the equations for the intended use correctly?

Challenge: Often unsettling when modeling highly nonlinear, chaotic mechanical systems

UQ

Uncertainty Quantification

What is the effect of input uncertainties on QoIs?

- Uncertainty inventory and characterization of input uncertainties
- Formal UQ; propagate characterized uncertainties through the model
- Experimental uncertainty

VAL

Validation

Validation hierarchy

How well do model predictions match experimental data?

CompSim Model Ensemble Plan

SVER

Solution Verification - Estimate numerical error with respect to element size

- *Comparative model:* in asymptotic region but reduced accuracy for optimization (faster solution)
- *Predictive model*: Most accurate refinement practical to run for UQ; numerical error estimated
- Credible numerical controls for different CompSim goals

Design Optimization - Minimum weight configuration subject to design constraints

- Under all operating conditions
- Reduced accuracy model used (*comparative*)

SVER

Deterministic Sensitivity - Perturbing each variable by a fixed amount; response trend analysis; variable sensitivity ranking

UQ

Uncertainty Informed Sensitivity - Perturbations tied to characterized uncertainties; variable importance ranking

UQ

Latin Hypercube Sampling - Response histograms, statistical moments, correlation analysis

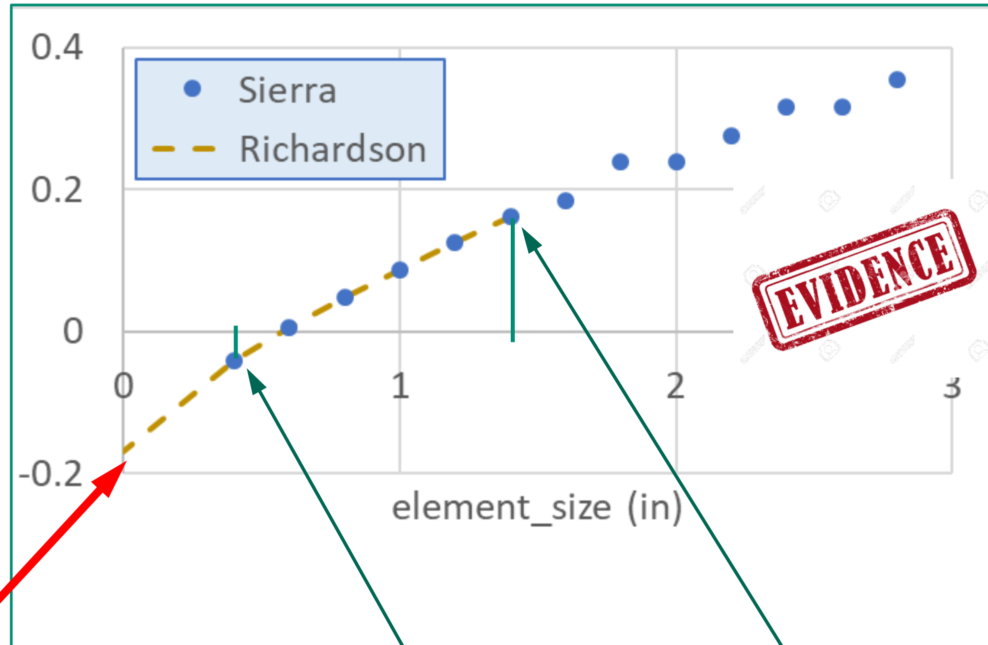
UQ

Quantification of Margins and Uncertainties – UQ for quantifying probability of rare events (margin violation)

Rapid studies, visual results support agile design and credible margin definition

Dakota Visual Results – Solution Verification, Stress Margin

What level of mesh refinement is appropriate?
What is the estimated numerical error?



