Classification Systems for V&V Benchmark Data

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Where Do Simulation Error Bars Come From?

Ideally, simulation error bars include:

- Numerical error (solution verification)
- Parametric uncertainty (uncertainty quantification)
  - Numerical method parameters
  - Model parameters
  - Parameters related to the flow configuration ←Today's topic

Ideally, we distinguish between these and can track them separately.

In validation, we are trying to determine (or bound) the model form error; to do so we must account for numerical errors and parametric uncertainties.

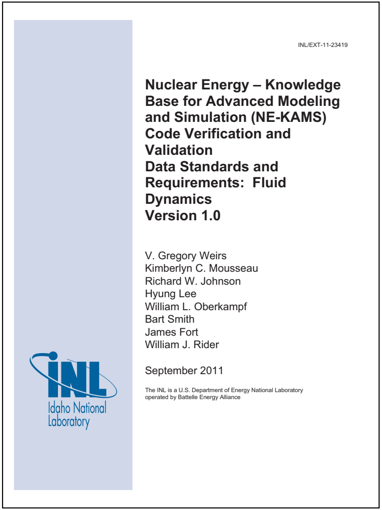
Why Data Standards? Why a Classification System?

There are many motivations for the current work, but start with this one:

A request from a computational analyst performing a validation study to the experimentalist.

- I want my validation effort to be conclusive.
- I don't want to make any unnecessary assumptions.
- I am relying on your expertise.

"NE-KAMS Data Standards" – A Classification System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Nuclear Energy – Knowledge Base for Advanced Modeling and Simulation (NE-KAMS) Code Verification and Validation Data Standards and Requirements: Fluid Dynamics Version 1.0

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The INL is a U.S. Department of Energy National Laboratory operated by Battelle Energy Alliance

Developed under NE-KAMS and focuses on fluid dynamics for nuclear power applications. Three main sections:

- Overarching framework for V&V
- Specific frameworks for code verification and validation, patterned broadly after PCMM

Version number acknowledges that ideas will be refined

NE-KAMS Validation Data Standards

The validation data standards were developed by Bill Oberkampf and Bart Smith; see the NE-KAMS report and the upcoming paper "Assessment Criteria for Computational Fluid Dynamics Validation Benchmark Experiments" (AIAA SciTech Conference, Jan. 2014) for a complete description

The validation data standards:

- clarify reporting and documentation requirements for validation experiments
- emphasize completeness of information provided
- help computational analysts set up simulations of the experiment

NE-KAMS Validation Data Standards Table (Partial)

COMPLETENESS / ATTRIBUTES	Completeness Level 0	Completeness Level 1	Completeness Level 2	Completeness Level 3
1. Experimental Facility	• Little or no description of the facility or its operation	• Some information on the functional operation of the facility and its operating procedures • Some information on the geometric and equipment features of the facility	• Detailed information on the functional operation of the facility and its operating procedures • Detailed information of the geometric and equipment features of the facility • Some information on the calibration procedures and reference standards for the facility • Some information on the calibration results and characterization of the facility	• Detailed information of the fine-scale flow features/environment inside the test section • Some information of the fine-scale flow features or physical processes upstream and downstream of the test section • Detailed information on the calibration procedures and reference standards for the facility • Detailed information on the calibration results and characterization of the facility • Information on the inspection, maintenance, and repairs of the facility
2. Analog Instrumentation and Signal Processing	• Little or no information on sensors and calibration procedures • Little or no information on instrumentation • Little or no information on signal processing	• Some information on sensors and calibration procedures • Some information on transducers • Some information on signal processing	• Detailed information on sensors and calibration procedures • Detailed information on transducers • Detailed information on signal processing • Some assessment of instrument performance and suitability	• Use of independent sensors and calibration procedures • Use of independent/alternative signal processing procedures • Detailed assessment of instrument performance and suitability
3. Boundary and Initial Conditions	• Little or no information on boundary conditions • Little or no information on initial conditions • Little or no	• Some inflow quantities measured • Some wall quantities measured • Some initial conditions measured • Detailed model-design	• Most inflow quantities measured • Most wall quantities measured • Most initial conditions measured • Detailed as-built model dimensions measured • Some outflow and reverse flow quantities measured	• Fine-scale inflow quantities measured • Fine-scale wall quantities measured • Fine-scale outflow quantities measured • Fine-scale initial conditions

Attributes and Completeness Levels

Attributes: Categories of information, aspects of an experiment aligned to establish a computational model

- Experimental facility
- Analog instrumentation and signal processing
- Boundary and initial conditions
- Fluid and material properties of the walls
- Test conditions
- Measurement of experimental responses

Levels: From 0 to 3, increasing amount of information for each attribute

Experimental Facility

How does the facility work, how are flow conditions are controlled, and how was it operated for the particular experiment?

Level 0:

- Little or no description of the facility or its operation

Level 1:

- Some information on the functional operation of the facility and its operating procedures
- Some information on the geometric and equipment features of the facility

Experimental Facility (2)

Level 2:

- Detailed information on the functional operation of the facility and its operating procedures
- Detailed information of the geometric and equipment features of the facility
- Some information on the calibration procedures and reference standards for the facility
- Some information on the calibration results and characterization of the facility

Experimental Facility (3)

Level 3:

- Detailed information on the fine-scale flow features/environment inside the test section
- Some information on the fine-scale flow features or physical processes upstream of the test section
- Detailed information on the calibration procedures and reference standards for the facility
- Detailed information on the calibration results and characterization of the facility
- Information on the inspection, maintenance, and repairs of the facility

Analog Instrumentation and Signal Processing

What sensors and diagnostic equipment are used, how are they calibrated, where are they located, and how are the raw measurements processed to arrive at the results reported?

