# V&V 2016
## ASME VERIFICATION AND VALIDATION SYMPOSIUM

CONFERENCE
May 18-20, 2016
The Westin Las Vegas, Las Vegas, Nevada

# Program

www.asme.org/events/vandv

ASME
SETTING THE STANDARD

The American Society of Mechanical Engineers (ASME)

# Welcome

## to ASME's 2016 Verification and Validation Symposium!

Dear Colleagues:

Thank you for participating in ASME's annual Verification and Validation Symposium, dedicated entirely to verification, validation and uncertainty quantification of computer simulations. The outstanding response to the call for abstracts has allowed us to create a technical program that has improved each year by bringing together engineers and scientists from around the world and from diverse discipline: all of whom use computational modeling and simulation.

Our goal is to provide you and your fellow engineers and scientists—who might normally never cross paths—with the unique opportunity to interact by exchanging ideas and methods for verification of codes and solutions, simulation validation and assessment of uncertainties in mathematical models, computational solutions and experimental data.

The presentations have been organized both by application field and technical goal and approach. We are pleased that you are here with us and your colleagues to share verification and validation methods, approaches, successes and failures and ideas for the future.

Thanks again for attending. We look forward to your valued participation.

Sincerely,

Symposium Co-Chairs

**Symposium Co-Chairs**


**Ryan Crane**

ASME

New York, NY, United States



**Scott Doebling**

Los Alamos National Laboratory

Los Alamos, NM, United States



**Christopher Freitas**

Southwest Research Institute

San Antonio, TX, United States

# Contents

# General Information

## REGISTRATION HOURS AND LOCATION

Registration is in the Casuarina Foyer, 2nd Floor.

Registration Hours:

| | |
|---|---|
| Tuesday, May 17: | 5:00pm – 7:00pm |
| Wednesday, May 18: | 7:00am – 6:00pm |
| Thursday, May 19: | 7:00am – 6:00pm |
| Friday, May 20: | 7:00am – 12:30pm |

## HOTEL BUSINESS SERVICES

The business center is located on the first floor in the lobby.

Business hours are:

| | |
|---|---|
| Monday – Friday: | 7:00am – 6:00pm |
| Saturday: | 9:00am – 12:00pm |
| Sunday: | Closed |

## ACKNOWLEDGEMENT

The Verification and Validation Symposium is sponsored by ASME. All technical sessions and conference events will take place at The Westin Las Vegas. Please check the schedule for event times and locations.

## REGISTRATION FEES

Full Registration Fee includes:

- Admission to all technical sessions.
- All scheduled meals.
- Symposium program with abstracts.

One-day Registration Fee includes Admission to events above for that day.

## NAME BADGES

Please wear your name badge at all times; you will need it for admission to all symposium functions unless otherwise noted. Your badge also provides a helpful introduction to other attendees.

## TAX DEDUCTIBILITY

Expenses of attending a professional meeting such as registration fees and costs of technical publications are tax deductible as ordinary and necessary business expenses for U.S. citizens. Please note that tax code changes in recent years have affected the level of deductibility.

## FREE ASME MEMBERSHIP

Non-ASME Members who pay the non-Member symposium registration fee, including students who pay the non-Member student fee, will receive a FREE one-year ASME membership. ASME will automatically activate this complimentary membership for qualified attendees. Please allow approximately 4 weeks after the conclusion of the conference for your membership to become active. Visit www.asme.org/membership for more information about the benefits of ASME Membership.

## INTERNET ACCESS IN THE HOTEL

High-speed wireless internet is included in your guest room at The Westin Las Vegas. Free Wi-Fi is also available in the lobby of The Westin. Check the ASME registration desk for other Wi-Fi options.

## EMERGENCY

In case of an emergency in the hotel, pick up any house phone which rings directly to Service Express. From there, operator can then dispatch.

## ACCESSIBILITY AND GENERAL QUESTIONS

Whenever possible, we are pleased to accommodate attendees with special needs. Advanced notice may be required for certain requests. For on-site assistance related directly to the conference events and for general conference questions, please visit the ASME registration desk. For special needs related to your hotel stay, please visit the Planet Hollywood concierge or front desk.

## NETWORKING RECEPTION AND ASME V&V COMMITTEE MEETING SCHEDULE

All meetings are open to the public and Symposium attendees are welcome to attend.

**Networking Reception followed by the Vs&V Standards Committee Meeting**
**Wednesday, May 18, 6:00pm-8:00pm**
**Casuarina Ballroom, 2nd Floor**

- V&V Standards Committee on Verification and Validation in Computational Modeling and Simulation
  - Charter: Coordinate, promote, and foster the development of standards that provide procedures for assessing and quantifying the accuracy and credibility of computational models and simulations
- Presentations and an open discussion on the standards development activities and future efforts

**Tuesday, May 17, 8:00am-5:00pm**

- V&V 10 Subcommittee on Verification and Validation in Computational Solid Mechanics – Mesquite 2, 2nd Floor
- V&V 20 Subcommittee on Verification and Validation in Computational Fluid Dynamics and Heat Transfer – Acacia B, 2nd Floor
- V&V 30 Subcommittee on Verification and Validation in Computational Simulation of Nuclear System Thermal Fluids Behavior – Mesquite 4, 1st Floor
- V&V 40 Subcommittee on Verification and Validation in Computational Modeling of Medical Devices – Acacia C-D, 2nd Floor
- V&V 50 Subcommittee on Verification and Validation of Computational Modeling for Advanced Manufacturing – Casuarina Ballroom, 2nd Floor

## ASME V&V STANDARDS DEVELOPMENT COMMITTEES

As part of this effort, the following ASME committees coordinate, promote and foster the development of standards that provide procedures for assessing and quantifying the accuracy and credibility of computational models and simulations.

ASME V&V Standards Committee – Verification and Validation in Computational Modeling and Simulation

ASME V&V 10 – Verification and Validation in Computational Solid Mechanics

ASME V&V 20 – Verification and Validation in Computational Fluid Dynamics and Heat Transfer

ASME V&V 30 – Verification and Validation in Computational Simulation of Nuclear System Thermal Fluids Behavior

ASME V&V 40 – Verification and Validation in Computational Modeling of Medical Devices

ASME V&V 50 – Verification and Validation of Computational Modeling for Advanced Manufacturing

Interested applicants should contact Ryan Crane at craner@asme.org

**WEDNESDAY, MAY 18**
**8:00am - 10:00am**
**Acacia D, 2nd Floor**

## PLENARY 1: INTEGRATION OF CALIBRATION, VERIFICATION AND VALIDATION RESULTS IN MULTI-LEVEL SYSTEMS

**Dr. Sankaran Mahadevan**
John R. Murray Sr. Professor of Engineering,
Vanderbilt University

Professor Sankaran Mahadevan has twenty-seven years of research and teaching experience at Vanderbilt University, in the areas reliability and risk analysis, design optimization, structural health monitoring, model verification and validation, and uncertainty quantification. His research has been extensively funded by NSF, NASA, FAA, DOE, DOD, DOT, NIST, General Motors, Chrysler, Union Pacific, American Railroad Association, and Sandia, Idaho, Los Alamos and Oak Ridge National Laboratories. He is the founder-director of graduate studies in risk, reliability and uncertainty methods at Vanderbilt, funded by the NSF-IGERT program. His research contributions are documented in more than 450 publications, including two textbooks on reliability methods and 200 journal papers. He has directed 40 Ph.D. dissertations and 24 M. S. theses, and has taught industry short courses on reliability and uncertainty analysis methods. His awards include the NASA Next Generation Design Tools award (NASA), the SAE Distinguished Probabilistic Methods Educator Award, and best paper awards in the MORS Journal and the SDM and IMAC conferences. He currently serves as Associate Editor for two journals (ASCE-ASME Journal on Risk and Uncertainty in Engineering Systems, and ASCE Journal of Engineering Mechanics), and as Co-Chair of the EMI 2016 and PMC 2016 Conferences. Professor Mahadevan obtained his B.S. from Indian Institute of Technology, Kanpur, M.S. from Rensselaer Polytechnic Institute, Troy, NY, and Ph.D. from Georgia Institute of Technology, Atlanta, GA.

**Abstract:** The presentation discusses recent developments in rolling up model verification, validation, and calibration results at multiple levels of the system hierarchy, in order to quantify the uncertainty in system-level prediction. Among multiple competing approaches for these activities, the approaches suitable for a roll-up methodology are identified. The individual models, their inputs, parameters, and outputs, experimental data, and various sources of model error are connected through a Bayesian network. The results of calibration, verification, and validation with respect to each individual model are integrated using the principles of conditional probability and total probability, and propagated through the Bayesian network in order to quantify the overall system-level prediction uncertainty. The relevance of each level of the system hierarchy to the overall system-level quantity of interest is also included in the roll-up framework. Novel strategies for sensitivity analysis are introduced, which facilitate optimum resource allocation decisions for testing and modeling activities at different levels of the system hierarchy.

## PLENARY 2: RESPONSES TO THE NASA LANGLEY UNCERTAINTY QUANTIFICATION CHALLENGE

**Dr. Luis G. Crespo**
Senior Research Engineer,
NASA Langley Research Center

Luis G. Crespo received a Bachelor and Masters degree from Universidad de Los Andes, Bogota, Colombia; and Ph.D. degree in Mechanical Engineering from University of Delaware in 2002. He currently serves as a Senior Research Engineer for the Dynamic Systems and Controls Branch of NASA Langley Research Center. He has worked for the Institute for Computer Applications to Science and Engineering (ICASE), the National Institute of Aerospace (NIA) and the Uncertainty Quantification, Model Verification and Validation Department of Sandia National Laboratories. His research interest are in the fields of dynamics and control, analysis and control of uncertain systems, and optimization under uncertainty. He is the author of over 80 publications in international journals and conferences.

**Abstract:** NASA missions often involve the development of new vehicles and systems that must be designed to operate in harsh domains with a wide array of operating conditions. These missions involve high-consequence and safety-critical systems for which quantitative data is either very sparse or prohibitively expensive to collect. Limited heritage data may exist, but is also usually sparse and may not be directly applicable to the system of interest, making uncertainty quantification extremely challenging. NASA modeling and simulation standards require estimates of uncertainty and descriptions of any processes used to obtain these estimates. The NASA Langley Research Center developed an uncertainty quantification challenge problem in an effort to focus a community of researchers towards a common problem. This challenge problem featured key issues in uncertainty characterization, sensitivity analysis, uncertainty propagation, extreme-case analysis, and robust design. Whereas the formulation is indeed discipline-independent, the underlying model, as well as the requirements imposed upon it, describes a realistic aeronautics application. This talk will cover the problem statement, the practical significance of the technical challenges raised and a summary of responses. Such responses are compiled in eleven journal publications led by discipline experts from Government agencies, industry, and academia.

**THURSDAY, MAY 14**
**8:00am-10:00am**
**Acacia D, 2nd Floor**

### PLENARY 3: TURBULENCE MODEL VERIFICATION AND VALIDATION

**Dr. Chris Rumsey**
Senior Research Scientist,
NASA Langley Research Center

Dr. Chris Rumsey has worked at NASA Langley Research Center in the area of computational fluid dynamics (CFD) since 1983. He received his doctoral degree in Aerospace Engineering from the University of Michigan in 1991. Throughout his career, he has focused in a variety of CFD areas, including numerical algorithms, unsteady flow applications, high lift, flow control, turbulence modeling, and verification and validation.

He has helped to lead the CFD General Notation System (CGNS) steering committee, which develops and supports an international standard for CFD data storage. In 2013, he received the AIAA Excellence in Aerospace Standardization Award for this work.

He has been an AIAA Fellow since 2011, and has served as Chair of the AIAA Hampton Roads Section and

President of the Peninsula Engineers Council.

About 8 years ago, in association with the AIAA Turbulence Model Benchmarking Working Group, Dr. Rumsey created the NASA Langley Turbulence Model Resource Website, which he still actively maintains. This widely-used site provides a central location where Reynolds-averaged Navier-Stokes turbulence models are documented, verified, and validated. In 2015, Dr. Rumsey received a NASA Agency Exceptional Service Medal for his work on the TMR website.

Dr. Rumsey is the author of over 55 journal articles and over one hundred conference papers and other CFD-related reports.

**Abstract:** CFD code verification is a necessary step in the code development process, but it is not always done. In the aerospace field, countless validation workshops have been undermined by the lack of participant code verification and the ensuing inevitable disparity between results. When one does not know if computed solution differences are due to turbulence model implementation details, coding bugs, discretization errors, or the models themselves, it is nearly impossible to draw any firm conclusions. Fortunately, a well-executed “verification by comparison” (or “inter-code comparison”) can help to establish confidence that a turbulence model has been implemented correctly, especially if at least one of the codes has also undergone a more rigorous exercise such as method of manufactured solution. This process, which involves a well-designed grid-convergence study, requires that any given solution characteristic approaches the same result for multiple codes as the grid is refined. This is one of the central ideas behind the NASA Langley Turbulence Modeling Resource (TMR), located at http://turbmodels.larc.nasa.gov. By providing grids and solutions for a variety of cases and turbulence models, the TMR encourages users to run their own CFD codes and verify by comparison. Although not 100% foolproof, this method continues to gain traction as more and more codes perform the posted studies and achieve the same results when using the same models. The TMR also documents the turbulence model equations, establishing naming conventions for many of the model variants found in the literature. Furthermore, the website provides many relatively simple validation cases, along with grids and solutions, in an effort to cover a wide variety of flow physics.

This talk will establish context by summarizing several previous RANS validation workshops. Then it will provide many details about the TMR website, including ways it has recently been employed at workshops and special technical sessions, toward the goal of achieving a broader landscape of verified CFD codes for aerospace applications.

### PLENARY 4: MATURATION OF MANUFACTURING PROCESS MODELS FOR AEROSPACE APPLICATIONS

**Dr. Mark D. Benedict**
Materials Engineer,
Air Force Research Laboratory

Dr. Mark D. Benedict is a computational materials scientist and program manager in the Propulsion, Structures & Industrial Technologies Branch, Manufacturing Technology Division, Materials and Manufacturing Directorate, Air Force Research Laboratory, Air Force Materiel Command, Wright-Patterson Air Force Base, Ohio in the area of Additive Manufacturing (AM) and Verification & Validation (V&V) of ICME models. Dr. Benedict conducts and directs research in the areas of metals and plastics additive manufacturing and is a recognized expert on additive manufacturing process modeling. He is currently a research active manager for several large and novel Data Science and AM programs in the areas of additive manufacturing variability assessment, analytics driven sustainment, and validation of electroslag remelting process models.

As part of his role as V&V lead for the Intergrated Computational Materials Science and Engineering IPT, he has helped to define directorate wide requirement for data management planning. Additionally he is the Vice Chair of the recently formed V&V 50 subcommittee on Verification & Validation of Computational Modeling for Advanced Manufacturing.

**Abstract:** Manufacturing Science and Technology programs within the Department of Defense have long supported the development and maturation of materials process modeling efforts to increase affordability and producibility of defense systems. The best practices identified by the Integrated Computational Materials Engineering (ICME) approach are central to recent efforts for materials model maturation within the Air Force Research Laboratory (AFRL), in particular, increased support for manufacturing focused uncertainty quantification and verification and validation efforts have led to improved confidence in the predictive power and utility of key manufacturing process models.

This talk will present two case studies intended to represent the diversity of verification, validation, and uncertainty quantification issues that AFRL is currently supporting, and provoke discussion about the challenges of material process model validation. The first case study highlights a large program designed to support model development in the area of Additive Manufacturing. It is primarily an uncertainty quantification effort that probes the “as manufactured” variability of a large number of AM

fabricated parts. Early findings will be presented including the correlation between best practice manufacturing factors and part variability. The second case study is a more conventional validation effort for a high-value metals refining process known as Electroslag Remelting (ESR). This four year effort highlights typical challenges for materials process model validation such as lack of publically available material property data, challenging to instrument processes, and relative scarcity of validation experiments.

**FRIDAY, MAY 20**
**8:00am - 9:00am**
**Acacia D, 2nd Floor**

### PLENARY 5: PERSPECTIVES ON CFD V&V IN NUCLEAR REGULATORY APPLICATIONS

**Dr. Christopher Boyd**
Senior Level Advisor for Computational Fluid Dynamics,
U.S. Nuclear Regulatory Commission

Dr. Boyd is a senior level advisor for computational fluid dynamics (CFD) at the Nuclear Regulatory Commission (NRC). This role provides a bird's eye view of the CFD analyses that are completed by and submitted to the NRC. During the 1990s, Dr. Boyd led the effort to bring commercial CFD tools and high performance computing to the NRC's Office of Research. Over the past two decades, he has continued to build upon these capabilities which have supported a variety of regulatory reviews and generic safety analyses. Dr. Boyd's interests are focused on CFD benchmarking and validation efforts aimed at understanding and reducing uncertainty with the overall goal of improving regulatory effectiveness for the NRC. Previously, he spent 9 years as a wind tunnel test engineer specializing in instrumentation, calibrations, and measurement techniques for the Naval Surface Warfare Center (NSWC) in White Oak, MD. Dr. Boyd received his Ph.D. in Mechanical Engineering from the University of Maryland after completing a Master's degree in Mechanical Engineering at Johns Hopkins University.

**Abstract:** The US Nuclear Regulatory Commission (NRC) is tasked with ensuring that the commercial use of nuclear materials in the United States is safe. This includes the review and evaluation of submitted analyses that support the safety justification for specific reactor system components. Typically these analyses involve codes that have been approved for the specific application of interest and this implies that the approach has a proven history of validation and acceptance in the regulatory environment. The application of computational fluid dynamics (CFD) has become common practice in many industries. This includes the use of CFD by the nuclear industry for design and safety analyses. CFD applications that support the licensing basis of nuclear power plants are less common and have only a limited history of acceptance. This lack of experience increases the time and resources required for licensees to submit CFD simulations as well as the time required for a regulator to ensure the results are valid. The anticipated higher cost for review and acceptance can become a deterrent to the submission of results from new approaches.

The ever increasing capacity of modern computers and the growing number of capable analysts ensures us that CFD applications will become more frequent in nuclear reactor safety analysis. The emergence of small modular reactors and high temperature gas cooled reactors creates new opportunities for CFD applications to enter into the regulatory process. The job of the regulator is to ensure that these tools are properly applied in order to build up the necessary evidence of validation and acceptance that is appropriate for nuclear safety. This process is more efficient if the industry follows well documented best practice approaches for modeling and validation. National and international efforts to develop best practice guidance, verification and validation methods, and CFD grade data bases are all positive developments. The regulator faces significant challenges, however, in a field where CFD quality benchmark data for reactor issues are limited, methods are not universal, and resource limitations and user experience can impact the quality of simulations. In this challenging environment, the regulator is tasked with deciding if a given CFD simulation is good enough for the intended application. Engineering judgement still plays a key role in balancing the level of confidence in a simulation against any potential risk to the public.

There is still a great amount of work to be done to build confidence in CFD methods. The nuclear community, both the regulator and the industry, should continue to refine and maintain best practice guidelines, support the development of CFD grade benchmark data, and push for more widespread adoption of practical verification and validation techniques. Through these efforts, it is anticipated that CFD methods will grow in acceptance for nuclear reactor safety applications.

# Session Chairs

## TRACK-1 CHALLENGE PROBLEM WORKSHOPS AND PANEL SESSIONS

1-1 V&V Benchmark Problem Session 1 -- Twin Jet Computational Fluid Dynamics (CFD) Numeric Model Validation

**Hyung Lee, Bettis Laboratory, West Mifflin, PA, United States**

**Yassin Hassan, Texas A&M University, College Station, TX, United States**

**Arthur Ruggles, University Of Tennessee, Knoxville, TN, United States**

**Richard Schultz, Consultant, Pocatello, ID, United States**

**Christopher Freitas, Southwest Research Institute, San Antonio, TX, United States**

**Ryan Crane, ASME, New York, NY, United States**

1-2 V&V Benchmark Problem Session 2 -- Twin Jet Computational Fluid Dynamics (CFD) Numeric Model Validation

**Hyung Lee, Bettis Laboratory, West Mifflin, PA, United States**

**Yassin Hassan, Texas A&M University, College Station, TX, United States**

**Arthur Ruggles, University Of Tennessee, Knoxville, TN, United States**

**Richard Schultz, Consultant, Pocatello, ID, United States**

**Christopher Freitas, Southwest Research Institute, San Antonio, TX, United States**

**Ryan Crane, ASME, New York, NY, United States**

## TRACK-2 DEVELOPMENT AND APPLICATION OF VERIFICATION AND VALIDATION STANDARDS

2-1 ASME V&V Standards Development Activities: Part 1

**Christopher Freitas, Southwest Research Institute, San Antonio, TX, United States**

**Scott Doebling, Los Alamos National Laboratory, Los Alamos, NM, United States**

2-2 Development and Application of Verification and Validation Standards

**Richard J. Peppin, Engineers for Change, Inc., Rockville, MD, United States**

2-3 ASME V&V Standards Development Activities: Part 2

**Christopher Freitas, Southwest Research Institute, San Antonio, TX, United States**

**Scott Doebling, Los Alamos National Laboratory, Los Alamos, NM, United States**

## TRACK-3 TOPICS IN VERIFICATION AND VALIDATION

3-1 Enhancements of V&V Thinking and Approaches

**Vikrant Aute, University Of Maryland, College Park, MD, United States**

**David Moorcroft, Federal Aviation Administration, Oklahoma City, OK,**

3-2 Topics in Verification and Validation

**David Hall, SURVICE Engineering Company, Carlsbad, CA, United States**

**William Rider, Sandia National Laboratories, Albuquerque, NM, United States**

## TRACK-4 UNCERTAINTY QUANTIFICATION, SENSITIVITY ANALYSIS, AND PREDICTION

4-1 Uncertainty Quantification, Sensitivity Analysis, and Prediction: Session 1

**Michael Shields, Johns Hopkins University, Baltimore, MD, United States**

**Ilias Bilionis, Purdue University, West Lafayette, IN, United States**

4-2 Uncertainty Quantification, Sensitivity Analysis, and Prediction: Session 2

**Arnaud Barthet, EDF, Villeurbanne, France**

**Mark Benedict, AFRl Mantech, WPAFB, OH, United States**

4-3 Uncertainty Quantification, Sensitivity Analysis, and Prediction: Session 3

**Cosmin Safta, Sandia National Labs, Livermore, CA, United States**

**Luis Crespo, NASA Langley Research Center, Hampton, VA, United States**

4-4 Uncertainty Quantification, Sensitivity Analysis, and Prediction: Session 4

**Brian Adams, Sandia National Laboratories, Albuquerque, NM, United States**

**Ryan Jamison, Sandia National Laboratories, Albuquerque, NM, United States**

## TRACK-5 VALIDATION FOR FLUID DYNAMICS AND HEAT TRANSFER

5-1 Validation for Fluid Dynamics and Heat Transfer: Session 1

**Dimitrios Tselepidakis, ANSYS Inc., Lebanon, NH, United States**

**Marian Heller, ASME, New York, NY, United States**

5-2 Validation for Fluid Dynamics and Heat Transfer: Session 2

**Guilherme Vaz, MARIN, Wageningen, Netherlands**

**Hessam Babaee, MIT, Cambridge, MA, United States**

## TRACK-6 VALIDATION METHODS

6-1 Validation Methods: Session 1

**Upendra Rohatgi, Brookhaven National Laboratory, Upton, NY, United States**

**Mark Benedict, AFRl Mantech, WPAFB, OH, United States**

6-2 Validation Methods: Session 2

**Ding Zhao, University of Michigan, Ann Arbor, MI, United States**

**William Rider, Sandia National Laboratories, Albuquerque, NM, United States**

## TRACK-8 VALIDATION METHODS FOR IMPACT, BLAST, AND MATERIAL RESPONSE

8-1 Validation Methods for Impact, Blast, and Material Response

**Nima Fathi, University of New Mexico, Albuquerque, NM, United States**

**Christopher Freitas, Southwest Research Institute, San Antonio, TX, United States**

## TRACK-9 VALIDATION METHODS FOR SOLID MECHANICS AND STRUCTURES

9-1 Validation Methods for Solid Mechanics and Structures: Session 1

**Thomas Paez, Thomas Paez Consulting, Sedona, AZ, United States**

**April Amaral , ASME, New York, NY, United States**

9-2 Validation Methods for Solid Mechanics and Structures: Session 2

**Parham Piroozan, California State Polytechnic University, Pomona, Pomona, CA, United States**

**April Amaral , ASME, New York, NY, United States**

## TRACK-10 VERIFICATION AND VALIDATION OF NUCLEAR POWER APPLICATIONS

10-1 Verification and Validation of Nuclear Power Applications

**Lane Carasik, Texas A&M University, Marietta, GA, United States**

**Nima Fathi, University of New Mexico, Albuquerque, NM, United States**

## TRACK-11 VERIFICATION FOR FLUID DYNAMICS AND HEAT TRANSFER

11-1 Verification for Fluid Dynamics and Heat Transfer: Session 1

**Simone Youngblood, The Johns Hopkins University Applied Physics Laboratory, Laurel, MD, United States**

**William Oberkampf, W L Oberkampf Consulting, Georgetown, TX, United States**

## TRACK-12 VERIFICATION METHODS

12-1 Verification Methods (Track)

**Scott Doebling, Los Alamos National Laboratory, Los Alamos, NM, United States**

12-2 Verification Methods: Session 2

**Luis Eca, IST, Lisbon, Portugal**

**Sez Atamturktur, Clemson University, Clemson, SC, United States**

12-3 Verification Methods: Session 3

**Christopher Roy, Virginia Tech, Blacksburg, VA, United States**

## TRACK-13 VERIFICATION AND VALIDATION OF MEDICAL DEVICES

13-1 Verification and Validation of Medical Devices

**Ali Kiapour, 4WEB Medical Inc., Newton, MA, United States**

**Marian Heller, ASME, New York, NY, United States**

## TRACK-17 VERIFICATION AND VALIDATION FOR ADVANCED MANUFACTURING

17-1 Verification and Validation for Advanced Manufacturing: Session 1

**Joe Hightower, The Boeing Company, Seattle, WA, United States**

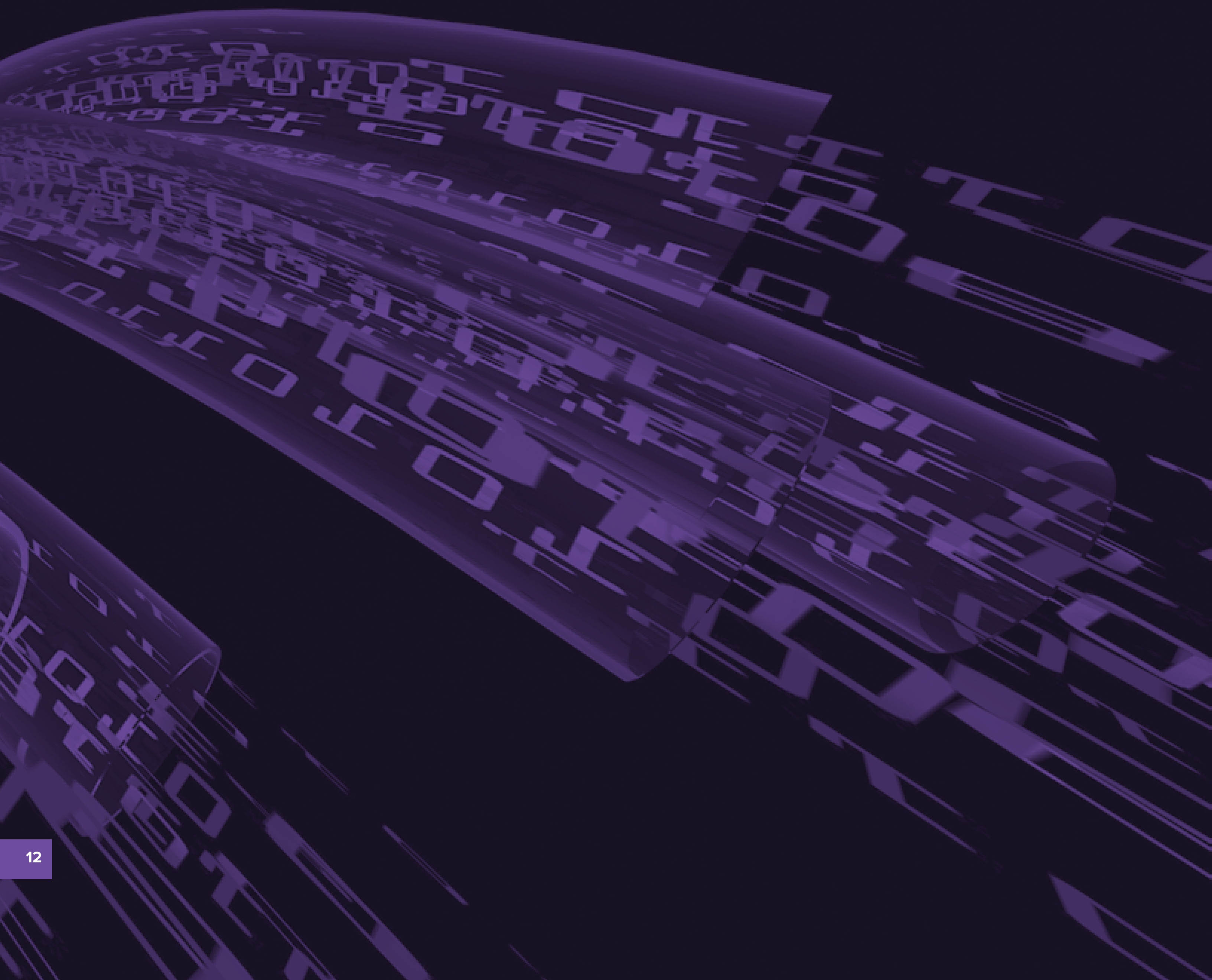
**Brian Weiss, National Institute of Standards and Technology, Gaithers-burg, MD, United States**

17-2 Verification and Validation for Advanced Manufacturing: Session 2

**Guodong Shao, NIST, Gathersburg, MD, United States**

**Huijuan Dai, GE Global Research, Niskayuna, NY, United States**

# Technical Program
# **Wednesday, May 18, 2016**



## TRACK 2 Development and Application of Verification and Validation Standards

**2-1**
**ASME V&V STANDARDS DEVELOPMENT ACTIVITIES: PART 1**
**2nd Floor, Acacia D** **10:25am - 12:30pm**

### VERIFICATION, VALIDATION AND UNCERTAINTY CONCEPTS AND THE APPLICATION OF ASME V&V STANDARDS

**Technical Presentation.** VVS2016-8946
10:25am-10:50am

**Christopher Freitas**, *Southwest Research Institute, San Antonio, TX, United States*

ASME Codes and Standards, Board On Standardization & Testing, Verification and Validation in Computational Modeling and Simulation Committee is the focus within ASME on the development of standards of practice in verification, validation, and uncertainty assessment methods for computational modeling and simulation. The V&V Committee has as its charter to coordinate, promote, and foster the development of standards that provide procedures for assessing and quantifying the accuracy and credibility of computational models and simulations. To date, the committee has created three standard or guide publications, identified as V&V10-2006, V&V20-2009, and V&V10.1-2012. Five additional publications are in progress with anticipated release dates in 2016 and 2017. To the computational modeler who wishes to learn more about "V&V&UQ", these different standards may be confusing as to where to start and what do they discuss. To address this concern, the V&V Committee is developing an additional publication with the objective to provide an introduction to ASME V&V Standards (a V&V 101, if you will). This V&V1 publication will describe (1) the mechanics and processes by which the Standards are developed, (2) provide a summary of the key definitions and concepts for V&V, (3) discuss the themes, connections and inter-relationship between the V&V publications, (4) define how to use the Standards in applications and in code accreditation, and (5) define the prerequisites or requirements if the user. This presentation will discuss the vision and objectives for the V&V1 Standard.

### V&V 20 VERIFICATION AND VALIDATION IN COMPUTATIONAL FLUID DYNAMICS AND HEAT TRANSFER

**Technical Presentation.** VVS2016-9998
10:50am-11:15am

V&V 20 Charter: Provides procedures for quantifying the accuracy of modeling and simulation in computational fluid dynamics and heat transfer. An update will be provided on the current activities of the subcommittee, including the V&V20 supplement and working group activities, including a conceptual Process for the assessment of prediction capability to support decision making, solution verification of unsteady flow calculations, and V&V concepts for non-deterministic simulations results and epistemic (lack of knowledge) uncertainties.

### REVISION OF THE "GUIDE FOR VERIFICATION AND VALIDATION IN COMPUTATIONAL SOLID MECHANICS"

**Technical Presentation.** VVS2016-8925
11:15am-11:40am

**James O'Daniel**, *USACE/ERDC, Vicksburg, MS, United States*

Since the original Verification and Validation (V&V) Committee 10 document, "Guide for Verification and Validation in Computational Solid Mechanics" was published in 2006, a considerable amount of work has been performed investigating aspects of V&V both by the committee as well as the community at large. This work, combined with the feedback that has been provided over the years, has led the committee to generate a revision to that original guide. The intent is to address multiple areas where the committee feels that the original document was ambiguous or did not adequately address a topic area. The guide will still remain an overarching document that is meant to introduce readers to the main concepts of V&V and provide high-level information about those concepts.

The committee has also produced, and is in the process of producing, several supporting documents that provide those details that the guide does not delve into. Through the development of these documents, better definitions of terms and other issues have arisen, and these generate input for the guide revision. Those documents include the publication of "An Illustration of the Concepts of Verification and Validation in Computational Solid Mechanics" and under development "Role of Uncertainty Quantification in V&V of Computational Solid Mechanics Models" and "Role of Validation Metrics in V&V of Computational Solid Mechanics Models".

An area where the original guide did not provide any information was for prediction using models after validation has been performed. While this is currently a research area, some basic knowledge is being inserted into the revision. While a complete covering of prediction is not possible, at least introducing some basic premises should aid the readers in the understanding of the role of prediction within the V&V process.

### V&V 10.3: ROLE OF VALIDATION METRICS IN COMPUTATIONAL SOLID MECHANICS

**Technical Presentation.** VVS2016-8923
11:40am-12:05pm

**David Moorcroft**, *Federal Aviation Administration, Oklahoma City, OK, United States*

The purpose of V&V 10.3: Role of Validation Metrics in Computational Solid Mechanics is to provide a primer on quantitative metrics used within the Validation process described in ASME V&V 10: The Guide for Verification and Validation in Computational Solid Mechanics. The Guide defines a validation metric as a mathematical measure that quantifies the level of agreement between simulation outcomes and experimental outcomes. An outcome is a response of interest extracted from either experimental data or simulation results, along with associated estimates of uncertainty. As such, any uncertainties in the system response quantities of interest or their features must be included in the metric calculation.

The document aims to provide background and illustrative examples rather than an exhaustive compendium of possible metrics. The user is encouraged to use this as a foundation for thoughtful establishment of metrics which highlight the properties of their model most relevant to the decision(s) to be supported by the model. The specification of the appropriate metrics and the corresponding accuracy requirements should be contained in the V&V plan and will typically depend on the types of data available and the complexity of the system to be modeled.

This talk will review response quantities and quantities with low-dimensional indicators of response, known as features, differentiate validation metrics from features, introduce different classes of metrics and provide application examples, identify the desirable characteristics of a validation metric, and provide guidance in the selection of validation metrics.

### THE ROLE OF UNCERTAINTY QUANTIFICATION IN VERIFICATION AND VALIDATION OF COMPUTATIONAL SOLID MECHANICS MODELS

**Technical Presentation.** VVS2016-8924
12:05pm-12:30pm

**Ben Thacker**, *Southwest Research Institute, San Antonio, TX, United States*

ASME V&V 10-2006, Guide for Verification and Validation in Computational

Solid Mechanics addresses an important need for a common language and process definition for V&V appropriate for analysts as well as their managers and customers. It was intended as an overview document to be followed by additional supplements containing more detailed treatments of selected topics and applications. For example, the ASME V&V 10.1-2012, An Illustration of the Concepts of Verification and Validation in Computational Solid Mechanics supplements the Guide with a simple example illustrating the key concepts in the Guide. Similarly, the purpose of this supplement is to expand upon the important role of uncertainty quantification (UQ) in the overall V&V process.

The Guide is clear that UQ plays a critical role in the model V&V process. It is generally recognized nowadays that model inputs and the form of the model itself are subject to uncertainties, which in turn leads to model predictions that are uncertain. Likewise, the experimental measurements being used in the validation also have uncertainties that must be considered. The goal, then, is to quantify the uncertainties in both the model predictions and experimental measurements such that the accuracy of the model can be assessed (validation) and the predictive accuracy of the model established quantitatively.

There are many different approaches, techniques and methods that can be used to quantify, model and manage uncertainties. Consistent with the approach taken in the Guide, this supplement will provide the groundwork for common language and process definitions associated with performing UQ in the V&V process. Where possible, the supplement will also provide discussion on how analysts might perform the UQ assessments as well as some of the primary issues and considerations to be aware of.
The main headings in the supplement will include:

1. Introduction
2. Background
3. Uncertainty Quantification in Modeling and Simulation
4. Uncertainty Quantification in Experimentation
5. Uncertainty Quantification in Model Validation Assessment
6. Model and Experiment Revision

Examples will be included, dispersed throughout the document, to demonstrate the approach or calculation (or both) being discussed.

## TRACK 4 Uncertainty Quantification, Sensitivity Analysis, and Prediction

### 4-1
### UNCERTAINTY QUANTIFICATION, SENSITIVITY ANALYSIS, AND PREDICTION: SESSION 1

**2nd Floor, Palo Verde A** **10:25am - 12:30pm**

**EXPLORING MODEL FORM UNCERTAINTY APPROACHES WITH A BURGERS' EQUATION EXAMPLE**
**Technical Presentation.** VVS2016-8833
10:25am-10:50am

**Benjamin Schroeder, Joshua Mullins**, *Sandia National Laboratories, Albuquerque, NM, United States*

Beyond considering uncertainty in model parameters and experimental data when quantifying predictive uncertainty, accounting for insufficiencies in the form of models has become an area of emphasis. Insufficiencies in the model form cause what is known as model form uncertainty, or the discrepancy between model predictions and the truth. Methods of accounting for model form uncertainty vary widely and no one method has been accepted across the VVUQ community. Model form uncertainty is known to cause identifiability issues when calibrating model parameters. Such issues have led many to incorporate model validation activities prior to making predictions. Using the 1D viscous Burgers' equation as an application example, a survey of a few methods of addressing model form uncertainty will be considered. Inadequacy in the model form for the example problem is introduced by using the linear convective diffusion equation as the model form, while the data is generated by the Burgers' equation. Implications on predictions for data types similar to that used for calibration as well as extrapolations to different data types will be considered. Methods considered in this analysis include those with Bayesian foundations as well as engineering bounds based. Through applying a diverse set of methods to a single test problem, analysis of the application and results can illuminate strengths and weaknesses of current approaches.

