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Advancing Model Credibility for Linked Multi-Physics Surrogate Models within a Coupled Digital Engineering Workflow of Nuclear Deterrence Systems

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ABSTRACT

Sandia National Laboratories' (SNL) digital engineering transformation initiative to accelerate product realization of nuclear deterrence (ND) systems has institutionalized quick turn modeling and simulation solutions. Surrogate modeling, coupled with model-based systems engineering (MBSE) using commercial-off-the-shelf (COTS) tools moves the start line forward to inform design and requirements. Yet, this paradigm shift poses a large challenge in a high-security environment: quick-turn credibility solutions and verification, validation, and uncertainty quantification (VVUQ) to match the rate at which models are developed.

This project demonstrates a model credibility process generating evidence to obtain buy-off from key stakeholders for rapidly developed (< 2-3 hours) surrogate models within MATLAB/Simulink that interface with SNL-developed codes and MBSE in an extended integrated digital engineering workflow. The pilot project under test of this process utilizes legacy higher fidelity and computationally expensive codes to inform mass/stiffness matrices for a structural and aero-dynamics trade study problem that verifies requirements—all on a standard desktop used by the customer vs. need for high-computing power and/or subject matter experts (SME's).

Our technical approach is directed at risk-informed decision-making for design engineers waiting on requirements, up to program leadership making key decisions. Steps include: 1) benchmarking against current VVUQ processes guided by SME's, 2) uncertainty inventory including source definition, quantification, and mapping (model form, parametric, numerical, and environmental boundary conditions), 3) mapping of uncertainties to modeling activities and 4) aggregation of evidence to fill gaps identified (e.g. peer review of methodology) or identify risks where additional testing or data may be required. This approach is underpinned by data engineering and configuration management that face need-to-know security challenges creating innovative capability adaptation for national security defense applications.

In summary, digital engineering workflows utilizing multi-physics surrogate models integrated with MBSE and data management are the way of the future for SNL—assuming associated credibility evidence, accessibility, and usability advances in parallel. Techniques discussed are an integral step in this process and how these types of models can help inform higher fidelity models, qualification, and beyond.

Keywords: Surrogate Model, Digital Engineering, Model Credibility, Multi-Physics Modeling

INTRODUCTION

Moving toward a digital engineering product lifecycle (Figure 1) in order to accelerate product realization of nuclear deterrence systems requires integrated and innovative, yet *credible,* capabilities within a model-based ecosystem that are usable and accessible. A generalized credibility process was created in order to address apprehension and challenges of using surrogate COTs-based models early in the design process (Phases 1 and 2) to support risk-informed decision making, quicker. Further, this process breaks down silos by integrating into the digital thread, including traceability to requirements

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via Model-Based Systems Engineering, creating an iterative environment that can be updated and matured as a product develops, ultimately informing higher fidelity model development and qualification. Challenges surrounding need-to-know and security remain but building an adaptable credibility evidence package for models *early* moves the goal of accelerating product realization at Sandia via digital engineering transformation one step closer.

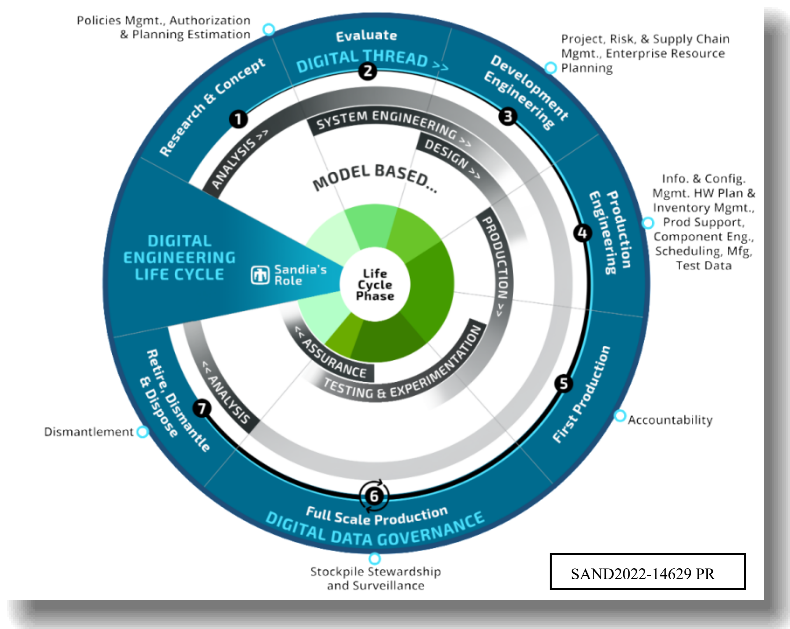

Figure 1: The Digital Engineering Product Lifecycle at Sandia National Laboratories

