INCORPORATING WORKFLOW FOR V&V/UQ IN THE SANDIA ANALYSIS WORKBENCH

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SAIC
Support the Design-To-Analysis process, capturing data in context

- DSM/ASM Development
- Analysis Model Development
- Simulation
- Results Processing
- Uncertainty Quantification / Optimization

PDM Database
SDM Database

Data Sources

Can I support my engineering assertion?
Can I re-execute models as computational capabilities continue to evolve?

How credible are my simulations?
Do I understand the pedigree of my analysis data?

1 2 3 4 5 6 7 8 9 10

Requirement

Material Characterization Test Data
Steel Mat Props
Mesh A
Mesh B
Mesh C
Mesh D
Mesh E
Mesh F
Simulation A
Simulation B
Simulation C
Simulation D
Simulation E
Simulation F
Analysis Conclusions

Design Solid Model
Analysis Solid Model
Input Deck A
Input Deck B
Input Deck C
Input Deck D
Input Deck E
Input Deck F

UNCLASSIFIED UNLIMITED RELEASE
SAW provides a unified view of distributed enterprise resources on the desktop

Multiple applications and tools combined into one, streamlining work and reducing complexity
SAW provides a unified view of distributed enterprise resources on the desktop.

- Simulation Data Management
- Eclipse Workbench
- Job Submission & Job Management
- Project Teaming
- Model Assembly
- Distributed File Management & Viz

Eclipse Workbench

Model Assembly

Distributed File Management & Viz
Parametric Analysis Workflow

- Automated process to execute and post process a single analysis – IT IS THE MODEL
- Driven by UQ/Optimization engine (DAKOTA at SNL)
  - **Efficiently**: leverage DAKOTA to manage concurrency
  - **Reliably**: resilient to random HPC (High Performance Computing) failures; report failure to UQ/Optimization engine for analysis instance retry
  - **Responsibly**: manage HPC utilization, manage disk space on file system; archive selected files after execution completes
  - **Platform independently**: environment fully parameterized
  - **Incrementally**: add post processing to existing design points as needed; evaluate QoIs and quantitative/qualitative credibility evidence
- **Required for UQ**
- **Supports analysis credibility evidence**
  Documents all computational steps from input parameters to responses
  Committed in repository
Open Source Workflow Platforms

- UC Davis, Santa Barbara, San Diego; graphical model builder, execution engine, Linux, Windows.
- Apache Incubator project; Written in Java, graphical model builder, provenance tracking through OPM, remote web services, cloud/grid capabilities.
- USC; distributed resilient scheduling on heterogeneous computing (desktop, workstation, cloud), Linux, Mac.
- DAWN/Passerelle; modular/dynamic platform for process automation. Wraps Ptolemy II (UC Berkeley) open-source platform for actor-based modeling.

Challenge: Correct make/buy decisions based on long-term ubiquitous adoption and commitment for support; some assembly required!
Current Status: Automatic Workflow Capture

User has a point and click interface to build workflow actions that extract common quantities of interest (no scripting needed).
Current Status: Automatic Workflow Capture

Generated workflows can be run in optimization loops or parameter studies using DAKOTA.
Workflow Architecture – Phase IV

User Workstation

SAW UI
- SAW Model
- Workflow Capture
- Workflow Editor

SAW Core
- Local Python Action
- Job Submission Action
- Remote Python Action
- APREPRO Action
- CUBIT Meshing Action
- User Defined Action

HPC

- Remote Simulation Process
- Cubit
- User Defined Process

Workflow Engine/Library

DAKOTA
Workflow Architecture – Phase V

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- Remote Simulation Process
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- Workflow Engine/Library
  - DAKOTA

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Proposed Scalable Workflow Architecture Directly Connects HPC Codes Using Available Comms

Port properties:
- Name ("Flow Field")
- Data type ("CSV")
- Connection types ("FILE", "NVRAM")

Connection properties:
- Type ("FILE")
- Parameters
  - PATH="/gscratch3/user"
  - NAME="field.csv"

Connection properties:
- Type ("NVRAM")
- Parameters
  - SEGMENT="0x00004332"
  - OFFSET="0x00002200"

Execute using COTS Workflow Engine

Tool 1
- "field.csv"
- 0x00004332
- 0x00002200

Tool 2
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