**SENSITIVITY ANALYSIS AND UNCERTAINTY QUANTIFICATION OF A MARS ASCENT VEHICLE MODEL**
**Technical Presentation.** VVS2016-8842
10:50am-11:15am

**Connor Noyes, Joel Benito, Lee D. Peterson**, *Jet Propulsion Laboratory, Pasadena, CA, United States*

A Mars Ascent Vehicle (MAV) is a rocket designed to put a Martian sample into orbit for a return mission to Earth. A MAV represents a challenging design problem because it must not only be capable of surviving the journey from Earth, landing at Mars, and enduring the harsh Martian atmosphere for up to a year but also of accurately inserting the sample into a specified orbit. There are a number of architectures available, and even among a single architecture there is significant design space. The key analysis goals are to improve the speed at which model uncertainty can be quantified and sensitivity to design space parameters can be estimated. If the computational effort involved in uncertainty quantification and sensitivity analysis can be reduced, then these factors can be coupled into the design iterations rather than simply performing such analyses after the design process.

Monte Carlo-based analysis is ubiquitous among engineering simulations due to its ease of implementation. It is well documented, however, that obtaining accurate statistics using Monte Carlo methods may require a large number of samples. As a result these methods are computationally expensive, even when run in parallel, and do not lend themselves well to rapid design iteration. Dakota, developed by Sandia National Labs, is a systems analysis toolkit for optimization, sensitivity analysis, uncertainty quantification, and more. A MAV represents an engineering problem wherein the design space is large and thus the opportunity exists to optimize in many ways. In addition, it is not intuitively clear as to which parameters are the most important. Which set of design choices exert the most influence on a MAV's performance? How do inherent uncertainties in the design space propagate through the model and what is their net effect on the system's performance metrics? Dakota provides multiple channels for answering these and related questions. The MAV simulation is coupled to Dakota via using the Integrated Modeling and Uncertainty Quantification software developed at JPL.

Preliminary results indicate that the statistics generated via Monte Carlo and Latin Hypercube sampling techniques can be obtained to similar accuracy via polynomial chaos expansions at a significantly reduced computational cost. There are yet other methods available in Dakota that may also prove useful. Although they may be expensive to create initially, surrogate models create a (cheaper to evaluate) approximate mapping of the input-output structure of the model. End-to-end 6DOF simulation of a MAV trajectory is computationally expensive so this manner of response surface modeling could allow for more rapid optimization of the design parameters as well as faster uncertainty quantification and sensitivity analyses. Dakota also implements reliability, epistemic, and Bayesian methods to be investigated for their suitability in enhancing design and analysis of a MAV. To the best of our knowledge, this effort marks the first attempt to make extensive use of non-Monte Carlo-based techniques to analyze high-fidelity ascent trajectory simulations.

**QUANTIFYING UNCERTAINTY IN MATERIAL MODEL SELECTION FOR FINITE ELEMENT ANALYSIS OF A HERMETIC CONNECTOR**
**Technical Presentation.** VVS2016-8846
11:15am-11:40am

**Brenton Elisberg**, *Sandia National Laboratories, Albuquerque, NM, United States*

Glass-to-metal seal (GTMS) connectors are used to feed electrical conductors through walls of hermetically sealed electronic packages. A typical GTMS connector consists of an outer metal shell that houses a glass element formed to surround an electrical conductor that passes through the metal shell. When the connector is brought to a sufficiently high temperature, typically hundreds of degrees Celsius above the glass transition temperature (Tg), the glass flows to create a seal before being cooled back to room temperature as part of the manufacturing process. Different types of seals can be created depending on the material set, but when the coefficient of thermal expansion (CTE) of the metal shell is greater than the CTE of the glass and conductor a 'compression seal' is created as the connector is cooled. High compression from the metal shell causes plastic deformation in the shell and conductor that leads to a nonlinear evolution of tensile stress in the glass that can muddle engineering intuition during the GTMS design process. Because the cost of producing a hermetic GTMS connector increases with design and material selection complexity, finite element analysis (FEA) tools are increasingly necessary during the design process to drive down cost and improve product yield.

This presentation will explore the complexities of simulating the manufacturing procedure of a hermetic GTMS connector using an amorphous Schott 8061 type glass, Alloy 52 conductors, and a stainless steel housing to produce a compression seal. Traditionally, GTMS simulations have been performed using modest constitutive models and an assumed stress free temperature of the connector close to the Tg of the glass. This has been used to predict qualitative trends in design alterations while neglecting thermal histories that can contribute to significant tensile stress in the hermetic seal. To increase quantitative fidelity, recently gathered material properties have been used to calibrate a viscoplastic constitutive model for the stainless steel and viscoelastic constitutive model for the amorphous glass. These models have been used to predict changes in the stress state of the hermetic seal due to different manufacturing histories and long-term storage of a connector. Various FEA predictions will be examined using combinations of elastic, viscoplastic, and viscoelastic constitutive models to determine the level of complexity needed for qualitative and quantitative accuracy.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

**USING A SENSITIVITY APPROACH IN ORDER TO MAKE A QUANTIFIED PIRT**
**Technical Presentation.** VVS2016-8848
11:40am-12:05pm

**Arnaud Barthet**, *EDF, Villeurbanne, France,* **Gaetan Constant**, *Datalyo, Lyon, France*

During the past two decades, CFD codes have become important partners to build up safety demonstrations for nuclear power plants. When using CFD for nuclear safety demonstration purposes, EDF applies a methodology based on physical analysis, verification, validation, application to industrial scale and uncertainty quantification (VVUQ), to demonstrate the quality of, and the confidence in results obtained.

By following this methodology, each step must be consistent with the others and with the final goal of the calculations. The physical analysis, based on a PIRT (Phenomena Identification and Ranking Table) dedicated to the specific CFD scenario, has a key role to achieve this consistency. The PIRT is normally built from three different sources: experiment, expert analysis and computation. The main purpose of the PIRT is to perform a physical analysis and rank the different input parameter by level of influence (High, Medium, Low). This rank gives an overview of the influence but not a precise value. The goal of this presentation is to achieve the PIRT approach with a quantification of the input parameters influence. A sensitivity approach based on Sobol coefficient computation is applied. The different steps are:
1) Build a design of experiment to run sensitivity thanks to the input parameters
2) Make a physical analysis from the previous results
3) Build a surrogate model if the number of computation are not enough
4) Compute the sensitivity coefficient with the Sobol coefficient approach

This strategy is tested on an industrial example of a CFD application: the main steam line break. The presentation will describe a first version of a classical PIRT which will be completed by the quantified PIRT approach.

**ALEATORY UNCERTAINTY OF THE MEAN: QUANTIFICATION AND CONVERGENCE**
**Technical Presentation.** VVS2016-8868
12:05pm-12:30pm

**Joris Brouwer**, *Marin, Wageningen, Netherlands*

New insights into the numerical behavior of the aleatory uncertainty of the mean (randomness) have cleared the path to its formal calculation. This presentation highlights information from several papers that have been published since 2013 and is intended to provide a basis for new UQ standards with respect to aleatory uncertainty contribution.

This presentation shows how the aleatory uncertainty of the mean converges with calculation time for statistically steady processes. Numerical methods are discussed to estimate this aleatory uncertainty from an actual realization. Using the estimated convergence of the uncertainty it can be judged whether a time series signal is actually statistically steady or not (yet). With this information, it can be analyzed how long the start-up transient in a computation influences the result of the mean and the most accurate estimate of the mean and its aleatory uncertainty can be found. Therefore, it becomes possible to quantify the effect of the length of the simulation time on the aleatory uncertainty.

The mathematics in this presentation can be extended to other statistical parameters besides mean. Work is well underway for aleatory uncertainty of standard deviation and it will be demonstrated. Hopes are that this paper establishes a fundament for proper UQ procedures with respect to quantifying aleatory uncertainty for mean, standard deviation and other statistical parameters.

## TRACK 5 Validation for Fluid Dynamics and Heat Transfer

### 5-1
### VALIDATION FOR FLUID DYNAMICS AND HEAT TRANSFER: SESSION 1

**1st Floor, Mesquite 2** **10:25am - 12:30pm**

**AIR-LIQUID BREAKUP MECHANISM IN A HIGH-SPEED FLOW CHAMBER**
**Technical Presentation.** VVS2016-8815
10:25am-10:50am

**Ryoichi Amano**, *University Of Wisconsin-Milwaukee, Glendale, WI, United States,* **Yi Hsin Yen**, *University Of Wisconsin-Milwaukee, Milwaukee, WI, United States*

To understand liquid breakup mechanism is an important role to improve the performance of solid rocket motor (SRM) since we could reduce the erosion mechanism near nozzle throat section from liquid states alumina that is the product after aluminum based solid fuel burns. Protection of the nozzle wall could be achieved by enhancing liquid breakup mechanism of the liquid alumina inside a combustion chamber before bulky alumina slug erodes the nozzle section. This paper presents a study of air and water two-phase straight channel experiment and the comparison of different Computational Fluid Dynamic (CFD) method based on the Large Eddy Simulation (LES) and Detached Eddy Simulation (DES). The experimental work provides validation information for the simulation study that can be used to predict liquefied alumina breakup mechanism in the propulsion chamber. The frequency analysis was carried out by capturing the image of the breakup droplets through a high-speed camera image processing technique along with the Welch frequency transform method. By comparing the results of the Welch analysis from experiment and different CFD method could help us to understand the character and capability of CFD in liquid breakup study.

### VALIDATION OF KINETIC-THEORY-BASED CONTINUUM MODELS WITH IDEAL NUMERICAL DATA OF PARTICLE CLUSTERING

**Technical Presentation.** VVS2016-8819
10:50am-11:15am

**William D. Fullmer, Christine M. Hrenya**, *University of Colorado, Boulder, CO, United States*

Understanding the behavior of solid particles suspended in a fluid is paramount to a variety of industrial and engineering fields. Unfortunately gas-solid flows are incredibly complex, yielding a variety of structural patterns that can span several orders of magnitude in size, ranging from the system scale down to a few particles. Numerical strategies to track the motion of individual particles, such as direct numerical simulation (DNS) or computational fluid dynamics-discrete element model (CFD-DEM), are able to faithfully reproduce the complicated behavior, but at a considerable computational cost. Continuum models that treat the particles as a continuous solids-phase coexisting with and interpenetrating the gas-phase (if considered), must be applied to simulate larger systems of engineering importance.

A common approach to derive continuum models relies on an analogy between the particles and the molecules which make up traditional fluids. Starting from the Enskog kinetic equation (Boltzmann equation for finite sized particles), a continuum theory for the solids-phase complete with explicit closure relations can be derived by employing a Chapman-Enskog perturbation method. Such an approach can be used to derive both granular (no interstitial fluid) and multiphase models. As should be expected, kinetic-theory-based models and their closures can be rather involved and validation is needed to confirm that they are able to accurately capture the discrete particle physics they are intended to model.

One of the most important examples of complex particulate behavior is the clustering instability. Unlike their molecular counterparts, macroscopic particles tend to form inhomogeneous structures of high concentration clusters surrounded by dilute regions which are both dynamic and persistent. Similar to turbulence in single-phase flows, clustering is so pervasive in gas-solid flows that it is more the rule, than an exception. Therefore, we prefer to validate continuum models against predictions of clustering, either conditions for critical stability or quasi-steady properties in clustered regimes, as this offers a stringent test of the theory.

Although experimental data on clustering does exist in the literature, comparisons to real systems are not the best place to start the process of validating such a model. In the derivation, many simplifying assumptions and approximations are required to make the kinetic theory approach tractable, e.g., the spatial gradients are small (low Knudsen numbers), particles collisions are uncorrelated (molecular chaos), instantaneous and binary, etc. In addition, the particles are frequently assumed to be perfectly spherical, monodispersed, smooth (no friction), cohesion-less and that the inelastic dissipation may be characterized by a constant coefficient of restitution. Furthermore, other (potentially) relevant physics are implicitly neglected, e.g., relative humidity, static electricity, compressibility effects, gas-phase turbulence, etc. Therefore, it is most natural to ask first whether the continuum theory can accurately model the clustering instability of ideal particles, before testing its accuracy against non-ideal (realistic) particles in the presence of a variety of neglected physics.

In this presentation, we will report recent validation studies of kinetic-theory-based continuum models by comparing clustering predictions to ideal DNS and CFD-DEM numerical data in the homogeneous cooling system (HCS) and unbounded fluidization/sedimentation (UF/S). In the HCS, predictions of the critical system size necessary for the onset of velocity vortex (a precursor to clustering) clustering instabilities are in excellent agreement with DEM data for granular (no gas) systems. Two-phase HCS comparisons to DNS data show qualitative agreement, but a larger degree of quantitative agreement than the granular counterpart. The UF/S system does not decay to a trivial state like the HCS and statistical steady-state comparisons are possible. In a large and small systems, comparisons to CFD-DEM and DNS data, respectively, show good agreement except at low density ratios - which is also explained and quantified.

### VALIDATION AND VERIFICATION OF A CFD MODEL FOR TURBULENT HEAT TRANSFER AT SUPERCRITICAL PRESSURES

**Technical Presentation.** VVS2016-8822
11:15am-11:40am

**Keke Xu**, *Zhejiang University, Hangzhou, Zhejiang, China,* **Hua Meng**, *Zhejiang University, Hangzhou, Zhejiang, China*

Supercritical-pressure turbulent heat transfer of various fluids, including carbon dioxide, water, and hydrocarbon fuels, play important roles in the fields of refrigeration, nuclear, and aerospace engineering. At supercritical pressures, although the phase-change phenomenon vanishes, significant thermophysical property variations, particularly in the transcritical region as the fluid temperature rises from the subcritical to supercritical state, make strong impact on the heat transfer processes and lead to peculiar features distinct from the low-pressure counterparts.

Comprehensive validation and verification of a computational fluid dynamic (CFD) model have been conducted for studying turbulent heat transfer at supercritical pressures. The model is based on the Reynolds averaged Navier Stokes (RANS) equations. The standard k-? turbulent model, with an enhanced wall treatment, is mainly used and examined for its applicability and accuracy in handling the turbulent fluid flows. Under conditions in which this turbulence model does not work well, other models, including the SST k-?, SA, V2F, and a number of the low-Re k-? models, are also tested in this paper. The extended corresponding state (ECS) principle is, in general, used to calculate thermophysical properties of the fluids at supercritical pressures, but a look-up table is used to obtain the thermophysical properties of water, based on the NIST data. For supercritical-pressure heat transfer of hydrocarbon fuels, once the fluid temperature reaches a threshold value, the endothermic chemical reactions of fuel decomposition occur. Therefore, chemical reaction mechanisms are further incorporated to treat fuel pyrolysis and surface carbon deposition.

A series of numerical studies are first carried out to analyze turbulent heat transfer of carbon dioxide and water in circular cooling tubes at supercritical pressures. Results are compared with the available experiment data. Under operating conditions in which the gravity effect is negligible, the calculated results are in good agreement with the experimental data. Under conditions with the gravity effect, the results are mixed. For the supercritical-pressure heat transfer in a horizontal tube, good match between the calculated results and experimental data is obtained. For the cases in a vertical tube, if the flow is in the same direction with the gravity force, numerical results can match the experimental data at low surface heat fluxes, but a large difference appears once the heat flux becomes higher. If the flow is in the opposite direction of the gravity force, however, the CFD model is incapable of accurately predicting the fluid flows and heat transfer processes, particularly as the physical phenomenon of heat transfer deterioration occurs. A number of other turbulent models are further tested, numerical results all show large differences from the experimental data.

The CFD model is next applied to study the fluid flows and heat transfer of hydrocarbon fuels at supercritical pressures, which play an important role in thermal protection of the propulsion and power generation systems. A one-step proportional product distribution (PPD) chemical model is applied to account for the mild thermal cracking of n-decane, and a detailed chemical reaction mechanism, which contains 18 species and 24 elementary reactions, is used to consider fuel pyrolysis and surface coking of the aviation kerosene, RP-3. The turbulent heat transfer of n-decane in a vertical tube is analyzed, with consideration of the gravity effect. The same conclusion as that drawn for carbon dioxide and water is again reached; numerical results can only match the experimental data under conditions in which the flow and gravity force are in the same direction. Numerical results indicate that the CFD model, without the gravity effect, is capable of accurately treating the heat transfer and pyrolytic chemical reactions at supercritical pressures.

**USING LASSO TO INFER A HIGH-ORDER EDDY VISCOSITY MODEL FOR K-EPSILON RANS SIMULATION OF TRANSONIC FLOWS**
**Technical Presentation.** VVS2016-8841
11:40am-12:05pm

**Jaideep Ray, Sophia Lefantzi**, *Sandia National Laboratories, Livermore, CA, United States,* **Srinivasan Arunajatesan, Lawrence J. Dechant**, *Sandia National Laboratories, Albuquerque, NM, United States*

We present a procedure by which we learn the functional form of a high-order eddy viscosity model (EVM) from experimental data and then calibrate it to estimate the EVM's parameters. This procedure is performed within the context of Reynolds Averaged Navier-Stokes (RANS) simulations and experimental data of an interaction of a supersonic jet with a transonic crossflow. The experimental data consists of mean flow (velocity) measurements on two planes in the flowfield and turbulent stresses on one plane. Previous calibration with a linear EVM (LEVM) had indicated that structural shortcomings of the LEVM led to poor predictions of turbulent stresses. While quadratic and cubic eddy viscosity models exist, their parameters are estimated from incompressible flow experiments. While a cubic eddy viscosity model properly calibrated for compressible flow would be ideal, it was unclear whether such a complex model could be calibrated to the limited experimental data at hand.

Our calibration procedure first establishes an acceptable functional form of the EVM. First, we fit a cubic EVM, computed using an approximate value of turbulent dissipation, to experimental measurements of turbulent stresses. The fitting is performed using LASSO to simplify the cubic EVM. We see that LASSO removes all high order terms in the model, except for one that is quadratic in vorticity; since JIC is a strongly vortical interaction, this is no surprise. However, due to the approximate dissipation rate used in the LASSO fit, the EVM parameter so estimated is not very trustworthy. Consequently, it has to be recalibrated in the second step.

The second step of the calibration involves using measurements of vorticity to calibrate three parameters of a k-epsilon RANS model, one of which is the EVM parameter. We first construct surrogate models for vorticity predictions and pose a Bayesian inverse problem to estimate the parameters. The inverse problem is solved using a Markov chain Monte Carlo (MCMC) and we construct probability density functions (PDF) for the three parameters. The PDFs capture the uncertainty in parameter estimation due to limited measurements and shortcomings of the k-epsilon RANS model. The calibrated model is tested for its ability to predict flow variables other than vorticity by performing posterior predictive runs.

**A PARALLEL MARKOV CHAIN MONTE CARLO METHOD FOR CALIBRATING COMPUTATIONALLY EXPENSIVE MODELS**
**Technical Presentation.** VVS2016-8856
12:05pm-12:30pm

**Jaideep Ray**, *Sandia National Laboratories, Livermore, CA, United States,* **Laura P. Swiler**, *Sandia National Laboratories, Albuquerque, NM, United States,* **Maoyi Huang, Zhangshuan Hou**, *Pacific Northwest National Laboratory, Richland, WA, United States*

Estimation of model parameters from experimental data is fundamental to predictive simulations. However, due to limited observational data and shortcomings of models, it is not always possible to infer them with precision. . One solution is to employ Bayesian estimation where the parameters are estimated as probability density functions (PDFs); it enables quantification of uncertainties in the inferred model parameters.

Bayesian estimation problems can be solved using Markov chain Monte Carlo (MCMC) methods. These methods describe a random walk in the parameter space, invoking the forward model repeatedly to gauge the quality of each step. A large number of steps are required to arrive at a 'converged' joint PDF and the model invocations are sequential; thus MCMC methods are phenomenally expensive. A parallel MCMC method consists of multiple Markov chains that share information among them as they explore the parameter space. Multiple chains can help reduce the run time by amortizing the sampling burden. Further, as the chains explore the parameter space, they can share information on the promising parts of the space where the peaks of the PDFs lie. In doing so, they reduce the number of MCMC steps towards convergence.

We describe SAChES (Scalable Adaptive Chain Ensemble Sampling), a multichain MCMC sampler that combines a genetic algorithm (differential evolution, DE) and an adaptive Metropolis-Hastings (M-H) sampler, to solve statistical inverse problems. The genetic algorithm is useful in the early epoch of the random walk when the chains have too few samples to allow efficient adaptation in the sample space. Starting with DE, SAChES evolves into an adaptive M-H sampler, where the chains pool their samples periodically to identify promising proposal distributions for their future steps. We will describe the parallel design of the sampler, which involves MPI-2/Remote Memory Access mechanisms. Passive target synchronization and active target synchronization with exposure epochs are used to ensure scalability to multiple processors and chains.

We test SAChES on sampling from analytical distributions with the aim of recovering the target distributions correctly. We also demonstrate its application through integration with a computationally expensive model, the Community Land Model, which has been widely used in climate change simulations.

## TRACK 17 Verification and Validation for Advanced Manufacturing

### 17-1
### VERIFICATION AND VALIDATION FOR ADVANCED MANUFACTURING: SESSION 1

**2nd Floor, Palo Verde B** **10:25am - 12:30pm**

**TILT MEASUREMENT OF ROLLERS IN CYLINDRICAL ROLLER BEARINGS USING TWO ULTRASONIC TRANSDUCERS**
**Technical Presentation.** VVS2016-8843
10:25am-10:50am

**Meng Li**, *Xi'an Jiaotong University, Xi'an, China,* **Cong Xu**, *Xi'an Jiaotong University, Xi'an, China,* **Heng Liu**, *Xi'An Jiaotong University, Xi'an, China,* **Li Chen, Minqing Jing**, *Xi'an Jiaotong University, Xi'an, China,* **Wei Chen, Shemiao Qi**, *Xi'an Jiaotong University, Xi'an, China*

Cylindrical roller bearings have been widely used as the key parts of rotating machineries in modern industry due to their carrying capacity and low-friction characteristics. The performances of line contacts in roller bearings have a great influence on the dynamic behavior of the rotating machines. In actual conditions, the line contact of the roller bearing often works under misaligned loads. And then the deflection effect and the potential arisen edge affection of the roller will invalidate the heavy tilting area of line contact earlier than the other. Many researches of roller crown design have been done in misalignment to improve the contact condition between roller and ring. However, it is very difficult to measure the tilt of rollers online in actual condition. Therefore, the validation of the crown design is lack of directly experimental data.

In this study, a new method is proposed to measure the tilt of rollers in cylindrical roller bearings. The stiffness distribution of the line contact is measured by two juxtaposed ultrasonic transducers and then the oil-film thickness distribution of the roller is got by the equivalent stiffness. The tilt of the roller can be observed from the difference between the minimum film thicknesses measured by two transducers. And the difference of stiffness distribution is related to the misaligned loads. A new ultrasonic pulser-receiver was described and used for the measurement of lubricant-film thickness distribution in a cylindrical roller bearing (type N2204). This device provided a maximum pulse repetition frequency of 100 kHz, so that the ultrasonic measurements could be used for high shaft speed. In order to avoid the effect of the rotor vibration, an accurate triggering signal has been used for the measurement, which is the reflection of the laser pulse from the reflective tape pasted on the bearing cage and the rotor. For a range of loads and speeds, the tilts of rollers are measured and the experimental results are verified with the bearing dynamics theory based on Gupta's method. The influences of the rotating speed and radial load on the tilt of rollers were consistent with the theoretical predictions. The limits of the pulse repetition rate used in measurements are discussed. The performance of the experimental system demonstrates that this new method has the potential for condition monitoring the tilt of rollers in an industrial application and then provides a good verification and validation of bearing dynamics theory and the crown design.

### A NEW METHOD TO MEASURE THE ROTATING SPEED OF BEARING CAGE AND ITS EXPERIMENTAL VERIFICATION

**Technical Presentation.** VVS2016-8865
10:50am-11:15am

**Zhixiang Liu**, *NanJing University of Aeronautics and Astronautics, Nanjing, Jiangsu, China,* **Heng Liu**, *Xi'An Jiaotong University, Xi'an, China,* **Minqing Jing, Meng Li**, *Xi'an Jiaotong University, Xi'an, China,* **Cong Xu**, *Xi'an Jiaotong University, Xi'an, China*

The skidding of roller in bearing is the one of important phenomenon when the rotating machinery is working at high rotating speed and light load. Actually many failures of the bearings are related to this phenomenon. Thus, many researchers have investigated this problem using many kinds of theoretical analysis and experiment methods before. Here the one of focus on this problem is how to measure the rotating speed of bearing cage accurately when the bearings are rotating. However, the optical measurement method of the rotating speed of bearing cage which has been used in laboratory widely meets some difficult of operation in actual condition, such as the arrangement of reflective material and path of ray. Therefore, it is the difficult mission in actual industrial environment.

This paper presents a new method to measure the cages rotating speed of bearings based on the technique of ultrasonic reflection measurement. Through emitting ultrasound signal inside from the bearing outer ring with high frequency and detecting its ultrasonic echo signal continuously, the time of each rollers passing by the measurement position can be recorded accurately by detecting the change of ultrasonic echo signal. Then the revolution rotating speed of the roller can be obtained by counting the passing frequency of the rollers, it is also the rotating speed of bearing cage. Comparing to the optical measurement method of the rotating speed of bearing cage, the new method do not need any special arrangement for the bearings and is not sensitive to environmental factors such as oil mist.

In order to verify the new method, a high repetition frequency ultrasonic pulser-receiver is used to measure the rotating speed of bearing cage of roller-bearings (type N2204) by this new method in our experiment rig. The ultrasonic echo signal indicates the time of each rollers passing by the measurement position clearly in experiment, and the revolution rotating speed of the roller is obtained accuracy. At the same time, the influence of different rotating speed and load are investigated additionally here.

### SIMULATION-INFORMED RELIABILITY ANALYSIS SUPPORTING PART ACCEPTANCE DECISIONS

**Technical Presentation.** VVS2016-8901
11:15am-11:40am

**Patricia D. Hough**, *Sandia National Labs, Livermore, CA, United States,* **Alix A. Robertson, Bruce L. Kistler, Scott T. Peterson, Kyle Allen**, *Sandia National Laboratories, Livermore, CA, United States*

Reliability of key parts that comprise a system is critical to the reliability of the overall system. Thus it is essential to minimize the risk that those parts fail. Given manufacturing variability, it is often the case that acceptance criteria are set on features of the part, such as size, that can be associated with failure. A question that might be asked, then, is: What is the risk that a part of an observed size will fail given uncertainties in material properties and operational conditions? In this talk, we describe an approach to answer such a question that combines the use of finite element simulation, computational sampling and optimization tools, response surfaces, statistical analysis tools, and reliability analysis. More specifically, computational sampling and optimization are used to explore the finite element model for a few specified part sizes in order to understand sensitivity to uncertainties and to identify extreme behaviors. A response surface is constructed using the data generated by the computational studies, enabling interpolation across the full range of part sizes. Statistical and reliability analyses are applied to the response surface in order to determine the risk of accepting a part of any given size and to inform a minimum acceptable size. We will illustrate this analysis approach on a demonstration problem. Such an analysis was successfully completed for a real problem, and the results were used to inform part acceptance for a high-impact project.

### DESIGN OPTIMIZATION ON MULTI-LAYER HDPE/EVOH FUEL TANK SYSTEM WITH MODEL BIAS PREDICTION

**Technical Presentation.** VVS2016-8903
11:40am-12:05pm

**Changsheng Wang, Haijiang Liu**, *Tongji University, Shanghai, China,* **Lin Jiang**, *YAPP Automotive Parts Co., Ltd., Yangzhou, China*

With the increasing regulation in automobile hydrocarbon emission, the components including plastic fuel tank) made of high density ethylene materials (HDPE) with ethylene vinyl alcohol copolymer (EVOH) that works as high-barrier film have been used more and more widely, which reduced the hydrocarbon emission significantly. Due to the complicated layer-structure material, some difficulties occur for the numerical simulations to evaluate the product performances in advance. Furthermore, there is few study of model validation or verification for the process of multilayer components such as plastic multilayer fuel tank, which results in too time-consuming to enhance non-risky design decisions. In this study, to correct the discrepancy and uncertainty of the simulated finite element model for plastic multilayer fuel tank, Bayesian inference-based method is employed to quantify model uncertainty and evaluate the prediction results based on collected data from real mechanical tests of plastic fuel tanks and FE simulations under the same boundary conditions. The advantages and disadvantages of the applied method are presented, and the effectiveness of the proposed approach is also demonstrated. It is shown that the accuracy and reliability of FE simulations of plastic multilayer fuel tank coupled with model bias prediction is increased apparently.

### PHYSICS-BASED MODELING AND SIMULATION (M&S) MATURITY MODEL FOR ADVANCED MANUFACTURING

**Technical Presentation.** VVS2016-8909
12:05pm-12:30pm

**Huijuan Dai**, *GE Global Research, Niskayuna, NY, United States,* **Matteo Bellucci**, *General Electric, Niskayuna, NY, United States,* **Adegboyega Makinde**, *GE Global Research, Niskayuna, NY, United States*

Modeling and simulation play increasingly important roles in advanced manufacturing. These models are used to optimize process parameters in order to minimize manufacturing defects, reduce the number of physical trials and consequently reduce cost. In design engineering, there are specific steps that a designer must take to ensure validity of numerical models for new product introduction and these steps have been codified into design practices within the various businesses at GE. However, for manufacturing process modeling, there are no such standards where the outcome of a

simulation model depends on the modeler?s experience and expertise. There is need to develop guidelines for manufacturing process simulation to ensure that the models are properly calibrated and validated in order to fully benefit from virtual manufacturing. These will enable us to:
(1) Identify manufacturing/sourcing risks and gaps much earlier
(2) Evaluate manufacturing and schedule impact on new product introduction
(3) Conduct producibility analysis
(4) Better estimate process development time and mature parts cost
(5) Rapidly attain yield level entitlement for the new manufacturing facilities (additive, casting, etc.)

In most manufacturing industries, a majority of process parameters is determined based on previous experiences and manufacturing process physics is rarely used to guide decisions. This makes it difficult to determine how much conservatism is built into processes. The resulting production costs of inefficiencies can be staggering. Many companies have started to develop what is called the smart factory where the different manufacturing processes for a component or product are linked in order to optimize the processes and minimize variability. Such smart factories require faster data feedback loops which can only be realized through the use of reduced order models coming from physics-based modeling. This means that the accuracy of modeling results is now more important than ever. In order to improve virtual process development and drive factory roadmaps, GE is developing a physics-based Modeling and Simulation (M&S) maturity model for advanced manufacturing. This model builds upon the Capability Maturity Model Integration (CMMI) framework which is used to define three focus areas and it is refined with highest maturity level end state in mind. We are going to describe current code verification/validation at GE-GRC, extending CMMI to include model selection, organization structure and talent training & development.

The M&S maturity model consists of three critical elements:
(1) M&S tools which are focused on process model representation, process physics fidelity, code/ algorithm/model integration, simulation verification & validation and uncertainty quantification.
(2) M&S procedures & methods including physics-based model selection, analysis set up/execution, result interpretation and application tutorial development
(3) M&S skills, training and motivation covering organization structure, workforce bench strength, training deployment plan, new product introduction and manufacturing / value engineering.

For each element, four levels of maturity and user categories are defined:
(1) Maturity level 0: empirical trial & error driven decisions, M&S used for manufacturing process scoping studies (user category: subject matter experts)
(2) Maturity level 1: expert M&S analyst driven decisions, M&S used for manufacturing process design support (user category: R&D engineers)
(3) Maturity level 2: operational M&S assisted decisions, M&S used for manufacturing process optimization (user category: R&D and process engineers)
(4) Maturity level 3: enterprise M&S driven decisions, M&S integrated into brilliant enterprise infrastructure (user category: enterprise workforce)

The tool provides guidelines to assess the maturity level of M&S effort in the manufacturing process, drive model & simulation rigor and product & process innovations.

## TRACK 2 Development and Application of Verification and Validation Standards

### 2-3
### ASME V&V STANDARDS DEVELOPMENT ACTIVITIES: PART 2
**2nd Floor, Acacia D** **1:30pm - 3:35pm**

**SCALING ANALYSIS AS A PART OF VERIFICATION AND VALIDATION OF COMPUTATIONAL FLUID DYNAMICS AND THERMAL-HYDRAULICS SOFTWARE IN NUCLEAR INDUSTRY**
**Technical Presentation.** VVS2016-8921
1:30pm-1:55pm

**Milorad Dzodzo**, *Westinghouse Electric Company, Cranberry Township, PA, United States,* **Arthur Ruggles**, *Univ Of Tennessee, Knoxville, TN, United States,* **Brian Woods**, *Oregon State University, Corvallis, OR, United States,* **Upendra Rohatgi**, *Brookhaven National Laboratory, Upton, NY, United States,* **Nam Dinh**, *North Carolina State University - Dept. Nuclear Engineering, Raleigh, NC, United States,* **Stephen Bajorek**, *U.S. Nuclear Regulatory Commission, Washington, DC, United States,* **Abdelghani Zigh**, *US Nuclear Regulatory Commission, Washington, DC, United States,* **Hyung Lee**, *Bettis Laboratory, West Mifflin, PA, United States,* **Yassin Hassan**, *Texas A&M University, College Station, TX, United States,* **Richard Schultz**, *Consultant, Pocatello, ID, United States,* **Christopher Freitas**, *Southwest Research Institute, San Antonio, TX, United States*

In Nuclear Industry one of the initial steps in the Evaluation Model Development and Assessment Process (EMDAP) is to identify and rank important phenomena in a Phenomena Identification and Ranking Table (PIRT) through a formalized consensus building process using a panel of subject-matter experts. A state of knowledge regarding highly and medium ranked phenomena is also established and ranked. The identification and ranking is performed in all relevant modules and subsystems of the nuclear power plant system and for all time sequences present during the particular postulated accident transient. However, the ranking developed in the PIRT is the subjective consensus of the experts. Application of Scaling Analysis can formalize and inform the ranking in the PIRT through a more detailed mechanistic analysis (in fact providing a quantification of ranking).

Scaling Analysis and Identification of existing and performing new experiments are parts of EMDAP Development of Assessment Base. Experiments may span a broad range of types and scope. Experiments of small and intermediate size examining behavior of one component during one time sequence of the transient addressing a single phenomenon, or smaller number of interacting phenomena are Separate Effects Tests (SET). More complex Integral Effect Tests (IET) might represent several modules, subsystems, or entire system of the nuclear power plant. Nuclear power plant systems are large and due to the cost of experimental facilities data from smaller scale SET and IET are used to assess the evaluation model. However, the entire plant (full scale) under transient accident conditions data is not available to assess the evaluation model and this lack of data for direct comparison is the main difference between V&V 20 and V&V 30 Standards. Therefore, V&V 30 Standard uses scaling analysis to guide selection and design of experiments used to generate validation data for Evaluation Models.

A review of current practice and recent contributions to scaling for nuclear power system evaluation models and validation experiments and status of development of Scaling Analysis document supporting V&V 30 Standard are presented.

**V&V40: VERIFICATION AND VALIDATION FOR COMPUTATIONAL MODELING OF MEDICAL DEVICES MEDICAL DEVICES**
**Technical Presentation.** VVS2016-8942
1:55pm - 2:20pm

**Carl Popelar**, *Southwest Research Institute, San Antonio, TX, United States,* **Tina Morrison**, *Food and Drug Administration, Silver Spring, MD, United States,* **Marc Horner**, *ANSYS, Inc., Evanston, IL, United States*

Computational modeling is used throughout the entire product life cycle to provide information related to the performance, safety and effectiveness of medical devices. Unlike other types of models, computational models can be used to assess aspects in vivo performance without subjecting patients to potential harm or unnecessary risk.

The credibility or trust in the predictive capability of a computational model to accurately represent reality can be of paramount importance due to the potential consequences of an incorrect assessment about the performance of a medical device. Attempts have been made to rate the maturity of the model by including additional factors such as the pedigree of the modeler. While model maturity and the pedigree of the analyst may facilitate achieving a credible model, the credibility of a computational model is nonetheless established through verification and validation (V&V) activities by demonstrating the ability to predict actual experimental data.

Although the V&V process is generally well-established, clinically-based V&V activities can be limited in the regulated medical device industry. Thus, the activities of the ASME V&V40 Subcommittee and the intent of this document is to provide guidance on ensuring that the V&V activities establish sufficient model credibility given the risk of using a computational model to predict device performance, safety and/or effectiveness.

**V&V 50 VERIFICATION AND VALIDATION (V&V) OF COMPUTATIONAL MODELING FOR ADVANCED MANUFACTURING**
**Technical Presentation.** VVS2016-8959
2:20pm-2:45pm

**Sudarsan Rachuri,** *Department of Energy, Washington, DC, United States,* **Mark Benedict***, Air Force Research Laboratory, Wright-Patterson Air Force Base, Ohio*

V&V 50 Verification and Validation (V&V) of Computational Modeling for Advanced Manufacturing

V&V50 Subcommittee Charter:
To provide procedures for verification, validation, and uncertainty quantification in modeling and computational simulation for advanced manufacturing.*
*Advanced Manufacturing, as defined in the PCAST report:
"Advanced manufacturing is a family of activities that (a) depend on the use and coordination of information, automation, computation, software, sensing, and networking, and/or (b) make use of cutting edge materials and emerging capabilities enabled by the physical and biological sciences, for example nanotechnology, chemistry, and biology. It involves both new ways to manufacture existing products, and the manufacture of new products emerging from new advanced technologies." --President's Council of Advisors on Science and Technology Report to the President on Ensuring American Leadership in Advanced Manufacturing

An update will be provided on the initial topics this subcommittee has identified for work, including: Terms, concepts, relationships, taxonomy for VVUQ in Advanced Manufacturing; Additive Manufacturing V&V Challenges; Modeling Problems; and Model Life Cycle.

**SCOPE AND VISION OF THE V&V 30 STANDARDS COMMITTEE**
**Technical Presentation.**
2:45pm-3:10pm

**Richard Schultz,** *Consultant, Pocatello, ID, United States,* **Hyung Lee***, Bettis Laboratory, West Mifflin, PA, United States*

The charter of the V&V 30 committee is to provide the practices and procedures for verification and validation of software used to calculate nuclear system thermal fluids behavior. The software of interest includes system analysis and computational fluid dynamics (CFD) numerical models, including the coupling of this software.

The V&V30 committee is working to achieve their objectives in accordance with the above charter by:

• Clarifying and normalizing the experiment design scaling approaches.
• Identifying the predominant differences and applications which distinguish the systems analysis and CFD software from one another. Additionally the widely-used historic nomenclature peculiar to the systems analysis codes will be normalized with that in common use today.
• Sponsoring a twin-jet benchmark problem to provide a baseline for how nuclear system CFD calculations are performed, verified, and validated.

