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PNNL-34506

Verification and Validation for Energy System Co-Design and Simulation

April 2023

Brent Daniel
Timothy Salsbury

U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

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Abstract

This project was only active for two months and was terminated due to a re-organization of the sponsoring initiative. The original purpose of the project was to develop and apply verification and validation (V&V) methodologies for the Energy System Co-Design with Multiple Objectives and Power Electronics (E-COMP) Initiative. This report summarizes the project and the work that was completed in the shortened time frame.

Summary

This project was focused on creating model development workflows that highlight validation needs early and at each stage of development activities, including conceptualization, simulation, optimization, etc. This process included potentially relevant V&V methods to be used in other E-COMP thrusts for ongoing, continuous model improvement.

Acknowledgments

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1.0 Introduction

Standard practices and workflows used in the research and development of scientific models sometimes leave verification and validation (V&V) until after the model development work has largely completed. Limited studies of operational validity are then reported in the scientific literature and evaluated against the standards of the academic community. The results of such models may, however, then be used to inform or support private, public, or governmental decisions or policies. A contentious, misinterpreted, or incorrect model result during those efforts can, then, lead to significant additional scrutiny of the V&V that was performed. This can leave researchers open to scientific criticism, reputational harm, and the degradation of stakeholder trust.

1.1 Project Aims

The project aimed to create model development workflows that highlight validation needs early and at each stage of development activities, including conceptualization, simulation, optimization, etc. This process includes potentially relevant V&V methods for ongoing, continuous model improvement. V&V insights learned would be assimilated into guidance and exercised in the context of the model development work being done on co-optimization, power electronics stability modeling, and agent-based models within other thrust areas of the initiative to identify challenges, shortcomings, and potential operational hurdles in the development of methods from theory to practice. Specific aims include:

- Provide V&V insight to other E-COMP projects accompanied with the development of tools to assist researchers in integrating rigorous, statistical validation of optimization and simulation tools.
- Quantification of the performance of co-optimization, power electronics stability modeling, and agent-based models will enable technology maturation towards operational use of PEL-enhanced grid simulations.
- Identification of methods and metrics and development into software algorithms to quantify operational validity in PEL-based power system models and co-design results.

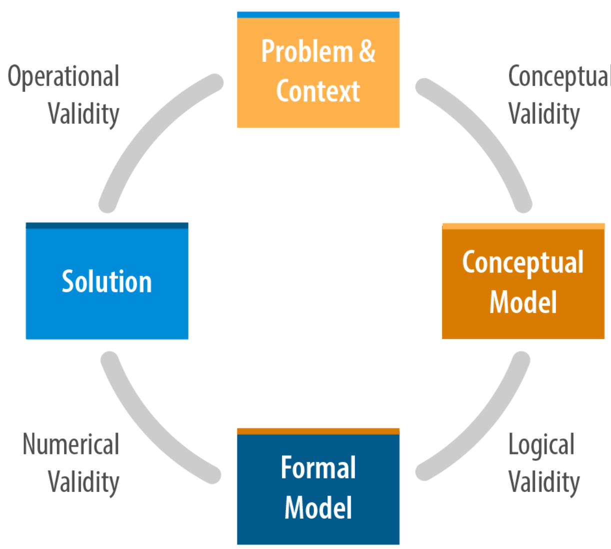
The first-year focus of the project was to develop methodologies for validating operational models and theorems of PEL-based systems developed in Thrust 1 of E-COMP and characterizing methodology for assessing optimality of solutions generated by a co-design engine (Thrust 2).

2.0 Research Approach

The cohesive integration of V&V efforts into the simulation and optimization methods and models development workflow would provide two key advantages: the early and holistic development of stakeholder trust in the models, model development processes, and results; and numerous opportunities to improve the models themselves. The work seeks to move validation science and implementation forward as a critical research thrust within E-COMP by developing the guidance and means to do this. (Note that in this proposal we take model to include the combination of mathematical equations, their numerical implementations, simulation/optimization algorithms, etc.)

E-COMP is well-suited to motivate this effort as many objectives within the Initiative have diverse and challenging validation needs, including: developing new theories and models of PEL-based devices and their incorporation into grid systems in Thrust 1; the solving of multi-objective optimization problems co-design in Thrust 2; the development of a broad energy system simulation and the integration of the co-design efforts with that model in Thrust 3; the integration of multiple modeling formalisms; and the many challenges associated with working at a wide breadth of spatiotemporal scales (across all Thrusts).

