

CONFERENCE May 3–5, 2017

The Westin Las Vegas, Las Vegas, Nevada

# Program



www.asme.org/events/vandv

The American Society of Mechanical Engineers® (ASME®)

## Welcome

Welcome to ASME's 2017 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 each year brings together engineers and scientists from around the world and from diverse disciplines: 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 Organizing Committee

#### Symposium Organizing Committee

Chris Freitas Southwest Research Institute

Scott Doebling Los Alamos National Laboratory

Ryan Crane ASME

Kevin Dowding Sandia National Laboratories

**Chris Roy** Virginia Tech

Marian Heller ASME

Mark Benedict Air Force Research Laboratory

Luis Eca Instituto Superior Tecnico

Ali Kiapour 4WEB Medical

Hyung Lee Bettis Laboratory

Carl Popelar Southwest Research Institute

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### **General Information**



#### REGISTRATION HOURS AND LOCATION

### Registration is in the Casuarina Foyer, 2nd Floor.

#### **Registration Hours:**

Tuesday, May 2:	5:00pm – 7:00pm
Wednesday, May 3:	7:00am – 6:00pm
Thursday, May 4:	7:00am – 6:00pm
Friday, May 5:	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.

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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 conference 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 conference registration fee, including students who pay the non-Member student fee, will receive a one-year FREE 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.

### **Committee Schedule**

#### ASME V&V COMMITTEE MEETING SCHEDULE

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

#### **TUESDAY, MAY 2, 8:00AM-5:00PM**

V&V 10 Subcommittee on Verification and Validation in Computational Solid Mechanics, Mesquite 5, 1st 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.

#### WEDNESDAY, MAY 3, 6:30PM-7:30PM

V&V Standards Committee on Verification and Validation in Computational Modeling and Simulation, Casuarina Ballroom, 2nd Floor

6:30pm–7:30pm – Meeting 7:30pm–9:00pm – Reception

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.

#### THURSDAY, MAY 4, 6:00PM-9:00PM

V&V 50 Subcommittee on Verification and Validation of Computational Modeling for Advanced Manufacturing, Acacia C, 2nd Floor.

#### FRIDAY, MAY 5, 1:00PM-5:00PM

V&V 50 Subcommittee on Verification and Validation of Computational Modeling for Advanced Manufacturing, Acacia C, 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

Interested applicants should contact Ryan Crane, CraneR@asme.org

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

Interested applicants should contact Fred Constantino, ConstantinoF@asme.org

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

Interested applicants should contact Marian Heller, HellerME@asme.org

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

Interested applicants should contact Ryan Crane, CraneR@asme.org

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

Interested applicants should contact Ryan Crane, CraneR@asme.org

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

Interested applicants should contact Marian Heller, HellerME@asme.org

#### ASME V&V 60 - Verification and Validation of Computational Modeling for Energy Systems

Interested applicants should contact the Committee Secretary, which are:

V&V 10 – Fred Constantino, ConstantinoF@asme.org V&V 20 and V&V 50 – Marian Heller, HellerME@asme.org V&V 30, V&V 40, and V&V 60 – Ryan Crane, CraneR@asme.org

### Workshops

#### TWO-DAY SEMINARS HELD IN CONJUNCTION WITH THEASME V&V SYMPOSIUM ON MAY 1-2, 2017

### VERIFICATION AND VALIDATION IN SCIENTIFIC COMPUTING (MC133)

#### Presented by: Dr. William Oberkampf and Prof. Christopher Roy

This seminar presents modern terminology and effective procedures for verification of numerical simulations, validation of mathematical models, and an introduction to uncertainty quantification of nondeterministic simulations. The techniques presented in this course are applicable to a wide range of engineering and science applications, including fluid dynamics, heat transfer, solid mechanics, and structural dynamics.

For more information and to register, go to http://go.asme.org/mc133

#### PROBABILISTIC AND UNCERTAINTY QUANTIFICATION METHODS FOR MODEL VERIFICATION & VALIDATION (MC146)

#### Presented by: David Riha and Ben Thacker, Southwest Research Institute

This seminar presents the concepts, methods, approaches, and strategies for characterizing and managing uncertainties within the context of model verification and validation (V&V). Uncertainty quantification methods are presented in-depth followed by simple exercises to reinforce the material. Attendees will learn to use the NESSUS probabilistic analysis software and will apply it throughout the course to gain experience in problem formulation, results interpretation and communication. V&V case studies are discussed to illustrate model development within a V&V framework.

For more information and to register, go to http://go.asme.org/mc146

### **PLEASE JOIN US**

### V&V STANDARDS COMMITTEE ON VERIFICATION AND VALIDATION IN COMPUTATIONAL MODELING AND SIMULATION

FOLLOWED BY A NETWORKING RECEPTION

WEDNESDAY, MAY 3 CASUARINA ROOM, 2<sup>ND</sup> FLOOR THE WESTIN LAS VEGAS MEETING 6:30PM – 7:30PM RECEPTION 7:30PM – 9:00PM

PLEASE JOIN US FOR PRESENTATIONS AND AN OPEN DISCUSSION ON THE STANDARDS DEVELOPMENT ACTIVITIES AND FUTURE EFFORTS FOLLOWED BY A NETWORKING RECEPTION WITH REFRESHMENTS AND LIGHT FARE.