Extrapolated margin at zero element size infeasible

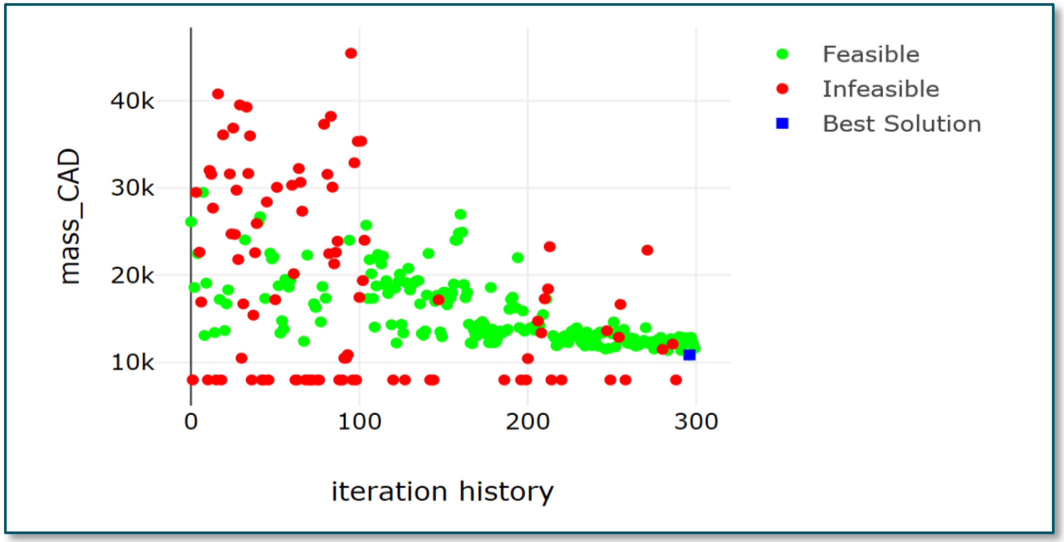
For prediction

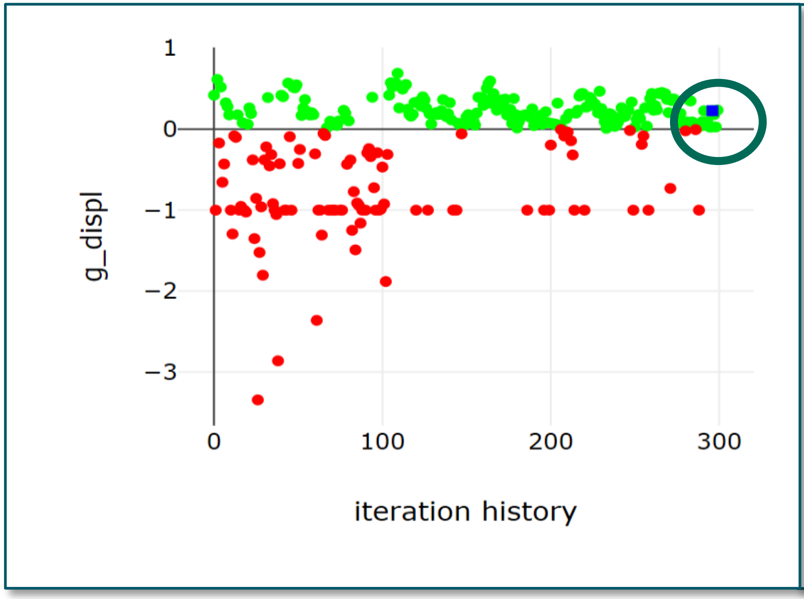
For scoping

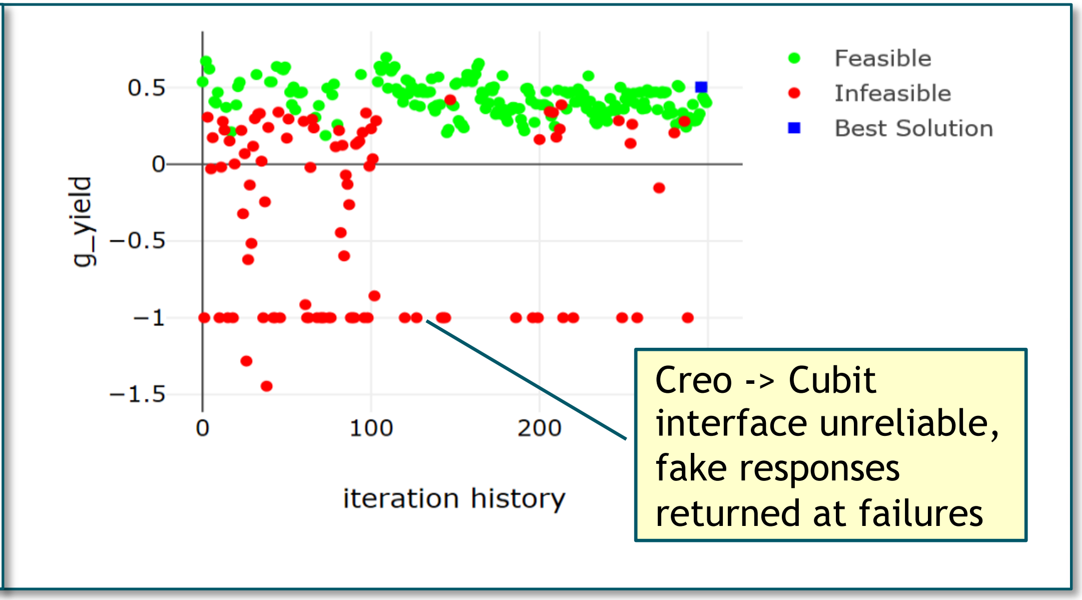
Different convergence behavior is likely at different loads/environments

Dakota Visual Results - Design Optimization

What is the lightest design that meets system requirements?





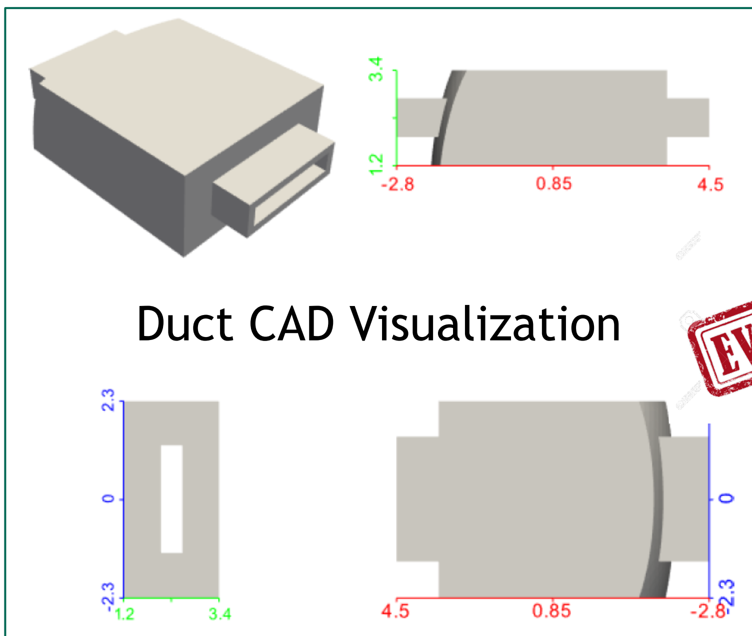


Best point at boundary of infeasibility of displacement constraint; implications for UQ

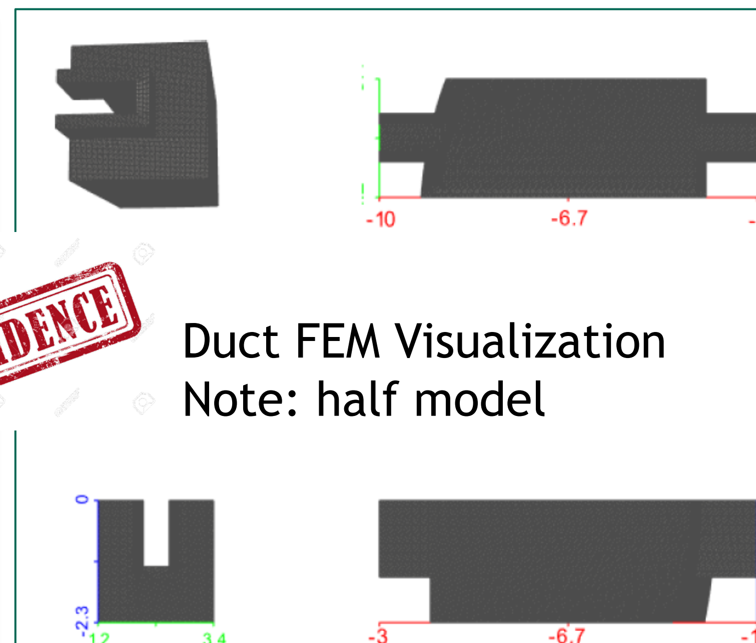
Geometric Fidelity Reported by ARG

CAD part	CAD mass	FEM mass	relative error
case	0.214743	0.214662	0.0%
crusher	4.7304	4.7304	-0.0%
plug	0.00789768	0.0078704	0.3%
lid	0.00105092	0.00105082	0.0%
target	4.7304	4.7304	-0.0%
post	0.000850239	0.000912318	-7.3%
weld	0.000341763	0.000341685	0.0%
foam	0.0217941	0.0217518	0.2%
box_shell	0.01194	0.0105475	11.7%
duct	0.0134568	0.0134448	0.1%

Is geometry captured sufficiently for intended purpose?