The research approach of this project takes a comprehensive view of an integrated model development and validation process, as shown in the figure below. The figure lays out the standard model development tasks, from the characterization of the problem to the early development of a conceptual model of it, the translation of that conceptual model into formal mathematics or numerical code, and the eventual solution of that model to obtain results that may drive stakeholder decisions or model improvements.



Adapted from: Landry et al. / *Model Validation in Operations Research*, 1983

Figure 1: Model development workflow and associated types of validation at each stage of the model development process.

At each stage of this integrated development process there are opportunities and needs for a variety of different validation types. Efforts to establish conceptual validity can help ensure that the model being developed addresses the right problem, can be used to answer relevant analytical questions, and is driven by appropriately targeted use cases or scenarios. Background efforts here may also seek to assure stakeholders that the problem is, at least in principle, solvable and any requisite supporting data or information measurable and obtainable. Logical validation ensures that the translation from conceptual model to logical model has been correctly performed. Tests of self-consistency and asymptotic behavior can be illuminating, but broader questions associated with epistemic issues, such as structural uncertainty, should also be considered.

Numerical validation should evaluate the degree to which the code and/or solvers yield repeatable results, are of sufficient computational efficiency and scalability to address the problem at hand, and whether they include guarantees of accuracy or optimality. Finally, operational validity incorporates what we normally think of as model validation, where model forecasts are compared to empirical or reference observations. Many additional questions arise here, though, in terms of the levels of aleatoric uncertainty in the observations and results, the potential non-stationarity of reference data, and the measurability or obtainability of the data most valuable to validation efforts. All these issues must be addressed in the context of questions about how success will quantitatively be gauged, and what this implies as to the accuracy/precision required of the model, its inputs, and the empirical observations it will be compared to, to claim success.

Key parts of the originally planned scope are itemized below.

- Developing guidance and tools to allow researchers to identify and implement cohesive validation and model development best practices. It is intended that the application of the guidance will make trust-building an integral part of the model development process; yield stronger, better understood, and potentially more insightful models; and reduce the likelihood of unwelcome discoveries or unanticipated questions cropping up after models have been used to inform policy decisions.
- Work collaboratively to apply this guidance to ongoing model development efforts in other Initiative Thrust areas to identify shortcomings of the guidance and improve its applicability, useability, and utility. It is intended that these cross-cutting efforts should also provide significant value to the other Thrust areas, helping them to identify opportunities and means to incorporate validation efforts into their workflows as early and consistently as possible.
- Development of a proof-of-concept software framework to assist researchers across all E-COMP projects in quantitatively assessing PEL-based grid models' operational validity. Sample reference data from hardware-in-the-loop simulations and/or existing systems will be acquired along with the anticipated outputs and formats from Initiative optimization modeling efforts. These sample data will allow us to develop the computationally efficient means to operationally

validate modeling results by several different measures. This work is intended to reduce the hurdles necessary to incorporate validity checks into model development as well as serve as a steppingstone on the path to more automated assessment. The development work will leverage an existing PNNL toolset called the *DataCube* that allows developers to rapidly integrate different types of geospatial and tabular information; define complex, multi-source metrics; and perform sophisticated analyses of the results.

Note that the only part of this work that was completed was developing general guidelines and a conceptual framework for the V&V process.

3.0 Results

The project got to the point of developing a framework for understanding the V&V needs for Thrusts 1 and 2 as depicted in Figure 2.