#### MONDAY, MAY 01, 2017

ТІМЕ	SESSION #	PAGE	SESSION	
08:00 AM – 05:00 PM		6	Verification and Validation in Scientific Computing	
08:00 AM – 05:00 PM		6	Probabilistic and Uncertainty Quantification Methods for Model Verification & Validation	

#### TUESDAY, MAY 02, 2017

TIME	SESSION #	PAGE	SESSION
05:00 PM – 07:00 PM			Registration
08:00 AM – 05:00 PM		6	Verification and Validation in Scientific Computing
08:00 AM – 05:00 PM		6	Probabilistic and Uncertainty Quantification Methods for Model Verification & Validation
08:00 AM - 05:00 PM			V&V 10 Subcommittee on Verification and Validation in Computational Solid Mechanics
08:00 AM – 05:00 PM			V&V 20 Subcommittee on Verification and Validation in Computational Fluid Dynamics and Heat Transfer
08:00 AM – 05:00 PM			V&V 30 Subcommittee on Verification and Validation in Computational Simulation of Nuclear System Thermal Fluids Behavior
08:00 AM – 05:00 PM			V&V 40 Subcommittee on Verification and Validation in Computational Modeling of Medical Devices
05:00 PM – 07:00 PM			V&V Standards Committee (Closed Session)

#### WEDNESDAY, MAY 03, 2017

TIME	SESSION #	PAGE (S)	SESSION
07:00 AM – 06:00 PM			Registration
07:00 AM – 08:00 AM			Continental Breakfast
08:00 AM - 10:00 AM			Opening Address and Plenary Presentions
10:00 AM - 10:30 AM			Coffee Break
10:25 AM - 12:30 PM	2-1	17	2-1 ASME V&V Standards Development Activities
10:25 AM - 12:30 PM	4-1	19	4-1 Uncertainty Quantification: Theory Part 1
10:25 AM - 12:30 PM	11-1	21	11-1 Verification for Fluid Dynamics and Heat Transfer
12:30 PM - 01:30 PM			Lunch
01:30 PM - 03:35 PM	4-2	23	4-2 Uncertainty Quantification: Theory Part 2
01:30 PM - 03:35 PM	5-1	25	5-1 Validation for Fluid Dynamics and Heat Transfer
01:30 PM - 03:35 PM	13-1	27	13-1 Verification and Validation of Medical Devices
03:30 PM – 04:00 PM			Coffee Break
04:00 PM - 06:05 PM	1-1	29	1-1 V&V Benchmark Problem Twin Jet Computational Fluid Dynamics (CFD) Numeric Model Validation
04:00 PM - 06:05 PM	4-3	31	4-3 Uncertainty Quantification: Application Part 1
04:00 PM - 06:05 PM	6-1	33	6-1 Validation Methods
06:00 PM – 08:00 PM		7	V&V Standards Committee on Verification and Validation in Computational Modeling and Simulation (followed by a Networking Reception)

TRACK	ROOM
(MC133)	Acacia A
(MC146)	Pinon

TRACK	ROOM
	Registration Desk (Foyer)
(MC133)	Acacia A
(MC146)	Pinon
	Mesquite 5
	Acacia B
	Mesquite 4
	Acacia C-D
	Mesquite 1

TRACK	ROOM
	Registration Desk (Foyer)
	Casuarina and The Loft
	Acacia D
	Pre-function, 2nd Floor
Development and Application of Verification and Validation Standards	Palo Verde A
Uncertainty Quantification, Sensitivity Analysis, and Prediction	Palo Verde B
Verification for Fluid Dynamics and Heat Transfer	Mesquite 2
	Casuarina Room
Uncertainty Quantification, Sensitivity Analysis, and Prediction	Palo Verde B
Validation for Fluid Dynamics and Heat Transfer	Palo Verde A
Verification and Validation of Medical Devices	Acacia D
	Pre-function, 2nd Floor
Challenge Problem Workshops and Panel Sessions	Acacia D
 Uncertainty Quantification, Sensitivity Analysis, and Prediction	Mesquite 2
Validation Methods	Palo Verde B
	Casuarina Room

#### **THURSDAY, MAY 04, 2017**

TIME	SESSION #	PAGE	SESSION
07:00 AM - 06:00 PM			Registration
07:00 AM - 08:00 AM			Continental Breakfast
08:00 AM - 10:00 AM			Plenary Presentations
10:00 AM - 10:30 AM			Coffee Break
10:25 AM - 12:30 PM	3-2	37	3-2 Topics in Verification and Validation: Part 1
10:25 AM - 12:30 PM	4-4	39	4-4 Uncertainty Quantification: Application Part 2
10:25 AM - 12:30 PM	12-1	41	12-1 Discretization Error Estimation
12:30 PM - 01:30 PM			Lunch
01:30 PM - 03:35 PM	3-1	42	3-1 V&V Workflow Development and Applications
01:30 PM - 03:35 PM	10-1	44	10-1 Verification and Validation of Nuclear Power Applications: Part 1
01:30 PM - 03:35 PM	12-2	47	12-2 Verification Test Suites
03:30 PM - 04:00 PM			Coffee Break
04:00 PM - 06:05 PM	2-2	48	2-2 Application of Standards
04:00 PM - 06:05 PM	2-3	50	2-3 NAFEMS Standards Development Activities
04:00 PM - 06:05 PM	10-2	50	10-2 Verification and Validation of Nuclear Power Applications: Part 2
06:00 PM - 09:00 PM			V&V 50 Subcommittee on Verification and Validation in Computational Modeling for Advanced Manufacturing

#### FRIDAY, MAY 05, 2017

ТІМЕ	SESSION #	PAGE	SESSION
07:00 AM - 12:35 PM			Registration
07:00 AM - 08:00 AM			Continental Breakfast
08:00 AM - 10:05 AM	1-2	54	1-2 Workshop on Iterative Errors in Unsteady Flow Simulations
08:00 AM - 10:05 AM	9-1	54	9-1 Validation Methods for Solid Mechanics and Structures
08:00 AM - 10:05 AM	17-1	56	17-1 ASME V&V 50 Verification and Validation of Computational Modeling for Advanced Manufacturing
10:00 AM - 10:30 AM			Coffee Break
10:30 AM - 12:35 PM	1-3	58	1-3 Workshop on Estimation of Discretization Errors Based on Grid Refinement Studies
10:30 AM - 12:35 PM	3-3	60	3-3 Topics in Verification and Validation: Part 2
10:30 AM - 12:35 PM	8-1	62	8-1 Verification & Validation for Impact, Blast, and Material Response
01:00 PM - 05:00 PM			V&V 50 Subcommittee on Verification and Validation in Computational Modeling for Advanced Manufacturing