Level 3:

- Use of independent sensors and calibration procedures
- Use of independent/alternative signal processing procedures
- Detailed assessment of instrument performance and suitability

Boundary and Initial Conditions

What are the conditions at all the domain boundaries a computational analyst might consider? If an analyst might assume some conditions, what information is provided to justify these assumptions?

Level 2:

- Most inflow quantities measured
- Most wall quantities measured
- Most initial conditions measured
- Detailed as-built model dimensions measured
- Some outflow and reverse flow quantities measured

Level 3:

As level 2, but for fine-scale (turbulent) quantities

Fluid and Material Properties of the Walls

What are the properties and conditions of the fluid? What are the properties and conditions of the domain boundaries?

Level 3:

- All thermodynamic, transport, and optical properties of the fluid(s) are provided, as well as how these are determined
- Thermal, mechanical, and optical properties of the wall(s) are provided
- Detailed description of additional phases is provided, plus size distribution statistics

Test Conditions

What are the properties and conditions of the fluid? What are the properties and conditions of the domain boundaries?

Level 3:

- Detailed description of operational procedures for setting and controlling test conditions
- Detailed measurement of time and spatial variation of test conditions

Examples: temporal variation of the temperature of the fluid over a long running experiment, or ambient room conditions, or bubble concentration in a recirculating water tunnel

Measurement of Experimental Responses

For the quantities of interest, what information is given about the their variability and uncertainty? How extensive is the spatial coverage of the QoIs? How extensive is the variety of the QoIs?

Level 3:

- Use of independent data acquisition procedures
- Description of sensitivity of experimental responses to control of test conditions
- Video recording of measurement procedures and data acquisition provided
- All experimental responses reported with estimated bias and random uncertainties, including correlated uncertainties

Let's Do An Experiment

Nice ideas. Do they really work?

Two experiments were assessed to try out the NE-KAMS Data Standards. For these initial assessments:

- focus on the process and the standards, not the experiments and the particular levels achieved
- actual process used was ad hoc, but still informative

Example 1: ERCOFTAC QNET-CFD Knowledge Base

ERCOFTAC: European Research Community on Flow, Turbulence, and Combustion

The QNET-CFD Knowledge Base has evolved over 20 years.

- A case in the "Gold" domain "has been carefully checked and therefore satisfies high quality standards" and also includes a quality review as contributed by one or more reviewers
- A case in the "Silver" domain "is less mature" and is "still under discussion and open for improvement"

Example 1: QNET-CFD Format

Case structure

- Front Page
- Description
- Test Case Studies
- Evaluation
- Best Practice Advice
- References
- Quality Review (gold)

Essentially, a canonical format for a journal article

Example 1: Case UFR 3-30, "2D Periodic Hill Flow"

QNET-CFD Quality Level: "Silver domain plus gold star"

Attribute	Level
Experimental facility	0
Analog Instrumentation and Signal Processing	1
Boundary and Initial Conditions	1
Fluid and Material Properties of the Walls	0
Test Conditions	1
Measurement of Experimental Responses	1

Experiment is high quality; reporting is as good as any other case in QNET-CFD

QNET-CFD case format was not designed for level of validation rigor needed today.

Example 2: Argonne MAX

- Currently operational experiment; producing data for about one year
- Data provided directly by experimentalist
- Examples of results data were provided due to amount of data
- Data was provided for a different purpose, not guided by NE-KAMS data standards or a detailed request

Sample artifacts:

- LabVIEW documentation
- LabVIEW virtual instrument files
- LabVIEW results flow and temperature data
- post processed LabVIEW results spreadsheet
- example PIV image pairs
- example PIV instantaneous and average velocity fields

Example 2: Initial Assessment

Attribute	Level
Experimental facility	2
Analog Instrumentation ans Signal Processing	2
Boundary and Initial Conditions	0
Fluid and Material Properties of the Walls	1
Test Conditions	0
Measurement of Experimental Responses	2

More data available; would improve completeness levels attained

Interaction could be more like a collaboration – synergy

Need a system for collecting, maintaining, finding, and distributing artifacts of the experiment – NE-KAMS

Lessons Learned: NE-KAMS Data Standards

- Consider adding information about the intent of the experiment, either as an attribute or separate item.
- Depending on the experiment, some attributes are less relevant.
- Completeness levels should not be viewed as a linear scale.
- It is difficult to identify all the critical information; this is why validation collaborations are more effective.
- Consider completeness levels for each diagnostic or each experimental response, if applicable.

Data Standards – Why Do It?

Is this a lot more work for experimentalists?

Yes:

- It's hard enough to collect the information I report now, this is a lot more.
- There are no tools to collect and distribute this information.

No:

- Good experimentalists are already chasing down a lot of issues to make the experiment successful. Document it and get credit for it.
- Better documentation and more transparency will distinguish better work.
- Your data will be used by more computational analysts if it is well documented.

Better documentation raises the bar on the simulation side as well.