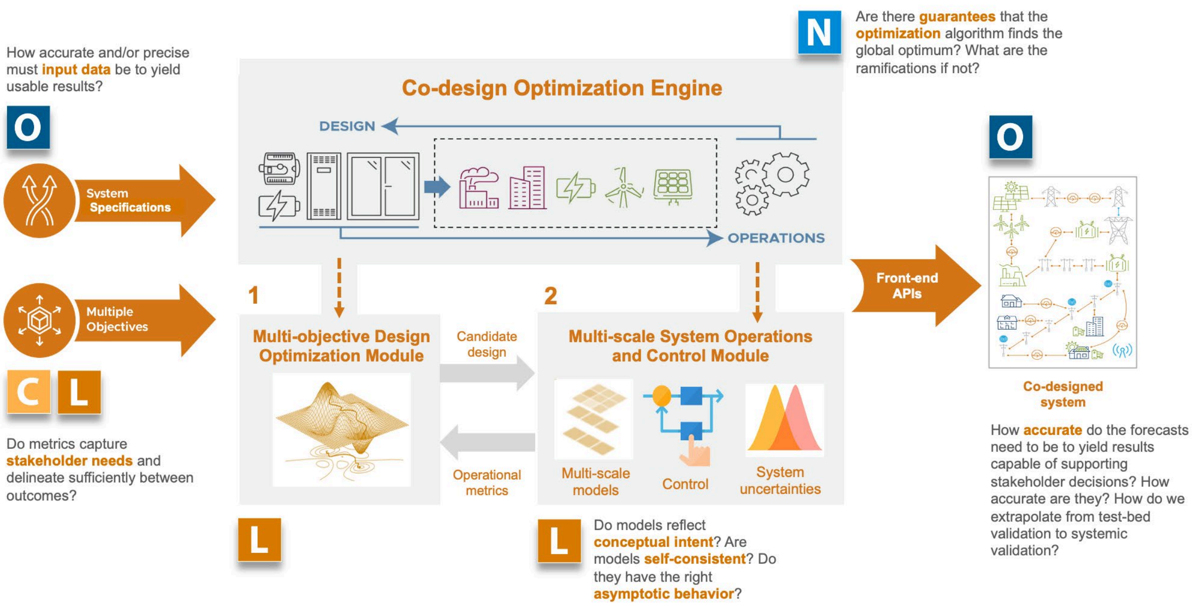


Figure 2: Initial application to Thrusts 1 & 2

A general set of validation steps were also identified as detailed below and which are also shown in a flow chart form in Figure 2.

Conceptual Validation – Problem specification, analytic questions, applicable use cases, key inputs/parameters; does conceptual solution address these considerations.

Logical Validation – Faithfulness of mathematical model, self-consistency, asymptotic behavior, epistemic uncertainty in structure and context

Numerical Validation – Local vs globally optimal solutions, solver efficiency and accuracy, repeatability, scalability

Operational Validation – Aleatoric uncertainty, exogenous variables, non-stationarity, availability of data for comparison, validation metrics, acceptable error

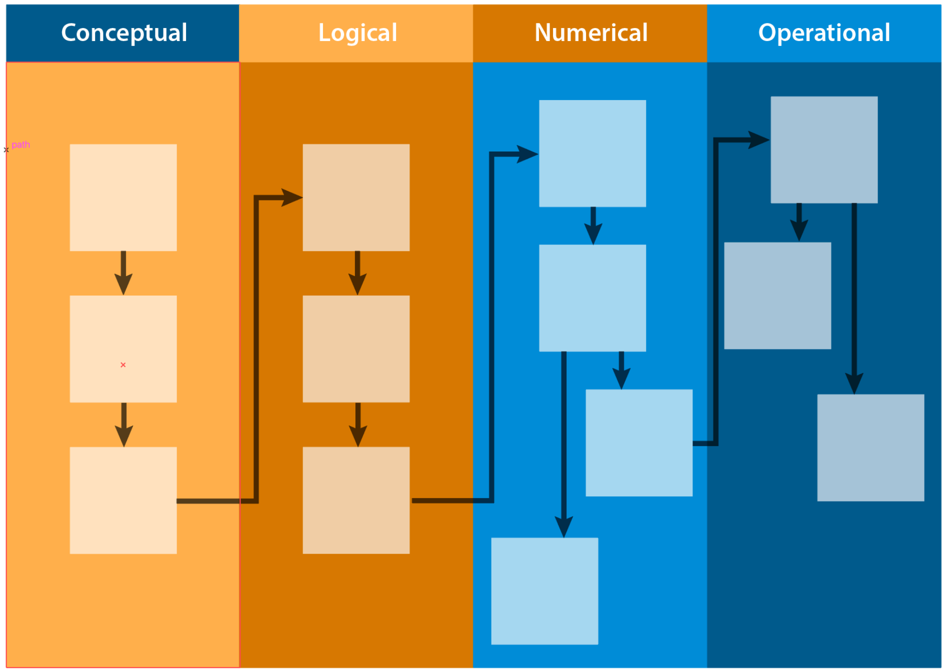


Figure 3: Develop multistage V&V prompts and guidance to highlight relevant V&V needs, methods, and measures at each stage of model development.

The work that was completed also identified several challenges to performing scientific validation:

- **Validating Authority**
    - Validation by **model developers** – with or without user involvement (for smaller working groups)
    - Model validation by an **independent third party** (concurrent or post-facto, for large projects).
- **Validation Risks & Consequences**
    - **Risk** is a function of system importance and intended use of models, e.g., video games vs autopilots.
    - Incomplete or **improper validation poses risks** to both users and model developers.
- **Unique Challenges**
    - Sensitivity to initial conditions
    - Emergent behavior
    - Artificial system boundaries
    - Feedback loops
    - Nonlinear relationships
    - Complex, spatiotemporally heterogeneous results

These validation challenges are also coupled with those related to the operational aspect as listed below.

