



Workshop #7

Improving the Verification and Validation Process

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The widespread employment of large, complicated simulation codes for physical phenomena in computational science and engineering requires a vigorous effort to insure the correctness of these simulation codes. This insurance comes from the verification and validation (V & V) process employed by the designers of the simulation codes. The V&V process can be almost as time consuming as the original code development process. The purpose of this workshop is to show how automatic differentiation (AD) and statistical experiment augmentation tools can improve the V&V process. In the workshop, we will focus on 4 elementary, but important techniques.

Specifically, we will look into:

- 1) Validation using calibrate-and-regress. Specifically, the calibration portion of this process can be made to go faster.
- 2) Verification using Method-of-Manufactured-Solutions (MMS). It is possible to automate a fair portion of this technique, using AD tools.
- 3) Uncertainty Quantification using Method of Moments. For "small" uncertainty regions, AD tools make it possible to compute mean and variance of outputs reasonably automatically and efficiently.
- 4) Simulation-based Augmentation of Experiments By augmenting experiments with detailed simulation-based physical models, one can greatly leverage the amount of information that even a limited set of experiments can provide. This part of the workshop will discuss approaches and methods for combining experimental information with simulation runs to calibrate unknown model parameters, quantify uncertainty in predictions, and to characterize systematic discrepancies between model and experiment.