BACKGROUND

Historically, most of the Modeling and Simulation (M&S) at Sandia has focused on high-fidelity computational codes developed by SME's geared toward areas where physical test and qualification is not possible. Hence, the Predictive Capability Maturity Model (PCMM) [1] displayed in Figure 2, along with other extensive VVUQ and credibility processes were established for evaluating model credibility. As surrogate and other reduced-order modeling efforts increased, including the increased use of COTs codes, the need for adapting current processes was apparent. An initial exercise of applying historic processes to a SOLSTICE[1] surrogate aerodynamics and structural dynamics highlighted the following:

- The PCMM can be used as a technical basis for elements to consider for surrogate multi-physics credibility (e.g. model form error when test data is available, which oftentimes is not the case)
- Uncertainty Quantification and Sensitivity Analysis techniques can be applied, but often performed by built-in toolboxes within MathWorks products (for the SOLSTICE example) which may require additional tool verification
- Code commenting and documentation, peer review (expert judgement and customer feedback), model boundary conditions, and interfaces with other codes are gaps that must be considered
- Credibility evidence evolves over time along with the model and must be a dynamic and flexible process
- A VVUQ expert is often required, slowing down the process due to funding and resource constraints

Based on this benchmarking exercise, a hybrid approach was developed for such models, enabling modelers to establish credibility quickly (<2-3 hours) and without need for an expert (other than consultation), that can be passed along to design

[1] SOLSTICE is an acronym for Simulation of Linked multi-physics Surrogate Time-domain models In Combined Environments, a modeling methodology used at Sandia National Laboratories.

engineers. The intended use is for quick-turn surrogate COTs-based models used early in the design phase of the product lifecycle and not to replace current processes, but provide alternative solutions based on the application and use of the model.