TRACK	ROOM
	Registration Desk (Foyer)
	Casuarina and The Loft
	Acacia D
	Pre-function, 2nd Floor
Topics in Verification and Validation	Acacia AB
Uncertainty Quantification, Sensitivity Analysis, and Prediction	Palo Verde A
Verification Methods	Palo Verde B
	Casuarina and The Loft
Topics in Verification and Validation	Acacia AB
Verification and Validation of Nuclear Power Applications	Acacia D
Verification Methods	Palo Verde A
	Pre-function, 2nd Floor
Development and Application of Verification and Validation Standards	Palo Verde A
Development and Application of Verification and Validation Standards	Palo Verde B
Verification and Validation of Nuclear Power Applications	Acacia D
	Acacia C

ТРАСК	ROOM
	Registration Desk (Foyer)
	Casuarina and The Loft
Challenge Problem Workshops and Panel Sessions	Palo Verde A
Validation Methods for Solid Mechanics and Structures	Palo Verde B
Verification and Validation for Advanced Manufacturing	Acacia D
	Pre-function, 2nd Floor
Challenge Problem Workshops and Panel Sessions	Palo Verde A
Topics in Verification and Validation	Acacia AB
Validation Methods for Impact, Blast, and Material Response	Palo Verde B
	Acacia C

### **Session Chairs**

### TRACK-1 CHALLENGE PROBLEM WORKSHOPS AND PANEL SESSIONS

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

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

#### 1-2 Workshop on Iterative Errors in Unsteady Flow Simulations

Luis Eca, IST, Lisbon, Portugal

**1-3 Workshop on Estimation of Discretization Errors Based on Grid** *Refinement Studies* 

Luis Eca, IST, Lisbon, Portugal

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

#### 2-1 ASME V&V Standards Development Activities

David Moorcroft, Federal Aviation Administration, Oklahoma City, OK, United States Tina Morrison, Food and Drug Administration, Silver Spring, MD, United

States

#### 2-2 Application of Standards

Lane Carasik, Texas A&B University, College Station, TX, United States Brian Weiss, National Institute of Standards and Technology, Gaithersburg, MD, United States

#### 2-3 NAFEMS Standards Development Activities

Andrew Wood, NAFEMS, Granville, OH, United States William L. Oberkampf, W.L. Oberkampf Consulting, Georgetown, TX, United States

#### **TRACK-3 TOPICS IN VERIFICATION AND VALIDATION**

#### 3-1 V&V Workflow Development and Applications

Christopher Freitas, Southwest Research Institute, San Antonio, TX, United States Qiang Yu, ANWISE Technology Ltd., Beijing, China

#### 3-2 Topics in Verification and Validation: Part 1

Mahmood Tabaddor, UL, LLC, Northbrook, IL, United States Tae-Won Park, Ajou Univeristy, Suwon-si, Korea (Republic)

#### 3-3 Topics in Verification and Validation: Part 2

Joe Hightower, The Boeing Company, Seattle, WA, United States Denis F. Hinz, Kamstrup A/S, Skaderborg, Denmark

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

#### 4-1 Uncertainty Quantification: Theory Part 1

Ronay Ak, National Institute of Standards and Technology, Gaithersburg, MD, United Statesz Joshua Mullins, Sandia National Laboratories, Albuquerque, NM, United States

#### 4-2 Uncertainty Quantification: Theory Part 2

Mark Benedict, AFRL Mantech, WPAFB, OH, United States James Sobotka, R. C. McClung, Southwest Research Institute, San Antonio, TX, United States

#### 4-3 Uncertainty Quantification: Application Part 1

Jeff Harris, Applied Research Lab, Pennsylvania State University, Bellefonte, PA, United States Suchandra Ghosh, U.S. Nuclear Regulatory Commission, Rockville, MD, United States

#### 4-4 Uncertainty Quantification: Application Part 2

Leonid Gutkin, Kinectrics, Inc., Toronto, ON, Canada M. Giselle Fernández-Godino, University of Florida, Gainesville, FL, United States

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

#### 5-1 Validation for Fluid Dynamics and Heat Transfer

Arnaud Barthet, EDF R&D, Chatou, France Thomas Frank, ANSYS Germany GmbH, Otterfing, Bavaria, Germany

#### **TRACK-6 VALIDATION METHODS**

#### **6-1 Validation Methods**

Ali Kiapour, 4WEB Medical, Newton, MA, United States Santhosh Seshadhri, Medtronic, Hyderabad, Telangana, India

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

#### 8-1 Verification & Validation for Impact, Blast, and Material Response

Joanne Budzien, Los Alamos National Laboratory, Los Alamos, NM, United States

Bahram Notghi, Baxter Healthcare, Round Lake, IL, United States

### **Session Chairs**

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

#### 9-1 Validation Methods for Solid Mechanics and Structures

Isaac Asher, General Electric, Co., Niskayuna, NY, United States George Orient, Sandia National Laboratories, Albuquerque, NM, United States

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

#### 10-1 Verification and Validation of Nuclear Power Applications: Part 1

Joshua Kaizer, U.S. Nuclear Regulatory Commission, Germantown, MD, United States

Roberto Zanino, Dipartimento Energia, Politecnico, Di Torino, Torino, Italy

#### 10-2 Verification and Validation of Nuclear Power Applications: Part 2

Heng Ban, Utah State University, Logan, UT, United States Janusz Edward Kowalski, Canadian Nuclear Society Commission, Ottawa, ON, Canada

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

#### 11-1 Verification for Fluid Dynamics and Heat Transfer

Christopher Roy, Virginia Tech, Blacksburg, VA, United States Avinash Vaidheeswaran, National Energy Technology Laboratory, Morgantown, WV, United States

#### **TRACK-12 VERIFICATION METHODS**

#### 12-1 Discretization Error Estimation

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

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

#### **12-2 VERIFICATION TEST SUITES**

Scott Doebling, Los Alamos National Lab, Los Alamos, NM, United States Dennis Hinz, Kamstrup A/S, Skanderborg, Denmark

