SAND2020-4946C

Credibility Framework – an End-to-End Credibility Workflow Platform

George E. Orient, Robert Clay (SNL)

Didier Verstraete (NexGen Analytics)

ASME V&V 2020 Symposium

May 20-22, 2020

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Credibility Overview

Credibility Framework (CF) Requirements

CF Software Process

PIRT (Phenomena Identification and Ranking Table) Tool

PCMM (Predictive Capability Maturity Model) Tool

Summary, Current Work and Plans

Modeling and Simulation Credibility Process

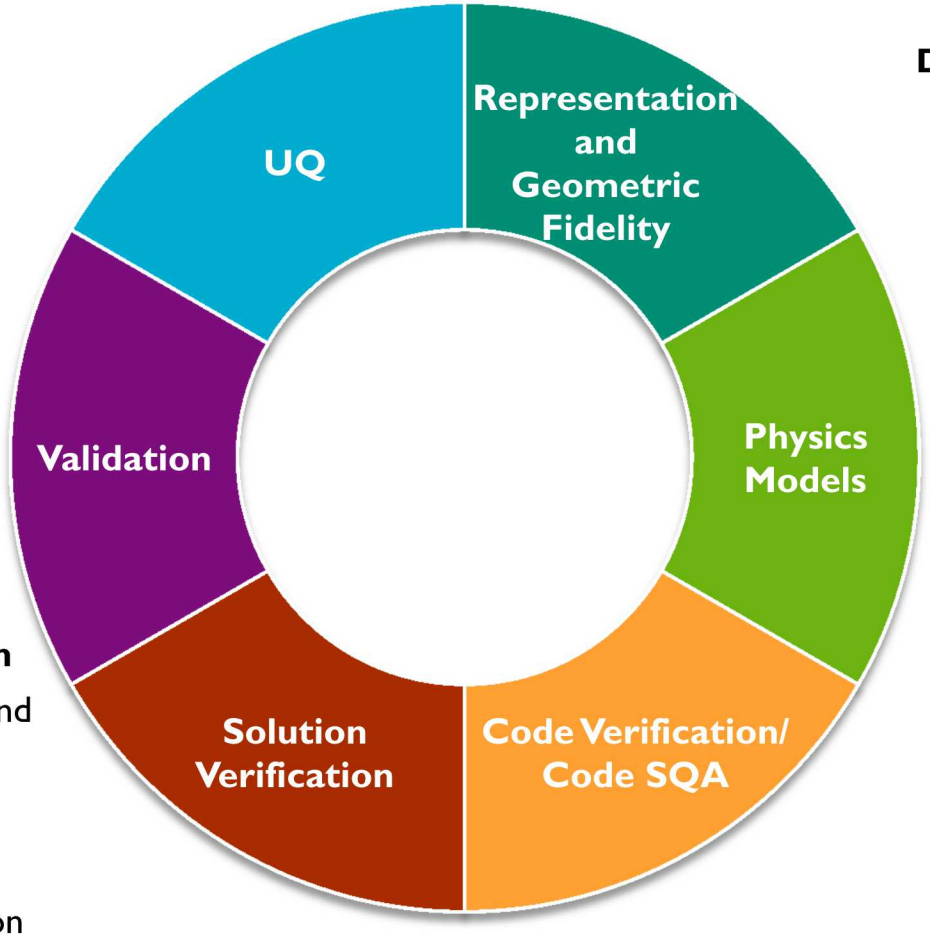
- The process of assembling and documenting **evidence** to ascertain and communicate the **believability** of **predictions** that are produced from computational simulations
- Quality process for ModSim

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 and 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

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 evidence

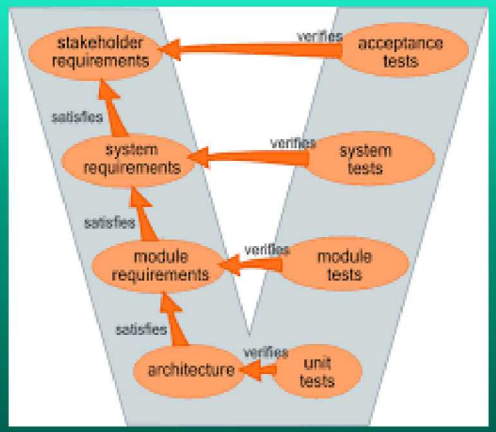
- PCMM (Predictive Capability Maturity Model) - SME elicitation process designed to characterize and communicate the completeness and rigor of the Comp/Sim process. Quantitative but "circumstantial"
  - Includes UQ, calibration and validation