MATURITY / ELEMENT	Maturity Level 0 Low Consequence, Minimal M&S Impact, e.g. Scoping Studies	Maturity Level 1 Moderate Consequence, Some M&S Impact, e.g. Design Support	Maturity Level 2 High-Consequence, High M&S Impact, e.g. Qualification Support	Maturity Level 3 High-Consequence, Decision-Making Based on M&S, e.g. Qualification or Certification
Representation and Geometric Fidelity What features are neglected because of simplifications or stylizations?	• Judgment only • Little or no representational or geometric fidelity for the system and BCs	• Significant simplification or stylization of the system and BCs • Geometry or representation of major components is defined	• Limited simplification or stylization of major components and BCs • Geometry or representation is well defined for major components and some minor components • Some peer review conducted	• Essentially no simplification or stylization of components in the system and BCs • Geometry or representation of all components is at the detail of "as built", e.g., gaps, material interfaces, fasteners • Independent peer review conducted
Physics and Material Model Fidelity How fundamental are the physics and material models and what is the level of model calibration?	• Judgment only • Model forms are either unknown or fully empirical • Few, if any, physics-informed models • No coupling of models	• Some models are physics based and are calibrated using data from related systems • Minimal or ad hoc coupling of models	• Physics-based models for all important processes • Significant calibration needed using separate effects tests (SETs) and integral effects tests (IETs) • One-way coupling of models • Some peer review conducted	• All models are physics based • Minimal need for calibration using SETs and IETs • Sound physical basis for extrapolation and coupling of models • Full, two-way coupling of models • Independent peer review conducted
Code Verification Are algorithm deficiencies, software errors, and poor SQE practices corrupting the simulation results?	• Judgment only • Minimal testing of any software elements • Little or no SQE procedures specified or followed	• Code is managed by SQE procedures • Unit and regression testing conducted • Some comparisons made with benchmarks	• Some algorithms are tested to determine the observed order of numerical convergence • Some features & capabilities (F&C) are tested with benchmark solutions • Some peer review conducted	• All important algorithms are tested to determine the observed order of numerical convergence • All important F&Cs are tested with rigorous benchmark solutions • Independent peer review conducted
Solution Verification Are numerical solution errors and human procedural errors corrupting the simulation results?	• Judgment only • Numerical errors have an unknown or large effect on simulation results	• Numerical effects on relevant SRQs are qualitatively estimated • Input/output (I/O) verified only by the analysts	• Numerical effects are quantitatively estimated to be small on some SRQs • I/O independently verified • Some peer review conducted	• Numerical effects are determined to be small on all important SRQs • Important simulations are independently reproduced • Independent peer review conducted
Model Validation How carefully is the accuracy of the simulation and experimental results assessed at various tiers in a validation hierarchy?	• Judgment only • Few, if any, comparisons with measurements from similar systems or applications	• Quantitative assessment of accuracy of SRQs not directly relevant to the application of interest • Large or unknown experimental uncertainties	• Quantitative assessment of predictive accuracy for some key SRQs from IETs and SETs • Experimental uncertainties are well characterized for most SETs, but poorly known for IETs • Some peer review conducted	• Quantitative assessment of predictive accuracy for all important SRQs from IETs and SETs at conditions/geometries directly relevant to the application • Experimental uncertainties are well characterized for all IETs and SETs • Independent peer review conducted
Uncertainty Quantification and Sensitivity Analysis How thoroughly are uncertainties and sensitivities characterized and propagated?	• Judgment only • Only deterministic analyses are conducted • Uncertainties and sensitivities are not addressed	• Aleatory and epistemic (A&E) uncertainties propagated, but without distinction • Informal sensitivity studies conducted • Many strong UQ/SA assumptions made	• A&E uncertainties segregated, propagated and identified in SRQs • Quantitative sensitivity analyses conducted for most parameters • Numerical propagation errors are estimated and their effect known • Some strong assumptions made • Some peer review conducted	• A&E uncertainties comprehensively treated and properly interpreted • Comprehensive sensitivity analyses conducted for parameters and models • Numerical propagation errors are demonstrated to be small • No significant UQ/SA assumptions made • Independent peer review conducted

Figure 2: General Descriptions for PCMM table entries which act as part of Sandia's current process.

PROCESS

A generalized credibility process was created for use when creating and implementing surrogate models within a Digital Engineering workflow, as in Figure 3 below. While not limited to this framework, a SOLSTICE model is used to demonstrate the necessary elements of this process, and the upstream / downstream effects of credibility based on the many integrations and interfaces. Model-Based Systems Engineering (MBSE), described as a 'Descriptive Model' below, provides a means of tracing and providing requirements for verification activities, whether it be through M&S (e.g. SOLSTICE) or test data.

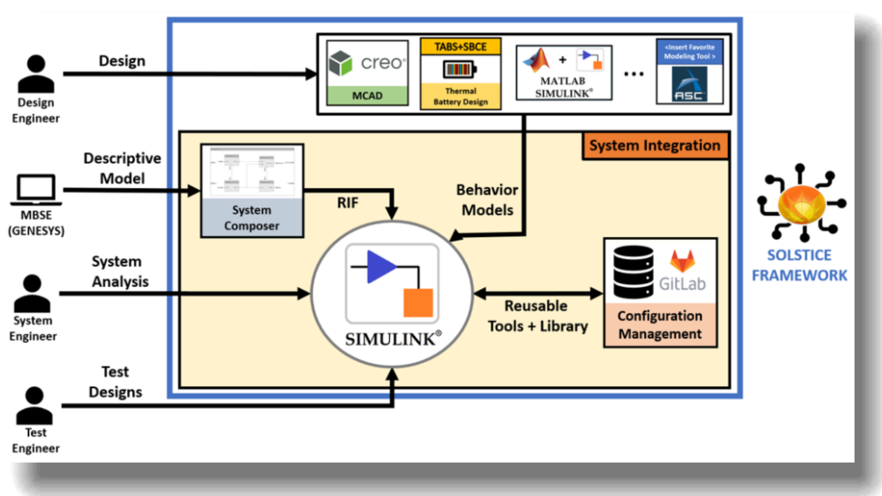

Figure 3: SOLSTICE Framework within the Digital Engineering Workflow

The process as applied to a SOLSTICE aerodynamics / structural dynamics model is as follows:

Part 1: Create Model Credibility Document

- If within MATLAB/Simulink, model preparation includes adding all variables and parameters to the workspace and ensuring no errors are present. The model credibility script can then be run (in less than 2 minutes!), which generates a document printout. The following sections are then completed:
- **Introduction:** includes customer needs, scope of model, and optimal use case for decision-making with the model, important to defining boundary conditions around model usage
- **Model Overview:** describes basic functions, including inputs, outputs, toolboxes used (e.g. Simulink blocks, Matlab commands, etc.) and other code interfaces or origins of the surrogate model (CAD, for instance, or other higher-fidelity models)
- **Model Equations and Assumptions:** all equations and behaviors modeled to generate output are listed along with all variables and units defined. Assumptions are documented for each equation, including why it was made, and how the model might improve if such assumptions are addressed. Additionally, this is where simplifications to improve run time are documented and uncertainties surrounding the simplification are quantified—for instance, if model is a surrogate of a higher fidelity model, associated uncertainties inherited from that model are provided here.
- **Model Parameters:** a table is created by the model credibility script, listing all parameters (inputs) with names, units, and values used to create outputs
- **Sensitivity Analysis:** evaluates how input parameters of a model influence the model output or specific design requirements. For this use case (or any MATLAB/Simulink model), MATLAB's Sensitivity Analyzer[2] can be used to perform this analysis. Steps include 1) Selecting the input parameters that will be used in the analysis and generate N number of samples for each parameter depending on a selected mean and standard deviation, 2) performing Monte Carlo simulations to evaluate design requirements at parameter values, and 3) using visual analysis to plot cost function evaluations against parameter samples in order to identify trends. Statistical analysis (correlation, partial correlation, and standardized regression) is then used to compute correlation coefficients quantifying the relations with either linear (Pearson) analysis or ranked (Spearman) analysis, depending on whether the relationship between the cost function and parameter values are linear or nonlinear monotonic relationships. A tornado plot visualizes the results (see Figure 4 as an example), showing parameters with most influence (and magnitude). Results are used to make decisions about the model and each parameter, including use of the parameter estimation tool to optimize the model.

[2] Reference MathWorks documentation on sensitivity analysis: https://www.mathworks.com/help/sldo/sensitivity-analysis.html.