- Are the critical aspects of the modeled system **observable**?
- **Data availability** and validity/uncertainty
- **Non-stationarity** of modeled system

- **Aleatoric parameter uncertainty**, exogenous variables
- Appropriate **validation metrics** that capture mission or user-specific criteria
- What is the **requisite accuracy** level?
- **How long** is validation good for?
- **Research-grade** versus **commercial** versus **regulatory** validation (level of trust)

It was also identified that to achieve a good V&V outcome, certain coding practices should be observed with the objective of developing a clear, practical guidance on how coding practices can be implemented on E-COMP projects and systems, specifically:

- R&D code development has **different software quality assurance needs** than large commercial products or high assurance software.
- Proposed coding practices must be **streamlined** enough that researchers will adopt them while providing sufficient validation to **reduce risk** to staff and customers to acceptable levels.
  - What can be **automated**?
    - **Testing**, **documentation**, continuous integration
  - What can be integrated into the existing **workflows**?
    - **Version control** systems, architectural and naming **standards**
- Well-defined processes can produce more **robust**, **reusable products** that can more easily be combined into larger systems.

The goal should be to Identify and evaluate **best practices** that enable agile development of high-quality models and frameworks addressing the following key areas:

- **Maintainability**
  - Coding standards
  - Naming conventions
  - Refactoring
  - Code reviews
  - Version control systems
  - Documentation & comments
- **Robustness**
  - Automated testing
  - Test-driven development
  - Continuous integration
  - Error handling
- **Collaboration**
  - Code re-use and modularization

Finally, basic guidelines for validation metrics were outlined as follows:

- Validation metrics are **context dependent.**
- They should **highlight relevant characteristics** w.r.t. addressing the use cases and analytic questions of interest (e.g., Thrust 3)
- Help drive understanding of requisite, context-dependent **accuracy.**

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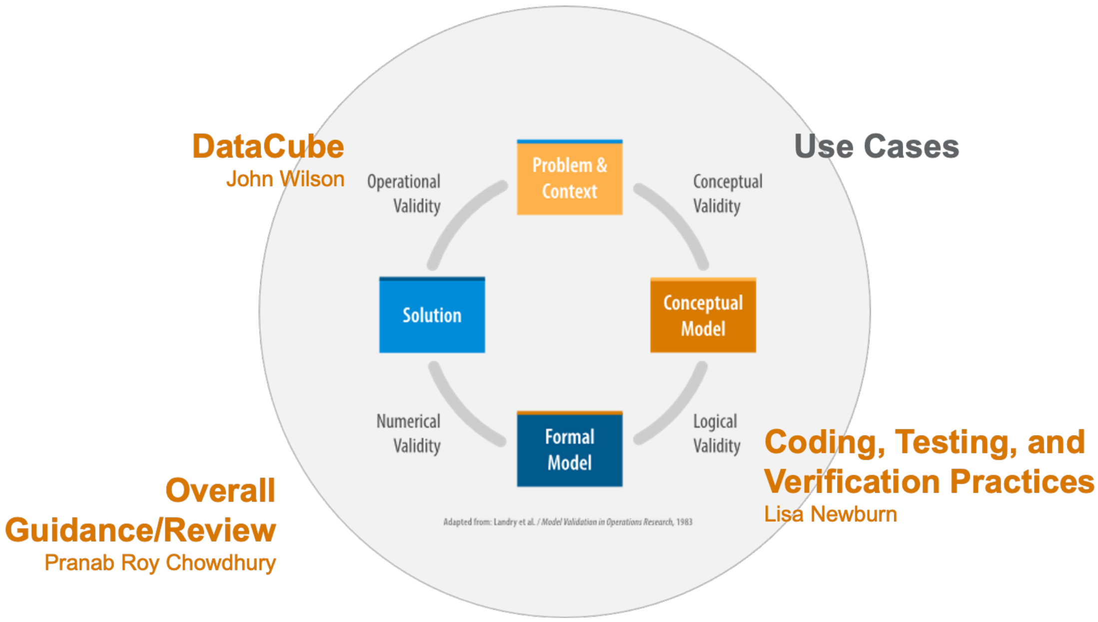
Appendix A – Standard V&V model linked to guidelines



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