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

CF - Credibility Framework and the CompSim Ecosystem

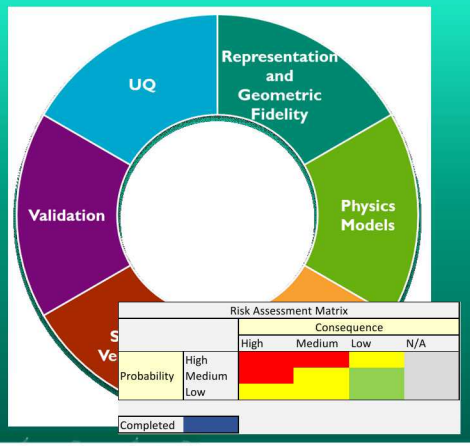
Requirements



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

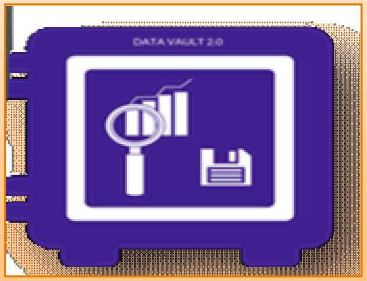
PCMM/Risks



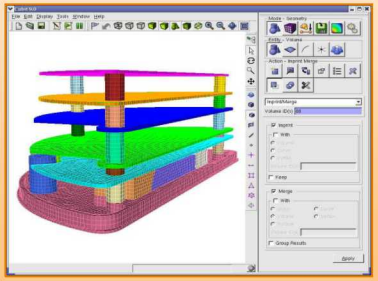
Reviews

EVIDENCE

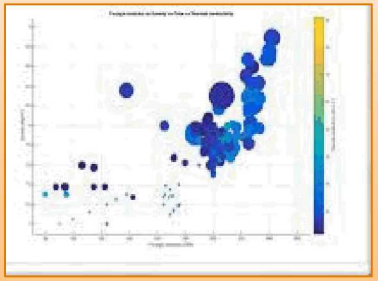
Simulation Data Management



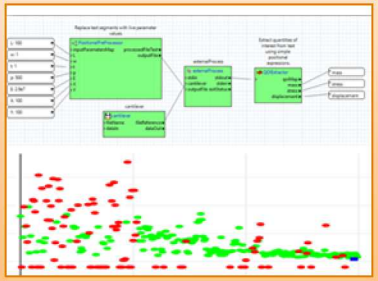
CAD and Model Building



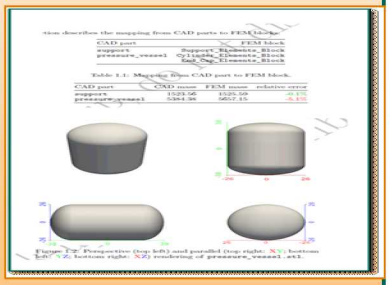
Materials (Granta)



Ensemble Workflows



Report Generation



Platform for answering: Why should the customer believe predictions?
What is the risk of making decisions based on CompSim?