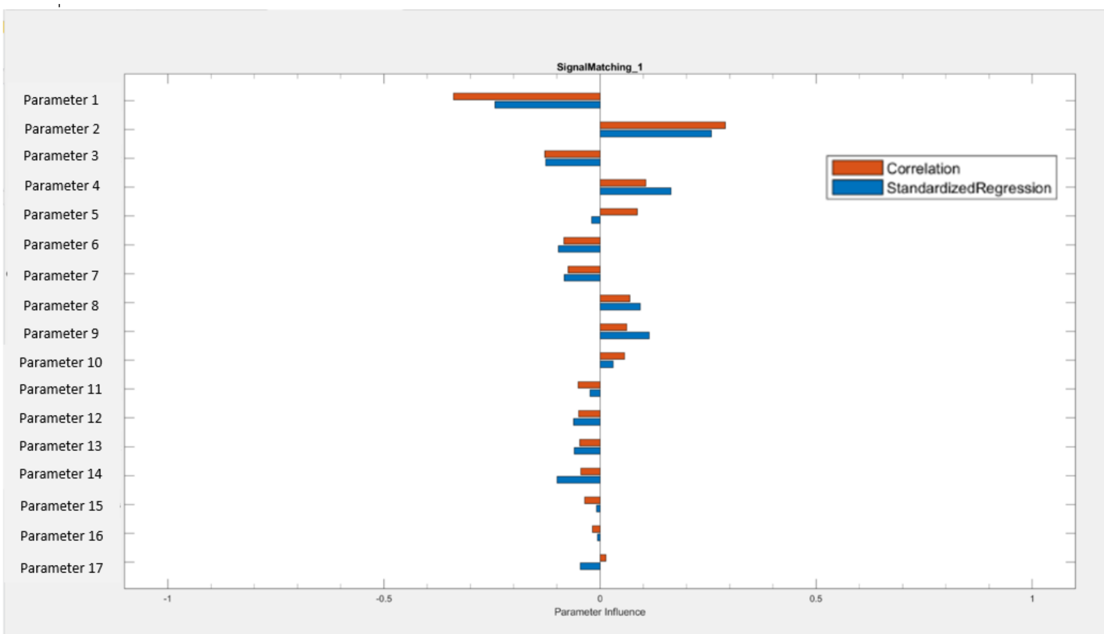

Figure 4: Example tornado plot with statistical analysis of the sensitivity analysis showing correlation coefficients between each parameter and the requirement (red) and the normalized regression slope of the parameters vs. requirement (blue).

- **MATLAB / Simulink Simulation Form Error:** runs the model with various time-steps, solvers, and relative tolerances to get simulation run time, providing insight to optimal model use based on customer needs. If test data is available to compare simulation results, the root-mean squared error (RMSE) is also included. The following table is outputted from the script to discover large discrepancies in run time or RMSE based on choice of solver, time-step, or relative tolerance (note, 'Time-Step' is replaced with solver, or relative tolerance).

Table 1: Sample table output from executing model credibility script within a SOLSTICE model

Time-Step	Run-Time (s)	RMS Error (Power)
Baseline (Fixed step 10^{-6}s)	57.23	-
Fixed step (1s)	0.48	3.68e44
Fixed step (0.1s)	0.59	2.24e36
Fixed step (0.01s)	0.63	1.37e-2
Fixed step (0.001s)	0.71	4.32e-4
Variable step (max 1s)	0.60	8.98e-3
Variable step (max 0.1s)	0.72	3.92e-3
Variable step (max 0.01s)	0.64	1.36e-3
Variable step (max 0.001s)	1.06	4.32e-4

- **Optimal Selections for Simulation Solver Options:** Evaluate the recommended options for time-step, solver, and relative tolerance when running the model. Inform these decisions from information obtained. Document any SME judgement or peer review required in making these decisions.

Part 2: Simulink Report Generator: A Graphical User Interface (GUI) was created and is used to auto-generate a customizable system design description and report on Simulink models within a preferred format (PDF, Word, HTML) documenting the model in detail from all blocks used, system, sub-system, components, properties, formulas, code comments, inputs, outputs etc. top supplement the model overview and assumption sections with the credibility document. Impact includes near-automatic model documentation to provide to the model customer, stakeholder, or any individual that may not understand the model details without the need to install Simulink.

Part 3: Model User Guide: generated based on outputs of the model credibility process in order to provide model usage details and limitations that were discovered (for instance, most sensitive parameters, optimal model solvers and analysis tolerances or time-steps) to the user or customer so that they can make the most optimal risk-informed decisions based on the model.

Additional credibility elements include model peer review of methodology, traceability to all data sources and/or other code or interfaces and configuration management of the model and simulation results as visualized within Figure 3.

CONCLUSION

Creation of a quick-turn hybrid generalized credibility process (derived from historic VVUQ techniques at Sandia) enables a model credibility document to be generated for any SOLSTICE model (or, more general, a surrogate model) within minutes. This greatly impacts the ability to accelerate product realization by providing design engineers, key stakeholders, and program leadership a means to make risk-informed decisions early in design without the need for higher fidelity models and/or physical tests. Additionally, this process can be iterated as often as needed based on changes upstream/downstream within the digital thread and/or requirements. The process is currently being piloted and in use for aerodynamic / structural dynamics and thermal battery applications at Sandia, with the goal to increase the user base exponentially as programs work through the digital engineering product lifecycle and digital engineering becomes the way of the future at Sandia.

ACKNOWLEDGEMENTS

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REFERENCES

[1] William L. Oberkampf, Martin Pilch, and Timothy G. Tucano, "Predictive Capability Maturity Model for Computational Modeling and Simulation" prepared for *Sandia National Laboratories*, SAND2007-5948, October 2007