#### TRACK-13 VERIFICATION AND VALIDATION OF MEDICAL DEVICES

#### 13-1 Verification and Validation of Medical Devices

Tina Morrison, Food and Drug Administration, Silver Spring, MD, United States

**Carl Popelar,** Southwest Research Institute, San Antonio, TX, United States

#### TRACK-17 VERIFICATION AND VALIDATION FOR ADVANCED MANUFACTURING

#### 17-1 ASME V&V 50 Verification and Validation of Computational Modeling for Advanced Manufacturing

Sudarsan Rachuri, Dept. of Employment, Frederick, MD, United States Marian Heller, ASME, New York, NY, United States Mark Benedict, AFRL Mantech, WPAFB, OH, United States

### **Plenary Sessions**

#### WEDNESDAY, MAY 3 · 8:00AM - 10:00AM · ACACIA D, 2ND FLOOR

PLENARY 1: EXPERIENCES IN ESTABLISHING CREDIBILITY FOR "REGULATORY GRADE" MODELS IN THE MEDICAL DEVICE INDUSTRY



#### Jeff Bodner

Senior Principal Engineer and Technical Fellow in the Restorative Therapies Group at Medtronic, Inc.

Jeff Bodner is a Senior Principal Engineer and Technical Fellow in the Restorative Therapies Group at Medtronic, the world's largest dedicated manufacturer of medical devices. During his 10 years at Medtronic, his work has primarily supported the targeted drug delivery business, which includes chronically implanted drug infusion systems. His professional interests include improving the understanding of the mechanical interface between an implanted device and the patient, including soft tissue biomechanics and drug bio-transport, using a combination of in *vivo, in vitro*, and *in silico* (i.e. computational) methodologies. His prior experience in the medical device industry includes a nine-year tenure at Guidant, now part of Boston Scientific, where he focused on the design of cardiac pacemaker leads.

Jeff is a member of ASME and has been a member of the V&V40 subcommittee since 2011. He has a Bachelor's and Master's degree in Mechanical Engineering from Case Western Reserve University and a Master's degree in Biomedical Engineering from the University of Minnesota, Twin Cities. He is an inventor on 12 US patents related to medical device design.

**Abstract:** There is increased interest in the use of modeling and simulation (M&S) in the medical device industry resulting from the continuing need to develop safer and more efficacious devices that reach patients faster. The rising costs of the evidence submitted to regulatory bodies worldwide and healthcare in general are also strong motivators for the increased use of M&S where in vitro and in *vivo* tests have traditionally been used.

This presentation will provide details of the experience of a non-expert V&V practitioner establishing the credibility of a computational model for the first time together as part of a high-consequence project where patient safety was at issue. In order to generate a "regulatory grade" model, a V&V plan was developed that strictly followed the existing ASME standards, including code verification, solution verification, and uncertainty quantification. Further, the submission to the US Food and Drug Administration (FDA) complied with recent guidance issued by the agency on reporting model results. To our knowledge, this is the first submission to FDA that included strict adherence to the V&V framework described in those standards, utilized FDA's new guidance, and incorporated some philosophical elements of the draft ASME V&V40 standard. As such, it is a benchmark for how the industry expects to submit M&S to regulators in the future.

To further improve the credibility case, a pilot program was initiated through the Medical Device Innovation Consortium (MDIC), a publicprivate partnership whose mission is to improve regulatory science in the medical device industry. As part of this program, a panel of independent experts in V&V was established by MDIC to review the credibility evidence for compliance to the ASME standards. The panel's report was submitted to the FDA along with Medtronic's normal documentation. The successes and challenges of the MIDC pilot will be described. One lesson learned from that experience is that for credibility evidence to be impactful, stakeholders must have sufficient technical background to properly interpret the results. Broader familiarity in the concepts of VVUQ will be needed across a spectrum of internal and external stakeholders if the shared vision for increased use of M&S is to be realized in the medical device industry.

#### PLENARY 2: VALIDATION AND VERIFICATION IN A MULTI-DISCIPLINE, MULTI-ROLE, MULTI-SCALE VIRTUAL AND REAL WORLD



Michael J. Doyle Validation and Verification in a Multi-discipline, Multi-role, Multi-scale Virtual and Real World

Dr. Michael J. Doyle is principal scientist at Dassault Systèmes BIOVIA. He is responsible for advising on the future direction of BIOVIA, especially as regards strategic technology acquisition and platform development. He has developed and implemented scientific innovation and information lifecycle initiatives and overseen strategic relationships with Shell, Exxon-Mobil, P&G, Unilever, Dow and Chevron. He has managed the Executive Petrochemical Advisory Council and lead the architecture teams for Shell (Criterion Catalysts), and Exxon (EMCC and EMRE) informatics projects. Dr. Doyle holds a Ph.D. in Chemistry from Cambridge University and is Charter Chemist from the RSC.

Abstract: "Small opportunities are often the beginning of great enterprises." (Demosthenes)

Digital technology, which pervades our society in so many diverse and different ways, clearly has the power to enhance or even transform materials based industries. The impact of this transformation ranges across all of the business stages of discovery, design, development and delivery to manufacturing.

To transform manufacturing and process industries digital solutions have begun to democratize information historically limited to a small group of experts. The increased use of platforms with integrated analytics to digitize and automate complex processes is enabling more users to run and create more complex processes. As this information becomes available to large groups of people within the organization, experts will be challenged to ensure information quality. Why is verification and validation important? What are the key innovation and business drivers that will continue to make verification increasingly important? What is the next generation of simulation and modeling?

Dassault Systems BIOVIA and SIMULIA are focused on science and engineering and are committed to facing these challenge with its next generation tools and technology.