Credibility Overview

Credibility Framework (CF) Requirements

CF Software Process

PIRT (Phenomena Identification and Ranking Table) Tool

PCMM (Predictive Capability Maturity Model) Tool

Summary, Current Work and Plans

General Functional Requirements for the Credibility Framework

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

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

Credibility Overview

Credibility Framework (CF) Requirements

CF Software Process

PIRT (Phenomena Identification and Ranking Table) Tool

PCMM (Predictive Capability Maturity Model) Tool

Summary, Current Work and Plans

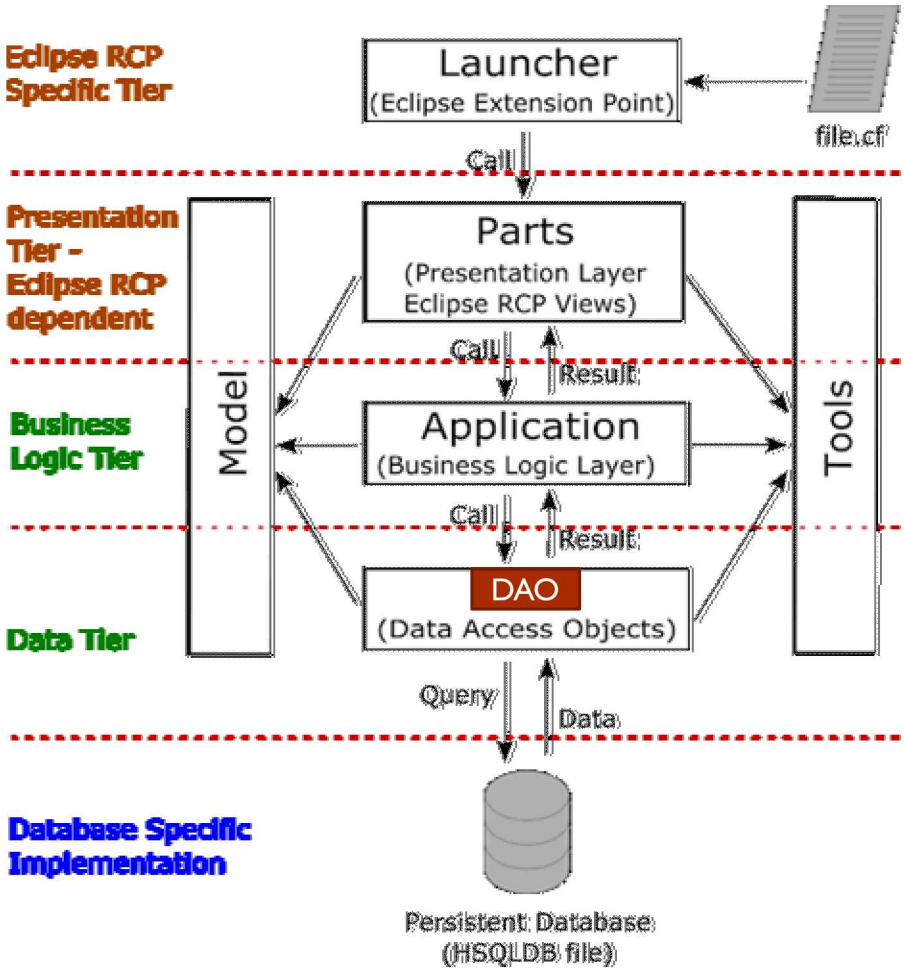
CF Software Architecture

N-tiered:

- **Launcher:** used to start plugin and load configuration
- **Presentation:** contains plugin GUI
- **Business Logic:** contains business logic, coordinates plugin behavior, performs calculations, makes logical decisions and processes commands
- **Data:** queries persistent data from database or files
- **Model:** used to transmit data (in memory) to other layers
- **Tools:** contains functions and methods used across whole application

Benefits:

- Easy to manage
- Scalable,
- Flexible,
- Reusable



File management and Database

Main requirements for CF plugin:

- Persistence through an open source database
- Configurable by non-programmers through familiar Excel spreadsheets

- Configuration files:
  - PIRT and PCMM **data schema** are **Excel** files
  - A **macro** converts these files to **YAML files** to be ingested by CF plugin
  - These YAML files are **necessary** to **configure** the project when creating new CF instance

- Database:
  - Use of **Java Persistence** API; **EclipseLink** for object-relational mapping (ORM) implementation
  - **HSQLDB** used to locally store data into workspace (open source and developed in Java)

- Credibility file (.cf) file format:
  - **Single .cf file** to store CF process data within the workspace
  - A **zip file** of both database and configuration files (as done by e.g. Word):
    - Easy to manage
    - Convenient to commit/ retrieve
  - When **opening** a CF project, its .cf file is **unzipped** in a workspace temporary folder
  - Modifications to .cf may be **rolled back** (if not saved)

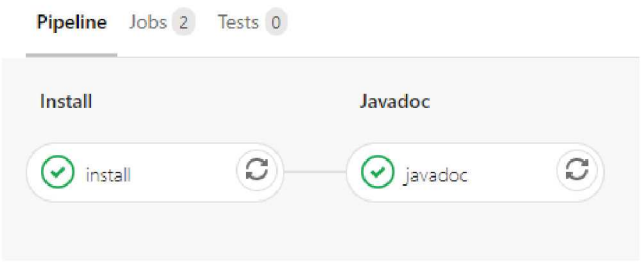
CF Software Process, Testing, and CI

GitLab-based continuous integration

- Testing
  - **Unit tests:** contained in separate plugin to test CF plugin features w/o including tests in installation package
  - **Integration tests** performed with Maven Tycho
  - **SWTBot** will be used to test the GUI (work in progress)

- Built with Maven Tycho
  - **Single-command** tool to **«** clean, compile, test and package **»**
  - Makes it easy to:
    - i**mport project in Eclipse** for development
    - **automate** build tasks

- Gitlab CI
  - Build, integration and unit tests launched at **each commit**, **merge request** or **manually**
  - **Commits linked** to project management & tracking
  - **Automation** of Javadoc generation
  - **Daily reports** @ GitLab.com and/or by email



CF Platform Requirements & Dependencies

CF plugin can be integrated into:

- an Eclipse product such as NGW/SAW
- plain vanilla Eclipse

Packaged as an **Eclipse Update Site:**

- **Contains CF feature**, its requirements and dependencies
- **Compatible with all Eclipse products** (Eclipse release versions must match)
- Easy to install/uninstall
- Can be easily deployed on a web server to facilitate download and make plugin more visible

Based on third-party open source software (OSS):

- Java dependencies: HSQLDB (database), JPA and EclipseLink (database access), Logback and Slf4j (logger), Mockito (unit tests), snakeyaml (Yaml to Java library)
- Eclipse dependencies: Opcoach E4Preferences (Eclipse Preferences GUI), JFreeChart, SwtGraphics2D (draw graphics), Nebula (GUI Components)

Credibility Overview

Credibility Framework (CF) Requirements

CF Software Process

PIRT (Phenomena Identification and Ranking Table) Tool

PCMM (Predictive Capability Maturity Model) Tool

Summary, Current Work and Plans

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 opinion for a particular intended use. The intended use is specific to the application driver, technical issue, scenario, and analysis objective, such as the performance or safety of a nuclear reactor.