The committee intends to build on the above efforts by sponsoring subsequent benchmark studies to provide a medium for verification and validation standards relevant to nuclear system analyses. An important ingredient in the subsequent benchmark studies is the inclusion of high fidelity experiment design scaling techniques to relate experiment geometry and boundary conditions to the subject nuclear reactor prototypes.

The above topics will be addressed in this scope and vision presentation.

## TRACK 4 Uncertainty Quantification, Sensitivity Analysis, and Prediction

### 4-2
### UNCERTAINTY QUANTIFICATION, SENSITIVITY ANALYSIS, AND PREDICTION: SESSION 2

**2nd Floor, Palo Verde A** **1:30pm - 3:35pm**

**EFFICIENT PROPAGATION OF IMPRECISE PROBABILITIES FOR MODEL VALIDATION**
**Technical Presentation.** VVS2016-8879
1:30pm-1:55pm

**Michael Shields, Jiaxin Zhang***, Johns Hopkins University, Baltimore, MD, United States*

Physics-based computational models are often complicated by uncertainties that are not easily quantified. These uncertainties typically stem from incomplete, imprecise, or otherwise inadequate data necessary to assign known probability distributions to stochastic system parameters. One avenue through which to quantify this uncertainty is the theory of imprecise probability wherein probability distributions are assigned with variable parameters that may be described through separate probability distributions, intervals, or other mathematical theories. However, propagation of these imprecise probabilities is a major challenge for both uncertainty quantification and model validation purposes, requiring nested Monte Carlo simulations that are prohibitively expensive.
We present a novel Bayesian importance sampling approach that allows the propagation of uncertain probability distributions through a single Monte Carlo analysis. The process is enabled by identifying, through optimization, a single importance sampling distribution that spans the range of possible distributions of interest. By propagating this optimal sampling distribution and re-weighting the samples according to the importance sampling method, we effectively propagate sets of numerous distributions. The results can be presented in the form of p-box or uncertain probability distributions on response that can be used to quantify "total" parametric uncertainty and validate computational models.

**EXPERIMENTAL DATA UNCERTAINTY, CALIBRATION AND VALIDATION OF A VISCOELASTIC POTENTIAL ENERGY CLOCK MODEL FOR INORGANIC SEALING GLASSES**
**Technical Presentation.** VVS2016-8882
1:55pm-2:20pm

**Ryan Jamison, Vicente Romero, Mark Stavig**, *Sandia National Laboratories, Albuquerque, NM, United States,* **Thomas Buchheit**, *Sandia Natl Laboratories, Albuquerque, NM, United States,* **Clay Newton**, *Sandia National Laboratories, Albuquerque, NM, United States*

Sealing glasses are ubiquitous in high pressure and temperature engineering applications, such as hermetic feed-through electrical connectors. A compression seal is a typical hermetic electrical connector. In a compression seal, the housing of the connector, typically an alloy, compresses a sealing material, such as amorphous glass, and electrical connectors due to thermal strain mismatch between the alloy and sealing material. The compression from the housing can lead to unfavorable tensile stress in the sealing glass. Reliable hermetic connector designs require material models that can accurately predict the response of the sealing glass to mechanical and temperature loadings over prolonged periods. A nonlinear viscoelastic simplified potential energy clock (SPEC) model has been previously developed for glassy thermosets and was found to be applicable to inorganic sealing glasses such as Schott 8061. Multiple material characterization tests are required to define the 30+ parameters found in the SPEC material model. Given the complexity of the SPEC material model, it is desired to understand and incorporate the uncertainty associated with the material model parameters and their effect on predicted stress in a hermetic connector application.

Through a brittle materials verification and validation program currently underway, multiple data sets have become available to enable calibration of the SPEC material model to ensemble data sets. Functional forms of the shear master curve and thermal strain were developed. These require estimation of the Williams-Landel-Ferry (WLF) coefficients and rubbery and glassy shear moduli, as well as the bulk moduli and the coefficients of the stretched exponential representing the volumetric response of the glass. Variability in the ensemble experimental results yields multiple sets of inferred calibration parameters.

For model validation, the ensemble of calibration parameters is propagated to model predictions at new validation conditions where experimental validation data exists. Model results are compared to results from a series of experiments performed on a simple hermetic connector in the form of a concentric glass-to-metal seal. The residual stresses of a concentric seal as determined through indentation methods are compared to model predictions. Specifically, the peak radial compression and tension in the concentric glass-to-metal seal is considered. Experimental and prediction uncertainties and associated discrepancies between model and experiment response statistics are quantified with the Real Space model validation methodology.

Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE- AC04-94AL85000.

**ASSESSMENT OF VALIDATION, CALIBRATION, AND PREDICTION TECHNIQUES FOR COMPUTATIONAL MODELING**
**Technical Presentation.** VVS2016-8890
2:20pm-2:45pm

**Christopher Roy, Ian Voyles, Jian-Xun Wang, Heng Xiao**, *Virginia Tech, Blacksburg, VA, United States*

There are many ways to use experimental data for uncertainty quantification and reduction in computational modeling. The most common way is through calibration of model parameters (e.g., parameter estimation, Bayesian updating) or of a model error/discrepancy term (e.g., the Kennedy and O?Hagan approach based on Gaussian Processes [1], the ASME V&V20 approach [2]). Alternatively, one could use the data to estimate the model form uncertainty (MFU) in the original (un-calibrated) model (e.g., the area validation metric [3,4]). Furthermore, there is a "middle ground" where elements of both calibration (i.e., model improvement) and validation (i.e., estimation of MFU) are combined together, possibly by segregating the data into a portion used for calibration and a portion used for validation.

We will examined are range of techniques for performing model validation and calibration. Three example problems will be examined using the Method of Manufactured Universes [5] which involves a 'truth' function which can be sampled to represent varying amounts of experimental measurements along with their uncertainty and a 'model' function with one or more uncertain inputs that are modeled probabilistically. The first example problem will be composed of simple 1D algebraic functions, the second will be composed of simple 2D algebraic functions, and the third is for turbulent flow over an airfoil which has a 'truth' function based on Reynolds-Averaged Navier-Stokes computations and the 'model' function based on thin airfoil theory with simple drag correlations [6]. We will examine how well each of the different methods for model validation and calibration capture the 'true' values in the presence of both parametric and experimental measurement uncertainty. In addition, we will investigate the effects of extrapolating the MFU and/or calibration parameters to conditions where no experimental data are available, i.e., to make model predictions.

References:
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**STATISTICAL CALIBRATION OF STRUCTURAL DYNAMIC MODELS**
**Technical Presentation.** VVS2016-8917
2:45pm-3:10pm

**Thomas Paez**, *Thomas Paez Consulting, Sedona, AZ, United States,* **Timothy Hasselman**, *Timothy Hasselman Consulting, Palos Verdes Estates, CA, United States*

Models of structural dynamic systems usually need to be calibrated because they contain features that can be accurately simulated only following calibration. Most critical among such features are mechanical joints and the parameters associated with energy dissipation.

One method used for the calibration of structural model parameters is the Bayesian approach. Among other advantages, it permits the incorporation of prior information into parameter estimates, along with experimental data, and it presents parameter estimates as jointly distributed random variables. The former advantage permits modelers to start with independently obtained data and information about the behavior of similar structures. The latter advantage incorporates an understanding of the uncertainty in parameters into the interpretation of a model and its predicted results.

In this presentation we seek to formalize some of the activities of practical Bayesian estimation using the ideas of statistical test of hypothesis. Specifically, nonlinear parameter estimation leads from the moments of a prior estimate of model parameters to a posterior estimate of those moments. Depending on the relative magnitudes of changes of parameters between the prior and posterior, it is usually found most advantageous to (1) accept the prior parameter estimates; (2) reject both prior and posterior estimates; or (3) reject the prior and accept the posterior parameter estimates. The qualitative criteria for the three choices are, respectively, (1) the prior estimates are accepted when the posterior estimates are all “near” the priors; (2) the priors and posteriors are both rejected when, at least, some of the posteriors are ‘far” from the priors; and (3) the posterior estimates are accepted when none are rejected for being too far from the priors, and the prior model is not accepted.

The rationale for these choices arises from the fact that Bayesian estimation provides parameter estimates that not only minimize the sum of differences between measured and predicted system response, but also the differences between prior and posterior parameter estimates, in a weighted least-squares sense where the inverse covariance matrices of the measurements and the prior parameter estimates are the weighting matrices. In other words, updates to the estimates are restrained by the prior estimates depending on how much credence is given to the prior estimates. If the credence in the prior estimates is high, more and/or stronger data are required to change the model, i.e. to reject the prior estimates in favor of the posterior estimates. Conversely, if credence in the prior model is weak, the posterior estimates are likely to move further from the prior estimates. However, if they move so far as to exceed the credible range of the prior estimates as determined by uncertainties assumed on the prior, then the posterior estimates should be rejected as violating the prior modeling assumptions. Finally, if the posterior estimates are so different from the prior that the prior model is rejected, and not so different as to reject the posterior model, then the posterior model has demonstrated acceptability.
The work reported here establishes test of hypothesis criteria for selecting the model parameter alternative, listed above, to be chosen. Two tests of hypothesis are performed using the T-squared statistic. The first test uses a null hypothesis that the posterior parameters come from the random source of the prior parameter estimates. If not rejected, at, say, a ninety-five percent level of significance, then action (1) is taken. If the first hypothesis is rejected because of the values of one or more components of the parameter vector, then a second test of hypothesis is performed. In this one, the null hypothesis is similar to the previous one, but the level of significance is raised, say, to ninety-nine percent. If this hypothesis is rejected, then action (2) is taken. Finally, if neither action (1) nor action (2) is taken, then action (3) is taken.

A numerical example is presented in which the parameters of a nonlinear model of a real aerospace system are estimated.

**STATE-AWARE CALIBRATION: PHYSICAL INTERPRETATION OF SYSTEMATIC BIAS IN COMPUTER SIMULTATIONS**
**Technical Presentation.** VVS2016-8947
3:10pm-3:35pm

**Sez Atamturktur, Garrison Stevens, Andrew Brown**, *Clemson University, Clemson, SC, United States,* **Cetin Unal**, *Los Alamos National Laboratory, Los Alamos, NM, United States*

Computational models developed to predict mechanical behavior of engineering systems define a representation of physics behavior linking the state variables (loads, temperature, etc.) to relevant output responses (deformation, stresses, etc.) with the goal of simulating the behavior of the system under various operational conditions. Representation of physics behavior requires additional input parameters to be defined that reflect the properties of the engineering system. Model calibration is the area concerned with determining the appropriate values of these input parameters.

Standard methods in computer model calibration treat the calibration parameters as constant throughout the domain of control inputs. In many applications, however, systematic variation not accounted for in the computer code may cause the best values for the calibration parameters to change between different experimental settings. Problems arise when such relationships are unforeseen or insufficiently understood. Often, such behavior tends to be ignored so that an overly simplistic model is used. This problem is exacerbated as the complexity of the system increases and as the available knowledge of the associated mechanistic behavior becomes increasingly insufficient.

In this work, we propose a framework for modeling the calibration parameters as systematic functions of the control inputs to account for a computer model’s incomplete system representation while simultaneously allowing for possible constraints imposed by prior expert opinion. We refer to this approach as State-Aware Calibration. In our proposed methodology, experiments are used to infer important relationships between model input parameters and state variables. Hence, State-Aware Calibration provides the capability to gain insight concerning the underlying and mechanistically-relevant physical processes absent from physics-based models.

The major benefit of state-aware calibration is that it can guide model developers by pinpointing the most influential, mechanistically-relevant processes that are absent from the models, thereby offering a definitive guide to the prioritization of future model developments as well as the efficient allocation of limited resources. Through state-aware calibration, we expect to further the engineer’s knowledge of the physics principles governing the system behavior of interest, as well as to significantly reduce the remaining systematic bias between model predictions and experimental observations. We demonstrate the feasibility and performance of our approach through simulation as well as application to a study of plastic deformation of a visco-plastic self-consistent material (5182 aluminum alloy) at varying temperatures. The numerical model used in this study omits the dependency of the model parameters on temperature. State-aware calibration is implemented to infer this relationship from measured stress and texture values.

## TRACK 5 Validation for Fluid Dynamics and Heat Transfer

### 5-2
### VALIDATION FOR FLUID DYNAMICS AND HEAT TRANSFER: SESSION 2

**1st Floor, Mesquite 2** **1:30pm - 3:35pm**

**ON THE APPLICATION OF A MULTIVARIATE METRIC FOR MULTIPLE SET POINTS IN VALIDATION EXERCISES OF RANS SOLVERS**
**Technical Presentation.** VVS2016-8878
1:30pm-1:55pm

**Luis Eca, Hugo Abreu, Rui Lopes**, *IST, Lisbon, Portugal,* **Filipe Pereira, Guilherme Vaz**, *MARIN, Wageningen, Select State/Province, Netherlands*

Computational Fluid Dynamics (CFD) has become a standard tool for the development of engineering projects. Although experimental fluid dynamics (EFD) is still the most common approach for assisting project decisions, it is undeniable that CFD is increasing its use as a complement of EFD. Therefore, the assessment of the quality of the mathematical models used in CFD is mandatory.

The most common way to address this problem is to perform Validation exercises, i.e. to estimate modeling errors of the selected mathematical models by comparing experiments and simulations taking into account experimental, numerical and parameter uncertainties. However, obtaining all the required information to make reliable estimates of the modeling error is not trivial.

In this presentation we focus on the Reynolds-Averaged Navier-Stokes equations, which are still the most common mathematical model for the simulation of wall-bounded turbulent flows at high Reynolds numbers. Our goal is to illustrate the use of the techniques proposed by the ASME V&V 20 Committee in practical test cases including flows around airfoils, cylinders and ships. In all these test cases, we present deterministic simulations with modeling errors estimated for functional and local flow quantities. Although we will not include parameter uncertainties in our estimates, the results demonstrate that quantifying modeling errors is much more demanding than the traditional graphical comparisons of experiments and simulations without any information of numerical and experimental uncertainties. Furthermore, we will illustrate how the recently proposed Multivariate Metric for Multiple Set Points can be used to quantitatively compare the performance of different turbulence models.

### VERIFICATION & VALIDATION OF CFD MODELS USED IN SHAPE OPTIMIZATION OF NOVEL AIR-TO-REFRIGERANT HEAT EXCHANGERS

**Technical Presentation.** VVS2016-8908
1:55pm-2:20pm

**Daniel Bacellar, Vikrant Aute, Zhiwei Huang**, *University of Maryland, College Park, MD, United States,* **Reinhard Radermacher**, *University Of Maryland, College Park, MD, United States*

The major limitation of air-to-refrigerant Heat eXchangers (HX) is the air side thermal resistance which can account for more than 90% of the overall thermal resistance. The current research on heat transfer augmentation extensively focuses on the secondary heat transfer surfaces (fins). The disadvantages of fins may include reduction of heat transfer potential due to temperature gradient, increased friction resistance, fouling and additional material consumption. On the other hand, fins contribute to reducing thermal resistance by adding significant secondary surface area. The heat transfer coefficient on the primary surfaces (tubes) is not sufficiently high in order to minimize the thermal resistance without significantly increasing the HX size. One contributing factor is the shape of the tube itself, which is generally limited to circular, oval, or flat. Another contributing factor is the tube size; the reduction of the refrigerant flow channel significantly improves performance and compactness. In this study we investigate two novel surface concepts, using NURBS, focusing on the airside tube shape with small flow channels aiming at the minimization or total elimination of fins. The study constitutes designing a 1.0kW air-to-water HX, using an integrated multi-scale analysis with topology and shape optimization methodology. Typically, such an optimization is unreasonably time consuming and computationally unaffordable. To overcome these limitations we leverage automated CFD simulations and Approximation Assisted Optimization (AAO), thus, significantly reducing the computational time and resources required for the overall analysis. In order to quantify the uncertainty of the CFD models, we employ the Grid Convergence Index (GCI) method. The Design of Experiments (DoE) encompasses of a Latin Hypercube Sampling (LHS) with 2500 designs including the boundaries of the design space. At the boundaries, as it has been demonstrated, that the uncertainties are fundamentally larger than for any other sample within the design space. The reason for that are the combinations of lower and upper bounds, which yield the most unrealistic computational domains, thus having a higher potential for poorer mesh elements in terms of size and aspect ratios. The GCI method carried out used constant grid refinement ratio of 1.3 and a factor of safety of 3.0. The results for heat transfer exhibited 96% of the cases with GCI less than 10%, with a median of 0.9% and an outlier maximum of 16.5%. The pressure drop, similarly, exhibited 91% with GCI less than 10%, with a median of 1.2% and a maximum outlier of 54.6%. The study also includes experimental validations for a proof-of-concept heat exchanger selected from the Pareto optimal designs. Validations show that the predicted heat capacity is within 5% of the measured values, and the airside pressure drop is within 10%. The new designs are expected to result in heat exchangers that are 20% lighter and smaller for residential air-conditioning applications.

### MODELING VERIFICATION AND VALIDATION OF THE STATE OF THE ART FLAMELESS OXYFUEL BURNER- PART ONE: EXPERIMENTAL AND NUMERICAL STUDY ON A SEMI-LAB SCALE FURNACE

**Technical Presentation.** VVS2016-8949
2:20pm-2:45pm

**Mersedeh Ghadamgahi**, *KTH Royal Institute of Technology, Stockholm, Sweden,* **Patrik Ölund**, *Ovako Sweden AB, hofors, Sweden*

Flameless oxyfuel combustion is proven to be one of the best solutions for reducing fuel consumption and reaching higher heating quality in industrial applications. Although a lack of study on these types of state of the art combustion systems makes it hard to be adjusted and implemented in current furnace configurations. In this study proper CFD models, according to the advisory in the literature, are selected and verified. Verification has been done by comparing the predicted results with experimental results on a 200 kW semi-lab furnace equipped with LPG fuel, flameless oxyfuel burner in AGA, Sweden. The experimental data that are taken with high accuracy suction pyrometer are: Local temperature, CO, CO2, O2 in 24 points inside the chamber. While selected CFD models are: k-? for turbulence, Discrete ordinates (DO) model for radiation and Probability density function (PDF) with equilibrium for combustion model.

Predicted and measured results show a very good agreement in temperature and gas species which verifies these selected models. The strongest un-similarities are visible in CO and CO2 volume fraction in the flame region which indicates the deficiency of using PDF combustion model and the simplifying assumption of equilibrium in this area.

### VALIDATION OF NATURAL CONVECTION MELTING ANALYSIS USING LATTICE BOLTZMANN METHOD

**Technical Presentation.** VVS2016-8954
2:45pm-3:10pm

**Jong Woon Park, Hyuk-Jin Song**, *Dongguk University, Gyeongju, Gyeongbuk, Korea (Republic)*

Convection melting is associated with applications such as metal processing, environmental engineering, thermal energy storage, nuclear reactor core safety, etc. Models of the convection melting need to account for thermally-driven flow coupled with a moving solid-liquid interface (melt front) where latent heat is absorbed during melting. The major variable interested is the melt front movement which describes the evolution of the system geometry. In the present paper, a multi-relaxation time lattice Boltzmann method (MRT-LBM) is formulated by using D2Q9 lattice model to couple pure solid melting and thermal convection in liquefied region and thus to describe momentum and heat transfer processes taking place in the liquid, mushy and solid regions as well as the melt front advancement. The LBM uses simple single set of formulations rather than complicated Navier-Stokes equations coupled with complicated multi-physics of melting. Also, compared with previous melt-front tracking methods such as adaptive grid or level set methods, the MRT-LBM can track the melt front by simply imposing positions with a specified liquid fraction as the interface. The liquid fraction is estimated from the Godunov enthalpy method using the temperature field obtained from the MRT-LBM. The flow boundary condition at the interface is treated with bounce-back mechanism generally and widely adopted in the MRT-LBM. Existing typical 9 cm x 4 cm vertical two-dimensional experiment of Gallium melting by Gau & Viskanta (1986) is used as a benchmarking case for melt front movement prediction using the present method. The initial temperature is set at 301.5 K and the left boundary of hot temperature is set at 311.5 K. All the four surfaces are assumed to be no slip. Melt fronts at 5, 8, and 12 mins are compared with the experiment. In order to confirm the transient flow field formation and variation which are not available from the experiment, they are analyzed using the rigorous Eulerian multiphase physics and the volume-of-fluid method contained in the STAR-CCM+ CFD code. In this computation, molten region physical properties are obtained from the two methods: slurry viscosity model for low values of solid fraction where the mixture is considered as a slurry and the mushy zone permeability model where a partially solidified stationary region is permeated with dendrites. The result from MRT-LBM and STAR-CCM+ is also compared with those from previous computations using finite element method (FEM). Reasonable agreement is achieved with regards to melt front propagation with upper-right skewing due to natural convection in the liquefied zone and the formation of multiple Bernard cells. Regardless of the simple physical basis and coding efforts, it can be concluded that the MRT-LBM approach is potentially well-suited and even very fast for computing convection melting processes and it is thus expected the method can be applied to engineering fields using more complicated and/or large media.

## TRACK 17 Verification and Validation for Advanced Manufacturing

### 17-2
### VERIFICATION AND VALIDATION FOR ADVANCED MANUFACTURING: SESSION 2
**2nd Floor, Palo Verde B** **1:30pm - 3:35pm**

**VariLink: An Investigation in Linking Variation and Uncertainty Quantification across the Product Lifecycle**
**Technical Presentation.** VVS2016-8926
1:30pm-1:55pm

**Thomas Hedberg**, *National Institute of Standards and Technology, Gaithersburg, MD, United States,* **Moneer Helu**, *National Institute of Standards and Technology, Silver Spring, MD, United States,* **Hui-Min Huang**, *National Institute of Standards and Technology, Gaithersburg, MD, United States*

Advances in information technology in industry have triggered a digital-manufacturing revolution that has the potential to reduce costs and improve productivity and quality. Using these innovations, manufacturing enterprises are changing how they communicate product definitions in the transition from paper-based drawings to digital models. This changeover has enabled improved simulation and analysis of products and processes, including the opportunity to model variation and uncertainty across the product lifecycle. Traditionally, quantifying the uncertainty of models, and the products and processes the models represent, has been understood at domain-specific levels (e.g., manufacturing, quality). Existing methods, such as error mapping and error budgeting in machine tools and inspection equipment, have provided the ability to determine the degree to which equipment errors affect the quality of a part. It remains challenging, though, to determine how the individual types of uncertainties and variations aggregate into a total uncertainty understanding for the entire product lifecycle.

More stringent requirements for time-to-market, quality, and cost have required industry to develop diagnostic and prognostic methods that can be applied in near-real time to remedy and improve errors. However, the increasing complexity of both products and process has made identifying potential errors before they occur difficult. The first step in developing appropriate diagnostic and prognostic methods is to explore how variation and uncertainty propagate and aggregate across the product lifecycle. We must also categorize the modes of variation that exist and where those modes are most likely to occur in the product lifecycle. These research areas can then support the use of sensing, monitoring, and control to minimize variation and uncertainty through decision-support systems and selection mechanisms.

Our proposed method, called VariLink, would link variation and uncertainty across the lifecycle using a model-based approach. Such an approach has the advantage of using a formal representation that is rigorous in nature that facilitates extension, reuse, repetition, and reproduction of information. The represented information could be used for simulation of designs, manufacturing and inspection equipment, and associated lifecycle processes. We emphasize using open standards in the VariLink approach to reduce interoperability, traceability, and analysis errors. We anticipate that successfully linking variation and uncertainty quantification across the product lifecycle through VariLink can improve prediction, sensitivity analysis, and robust design.

**VALIDATION OF MICROSTRUCTURE CONTROL IN ADDITIVE MANUFACTURING PROCESSES USING NUMERICAL MODELING TECHNIQUES AIDED BY HIGH PERFORMANCE COMPUTING**
**Technical Presentation.** VVS2016-8939
1:55pm-2:20pm

**Narendran Raghavan**, *University of Tennessee Knoxville, Knoxville, TN, United States,* **John Turner**, *Oak Ridge National Laboratory, Oak Ridge, TN, United States,* **Srdjan Simunovic**, *Oak Ridge National Lab, Oak Ridge, TN, United States,* **Michael Kirka, Ryan Dehoff**, *Oak Ridge National Laboratory, Oak Ridge, TN, United States,* **Suresh Babu**, *ORNL/UTK, Knoxville, TN, United States*

Additive Manufacturing (AM), also known as 3D printing, is the fabrication of functional 3D components from CAD models. It is a disruptive technology that is transforming conventional manufacturing industries. Understanding the transient phenomena of repeated melting and solidification is vital for site-specific microstructure control. The effect of solidification microstructure on the mechanical properties of engineering components is well understood, and AM processes provide the ability to locally control conditions and hence grain structure. Columnar or epitaxial grain growth is a common phenomenon observed in all additive manufacturing processes. Columnar grains are well suited for applications involving unidirectional stresses. In some cases, where omnidirectional stresses are involved, columnar grains are detrimental to the life span of the component. In such cases, equiaxed grains are preferred to get isotropic mechanical properties of the part fabricated. For a given alloy composition, evolution of solidification microstructure in rapid solidification conditions is primarily determined by the temperature gradient (G) and velocity (R) at the liquid-solid interface during the solidification of the meltpool. Robust understanding of highly transient (3D) spatiotemporal G and R through experimental strategy is nearly impossible. Experimental difficulties arise due to smaller space (microns) and time scales (milliseconds) involved during the rapid solidification of molten pool in the process. Hence, it is vital to employ numerical modeling techniques to better understand and quantify the influence of the heat source parameters and scan strategies on the melt pool dynamics. In this study the Truchas code, developed by Los Alamos National Laboratory (LANL) for casting and welding simulation and compatible of running in parallel across multiple processors, is used to simulate the transient thermal behavior and understand the spatiotemporal variation of solidification parameters of thermal gradient (G) and velocity (R) as a function of process parameters. Depending on the alloy system used, the volume fraction of equiaxed grains formed can be expressed as a function of G and R at the liquid-solid interface. Statistical analysis is then used to identify and quantify the effect of different parameters on the volume fraction of equiaxed grains formed. The modeling results are validated by demonstrating columnar to equiaxed transition (CET) in electron beam AM (Arcam®). Results of this study will help to reduce the number of experimental trials required during process parameter development for new materials. Furthermore, results of this study are generic and can be applied to different materials and most additive manufacturing processes. It also demonstrates the potential of numerical modeling techniques to validate the evolution of solidification microstructures in AM processes.

**A COMPARATIVE ANALYSIS OF REGRESSION MODELS FOR ENERGY PREDICTION OF MILLING MACHINE TOOLS**
**Technical Presentation.** VVS2016-8943
2:20pm-2:45pm

**Ronay Ak, Daniel Samarov**, *NIST, Gaithersburg, MD, United States,* **Raunak Bhinge**, *UC Berkeley, Berkeley, CA, United States*

Uncertainty quantification (UQ) plays a critical role in the characterization of variability from known and unknown sources in predictive analytics applications. As such, any model used for predicting a quantity of interest should be capable of providing UQ for those predictions so that informed decision-making can be made. However, quite frequently statistical techniques used in engineering applications provide only point predictions without consideration for the uncertainties in the model parameters and input data, or the lack of knowledge of the associated physical processes. One way to quantify uncertainty in predictions is to provide prediction intervals (PIs), i.e., confidence bounds for new observations, which are used to convey the uncertainty in the predictions, accounting for both the uncertainty in the model parameters and noise in the new data.

In this work, we perform a comparative analysis of sparse (additive) regression [1] and Gaussian process regression [2] for energy consumption during a manufacturing process. A comparison of predictive performance is done using the root mean squared error (RMSE) associated with predictions against an external validation set. In order to quantify the uncertainty in the predictions, accounting for both the uncertainty in the model parameters and noise in the new data, we provide confidence bounds for new (unseen) observations. Manufacturing process data used in the case study has been collected from a Mori Seiki NVD1500 DCG milling machine tool with experiments that cover a large parameter space. The data resulting from these experiments, which includes 18 different parts covering a wide range of process parameters, have been used to build the regression function to predict the energy consumption of the milling machine tool and is then tested on a part with a different geometry and with different process parameters to better understand the robustness of these approaches.

Energy prediction modeling and characterization of machine tools is a topic of research that finds significant impact and interest in the manufacturing industry. Applying predictive analytics using manufacturing data is a promising way to improve efficiency of manufacturing systems as well as reducing cost of production at every manufacturing level [3], [4]. Several machine learning approaches [4]-[6] have been used in metal manufacturing industries to study the relationship between process parameters and machine tool conditions. Accurate prediction of required energy consumption for machine tool operations enables manufacturers to improve operating efficiency and reduce cost, respond to new regulations and business drivers (e.g., the Smart Grid, carbon cap and trade policy), and develop useful process monitoring [5], [6] approaches relying on the predicted results. Moreover, degradation of cutting tools and the machine tool itself can be characterized using an adaptive energy prediction model and this can in turn lead to energy-efficient toolpath generation and planning.

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Acknowledgments and Disclaimer:
The authors would like to acknowledge the support of Jinkyoo Park from Stanford University, US in collecting, preparing and providing machine operation data. Certain commercial systems are identified in this paper. Such identification does not imply recommendation or endorsement by NIST; nor does it imply that the products identified are necessarily the best available for the purpose.

**MEASUREMENT SCIENCE FOR PROGNOSTICS, HEALTH MANAGEMENT, AND CONTROL**
**Technical Presentation.** VVS2016-8957
2:45pm-3:10pm

**Brian Weiss, Greg Vogl**, *National Institute of Standards and Technology, Gaithersburg, MD, United States,* **Moneer Helu**, *National Institute of Standards and Technology, Silver Spring, MD, United States,* **Guixiu Qiao**, *National Institute of Standards and Technology, Gaithersburg, MD, United States*

Early implementations of smart manufacturing technologies have enabled manufacturers to use equipment and process data to provide decision-makers with information on many performance-related measures (e.g., machine status and utilization) and overall process health. There is increasing interest to leverage the same data to generate diagnostic and prognostic intelligence at the machine, process, and system levels. Complex system, sub-system, and component interactions within smart manufacturing systems make it challenging to determine the specific influences of each on process performance, especially during disruptions. The simultaneous operation of complex systems within the factory increases the difficulty to determine and resolve failures due to ill- and/or undefined information flow relationships. There is no uniform process that guides sensing, prognostics and health management (PHM), and control at all levels (from the component to the system to the enterprise level). Proprietary solutions exist that integrate some manufacturing systems, but they apply to systems from one vendor and are often expensive and inaccessible to many manufacturers. The National Institute of Standards and Technology’s (NIST?s) Prognostics, Health Management, and Control (PHMC) project is aimed at advancing the measurement science (e.g. performance metrics, test methods, reference datasets, guidelines/standards, etc.) to promote the evolution of health monitoring, diagnostic, prognostic, and control strategies within smart manufacturing environments. The advancement of these capabilities will result in improved decision-making support and greater automation with a focus on vendor-neutral approaches and plug-and-play solutions. Specifically, the PHMC project will develop and output measurement science products as a means of providing the manufacturing community a way to verify and validate their own PHM technologies and strategies. To date, NIST has output several measurement science products in the form of published industry case studies and a comprehensive roadmapping report (output from an intense, two-day workshop hosted at NIST) that identify key challenges and barriers to be overcome in specific research domains within PHM.

The PHMC project has three key research thrusts: Machine Tool Linear Axes Diagnostics and Prognostics (at the component level), PHM for Robot Systems (at the work cell level), and Manufacturing Process and Equipment Monitoring (at the system level). Each research thrust is supported by a specific test bed that serves as a platform to develop test methods, use case scenarios, reference datasets, and supporting software/tools. As this research continues to evolve, the NIST team is looking to develop a set of guidelines/standards that will promote the adoption, implementation, verification, and validation of PHM technologies within smart manufacturing environments. This presentation will present the PHMC project’s efforts, to date, and lay out the planned future efforts to develop the necessary measurement science to verify and validate manufacturing PHM technologies and strategies.

**PHYSICS-BASED MODELING AND SIMULATION (M&S) MATURITY MODEL FOR ADVANCED MANUFACTURING**
Technical Presentation. VVS2016-9999
3:10pm-3:35pm

**Huijuan Dai, Matteo Bellucci, Ade Makinde,** *GE Global Research, Niskayuna, NY, United States*

Modeling and simulation play increasingly important roles in advanced manufacturing. These models are used to optimize process parameters in order to minimize manufacturing defects, reduce the number of physical trials and consequently reduce cost. In design engineering, there are specific

steps that a designer must take to ensure validity of numerical models for new product introduction and these steps have been codified into design practices within the various businesses at GE. However, for manufacturing process modeling, there are no such standards where the outcome of a simulation model depends on the modeler's experience and expertise. There is need to develop guidelines for manufacturing process simulation to ensure that the models are properly calibrated and validated in order to fully benefit from virtual manufacturing. These will enable us to:
(1) Identify manufacturing/sourcing risks and gaps much earlier
(2) Evaluate manufacturing and schedule impact on new product introduction
(3) Conduct producibility analysis
(4) Better estimate process development time and mature parts cost
(5) Rapidly attain yield level entitlement for the new manufacturing facilities (additive, casting, etc.)

In most manufacturing industries, a majority of process parameters is determined based on previous experiences and manufacturing process physics is rarely used to guide decisions. This makes it difficult to determine how much conservatism is built into processes. The resulting production costs of inefficiencies can be staggering. Many companies have started to develop what is called the smart factory where the different manufacturing processes for a component or product are linked in order to optimize the processes and minimize variability. Such smart factories require faster data feedback loops which can only be realized through the use of reduced order models coming from physics-based modeling. This means that the accuracy of modeling results is now more important than ever. In order to improve virtual process development and drive factory roadmaps, GE is developing a physics-based Modeling and Simulation (M&S) maturity model for advanced manufacturing. This model builds upon the Capability Maturity Model Integration (CMMI) framework which is used to define three focus areas and it is refined with highest maturity level end state in mind. We are going to describe current code verification/validation at GE-GRC, extending CMMI to include model selection, organization structure and talent training & development.

The M&S maturity model consists of three critical elements:
(1) M&S tools which are focused on process model representation, process physics fidelity, code/ algorithm/model integration, simulation verification & validation and uncertainty quantification.
(2) M&S procedures & methods including physics-based model selection, analysis set up/execution, result interpretation and application tutorial development
(3) M&S skills, training and motivation covering organization structure, workforce bench strength, training deployment plan, new product introduction and manufacturing / value engineering.

For each element, four levels of maturity and user categories are defined:
(1) Maturity level 0: empirical trial & error driven decisions, M&S used for manufacturing process scoping studies (user category: subject matter experts)
(2) Maturity level 1: expert M&S analyst driven decisions, M&S used for manufacturing process design support (user category: R&D engineers)
(3) Maturity level 2: operational M&S assisted decisions, M&S used for manufacturing process optimization (user category: R&D and process engineers)
(4) Maturity level 3: enterprise M&S driven decisions, M&S integrated into brilliant enterprise infrastructure (user category: enterprise workforce)

The tool provides guidelines to assess the maturity level of M&S effort in the manufacturing process, drive model & simulation rigor and product & process innovations.

## TRACK 2 Development and Application of Verification and Validation Standards

### 2-2
### DEVELOPMENT AND APPLICATION OF VERIFICATION AND VALIDATION STANDARDS

**2nd Floor, Acacia D** **4:00pm - 6:05pm**

**DEVELOPMENT AND IMPLEMENTATION OF NUCLEAR ENERGY KNOWLEDGEBASE AND SIMULATION CODE VALIDATION SYSTEM**
**Technical Presentation.** VVS2016-8825
4:00pm-4:25pm

**Weiju Ren**, *Oak Ridge National Laboratory, Oak Ridge, TN, United States*

To establish trust in simulation results, evidence must be systematically collected to validate simulation code for intended applications. The validation encounters significant challenges that require years of research and development (R&D). A plan is created to establish the Nuclear Energy Knowledgebase for Advanced Modeling and Simulation (NE-KAMS) to support the validation R&D under the direction of the Department of Energy's Nuclear Energy Knowledge and Validation Center (NEKVAC).

Perceived as a framework for collaborative research, NE-KAMS will consist of a Resource Portal to network resources worldwide for project cooperation, and a Validation Portal to develop knowledge management and software tools for code validation. For effective NEKVAC operation, NE-KAMS must develop the capacities for validation of single and multi-physics modeling and simulation to cover reactor physics, thermal-hydraulics, fuels performance, structural materials behavior, and chemistry of nuclear systems individually and coupled. Academics and researchers, reactor designers and vendors, regulators and operators would all benefit from this deployment and availability. NE-KAMS would facilitate participation of the networked resources and stakeholders in research and funding opportunities, and also support international collaborations and receive contributions such as those executed under joint international projects of the Nuclear Energy Agency.

Key characteristics required for NE-KAMS to develop the desired capacities include managing data at the lowest meaningful information element levels for effective data processing; maintaining relations among the information elements for data integrity; modularizing its structure for schema customization for different information domains; enabling data comparison along with a library of benchmarks, exact solutions, and other comparison bases; automating data transfer between database and simulation software; providing version control to track data evolution; and implementing access control to define user privileges.

In the initial development, the Resource Portal will be focused on modules for validation resources, terminology definitions, operation instructions, technical issues, NEKVAC documents, and research projects; while the Validation Portal on modules for R&D reports, experiment definitions, experiment units, material properties, fluid properties, test data, quality assurance, quality assessments, and data permits. As new requirements emerge from NEKVAC operations, more modules will be developed.

To enable timely data collection and effective data analysis and processing, NE-KAMS will consist of a Data File Warehouse that quickly archives original data files of different types and a Digital Database that efficiently manages data in various digitized information elements.

NE-KAMS will be developed and operated under the direction of the NEKVAC Directorate committees, which organize project identification, planning, approval, and implementation.

**IMPROVED STATISTICAL APPROACH FOR CERTIFICATION OF CFD CODES WITH EXAMPLES**

**Technical Presentation.** VVS2016-8832
4:25pm-4:50pm

**Frederick Stern**, *University Of Iowa, Iowa City, IA, United States,* **Matteo Diez**, *INSEAN, Rome, Italy,* **Seyed Hamid Sadat Hosseini**, *IIHR, Iowa City, IA, United States*

Improved Statistical Approach for Certification of CFD Codes with Examples

Stern et al. (2006) and Stern (2007) proposed a statistical approach for certification of CFD codes based on earlier statistical approach for estimating intervals of experimental facility biases (Stern et al., 2005) and extension of N-version testing (Hemsch, 2004). Approach includes consideration of systematic uncertainties (solution V&V), use of reference values (experimental data and uncertainties) and random uncertainty based on N-version testing standard deviation for estimating interval of certification. Certification is a process for assessing probabilistic confidence intervals for CFD codes for specified benchmark applications and certification variables. Certification of CFD codes is at the multiple codes or users, models, grid types, etc. level (code level). Multiple users are appropriate for many user codes, whereas multiple codes are appropriate for various few user codes (often case for industrial applications). Differences between versions and implementations are due to myriad possibilities for modeling, numerical methods, and their implementation as CFD codes and simulations.