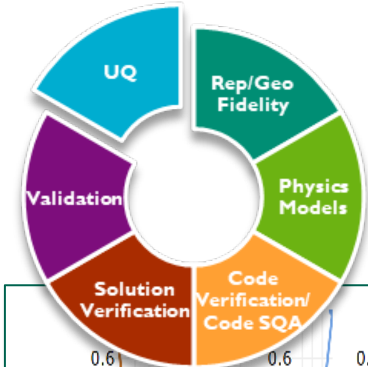
Duct CAD Visualization

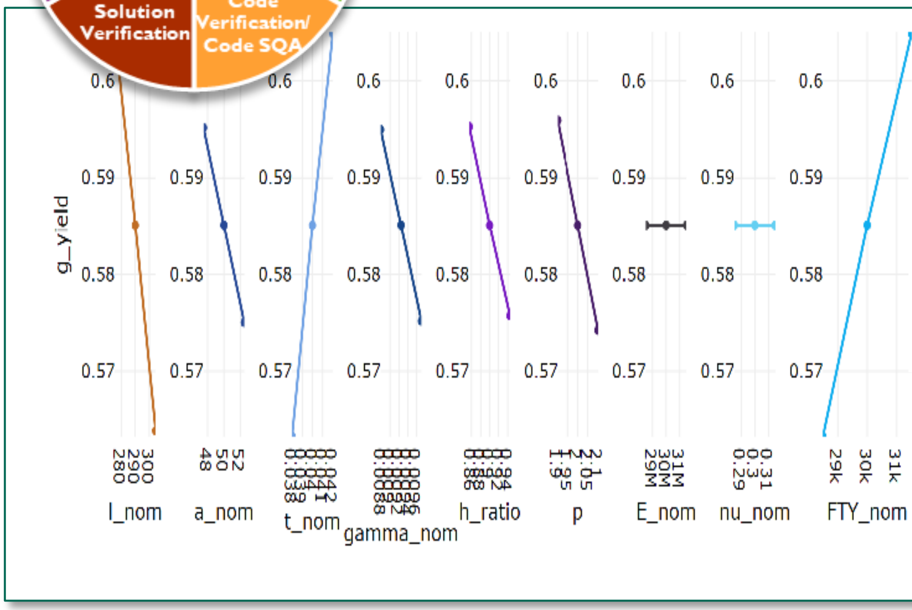


Duct FEM Visualization
Note: half model

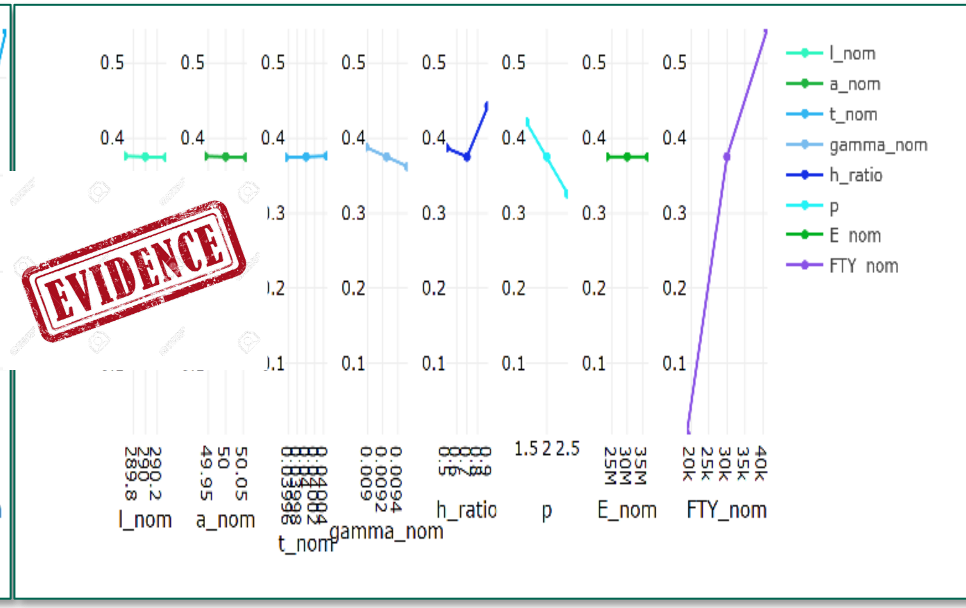
Dakota Visual Results - Sensitivity Analysis

Which variables are the most sensitive and most important?
Do predicted trends make sense?





Local deterministic sensitivity



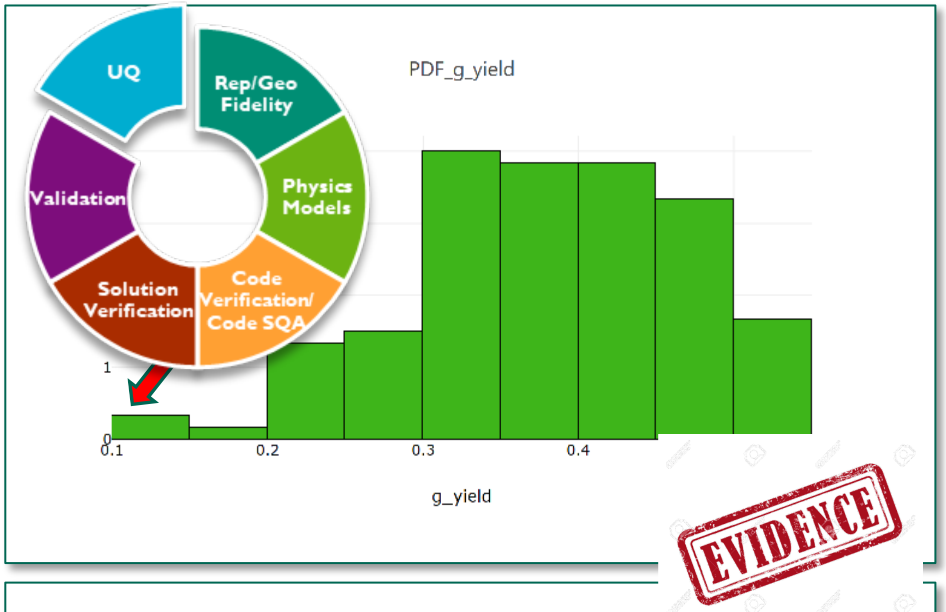
Local uncertainty informed sensitivity

Most ***sensitive*** variables: geometry, material yield stress (aleatory)

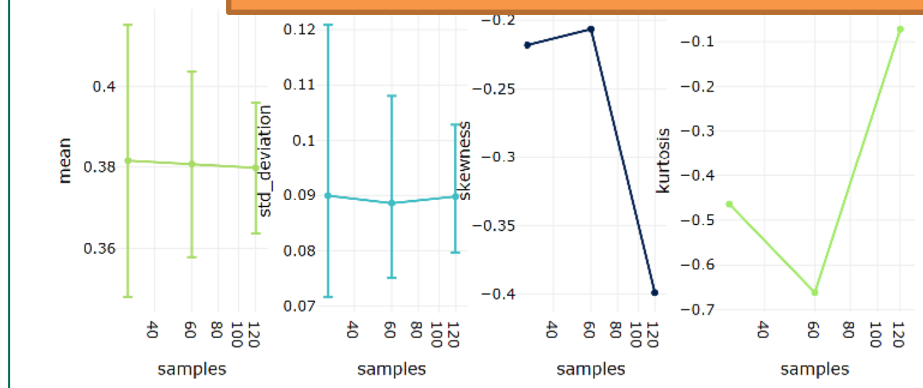
Most ***important*** variables: material yield stress (aleatory), loading (epistemic); how full is the vessel

Sensitive variables - "design tuning"; important variables - fabrication, operations

Dakota Visual Results - UQ, LHS Sampling



Do we have sufficient margins under uncertainty?