CF PIRT Tool

CompSim Credibility Process

Quantities of Interest and their PIRT tables

Model Description

Application	Storage Tank
Contact	

+ Add

Creation Date	Name	Tagg...	Tag Date	Tag Description
February 19, 2020 12:24:21	g_yield (stress margin)	False		
February 19, 2020 13:13:00	g_displ (displacement margin)	False		

QoI Home | g_yield (stress margin) | g_displ (dis

CompSim Credibility Process

Phenomena

g_yield (stress margin)

Quantity of Interest	g_yield (stress margin)
Creation Date	February 19, 2020
Tag	False
Tag Date	
Tag Description	
Assessment Team	
Contact	

ID	Phenomena	Importa...	Math. Model Formulation	Code Implementation	Validation	Model Parameter	Comments
A	**Metal Constitutive Behavior**						
A1	Uniaxial elastic deformation	H	H	H	N/A	H	
A2	Transverse deformation under uniaxial load	M	H	H	N/A	H	
A3	Anisotropy	L	M	H	N/A	L	
A4	Yielding	M	H	H	N/A	M	High required factor of safety assures elastic deformation
B	**Deformation of Slender Structures**						
B1	Nonlinear coupling between stress and displacement	M	H	H	N/A	N/A	
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	

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

Credibility Overview

Credibility Framework (CF) Requirements

CF Software Process

PIRT (Phenomena Identification and Ranking Table) Tool

PCMM (Predictive Capability Maturity Model) Tool

Summary, Current Work and Plans

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, ES derivation, 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

Code Verification

Analysis code reproduces closed-form results

Physics and Material Model Fidelity

Are "closure models" (constitutive etc.) credible?

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

Representation and Geometric Fidelity

Is the geometric abstraction acceptable?

Solution Verification

Code solves the equations for the intended use correctly?

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

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

Validation

Validation hierarchy

How well do model predictions match experimental data?

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
Assess
Aggregate
Stamp

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

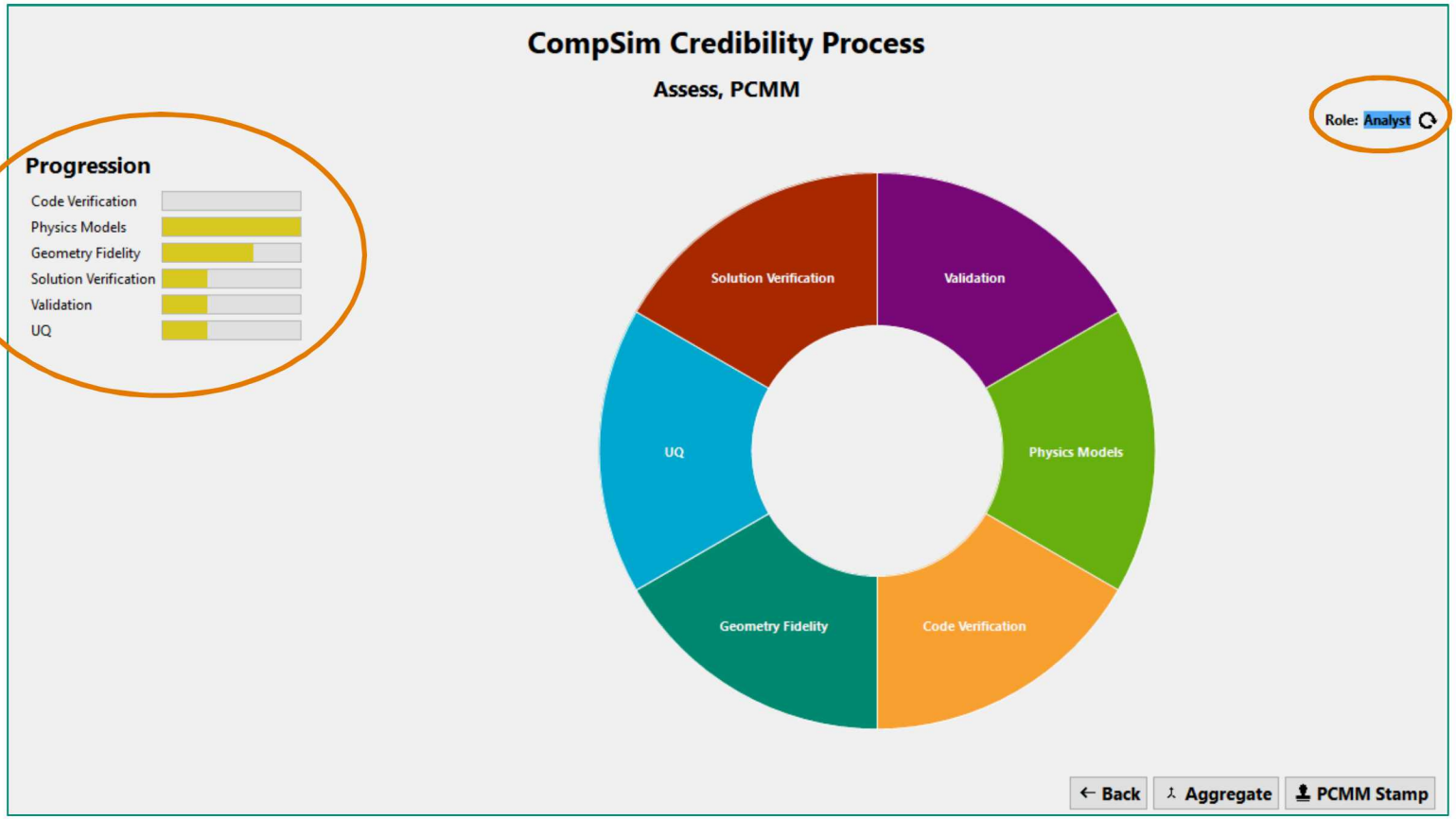
Activities
Evidence
Assess
Aggregate
Stamp