One drawback of the approach is the use of mean code comparison error and standard deviation based on signed values as opposed to absolute values. The improved approach uses absolute values, which provides more conservative error estimates and possibility for certification at reduced intervals. Examples are provided for ship hydrodynamics using previous Gothenburg 2000 and Tokyo 2005 and most recent Tokyo 2015 CFD Workshop results. Role of individual code V&V vs. N-version testing are discussed along with opportunities and challenges for achieving consensus on standard V&V and certification methodology and procedures.

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**ON THE QUALITY CONTROL OF CFD CODE REFRESCO USING V&V STANDARDS**

**Technical Presentation.** VVS2016-8880
4:50pm-5:15pm

**Guilherme Vaz, Christiaan Klaij, Douwe Rijpkema**, *MARIN, Wageningen, Netherlands,* **Luis Eca**, *IST, Lisbon, Portugal*

V&V standards, and all its components (code verification, solution verification and solution validation), have been applied within the development of the CFD code ReFRESCO (www.refresco.org), since its beginning in 2009. ReFRESCO is an incompressible, multi-phase, viscous-flow code targeted, verified and validated for Maritime applications (ships, submarines, offshore platforms, renewable energy systems). Development and application take place within a community of developers and users spread around the world. In order to meet the high accuracy demands of the Maritime industry (errors below a few percent), it’s necessary to control and minimize not only human errors, but also coding, discretization, and modeling errors. Therefore the ReFRESCO community has the policy to verify and validate each new type of application before releasing the code to the end users interested in that specific purpose. This is not self-evident: all too often the burden of V&V is placed solely on the end user side.

The challenge arising from this policy is that V&V standards must be applied to real-life industrial problems and not only to simplified academic test-cases. In addition, it must be done in a sustainable and automatic way, for each code version, for all major features and applications. The procedure must fit within the rapid code development cycle involving several developers situated in different countries, using a variety of IT tools and platforms, and be suitable for heavy real-life cases.

In this presentation, we discuss the mechanisms and tools used within ReFRESCO to address these challenges. Several automated benchmark “suites” used to perform scalability studies, code verification, solution verification and solution validation are presented, both for academic and industrial relevant test cases.

**NAFEMS DOCUMENT: “VERIFICATION, VALIDATION, AND UNCERTAINTY QUANTIFICATION FOR MANAGERS”**

**Technical Presentation.** VVS2016-8918
5:15pm-5:40pm

**William Oberkampf**, *W L Oberkampf Consulting, Georgetown, TX, United States,* **Martin Pilch**, *M. Pilch Consulting, Tijeras, NM, United States*

The Analysis Management Working Group is the primary Working Group in NAFEMS that is responsible for the development and promotion of the activities of verification, validation, and uncertainty quantification (VVUQ) for simulation models. One of the documents in preparation by the AMWG is titled “Verification, Validation, and Uncertainty Quantification for Managers” to be authored by W. L. Oberkampf and M. Pilch. The primary focus of the document will be management personnel in both private and government organizations who use, develop, or procure simulation capabilities and results. This would include not only managers and decision makers within the organization generating simulation results, but also managers, customers, and regulatory authorities who use simulation results in their organizations for product design, safety and performance decisions, regulatory control, and policy formation for engineering and environmental systems. The document will be written so that much of the material could be understood by managers and decision makers who do not have technical training in mathematics, science, and engineering.

The document is planned as a two-part document. The primary part of the document would concentrate on: (a) the stunning breadth of simulation-informed decision making in private organizations and governments, (b) the value proposition of VVUQ, (c) the trade-offs between VVUQ and loss of credibility of simulation results, (d) the responsibilities and risks of simulation capability developers, simulation producers, simulation customers, and simulation stakeholders, (e) the cost, schedule, and resource requirements needed for VVUQ activities, and (f) how producers and consumers of simulation results could balance trade-offs between simulation confidence and potential adverse consequences of ill-informed decisions based on simulation information. It will be stressed that there is no universal answer to the question “How much VVUQ is sufficient”? The answer should depend on the importance of simulation results in the decision-making process, the cost and schedule trade-off with other potential sources of credible information, and the potential adverse consequences of an ill-informed decision. It will be pointed out that adverse consequences can be very difficult to identify because they the are both near term and long term, and they can be thought of as local, e.g., the individual computational analyst or the decision maker, or thought of as comprehensive, e.g., the organization or public safety and welfare.

The second part of the document will be the appendices. The appendices will briefly discuss the basic approaches, procedures, technical personnel, facilities, costs, and schedules associated with VVUQ activities. Specific topics to be addresses are: (a) setting simulation requirements relative to customer needs, (b) code verification, (c) solution verification, (d) validation experiments and model accuracy assessment, (e) total uncertainty estimation in a simulation, (f) the use of sensitivity analyses, and (g) simulation planning and management.

**CALIBRATION ISSUES AND UNCERTAINTY**
**Technical Presentation.** VVS2016-8801
5:40pm-6:05pm

**Richard J. Peppin**, *Engineers for Change, Inc., Rockville, MD, United States*

Calibration is often required when using precision measuring instrumentation. This paper, while focusing on acoustical instrumentation, can be generalized to all instruments where the results of measurements are of major concern. This paper critically examines field and lab calibrations and the intervals used for recalibration. For example, concentrating on ommunity noise- in some community noise ordinances a section might say "instrument must be calibrated within the last year." Where did that "year" come from? What happens if it gets calibrated, whatever that means, and the day after receipt, the instrument is dropped? Can you wait a year? When instruments are sent to a calibration lab they often come back with some sort of certificate, the "calibration certificate." There are some points to discuss about that certificate. 1) Was it done by an "accredited" laboratory? If so, you may have noticed there is no "calibration due date." (Or there shouldn't be, unless you tell the lab you want it on and what that date is to be.) When to calibrate is an issue that, really, is independent of using a calibration lab or not. How often to calibrate? (Calibration is NOT just using an acoustical calibrator to check sensitivity.) 2) To what degree of accuracy does the lab check the instruments? There really is no choice here because often the instrument standard (like for a Class 1 or 2 system) is specified in the corresponding IEC or ANSI standards. But is it necessary? So, there are at least two issues in the area of acoustical measurements that are of importance: 1) how important is calibration and to what level of accuracy and 2) how frequently must we calibrate our instruments and how do we determine it. This paper discusses both these concerns. Specifically I discuss if the 0.01 dB sensitivity resolution makes any sense, if yearly calibration is "right," and, most importantly, how we can make reasonable decisions on instrument calibration intervals.

## TRACK 3 Topics in Verification and Validation

### 3-1
### ENHANCEMENTS OF V&V THINKING AND APPROACHES
**1st Floor, Mesquite 2** **4:00pm - 6:05pm**

**UNCERTAINTY IN UNCERTAINTY QUANTIFICATION AND THE VALIDITY OF VALIDATION**
**Technical Presentation.** VVS2016-8821
4:00pm-4:25pm

**Daniel Segalman**, *Michigan State University, East Lansing, MI, United States,* **Thomas Paez**, *Thomas Paez Consulting, Sedona, AZ, United States*

Uncertainty quantification (UQ) is the process of characterizing all uncertainties in a model or experiment and of quantifying their effect on the simulation or experimental outcomes. The process of uncertainty quantification is usually performed only to assess the chances of high stakes events, especially when those events are expected to be rare. The usual sort of conclusion one draws from such an analysis is expressed along the lines of "the probability of a fatal accident is less than 1 in ten to the fifth". When UQ is performed with a model, it is usually assumed that the model has been validated; the rub is that models are never perfectly "validated" as being quantitatively correct and the probability distributions of the model parameters are known only in regimes easy to observe. The goal of employing uncertainty quantification to estimate the probability of very unlikely events is flawed from the get-go.

In this talk both the issues - quantitative model validation and poor resolution on probability distributions of model parameters - are addressed through mappings from regions where parameter properties and model fidelity are unknown or unclear to regions in parameter space where those issues are understood much better. The resulting formulation "though more difficult to implement" has firm theoretical foundation and yields conclusions expressed more squarely on engineering considerations.

This approach is substantially more conservative than that conventionally employed. Instead of asserting the correctness of models from experiments in conveniently testable regimes and then applying those models in other regimes, in this approach one employs the validation experiments to calculate quantitative error bounds in the tested regime. This quantitatively validated model is then employed to assess and quantify the uncertainty of model predictions and in a way that accounts for the measured error of the model and the uncertainty in the parameter distributions.

**A HOLISTIC APPROACH TO CREDIBILITY AND UNCERTAINTY ASSESSMENT**
**Technical Presentation.** VVS2016-8836
4:25pm-4:50pm

**William Rider**, *Sandia National Laboratories, Albuquerque, NM, United States,* **Kenneth Hu, Walter Witkowski**, *Sandia National Laboratories, Albuquerque, NM, United States*

When modeling and simulation is used as part of a decision-making process the requirements and demands for credibility and uncertainty assessment become far more refined. In the past several decades modeling and simulation has become an integral part of many decision-making processes yet the assessment of the quality has not kept pace with this integration. Moreover the complexity of defining credibility and uncertainty makes any assessment incomplete. The lack of completeness is a trap that most credibility and uncertainty assessments fall into that gives most analysts the excuse to short-change the exercise. In other words any assessment of credibility and uncertainty will be incomplete, but this in no way means such an endeavor should not be engaged. Instead the depth of complexity is the very reason such assessments need a vigorous engagement. Moreover they provide perspective and depth of understanding necessary for improving the quality of existing work. Without such focus, progress inevitably stagnates.

We suggest basing the overall assessment of the modeling and simulation credibility on three basic activities that reinforce one another in their execution. The first activity is the identification of the reasons for conducting the modeling and simulation, its role in any decision-making and the quantities of interest to be used. The second activity is the formal assessment of credibility, which we suggest be arranged around the completion of a PIRT and PCMM for the analysis and any computational tools utilized in its conduct. The credibility is founded on mapping the computational tools and modeling to the intended use and requirements for the simulated results. We believe this provides a structural basis for defining the credibility of the analysis. Finally the third step is completing an overall uncertainty assessment for the combination of the modeling and simulation with any testing or experiment. Too often in such uncertainty assessments key aspects of the uncertainty are not explored and the analyst assigns an uncertainty of zero (often implicitly). The reality is that this uncertainty should almost always be much larger and certainly not zero. If executed on a regular basis these three steps can provide the basis for far better delivery of modeling and simulation results with credibility in a form suitable for decision making. The entire process should ideally be iterative with a firm engagement with previous results in conducting future work. An objective to strive toward is the actual quantitative decrease in uncertainty as more work is conducted to assess it. In most cases the exact opposite occurs almost as a matter of course. Today doing no work at all is typically rewarded by the assignment of the value of identically zero for the uncertainty.

We will provide a set of concrete steps for presenting credibility and producing a holistic uncertainty assessment. The credibility will be provided by a concise definition of the use of the simulation results, the quantities of interest examined and their origin whether computed or measured through experiment or observation. The credibility statements are bridged to experiments via the PIRT, and to the computational tools through PCMM. Finally these sources of information are engaged to provide concrete assessments of uncertainty. In cases where the information is not sufficient to provide a concrete assessment of uncertainty subject matter experts should be consulted, and this deficiency should be addressed as soon as possible. The goal of the work is to make the strengths and weaknesses of the modeling and simulation activity as explicit as possible. Future work can be defined from the product of this exercise.

**THOUGHTS AND DEVELOPMENTS TOWARD THE 2ND LAW OF MODELING AND SIMULATION AND ITS IMPLICATIONS**
**Technical Presentation.** VVS2016-8910
4:50pm-5:15pm

**Vicente Romero**, *Sandia National Laboratories, Albuquerque, NM, United States*

"All models are wrong, some are useful 'the practical question is how wrong do they have to be to not be useful'? These well-recognized statements by the eminent statistician George Box are considered by the author of this talk to be partial statements of a proposed "2nd Law" of Modeling and Simulation. Box was presumably referring to mathematical and statistical analytical models at the time, and not to numerical/computational physics models, but his statements are also applicable to computational physics models. The author proposes the following as another partial statement of the 2nd Law of M&S (2LMS). "Modeling and simulation can only provide inequality statements about reality, as opposed to equality statements." This expression of 2LMS perhaps makes more clear the implications, challenge, and action implied: "Provide suitable inequality statements with your M&S results."

The author recognizes that the sentiment that all models are imperfect has been expressed in various ways by countless scientists and engineers in the past, and is not foreign to many or most M&S practitioners. But it appears there is a need and advantage to consolidate the various expressions of this sentiment via a common recognizable vessel here proposed as the 2nd Law of Modeling and Simulation. Indeed, the sentiment should be taught at the undergraduate level of technical disciplines and presented as a Law that exists as a constraint on what modeling and simulation are capable of and not capable of, just as the Second Law of Thermodynamics is taught as a constraint on the relationship between work and heat. The implications of universally recognizing the 2nd Law of M&S and the fact that M&S (and experiments) can only provide inequality statements about reality, rather than equality statements, should be present more centrally in engineering and science education and practice.
Uncertainty can be used to express inequality statements of the type discussed here. Uncertainty is a mechanism for bridging the gap between physical reality and experiments, mathematics, computers, simulations, and inferences. Of course, uncertainty models and procedures are also subject to 2LMS and are imperfect as well. The talk will consider implications of these observations, as well as developments toward the challenge of providing suitable uncertainty procedures and inequality statements subject to institutional objectives and risk postures.

**THE FALLACIOUS PROMISES OF V&V**
**Technical Presentation.** VVS2016-8922
5:15pm-5:40pm

**Francois Hemez, Kendra Van Buren**, *Los Alamos National Laboratory, Los Alamos, NM, United States*

The accelerated pace at which challenges in global security, ecology, economy, and welfare of the citizen have been "globalized" in the last two decades is yielding profound alterations in the manner in which decisions are supported. One of the most significant changes is the ever-increasing reliance on first-principles modeling and simulation. Examples include supporting decision-making in public health or energy security, anticipating the effects of climate change, and meeting global security challenges. The activity of simulating, however, introduces modeling assumptions that should be validated and sources of uncertainty whose effects on decisions should be managed. Doing so is the responsibility of the Verification and Validation (V&V) community. The question posed is: Has V&V delivered its promise of achieving "better" models in computational sciences and engineering? Drawing from the authors' world-renowned experience at Los Alamos National Laboratory and other institutions, a three-point critique is articulated. Our discussion starts with the recognition that the validation domain, where physical measurements are available to assess the accuracy of numerical predictions, is often disjoint from the forecasting domain where predictions are sought to support decision-making. It is our contention that the discipline of V&V has largely failed to recognize this fundamental distinction between validation and forecasting domains. Consequently, much of the technology currently developed to support V&V efforts, such as test-analysis correlation and statistical discrepancy functions, is inappropriate to assess forecasting accuracy. This primal sin results in the failure to establish what makes a "correct" decision, which is the second point of our critique. Thoughts are offered on how V&V could more effectively contribute to decision-making. The third point is the inappropriate structure of V&V programs at large institutions, such as National Laboratories, which foster standardization and compliance at the expense of integration and innovation. The presentation concludes by discussing what it would take to reach "confident" decisions, which is ultimately what stakeholders and decision-makers care about.

**M&S REQUIREMENTS AND VV&A REQUIREMENTS: WHAT'S THE RELATIONSHIP?**
**Technical Presentation.** VVS2016-8940
5:40pm-6:05pm

**David Hall**, *SURVICE Engineering Company, Carlsbad, CA, United States,* **James Elele**, *Naval Air Systems Command, Patuxent River, MD, United States,* **Allie Farid, Mark Davis, David Turner, John Madry**, *SURVICE Engineering Company, Lexington Park, MD, United States*

Requirements for software development should be driven by the anticipated uses of the software. In the particular case of modeling and simulation (M&S) tools, Verification, Validation and Accreditation (VV&A) activities also are driven by those same intended uses. In our experience, VV&A activities help to refine the software requirements for M&S by tying them more closely with the needs of the intended use.

Three basic criteria influence the credibility of a simulation and whether it is acceptable for the intended uses:
Capability - the functions it models and the level of detail with which they are modeled should support its anticipated uses.
Accuracy - how accurate it must be should depend on the risks involved if the answers are incorrect.
Usability - the extent of available user support to ensure it isn't misused should also derive from the importance of its application.

M&S acceptability criteria must be derived from the requirements that support the intended uses. Whether an M&S is acceptable for an application (intended use) is determined by how well it meets the requirements of that intended use. How well it meets those requirements has to be determined by an assessment method, with criteria identified as to how the user will decide if it passes or fails. The assessment criteria can be subjective or objective, depending on the assessment method. Accreditation activities are focused on assessments of capability, accuracy and usability as compared with acceptability criteria established for the intended uses.

VV&A activities thus expand on and supplement the software requirements to address the five questions posed below for each of those uses.
What are the users' needs for the M&S (i.e., what questions do they need to answer)?
How does the user anticipate that such a model might help meet those

needs (i.e., what outputs will be used to help answer those questions)?
What characteristics must the M&S have in order to meet those needs (capability, accuracy, and usability - how accurate must the answers be, and what functionality and fidelity are required to ensure an adequate answer to the questions)?
What information will be required in order to determine if the M&S meets those needs (documentation, V&V results, results of previous uses, etc.)?

We will show examples of how VV&A activities improved upon and refined the requirements originally developed for M&S tools, and how focusing on capability, accuracy and usability requirements helps develop better software requirements and ultimately better M&S tools.

## TRACK 4 Uncertainty Quantification, Sensitivity Analysis, and Prediction

### 4-3
### UNCERTAINTY QUANTIFICATION, SENSITIVITY ANALYSIS, AND PREDICTION: SESSION 3

**2nd Floor, Palo Verde A** **4:00pm - 6:05pm**

**AUTOMATIC DIMENSIONALITY REDUCTION VIA DEEP ARCHITECTURES AND APPLICATIONS TO HIGH-DIMENSIONAL UNCERTAINTY QUANTIFICATION**
**Technical Presentation.** VVS2016-8861
4:00pm-4:25pm

**Rohit Tripathy, Ilias Bilionis**, *Purdue University, West Lafayette, IN, United States*

Uncertainty Quantification (UQ) is a burgeoning field, the ultimate goal of which is to develop reliable predictive models for complex physical phenomena. Owing to the curse of dimensionality, the cost of performing UQ increases exponentially with the number of model parameters. This problem is compounded by the fact that computational models are becoming increasingly more sophisticated so as to better capture the underlying physics. Thus, despite rapid advances in computer hardware, there is a significant cost associated with evaluating state-of-the-art computer codes. In order to mitigate this high computational cost, one typically resorts to building a surrogate of the computer code. However, traditional surrogate models do not scale well in high input dimensions. The curse of dimensionality is typically addressed by looking for special structure in the high dimensional design space. In this work, we look for a low dimensional manifold embedded in the input parameter space, which captures most of variability of the response. We demonstrate recent advances in gradient-free active subspace discovery and exploitation using Gaussian process (GP) regression to study both the uncertainty propagation problem (quantifying output uncertainties given input uncertainties) as well as the inverse problem (learning system properties such as porosity and permeability from historic production data) based on a finite number of evaluations of the computer code. The results will be compared systematically to deep convolutional neural networks which, given the recent successes in the field of image classification, seem to be the natural way to extend our methodology to account for non-linear features connecting the input to the output.

In our application, we study flow through porous media which has gained significant attention due to its extensive applications in several areas of applied fluid mechanics. Specifically, we consider the problem of two-phase flow in an oil reservoir. The dynamics of porous media flow are governed by Darcy's Law, which is parameterized by the permeability tensor and viscosity of the porous medium. Uncertainties about the soil structure and its material properties lead to uncertainties in the permeability and porosity of the media. Naturally, any robust predictive simulation model must necessarily be probabilistic, accounting for uncertainties in the permeability and porosity of the system. The permeability tensor is characterized by a very large number of random parameters, making it an ideal benchmark for the proposed methodological developments.

**RECENT ADVANCES IN DAKOTA SA, OPTIMIZATION, AND UQ SOFTWARE**
**Technical Presentation.** VVS2016-8884
4:25pm-4:50pm

**Brian Adams**, *Sandia National Laboratories, Albuquerque, NM, United States*

Sandia National Laboratories? Dakota software (http://dakota.sandia.gov) delivers advanced parametric analysis techniques enabling quantification of margins and uncertainty, risk analysis, model calibration, and design exploration with computational models. Its methods include optimization, uncertainty quantification, parameter estimation, and sensitivity analysis, which may be used individually or as components within surrogate-based and other advanced strategies. Available publicly under an open source license, Dakota is used broadly by academic, government, and corporate institutions and plays a critical role in DOE ASC, Office of Science, and Office of Nuclear Energy Programs. This presentation will survey Dakota's capabilities, interfaces, and algorithms. It will then highlight recent developments, including architecture improvements and algorithm R&D that aim to make these analyses practical for complex science and engineering models. Growth directions such as architecture modularity, graphical user interfaces, and improved algorithms for sensitivity analysis, surrogate modelling, and Bayesian inference, will be reviewed.

**DEALING WITH MISSING DATA IN MULTI-INTELLIGENCE STATISTICAL MODELS**
**Technical Presentation.** VVS2016-8935
4:50pm-5:15pm

**Kendra Van Buren, Francois Hemez**, *Los Alamos National Laboratory, Los Alamos, NM, United States*

In the discipline of verification and validation (V&V), statistical models are used for a wide range of purposes, including empirical model development, test-analysis correlation, and sensitivity analysis. In data-driven analysis, however, the development of statistical models can be hindered due to the lack of data availability, especially when dealing with experimental observations from multiple sources or sensors where there may be lapses in data collection. For example, sensors are often deployed to measure temperature variations, pressure profiles, and vibration response. It is important, however, to have a complete dataset because many methods for analyzing data, such as principal component analysis, clustering, and supervised machine learning, require it. In many applications, significant gaps in data can occur due to battery failure of the sensors, environmental effects that result in intermittent collection of data, or decisions to change the sensor setup. The most common method for dealing with missing data is to restrict the analysis to observations with complete data, ignoring those with partial information.

We present an application that represents multiple sensors collecting data around a technical facility, where one or more data streams were not observed during 75% of the analysis time frame. It is clearly desirable to find a way to utilize all of the data that are collected in the development and validation of statistical models. Herein, we pursue two techniques to estimate feature streams where no raw data was available due to lapses in the collection effort. The first technique, referred to as median imputation, is commonly employed in the gene analysis literature. The second technique is a novel method that attempts to estimate trends that would have been observed had the data been collected. This technique is based on the assumption that if data streams are monitoring a similar activity but in a different manner, the streams will likely be correlated. Since we expect the different streams to vary similarly over time, we are using the potentially complicated correlations of the streams to produce a reasonable estimate of the unobserved stream.

Finally, we generate uncertainty bounds of the unobserved data to account for our incomplete knowledge of the missing data values. We show that the uncertainty bounds can then be propagated through to subsequent analyses to prevent unobserved values from having the same weight on the conclusions as those that were collected experimentally.

**CM&S AND VVUQ OF COMPLEX SYSTEMS USING "DIGITAL TWIN" AND "DIGITAL THREAD" FRAMEWORKS**
**Technical Presentation.** VVS2016-8945
5:15pm-5:40pm

**Sanjeev Kulkarni**, *VEXTEC Corporation, Brentwood, TN, United States,* **Robert Tryon**, *VEXTEC, Brentwood, TN, United States,* **Animesh Dey**, *VEXTEC Corporation, Brentwood, TN, United States*

The future vision of the United States Air Force (USAF) includes the "Aircraft Digital Twin", i.e. virtual simulations offering real time, high-fidelity operational decisions for individual aircraft by tail number - an actual inspection of the aircraft updates the Digital Twin model including any detected flaws. The framework that makes the "Aircraft Digital Twin" a reality is the concept of a "Digital Thread". The "Digital Thread" is the backbone system with continuous updates to allow dynamic, real-time assessment of the system's current and future capabilities to make informed decisions. The key components of the "Digital Thread" framework are a) a physics based microstructural material modeling and b) a methodology for uncertainty quantification tied together by a Monte Carlo simulation engine that leverages all existing knowledge (test and models). The simulation engine itself incorporates multi-scale statistical characterization using probabilistic and parallel computational simulation techniques.

VEXTEC's representation of the above described framework is, Virtual Life Management® (VLM®). The VLM tool is a method that combines testing with computational simulation to address device reliability and product certification. It is a modeling and simulation capability that predicts product durability at the material microstructural level, while accounting for the inherent variability of material processing, product manufacturing and changes in in-service usage conditions. VLM has been successfully applied to metals, laminated composites, and ceramics used in structural, mechanical and electrical products. The key strength of VLM is to understand the reasons for variability, for correlating the impact of the uncertainty on the output result and providing broader insights.

Further, this probabilistic framework sits on top of and works integrally with commercially available finite element software such as, DS Simulia, ANSYS and Nastran that leverages the structural analysis output with material microstructural damage simulation to develop a durability prediction model with higher confidence. The technology is in the form of a software tool and aligns with Integrated Computational Materials Engineering (ICME) and the Materials Genome.

A cornerstone of implementation is the Verification & Validation as well as the Uncertainty Quantification. Such VVUQ is required at multiple scales and hierarchical levels. VVUQ has been demonstrated for complex analyses. The basis of the technology, its implementation and VVUQ protocol is the topic of this presentation. As a highlight, broad applications in multiple industries (Automotive, High-Tech and Medical Devices) will also be discussed - applications ranging from analyzing fleet level risk to predicting failure in components and complex systems, from reducing time and resources to develop new products to optimizing maintenance schedules.

**STOCHASTIC MULTI-OBJECTIVE OPTIMIZATION ON A BUDGET: APPLICATION TO MULTI-PASS WIRE DRAWING WITH QUANTIFIED UNCERTAINTIES**
**Technical Presentation.** VVS2016-8862
5:40pm-6:05pm

**Piyush Pandita, Ilias Bilionis, Jitesh Panchal**, *Purdue University, West Lafayette, IN, United States,* **Amol Joshi, Pragmod Zagade**, *TCS, Pune, Maharashtra, India*

Design optimization of engineering systems with multiple competing objectives is a painstakingly tedious process especially when the objective functions are "expensive-to-evaluate" computer codes with parametric uncertainties. The effectiveness of the state-of-the-art techniques, like goal programming, goal attainment approach, weighted-sum method and heuristic methods like genetic algorithms, is greatly diminished mainly due to the following lacuna: 1) they generate solutions that are "dominated" or not "Pareto optimal" and; 2) they require large number of objective evaluations, which makes them impractical for realistic problems. Bayesian global optimization (BGO), has been relatively successful in dealing with the above challenges in solving single-objective optimization problems and has recently been extended to multi-objective optimization (MOO). BGO models the objectives via probabilistic surrogates and uses the epistemic uncertainty to define an information acquisition function (IAF) that quantifies the merit of evaluating the objective at untried designs. The expensive objective is evaluated at the design corresponding to the maximum value of the IAF, and the latest observation is used to update the surrogate. This iterative process continues until a stopping criterion is met. The most commonly used IAF is the Expected improvement (EI), which extends to the Expected improvement over the dominated Hyper volume (EIHV) when solving MOO problems. Unfortunately, the current versions of EIHV are unable to deal with parametric uncertainties or uncertainties in measuring the objectives. In this work, we provide a systematic reformulation of EIHV to deal with the problem of stochastic MOO. An addendum of the probabilistic nature of our methodology is that it enables us to characterize our confidence about the predicted Pareto front and use this information to formulate a stopping criterion. We verify and validate the proposed methodology by applying it on synthetic test problems with known solutions. We demonstrate our approach on a real engineering problem of die pass design for a multi-pass steel wire drawing where the physical process is represented by an expensive Finite element solver (developed at TRDDC, Pune, India). The competing objectives in this problem are the ultimate tensile strength and the strain non-uniform factor of the drawn wire. The reduction ratios and the die angles at each pass are the design/process variables which have associated uncertainties due to unavoidable manufacturing tolerances as well as die wear during the process. The methodology provides flexibility to the designer to design the die parameters while quantifying the associated uncertainties.

## TRACK 12 Verification Methods

**12-1**
**VERIFICATION METHODS (TRACK)**
**2nd Floor, Palo Verde B** **4:00pm - 6:05pm**

**DISCRETIZATION ERROR TRANSPORT FOR UNSTRUCTURED CFD**
**Technical Presentation.** VVS2016-8888
4:00pm-4:25pm

**Brian Carnes**, *Sandia National Laboratories, Albuquerque, NM, United States*

Estimation of discretization error is an important test for verification of computer simulations. For CFD codes, this is often accomplished by performing a grid refinement study. Recently the concept of discretization error transport has been studied by various authors, with the goal of computing an estimation of the discretization error using a single mesh, with only the cost of another flow solve. We present work on a novel method to generate the source term for discretization error transport in the context of unstructured vertex-based finite volume flow solvers. Results include verification of the computed error indicator and application to mesh adaptivity.

**VERIFICATION AND VALIDATION OF THE NAVY ENERGETIC MODELING ORACLE (NEMO)**
**Technical Presentation.** VVS2016-8913
4:25pm-4:50pm

**Badri Hiriyur**, *Thornton Tomasetti - Weidlinger Applied Science, New Providence, NJ, United States,* **Paul Hassig**, *Thornton Tomasetti - Weidlinger Applied Science, New York, NY, United States,* **John Gilbert**, *NSWCCD, Bethesda, MD, United States,* **Michael Miraglia**, *Naval Surface Warfare Center Carderock Division, Bethesda, MD, United States,* **Jonathan Stergiou**, *Naval Surface*

*Warfare Center, Carderock Division, West Bethesda, MD, United States,* **Najib Abboud**, *Thornton Tomasetti - Weidlinger Applied Science, New York, NY, United States,* **Erwin Moyer**, *NSWCCD, West Bethesda, MD, United States*

NEMO is a CFD hydrocode under development at NSWC Carderock Division and is focused on providing a modern platform for underwater fluid-structure coupled shock analyses. It specifically aims to provide a platform for convenient and rapid prototyping of new and candidate algorithms that can enhance Navy capabilities while assessing their robustness and their readiness for production-level analyses. For simulations involving fluid-structure interactions, NEMO is coupled with Sierra Mechanics, a suite of computational solid mechanics tools developed by Sandia National Laboratories, within the Navy Enhanced Sierra Mechanics (NESM) toolkit. This talk focuses on V&V of NEMO and covers three topics: The first part, which is the primary focus of this talk, covers code verification and assessment of (a) the order-of-accuracy of the solution of Euler equations in the fluid flowfield and (b) the order-of-accuracy of the pressure loads conveyed to NESM in a coupled simulation. The second part covers validation of NEMO/NESM by comparing the results of a series of coupled simulations with respect to benchmark experimental data. Finally, we briefly discuss a couple of tools that aid in the software QA process with a discussion of (a) NUnit - a framework for unit testing NEMO code modules, and (b) NERT - a framework for automated regression testing of NEMO and NESM.

Acknowledgement: This work is funded under a Naval Surface Warfare Center - Carderock Division contract N00167-11-D-0008

### VERIFYING DIFFERENT METHODS FOR THE INCLUSION OF MOTIONS IN THERMAL FE-ANALYSES OF STRUCTURES

**Technical Presentation.** VVS2016-8809
4:50pm-5:15pm

**Marian Partzsch, Michael Beitelschmidt**, *Technische Universität Dresden, Dresden, Germany*

The German Collaborative Research Center/Transregio 96 “Thermo-energetic design of machine tools” (CRC/TR96) aims to decrease the thermally caused production defect of machine tools in an energy efficient way. Various simulation-based methods are developed which either should correct the thermal error online during the production process itself or should previously compensate it by an innovative design of the machine tool during its development phase. Therefore, the underlying numerical analyses are of distinct characters because they need to meet several application-oriented requirements. Furthermore, in order to predict the thermo-elastic deformation more precisely, these analyses should especially consider the structural variabilities of the simulated systems as well as the position depended interactions between the motion-involved bodies, which both are of a certain relevance in the field of machine tool engineering.

In detail, we will talk about a sequential thermo-elastic finite-element analysis of these structural variable systems carried out with the open-source FE-software AMDiS. This approach allows a flexible treatment and customization of the desired analysis especially with regard to the inclusion of the motions and by making it accessible for multicore HPC or allowing the usage of a problem focused integration scheme. With this, a very beneficial ratio between the effort of calculation time and the result quality is obtained, so that the AMDiS-approach can serve as the base for developing the compensation methods as well as an overall reference for long term calculations within the research activities of the CRC/TR96 itself. Its effectivity is furthermore improved by incorporating the so called Defect Corrected Averaging method (DCA) within the analysis which significantly reduces the needed calculation time by taking advantage of the often occurring periodicity of the mapped motions.

We will also talk about an approach using a Model Order Reduction (MOR) of the given FE system matrices to enable an online computation of the thermal defect on the limited hardware of an ordinary machine tool control unit. In this approach, the structural variability is represented by an individual parameter that the system matrices are dependent of, whereby their parameter affine representation is used for determining the projection matrices between original and reduced system.

Now the inclusion of motions by these novel and mathematically more sophisticated approaches need a reliable references to be verified with. Therefore, a further approach within the commercial and common used FE-software ANSYS has been developed, which uses the very intuitive method of discretely adjusting the position within the time steps of a transient analysis.

In this technical presentation, we will shortly introduce the theoretical basics of how the structural variabilities are included within the single simulation approaches. Thereafter, we briefly demonstrate the systematical verification of each approach against the results of a related reasonable method, whereby the ANSYS approach will serve as the basic numerical reference. The performance of the ANSYS-approach is finally verified against the analytical JAEGER-solution for the temperature field of a semi-infinite solid exposed to a constantly moving source of heat.

The research activities within the CRC/TR96 are funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation). Therefore, we would like to extend our deepest appreciation for their support.

### VERIFICATION OF A HIGH-ORDER COMPRESSIBLE FINITE ELEMENT-BASED EULER/NAVIER-STOKES CODE USING THE METHOD OF MANUFACTURED SOLUTIONS

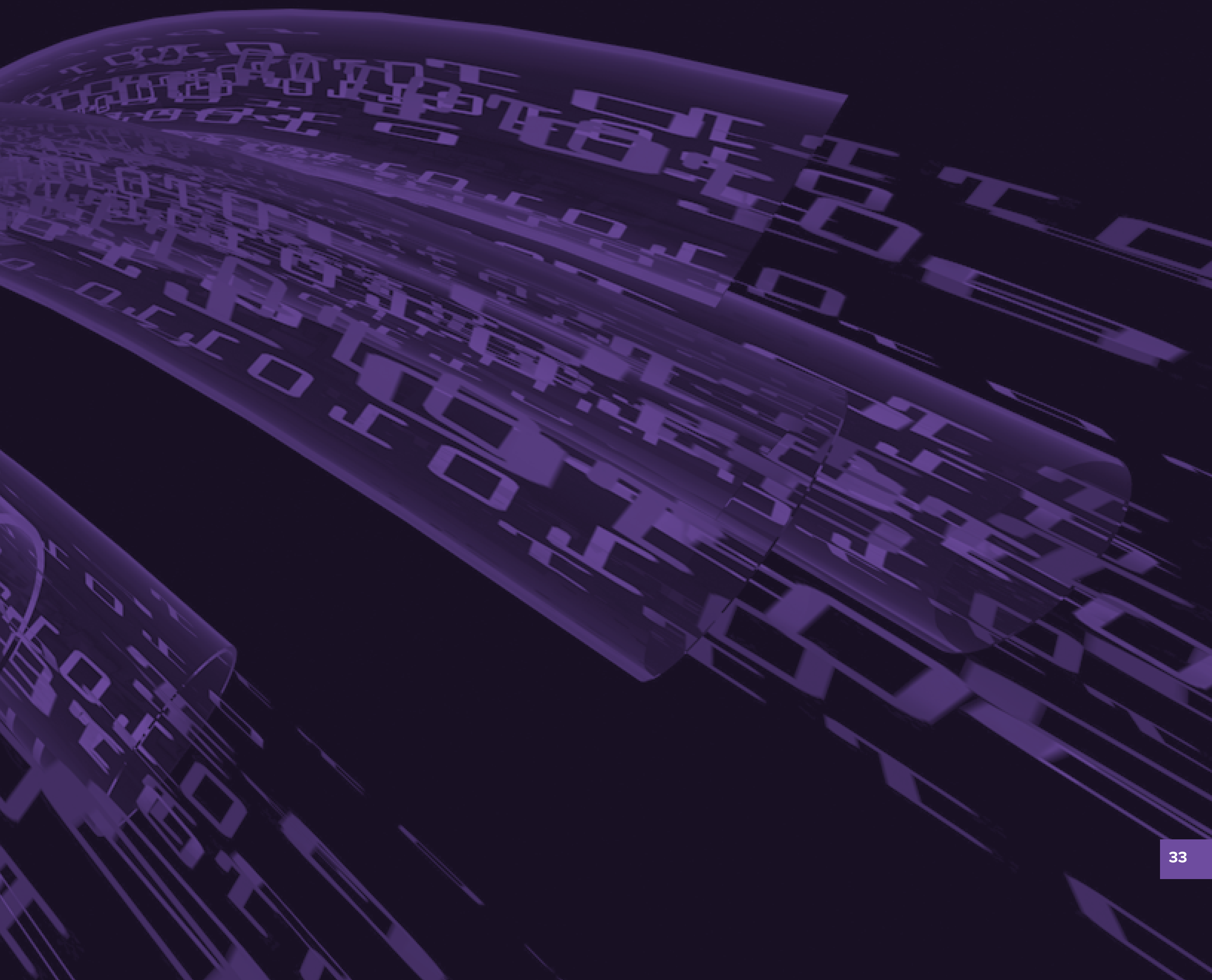
**Technical Presentation.** VVS2016-8816
5:15pm-5:40pm

**Seyi Olatoyinbo**, *National Space Research and Development Agency, Abuja, FCT, Nigeria,* **Abdelkader Frendi**, *University of Alabama in Huntsville, Huntsviile, AL, United States*

A high-order computational fluid dynamics (CFD) code was developed “in-house” to solve compressible turbulent flow and acoustic problems using a mixed explicit-implicit numerical scheme, namely the Flowfield Dependent Variation (FDV) method implemented in a Finite Element Method (FEM) framework that supports arbitrarily high-order, unstructured, isoparametric elements in one-, two- and three-dimensional geometries. The FDV method is fundamentally derived from the Lax-Wendroff Scheme (LWS) by replacing the explicit time derivatives in LWS with a weighted explicit and implicit time derivatives. The increased implicitness and the intrinsic numerical dissipation of FDV contribute to its numerical stability, as well as monotonicity. The finite element code employs linear, quadratic and cubic isoparametric two-dimensional (2-D) quadrilateral and three-dimensional (3-D) hexahedral Lagrange elements with corresponding piecewise shape functions which are formally second-, third- and fourth-order accurate in space, respectively. This paper presents the results of observed order-of-accuracy of the implemented FDV-FEM scheme involving grid and polynomial order refinements on uniform Cartesian grids. The Method of Manufactured Solutions (MMS) is used to “manufacture” exact solutions to the governing equations and to generate additional source terms. The exact (manufactured) solutions are then utilized to calculate the discretization error in the numerical solutions. The MMS approach is applied to 2-D inviscid Euler and laminar Navier-Stokes equations along with the analytical source terms, spanning both subsonic and supersonic flow regimes. By employing global discretization error analyses, the spatial order-of-accuracy of the FDV-FEM scheme is observed to be nearly equal to the order of the shape function polynomial plus one, for the four test cases investigated, in good agreement with theory. This procedure gives a high level of confidence that the code is free from programming errors in the spatial discretization. Furthermore, the wider applicability of the MMS approach in the verification of spatial order-of-accuracy of a higher order CFD method is established.