PartialRankCorrelation

	l unc	a unc	t unc	E unc	FTY unc	h ratio	gamma unc	p
g displ	-0.079	0.011	-0.014	0.604	0.169	0.904	-0.278	-0.025
g yield	-0.113	-0.003	0.043	0.112	0.978	0.67	-0.338	-0.861

- There is a concern about violating yield constraint
- Higher statistical moments not yet converged
- Correlation structure confirms uncertainty informed sensitivity analysis conclusions

Program decision alternatives

- Live with plausible negative margin
- Quantify p(margin<0)
- Negotiate criteria
- Tune design; deterministic sensitivities on controllable variables

Basis for credible risk informed decision - program agility through CompSim workflow

CF PCMM Configuration by Non-Programmers

Excel spreadsheets familiar to V&V practitioners

	Element
CVER	Code Verification
PMMF	Physics and Material Model Fidelity
RGF	Representation and Geometric Fidelity
SVER	Solution Verification
VAL	Validation
UQ	Uncertainty Quantification (UQ)

Solution Verification (SVER)		Return to Elements
	Descriptor	Outcome
Low	Have an SQE process in place, discuss bugs/errors	Memo documenting/referencing the SQE process
Medium	Test feature Coverage	FCT report
High	Coordinate with code team on known deficiencies and status	Document/release notes with deficiency information

Levels	
Low	
Medium	
High	

Activities
Evidence

Roles
Customer
System Engineer
Analyst
Experimentalist

Low Rigor

	Element/Subelement
CVER	Code Verification
CVER1	Apply Software Quality Engineering (SQE) processes
CVER2	Provide test coverage information
CVER3	Identification of code or algorithm attributes, deficiencies and errors
CVER4	Verify compliance to Software Quality Engineering (SQE) processes
CVER5	Technical review of code verification activities
PMMF	Physics and Material Model Fidelity
PMMF1	Characterize completeness versus the PIRT
PMMF2	Quantify model accuracy (i.e., separate effects model validation)
PMMF3	Assess interpolation vs. extrapolation of physics and material model

Solution Verification (SVER)		
SVER1: Quantify numerical solution errors		Descriptor
SVER1	Level 0	Errors due to mesh size not examined
SVER1	Level 1	Sensitivity, or robustness, of one or more computed quantities of (QoI) to mesh resolution and numerical solution parameters is stu and presented. Quantification as a computational "error" is not re or expected. Conclusions may be qualitative.
		Computational errors, due to mesh resolution and choice of nume

Levels	
Level 0	
Level 1	
Level 2	
Level 3	

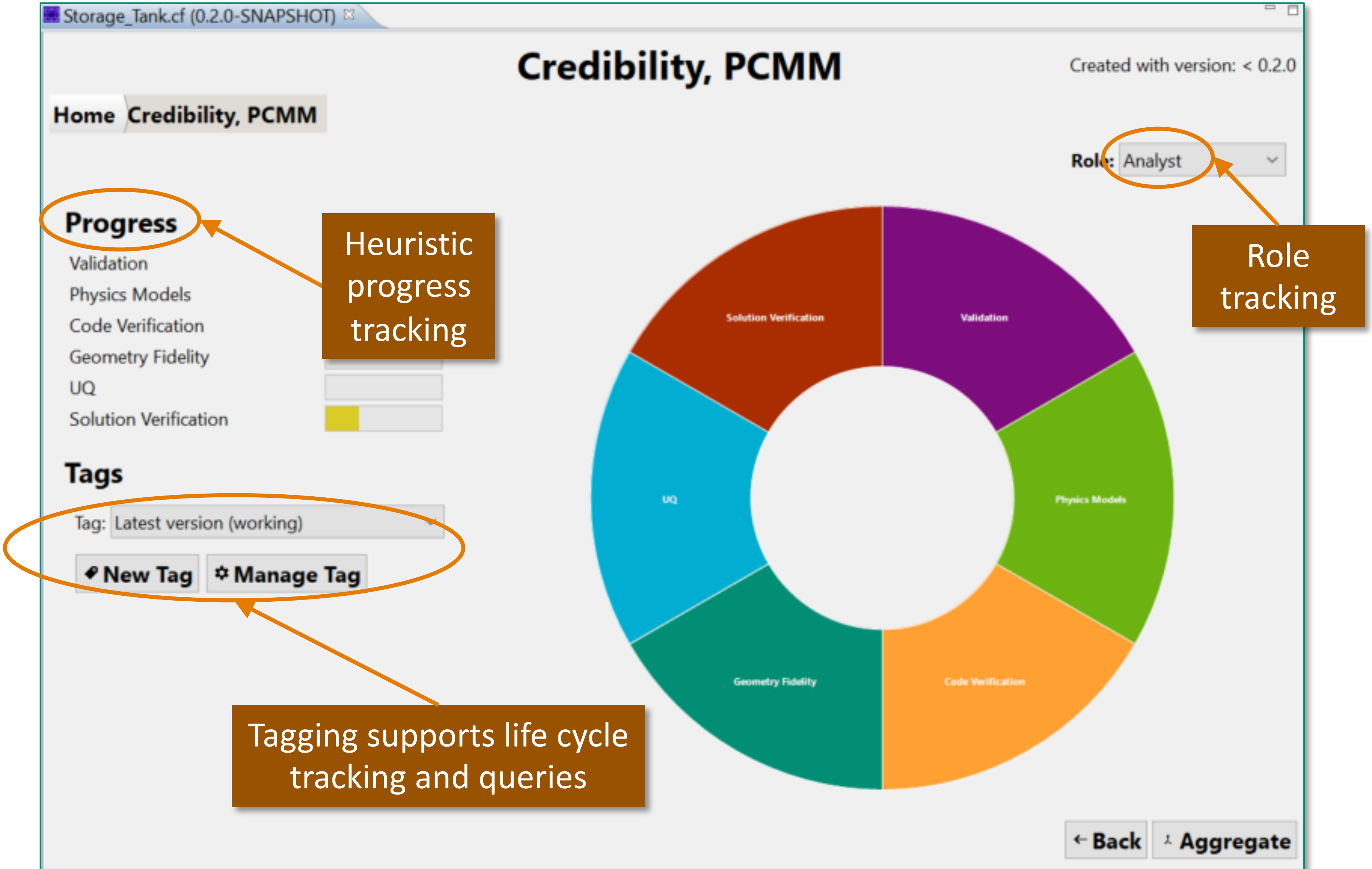
Activities
Evidence
Assess
Aggregate
Stamp

Roles
Customer
System Engineer
Analyst
Code Developer
Experimentalist
V&V Partner