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

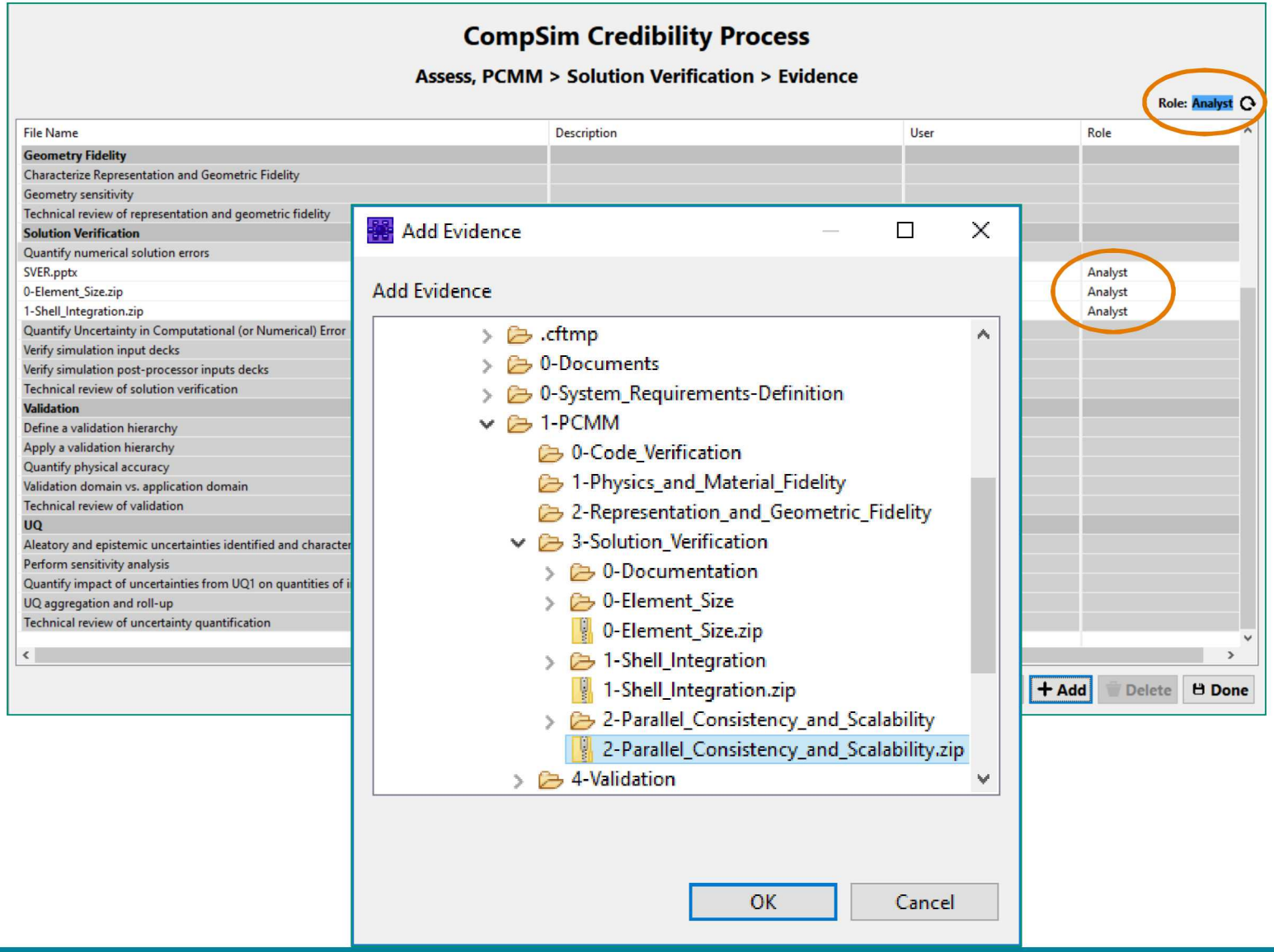
High Rigor

Agile adaptivity to organizational requirements

CF PCMM Tool


CompSim Credibility Process
Assess, PCMM
Role: Analyst
Progression
Code Verification
Physics Models
Geometry Fidelity
Solution Verification
Validation
UQ
Solution Verification
Validation
UQ
Physics Models
Geometry Fidelity
Code Verification
← Back
Aggregate
PCMM Stamp