Technical Program

# Thursday, May 19, 2016



## TRACK 3 Topics in Verification and Validation

### 3-2
### TOPICS IN VERIFICATION AND VALIDATION
**2nd Floor, Acacia D** **10:25am - 12:30pm**

**DEVELOPMENT AND INTEGRATION OF ENVIRONMENTAL SENSORS MODELS FOR DRIVER ASSISTANCE SYSTEMS IN A REAL-TIME HIL-BASED SIMULATION ENVIRONMENT**
**Technical Presentation.** VVS2016-8834
10:25am-10:50am

**Mohamed Elgharbawy**, *Daimler AG, Stuttgart, Germany*

The paper contains the conceptual design for sensor simulation in a hardware-in-the-loop test bench. Starting from the conflict between realism and computational effort a compromise is worked out. This compromise considers both high real-time requirements of the test bench and demands on the sensor models. As a first step to develop the compromise a requirements analysis of the test bench, the assistance functions and the real sensors is done. The derived conditions of this analysis form the starting point for the conceptual design of a sensor model. The concept contains both the structural design and a time-efficient integration into the test bench. Following, the concept is applied to a radar- sensor and a camera sensor. Additionally, it is implemented into the test bench. To validate the algorithms and the temporal analysis the sensor models are proved by using test scenarios.

**TEST SELECTION FOR MODEL CALIBRATION AND VALIDATION**
**Technical Presentation.** VVS2016-8875
10:50am-11:15am

**Chenzhao Li, Sankaran Mahadevan**, *Vanderbilt University, Nashville, TN, United States*

Model calibration and model validation are two activities in the system response prediction, and both of them make use of test data. The test can be conducted on different components or sub-systems, meaning multiple types of test. Due to the variability in test outcomes, two sets of test data of the same size may give distinct predictions even if the same framework of model calibration/validation is followed. The test selection in this research aims to identify the number of each type of test under budget constraint to achieve consistent predictions under different test outcomes, which means 1) small uncertainty of the prediction mean, i.e., the PDFs of these predictions have close locations; and 2) small uncertainty of the prediction variance, i.e., the PDFs of these predictions have similar shapes.

Test selection is required before any actual test thus can only use synthetic data. The generation of synthetic data simulates the process to obtain test data. However, the synthetic data has a new uncertainty source which is the epistemic uncertainty in selecting the value of model parameters. This uncertainty source does not exist in the test data since the real test fixes the value of model parameters at their unknown true values.

The proposed method in this research is as follows. For the prediction using synthetic data, the proposed method aims to find the number of each type of test to maximize the contribution of the new uncertainty towards the uncertainty in the prediction mean and variance. As the test data eliminate this dominant uncertainty source by fixing the model parameters at their true values, the predictions using test data will have a small uncertainty in the their mean and variance, thus consistent predictions under different test outcomes can be achieved.

To quantity the contribution of this new uncertainty source, this research uses the Sobol index. An optimization formulation is established where 1) the design variables are the number of each type of test, 2) the objective is to maximize the Sobol index of the new uncertainty source, and 3) the constraint is the budget limit. A simulated annealing algorithm is applied to solve this discrete optimization problem. The proposed method is suitable for any system response prediction framework, no matter whether only model calibration is considered or both model calibration and model validation are considered. Two numerical examples are provided to demonstrate the proposed approach, including a illustrative example and the dynamics challenge problem provided by Sandia National Laboratories.



**FUNDAMENTALS AND APPLICATION OF THE MODELING AND SIMULATION USE RISK METHODOLGY (MURM)**
**Technical Presentation.** VVS2016-8931
11:15am-11:40am

**Simone Youngblood, Peter Pandolfini, Lee Hendrix**, *The Johns Hopkins University Applied Physics Laboratory, Laurel, MD, United States*

The Modeling and Simulation Use Risk Methodology (MURM) was developed to provide a mathematically coherent paradigm for the assessment of model and simulation Use Risk as well as to address the need for an integrated methodology for planning, tailoring, and conducting VV&A of model(s), simulation(s), and the associated data (hereinafter referred to collectively as “M&S”). The methodology seeks to provide insightful information that contributes to minimizing the risk that users incur when applying M&S to their intended uses. The objective of this risk-based methodology is to optimize VV&A resources while minimizing the risks of using an M&S. The VV&A resources include the information available to support the gathering and analysis of verification and validation (V&V) evidence, the personnel required to execute VV&A activities and tasks, and the time available within which to perform the VV&A activities. M&S Use Risks arise from many factors, including uncertainties in the representations of the M&S, uncertainties in the V&V evidence itself, and the consequences that result from using an M&S for an intended use. The uncertainties, if left uncharacterized, could lead the M&S User to either believe M&S results are correct when they are not or judge M&S results as incorrect when, in fact, they are correct. Either of these two errors could lead to adverse consequences for the M&S User or those whom they represent.

At present, M&S may be developed and used without a comprehensive appreciation for the risks associated with the use of the M&S and the M&S results. MURM is a methodology that goes beyond the scope of a standard V&V analysis by mathematically calculating and displaying the risk of M&S use for decision-making. The methodology is flexible in that it can be employed throughout the M&S lifecycle. By applying established concepts that include probability theory (the product and sum rules), a Bayesian concept of prior probability, and by leveraging the concept of maximum information entropy to establish influences, the resulting methodology helps to preclude unintended bias and allows full use of all available information. MURM involves assessing the logical atoms for all M&S requirements, calculating their resultant use risks and simultaneously displaying all of the risks to visualize the broader M&S use risk picture. Subsequent iterative MURM analysis may then be used to identify remedial courses-of-action and their expected reductions of use risk.

In order to demonstrate the capability and applicability of the MURM, the authors collaborated with the Sandia National Laboratory V&V, UQ and Credibility Processes Department to apply the MURM to one of the responses to the SNL 2014 V&V Challenge Problem. Application of the MURM illustrates its efficacy to assess a state-of-risk for the model or simulation on a requirement-by-requirement basis while also demonstrating how it can be used to guide VV&A activities to reduce risk for the intended use of the M&S.

This paper describes the MURM, its fundamental concepts, and the lessons learned garnered from application of the MURM concepts.

**DETERMINATION AND VALIDATION OF REDUNDANT CONTACT FORCES IN RIGID-BODY SYSTEMS**
**Technical Presentation.** VVS2016-8938
11:40am-12:05pm

**Alfonso Callejo, Farnood Gholami, Jozsef Kovecses**, *McGill University, Montreal, QC, Canada*

A very common assumption within rigid-body dynamics is that bilateral constraints are independent, especially when reaction forces are computed from Lagrange's equations of the first kind. The presence of redundant (dependent, compatible) constraints results in overconstrained systems. In other words, the Jacobian matrix of constraint equations will not have full rank, which means that the reaction forces are not unique and there are infinite possible solutions. In these cases, authors often discard the extra constrains either manually or mathematically, or else introduce compliance/relaxation in the constraints, so that the reactions can be univocally determined. In any case, the system motion is not affected by this phenomenon, because the generalized accelerations and constraint forces can still be univocally computed using, for instance, an index-1 version of the dynamic equations or a semi-implicit, velocity-level formulation.

Discarding constraints is equivalent to modifying the mechanical system, and introducing stiffness coefficients in the constraints requires additional information about the structural properties of the system. An alternative approach is to find the so-called minimum norm solution, which is the 'smallest' solution among the infinite possible solutions. This often involves a diagonal weighting matrix that can be used to scale the reaction forces. This way, the original system definition is preserved and constraints are considered to be perfect. Physically speaking, self-equilibrating constraint forces (pre-loads, assembly defects, thermal stresses, etc.) are neglected. This solution to the reaction forces is often computed through the Moore-Penrose pseudoinverse.

The minimum norm solution is especially attractive for contact problems with redundant unilateral or bilateral constraint equations. Often, the user cannot or will not define a compliance factor for each contact constraint. This paper extends the concept of minimum norm solutions to the solution of redundant contact problems with bilateral and unilateral constraints and Coulomb friction. Specifically, we study the conditions under which the pseudoinverse can be computed. We also analyze the physical interpretation of such reaction forces, which is rarely addressed in the literature when the constraints are discarded or the minimum norm solution is used. This raises interesting questions about the validation of dynamic simulations where the solution of reaction forces affects the forward dynamics, which is the case with Coulomb friction.

Finally, we propose benchmark problems to assess the existence, uniqueness and validity of reaction forces. The first numerical case that has been investigated is a three-body system with bilateral constraints and Coulomb friction that was proposed in the literature. It consists of a two-dimensional sliding bar under the effect of gravity and connected to two sliders. The second case consists of a benchmark problem for redundant unilateral contact with friction. The system is a ten-link cable made up of linear segments resting on the ground and under the effect of gravity.

#### DISCRETIZATION ERROR ANALYSIS WITH UNFAVORABLE MESHES - A CASE STUDY

**Technical Presentation.** VVS2016-8953
12:05pm-12:30pm

**Denis F. Hinz, Mario Turiso**, *Kamstrup A/S, Skanderborg, Denmark*

For industrial applications, the ideal verification and validation procedure should be robust, universal, and applicable to a wide range of problems. However, established verification and validation procedures to estimate the numerical uncertainties in computational fluid dynamics (CFD) simulations are formally limited to strong prerequisites including structured and geometrically similar meshes, large enough refinement ratios, and simulation results in the asymptotic range. Yet, some investigations suggest that various formal prerequisites can be relaxed such that grid convergence methods can also be applied for meshes that are not geometrically similar and structured. Further, the ASME Standard for verification and validation in computational fluid dynamics and heat transfer (ASME V&V 20-2009) provides only limited guidance on prerequisites for meshes and it remains unclear which methods (if any) can be applied for cases with unstructured meshes.

In this research project, we test different methods to estimate the discretization error and estimate the numerical uncertainty in industrial CFD simulations with unfavorable prerequisites. The goal of this project is to identify if any of the established procedures has potential to be applied for simulations with the finite volume code OpenFOAM in combination with the unstructured mesh generator SnappyHexMesh. As realistic and industrially relevant test case we simulate the turbulent flow downstream of an asymmetric swirl disturbance generator that is used for assessing the robustness of flow meters. We test the grid convergence index method (GCI) as established in the ASME V&V 20-2009 as well as the least-squares approach according to Eça and Hoekstra (Comput. Fluids 38 (2009) 1580).

The convergence study over 5 different grids with refinement ratios between 1.30 and 1.38 produces oscillatory behavior in most monitored variables. Our results indicate that the CGI approach cannot provide realistic estimations of the order of convergence for the present scenario. We find that the least-squares approach is more robust for estimating the order of convergence than the standard CGI approach. In turn, the estimation of the order of convergence with the least-squares approach can also depend on (mostly arbitrary) choices on procedural details including choices on admissible ranges for fitting variables and weighting factors.

## TRACK 4 Uncertainty Quantification, Sensitivity Analysis, and Prediction

### 4-4
### UNCERTAINTY QUANTIFICATION, SENSITIVITY ANALYSIS, AND PREDICTION: SESSION 4

**2nd Floor, Palo Verde A** **10:25am - 12:30pm**

#### A MULTI-FIDELITY FRAMEWORK FOR CONSTRUCTING STOCHASTIC RESPONSE SURFACES BY COMBINING EXPERIMENTAL MEASUREMENTS AND NUMERICAL SIMULATIONS

**Technical Presentation.** VVS2016-8837
10:25am-10:50am

**Hessam Babaee**, *MIT, Cambridge, MA, United States,* **Paris Perdikaris, Chryssostomos Chryssostomidis**, *MIT Sea Grant, Cambrdige, MA, United States,* **George Karniadakis**, *Brown University, Providence, RI, United States*

We present a general multi-fidelity framework for constructing a stochastic response surface for quantities of interest by blending previously developed experimental correlations/measurements (low-fidelity model) with accurate numerical simulations (high-fidelity model) using modern tools from machine learning namely Kriging/co-Kriging. In this framework the high-fidelity model is sampled only a few times, while the inexpensive empirical correlation is sampled at a very high rate. We obtain the quantities of interest directly from the stochastic response surface. In addition we quantify the uncertainty associated with these predictions. While in this work we present new results on the thermal mixed convection, this information-fusion framework provides a new paradigm that could be used in many different contexts in fluid mechanics including heat and mass transport, but also in combining various levels of fidelity of models of turbulent flows.

#### ACCELERATED EVALUATION OF AUTOMATED VEHICLES

**Technical Presentation.** VVS2016-8852
10:50am-11:15am

**Ding Zhao, Huei Peng, Henry Lam**, *University of Michigan, Ann Arbor, MI, United States,* **David Leblanc**, *Um Transportation Research, Ann Arbor, MI, United States*

Automated Vehicles (AVs), which monitors the driving environment and conduct some or all of the driving tasks, must be evaluated thoroughly before their release and deployment. The challenges of AV evaluation stem from two facts. i) Crashes are exceedingly rare events. In the U.S., one needs to drive on average 530 thousand miles to experience a police-reported crash and nearly 100 million miles for a fatal crash. The low exposure to safety-critical scenarios makes the Naturalistic-Field Operational Test (N-FOT) approach very time-consuming and expensive to conduct, in which prototype AVs are distributed to volunteers or driven by test drivers for daily usage. ii) AVs can "cheat" to pass pre-announced tests. Traditionally, vehicle test protocols are published and the test conditions are fixed. This is not a problem when the vehicle is "dumb", but becomes a problem when the vehicle is intelligent and can be customized to excel only in the selected tests, but not other conditions. An evaluation approach that represents the real world but not as time-consuming as the N-FOT can help to address the problems mentioned above.

In this research, we proposed an "Accelerated Evaluation" concept to accelerate the evaluations of AV by several orders of magnitude. The interactions with surrounding Human-controlled Vehicles (HVs) are taken as the major challenge of AV, which are modeled based on the naturalistic driving data collected by the University of Michigan Transportation Research Institute in the Safety Pilot Model Deployment Program and the Integrated Vehicle-Based Safety Systems Program. Probabilities of the conflict, crash, and injury occurrence are calculated in the "accelerated" tests as metrics to assess the safety of specific AV designs. In general, Accelerated Evaluation consists of six steps. 1) Collect a large quantity of naturalistic driving data. 2) Extract events that have potential conflicts between an AV and surrounding HVs from this data. 3) Model the conflict driving scenarios with stochastic models. 4) Reduce the non-safety-critical events by skewing the probability density functions. 5) Conduct Monte Carlo simulations with the skewed (accelerated) probability density function, resulting in more intense interactions between the AV and HVs. 6) "Skew back" the results of the accelerated tests to understand the performance of AVs under naturalistic driving conditions. The proposed approach can be used in computational simulation, human-in-the-loop tests with driving simulators, hardware-in-the-loop tests, or on-track tests.

Four methodologies were developed to enrich the Accelerated Evaluation concept. The first method is based on the likelihood analysis of the naturalistic driving. The test scenarios are built as a probabilistic model based on the time series driving data. The evaluation procedure is accelerated by reducing the relatively safe events that have a high likelihood of occurring. The second method provides a mathematical basis for the "skewing back" mechanism in step 5) based on the Importance Sampling theory, such that the statistical equivalence between the accelerated tests and naturalistic driving tests can be rigorously proved. The third method, the "Adaptive Accelerated Evaluation", provides a procedure to recursively find the best way to skew the probabilistic density functions of HVs to maximally reduce the evaluation duration. Finally, the Accelerated Evaluation approach to analyzing the dynamic interactions between AVs and HVs were developed based on stochastic optimization techniques.

Simulation results show that the accelerated tests can reduce the evaluation time of crash events by as much as 10,000 to 100,000 times. In other words, driving for 1,000 miles will expose the AV with challenging scenarios that will take 10 to 100 million miles in the real-world to encounter. This technique thus has the potential to dramatically reduce the development and validation time of AVs.

### BAYESIAN ESTIMATION OF THERMAL CONDUCTIVITY PARAMETERS FOR A POLYURETHANE FOAM

**Technical Presentation.** VVS2016-8881
11:15am11:40am

**Cosmin Safta**, *Sandia National Labs, Livermore, CA, United States,* **Leslie Phinney**, *Sandia National Labs, Albuquerque, NM, United States,* **Victor Brunini**, *Sandia National Labs, Livermore, CA, United States,* **Robert Garcia**, *Sandia National Labs, Albuquerque, NM, United States,* **Ryan Keedy, Patricia D. Hough**, *Sandia National Labs, Livermore, CA, United States*

In this work we present alternative approaches for estimating the parameters of a thermal conductivity model in a Bayesian framework. Specifically, we compare conventional approaches to account for model error, e.g. model the discrepancy as a Gaussian process, with a novel approach [1] where this error is subsumed in the definition of the model parameters. We highlight the benefits of the latter formulation to model the thermal conductivity as a function of density and temperature for a polyurethane foam. Further, we examine, in a Bayesian context, whether the foam requires conductivity models tailored to specific ranges in the experimental conditions or if one overall model is sufficient to cover the entire experimental range. Lastly, we will make use of the proposed conductivity model in a practical heat transfer application.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

[1] K.Sargsyan, HN Najm, R Ghanem, International Journal of Chemical Kinetics, Vol 47, pages 246-276, (2015)

### PREDICTING THE BEHAVIOR OF A MODULAR MULTILEVEL CONVERTER BASED ON A SINGLE-MODULE CONVERTER VALIDATION EXPERIMENTS

**Technical Presentation.** VVS2016-8886
11:40am-12:05pm

**Niloofar Rashidi**, *Vigrinia Tech, Blacksburg, VA, United States,* **Rolando Burgos**, *CPES - Virginia Tech, Blacksburg, VA, United States,* **Christopher Roy**, *Virginia Tech, Blacksburg, VA, United States,* **Dushan Boroyevich**, *CPES- Virginia Tech, Blacksburg, VA, United States*

The modular multilevel converter (MMC) has received increased attention over time due to its interesting features such as inherent modularity, and voltage and current scalability. The power cells of an MMC are connected in series/parallel, in order to achieve practically any desired current/voltage/power level and therefore can be used in a variety of applications. Modeling and simulation as a set of design and development tools play a key role in the design of MMCs. As opposed to simulation models in other technical fields, however, power converter simulation models are used jointly with laboratory prototypes, as simulation itself has not been looked upon as a true substitute for experimental results.

In this study, experimental results of a single-module converter prototype is used to calculate the model form uncertainty of the simulation model of an MMC with one power cell per arm. This model form uncertainty is then extrapolated to the condition with more power cells per arm in order to predict the behavior of an MMC. As a result, the modeling and simulation tool is empowered in the study of this type of converter without having the experimental prototype of the converter with more power cells.

### ON THE RELATION BETWEEN NUMERICAL AND PARAMETER UNCERTAINTIES

**Technical Presentation.** VVS2016-8877
12:05pm-12:30pm

**Luis Eca**, *IST, Lisbon, Portugal,* **Guilherme Vaz**, *MARIN, Wageningen, Netherlands*

The quantification of the modeling error of the mathematical models solved by Computational Fluid Dynamics (CFD) requires the estimation of the experimental, numerical and parameter uncertainties. In the procedure proposed by the ASME V&V 20 Committee these three quantities can be assumed to be independent. Parameter uncertainty is typically originated by lack of knowledge of exact values for the boundary conditions and/or fluid properties and its evaluation is handled by the broad field of uncertainty quantification. However, this evaluation requires simulations that are necessarily affected by numerical errors. Therefore, it may be questionable if parameter and numerical uncertainties are really independent or, alternatively, how small must be the numerical uncertainty to estimate parameter uncertainties without its influence.

In order to address the relation between parameter and numerical uncertainties, we have selected as test case the transition from laminar to turbulent flow on a flat plate boundary-layer simulated with the Reynolds-Averaged Navier-Stokes equations supplemented by the Wilcox k-w two-equation, eddy-viscosity turbulence model with and without low Reynolds number corrections. The quantities of interest are the skin-friction coefficients Cf in the transition region. The parameter uncertainty of Cf is estimated using the local sensitivity method and finite-differences, which is the simplest technique available. Numerical and parameter uncertainties are estimated for simulations performed with different levels of numerical error (grid refinement). The simplicity of the selected geometry allows us to reach extremely fine grids and so a reference solution can be obtained to obtain reliable estimates of the numerical uncertainty. Therefore, it is possible to evaluate parameter uncertainties for different levels of numerical uncertainty and determine the relation between these two quantities.

## TRACK 9 Validation Methods for Solid Mechanics and Structures

### 9-1
### VALIDATION METHODS FOR SOLID MECHANICS AND STRUCTURES: SESSION 1

**1st Floor, Mesquite 2** **10:25am - 12:30pm**

#### MODAL FREQUENCY ANALYSIS OF ISOGRID STRUCTURES FOR USAGE IN MICROSATELLITES

**Technical Presentation.** VVS2016-8808
10:25am-10:50am

**Subham Gupta**, *SRM University, Kanchipuram, Tamil Nadu, India,* **Aryan Kothiyal**, *SRM University, Chennai, Tamil Nadu, India*

Microsatellites are spacecrafts which have mass in the range of 1-100 kg and have grown by a great extent in the near past and have become an efficient means of performing various missions in Low Earth Orbits (LEO). These microsatellites are also being developed for Deep Space Exploration Missions such as exploration in Low Lunar Orbit (LLO). Now microsatellites are just a miniaturised variant of a large satellite intended to perform the same tasks with a lot of imperatives added to it. Deep Space exploration requires On-board ignition/space propulsion hence the mass of the spacecraft is a problem. Isogrids are grid stiffened structures with ribs/stiffeners intersecting as lattices of equilateral triangles. Isogrid structures are isotropic in nature i.e. they have the same mechanical properties in all directions. Isogrids are known for their weight reduction and strength retention properties. Since an isogrid is milled out from a single metal sheet it reduces the mass of the satellite by 70-75% and its stiffeners are responsible for retaining the strength of the structure. Now before these isogrid structures can be used in space applications, they must be validated for mechanical stabilities. When a spacecraft is being carried by a Launch Vehicle it induces some mechanical vibrations in the satellite. If the frequency of these vibrations matches the natural frequency of the satellite, there will be an occurrence of Dynamic Coupling which causes the structure to resonate. Resonance will cause the structure to vibrate violently with its maximum amplitude and thus it may cause mechanical failures in the structure. Therefore, a modal analysis must be performed on the structures with proper constraints in order to examine its natural frequency and hence its validation to be used in various applications. This abstract deals with analysing the isogrid structure by converting the isogrid into an equivalent plate and hence analysing the isogrid structure as a plate as examining a plate is much simpler. The paper deals with the analysis of plate vibrations and then analysing the isogrid structure analytically and then analysing it on a computer using numerical methods after converting the isogrid into an equivalent plate. The material used for the test was Aluminium-6061 T6. Various modes of vibrations of plate and isogrid are intended to be shown in the paper and the analytical result is also compared with the numerical result. An attempt was made to restrict the error below 5% of the analytical result. Maximum deflection and Stress were noted for each mode of vibration and validated after comparing with Yield Strength and Ultimate Tensile Strength.

#### A SUMMARY OF THE COMPUTATIONAL METHODOLOGIES AND VALIDATION TECHNIQUES EMPLOYED TO DEVELOP UPDATED WELD RESIDUAL STRESS GUIDANCE IN API 579-1/ASME FFS-1 FITNESS-FOR-SERVICE

**Technical Presentation.** VVS2016-8820
10:50am-11:15am

**Phillip E. Prueter, P.E.**, *The Equity Engineering Group, Inc., Shaker Heights, OH, United States,* **Dave Dewees**, *Babcock & Wilcox, Barberton, OH, United States*

Residual stresses associated with welding can contribute to crack initiation and even brittle fracture in fixed pressure retaining equipment. Understanding the weld residual stresses (WRS) in pressure vessels, piping, and other structures is an essential part of designing reliable equipment and establishing component critical flaw sizes in the petrochemical, chemical, and nuclear industries, among others. Furthermore, in recent years, the evolution of parallel computing technology, and overall improvements in computer performance have made detailed computational weld residual stress analysis feasible. Additionally, recent enhancements of commercial finite element software programs have enabled the implementation of complex weld simulation techniques. More recently, the focus on Verification and Validation (V&V) techniques has extended to welding simulation and represents a critical aspect of ensuring the quality of analysis results. Also, other formal efforts aimed at standardization of weld simulation methodologies have ensued. In this paper, detailed V&V is applied to a few benchmark problems, such that the general computational approach itself is verified and validated. Detailed welding simulation methods, such as the ones presented in this study, can ultimately be used to verify and validate analysis simplifications, which compliment simpler, more fundamental validations.

A recent Materials Properties Council (MPC) Joint Industry Program (JIP) investigated the WRS guidance in the current (2007 Edition) of API 579-1/ASME FFS-1 Fitness-For-Service (FFS-1) and other European Standards and is summarized herein. The primary goal of this JIP was to simplify, enhance, and reduce any undue conservatism associated with the existing weld residual stress guidance and to incorporate updated guidelines into the upcoming release of FFS-1. Explicit computational weld residual stress simulation is employed, and results are compared against experimental weld residual stress data obtained primarily from the published European Network on Neutron Techniques Standardization for Structural Integrity (NeT) benchmarks. This includes consideration for the effects of heat input and ultimately comparison of through-wall weld residual stress distributions for different weld geometries. Thermal-mechanical finite element analysis (FEA) results are presented that show excellent agreement with published experimental data and provide a foundation for understanding the procedures and nuances associated with accurately simulating the heat transfer and ensuing non-uniform plastic strains associated with the welding process. In particular, a discussion on non-linear material modeling techniques, including formulations for implementing cyclic plasticity, is offered, and comparisons between isotropic, kinematic, and combined hardening material models are rendered. A summary of the comprehensive underlying analyses used to update and ultimately validate the weld residual stress guidance for pressure vessels and piping components that will be included in the upcoming release of FFS-1 is provided.

#### CHARACTERIZATION, VERIFICATION, AND VALIDATION PROCESS FOR THE IMPLEMENTATION OF A SPEC MATERIAL MODEL FOR STRUCTURAL DYNAMICS RANDOM VIBRATION ANALYSIS

**Technical Presentation.** VVS2016-8850
11:15am-11:40am

**Nathan Spencer**, *Sandia National Laboratories, Livermore, CA, United States*

A finite element model of a container, polyurethane foam packaging material, and an asset is generated to predict the random vibration response of the asset during transportation. A typical approach to such a problem is to perform a modal analysis of the finite element model, followed by a random vibration analysis based on a power spectral density loading. The modal analysis requires a linear material stiffness, which is typically satisfied for small deflections during vibration. However, in the case of flexible polyurethane foam, test data has shown stiffness dependency on the loading rate and frequency within the regime of interest for the transportation environment. In order to capture the change in stiffness at different frequencies, a Simplified Potential Energy Clock (SPEC) material model is used for the foam. Desired features of the SPEC model include time, frequency, and temperature dependent material properties. The temperature dependency is also important to the application because shipping requirements include temperatures above and during the glass transition of the polyurethane foam, allowing for the possibility of order of magnitudes difference in the shear modulus. The SPEC material model is characterized based on a number of material compression, torsional, and cyclical tests at different temperatures above and during the glass transition of the foam. Once characterized, the material model is then used to capture the behavior of the foam in the system level model. Due to the nonlinear response of the SPEC model, modal extraction is not performed, rather a synthesized acceleration time history derived from the desired power spectral density input is applied to the model as a prescribed acceleration in an explicit dynamics simulation. The use of explicit dynamics also facilitates the use of other capabilities such as sliding contact at interfaces, with the main drawback being required extended simulation time. Other steps in the analysis process include a desired quasi-static preload step and temperature ramp. The implementation of the SPEC model into the analysis process motivated verification of its usage in the system level model. Mesh refinement is performed to demonstrate spatial convergence. Time convergence is performed for the quasi-static and explicit time stepping. Due to the nature of the SPEC model, convergence of the temperature ramp rates is also investigated. The final results using the SPEC model in an explicit dynamics solution is compared with those generated from an implicit solution based on the traditional modal extraction and random vibration method. These solutions are also compared to currently available system level test data for initial validation.

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### PREDICTING AND VALIDATING ASSEMBLY FORCES OF CYLINDRICAL SNAP-FIT JOINTS BY COMPARING CLOSED-FORM SOLUTIONS TO COMPUTATIONAL METHODS

**Technical Presentation.** VVS2016-8869
11:40am-12:05pm

**Linda Knudsen**, *Syncroness, Westminster, CO, United States,* **Bobby Truitt**, *Syncroness, Inc., WESTMINSTER, CO, United States*

Cylindrical snap-fit joints are commonly used for connections and fastening; however, the assembly forces are notoriously hard to predict. Closed-form equations determine the required assembly force reasonably well for cylindrical snap-fit joints with simple geometry and uniform wall thickness. Unfortunately, the closed-form equations do not adequately address components with complex geometry. At the same time, compressed product development schedules reduce the time engineers have to analyze snap-fit joints. Further, the mechanical properties of additive manufacturing materials do not yet mimic the feel and assembly force of molded components, which means that rapid prototype testing does not provide useful results for snap-fit joint design.

Based on a case study in which a slip-fit, epoxy-bonded connection in a medical device was redesigned to a less costly, permanent, cylindrical snap-fit joint, this technical presentation compares closed-form solutions to results from computational methods for determining the assembly force for a given snap-fit design. Following ASME V&V 10 validation methodology of uncertainty quantification, we also consider the relative impact of material properties and component dimensions on the maximum assembly force for a given snap-fit design. After iterating and comparing solutions, we delineate the fastest way to get meaningful results.

Motivated by expediency, engineers often use the closed-form cylindrical-snap fit equations without reviewing its underlying assumptions. We reviewed those assumptions and compared the closed-form equations' experimentally-correlated assembly forces to analytical results. The closed-form equations assume that the components have straight walls of uniform thickness. For these idealized components, the closed-form equations' assembly force was compared to the nonlinear FEA-predicted assembly force profile.

We reran the FEA using components that had walls with a 2 degree draft for injection molding and overlaid the force profile on the straight-walled components' force profile, showing that small changes in geometry result in increased assembly force.

The closed-form equations also assume that one component is rigid and the other is elastic. In our case, the cover (outer component) and the hollow shaft (inner component) of the design evaluated were made of semi-rigid thermoplastic material. Therefore, to use the equations, we graphed the force versus deflection curve for each component and estimated the transverse force to be at the intersection of the two curves. Capturing the components' true geometry, the FEA results predicted a greater assembly force.

The results of this work allow engineers to consider the complexity of a proposed cylindrical snap-fit joint design and, subsequently, to follow an efficient method for predicting the assembly force.

References: Two commercial software packages – PTC Mathcad Prime® 3.0 and SOLIDWORKS Simulation Premium 2015 nonlinear Finite Element Analysis (FEA) - were used without user-modifications.

### VERIFICATION AND VALIDATION OF FINITE ELEMENT ANALYSIS OF A DISK SUBJECTED TO DIAMETRICAL COMPRESSION BY USING A REFLECTION POLARISCOPE

**Technical Presentation.** VVS2016-8892
12:05pm-12:30pm

**Parham Piroozan, Matthew Lowry, Maribel Carrera, Cristian Galvan**, *California State Polytechnic University, Pomona, Pomona, CA, United States*

Compression tests on disks provide useful information needed in many metalworking processes such as in forging, rolling, and extrusion, where the workpieces are being subjected to compressive forces. For brittle materials, a disk test has been developed in which the disk is subjected to diametrical compression between two flat platens. This paper describes how the finite element method (ANSYS) was used to analyze the stresses in a disk subjected to diametrical compression, as well as how the results were verified with experimental results obtained by using a reflection polariscope.

A reflection polariscope is an optical instrument that creates full-field fringe patterns on a stressed body. The body which was selected for stress analysis in this investigation was a disk subjected to diametrical compression. The disk was made of 6061-T6 aluminum with a diameter of 2.5 inches and a thickness of 0.25 inches. Surface of the disk was covered with a reflective coating and a birefringent material with a thickness of 0.122 inches. The disk was loaded diametrically by a compressive force of up to 3,000 pounds and was viewed with a reflection polariscope and a CCD camera (Figure attached). Bands with different colors, which were created on the surface of the disk, represent shear stress distribution on the disk. The isochromatic fringe patterns on the surface of the disk represent contours of points with constant maximum shear stress values. These fringes were used to find the shear stresses along the horizontal and vertical diagonal lines on the surface of the disk, and were used for comparison with the results obtained from the finite element analysis. In addition, a video was created that shows the formation and motion of fringes during the loading and unloading of the disk. Starting with the unloaded disk, the video shows the fringes appearing at the most highly stressed points (contact points). As the load was increased, new fringes appeared, pushing the earlier fringes toward the areas of lower stress. Direction of movement of fringes instantly identify critical areas, as well as the overstressed and understressed regions on the disk.

Finite element analysis (FEA) of the disk was carried out by using the commercial software ANSYS (version 16.1, ANSYS, Inc.). A two dimensional model was used for the disk which was placed between two flat platens. Frictional contact elements were used between the disk and the platens. This type of element introduces contact nonlinearities and uses large displacement theory. Contours of maximum shear stress on the surface of the disk were compared with the experimental results obtained by using the reflection polariscope. In addition, stresses along the horizontal and vertical diagonal lines were compared with the experimental results. The FEA results were in good agreement with the experimental results, with a difference of less than 5% in the maximum shear stress values.

## TRACK 12 Verification Methods

### 12-2
### VERIFICATION METHODS: SESSION 2
**2nd Floor, Palo Verde B** **10:25am - 12:30pm**

**CONVERGENCE CHECKS FOR STRESS ANALYSIS WITH FINITE ELEMENTS IN THE PRESENCE OF NONMONOTONIC CONVERGENCE**
**Technical Presentation.** VVS2016-8828
10:25am-10:50am

**Glenn Sinclair**, *Louisiana State University, Baton Rouge, LA, United States,* **Jeff Beisheim**, *ANSYS, Inc., Canonsburg, PA, United States*

Convergence checks with finite elements offer stress analysts a means of estimating errors and thereby verifying results. Such checks generally work well when convergence is monotonic: however, they can be problematic when it is not. When convergence is nonmonotonic in stress analysis, typically errors in stresses initially reduce in magnitude with mesh refinement and go to zero, then change sign and increase in magnitude before ultimately reducing again. Under these circumstances, estimating corresponding errors by monitoring changes in stress values with mesh refinement is a process that itself can be fraught with error because the stress increments attending mesh refinement go to zero when the actual error is not zero, in fact, when the actual error is at a local maximum value.

Here we offer some means for guarding against underestimating errors when nonmonotonic convergence occurs. These modified checks and companion a posteriori error estimates are applied to six 3D test problems that have exact solutions that feature concentrated stresses to challenge finite element analysis. All six exhibit nonmonotonic convergence in their finite element analysis. Nineteen error estimates for peak stresses are obtained with the modified checks. These error estimates are classified as being at the following levels: 1-5%, satisfactory; 1/5-1%, good; and <1/5%, excellent. Then error estimates are at the same level as actual exact errors on six occasions, and are at a higher level, hence conservative, on thirteen. They are never lower and nonconservative. For the same test problems without the modifications, there are eight instances of error estimates being lower than actual errors. All told, therefore, a demonstration of the effectiveness of the modified convergence checks in avoiding nonconservative error estimates in the presence of nonmonotonic convergence.

**IMPROVED TUNED TEST PROBLEMS FOR VERIFYING FINITE ELEMENT ANALYSIS OF STRESS CONCENTRATIONS**
**Technical Presentation.** VVS2016-8829
10:50am-11:15am

**Glenn Sinclair, Boliang Zhang, Yi Zhang**, *Louisiana State University, Baton Rouge, LA, United States*

The construction of Tuned Test Problems (TTP) is a variation of the method of manufactured solutions that seeks to tune test problems to applications while yet having solutions that comply exactly with governing field equations and local boundary conditions. Here we offer a straightforward means of developing such TTP for applications seeking elastic stress concentrations with finite elements. In particular, for stress concentrations occurring at local features with stress-free surfaces having a single radius of curvature. The approach employs some simple stress and displacement fields that satisfy the two-dimensional equations of elasticity and the local, stress-free, boundary conditions. These fields are taken to be active throughout the entire region occupied by the originating application. On the boundaries of this region away from the local stress-free portion, boundary conditions in TTP are taken to be whatever displacements the fields realize thereon. For the improved TTP offered here, these fields contain four adjustable parameters. These parameters are selected so as to generate a slightly larger (+10%) stress concentration at the same location as that expected in the application ? such expectations result from preliminary finite element analysis of the application. The parameters are also selected so as to promote slightly larger stress gradients as the stress concentration is approached. Then by analyzing TTP of this ilk with the same finite element meshes as used on corresponding applications, the stress analyst can gain an appreciation of the local mesh refinement needed to attain their desired levels of accuracy. To check that an appreciation of this nature can be so obtained, the approach is applied to fourteen applications with stress concentration factors spanning a wider range than that usually encountered in practice. Finite element analysis of the applications and companion TTP employs low-order and higher-order elements, as well as a variety of mesh generation approaches for initial meshes. Mesh refinement throughout is undertaken by halving element extents. Exact errors for the TTP then establish the degree of refinement required to meet different accuracy levels for all fourteen test problems. Furthermore, when effective convergence checks and an a posteriori error estimate are applied to the TTP, essentially the same levels of mesh refinement are indicated, thereby confirming the use of such error estimates to establish refinement levels in the actual original applications.