#### THURSDAY, MAY 4 · 8:00AM - 10:00AM · ACACIA D, 2ND FLOOR

#### PLENARY 3: ANALYTICAL METHODS IN AEROSPACE APPLICATIONS: CERTIFICATION DECISION MAKING



#### Joseph Pellettiere

Chief Scientific and Technical Advisor for Crash Dynamics, Federal Aviation Administration

Joseph Pellettiere is the Chief Scientific and Technical Advisor for Crash Dynamics at the Federal Aviation Administration. Dr. Joseph Pellettiere supports the development of occupant injury criteria as they apply to Aerospace systems and the application of these criteria to the certification of aircraft structure, seats, and cabin interiors. He has been heavily involved in the development of processes and procedures of analysis methods within the certification process with the ultimate goal of seat certification by analysis. Dr. Pellettiere has also supported transport, rotorcraft and small airplane certification programs. Current focal projects include the investigation of full scale test methods and analytical techniques to support system level crash worthiness for both metallic and composite aircraft. Dr. Pellettiere spent over 17 years working for the United States Air Force as a part of the Air Force Research Laboratory in the Human Effectiveness directorate. While working for AFRL, he lead many research programs including the effects of helmet supported mass, the development of tensile neck injury criteria, and the development of modeling and simulation tools for crash safety. He supported several accident investigation boards and large acquisition programs such as the joint strike fighter.

Abstract: The Federal Aviation Administration (FAA) has a standards and regulations that are designed to protect aircraft occupants in the event of a crash. These regulations focus on the occupant, restraint and seat in a longitudinal and a combined longitudinal and vertical direction. These requirements are typically met through deterministic testing to certify the part as meeting the airworthiness requirements. In recent years, there has been interest in supplementing the testing with Modeling and Simulation to reduce the number of required tests. If Certification by Analysis is to be realized, the analyst must understand the certification process and the needs of the decision maker, such as what level of Verification and Validation is necessary and how can the goals of meeting the safety requirements be met while still exhibiting conservatism. FAA has written guidance on this topic and has been heavily involved in standards development and hosting workshops to discuss these topics.

#### PLENARY 4: BUSINESS AND REGULATORY PERSPECTIVES OF VERIFICATION, VALIDATION AND UNCERTAINTY QUANTIFICATION



Dr. William L. Oberkampf Consulting Engineer, W. L. Oberkampf Consulting

Dr. Oberkampf earned his PhD in Aerospace Engineering at the University of Notre Dame in 1970. He has conducted research and development in fluid mechanics, heat transfer, and solid mechanics, and during the last 25 years he has focused on advancing the state of the art and practice of verification, validation, and uncertainty quantification. He served in staff and management positions at Sandia National Laboratories for 29 years and early in his career served on the faculty of the Department of Mechanical Engineering at the University of Texas at Austin for 9 years. He contributed to the formation of the ASME Standards Committee on Verification and Validation in Computational Solid Mechanics and continues as an active member. He is also an active member of the Analysis Management Working Group for NAFEMS and the AIAA Committee on Standards for Verification and Validation in Computational Fluid Dynamics. He has published over 140 journal articles, book chapters, and conference papers, and co-authored the book "Verification and Validation in Scientific Computing," Cambridge University Press. He has presented over 50 short courses on verification, validation, and uncertainty quantification in the United States and the United Kingdom. He is a Fellow of the American Institute of Aeronautics and Astronautics.

Abstract: Computer simulations are increasingly relied upon to inform business management and regulatory decisions ranging from product innovation to certification of complex, high-consequence systems. Businesses and regulatory authorities routinely utilize a combination of simulation and experimental testing when making design, performance, and safety decisions. When simulation integrates with physical testing, the decision-making process is said to be *simulation-informed*. Regardless of the balance between simulation and experiment, computer simulation should be viewed as an information product that (a) supports a specific decision-making process and (b) provides an improved understanding of the uncertainties and risks incurred by the user of the simulation results. When viewed as an information product, traditional attributes of information quality should be considered, such as, correctness, objectivity, completeness, interpretability, and timeliness. Additionally, the information quality must be judged with regard to a specific decision context, for example, the magnitude of the potential risk or gain to the business activity, or the risk to public safety from the perspective of a regulator.

NAFEMS, under the sponsorship of the Analysis Management Working Group, has recently published a booklet for managers that introduce the concepts of verification, validation, and uncertainty quantification (VVUQ) in computational simulation. Managers with little or no training in science or engineering will be able to understand the technical concepts and why VVUQ add value to simulation credibility. The presentation discusses this booklet, as well as the roles, responsibilities, and implementation costs of simulation developers, producers, and customers. Since time and resources are required for VVUQ, rationale is presented for the value added to the correctness and completeness of the information provided by simulation. The value proposition of conducting VVUQ should be viewed as a trade-off between increased confidence in simulation results versus increased risk by management and regulators of using simulation results with unknown or unsupported credibility. Since business management is understandably resistant to increased time and costs of VVUQ activities, examples will be given of what has motivated organizations in the past.

## Technical Program Wednesday, May 3, 2017

### Wednesday Technical Program

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

### 2-1 ASME V&V STANDARDS DEVELOPMENT ACTIVITIES 2ND FLOOR, PALO VERDE A 10:25AM - 12:30PM

#### V&V 60 Subcommittee on Energy Systems and Applications

Technical Presentation. VVS2017-4126

Christopher Freitas, Southwest Research Institute, San Antonio, TX, United States, Ryan Crane, ASME, New York, NY, United States

An introduction to the new V&V Subcommittee which is focused on verification and validation in modeling and simulation focused on energy systems and applications. The specific energy technologies are oil & gas, renewal energy, big data, and big data analytics.