High Rigor

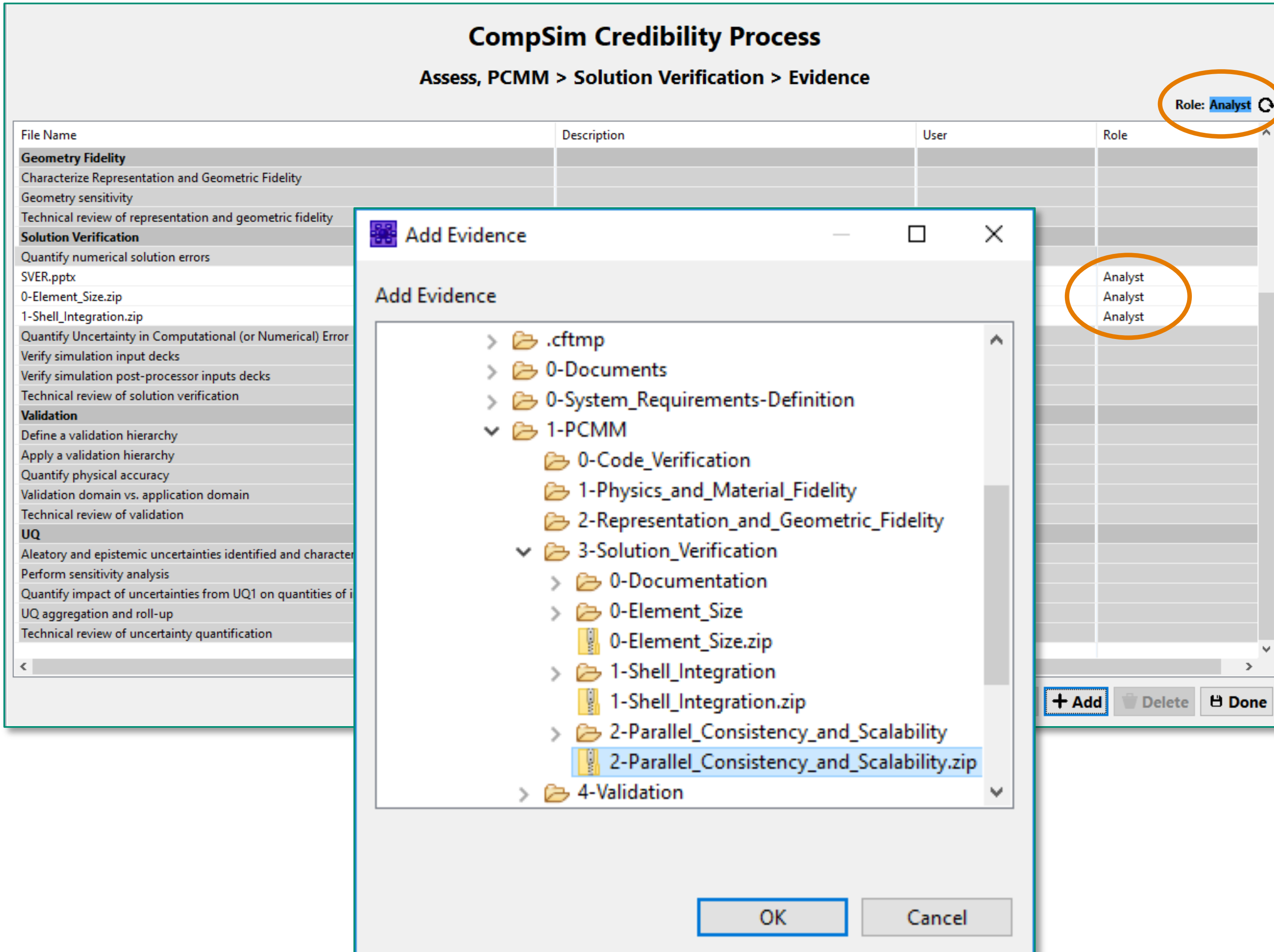
Agile adaptivity to organizational requirements

CF PCMM Tool



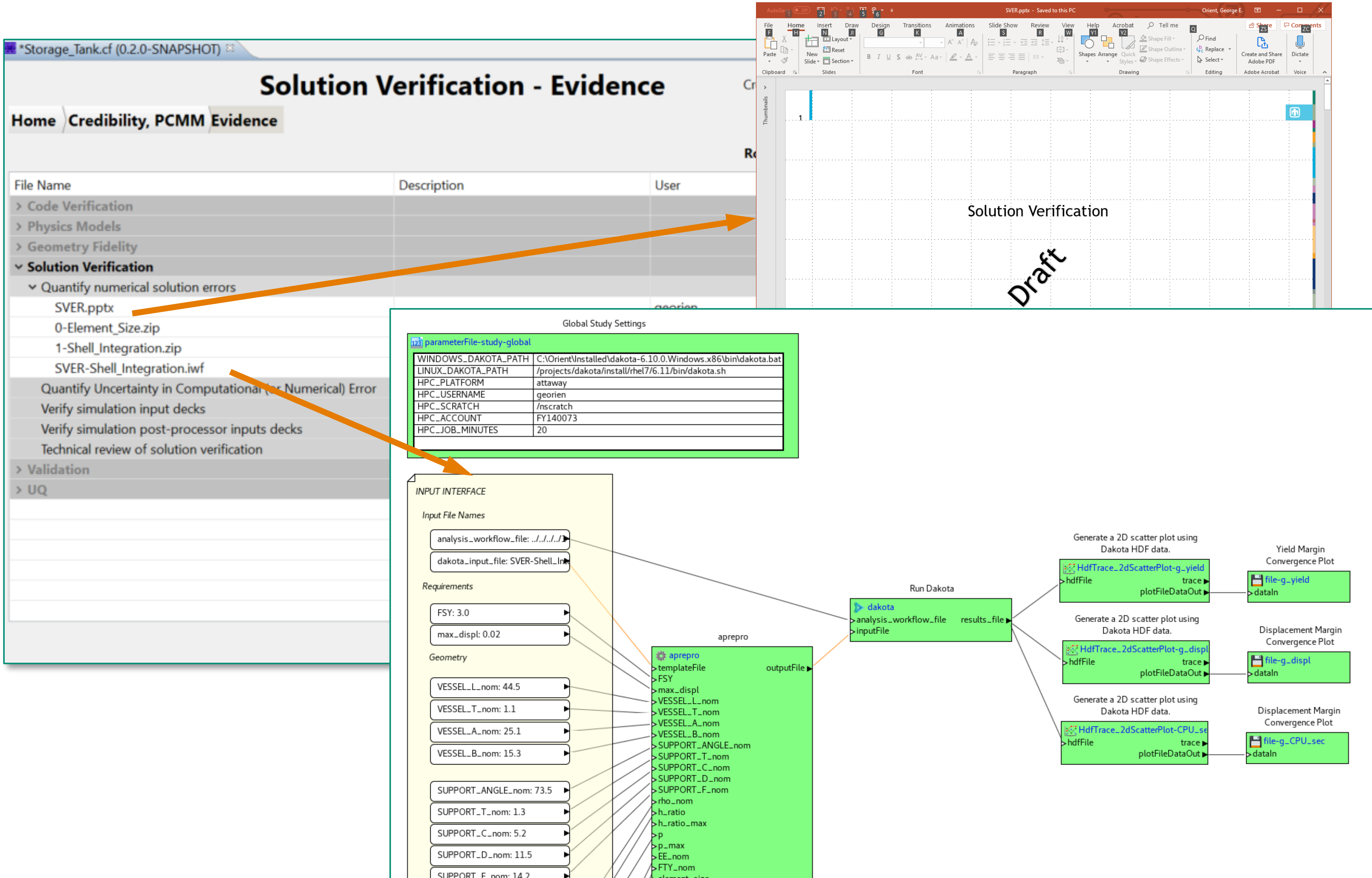
Progress and role of the actor are recorded