**EXACTPACK: AN OPEN-SOURCE SOFTWARE PACKAGE FOR CODE VERIFICATION**
**Technical Presentation.** VVS2016-8845
11:15am-11:40am

**Scott Doebling, Daniel Israel, Robert Singleton, Jr., C. Nathan Woods,** *Los Alamos National Laboratory, Los Alamos, NM, United States*

ExactPack is an open-source software package that has been developed for the verification & validation community. The package has two major capabilities: (1) the generation of exact solutions for common exact-solution benchmark problems in computational physics; and (2) the analysis of computational physics code output to assess solution accuracy and convergence rate. ExactPack is written in Python and has the ability to access compiled code written in other languages (currently many of the solver implementations are in Fortran). ExactPack is built as a Python package and is designed to be object-oriented to enable class hierarchies, property inheritance, modularity, and other desirable attributes.

The talk will describe the architecture and current solver contents of the package. Several demonstrations of the package capabilities will be presented. ExactPack was intended to be used to verify computational physics codes, and so its default solver classes include many common test problems in hydrodynamics (Noh, Sedov, Riemann), reactive flow (escape of HE products, programmed burn timing, steady detonation reaction zone), and solid mechanics (Blake).

The analysis capabilities of ExactPack include the import of data from computational physics codes, calculation of error norms between the exact solution and the computational physics results, and the calculation of spatial convergence rates. The analysis tools follow the V&V standards defined by ASME.

The package is designed to be easily extended and the community is welcome to contribute solvers and extend the analysis capabilities. The package is fully documented, and a developer's manual describes the required and desired attributes of contributed content. The package is available for download and collaboration at www.github.com/losalamos. This abstract has been approved for unlimited release with release number LA-UR-15-29615.

**MULTIVARIATE MODEL VERIFICATION USING RELATED MODEL DATA**
**Technical Presentation.** VVS2016-8871
11:40am-12:05pm

**Byoung Kim**, *PC Krause & Assoc., Wright-Patterson AFB, OH, United States,* **Jon T. Zumberge, Mark O. Bodie**, *Air Force Research Laboratory, Wright-Patterson AFB, OH, United States*

Model development and integration are increasingly important in the complex systems fielded by both military and commercial entities. However, model developers and users, including the decision makers utilizing information from the models and people affected by the assessment from the decision makers, have been concerned with whether a model and its results are "really" correct.

Models describe the systems by providing a characterization of the nature and working process to explain real-world tasks and events. In addition, models can be developed to predict future events and provide direction about the proper course of action by utilizing the appropriate output of the models. Due to the importance of the "correct" model outputs and the potentially high cost of failure, verification and validation (V&V) of the model development and integration is critical.

Model verification is the first stage of V&V and its purpose is to determine that given model implementations and their associated data accurately represent the model developer's conceptual description and specifications. There are a number of verification types and techniques addressed by the Air Force Research Laboratory (AFRL). We are particularly interested in model verification when we have a related verified model. Models given for this task include the multivariable data with internal states to be analyzed with multiple operational cases to be considered. Therefore, the conventional univariate approach that considers only one behavioral measure can't be applied and it results in inspiring us to consider a multivariate statistical test approach.

In order to solve the problem at hand by utilizing and improving the existing terminology and techniques, we present a multivariate statistical test approach for a model verification study. The initial approach utilizes popular multivariate techniques such as chi-square test statistic to provide the level of significance with probability by estimating how closely a distribution of model data matches a distribution of related model data.

Another approach is based on error intervals obtained by metrics estimating parameters in the range of acceptable values. The error intervals for each of these parameters are applied to compare the model and related model, and if it exceeds intervals, we mark this parameter as "Not passed" and show the stacked results for model verification. Based on the results obtained from our metrics, we also provide other valuable information with a Pareto chart showing the magnitude and frequency of each parameter showing the number of cases and the degree of error intervals for model verification procedures. To evaluate and answer the effectiveness of this approach, the corresponding application study is shown with acceptable errors for each parameter defined by Subject Matter Experts (SMEs). We believe this multivariate approach allows us to answer the operational correctness of the given model by specifying the associated range of verification and model tolerances.



**SOLUTION VERIFICATION FOR FIELD VARIABLES**
**Technical Presentation.** VVS2016-8897
12:05pm-12:30pm

**V. Gregory Weirs**, *Sandia National Laboratories, Albuquerque, NM, United States*

Solution verification uses Richardson extrapolation, solutions computed on a mesh sequence, and knowledge about the numerical method to estimate the numerical error of a quantity of interest (QoI). The QoI is usually a scalar value - a quantity integrated over all or part of the domain, or the value at a particular location and time – and may be a functional of the numerical solution. Solution verification estimates of QoIs rely on a number of assumptions that are often violated in practice. In this work solution verification is applied to field variables, which may rely on fewer assumptions. The estimated numerical error field may inform the accuracy of traditional QoIs, but is also useful in and of itself.

## TRACK 1 Challenge Problem Workshops and Panel Sessions

### 1-1
### V&V BENCHMARK PROBLEM SESSION 1 — TWIN JET COMPUTATIONAL FLUID DYNAMICS (CFD) NUMERIC MODEL VALIDATION

**1st Floor, Mesquite 2** **1:30pm - 3:35pm**

**V&V BENCHMARK PROBLEM SESSION 1 —TWIN JET COMPUTATIONAL FLUID DYNAMICS (CFD) NUMERIC MODEL VALIDATION**
**Technical Presentation.** VVS2016-8911

**Hyung Lee**, *Bettis Laboratory, West Mifflin, PA, United States,* **Ryan Crane**, *ASME, New York, NY, United States,* **Yassin Hassan**, *Texas A&M University, College Station, TX, United States,* **Arthur Ruggles**, *University Of Tennessee, Knoxville, TN, United States,* **Richard Schultz**, *Consultant, Pocatello, ID, United States,* **Christopher Freitas**, *Southwest Research Institute, San Antonio, TX, United States*

The ASME Verification and Validation in Computational Nuclear System Thermal Fluids Behavior Committee (ASME V&V30 Standards Committee) is initiating a series of verification and validation (V&V) benchmark problems designed to:

Study the scope and key ingredients of the V&V30 Committee's charter,
Achieve the above objective by using new, high-quality, state-of-the-art validation data sets obtained specifically for this purpose, and
Achieve the above objectives using a stepwise, progressive approach characterized by focusing on each key ingredient individually in a benchmark problem designed for that purpose.

The first V&V benchmark problem in the series was conducted as the part of the 2016 ASME V&V Symposium. The results and findings from the first V&V benchmark problem will be presented and discussed in this session. The full spectrum of upcoming benchmark problems to be considered will also be introduced.

A Summary Description of the First Problem: In the context of investigating the mixing between and the penetration of two parallel twin jets which are typical for an advanced liquid metal-cooled reactor a scaled twin-jet experiment was designed to obtain validation data at Reynolds numbers typical of operational conditions in the upper plenum of the liquid metal-cooled reactor. These data may also characterize twin-jet behavior in the lower plenum of a very high temperature reactor. In addition, the test facility may also be used to obtain natural circulation data characterizing twin-jet behavior in the upper plenums of both a liquid-metal cooled reactor and the very high temperature gas-cooled reactor. In the experiment, the working fluid is water and the velocity field was measured in detail using advanced particle image velocimetry (PIV) and laser Doppler anemometry (LDV) with measurement uncertainties estimated using accepted ASME practices for experimental uncertainty (ASME PTC 19.1 Test Uncertainty).

Objective of the First Problem: Using a select set of data from the twin-jet experiment (provided by the ASME and organizers), apply the V&V practices necessary to ensure an appropriately validated computational solution is obtained. For those participants from the nuclear community, the V&V30 Committee encouraged them to use whatever V&V practices they would normally use in the context of preparing a document which they might submit to the U.S. Nuclear Regulatory Commission for review.

Protocol for Participating in the First Problem: The participating organization or individual was required to register to take part in the benchmark exercise and requested that they perform their V&V assessment using the standard protocol and procedures accepted by their engineering community and sponsoring organization. It was noted that this benchmark effort was not intended as a competition among companies or individuals, but rather was intended as a demonstration of the state of the practice in using and applying computational tools to support U.S. Nuclear Regulatory Commission or other regulatory reviews. The expected outcomes of this first benchmark effort will be lessons learned, review of V&V methods, and effectiveness of V&V methods to support modeling and simulation reviews.

The results of the various participants will be summarized and compared in a subsequent report to be presented by the benchmark problem committee at the 2017 V&V Symposium.

### COMPUTATIONAL FLUID DYNAMICS VALIDATION OF TWO PARALLEL RECTANGULAR JETS USING OPENFOAM

**Technical Presentation.** VVS2016-8905

**Han Li, Huhu Wang, N. Anand, Yassin Hassan**, *Texas A&M University, College Station, TX, United States*

Two or multiple parallel jets are examples of shear flow phenomena that widely existing in many industrial applications. The mixing feature of parallel jets has many engineering applications, such as, in Generation IV conceptual nuclear reactors, wherein the coolants merge in upper or lower plenum after passing through the reactor core. The interaction between turbulence jets enables fast and thorough mixing of two fluids, however, the physics of such interaction is rich and yet to be fully understood. Computational Fluid Dynamics (CFD) simulations are extensively incorporated when it comes to studying parallel jets mixing phenomenon. Therefore, validation of varied turbulent models is of importance to make sure that the numerical results could be trusted and serve as a guide for the future design. OpenFOAM as an open source CFD toolbox is able to fulfill both academic and industrial needs by achieving large-scale computational capability with a variety of physical models as well as grants users the full control of the source code with complete freedom of customization such as implementing a new turbulence model. The purpose of this study is to validate Reynolds Averaged Navier- Stokes Equations (RANS) models using the open source code OpenFOAM for two submerged parallel jets issuing from two rectangular channels. Fully hexahedron multi-density mesh is generated using blockMesh utility to ensure velocity gradients are properly evaluated. A generalized multi-grid solver is used to enhance convergence. A grid independence study was performed to quantify errors in this simulation. Realizable k-epsilon model is selected to perform simulation using the SIMPLE algorithm. In order to validate turbulence models, experiments have been performed at Thermal-Hydraulic Lab of Texas A&M University using particle image velocimetry (PIV) method and laser Doppler velocimetry (LDV) method respectively. Simulations were carried out based on boundary conditions obtained from experiments in terms of mean velocity as well as turbulence statistics such as root mean square (RMS) velocity. Mean velocity and vorticity were considered in comparisons. Besides, a number of turbulent characteristics had been accounted to compare with experiments, such as turbulent intensity, Reynolds stress components. Boundary condition sensitivity study also included in this study by comparing two jets inlet boundary conditions, mass flow rate, and the PIV mean velocity profile. It was found that for stream-wise mean velocity and lateral mean velocity profiles, realizable k-epsilon model exhibits a good agreement with experiments data. However, for root mean square velocity fluctuations and turbulence intensities, simulation results showed certain discrepancy at the region between the merging point and combining point.

### TWIN JET COMPUTATIONAL FLUID DYNAMICS (CFD) NUMERIC MODEL VALIDATION

**Technical Presentation.** VVS2016-8932

**Sasan Salkhordeh, Corey Clifford, Mark Kimber**, *Texas A & M University, College Station, TX, United States*

Over the last 30 years, an industry-wide shift within the nuclear industry has led to increased utilization of computational fluid dynamics (CFD) to supplement nuclear reactor safety analyses. Although several "best practice" guidelines exist for individual safety evaluations, verification of these CFD simulations and validation against analogous experimental data must occur to ensure the dependability and accuracy of these numerical models. One such area of significant interest to the nuclear thermal-hydraulics community, specifically to those analyzing next-generation high-temperature gas and sodium-cooled reactors, is the capacity of current computational models to accurately capture the thermal mixing of adjacent, turbulent jets. In order to combat the need for a more robust, experimentally-validated computational framework capable of predicting these types of phenomena, the present investigation performs a gamut of computational simulations and compares numerical system response quantities (SRQs) to CFD validation data collected from a scaled twin-jet experiment. The present study employs two different computational methodologies: (1) unsteady Reynolds-averaged Navier-Stokes (URANS); (2) large-eddy simulations (LES). A detailed assessment of possible sources of numerical uncertainty is conducted to ensure valid comparisons between computational data and analogous experimental SRQs. For both the URANS and LES simulations, a 'precursor' model of the region upstream of the twin-jet exhaust is constructed and analyzed to obtain high-resolution temperature, velocity, and turbulent quantities at the inlet of the experimental facility. By including the results of the precursor simulations at the inlet of the numerical model of the experimental facility, both computational methodologies produce substantially more accurate predictions of the measured field variables, highlighting the need to quantify upstream flow conditions when downstream mixing is the phenomenon of interest.

### VALIDATION AND VERIFICATION OF CFD SIMULATIONS INVOLVING TWIN RECTANGULAR JETS USING STEADY AND UNSTEADY RANS IN STAR-CCM+

**Technical Presentation.** VVS2016-8906

**Lane Carasik**, *Texas A&M University, Marietta, GA, United States,* **Huhu Wang, Yassin Hassan**, *Texas A&M University, College Station, TX, United States*

Rectangular turbulent jets are encountered in many types of engineering applications and provide a challenge in nuclear reactor systems. Reactor systems such as the upper and lower plenums of a Sodium Fast Reactor (SFR), compact heat exchangers, and the Reactor Cavity Cooling System (RCCS) experience these types of turbulent flows. To analyze this applications of turbulent jets, Computational Fluid Dynamics (CFD) tools are required for the significant insight into the flow behavior. These codes require benchmark problems for validation and verification to ensure the predictions are reasonable representations of reality. The data from these benchmark problems take form as both experimental and computational data sets that should be developed using high temporal and spatial resolution methodologies and measurements. The Twin Jet Water Facility (TJWF) designed and built at the University of Tennessee, Knoxville [1], was created for this purpose. The facility features two vertical parallel rectangular jets injecting fluid into a large transparent tank to study a large variety of thermal fluid phenomena. The two jets' full geometry features separated stagnation boxes that feed into the individual jets. Recent experimental studies conducted by Texas A&M [2] using high resolution experimental techniques provide useful information about the jets behavior as compared to previous works. The velocity, turbulence intensity, Reynolds stresses and other parameters acquired enable a thorough comparison to CFD simulations for V&V efforts of the same facility and boundary/initial conditions. The effort encompassed in the current study involves an analysis of the appropriate implementation of boundary/initial conditions, meshing techniques, and turbulence modeling. This work was conducted using the CD-Adapco's Star-CCM+ v10.04 CFD code [3] using both steady and unsteady Reynolds Averaged Navier Stokes (uRANS) formulations to simulate the behavior. The differences of the predictions between the two formulations will be shown in an effort to see which is most appropriate for different applications. These applications are differentiated by the requirements from industry (design) or research (development) that utilize CFD codes. The simulation results are compared with high resolution experimental results created in the Texas A&M Thermal Hydraulic Research Laboratory using a Verification and Validation approach.

[1] M. Crosskey and A. Ruggles, "UTK Twin Jet Water Facility Computational Fluid Dynamics Validation Data Set." ICAPP 2014, April 2014.
[2] Huhu Wang, Saya Lee, Yassin A. Hassan, Arthur E. Ruggles. (2016) Laser-Doppler measurements of the turbulent mixing of two rectangular water jets impinging on a stationary pool. International Journal of Heat and Mass Transfer 92, 206-227
[3] CD-Adapco STAR-CCM+ 10.04.011 User's Guide, www.cd-adapco.com

### NUMERICAL SIMULATIONS OF TWIN RECTANGULAR JETS USING ANSYS-CFX FOR VERIFICATION AND VALIDATION

**Technical Presentation.** VVS2016-8929

**Giacomo Busco**, *Texas A&M University, College Station, TX, United States,* **Lane Carasik**, *Texas A&M University, Marietta, GA, United States,* **Yassin Hassan**, *Texas A&M University, College Station, TX, United States*

A Verification and Validation (V&V) study of Twin Rectangular Jets has been performed using the Computational Fluid Dynamic software tool, ANSYS-CFX within the Twin Jet Water Facility (TJWF). The TJWF, which resides in the Thermal-Hydraulic Research Laboratory of Texas A&M University, has had experimental data obtained using measurement techniques such as Particle Image Velocimetry (PIV) and Laser Doppler Velocimetry (LDA). The scope of these measurement activities was to obtain high-fidelity experimental data sets for benchmarking different numerical models in advanced reactor technologies. The motivation of this study is related to the coolant/structure interaction issues found in advanced nuclear reactor technologies. Particular attention is focused on the structural integrity of reactor components. An illustration of this phenomenon is the induced thermal fatigue in the core coolant exit plenum of a gas cooled reactor or sodium cooled reactor, experienced during operational transients. An inefficient amount of coolant mixing could lead to random temperatures fluctuations (thermal striping), which leads to high cycle thermal fatigue and potential crack initiation at the surface level. For these reasons, mixing condition of the core coolant exit plenum needs to be accurately evaluated and fully understood. Massive computational work, involved in the design process, necessitate high-fidelity experimental data sets for benchmarking simulation results. Application of the V&V best and advanced practices will, in the near future, offer the possibility of using CFD simulations as a robust tool to be used for supporting the reactor design. The CFD study was conducted to simulate the mixing and the penetration flow of two vertical rectangular adjacent slot jets in a large volume of water at atmospheric pressure and temperature. The twin rectangular jets are characterized by the formation of a sub-atmospheric pressure region, near the inlet region, due to the high imposed velocity field. This causes the mutual entrainment of the two jets to converge into each other, which results in jet behaving as a single jet. The Control-Volume-Based Finite Element code ANSYS CFX was used to solve the steady, Reynolds-Averaged Navier-Stokes equations in this flow situation. The computational domain was defined by a hexahedral grid using ANSYS ICEM-CFD, whose grid density is proportional to the desired physical resolution of the problem. Different RANS turbulence model were applied, some of them based on the Boussinesq approximation and others that do not make use of the Boussinesq approximation, defining transport equations for each of the six independent components of the turbulent stress tensor.

The numerical simulations results have been verified and the different models validated with the high resolution experimental results. This was done in accordance with current best V&V practices.

## TRACK 6 Validation Methods

**6-1**
**VALIDATION METHODS: SESSION 1**
**2nd Floor, Acacia D** **1:30pm - 3:35pm**

### VARIABILITY ESTIMATION AND A VALIDATION METRIC FOR FREQUENCY RESPONSES IN P-BOX APPROACH

**Technical Presentation.** VVS2016-8810
1:30pm-1:55pm

**Dooho Lee**, *Dongeui University, Busan, Korea (Republic)*

Many performances on noise and vibration in a passenger car are represented in frequency responses. In a finite element (FE) model of passenger car, the input parameters usually have both aleatory and epistemic uncertainties. Probability-box (p-box) is a useful representation of the response uncertainties due to the mixed input uncertainties propagated through the dynamic system. In this paper, using a newly introduced area metric for the p-box approach and additional tools in the frequency domain, the variability of an FE model for a passenger car is estimated. The practical tools include p-box color map over the frequency band and a u-pooling p-box for frequency band of concern.

The area metric quantitatively represents the difference in the responses between the simulation and experimental results considering the uncertainties in the input parameters. For frequency responses, the area metric has different values at each frequency; i.e., both the area metric and the p-box depend on the frequency. To assess the numerical model properly, both the area metric and the area of the p-box should be examined simultaneously. Thus, p-boxes in the frequency domain are transformed into a color map in which the plotted values are obtained by adding the left-hand-bound cumulative density function (CDF) and the right-hand-bound CDF, and by subtracting the added value from the maximum (i.e., 2) if the added value is greater than one. In the colour map the vertical length of the central value is the approximated width of the p-box which indicates the variability of the freqeuncy responses due to the epistemic uncertainty at each frequency. The vertical lengths from zero to one and from one to zero also approximately represent the variability of the frequency responses due to the aleatory uncertainties. Therefore, this transformation enables us to assess the numerical model over the frequency range of concern while retaining the main characteristics of the p-box. The colour map clearly illustrates that the uncertainty of the responses over the frequency band is due to the epistemic input parameters while the aleatory uncertainties are dominant in the other frequency band.

At each frequency, the noise and vibration responses have different distributions. Thus, u-pooling for all frequency responses over the frequency range of concern will provide a wealth of information pertaining to the validity of the numerical model. Similar to the p-box at a specific frequency, the area metric between the u-pooling CDFs and the reference uniform CDF represents the discrepancy between the numerical model and the experimental measurements in an overall sense. The u-pooled CDFs consist of two curves due to the epistemic uncertainties. When the numerical model contains only aleatory uncertainty, the two CDFs will be merged into one CDF. Less epistemic uncertainty leads to a shorter distance between the two CDF curves. The area metric of the u-pooling p-box considers only the propagated variability of the numerical model due to the uncertainties in the aleatory input. The influence of the epistemic uncertainty on the overall agreement is represented by the area between two u-pooling CDFs.

The proposed validation framework was applied to a vibro-acoustic FE model for a passenger car. The color map of the p-boxes over the frequency band, the u-pooling p-box for the frequency band of concern and the p-boxes at different frequencies were proven to be suitable for assessing the model error and for making quantitative contributions of the aleatory and epistemic input parameters to the overall variability of the responses in the frequency domain.

### SIMULATION TIME HISTORY VALIDATION VIA MULTIVARIATE HYPOTHESIS TESTING OF FOURIER COEFFICIENTS

**Technical Presentation.** VVS2016-8844
1:55pm-2:20pm

**Jeffry Sundermeyer**, *Caterpillar, Inc., Mossville, IL, United States,* **Juan F. Betts**, *Front End Analytics, LLC, Boston, MA, United States,* **Mark A. Walker**, *Front End Analytics, LLC., Boston, MA, United States*

Some of the most common outputs of product development simulations are time histories that are relevant to some aspect of product operation. Quite often, these time histories in a physical test or customer usage environment exhibit considerable variability while at the same time maintaining some qualitative similarities. From a simulation validation perspective, the natural question to ask is whether it is plausible that a candidate set of simulation time history(ies) belongs to the same population from which a collection of reference (physical test) time histories were randomly sampled. The very nature of this question is suggestive of the concept of hypothesis testing. In this work, all curves in the candidate and reference sets were expressed via discrete Fourier series, and then the chosen coefficients were compared via a multivariate hypothesis testing process. Two different classes of problems are considered.

The first class of problem is one in which the event under consideration is a finite-duration non-stationary random process. Each physical test example of the event has a somewhat different duration. Fourier coefficients are grouped together in the hypothesis testing process according to their corresponding integer multiple of the fundamental frequency. Magnitude and phase (or alternatively, real and imaginary) are both utilized in the multivariate hypothesis testing process.

The second class of problem is one in which the event is more of a quasi-stationary random process of arbitrary length. In this class of problem Fourier coefficients are simply grouped together according to their associated frequency in the hypothesis testing process. Only magnitude is utilized in this case.
Both classes can be further subdivided into the subcases of one candidate time history versus many reference time histories, and many candidate curves versus many reference curves. In the first subcase, the question of plausible membership is addressed via the multivariate hypothesis testing process. In the second subcase, there is a more demanding comparison of mean column vectors and a comparison of covariance matrices.

A number of examples of the two different classes of problems for both subcases are illustrated. In some of the examples, it is known ahead of time that the candidate curve(s) are members of the reference population, and it is shown that this assertion is supported by the results of the hypothesis test. In other examples, candidate time histories are corrupted in some way via the introduction of noise or other means, and it is shown that the probability of rejection increases with the degree of signal corruption.

### VALIDATION OF AN AIR CYCLE MACHINE

**Technical Presentation.** VVS2016-8853
2:20pm-2:45pm

**Jon Zumberge, Thierry Pamphile**, *AFRL, Wright Patterson AFB, OH, United States,* **Mark Bodie**, *P.C. Krause and Associates, Wright Patterson AFB, OH, United States*

Cost and performance requirements are driving military and commercial systems to highly integrated, optimized systems which require more sophisticated, highly complex controls. To realize benefits of those complex controls and make confident decisions, the validation of both plant and control models becomes critical. To quickly develop controls for these systems, it is beneficial to develop plant models and determine the uncertainty of those models to predict performance and stability of the control algorithms. Validation for an air cycle machine model based on acceptance sampling and tolerance interval is presented here. The validation process described in this presentation is based on MIL-STD 3022 with emphasis on requirements settings and the testing process.

The process for model validation to be presented is discussed in more detail in [1] and [2]. The hypothesis test used in the validation process is based on acceptance sampling using a single-sampling plan from statistical quality control [3], [4], and [5] that ensures Type I and Type II risk levels are met. The acceptance sampling technique is based on satisfying the following two probabilities P(p1) >>= (1 - alpha) P(p2) <= beta where p1 is called the acceptable quality level (AQL), and p2 is the rejectable quality level (RQL) or lot tolerance percent defective (LTPD). In words, the sampling plan ensures the probability of acceptance at the AQL is higher than 1 - alpha, and lower than beta at the RQL. The binomial distribution is used here as the population of possible computations (i.e., simulations) is large and effectively samples can be pulled with replacement. The two probabilities are binomial distribution that can be optimized over number of test runs and number of allowed bad points/rejects (see [2] and [3] for more information on the optimization).

The confirmation tests, the number of tests executed, and the critical number protect against identifying a good model as bad, but also identifying a bad model as good. Each confirmation test is randomly chosen (i.e., the operating conditions are randomly chosen) and evaluated against a pre-determined metric. For example, each confirmation test may measure the amount of error in a given output and if that error exceeds a pre-determined threshold then the individual confirmation test fails. If the number of confirmation test fails exceeds the critical number than the hypothesis fails.

The system under study is an air cycle machine that is composed of a heater, regulation valve, turbo-charger, heat exchanger, and ducting. Ordinary differential equations are used to represent the physics of the individual components and those models will first be validated individually and then a system validation will be performed. In the presentation, only the regulation valve validation will be documented.

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### VALIDATION OF MULTI-BODY DYNAMICS APPLICATIONS FOR RAIL VEHICLE CERTIFICATION

**Technical Presentation.** VVS2016-8867
2:45pm-3:10pm

**Gernoth Götz**, *Berlin Institute of Technology, Berlin, Germany,* **Oldrich Polach**, *Bombardier Transportation, Winterthur, Switzerland*

Continuous development of multi-body dynamics programs and capable information technology enable broad application fields for all industry sectors.

Within the application in the railway industry, multi-body simulation programs are used during design and development as well as for investigating various vehicle-track interaction issues [1]. Nowadays, time consuming and cost-intensive on-track tests are mandated for the certification of rail vehicles. The use of multi-body simulations to reduce the amount of testing is increasingly recognised as a possible mean to reduce costs and efforts of this certification. The application of simulation instead of physical testing, however, requires a reliable validation of the simulation model.

All rail vehicle model validation approaches follow the common attempt to compare simulations with measurement results. The testing for the acceptance of running characteristics of rail vehicles consists of stationary and on-track tests. Although rail vehicles are equipped during testing with several measurement devices (e.g. force measurement wheelsets, accelerometers, devices for rail profiles and track irregularity recording), there are several uncertain parameters such as the friction coefficient between wheel and rail, which can hardly be measured. The resulting scatter of possible influencing quantities and similarly the question of repeatability of measurements lead to difficulties in the selection of quantities and in the definition of threshold values for model validation.

Different model validation approaches have been developed within the last years. The European approach used in UIC 518:2009 [2] and incorporated in the recent revision of European standard EN 14363:2016 [3] is predicated on early experience with model validation in the UK using stationary tests. This validation method contains proposals for possible comparisons between simulation and measurement but threshold values are not defined. Thus, an approval by an independent reviewer is required. To overcome this gap, the development of a new validation method with explicit threshold values was one of the objectives of the European research project DynoTRAIN [4]. The result of this project considers comparisons of simulations with measurement results from the on-track tests. A statistical approach has been selected to assess an overall agreement calculating mean value and standard deviation of differences between simulation and measurement for 12 specified quantities for a minimum of 12 test sections representing the conditions for vehicle acceptance. The recently developed US model validation approach follows a two-step assessment [5]. Comparisons between testing and simulation are carried out by means of three static tests (static lean test, wheel load equalization test, modal) to validate principal vehicle parameters followed by a dynamic on-track test to validate observed nonlinear motions of the rail vehicle during testing. The nonlinear motions are excited with a "virtual excitation track" including large enough track irregularities. Other model validation approaches such as signal comparisons in the frequency domain or the use of validation metrics are presently being studied.

The presentation will give an overview and a critical discussion about existing methods for model validation considering the repeatability of measurements and the scatter of uncertain experiment's parameters. Furthermore, the presentation will include also new investigations regarding the reliability of the validation method developed in the DynoTRAIN project with respect to section length, number, and selection of sections being used for the model validation as well as varying parameters of the simulation model.

References:

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### A METHOD FOR QUANTITATIVE COMPARISON OF VALIDATION DATA FOR FINITE ELEMENT MODELS OF THE HUMAN HEAD

**Technical Presentation.** VVS2016-8895
3:10pm-3:35pm

**Logan Miller**, *Wake Forest University, Winston Salem, NC, United States*

Each year, approximately 1.7 million people in the United States suffer from traumatic brain injury (TBI). To prevent and treat these types of injuries, the fundamental injury mechanisms need to be well-characterized and understood. Finite element models (FEMs) are powerful tools for studying brain injury because they can provide spatial and temporal distributions of stresses and strains over the problem domain. Finite element models with varying degrees of anatomical accuracy, element size and material properties have been developed. The experimental validation of such FEMs is a critical step in model development before results from these models can reliably be applied in fields such as injury prediction. The current standard for brain model validation is evaluating the temporal strain response throughout the model following impact and comparing to experimental data. To date, there has been no reliable quantification of time-varying model performance or quantitative comparison of different models. The objective of the current study is two-fold. The first objective is to present validation results using data from three experimental tests for the following six previously published brain FEMs: Atlas-Based Brain Model (ABM), Simulated Injury Monitor (SIMon), Global Human Body Models Consortium (GHBMC) head model, Total Human Model for Safety (THUMS) head model, Kungliga Tekniska Högskolan (KTH) model, and the Dartmouth Head Injury Model (DHIM). The second objective is to perform a quantitative comparison of model performance using an objective rating method called CORA (CORrelation and Analysis).

The three experimental tests used in the current study are cadaver impact tests conducted in frontal, occipital, and parietal configurations. These three tests were chosen for validation purposes because they cover a range of impact velocities and directions. In each of these experiments, between 10 and 15 neutral density targets (NDTs) were implanted in the cadaver brain and their motion relative to the head center of gravity (CG) was tracked using high-speed biplanar X-ray video. Results for the ABM, SIMon, GHBMC, and THUMS models were obtained through finite element simulation in LS-DYNA and localized brain motion quantified using nodal displacements. Results for the KTH and DHIM models were obtained from published literature. Model performance is evaluated by comparing experimental displacements at each NDT to the displacements predicted by each model. The similarity of time-varying curves is quantified in the current study using CORA, an objective rating method that combines two independent sub-methods, a corridor rating and a cross-correlation rating. These two ratings range from 0 to 1 and are averaged to determine the CORA rating (1 indicates a perfect match). The corridor method computes a rating based on where the simulated curve falls in relation to corridors around the experimental curve. The cross-correlation method is based on ratings for the phase shift, size and shape of time-shifted curves.

For each model, a CORA score was computed at each NDT and averaged to compute an overall CORA score per model for each of the three configurations. Of the models examined, the highest CORA scores for the frontal, occipital, and parietal cases were observed for the DHIM, KTH, and ABM models, respectively. Looking at the average CORA rating between the three impacts, the ABM has the highest CORA score. This result indicates that of the models considered, the ABM demonstrates the strongest ability to predict local brain deformations under a range of impact severities and directions.

## TRACK 8 Validation Methods for Impact, Blast, and Material Response

### 8-1
### VALIDATION METHODS FOR IMPACT, BLAST, AND MATERIAL RESPONSE

**2nd Floor, Palo Verde A** **1:30pm - 3:35pm**

#### DEVELOPING, VERIFYING, AND VALIDATING VARIABLE AXIAL LOADING IN THICK WALLED PRESSURE VESSELS

**Technical Presentation.** VVS2016-8818
1:30pm-1:55pm

**Lucas Smith, Davin Alfano**, *Benét Laboratories, Watervliet, NY, United States*

Traditional hydraulic fatigue testing is performed quasi-statically on open ended cylindrical sections of pressure vessels to establish their fatigue life. Typically, only hoop loading of the pressure vessels is required to determine fatigue life. However for some specific geometries and service conditions a more complex test is required. This has been confirmed, whereby, certain geometries have experienced circumferential cracking because of combined, nearly equivalent axial loading and hoop loading. Consequently, a test fixture was engineered, designed, built and tested by US Army - Benét Laboratories / ARDEC to replicate the service loading condition and verify the finite element analysis (FEA) modeling of the system. Simultaneous axial / hoop fatigue testing in a lab environment can validate the FEA model to ensure the test fixture design is a realistic representation of loading conditions.

Thick walled pressure vessels subject to high axial loads were instrumented with strain gages during field loading conditions, and the resulting strain output has shown the axial and hoop components are equivalent in certain sections. These sections have specific geometric design constraints. After various design iterations through FEA and review, a test fixture was manufactured to test thick walled pressure vessels in a laboratory environment in order to duplicate field loading conditions. To verify the test fixture in the laboratory environment, strain gages were applied to representative sections as done in field loading. Upon review of the test sections at test pressure, the strain gage data was able to validate the FEA as well as ensure the representative field loading could be duplicated.

#### VALIDATION OF VEHICLE UNDER-BODY BLAST METHODOLOGY

**Technical Presentation.** VVS2016-8883
1:55pm-2:20pm

**Andrew Drysdale**, *US Army Research Laboratory, Aberdeen Proving Ground, MD, United States,* **Raquel Ciappi, Brian Benesch**, *SURVICE Engineering, Aberdeen Proving Ground, MD, United States*

The UBM Program was started to develop the Army's capability for simulating under-body blast attacks against ground vehicles. The current UBM toolset uses physics-based modeling and simulation to predict occupant injury from accelerative loading to support Live Fire Test & Evaluation (LFT&E). The use of these tools combined with subject matter expertise derived from extensive experience in system-level testing and theater event analyses is intended to enable accurate and efficient predictions of vehicle damage and occupant injuries.

The first official use of the UBM toolset will be for the upcoming LFT&E of the Joint Light Tactical Vehicle (JLTV). The V&V is focused on the UBM tools which will be used for the JLTV analysis. These include Arbitrary Lagrangian-Eulerian loading, a detailed finite element model of the JLTV, and two occupant sub-models representative of the JLTV (i.e. floor and seat design). Injury assessments are performed using the Analysis of MANikin Data (AMANDA) model, which is being independently verified and validated this fiscal year.

A unique challenge for this V&V/accreditation effort is overcoming the sporadic nature of relevant experimental data that is suitable for validation. System-level live-fire tests are inherently expensive, chaotic, and difficult to instrument efficiently. This leads to persistent uncertainties in both the modeling predictions and the baseline data that the model is checked against. Several strategies for overcoming this obstacle are presented, as well as an overall V&V plan for validating the end-to-end UBM process.

#### CAE MODEL SIMPLIFICATION AND VALIDATION STRATEGIES FOR COMPLEX ENGINEERING APPLICATIONS

**Technical Presentation.** VVS2016-8900
2:20pm-2:45pm

**Nanliang Jiang, Zhenfei Zhan**, *Chongqing University, Chongqing, China,* **Jie Zheng**, *Siemens Ltd., China, Beijing, China,* **Yucheng Tang**, *Siemens Energy, shanghai, China,* **Junqi Yang, Xin Yang**, *Chongqing University, Chongqing, China*

Computer aided engineering (CAE) has become a vital tool for product development in various industry. However, computational time increases significantly with the ever growing complexities of engineering systems. Hence, how to effectively simplify the models without lose necessary accuracy attracts lots of researchers' attentions. Take automotive crashworthiness analysis for example, as it mainly focuses on the longitudinal dynamic characteristics during crash, it is viable to simplify the vertical and lateral features of vehicle model to save computational costs. For such purpose, the medial surface (midsurface) of model, which is regarded as the skeletal of a solid shape, can be extracted for CAE model simplification.

In this study, a midsurface extraction based dimensional reduction method is adopted to simplify Finite Element (FE) model, so that to improve the computational efficiency. The solid model is firstly decomposed into less complex solid sub-models using the splitting planes or created surfaces. The decomposed sub-models are considered as primitives. The distance between the two surfaces to be simplified is then measured to test whether the designed simplification requirements are satisfied. Through the procedure, the solid element can be simplified into 2-dimensional midsurfaces which reduces the population of the mesh and saves time in the following analysis.

To evaluate the predictive capability of the simplified model, the Enhanced Error Assessment of Response Time Histories (EEARTH) metric is employed. EEARTH metric employs dynamic time warping (DTW) to separate the interaction of phase, magnitude, and shape errors. It aligns peaks and valleys as much as possible by expanding and compressing the time axis according to a given cost (distance) function and employs a linear regression method to combine the three errors into one score for quantitative error assessment.

The proposed strategies are implemented on a CAE based vehicle design problem. The results show that the proposed method is able to greatly improve the computational efficiency and facilitate the CAE model. The simplified model is able to demonstrate the deformation visually. Moreover, longitudinal directional analysis avoids the unnecessary modifications on vertical and lateral features, and enhances the potential model calibration process. Further study will be on the analysis of adaptive boundary conditions, the method of adaptive dimensional reduction, and their integrations with the proposed strategies.

#### CRASH BOX RESPONSE TO A DROP WEIGHT IMPACT TESTER

**Technical Presentation.** VVS2016-8928
2:45pm-3:10pm

**Khaled Asfar, Salman Deilat, Mai Qudeh,** *Jordan University of Science & Technology, Jordan, Irbid, Jordan*

The performance of a crash box/attenuator in a drop weight impact testing machine is simulated by finite elements. The crash box/attenuator is a structure that is located in front of vehicles and used to absorb collisions and decelerate the vehicle to a complete stop. They can be placed on vehicles or on road barriers to absorb high impact in order to protect and minimize damages to frames and people. The simulation is carried out using ANSYS where several attenuator geometries and materials such as copper, aluminum and steel were investigated. Deceleration properties and deformations were analyzed due to free drop weight testing. Three dimensional finite element models were developed for a pyramid- like crash box shape and other configurations. This program could depict the nonlinear behavior during impact. The Creo parametric ProEngineer were used to generate the geometric lattice configuration which was fed to the finite elements ANSYS code. Optimized element size was used in the calculations. A scaling method was also used which lead to more accuracy and less processing time. Impact of the drop weight was simulated from falling from zero height with an initial impact velocity calculated from the desired mass initial height. Results indicated whether the attenuator fractures during or after impact if it does. Verification of the finite element solution is done through experiments.