#### V&V 10: Verification and Validation in Computational Solid Mechanics

Technical Presentation. VVS2017-4125

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

The charter of the ASME Verification and Validation in Computational Solid Mechanics (V&V 10) subcommittee is to provide procedures for assessing the correctness and credibility of modeling and simulation in computational solid mechanics. The group was originally formed in 1999 as an ad-hoc committee under the auspices of the United States Association for Computational Mechanics and granted official ASME committee status in 2001 as PTC 60 under the Board on Performance Test Codes. In 2010, an overarching V&V Standards Committee was formed and V&V 10 become a subcommittee. The subcommittee has two published standards: V&V 10-2006 Guide for Verification and Validation in Computational Solid Mechanics and V&V 10.1-2012 An Illustration of the Concepts of Verification and Validation in Computational Solid Mechanics. Two new documents are underway: V&V 10.2 Role of Uncertainty Quantification in Verification and Validation of Computational Solid Mechanics Models and V&V 10.3 Role of Validation Metrics in Verification and Validation of Computational Solid Mechanics Models. The purpose of the Uncertainty Quantification (UQ) supplement is to expand upon the important role of uncertainty quantification in the V&V process and address the need for a common language and process of UQ in Computational Solid Mechanics, particularly as it may relate to how analysts perform UQ as well as how they subsequently communicate results, conclusions and recommendations to a decision maker. The purpose of the metrics supplement is to provide a primer on quantitative metrics used within the Validation process described in the 2006 Guide. This presentation will discuss the ongoing revisions to the 2006 Guide and 2012 Illustration as well as the draft content of the two new documents.

#### **ASME V&V 20 Activities**

Technical Presentation. VVS2017-4144

Leonard Peltier, Bechtel National, Inc., Reston, VA, United States, Dawn Bardot, Medical Device Innovation Consortium, Minneapolis, MN, United States, Kevin Dowding, Sandia National Laboratories, Albuquerque, NM, United States

V&V 20 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 committee, with a discussion of a draft supplement detailing multivariate techniques, and on future directions, which include conceptual frameworks 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.

#### Scope and Vision of the V&V 30 Standards Committee

Technical Presentation. VVS2017-4129

Hyung Lee, Bettis Laboratory, West Mifflin, PA, United States, Richard Schultz, Consultant, Pocatello, ID, 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 V&V benchmark problems 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.

The ASME Verification and Validation in Computational Nuclear System Thermal Fluids Behavior Committee (ASME V&V 30) is supporting 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

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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 initiated for the 2016 ASME V&V Symposium and the results and findings from the first V&V benchmark problem were presented and discussed during the conference session. The full spectrum of upcoming benchmark problems are currently being considered.

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&V 30 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 outcomes of this first benchmark effort are 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.

#### Assessing Credibility of Computational Models through Verification and Validation: Application to Medical Devices

Technical Presentation. VVS2017-4093

Tina Morrison, Food and Drug Administration, Silver Spring, MD, United States

Computational modeling can be used throughout the product life-cycle to provide information about the technical performance, safety and effectiveness of medical devices. Computational models can also be used to assess aspects of in vivo performance without subjecting patients to potential harm or unnecessary risk. The potential consequence of an incorrect assessment elevates the importance of being able to establish the credibility or trust in the predictive capability of a computational model. Although methods for V&V are well-established, guidance is lacking on assessing the adequacy of the V&V activities for computational models used to support medical device development and evaluation. Given the inherent risk of using a computational model as a basis for predicting medical device performance, a risk-informed credibility assessment framework has been developed. The framework centers on establishing that model credibility is commensurate with the risk associated with a decision based in part on the computational model. Thus, the intent of this standard is to provide guidance on how to establish the credibility requirements of computational models based on risk, and then determine and communicate the credibility of computational models used in the evaluation of medical devices through V&V activities.

This presentation will provide a high-level overview of the risk-informed credibility assessment framework, focusing on the new concepts that V&V 40 is introducing into the ASME V&V family of documents.

#### V&V 50 Advanced Manufacturing Subcommittee Update

Technical Presentation. VVS2017-4148

### Mark Benedict, AFRL Mantech, WPAFB, OH, United States, Sudarsan Rachuri, Dept. of Employment, Frederick, MD, United States

While many of the earliest efforts within ASME to define best practices for verification and validation focused on particular computational models, such as Finite Element Analysis or Computational Fluid Dynamics, more recent efforts have focused on contextualizing these concepts to particular communities of practice such as the nuclear energy industry, the medical device community, the petroleum industry, or the advanced manufacturing community. The area of advanced manufacturing is a family of activities that involves using a combination of physics-based and data-driven models to aid in the manufacture of desired end items. This reliance on a mix of modeling approaches greatly complicates the application of conventional verification and validation techniques, hence a new subcommittee, the ASME V&V 50 subcommittee on Advanced Manufacturing, was formed to explore these issues. This session will provide an update on the plans of the subcommittee including:

VVUQ Applications in Process Technologies

Terminology, Concepts, Relationships and Taxonomy for VVUQ in Advanced Manufacturing

V&V Interactions with the Model Life Cycle

VVUQ Challenges and Methods in Systems of Models

VVUQ Methods in Data-driven and Hybrid Models

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

### 4-1 UNCERTAINTY QUANTIFICATION: THEORY PART 1 2ND FLOOR, PALO VERDE B 10:25AM - 12:30PM

#### **Convolutional Neural Networks for Frequency Response Predictions**

Technical Presentation. VVS2017-4024

#### 10:25am - 10:50am

Andrew Wilson, Daniel Wade, Department of Army AMRDEC, Redstone Arsenal, AL, United States, Julia Ling, Stanford University, Oakland, CA, United States, Kamaljit Chowdhary, Sandia National Labs, Livermore, CA, United States, Warren L. Davis IV, Matthew Barone, Jeffrey Fike, Sandia National Labs, Albuquerque, NM, United States

We report on the use of convolutional neural networks to provide efficient and accurate models using frequency response data. Machine learning methods have tremendous potential to provide data-driven models for physics systems. They can scale to high-dimensional data sets to learn underlying structures and patterns in the data. Convolutional neural networks are of particular interest because they can leverage the notion of adjacency in frequency space. These data-driven models provide a method of using experimental data and simulation results to inform model predictions.

We apply convolutional neural networks to two different test cases. The first application is in fluids-structure interactions, in which a model for the pressure power spectrum at the wall is sought. Current models struggle to correctly predict wall pressure fluctuations. We apply convolutional neural networks to predict the wall pressure power spectrum with promising results. We demonstrate that the pressure spectra away from the wall can be used to reconstruct the pressure spectra at the wall. This approach could be used to assess the uncertainty in wall pressure fluctuation predictions.