CF PCMM Tool – Adding Evidence



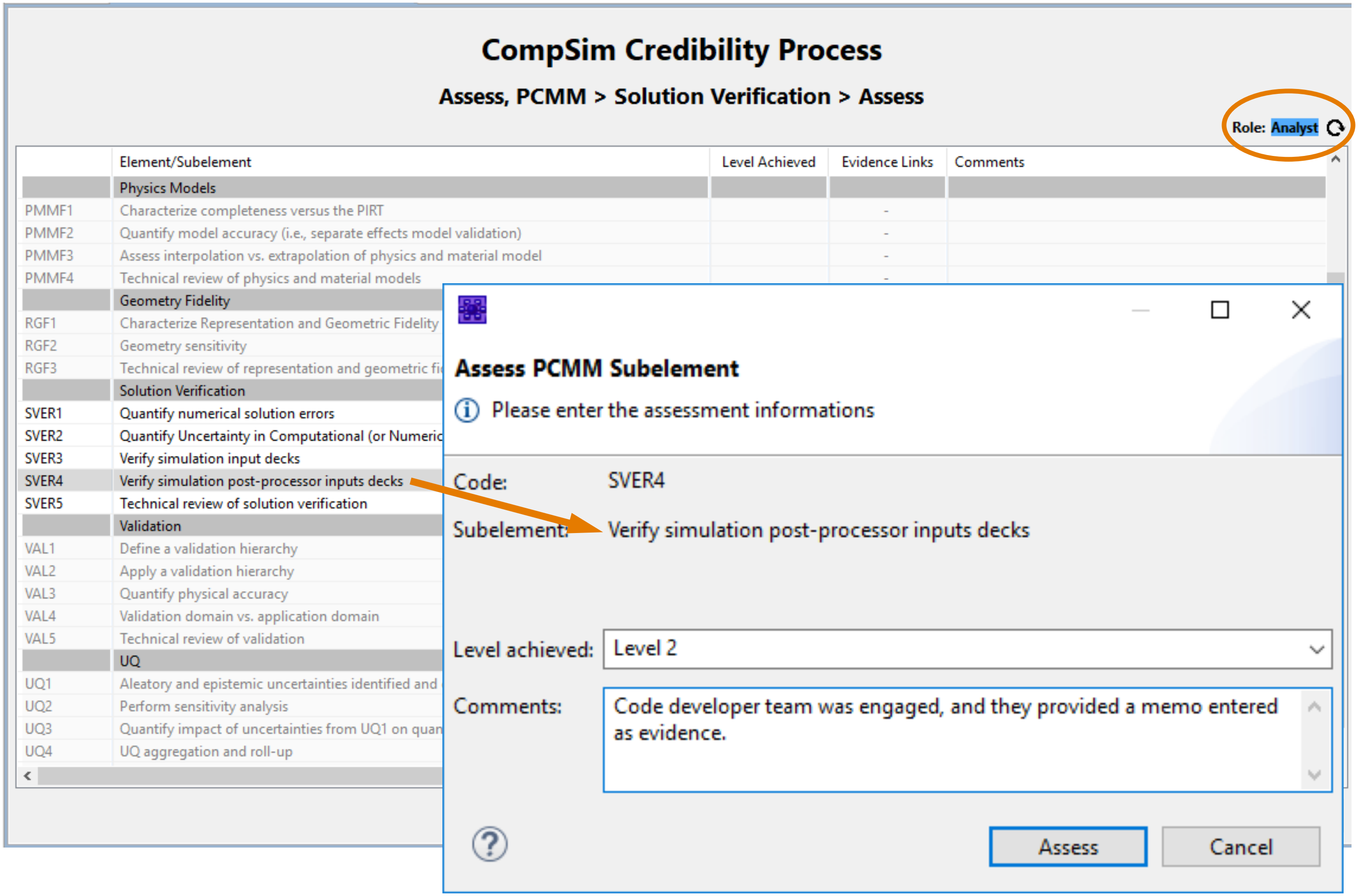
Recommended folder structure contains artifacts employed as evidence generated

CF PCMM Tool – Examining Evidence



Evidence is opened with associated editor

CF PCMM Tool – Assess (Optional)



Role is associated with assessment

CF PCMM Tool – Aggregate (If Assessment Done)