The impact testing machine was designed to perform low speed impact tests, i.e. impact velocities less than 15 m/s. The machine is able to accommodate impact tests on specimens of various cross sectional geometry with maximum outer geometry of 350 mm and maximum height of 350 mm. In the design, a specimen attenuator was fixed to a heavy steel base. An impactor mass of 230 kg is raised to a certain height using a winch such that its desired impacting speed is based on this height. The kinetic energy of the falling mass is absorbed by the progressive folding of the attenuator wall which reduces the kinetic energy of the impacting mass till it finally stops. The crushing force on the attenuator is sensed and recorded by a load cell which is placed between the specimen and the steel base. The variation of acceleration with time is detected and filtered to remove noise and vibration. The crushing force data, the dropped weight mass and impact speed are all used in the validation of the numerical analysis.

## TRACK 12 Verification Methods

### 12-3
### VERIFICATION METHODS: SESSION 3

**2nd Floor, Palo Verde B** **1:30pm - 3:35pm**

**VERIFICATION OF SHOCK-CAPTURING CODES USING MANUFACTURED SOLUTIONS**

**Technical Presentation.** VVS2016-8904

1:30pm-1:55pm

**C. Nathan Woods, Scott Doebling**, *Los Alamos National Laboratory, Los Alamos, NM, United States*

The theory of code verification has been revolutionized by the introduction of the method of manufactured solutions (MMS), though widespread adoption has been slow in coming. One reason for this is that MMS encounters difficulties when dealing with shock-capturing codes, which are extremely important for many fields for which verification is critical, such as hypersonic aerodynamics, explosives modeling, and astrophysics. We investigate a means of resolving these difficulties based on an integral formulation of the MMS methodology.

MMS struggles to represent shocked (discontinuous) solutions because of a fundamental inconsistency between the way it is formulated and the way shocked solutions arise in physical models. MMS is formulated in the context of differential equations, where the strong (differential) mathematical model is operated on an analytical manufactured solution in order to yield analytical source terms. Shocked solutions, in contrast, are not solutions to strong models at all, but related weak (integral) models, which do not require differentiable solutions. As a result, strong-form formulations of MMS must be smoothed, via the addition of artificial viscosity terms. Although artificial viscosity is included in many codes, it is not part of the mathematical model upon which these are based. As a result, including them in MMS formulations leads to a situation where a code is verified against a specific viscosity model, rather than an actual physical model.

Once we understand that the problems with shock-capturing MMS arise from this fundamental mismatch, it is reasonable to assume that they may be resolved by reformulating MMS itself into weak form. This reformulation is straightforward, but computing manufactured source terms requires the evaluation of complicated, multidimensional, integrals, which likely contain shock interfaces. As a result, numerical integration techniques must be found that are both sufficiently accurate for the purposes of code verification and fast enough to be usable over a reasonable discretization of space and time, even in the presence of jump-singular integrand functions.

We have developed a new method for integrating discontinuous functions based on a technique we call discontinuity tracking. Using a priori knowledge of the shape and location of the shocks, we are able to eliminate the numerical difficulties associated with the jump singularity for n-dimensional integrals. The results are extremely accurate for test problems, although discontinuity tracking does come with significant computational costs. We have used this method to demonstrate integral MMS with a prototype fluid dynamical code, and we have obtained convergence rates that are similar to those associated with both differential MMS and exact solutions. The computational cost of discontinuity tracking is problematic, because verification is already an inherently expensive operation that must be done at scale in order to be effective. As a result, our integration method is limited to small verification problems. However, the availability of a highly accurate integrator, albeit an expensive one, many new possibilities for the evaluation of faster routines, and we are evaluating these for future development of integral MMS. Once the integration problem is successfully resolved, integral MMS will enable code verification for shock capturing codes and extend rigorous verification procedures to fields where they have never been available before.

**A NEW APPROACH TO FINITE ELEMENT METHOD ERROR ESTIMATION USING A NONLINEAR LEAST SQUARES LOGISTIC FIT OF CANDIDATE SOLUTIONS**

**Technical Presentation.** VVS2016-8912

1:55pm-2:20pm

**Jeffrey T. Fong**, *National Inst. of Standards & Technology, Gaithersburg, MD, United States,* **James J. Filliben, N. Alan Heckert**, *NIST, Gaithersburg, MD, United States,* **Pedro V. Marcal**, *MPACT, Corp., Oak Park, CA, United States,* **Robert Rainsberger**, *XYZ Scientific Applications, Inc., Pleasant Hill, CA, United States*

Errors and uncertainties in finite element method modeling and computing are known to originate from at least seven sources: (1) The computer code or “platform“ of the finite element method using a specific numerical algorithm of approximation for solving a system of partial differential equations with initial and boundary conditions; (2) the choice and design of the finite element mesh using one or more element types; (3) the “quality“ measures of the finite element mesh such as the mean aspect ratio; (4) the uncertainties in the geometric parameters of a model; (5) the uncertainties in the physical and material property parameters of a model; (6) the uncertainties in the loading parameters, and finally (7) the uncertainty in the choice of the governing equations of a correct model. In this paper, we will address the errors and uncertainties due to the first three sources, namely, (1) the platform, (2) the dominant element type, and (3) the mean aspect ratio. Our approach is to design a family of meshes of increasing degrees of freedom for a specific element type and mean aspect ratio, and solve them using at least two different platforms in order to estimate the errors and uncertainties due to the approximate nature of the finite element method. To obtain an estimate of the “correct“ solution at infinite degrees of freedom, we introduce a nonlinear least squares fit algorithm based on a 4-parameter logistic distribution and apply to a sequence of at least five candidate solutions for a specific platform, element type, and mean aspect ratio. The predicted “correct“ solutions with uncertainties and error convergence rates at infinite degrees of freedom are then compared with one another to yield a ranking of the solutions from the “most“ to the “least“ accurate, based on the preference of least uncertainty and maximum error rate of convergence. To illustrate this approach, we introduce five numerical examples, of which the first two have known analytical solutions: (1) The elastic bending of a cantilever beam due to an end load; (2) the first bending resonance frequency of a simple, isotropic, elastic cantilever beam; (3) the elastic deformation of a barrel vault; (4) the elastic deformation of a cylindrical pipe with a circumferential surface crack; and (5) the elastic deformation of a pipe elbow with two welds and a circumferential surface crack at one of the two welds. The significance and limitations of our new approach as a tool for verification and validation of the finite element method are presented and discussed.

**METHOD OF NEARBY PROBLEMS FOR MULTI-MATERIAL SOLID ANALYSIS**
**Technical Presentation.** VVS2016-8919
2:45pm-3:40pm

**Takahiro Yamada**, *Yokohama Nat'l University, Yokohama, Japan*

The method of nearby problems developed by Roy el al. is a sophisticate verification procedure, in which the problems with exact solutions near the target problem of interest can be generated by a curve fitting of a numerical solution to a continuous function. To apply this method to solid problems in the conventional procedure, spatial derivatives of stresses derived from given displacement solutions, which is hardly calculated for general constitutive laws, are required to calculate body forces in the nearby problem. Therefore they have been not popular in solid mechanics. To circumvent such difficulty, the author developed an alternative procedure to calculate equivalent nodal vectors of body forces without calculation of the spatial derivative of stresses. It is based on the weak formulation of the problems of solid and the actual procedure to calculate equivalent nodal force vectors is similar to evaluation of internal force, in which the work product of the stress and virtual strain is integrated over the domain.

In our previous work, problems of a single material are considered and nearby solutions are constructed by the projection of a finite element solution of displacement onto an approximating function space using the inner product in the Sobolev space H1. For the approximating function space, the uniform tensor product B-spline functions are employed and complex geometry is modeled by using the fictitious domain approach.

In this work, we consider multi-material problems, in which discontinuity of strains emerges on the interface of different materials. In this situation, highly continuous function on the whole domain that is defined by the spline bases is not suitable to represent such strain fields. Therefore, weighted spline function proposed by Hollig et al. is employed to deal with such discontinuity. The weighted spline function is originally designed to impose Dirichlet boundary conditions on the domain of complex shape. We adapt this function to attain continuity on the material interface, in which displacements are continuous and strains are discontinuous. Although discontinuous strain fields can be expressed by the weighted spline function, continuity of stress vectors on the material interface may not be satisfied. Such unmatched stress vectors result in residual traction on the interface. In the conventional procedure for method of nearby problems, such tractions need to be calculated from boundary values of stress field on the interface in addition to body forces. On the other hand, tractions are automatically included in the process to evaluate nodal force vector from stress fields of nearby solutions thanks to the weak formulation in the present approach.

Several representative numerical results are presented to show the validity of the present approach.

## TRACK 1 Challenge Problem Workshops and Panel Sessions

### 1-2
### V&V BENCHMARK PROBLEM SESSION 2 — TWIN JET COMPUTATIONAL FLUID DYNAMICS (CFD) NUMERIC MODEL VALIDATION

**1st Floor, Mesquite 2** **4:00pm - 6:05pm**

**V&V BENCHMARK PROBLEM SESSION 2 —TWIN JET COMPUTATIONAL FLUID DYNAMICS (CFD) NUMERIC MODEL VALIDATION – PANEL DISCUSSION AND PRESENTATIONS**
**Technical Presentation.** VVS2016-8002

**Hyung Lee**, *Bettis Laboratory, West Mifflin, PA, United States,* **Ryan Crane**, *ASME, New York, NY, United States,* **Yassin Hassan**, *Texas A&M University, College Station, TX, United States,* **Arthur Ruggles**, *University Of Tennessee, Knoxville, TN, United States,* **Richard Schultz**, *Consultant, Pocatello, ID, United States,* **Christopher Freitas**, *Southwest Research Institute, San Antonio, TX, United States*

The ASME Verification and Validation in Computational Nuclear System Thermal Fluids Behavior Committee (ASME V&V30 Standards Committee) is initiating a series of verification and validation (V&V) benchmark problems designed to:

Study the scope and key ingredients of the V&V30 Committee's charter,
Achieve the above objective by using new, high-quality, state-of-the-art validation data sets obtained specifically for this purpose, and
Achieve the above objectives using a stepwise, progressive approach characterized by focusing on each key ingredient individually in a benchmark problem designed for that purpose.

The first V&V benchmark problem in the series was conducted as the part of the 2016 ASME V&V Symposium. Some of the results and findings from the first V&V benchmark problem were presented and discussed in Session 1. In this session, the presentation and discussion of the first V&V benchmark problem continues as a part of an open-forum panel discussion in a broader context of demonstrating the state of the practice in using and applying computational tools to support U.S. Nuclear Regulatory Commission or other regulatory reviews. It is hoped that through these open-forum discussions, the envisioned outcomes of lessons learned, review of V&V methods, and effectiveness of V&V methods to support modeling and simulation reviews can be captured and documented.

The results of the various participants and open-forum discussion findings will be summarized and documented in a subsequent report to be presented by the benchmark problem committee at the 2017 V&V Symposium.

## TRACK 6 Validation Methods

### 6-2
### VALIDATION METHODS: SESSION 2

**2nd Floor, Acacia D** **4:00pm - 6:05pm**

**ESTIMATION OF CARBON MONOXIDE LEVELS AND ITS REMOVAL IN CARPARK BY INCORPORATING PROPER HVAC SYSTEM BY USING CFD**
**Technical Presentation.** VVS2016-8902
4:00pm-4:25pm

**Nirav Parikh**, *Parul University, Vadodara, Gujarat, India*

With the rise in number of automobile users there is an immense rise in number of car park built all around. Immense number of vehicles can be seen at the parking areas where the movement of air is less and the carbon monoxide (CO) gets accumulated at the level of earth. Automobile parking area can be partially open or fully enclosed. Partially open garages are typically above-grade with open sides and generally do not need mechanical ventilation. However, fully enclosed parking garages are usually underground and require mechanical ventilation. Indeed, in the absence of ventilation, enclosed parking facilities present several indoor air quality problems. The most serious is the emission of high levels of CO by cars within the parking garages and other parking plots.

Many studies of air quality have focused on Carbon Monoxide (CO) because it is generally considered to have severe impact; CO is colourless, odourless, and highly toxic gas, emitted as a product of incomplete combustion of hydrocarbon-based fuels. When CO is inhaled, it combines preferentially with haemoglobin (Hb), the oxygen carrier of the blood, to produce carboxy haemoglobin (COHb), displacing oxygen and reducing system arterial oxygen content. Its toxicity is due to the fact that it binds reversibly to haemoglobin with an affinity 200-250 times that of oxygen. This makes CO dangerous even at low concentrations.

The objective of the paper is to analyze permissible carbon monoxide levels in the enclosed car parks and design a proper mechanical ventilation system to reduce the CO concentration to the permissible levels with the help of CFD analysis. This Project aims to verify whether the flow rates prescribed by client are able to efficiently eliminate CO without using jet fans or is there a need to run jet fans to remove excess CO concentration. Project also tries to verify at what percentage of speed thus the extract fans be used 30% or 60% or at full speeds.

Computational Fluid Dynamics (CFD) is the use of computer-based simulation to analyse systems involving fluid flow, heat transfer and associated phenomena such as chemical reaction. A numerical model is first constructed using a set of mathematical equations that describe the flow. These equations are then solved using a computer programme in order to obtain the flow variables throughout the flow domain. Since the advent of the digital computer, CFD has received extensive attention and has been widely used to study various aspects of fluid dynamics. The development and application of CFD have undergone considerable growth, and as a result it has become a powerful tool in the design and analysis of engineering and other processes.

This paper considers basement-1 and basement-2 for case study. Paper deals with natural inlet source as ramp opening and mechanical extract fans for base -1 & complete mechanical supply and extract system for base-2. CO levels have been monitored for both basements and excess CO has been evacuated by use of jet fans. It has found Basement-1 with natural inlet requires lesser effort to evacuate CO when compared to basement-2. Effective arrangement of Jet fan locations to remove CO effectively is also shown explicitly in this paper.

### VALIDATION OF INTENTIONAL AND NON-INTENTIONAL ACOUSTIC SOURCES WITH SCANNING LASER VIBROMETRY

**Technical Presentation.** VVS2016-8941
4:25pm-4:50pm

**Tim Gladwin**, *Harman International, Northridge, CA, United States*

Scanning LASER vibrometry is a relatively mature practical measurement technique in speaker design for examining transducer diaphragm and surround vibration issues. However, its greatest potential may be to validate FEA models of both intentional acoustic sources such as transducers, and also of enclosures and other unintentional acoustic sources. The Klippel LASER scanner can accurately predict acoustic contributions from the parasitic vibrations of unintentional sources excited by the high ambient SPL from transducers.

The proliferation of excellent simulation tools, such as FEA and BEA, has revolutionized product design; but the results can be misleading if not validated by measurement. One of the difficulties is that library material parameters are measured using essentially static (DC) methods, or at low frequencies for dynamic measurements, and the materials are typically measured in a raw state. Key parameters such as Young's Modulus and Damping Factor are usually frequency dependent and are altered by forming methods.

In one case study, the development of flat-ish thin aluminum diaphragms for a high-end audiophile loudspeaker client was undertaken both experimentally and through FEA, in cooperation of an acoustic FEA vendor and a Scanning Vibrometer vendor. The objective was to demonstrate the effectiveness of the FEA tool to gain insight for shortening the development time, and to produce a paper to that effect. Unfortunately, the FEA results did not match the measured vibration pattern or SPL, that is, until the LASER scans were provided to the FEA vendor. The FEA vendor then tweaked the FEA material properties to be frequency dependent so that the simulation matched the measured results. Once the material properties were adjusted, changes to the diaphragm design could be predicted from FEA with good correlation. This led to a software tool that determines the frequency dependent Young's Modulus and Damping Factor by automatically converging FEA results with measured data.

As the consumer market demands products with audio that are smaller and lower cost, parasitic vibration of enclosures and other unintentional radiators is a growing concern. Product designers, often with minimal acoustic experience, are required to minimize enclosure wall thickness, implement acoustically-challenged industrial design, and work with unfavourable lowest-cost materials. The resulting enclosure vibration and resonance contributes to the overall sound of the product, usually in a negative way.

In a further case studies, the acoustic output of non-intentional sources is measured in isolation by vibrometry so that the contribution to the total SPL may be gauged. Three unintentional acoustic sources will be examined in order to show the effects of ribbing a loudspeaker baffle, the effects of enclosure material choice, and the effects of design defects in smartphone design.

Scanning Laser Vibrometry precisely measures and visualizes enclosure vibration; from this the software determines the SPL of the surface independently of the SPL from the speaker. The correlation between the measured speaker SPL(f) curve and the SPL(f) predicted from the vibration measurement can be readily checked.

Benefits of Scanning Laser Vibrometry include the ability to quantify the impact of intentional and parasitic vibration, the knowledge to mitigate resonances with surgical precision and the ability to validate simulation results. This expedites better products to market.

### A ROBUST APPROACH TO QUANTIFYING FORECASTING PRECISION USING PROXY SIMULATIONS

**Technical Presentation.** VVS2016-8936
4:50pm-5:15pm

**Kendra Van Buren**, *Los Alamos National Laboratory, Los Alamos, NM, United States,* **Scott Cogan**, *University of Franche-Comté, Besançon, France,* **Francois Hemez**, *Los Alamos National Laboratory, Los Alamos, NM, United States*

When using numerical models, analysts are often confronted with the situation whereby simulation predictions are used to inform decision-making in a domain where experimental data are unavailable. In such cases, the numerical model is trusted to predict in the forecasting domain simply because it has been shown to be trustworthy in the validation domain, where experimental data are available. Although the inherent dangers of this prediction extrapolation are widely recognized, few methods are available to actually establish its credibility for a given application. In this paper, the authors propose a diagnostic tool to quantify the robustness of forecasting precision to uncertainties in the calibration process resulting from compensating effects and measurement errors. Since no experimental data are available in the forecasting domain, proxy simulations are used. Moreover, in this context only forecasting precision can be quantified and forecasting accuracy can no longer be evaluated. By comparing the isocontours of equivalent fidelity in the parameter space between the two domains, a robustness indicator can be formulated quantifying the degree of calibration errors that can be tolerated while still insuring a critical level of forecasting precision. Clearly if only small errors can be tolerated then this suggests that extrapolation should be avoided. The proposed methodology is illustrated using an academic portal frame structure with a nonlinear interface.

**SMARTUQ: AN UNCERTAINTY QUANTIFICATION TOOL FOR COMPLEX PROBLEMS**
**Technical Presentation.** VVS2016-8960
5:15pm-5:40pm

**Mark Andrews, Brian Leyde,** *SmartUQ, LLC, Madison, WI, United States*

We present SmartUQ, a new Uncertainty Quantification software package with a novel approach to building accurate emulators based on statistical interpolators. SmartUQ allows emulator fitting for univariate, multivariate, and functional responses for large data sets and high dimensional problems with minimal computational effort. Combined with advanced sampling techniques, such as adaptive design, this new approach permits analysts to carry out large-scale UQ tasks on laptop-sized resources. This approach has now been integrated into user friendly tools for tasks such as such as design optimization, sensitivity analysis, calibration, inverse analysis, and propagation of input uncertainty. The emulators generated by this approach may also be used to carry out UQ analysis when dealing with missing data such as a broken sparse grid DOE.

Several examples demonstrating the application of this approach and the utility of UQ techniques to physics simulations are presented. Large-scale examples of various UQ tasks such as stochastic design optimization, sensitivity analysis, calibration, and propagation of input uncertainty are also presented along with a comparison of recent techniques, our framework, and more traditional UQ techniques such as Monte Carlo simulations.

**THE ABAQUS LIVING HEART: COMPARISON TO STATIC AND DYNAMIC IN VIVO MEASUREMENTS**
**Technical Presentation.** VVS2016-8001
5:40pm-6:05pm

**Paul Briant***, Exponent Inc., Menlo Park, CA* , **Steven Kreuzer***, Exponent Inc., Menlo Park, CA,* **Jorge Ochoa***, Exponent Inc., Menlo Park, CA*

Finite element analysis is widely used in the medical device industry to analyze the stresses and strains in devices throughout their product life time. One of the most difficult problems in analyzing an implantable medical device is estimating the in vivo loads to the device. Commonly, the motion and stiffness of the tissues at the implantation site are estimated from measurements in the published literature and used to load the device. However, the load balance between the device and the surrounding tissue can be especially difficult in regions with complex motions or regions of active muscle, such as in and around the heart. To better capture the loads applied to devices implanted in and on the heart, DS Simulia, Inc. is developing the Abaqus Virtual Living Heart (LH), a finite element model of the human heart.

The LH is devein in load control by electrical pulses within the heart wall tissue and can be used to load such devices as heart valve implants or coronary stents. However, the resulting motion of the LH valves and chamber diameters have not been directly compared to in vivo measurements of heart motion to validate the LH motion. The purpose of this study was therefore to compare the motion of the LH without a device implanted to dynamic heart motion measurements reported in the published literature.

The primary metrics used to compare the LH against literature were the mitral valve diameter, the aortic valve diameter, the tricuspid valve diameter, diameter of the left atrium along with its height, and the diameter and volume of the left ventricle during the cardiac cycle. Both mean (static) dimensions of each of these structures, as well as the dynamic motion of the structures were compared between the LH and experimental data.

The analysis results indicate that overall the mean (static) dimensions of the LH ranged from comparable to average experimental measurements to being larger than average experimental measurements (up to 17% larger than reported average dimensions). Correspondingly, the dynamic motions of the LH were also generally larger than those reported in the literature, ranging from 10% higher cyclic motion for the left ventricle volume to approximately 80% more cyclic motion for the mitral valve diameter. Taken together, the analysis results indicate that the LH represents a generally larger heart (but within expected size ranges for coronary devices) and that the LH would subject a device to conservative in vivo loading conditions.

## TRACK 13 Verification and Validation of Medical Devices

### 13-1
### VERIFICATION AND VALIDATION OF MEDICAL DEVICES
**2nd Floor, Palo Verde A** **4:00pm - 6:05pm**

**COMPUTER MODELING OF TRANSPORT PHENOMENA IN RF ABLATION**
**Technical Presentation.** VVS2016-8840
4:00pm-4:25pm

**Adriana Druma***, Aavid Thermalloy, San Jose, CA, United States,* **Calin Druma***, Medtronic, Inc., Milpitas, CA, United States*

One of the most common causes for severe pain in patients with cancer comes from cancer metastases. Once the cancer metastasized, the patients often experience chronic pain or other related effects (SRE). Even though radiotherapy and chemotherapy is the standard of care for cancer patients, approximately 25% of those patients do not get pain relief. There are currently several treatment options for painful metastatic disease with RF ablation being the most mature treatment option. The principles of the RF ablation rely on the ionic heating effect. As an electromagnetic wave at high frequency travels through a biological tissue the tissue gets heated at temperatures above 45°C causing cell death. One of the disadvantages of RF ablation is its reliance on conduction to spread the heat from the ablation probe to the surrounding tissue. Typical RF ablation probes consist of an either monopolar or bipolar applicator that has no internal cooling. One of the disadvantages of the uncooled RF applicators is the presence of charring at the surface of the applicator (where current densities are higher). Charred tissue deters the growth of the ablation zone due to its poor thermal conductivity.

A multiphysics simulation was used to model a water-cooled RF applicator used in the OsteoCool Ablation System. A coupled electromagnetic 'CFD' heat transfer analysis was conducted on several applicator designs in order to understand the physics behind lesion formation and provide a platform for the new device design. The main purpose of the study was to compare the computer model to the experimental data gathered by the product development team. Once a good agreement between the experimental data and the computer model was reached, the product development team has another tool to aid in quickly iterate new designs for future development as the clinical needs will undoubtedly be expanded after using OsteoCool to treat patients.

Part of the FDA submission, the product development team worked closely with the agency to ensure that the ablation lesion (defined as the spatial region surrounding the applicator that experiences temperatures above 45°C for extended time periods) guidance relayed to the physicians are based on comprehensive benchtop testing. In vitro testing involved both cadaveric tissue that was brought to 37°C temperature to simulate physiological conditions and homogeneous animal tissue. The procedure used to determine the lesion size is outlined in the OsteoCool IFU (http://www.medtronic.com/manuals) section "Ablation Size and Shape". Briefly, the procedure involved performing a series of in-vitro ablations while measuring the temperature of the adjacent tissue temperature using an independent temperature monitor until steady state conditions occurred. The 45°C isotherm was used to report the length and width of the ablation zone. The computer simulation model used an isotropic material model (electrical properties by C. Gabriel ?Compilation of the Dielectric Properties of Body Tissues at RF and Microwave Frequencies, Report N.AL/OE-TR- 1996-0037, Occupational and environmental health directorate, Radiofrequency Radiation Division, Brooks Air Force Base, Texas (USA), 1996.?) and constant thermal conductivity. The model predicted the ablation zone with high accuracy (error of approximately 10%) which was considered acceptable by the development team.

The RF Ablation System utilizes temperature-based control, which automatically controls the RF power delivery to maintain a certain target temperature. The maximum allowable power limit (on the actual device) is set through the control software at 20W. The simulation was performed on various RF powers and the size and shape of the lesion were analyzed.

### VALIDATION OF RANS USING THE SST K-W MODEL FOR THE TWINCAPS® DRY POWDER INHALER

**Technical Presentation.** VVS2016-8854
4:25pm-4:50pm

**Luis Eca, Nuno Enes**, *IST, Lisbon, Portugal,* **Joao Ventura, Conrad Winters**, *Hovione, Loures, Portugal*

Dry Powder Inhalers (DPIs) have been widely used in the treatment of pulmonary diseases and are expanding to emerging applications, such as to administer antibiotics or treat infectious diseases through inhaled drug delivery. The TwinCaps® (Hovione, Portugal) is a single use, disposable DPI currently marketed to deliver Inavir® (Daiichi Sankyo, Tokyo), an anti-influenza medication, which allows the treatment of the infectious agent while eliminating the potential for contamination by discarding the device after use. In operation, the patient pushes a shuttle comprising powder compartments into an actuation position, where air inlets become unblocked thus allowing the admission of air for dispersing the powder when the patient engages with the mouthpiece and performs the inhalation.

Our goal is to present a Validation exercise for the simulation of the flow through the TwinCaps® inhaler using the Reynolds-Averaged Navier-Stokes (RANS) equations supplemented by the SST k-w eddy-viscosity two-equation turbulence model. The numerical simulations are performed with the open source code RANS solver OpenFOAM. The quantity of interest is the mass flow rate for a given pressure drop between the inlet and outlet of the inhaler. Modeling errors are estimated with the procedure proposed by the ASME V&V 20 Committee. Experimental uncertainties are obtained from the standard deviation of the collected experimental data and numerical uncertainties are estimated from grid refinement studies. Parametric uncertainty is assumed to be zero. The results show that the mathematical model over predicts the mass flow rate and that reducing numerical uncertainties to negligible levels for this type of simulations may require grids a lot finer than those used in this study (finest grid includes 10.9E6 cells).

### TOWARDS ESTIMATING THE UNCERTAINTY ASSOCIATED WITH 3D GEOMETRY RECONSTRUCTIONS FROM MEDICAL IMAGE DATA

**Technical Presentation.** VVS2016-8855
4:50pm-5:15pm

**Marc Horner**, *ANSYS, Inc., Evanston, IL, United States,* **Kerim Genc**, *Simpleware Inc., Herndon, VA, United States,* **Stephen Luke**, *Simpleware Ltd., Exeter, United Kingdom,* **Todd Pietila**, *Materialise, Plymouth, MI, United States,* **Ross Cotton**, *Simpleware Ltd., Exeter, United Kingdom,* **Benjamin Ache**, *Micro Photonics, Inc., Allentown, PA, United States,* **Zachary Levine**, *National Institute of Standards and Technology, Gaithersburg, MD, United States,* **Kevin Townsend**, *Materialise, Plymouth, MI, United States,* **Philippe Young**, *Simpleware Ltd., Exeter, United Kingdom*

3D-image based geometries are increasingly used for patient-specific visualization, measurement, physics-based simulation and additive manufacturing. Computed Tomography (CT) is a common imaging modality used to obtain the 3D geometry of objects through X-ray images taken from different angles to produce cross-sectional images along an axis. Levine et al. (1,2) developed a reference phantom, or ?NIST phantom?, to help control for variations in scanner settings, noise and artifacts. Ideally, the geometry of the phantom would be extracted through the ISO 50 standard threshold-based segmentation, which states that the material boundary is set as the middle greyscale value between the background and material peaks in the greyscale value histogram (3). The purpose of this study is to examine the effects of image resolution on the uncertainty associated with 3D geometries reconstructed from idealized and real CT images.

An idealized spherical reference phantom of known diameter was generated in CAD format used by AutoCAD. A CAD voxelization process was used to convert the CAD sphere into 3D greyscale images at various resolutions. These images were then used to study the effect of image resolution on measurement accuracy of the sphere diameter, measured via a sphere-fitting method. Next, an image stack of the NIST phantom, generated using a SkyScan 1173 CT scanner (Bruker MicroCT N.V. Kontich, Belgium), was resampled to various resolutions to allow for a similar accuracy study. Image stacks generated from the voxelized CAD sphere were devoid of artifacts, and as such, an ISO50 thresholding approach could be used with confidence. A similar ISO50 technique was also applied to the segmentation of the NIST phantom data.

During the CAD sphere voxelization process, the uncertainty of measurement was 2% if 5 or more voxels were present across the sphere diameter. The measurement uncertainty degraded to approximately 4% for a similar degree of voxelization when resampling the CT scan data of the NIST phantom. The main source of this uncertainty appears to be related to the choice of segmentation threshold. Investigation of threshold choice suggests the ISO50 segmentation approach is not suitable for these CT images, which is in agreement with results in published literature (3).
Through an idealized image set (i.e. a perfect CT scan), we have shown that a measurement accuracy of 2% or less can be maintained down to a very coarse image resolution. Artifacts present in CT image data, whether from the physical object or the scanning process, can lead to worse accuracy. These artifacts may affect segmentation threshold choice during geometry reconstruction. In summary, this work is an important first step towards estimating the systematic uncertainty associated with 3-D geometry reconstructions that are utilized as part of image-based modeling applications.

Mention of commercial products does not imply endorsement by NIST.

References:
1. Levine ZH, J Res Natl Inst Stand Technol, 2008, Vol 113, 335-340.
2. Standard Reference Material 2087, www.nist.gov/srm.
3. Tan, Y. et al. 2011, Intl. symp. on digital industrial radiology and computed tomography, Berlin, Germany.

### CREDIBILITY OF COMPUTATIONAL METHODS IN HEALTHCARE: A COMPARISON OF COMMUNITY-BASED STANDARDS AND GUIDELINES

**Technical Presentation.** VVS2016-8874
5:15pm-5:40pm

**Marc Horner**, *ANSYS, Inc., Evanston, IL, United States,* **Lealem Mulugeta**, *Independent, Houston, TX, United States,* **Ahmet Erdemir**, *Cleveland Clinic, Cleveland Heights, OH, United States,* **Gary An**, *University of Chicago Medicine, Chicago, IL, United States,* **David Eckmann**, *University of Pennsylvania Medicine, Philadelphia, PA, United States,* **Jeff Bischoff**, *Zimmer, Warsaw, IN, United States,* **Anthony Hunt**, *UCSF School of Pharmacy, San Francisco, CA, United States,* **Joy Ku**, *Stanford Dept. of Bioengineering, Stanford, CA, United States,* **Donna Lochner**, *Food and Drug Administration, Silver Spring, MD, United States,* **William Lytton**, *SUNY Downstate Medical Center, Brooklyn, NY, United States,* **Vasilis Marmarelis**, *USC, Los Angeles, CA, United States,* **Jerry Myers**, *NASA Glenn Research Center, Cleveland, OH,* *United States,* **Grace Peng***, NIH/NIBIB, Bethesda, MD, United States,* **Martin Steele***, NASA, Kennedy Space Center, FL, United States,* **Marlei Walton***, Wyle, Houston, TX, United States*

The role of computational modeling and simulation (M&S) in the development and delivery of healthcare continues to grow at a rapid pace. Consequently, there is a demand within the healthcare community to establish standards and guidelines to ensure M&S will be developed and applied reliably in healthcare practice and research. However, the multidisciplinary nature of healthcare practice and biomedical research, combined with the multi-contextual use and highly diverse maturity levels of biomedical M&S, present significant challenges for establishing unified M&S credible practice standards and guidelines. This presentation will compare and discuss the synergistic efforts of two cross-disciplinary initiatives to identify overlaps and differences in the context of M&S credibility. The specific initiatives are the Committee on Credible Practice of Modeling & Simulation in Healthcare (CPMS hereafter) and the American Society of Mechanical Engineers (ASME) V&V40 Sub-Committee (V&V40 hereafter). All authors are members of CPMS and/or V&V40 from the early stages of both initiatives.

A comparative analysis identified similarities and differences in their mission statements, stakeholders, end-products, operational approach and credibility workflows. For example, the CPMS group aims to "establish credible practice guidelines, consistent terminology and proposed model certification process, as well as to demonstrate workflows and identify new areas of research for reliable development and application of M&S in healthcare practice and research", whereas V&V40 aims to "provide procedures to standardize verification and validation for computational modeling of medical devices". Thus, V&V40 has a greater focus on medical device development and regulatory review versus CPMS which has a broader focus. The results of this and the other comparisons makes it clear that the CPMS and V&V40 groups have similar goals with respect to their pursuit to establish procedures for credible application of M&S in medicine. However, they differ significantly with respect to their approach, end-products and target audience. The CPMS aims to establish guidelines, consistent terminology, and a model certification process that are broadly applicable to M&S in healthcare practice and research. Moreover, their work is largely driven by the research community. V&V40, on the other hand, is dedicated to developing procedures to standardize verification and validation for M&S of medical devices for medical device development and in regulatory applications. This is a direct result of the fact that the V&V40 initiative is largely driven by the medical device industry, and regulatory and standard bodies such as FDA and ASME.

Acknowledgements: The authors acknowledge all members of CPMS and V&V40. Further details about CPMS, V&V40, and the contributing authors can be found at http://wiki.simtk.org/cpms/CPMS_Members and https://cstools.asme.org/csconnect/CommitteePages.cfm?Committee=100108782.

### CODE-VERIFICATION BENCHMARKS TO EVALUATE THE IMPLEMENTATION OF POWER-LAW HEMOLYSIS MODELS IN COMPUTATIONAL FLUID DYNAMICS

**Technical Presentation.** VVS2016-8927
5:40pm-6:05pm

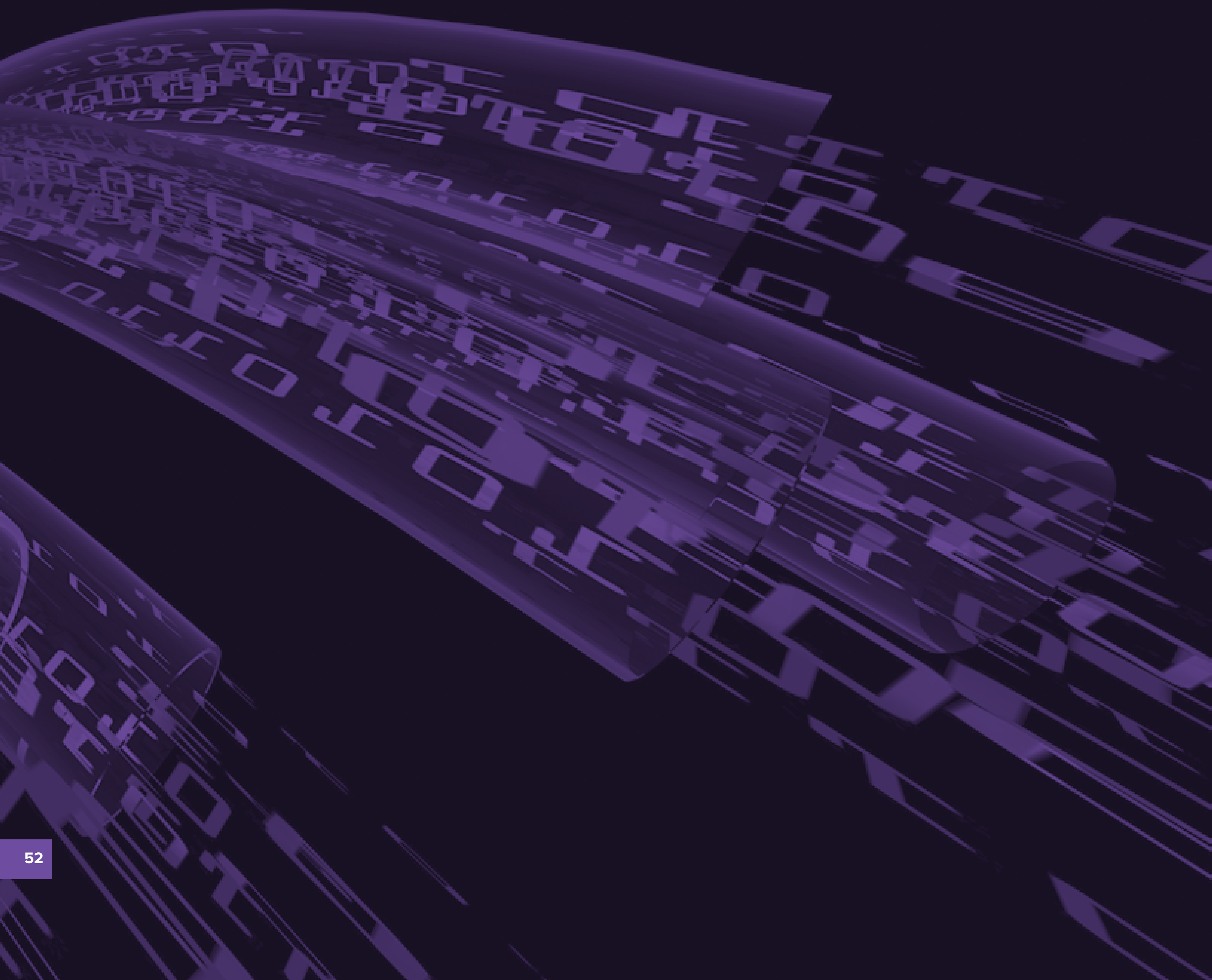
**Prasanna Hariharan***, FDA, Silver Spring, MD, United States,* **Matthew Myers***, FDA, Potomac, MD, United States,* **Gavin D'Souza***, University of Cincinnati, Silver Spring, MD, United States,* **Richard Malinauskas***, FDA, Silver Spring, MD, United States,* **Marc Horner***, ANSYS, Inc., Evanston, IL, United States*

Computer modeling is increasingly used at all stages of development to evaluate the safety and effectiveness of medical devices. While general-purpose simulation codes provide a broad spectrum of physical modeling capabilities, the unique nature of biological tissues, bio-fluids, etc. often necessitate the incorporation of custom code (i.e. user-defined functions) into the computational model. Numerous benchmark models exist for performing code verification on standard fluid-flow problems, but they have not been pursued for transport problems specific to the biomedical device industry. One common example is the utilization of computational fluid dynamics (CFD) for evaluating the risk of hemolysis— the release of hemoglobin caused by damage to the red blood cell membrane—in blood-contacting devices. The most common way to evaluate hemolysis is using an empirical power-law model which estimates the hemolysis index (HI) as a function of shear stress and exposure time. There are examples in the peer-reviewed literature of incorrect implementation of a power-law model into a CFD code, which results in inaccurate hemolysis prediction. These errors may have been avoided if the users had followed code verification best practices.