The second application is in helicopter vibrations, in which a model for vibration in an opposing axis is sought. Current fielded systems have two sensors in opposing axes at a single location, which may be unneeded. We apply convolutional neural networks to predict the vibration spectrum in one axis, given the vibration spectrum from the other axis. This approach can be used to evaluate the need for two sensors, determining whether the information from one sensor contains all information provided by both.

A major purpose of this work is to use the two applications as a means of developing verification and validation metrics and requirements for surrogate spectrum models. Traditional analytic and computational models are derived from physics models which have a large body of empirical evidence for validation. The derived models used for specific scenarios require verification to ensure the physics were derived and coded correctly, and validation to ensure that the assumptions underlying the specific model are a good fit for the scenario being modeled. By contrast, data-driven models do not make direct use of well-validated physics, instead relying only on the available data and a good training/ testing methodology.

We investigate the role of validation in the context of data driven models. This includes different methods for mathematically and statistically scaling spectrum data; various error metrics for model evaluation; and the use of training/validation/testing data sets. Finally, we discuss methodologies for validating that a surrogate spectrum-prediction model is of sufficient quality to justify its use in place of a higher-cost model.

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#### Heteroskedastic Gaussian Process Meta-models for Improved Predictive Uncertainties

Technical Presentation. VVS2017-4060

10:50am - 11:15am

Jesper Kristensen, General Electric Co. - Global Research, Niskayuna, NY, United States, Isaac Asher, Kevin Ryan, You Ling, Liping Wang, Arun Karthi Subramaniyan, General Electric Co., Niskayuna, NY, United States

Gaussian Processes (GPs) have proven to be powerful meta-modeling tools. The Bayesian nature of the GP enables it to effectively fit hyperparameter distributions. However, classical GPs rely on strict assumptions about the hyperparameter distributions. Common assumptions include constant length scales and constant noise parameters throughput the input domain space. This can lead to regions of over- and/or underfitting. Data from real-world engineering applications rarely adhere to the classical-GP assumptions. Fitting classical GPs to this data results in inconsistent predictive uncertainty estimates. Meta-model predictive uncertainty is the foundation for data analysis techniques such as robust design optimization and intelligent design and analysis of computer experiments. Engineering applications employing these techniques need accurate predictive uncertainties to ensure a safe and successful product or process.

To address the issue of inaccurate predictive uncertainty, we improve the classical GP model by allowing its noise hyperparameters to vary over the input domain space. The predictive error on the training data or the leave-one-out cross validation (LOOCV) should be adequate measures of local uncertainty. We collect the LOOCV distribution during the GP building phase to quantify and inform the noise hyperparameters as a function of the input domain.

We develop a method which can build GPs with input-domain-dependent noise hyperparameters. The GP is built with Markov Chain Monte Carlo while the LOOCV is computed. The LOOCV is used to define an additional regression model for the noise estimator. This non-linear regression model can be recursive in nature and we show how to solve it. The result is a heteroskedastic GP with an input-domain-space-dependent noise parameter.

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We demonstrate the effectiveness of heteroskedastic GPs on example problems. The heteroskedastic framework creates meta-models with more correct predictive uncertainty estimates. In areas where the data is plentiful error bars will not be unnecessarily large due to the influence of other regions with high noise. Conversely, in areas where data is noisy and/or sparse, predictive uncertainty will be increased to more accurately represent the larger local uncertainty.

#### **Bayesian Tolerance Intervals for Sparse Data Margin Assessment**

Technical Presentation. VVS2017-4087

11:15am - 11:40am

Benjamin Schroeder, Lauren Hund, Sandia National Laboratories, Albuquerque, NM, United States

Uncertainty in experimental data may be caused natural variability in a population, measurement uncertainties that are inseparable from measured values, as well as many other sources. Such uncertain data are often compared against system requirements in order to aid a decision making process. One example of this comparison applied at Sandia National Laboratories is known as quantification of margins and uncertainty (QMU). A typical QMU workflow includes the following steps. First, specifying a common distributional form to describe the variability in the data. Then, using a statistical goodness-of-fit hypothesis test such as the Anderson-Darling (AD) test to determine if sufficient evidence to reject the proposed distributional form is present. If the distributional form is not reject, the distribution is used to calculate desired distributional characteristics for comparison with a specified performance requirement. Typical distributional characteristics of interest include high reliability requirements such as the 0.9999 percentile and tolerance intervals are then be used to make confidence statements such as "there is 90% confidence that at least 99.99 percent of the underlying true variability is less than the specified tolerance bound." Comparison of the tolerance interval and performance requirement allow for quantification of margin and uncertainty for the system's performance.

Clearly, in contexts where this type of certainty is required, great care should be taken to ensure overly confident estimates are not provided based on incorrect assumptions. Issues can arise with the aforementioned QMU approach when applied to sparse data situations. Goodness-of-fit tests lack power in sparse data situations and incorrect distributional choices can lead to significant errors in distributional characteristic estimation. Real world data rarely conforms to typical statistical distributional forms.

Given that we acknowledge that a dataset is unlikely to follow a specified standard statistical distribution, how should we measure our confidence in making extrapolative percentile estimates? Non-parametric methods exist and allow distributional form assumptions to be avoided, but such methods are still unable to prescribe confidence in extrapolative percentile estimates. Instead of making percentile extrapolations based solely on distributional assumptions, additional information can be integrated into the estimations using a Bayesian tolerance interval estimation approach. Additional information sources such as computational simulation results and expert knowledge can be integrated into Bayesian tolerance interval estimation through prior specification and

likelihood formation. Using prior information to specify distributional forms such as mixtures of distributions, Bayesian statistical methods can explore the uncertainty in distributional parameters, resulting in tolerance interval estimates. Illustration of some of the issues with sparse data margin assessment and how Bayesian tolerance intervals can be implemented in this context will be shown.