CF PCMM Tool – Adding Evidence



Folder structure to contain artifacts employed as evidence generated by CF

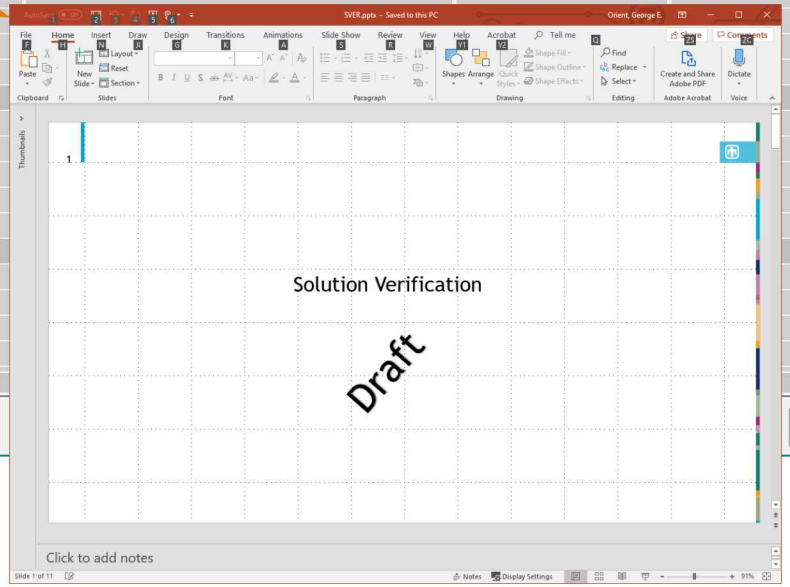
CF PCMM Tool – Examining Evidence

CompSim Credibility Process

Assess, PCMM > Validation > Evidence

Role: Analyst

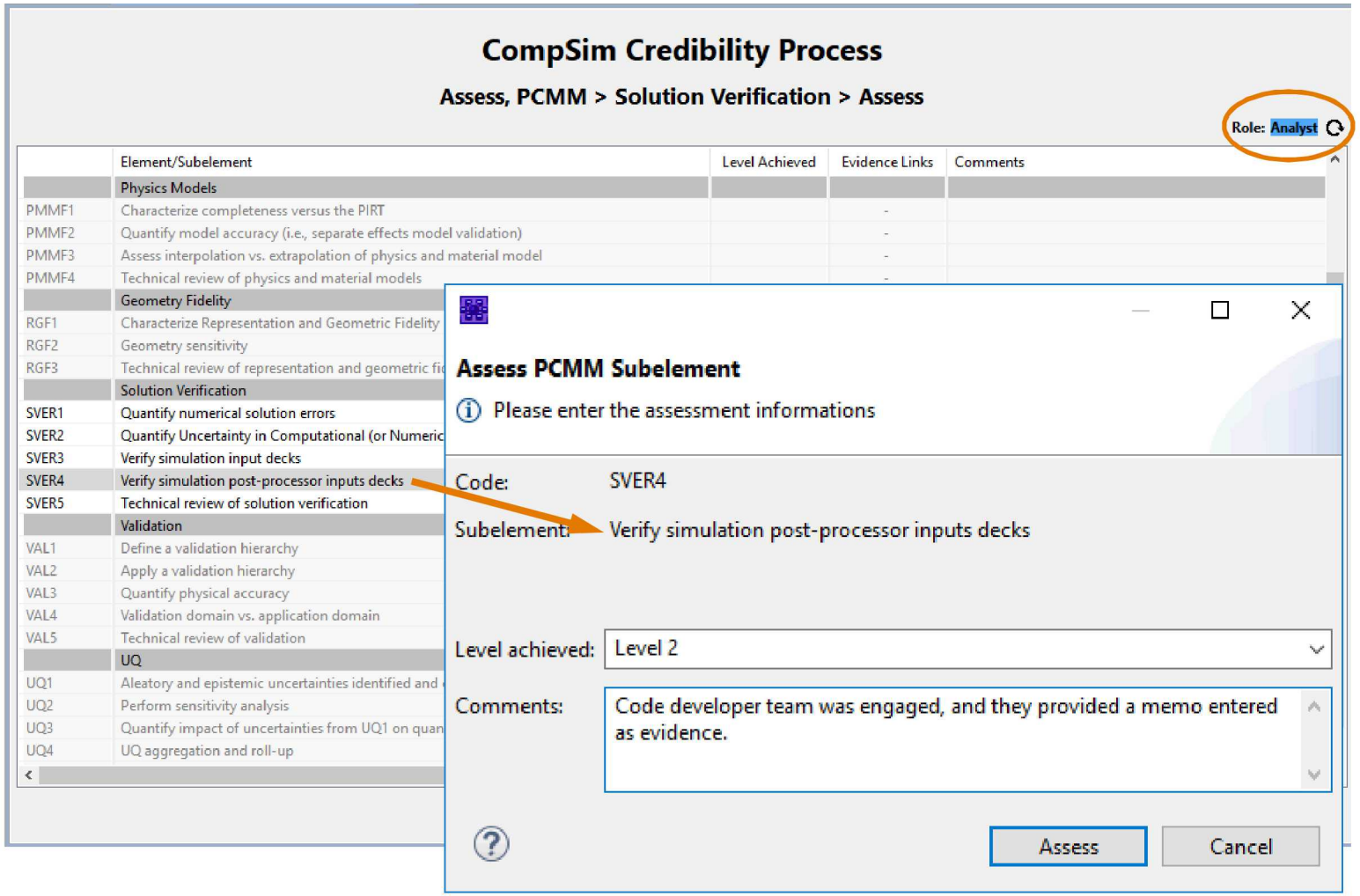
File Name	Description	User	Role
Assess interpolation vs. extrapolation of physics and material model			
Technical review of physics and material models			
Geometry Fidelity			
Characterize Representation and Geometric Fidelity			
Geometry sensitivity			
Technical review of representation and geometric fidelity			
Solution Verification			
Quantify numerical solution errors			
SVER.pptx		georien	Analyst
0-Element_Size.zip		georien	Analyst
1-Shell_Integration.zip		georien	Analyst