CompSim Credibility Process

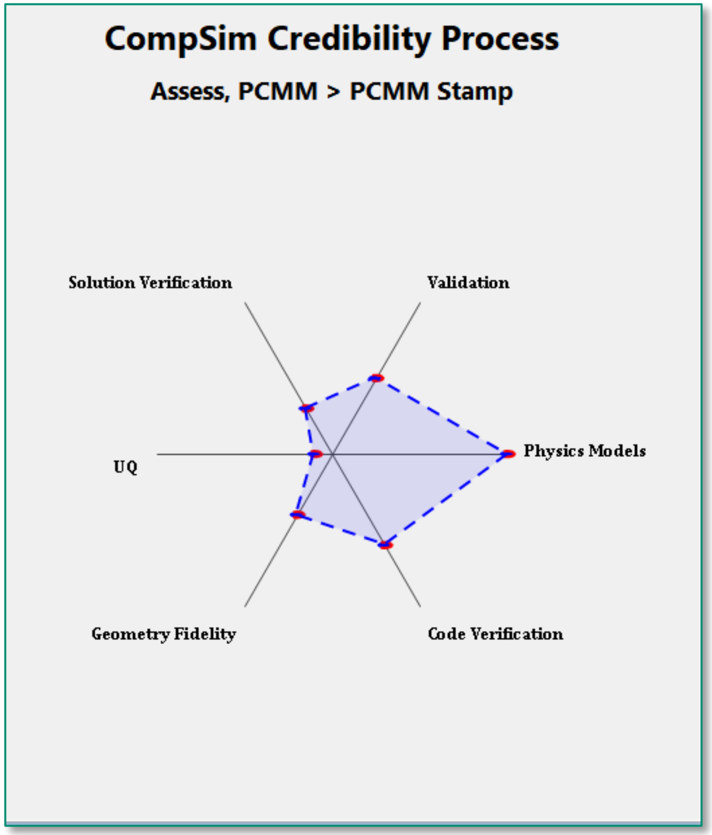
Assess, PCMM > Aggregate

Role: VV Partner

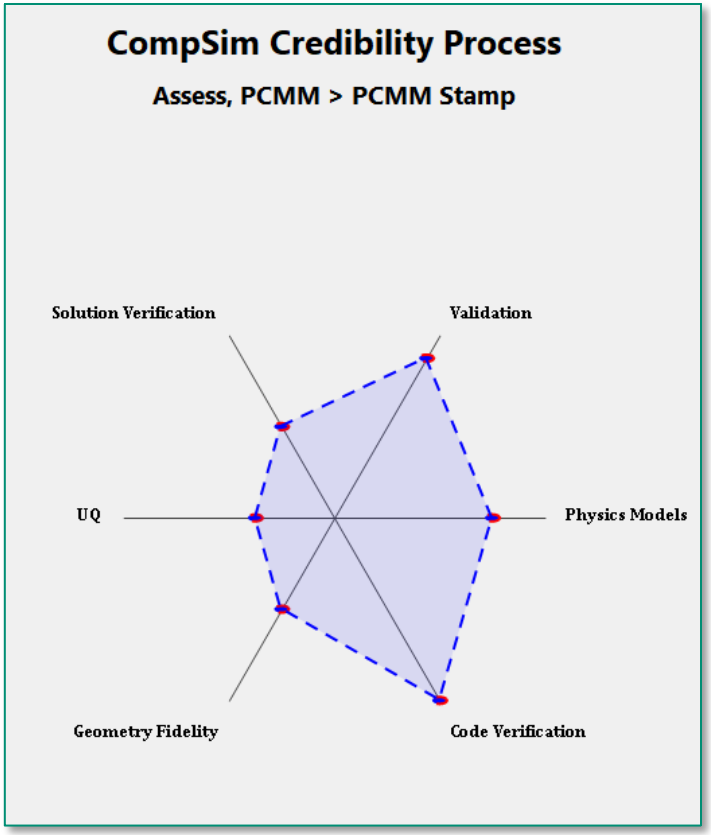
	Element/Subelement	Level Ach...	Evidence ...	Comments
	Code Verification	Level 1		
CVER1	Apply Software Quality Engineering (SQE) processes	Level 0	1 Evidence	
CVER2	Provide test coverage information	Level 1	1 Evidence	
CVER3	Identification of code or algorithm attributes, deficiencies and errors	Level 2	1 Evidence	
CVER4	Verify compliance to Software Quality Engineering (SQE) processes	Level 0	-	
CVER5	Technical_review of code verification activities	Level 0	-	
	Physics and Material Model Fidelity	Level 1		
PMMF1	Characterize completeness versus the PIRT	Level 2	1 Evidence	
PMMF2	Quantify model accuracy (i.e., separate effects model validation)	Level 1	-	
PMMF3	Assess interpolation vs. extrapolation of physics and material model	Level 0	-	
PMMF4	Technical review of physics and material models	Level 0	-	
	Representation and Geometric Fidelity	Level 1		
RGF1	Characterize Representation and Geometric Fidelity	Level 2	1 Evidence	
RGF2	Geometry sensitivity	Level 0	-	
RGF3	Technical review of representation and geometric fidelity	Level 0	-	
	Solution Verification	Level 2		
SVER1	Quantify numerical solution errors	Level 2	1 Evidence	
SVER2	Quantify Uncertainty in Computational (or Numerical) Error	Level 2	-	
SVER3	Verify simulation input decks	Level 2	-	
SVER4	Verify simulation post-processor inputs decks	Level 2	-	
SVER5	Technical review of solution verification	Level 0	-	
	Validation	Level 0		
VAL1	Define a validation hierarchy	Level 0	-	
VAL2	Apply a validation hierarchy	Level 0	-	
VAL3	Quantify physical accuracy	Level 0	-	
VAL4	Validation domain vs. application domain	Level 0	-	
VAL5	Technical review of validation	Level 0	-	
	Uncertainty Quantification (UQ)	Level 2		
UQ1	Aleatory and epistemic uncertainties identified and characterized.	Level 2	1 Evidence	
UQ2	Perform sensitivity analysis	Level 2	1 Evidence	
UQ3	Quantify impact of uncertainties from UQ1 on quantities of interest	Level 2	1 Evidence	
UQ4	UQ aggregation and roll-up	Level 2	1 Evidence	
UQ5	Technical review of uncertainty quantification	Level 0	-	

Average assessment of multiple respondents; consensus but retaining diversity

CF PCMM Tool – Quality Stamp (If Assessment Done)

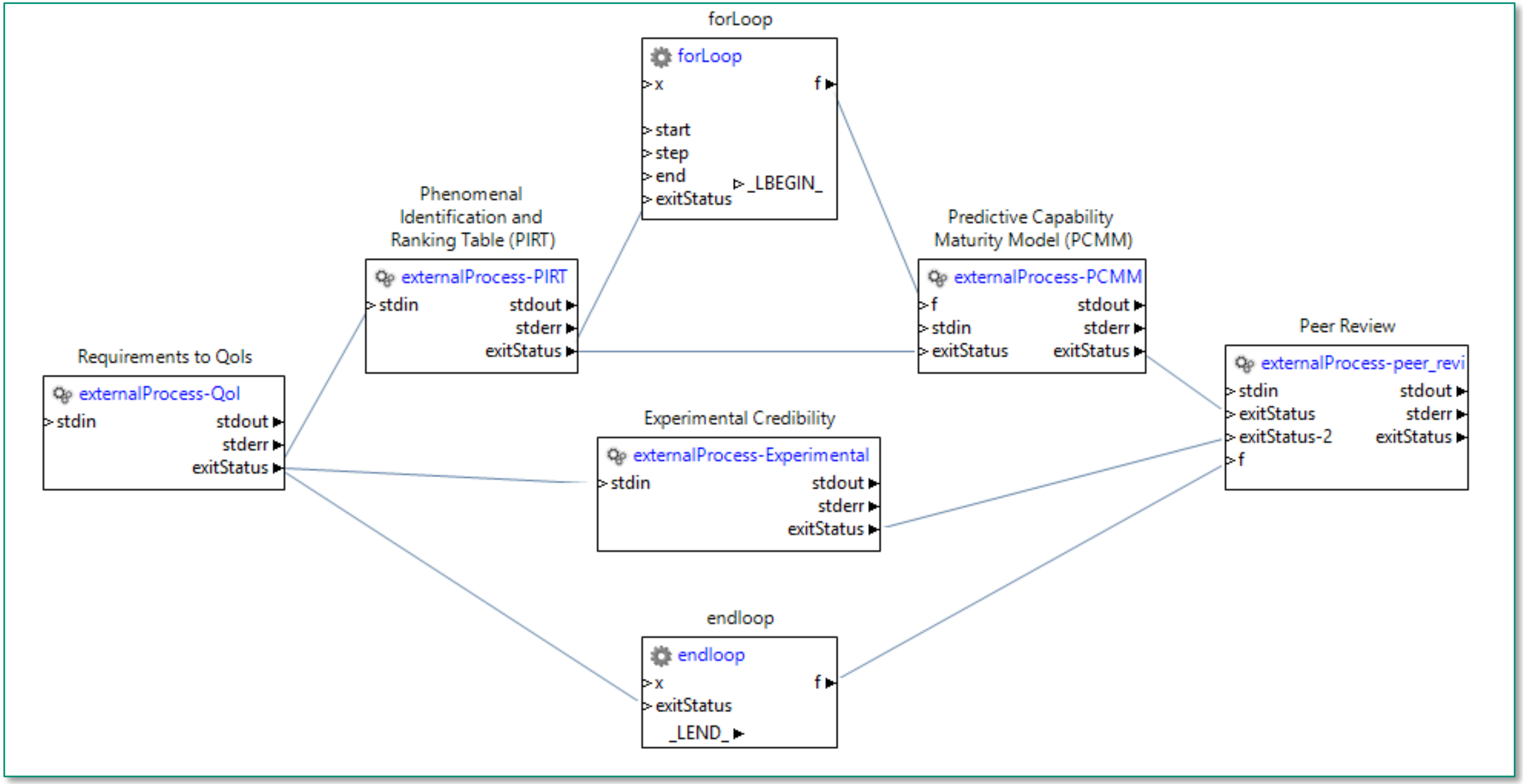


Investment



Simple visual representation of CompSim credibility evolution

Credibility Process Business Workflow in NGW



Flexible configuration mechanism leveraging NGW – Not yet implemented

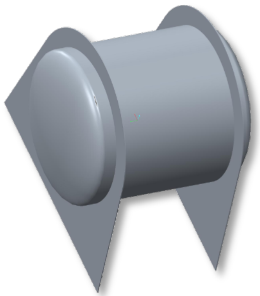
CompSim (Computational Simulation) Models and Credibility

