




# State of the Art in Validation for Low Temperature Plasma Simulations and Experiments



*Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & 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.*

Matthew Hopkins, Sandia National Laboratories

Workshop at the 73<sup>rd</sup> GEC

October 5, 2020

# Introduction

Ultimately, *validation* of a *verified* code is relied upon for claiming *predictivity*. This is rarely done in a strong formal manner, although some examples exist. Instead, various kinds of evidence are used (sometimes indirectly) to spin a story of confidence in results. This workshop will highlight some of the leading efforts in validation in the community. Apologies to other groups and efforts that were not included – there is only so much capacity!

- Verification = “Confirming the simulation tool is solving the mathematical model equations correctly”, “Solving the equations correctly”.
- Validation = “Comparing a simulation output to an experimental output”, “Solving the right equations”.
- A validation exercise must be focused on applying a particular code to a particular application; a code cannot be validated in general.

# Workshop Goals

Prompts for discussion and panel at the end:

- Consider the axis:

Qualitative → Quantitative → Predictive

- Qualitative: Reproducing a trend (e.g., ionization rate increases).
- Quantitative: Comparing specific numerical experimental measurements to simulation ones; Significant calibration.
- Predictive: Uncertainty estimates (standard deviations, error bars) for simulation and/or experiment output; Less or no calibration; Significant evidence of accuracy across parameter space.
- “We got a bad result/comparison” with good validation methodology (high confidence) is a better outcome than “We got a great result/comparison” with bad validation methodology (low confidence). The first is an actionable result.



# Workshop Goals

Prompts for discussion and panel at the end:

- What level of validation is appropriate for your work?
  - Internal working group expectations?
  - Journal expectations?
  - Customer expectations? (do they know this is a question?)
- Can you estimate the cost of validation?
- Recommendations for others? What do you consider a best practice?
- What next advances should be pursued?
- What are the significant gaps?