Quantify Uncertainty in Computational (or Numerical) Error			
Verify simulation input decks			
Verify simulation post-processor inputs decks			
Technical review of solution verification			
Validation			
Define a validation hierarchy			
Apply a validation hierarchy			
Quantify physical accuracy			
Validation domain vs. application domain			
Technical review of validation			
UQ			
Aleatory and epistemic uncertainties identified and characterized			
Perform sensitivity analysis			
Quantify impact of uncertainties from UQ1 on quantities of interest			
UQ aggregation and roll-up			



Done

Evidence is opened with associated editor

CF PCMM Tool – Assess



Role is associated with assessment

CF PCMM Tool – Aggregate

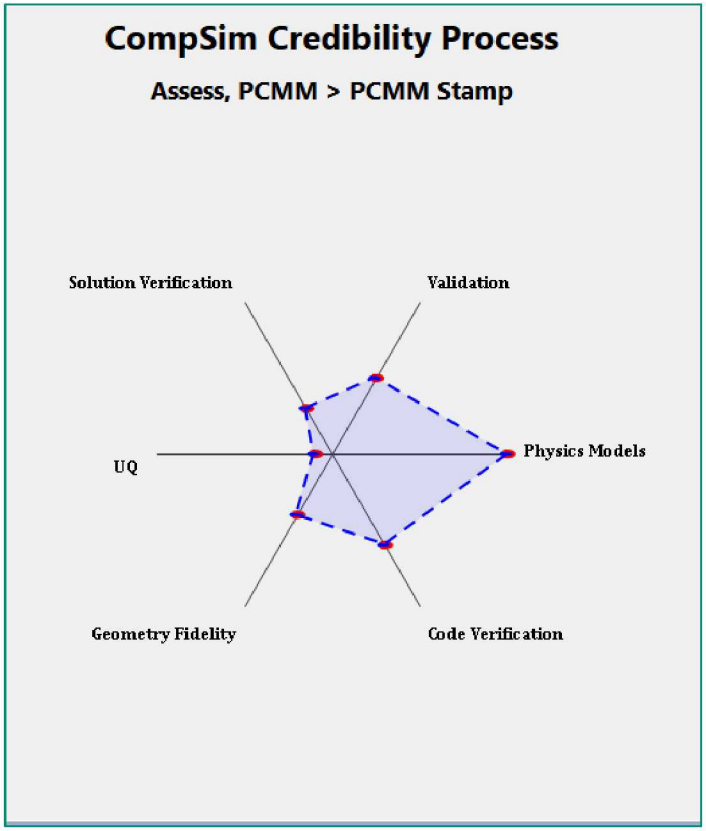
CompSim Credibility Process
Assess, PCMM > Aggregate