Enabling Capabilities

Credible Design through Analysis Exemplar

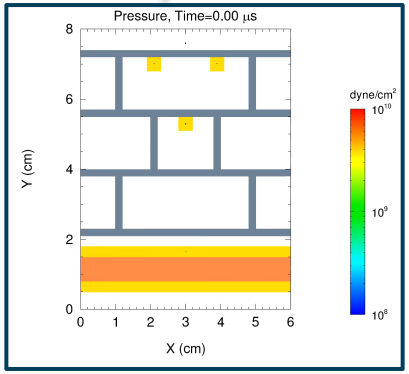
Summary

Exemplars Demonstrate Integrated Capabilities and Support Training



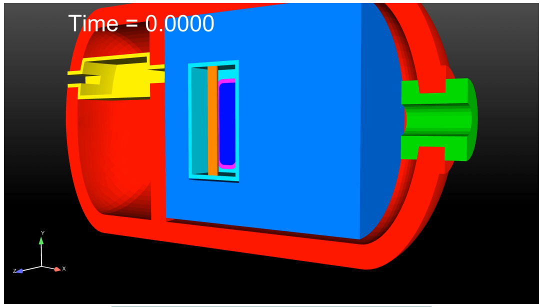
Tank assembly partially filled with liquid

- Parametric Creo (CAD) model connected to Cubit meshing and Sierra solution followed by ARG report.
- Solution verification, structural optimization, sensitivity analysis and UQ studies.



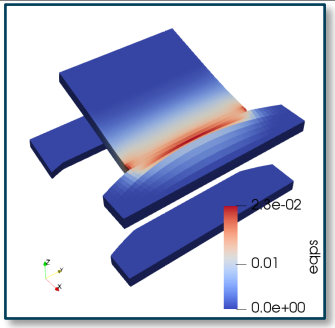
Explosion beneath a lattice structure

- CTH model illustrating generality of the framework; computationally intensive.
- Parallel consistency and scalability, sensitivity analysis and UQ studies.



Abnormal mechanical crush

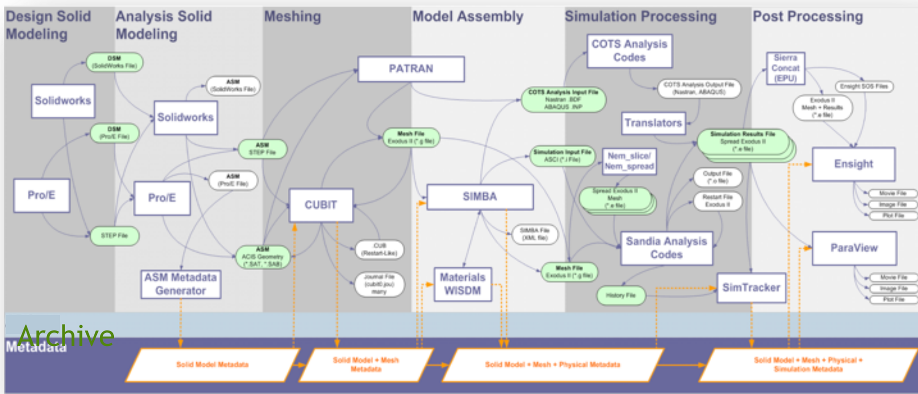
- Parametric Cubit meshing, Sierra explicit solution followed by quantitative Ensight and Python post processing summarized in an ARG report. Computationally intensive.
- Parallel consistency, scalability and mesh resolution studies.

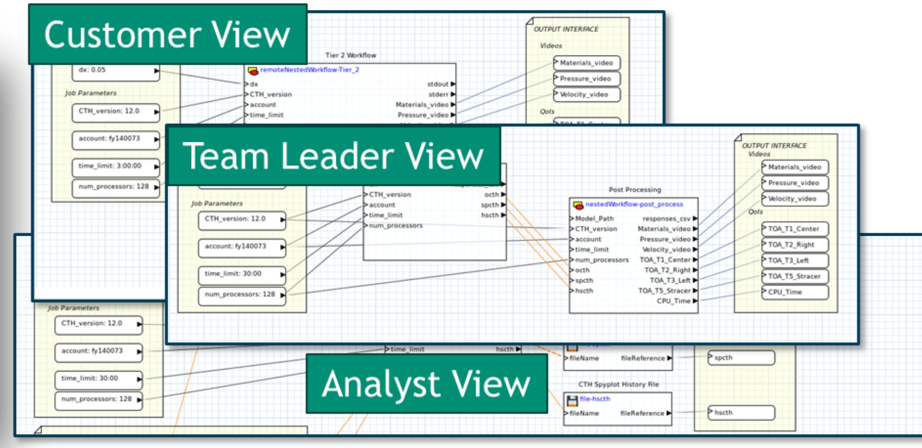


Flex cable assembly response V&V for KCNSC

- Fixed mesh, Sierra
- Parallel consistency and scalability, sensitivity analysis and UQ studies. Demonstration of agile V&V enabled by NGW and SAW.

ModSim Process – Current vs. Future States





Past Practice	Current Emerging Practice
Disconnected analysis components	Integrated analysis components
Opaque, no communication support	Clear and transparent, easy to communicate
Not reviewable	Fully reviewable by peers and customers
Lack of configuration control	Intrinsic configuration control
Specialized non-engineering expertise required	Minimal training, empowers all analysts
Effort not reusable	Reusable workflows shared
Lack of integration with other tools (CAD, Dakota)	Parametric CAD, Dakota wizard, integration with many tools
Doable but cycle time doesn't support program goals	Analysis workflow/study cycle time reduction:3-10X

Agility

Fundamental shift; agility through clear communication and high usability platform

Workflow is Foundational to Credibility and Agility

- Model development and V&V process through high usability integrated visual platform
- Credible models through ubiquitous and visually communicated sensitivity, optimization, UQ
- Graphical environment, repository of analysis workflows and individual tools enable
  - Analysis repeatability and traceability is central to credibility and V&V
  - Efficient inter-team communication and peer reviews
  - Enterprise knowledge retention and analysis governance
  - On-boarding new analyst, reduction of analyst-to-analyst variability
- Current state: management commitment and intensive training
- Plans: integrate experimental processes and data, CompSim model validation, SME judgment