To address this issue, we have developed idealized flow-based verification benchmarks to assess the implementation of commonly cited power-law based hemolysis models in CFD. The code verification process ensures that all governing equations are solved correctly and the model is free of user and numerical errors. Using an Eulerian blood damage formulation, an analytical solution for HI was obtained for i) parallel and inclined Couette flow, and ii) Newtonian and non-Newtonian pipe flow problems. CFD simulations of fluid flow and HI were performed and compared with the analytical solutions. For all the flow problems, the CFD results matched the analytical solutions within 5%. In addition, the analytical solution for the Eulerian model was compared with different Lagrangian hemolysis models to understand the inherent differences between their numerical formulations.

These benchmark examples have the potential to be used as standard test problems for verifying the blood damage models implemented in commercial and open-source CFD codes.

# Technical Program
# **Friday, May 20, 2016**



## TRACK 9 Validation Methods for Solid Mechanics and Structures

### 9-2
### VALIDATION METHODS FOR SOLID MECHANICS AND STRUCTURES: SESSION 2

**1st Floor, Mesquite 2** **9:30am-11:35am**

#### KERNEL DENSITY ESTIMATION BASED MODEL VALIDATION METHOD FOR STRUCTURAL DYNAMIC SYSTEMS

**Technical Presentation.** VVS2016-8898
9:30am-9:55am

**Jun Lu, Zhenfei Zhan**, *Chongqing University, Chongqing, China,* **Chen Xueqian**, *Institute Of Structual Mechanics/Caep, Sichwan, China,* **Xin'en Liu**, *Institute of System Engineering/Caep, Mianyang, China,* **Zhanpeng Shen**, *Institute of Structual Mechanics/Caep, Mianyang, China,* **Junqi Yang**, *Chongqing University, Chongqing, China*

Computer-based simulation is playing an increasing role in structural design and product development. Computer models are mathematic representations of real systems developed for understanding and investigating the systems. Before a computer model is ready for engineering design, it needs to be validated by comparing the computer outputs with physical observations, and if it does not meet the requirement, it needs to be further calibrated by adjusting internal model parameters in order to improve the agreement between the computer outputs and physical observations. The purpose of the model validation is to compare simulator predictions with observed experimental outcomes to assess the accuracy of a particular computer model.

As computer models become more powerful and popular, the complexity of input and output data raises new computational challenges. One of key obstacles in dynamic model validation is to deal with computer models with multivariate functional outputs. The simulation model obtained contains multiple output responses. It is difficult to assess the validity and judge whether the simulation model can be accepted or not, for the error of simulation results and test data is distinct for different responses. Multiple variety comparisons may give conflicting inferences. The dynamic responses are also highly correlated, which requires the multiple correlation analysis. Additionally, many computer experiment responses in dynamics are collected in a functional form, stepping up the difficulties. The feature of functional data and multivariate correlation quantities makes it infeasible to apply the traditional Bayesian approach. The available field data in dynamics are usually very limited, the Gaussian assumption sometime may not be appropriate.

To address the aforementioned issues, this paper proposes a systematic method to validate the structural dynamic systems. The dimension reduction utilizing kernel principal component analysis (KPCA) is used to improve the computational efficiency, and non-parametric kernel density estimation (KDE) method is utilized to establish the probability model. The differences between the test data and simulation results are extracted to further comparative validation. Based the established probability model, a classifier based on Bayesian decision theory with minimum error rate is then proposed to ultimate judgment for simulation accuracy. This new approach compared to the previous methods improves the processing ability to nonlinear problem to validation the dynamic model. The proposed method and process are successfully illustrated through an analytical example. The results demonstrate that the method of incorporate with KPCA, KDE and Bayesian decision is an effective approach to solve the dynamic model validation problem.

#### EXPERIMENTAL AND SIMULATION DYNAMICS OF A CAM AND FOLLOWER MECHANISM

**Technical Presentation.** VVS2016-8907
9:55am-10:20am

**LOUAY AL-ROOMI**, *Auburn University, Auburn, AL, United States*

A cam is a mechanical device used to transmit motion to a follower by direct contact. Many researchers have been studied the contact-impact problem, collision between cam and follower, and chaotic detection. In this study a cam and follower mechanism is analyzed. The proposed cam can be used for controlling valve and also on motor car camshafts to operate the engine valves. The dynamic analysis presents follower displacement driven by a cam rotating at a uniform angular velocity. There is a clearance between the follower and the guide. The follower with clearance has three degrees of freedom. The mechanism is analyzed using SolidWorks simulations taking into account the impact and the friction between the roller follower and the guide. A SolidWorks simulation is developed for the planar case using the block commands. The cam, follower, and guides are drawn in a SolidWorks program using the experimental dimensions of an existing mechanisms. Four different follower guide's clearances have been used in the simulations like 0.5, 1, 1.5, and 2 mm and compared for Largest Lyapunov Exponents during the follower motion in the vertical direction. Lyapunov exponents quantify the average exponential rate of divergence of neighboring trajectories in state space, and thus provide a direct measure of the sensitivity of the system. In simulation analysis, the spring force is added in the analysis and the linear displacements are varying with each position of the follower motion in the vertical direction. The cam, the follower, and the two guides are made from Polylactic Acid (PLA) plastic material that is manufactured by a 3D printing filament technique device to obtain the parts. Our rig is based on a radial cam with an oscillating roller follower. An experimental set up is developed to capture the general planar motion of the cam and follower. The measures of the cam and the follower positions are obtained through high-resolution optical encoders (markers) mounted on the cam and follower shaft with 500 frames per second. The signals are proposed and analyzed using MATLAB program. The effect of guide clearance is investigated for different angular velocities of the cam such as 100, 200, 300, 400, 500, 600, 700 and 800 R.P.M. Impact with friction is considered in our study to calculate the Lyapunov exponent. A computer algorithms is used to calculate the time delay and the embedding dimension for the nonlinear analysis. The global dimension indicates an appropriate embedding dimension for all-time series. The largest Lyapunov exponents for the simulated and experimental data are analyzed and selected.

#### UPDATING OF STRUCTURAL DYNAMICS MODEL WITH MODEL BIAS

**Technical Presentation.** VVS2016-8899
10:20am-10:45am

**Chen Xueqian**, *Institute Of Structual Mechanics/Caep, Sichwan, China,* **Shen Zhanpeng**, *Institute of systems engineering/CAEP, mianyang, China,* **He Qinshu**, *Institute of Systems Engineering, Mianyang, China,* **Liu Xinen**, *Institute of systems engineering/CAEP, mianyang, China*

Finite element (FE) methods have become a popular technique for structural analyses and design for more than three decades. The accurate modelling and simulating of a real-word structure is very important for structure design. However, this may still be considered a quite challenging task in many cases. For example, bolt or weld joints are commonly used in industries to connect two components/parts together. However, one may often find it difficult to directly model them in a FE analysis. Consequently, people make some kind of assumptions or simplifications in the FE model, which is one of the frequently mentioned causes for an unsatisfactory FE prediction.

In order to get accurate and reliable FE model for the structure design, the structural dynamic model updating technique has been rapidly developed based on the vibration and modal experiments data. But there are some biases in the updated model generally, which affect the reliability of predictions. It is necessary to study the FE modelling and updating is consideration of the model bias. Firstly, the optimization values of updating parameters is identified based on the response model. Secondly, the effect of model bias on updating parameters is identified by combining the response model and the sensitivity analysis. That is, the updating parameters is updated again, and then the updating parameter interval is obtained with model bias. Lastly, the proposed method has been validated by model updating on a cantilever beam, which proved the feasibility of the method. The results also show that it can improve the reliability of the structural response predictions when the model biases are considered.

### VALIDATION AND UNCERTAINTY QUANTIFICATION FOR V&V 10 EXAMPLE

**Technical Presentation.** VVS2016-8944
10:45am-11:10am

**Sanjeev Kulkarni**, *VEXTEC Corporation, Brentwood, TN, United States,* **Tsolag Apelian**, *Enertech, Nuclear Division - Curtiss-Wright, Brea, CA, United States,* **Robert Tryon**, *VEXTEC, Brentwood, TN, United States,* **Animesh Dey**, *VEXTEC Corporation, Brentwood, TN, United States*

The ASME V&V 10.1-2012 describes a simple example of verification and validation (V&V) to illustrate some of the key concepts and procedures presented in V&V 10. The example is an elastic, tapered, cantilever, box beam under non-uniform static loading. The validation problem entails a uniform loading over half the length of the beam. The response of interest is the tip deflection.

As the first half of the paper, the authors replicated the example step-by-step and followed the verification and validation framework and protocol as detailed in the example. There were some modifications - such as the beam used in this example was uniform. Specifically, a computational model of the beam was developed in ANSYS, model verification studies were completed (mesh refinement and multiple element types) and validation was completed using actual experiments. The reference document considered uncertainties to quantify the distribution of results due to unintended variations in material properties, construction of the test specimens, and test execution. Beyond that, virtual tests were conducted to characterize uncertainties in selected model input parameters, namely rotational support stiffness and elastic modulus. The present study considered uncertainties as well but used only one of two methods suggested by the reference document - namely - the uncertainty data was extracted from repeat tests and calculations. The same metric was employed to demonstrate the use of uncertainty information in the model test comparison, the metric being the measure of the relative error between the calculated and measured tip deflection of the beam. As it turned out, the validation effort was inconclusive as the suspected anisotropy of the material is speculated to play a role in the results variation when the beam is set up one way and then flipped over.

As the second half of the effort, a probabilistic structural analysis method, Virtual Life Management® (VLM®), was used to understand the reasons for the variation, for correlating the impact of the uncertainty on the output result and providing broader insights. The tool combines testing with computational simulation to address device reliability and product certification. It is a modeling and simulation capability that predicts product durability at the material level, while accounting for the inherent variability of material processing, product manufacturing and changes in in-service usage conditions. VLM has been successfully applied to metals, laminated composites, and ceramics used in structural, mechanical and electrical products. Verification and validation (V&V) of the technology has been validated on over 100 different product applications and is applied to explain the variability in the above results. The power of the method is to leverage a limited amount of test data and expand it to simulate a larger sample and population virtually. The impact of uncertainty of the tip deflection will be discussed by addressing the multi-scale level discontinuous definition of the material. Resulting outcomes are presented in terms of Probabilistic Density Functions (PDFs), Cumulative Distribution Functions (CDFs) and Weibull Charts.

### STRESS CONCENTRATION DECOMPOSITION OF FINITE ELEMENT RESULTS BY WAVELET MULTISCALE ANALYSIS

**Technical Presentation.** VVS2016-8937
11:10am-11:35am

**Walter Ponge-Ferreira**, *Escola Politécnica da Universidade de São Paulo, São Paulo, Brazil,* **Flavius Martins**, *Universidade de Sao Paulo, Sao Paulo, Brazil,* **Flavio C. Trigo**, *Escola Politécnica da Universidade de São Paulo, São Paulo, São Paulo, Brazil*

Wavelet multiscale analysis is used to decompose the stress field of structures with stress concentrations. First the analytical solution of plane stress structures is decomposed by wavelet multiscale analysis to separate the near field stress concentration from the far field. The wavelet decomposition separates the stress into different scales and locates the stress concentration position on the structure. According to the Saint Venant's principle, concentrated loads or abrupt geometric changes have negligible effects at sufficient large distances from the disturbance, suggesting that near and far stress fields are naturally described by different spatial scales. Therefore, they can be separated with the wavelet multiscale analysis. Hence, the rather practical or common-sense proposition of Saint-Venant's principle becomes an exact mathematical meaning. This approach was applied to the Kirsch's analytical solution of stress concentration at a circular hole. With wavelet decomposition, the stress around the hole could also be split into two components, as has been done by Kirsch's analytical solution. Further, the same procedure was applied to post-processing finite elements results of the circular hole problem, with different mesh refinements to represent the hole boundary. The finite elements results were then compared to the analytical model. Modeling error is fit to the wavelet multiscale representation of the stress field by least square method. Hence, the modeling error could be associated with different scales and locations, giving a spatial view of the error influenced zone. This technique can be used for model validation, improves the understanding and confidence of the analysis.

Summary of presentation: motivation, wavelet multiscale analysis, wavelet decomposition of Kirsch's solution of stress concentration at a circular hole, comparison to finite elements solution, modeling error fitting, conclusion.

## TRACK 10 Verification and Validation of Nuclear Power Applications

**10-1**
**VERIFICATION AND VALIDATION OF NUCLEAR POWER APPLICATIONS**
**2nd Floor, Palo Verde A** **9:30am-11:35am**

### THE BENCHMARK AND APPLICATIONS OF SINGLE-PHASE CFD MODELS USED IN AP1000® PLANT

**Technical Presentation.** VVS2016-8893
9:30am-9:55am

**Hong Xu, Richard Wright, William Moody**, *Westinghouse, Cranberry, PA, United States*

Computational Fluid Dynamics (CFD) analysis is a useful tool in determining the behavior of passive safety systems of the AP1000® design. During the design and analysis of these systems, CFD was used to address:
• Cold traps which are used to minimizer heat losses between the reactor coolant system and cold components connected with open piping
• Air flow resistance along the passive containment cooling system (PCS) flow path
• Complex flow fields within the reactor vessel upper head for design and implementation of a comprehensive vibration assessment plan (CVAP)
To provide confidence in the CFD results, it is best to validate the models against applicable test data. By continually adding to the validation basis, greater confidence can be gained using CFD for other applications. This paper documents the validation work for the water in stagnant piping which utilize cold traps to minimize the heat losses from the hot reactor coolant system, and water in the reactor vessel upper head during forced flow conditions. In addition, CFD is validated against air flow tests to determine the pressure drop in the AP1000 PCS.
Several tests were used to provide the validation basis including:
1. A scale-model test of the cold trap geometry was conducted at the Applied Research Laboratory (ARL) in State College, PA.

2. The Robust Containment Air Flow Test (RAFT) with 1:6 length scale, 1/32nd sector model of the PCS air flow path from the inlets to the chimney was conducted at Oregon State University.
3. The quantifying flow detail test in a prototypical AP1000® reactor vessel upper head region with a ¼-scale and 90° quadrant model was performed at ARL in State College, PA.
Utilizing the modeling needed to provide proper benchmarking against these tests allows for the confident use of CFD for plant design and safety analysis.

## VERIFICATION OF A FE MODELLING PROCEDURE FOR SECONDARY STRESS INDICES ON ELBOWS WITH STANCHION ATTACHMENTS

**Technical Presentation.** VVS2016-8824
9:55am-10:20am

**Joon Ho Lee, Hong Joo Park**, *KEPCO E&C, Gimcheon, Korea (Republic)*

Welded attachments on a piping system inevitably produce stress concentration on local areas, lead to decrease in the structural stability, and may cause fatigue failures due to locally occurred peak stress. ASME B&PV code, Sec. III provides methods for evaluating local stresses on straight pipes with hollow circular welded attachments via the issuance of Code Cases N391 and N392 for class 1 and class 2/3 piping respectively, but does not provide evaluation method for stress indices on elbows with circular attachments such as stanchions or trunnions. Hankinson et al.[1,2,3,4], whereas, have presented remarkable research results on elbows with stanchion or trunnion attachments based upon FEAs(Finite Element Analyses) or tests.

KNPP(Korean Nuclear Power Plant) has been reviewing the method for direct application of stress indices on elbows based upon the studies performed in References [1,2,3,4] instead of utilizing the existing Code Case N392. For this purpose, 27 FE models were produced and analyses were performed to demonstrate the validity of a FE modelling procedure used to determine the local stress indices on elbows with stanchions. Analyses were performed for each unit loading in static condition for FE models composed of homogeneous and isotropic shell elements which present linear-elastic behaviors.

Comparison between the results using secondary stress indices (CL: in-plane bending, CN: out-of-plane bending, CW: axial force) calculated from FEAs per KNPP procedure and the results from Reference [1] indicates that both results show good matches, i.e., the average ratios between the results from the two analyses for 27 models are 1.07 for CL, 1.19 for CN, and 0.88 for CW. In case of comparisons between the results of FEAs and N392, N392 is confirmed to be too conservative since the average ratios of stress indices calculated per N392 to FEAs are 1.2 for CL, 4.26 for CN, and 5.3 for CW. Comparison between the results from FEAs per KNPP procedure and those from Reference [4], on the other hand, shows FEAs are more conservative than Reference [4] from the average ratios of 1.61 for CL, 1.33 for CN, and 1.78 for CW. In addition to the above results, based on the facts that results of Reference [4] show the lowest stress indices among References [1,2,3,4] and are incorporated into the Reference [5], it can be concluded that the FE modelling procedure used for developing stress indices on elbows with stanchions in KNPP is verified to have a good validity.

References:
[1] Hankinson, R.F. et al., "Stress Indices for Piping Elbows with Trunnion Attachments for Moment and Axial Loads, " PVP, ASME, 1987.
[2] Rodabaugh, E.C., "Review of Data Relevant to the Design of Tubular Joints for Use in Fixed Offshore Platforms, " Welding Research Council Bulletin 256, January 1980.
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[4] Wais, E.A., et al., "Stress Indices for Elbows with Trunnion Attachments, " PVP-Vol.399, ASME, 2000.
[5] "Stress Indices for Elbows with Trunnion Attachments, " EPRI, TR-107453, December 1998

## APPLICATION OF STATISTICAL DESIGN OF EXPERIMENTS TO BEST ESTIMATE AND UNCERTAINTY ASSESSMENT OF RESISTANCE TO HYDRIDE-ASSISTED CRACKING IN CANDU PRESSURE TUBES

**Technical Presentation.** VVS2016-8826
10:20am-10:45am

**Leonid Gutkin**, *Kinectrics Inc., Toronto, ON, Canada*

In CANDU nuclear reactors, each one of several hundred fuel channels in the reactor core includes a Zr-2.5Nb pressure tube, containing nuclear fuel and heavy water coolant. In the course of reactor operation, the pressure tubes may become susceptible to hydride-assisted cracking at the locations of stress concentration, such as in-service flaws, where hydrided regions may develop and potentially fracture under internal pressure, thereby leading to crack initiation. Repeated formation, growth and fracture of hydrided regions may result in crack propagation by the mechanism of delayed hydride cracking and, eventually, in pressure tube rupture. Therefore, hydride-assisted cracking requires major attention in fitness-for-service assessments of CANDU reactor core. This presentation illustrates how the methodology of statistical design of experiments has been applied to best estimate and uncertainty assessments of the resistance of Zr-2.5Nb pressure tube material to hydride-assisted cracking. The discussion focuses on the material resistance to crack initiation due to hydrided region overloads, which occur during the reactor pressure transients.

At a flaw with an existing hydrided region, an overload event would occur within a given pressure transient when the flaw-tip stress applied at any time during this transient exceeds the stress at which the hydrided region is formed. The overload event would then result in crack initiation if the flaw-tip stress applied during the event exceeds the critical flaw-tip stress for overload crack initiation. Previous experiments had demonstrated that the resistance of pressure tube material to overload crack initiation is affected by the resistance of Zr-2.5Nb to the initiation of delayed hydride cracking, the magnitude of the applied stress during hydride formation, the flaw severity and potentially other factors related to the hydrided region morphology. In this work, the statistical design of experiments was used to establish a test matrix that would be executed to obtain a set of overload crack initiation data suitable for developing a multi-variable probabilistic model for the overload resistance. The scope of work was limited to six explanatory variables, and the preferred experimental design was selected to attain the best statistical resolution possible and to maximize the statistical power of effect detection, while taking into consideration the experimental constraints. The data set produced by implementing the selected experimental design was then successfully used to develop a multi-variable probabilistic model for the resistance of Zr-2.5Nb to overload crack initiation, which has been included in the recent revision (2015) of the Canadian Nuclear Standard CSA N285.8.

## APPLICATION OF AREA VALIDATION METHODS FOR UNCERTAINTY QUANTIFICATION IN VALIDATION PROCESS OF THERMAL-HYDRAULIC CODE FOR THERMAL FATIGUE ISSUE IN SODIUM-COOLED FAST REACTORS

**Technical Presentation.** VVS2016-8920
10:45am-11:10am

**Masaaki Tanaka**, *Japan Atomic Energy Agency, O-Arai, Ibaraki, Japan*

Thermal fatigue on a structure caused by thermal striping phenomena is one of the most important issues relating to structural integrity in design of sodium-cooled fast reactors (SFRs). A numerical simulation code MUGTHES has been developed to estimate thermal mixing phenomena and a thermal response in the structure. To simulate fluid-structure thermal interaction problem, MUGTHES has the thermal-hydraulics analysis module for the fluid part and the structure heat conduction analysis module to simulate unsteady heat conduction with conjugate heat transfer model in the structure part. Since verification and validation (V&V) process is indispensable in the code development and in use of the code, a practical procedure called V2UP in which the V&V process is combined with the numerical prediction process has been developed by referring to the existing guidelines. In the validation process of V2UP, uncertainty quantification is required by measuring the degree of agreement (difference) between the numerical and the experimental results. Therefore, application of the area validation metric (AVM) method and the modified AVM (MAVM) method has been considered in V2UP. They were examined with results of the numerical simulation of the water experiment of a T-junction piping system in advance. In this presentation, further application of the AVM and MAVM methods to results of numerical simulations of the PLAJEST experiment which is a sodium experiment to investigate thermal mixing phenomena of triple parallel jets will be presented. Test section of the PLAJEST had three rectangular discharge nozzles simulating a control rod channel at the center and neighboring two fuel assemblies on both sides. A cold jet and two hot jets flowed out vertically from the center and the neighboring nozzles, respectively. And also the stainless steel (SS316) plate was installed in the test section to investigate the heat transfer characteristics between fluid and structure regions. Numerical simulations of the PLAJEST using MUGTHES were performed. MUGTHES calculated simultaneously the thermal mixing phenomena in the fluid part and the unsteady heat conduction in the structure part under fluid-structure thermal interaction condition. In the numerical simulations by MUGTHES, the large eddy simulation approach with standard Smagorinsky model was employed. Through the examinations of the AVM and MAVM methods, values of the degree of agreement between the numerical and the experimental results were successfully estimated as uncertainty value and it was indicated the MAVM method could be a reference one in the validation process of V2UP.

#### THERMAL HYDRAULIC ANALYSIS METHODS: VERIFICATION, VALIDATION AND QUALITY ASSURANCE FOR NUCLEAR REACTOR PLANT DESIGN & JUSTIFICATION

**Technical Presentation.** VVS2016-8930
11:10am-11:35am

**Sam Treasure, Jonathan Adams**, *Rolls-Royce Power Engineering PLC, Derby, United Kingdom*

An element of the work undertaken within the nuclear division at Rolls-Royce Power Engineering PLC is the analysis to determine the performance of nuclear reactor plants through the application of thermal hydraulic analysis methods. These methods are used throughout the product introduction & lifecycle management process; beginning with exploring the performance potential of design options and ultimately providing the analysis to support the safety justification of the nuclear reactor plant.

It is imperative that a rigorous approach is taken in the verification, validation and quality assurance of the thermal hydraulic methods used for performance analysis since these methods are used to define limits used in the reactor protection system, define requirements for protective safety measures, determine the Loss of Coolant Accident (LOCA) protection limits and inform plant operating instructions.

Previously, thermal hydraulic methods were developed to address aspects of the design and justification depending on the important phenomena under consideration. This led to multiple methods, often with much overlap, each requiring on-going maintenance and development. This resulted in a substantial, costly (and repetitive) burden of undertaking verification, validation and quality assurance processes on multiple, similar analysis methods.

A new approach has been developed such that a full suite of performance analysis (pumped, non-pumped, critical, shutdown and LOCA) can be undertaken using a single thermal hydraulic analysis method, governed by a common set of verification, validation and quality assurance rules whilst still allowing the dominant phenomena to be appropriately addressed in different cases.

This innovative approach considers the analysis method more like a system of systems and places focus on the verification, validation and quality assurance on these constituent systems, the process of integration and of the analysis method as an integrated whole. Bespoke developments are therefore minimized and only occur on the system level where the maintenance overhead is correspondingly reduced. The result is a single analysis method that is suitable for a wider range of analyses with benefits of increased flexibility of the workforce, reduced overall maintenance overhead, with increased quality assurance and a simpler, but more robust, approach to verification and validation.



## TRACK 11 Verification for Fluid Dynamics and Heat Transfer

### 11-1
### VERIFICATION FOR FLUID DYNAMICS AND HEAT TRANSFER: SESSION 1

**2nd Floor, Palo Verde B** **9:30am-11:35am**

#### FLOW AND HEAT TRANSFER ANALYSIS OF VARIABLE DIAMETER CIRCULAR PILLAR DISC BRAKE ROTOR

**Technical Presentation.** VVS2016-8823
9:30am-9:55am

**Mahesh Chopade**, *MIT College of Engineering, Maharashtra, India,* **Avinash Valavade**, *Dhole Patil College of Engineering, Pune, India*

In the present work, ventilated disc brake rotors with variable diameter circular pillar configurations were analyzed to enhance the heat dissipation and obtain more uniform temperature distribution in the rotor. CFD code used in this work was validated with experimental results obtained by conducting experiments on a test rig. Experimental analysis was performed on existing taper radial vane (TRV) rotor to calculate the mass flow rate and heat transfer coefficient. Further, variable diameter circular pillar (VDCP) rotor with different configurations namely VDCP1, VDCP2 and VDCP3 were considered for the analysis. A 20° segment of rotor was considered for the numerical analysis due to its rotational symmetry. CFD results were in good agreement with the experimental analysis. The maximum deviation of numerical results were about 15% from the experimental results. It is found from the analysis that among all the rotor configurations; VDCP1 rotor configuration gives better rate of heat dissipation and more uniform temperature distribution in the rotor. Hence for modern high speed vehicles VDCP1 rotor configuration may be more appropriate.

#### COMPUTATIONAL VERIFICATION OF HYBRID LAMINAR FLOW DESIGN BY SUCTION METHOD

**Technical Presentation.** VVS2016-8830
9:55am-10:20am

**Abolghasem Zareshahneh**, *Cranfield University, Bedford, Bedford, United Kingdom*

Rise in the performance and therefore profit of airliners is a major challenge for aircraft designers. Here, the design of a Hybrid Laminar Flow Control system is considered and a computational verification has been done to show the performance of the system and by employing the fundamental equations required, it shown that required levels of suction across a wing to efficiently suppress flow is achievable. A novel system was designed that could be incorporated into the leading edge of large civil aircraft or adapted to suit alternative aircraft using a combination of active and passive suction methods. The active system uses electric or bleeds air powered turbocompressors to provide the required levels of suction, whereas the passive system automatically produces suction by introducing ducting from the high pressure region at the leading edge to the low pressure region at the underside of the wing. By this method the fuel saving of 5.5% is achievable. The outcome of the investigation shows a good meeting with computational analysis and the available source of validation. This method is recommended to be experimentally investigated.

### VERIFICATION STUDIES OF THE NOH PROBLEM

**Technical Presentation.** VVS2016-8859
10:20am-10:45am

**Sarah C. Burnett, Scott D. Ramsey, Kevin G. Honnell, Robert Singleton, Jr.,** *Los Alamos National Laboratory, Los Alamos, NM United States*

The Noh problem [1] is a well-studied and widely-used verification test problem in the field of computational hydrodynamics of compressible fluids. Typically, indeed almost universally, it is applied to an ideal gas fluid. In this work we review the general solution of the Noh problem, using Lie group methods, and then apply the general solution to two more realistic, non-ideal gas equations of state, the Clausius, the "stiff gas" and the Carnahan-Starling. The exact solutions for these non-ideal gases are then compared to the numerical results obtained using the Los Alamos hydrodynamic code Flag.

The Noh problem [2] consists of a strong shock forming as a piston pushes a compressible gas towards a rigid wall (in planar geometry) or as an outer wall compresses a gas towards a central axis (cylindrical) or point (spherical) in higher geometries. The problem is usually defined by specifying the geometry and the equation of state, initial velocity, density, and internal energy of the fluid. It is typically applied to an ideal gas initialized at zero pressure and energy/temperature, giving rise to an infinitely strong shock. In this paper we explore extensions of the Noh problem beyond these idealized conditions.

The analytical solution is first reviewed using Lie group methods to simplify one-dimensional Euler compressible flow equations in the form of partial differential equations to ordinary differential equations. The bulk modulus, indicative of a specific equation of state, is featured in the conservation of energy equation to represent the inverse compressibility. A general solution is achieved analytically by applying the Rankine-Hugoniot jump conditions and the conditions of the shocked and unshocked regions characteristic of the Noh problem that is the velocity being constant and inwardly directed in the unshocked region and zero velocity in the shocked region. In the planar case, this analysis shows that general solutions can be applied to any equation of state and do not necessarily have to exhibit strong shocks as the initial pressure can be greater than zero. For cylindrical and spherical geometries, it is necessary that the studies feature only strong shocks.

Two non-ideal equations of state, the two-parameter Clausius-like gas [3], the stiff gas [4], and the Carnahan-Starling gas [5] are examined using the Los Alamos Lagrangian hydrocode FLAG. Prediction for the pressure, density and internal energy as a function of time, position, and mesh resolution are compared with the exact solutions and with predictions for the ideal gas. First-order convergence with mesh size is observed with respect to spatial mesh size.

Our results suggest that use of non-ideal equations of state in verification studies can provide a more physically-realistic, but still computationally-tractable tool for verifying and validating complex hydrocodes.

References

[1] R. Axford, "Solutions of the Noh Problem for Various Equations of State Using Lie Groups, " Lasers and Particles Beams 18, 93 (2000).
[2] W. Noh, "Error for Calculations of Strong Shocks Using an Artificial Viscosity and an Artificial Heat Flux, " J. Comp. Phys. 72, 78 (1987).
[3] R. Clausius, "Über das Verhalten der Kohlensäure in Bezug auf Druck, Volumen und Temperatur, " Annalen der Physik und Chemie 9, 337 (1880).
[4] F.H. Harlow, A.A. Amsden, "Fluid Dynamics," LA-4700, Los Alamos Scientific Laboratory Monograph (1971).
[5] Norman F Carnahan and Kenneth E Starling. Equation of state for nonattracting rigid spheres. The Journal of Chemical Physics, 51(2):635-636, 1969.

### VERIFICATION OF ADVECTIVE BAR ELEMENTS IMPLEMENTED IN THE SIERRA/ARIA THERMAL RESPONSE CODE

**Technical Presentation.** VVS2016-8860
10:45am-11:10am

**Brantley Mills, Adam Hetzler**, *Sandia National Laboratories, Albuquerque, NM, United States*

A reduced order finite element model for 1D fluid flow convectively coupled with a 3D solid, referred to as the "advective bar" model, has been implemented in the Sierra/Aria thermal response code at Sandia National Laboratories. The primary advantage of this model is that energy advection in fluid flows can be integrated with very large existing 3D models without a significant increase in setup or computation time with acceptable physical accuracy. Historically, analysts have used either an empirical heat transfer coefficient correlation with constant reference temperature for the fluid or coupled a very computationally expensive 3D fluid flow model when modeling convection on surfaces. Instead, 1D bar elements are used to model the fluid volume whose nodes have been coupled with the nearest surfaces of the solid and act as a local reference temperature and velocity for use with the empirical heat transfer coefficient correlations. For relevant geometries, specifically those that feature unidirectional flow where accurate heat transfer coefficient correlations are available, this provides analysts a model that can provide satisfactory solutions without significant computation cost.

A suite of verification tests have been performed on the advective bar model using a simple pipe flow as a relevant geometry to demonstrate proper implementation in Aria. First, a visual analysis of the mapping of the nodes on the fluid elements for various meshes sizes is performed to ascertain if surfaces are being properly assigned. Then, solution convergence is demonstrated using local responses in both temperature and velocity in the model for a uniformly refined mesh. The method of manufactured solutions (MMS) is then applied to the governing equations to provide an exact solution for the problem investigated in order to demonstrate the appropriate order of convergence with spatial and temporal refinement. The energy advection in the fluid flow requires that a spatially first-order upwind scheme is coupled with the second-order 3D solid. This model also presents a unique challenge with MMS as the fluid flow is coupled to the solid through a source term in the energy equation and is not homogenous. The MMS tests are performed for an array of different boundary conditions and temperature-dependent properties. The result of these tests provides future analysts confidence in the implementation of this model.

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### VERIFICATION AND MODEL SENSITIVITY ANALYSES FOR COMPUTATIONAL FLUID DYNAMICS SIMULATIONS OF WIRE-WRAPPED NUCLEAR FUEL ASSEMBLIES

**Technical Presentation.** VVS2016-8889
11:10am-11:35am

**Daniel J. Leonard, R. Brian Jackson, K. Michael Steer**, *TerraPower, Bellevue, WA, United States*

TerraPower is participating in a cooperative project among industry, national lab, and university to perform verification and validation of Computational Fluid Dynamics (CFD) methods for predicting the flow and heat transfer within liquid-metal-cooled nuclear fuel assemblies with wire-wrapped fuel pins. This project, consisting of both experimental and numerical components, uses surrogate fluids and electrically heated fuel pins to substitute for liquid metal and nuclear fuel. The experiments include both unheated assemblies to measure velocities with Laser Doppler Velocimetry and Particle Image Velocimetry, and heated assemblies to measure temperatures with thermocouples. Both classes of experiments will also measure pressure drops with pressure probes. The numerical component involves high-fidelity Large-Eddy Simulation modeling and industrial-level Reynolds Averaged Navier-Stokes modeling of the experiments. This presentation describes the methods and results of the industrial-level CFD code and solution verification.

Preliminary code verification results of a commercial CFD software package are presented. A rigorous Order-of-Accuracy test, achieved with the implementation of the Method of Manufactured Solutions is presented for the two-dimensional steady Euler equations. The results converge to the exact solution with mesh refinement. Furthermore, the observed order of accuracy of the variables of interest approaches second order with mesh refinement, which is consistent with the formal order of accuracy of the discretized equations. This approach is currently being applied to more complex governing equations representative of the experiments.

CFD simulations of helically wire-wrapped fuel assemblies employ meshes of bare pins without wire-wrap in the bundle, where the effect of wire-wrapping on the flow is accounted for by way of a momentum source in the governing fluid equations. This methodology allows simplified geometry and mesh generation, and possible reductions in cell count, while still capturing the effects of the wire-wrapping. Solution verification is conducted through iterative and mesh convergence analyses of the variables of interest. Additionally, various turbulence models, mesh spacing in particular directions, and momentum source modeling coefficient values are investigated to assess their sensitivity. The observed order of accuracy is determined to be consistent with the formal order of accuracy of the discretized equations, proving that the asymptotic range has been achieved, and a Richardson extrapolation is employed to provide an estimate of the exact solution of the discretized equations. It is shown that the pressure drop across the bundle can display appreciable variation depending on the choice of turbulence model. In addition, it is concluded that the mesh level displaying convergence can be greatly coarsened in the axial direction without affecting the variables of interest.

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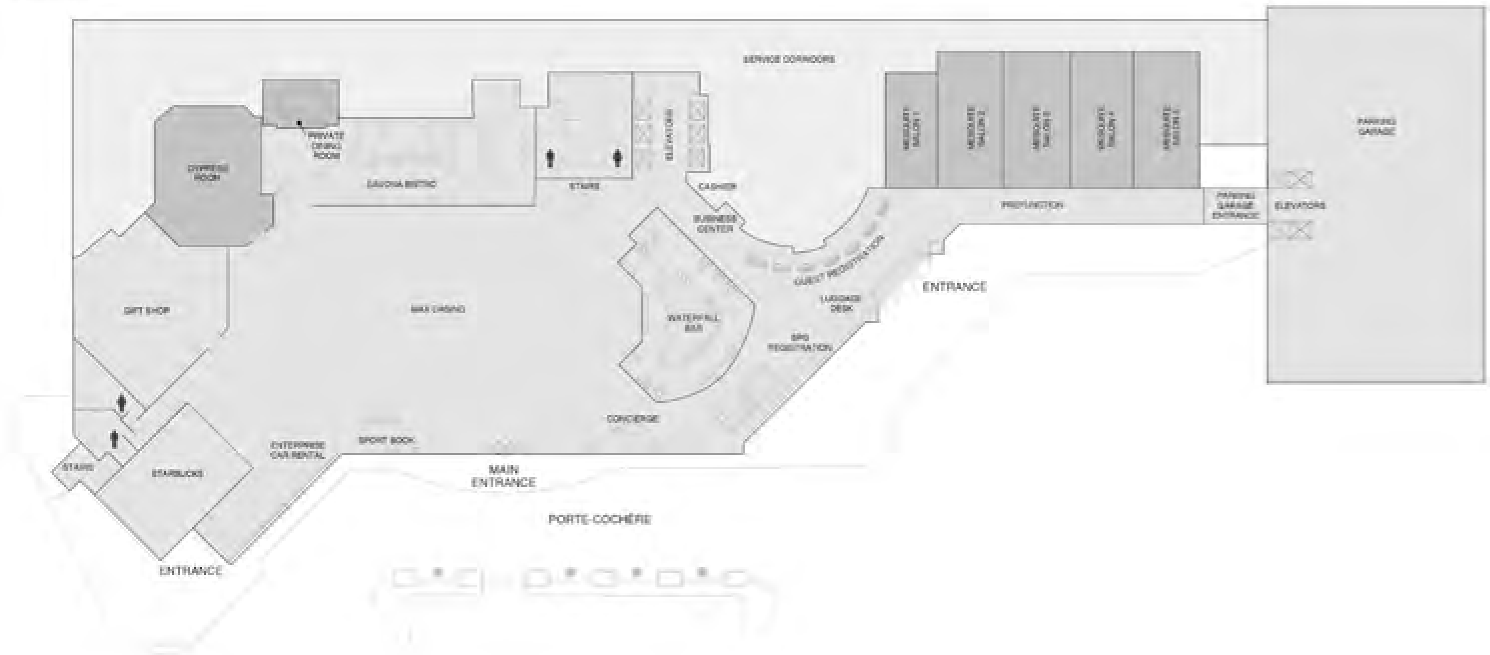


The Westin
Las Vegas
Hotel, Casino & Spa

## SECOND FLOOR


SERVICE CORRIDOR

HOTEL GUEST FACILITIES

MEETING / BANQUET FACILITIES

ASME

SETTING THE STANDARD

# V&V 2016

## ASME VERIFICATION AND VALIDATION SYMPOSIUM