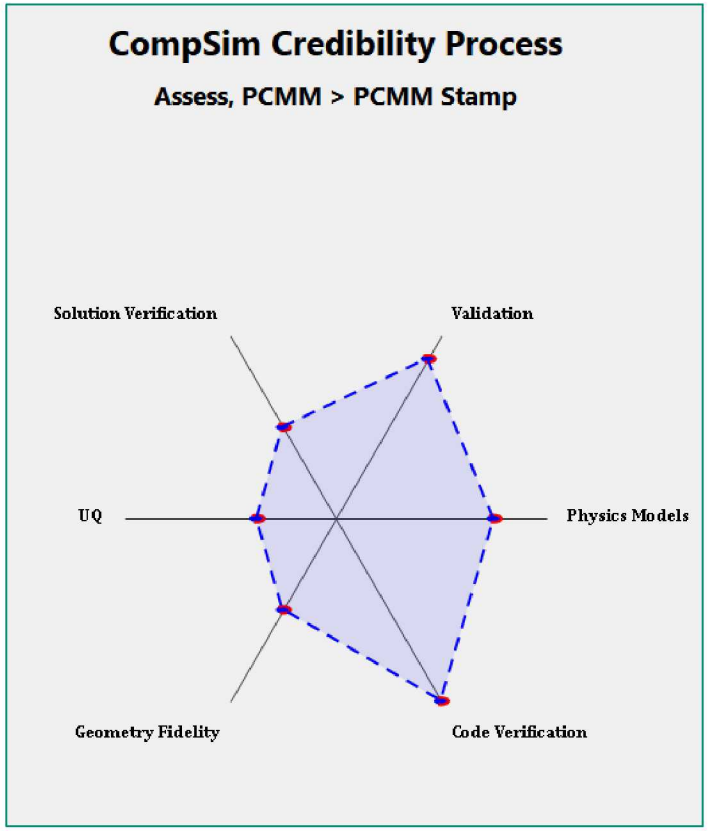
Role: VV Partner

	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

CF PCMM Tool – Quality Stamp





Simple visual representation of the credibility evolution of the CompSim effort

Credibility Overview

Credibility Framework (CF) Requirements

CF Software Process

PIRT (Phenomena Identification and Ranking Table) Tool

PCMM (Predictive Capability Maturity Model) Tool

Summary, Current Work and Plans

Credibility Framework - Summary

On-going work

- UI/UX testing started
- Early adoption on high consequence programs
- Engaging other organizations (KCNSC, different SNL ND programs) to test configurability of CF to match its behavior with their credibility process
- CF open source submission process started

Plans (FY21 and beyond)

- Queries (PIRT: "What phenomena had 'red' gaps at the preliminary design review?")
- Managing program requirements and evidence of meeting them
  - Likely to involve existing requirement management systems
- Experimental credibility
- Credibility risk management
- Peer review framework
- Credibility constructs at different consequence levels (design study, system test design, CompSim based qualification)
- Credibility report generation through ARG
- Evidence theory (belief-plausibility) and UQ based verification of program requirements

Backup Slides

Credibility Framework (CF)

What: Platform for answering: Why should the customer believe predictions? Open source implementation of Sandia credibility constructs and tools (Phenomena Identification and Ranking Table (PIRT), Predictive Capability Maturity Model (PCMM), Experimental Credibility, etc.). Version controlled credibility process for any engineering discipline; configurable by non-programmers for program specific organizational and program needs.

Current state: Several spreadsheets; evidence may be "hearsay"; no central access point. Final peer review team may spend considerable time collecting/organizing evidence

Future state: Reviewable tightly linked evidence package covering program requirements, computational and experimental credibility and risks communicated through an automatically generated human extensible report.

Stakeholders: High consequence programs need defensible credibility communication provenance tracking

Approach:

- Involve V&V practitioners, ModSim team members and UI/UX experts early
- Implementation by small business partner, NGA (Next Generation Analytics)

Risks: Lack of adoption (need analysis management support)