### Practical Challenges and Recommendations for Calibration, Validation, and Prediction under Uncertainty

Technical Presentation. VVS2017-4090

11:40am - 12:05pm

#### Joshua Mullins, Benjamin Schroeder, John R. Lewis, Lauren Hund, Sandia National Laboratories, Albuquerque, NM, United States

Across an array of engineering applications, a number of practical challenges arise when attempting to characterize and quantify uncertainty in calibration, validation, and prediction activities. These challenges stem largely from resource constraints that lead to sparse and/or imprecise data sets from which analysts are asked to inform high impact decisions. These data sets may either be from experiments (e.g., when hardware is expensive and/or challenging to replicate) or computational simulations (e.g., when simulations require extreme runtimes). In this presentation, we will discuss some of these common situations (providing some motivating examples) and offer recommendations for how best to cope with these real world constraints. Some common V&V/UQ approaches for handling these challenges will be discussed, noting the relevant strengths and weaknesses of each method. First, the topic of experimental uncertainty quantification will be addressed, including how the presence of this uncertainty should influence test selection and design of experiments. Second, the integration of experimental data into computational simulation activities such as sensitivity analysis and model calibration will be discussed with particular focus on how data uncertainty impacts the characterization of uncertainty in model inputs and parameters. Lastly, the contribution of uncertainty to model validation assessments will be considered. In particular, we comment on the effect of the validation result when extrapolating to predictions and making decisions such as systems margins assessments. This connection to decision making is particularly challenging in realistic applications since decision makers and analysts often have different goals and constraints.

#### Sequentially Refined Latin Hypercube Designs, with Application to Model Validation

Technical Presentation. VVS2017-4134

12:05pm - 12:30pm

Peter Qian, University of Wisconsin-Madison, Madison, WI, United States

Validation of a computer model often requires assessing output uncertainty with respect to a set of random inputs and computing sensitivity index of each input. Since computer models can be timeconsuming to run, it is desirable to minimize the sample size and in the

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meantime, achieve the most accurate uncertainty analysis. The Latin hypercube design has become very popular for conducting uncertainty analysis, sensitivity analysis and building surrogate or emulators for complex codes. For a given simulate code, it is often very difficult to fix the sample size of a Latin hypercube design. The use of iteratively enlarged Latin hypercube designs for verification and validation of a computer model has recently gained popularity. This approach conducts an initial experiment with a computer code using a Latin hypercube design and then runs a follow-up experiment with additional runs elaborately chosen so that the combined design set for the two experiments forms a larger Latin hypercube design. This augmenting process can be repeated multiple stages, where in each stage the augmented design set is guaranteed to be a Latin hypercube design. We provide a theoretical framework to put this approach on a firm footing. This new result shows that the sequential construction of Latin hypercube designs does not lose efficiency in sampling from the input distribution of a computer model. Examples are given to illustrate the sequential procedure, corroborate the derived theoretical results and demonstrate how the sequential procedure can be used for validation and calibration of computer codes in multiple stages.

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

### 11-1 VERIFICATION FOR FLUID DYNAMICS AND HEAT TRANSFER **1ST FLOOR, MESQUITE 2 10:25AM - 12:30PM**

On Issues Related to Estimation of Numerical Uncertainty in Transient Gas-Solid flow Simulations

Technical Presentation. VVS2017-4006

#### 10:25am - 10:50am

Ismail Celik, West Virginia University, Morgantown, WV, United States, Sofiane Benyahia, US DOE National Energy Laboratory, Morgantown, WV, United States, Sai S. Guda, MAE Dept., West Virginia University, Morgantwon, WV, United States, Madahava Syamlal, US DOE Morgantown Energy Technology Laboratory, Morgantown, WV, United States

Two-phase gas-solid flows simulations are usually performed in a transient manner (similar to large eddy simulations in single-phase flows) because they are more prone to chaotic dynamics arising from the presence of pseudo-turbulence even at very low Reynolds numbers. Here, "pseudo turbulence" is used in the context of having turbulence like structures with a high degree of randomness in flow parameters such as gas and solids volume fraction. This type of randomness cannot be classified as "turbulence" in the sense it is used for classical single-phase flows. There instabilities are triggered and eventual transition to turbulence occurs when a properly defined Reynolds number exceeds a threshold. Thus, transients in both the physical sense and in numerical implications play a significant role in estimation of numerical errors. The solutions can be periodic, semi-periodic with dominant frequencies related to for example bubbling motion, chaotic, and completely random. As such, the numerical

errors may consist of discretization errors superimposed by iteration errors, time or space averaging errors, and sometimes by interpolation errors. This study reports on segregation of the afore-mentioned errors and elucidation of their significance in calculation of the overall numerical uncertainty in a solution. This is done in the context of Richardson extrapolation and also using error transport equation approach. Based on the transient one-dimensional and two-dimensional simulation results it is found that discretization errors dominate the spatio-temporal occurrence of transition to chaotic flow regime, as well as the frequency and amplitude of periodic solutions. If this transition is not accounted for a priori, the scaling used in Richardson extrapolation becomes questionable. For pseudo-random solutions that resemble stationary turbulence, the starting time to avoid initial transients and the duration of the time averaging needed are difficult to predict, hence leading to non-negligible averaging errors which must be accounted for. The iteration errors in implicit calculations only exasperate the situation described above. Moreover, the techniques used in assessing the LES resolution of single-phase flows cannot be easily extended to transient multi-phase flow calculations. This is because the resolved turbulence depends not only on grid resolution, but also it is strongly influenced by the dynamic clustering of particles. As the grid is refined particle clustering may increase in certain regions which may lead to a decrease in turbulence in spite of the grid resolution being finer.

#### Uncertainty Quantification and Verification of Numerical Solutions for Water Flow over a Circular Cylinder in a Channel

Technical Presentation. VVS2017-4102

10:50am - 11:15am

Deify Law, California State University, Fresno, Fresno, CA, United States

In this present work, the effects of grid resolution and two-equation turbulence models such as k-epsilon and shear stress transport (SST) k-omega models on unsteady simulations of water flow over a circular cylinder in a channel are studied in ANSYS FLUENT. The channel is 18.02 inches (0.46 meters) in length, 3.05 inches (0.077 meters) in width, and 2 inches (0.05 meters) in height. The cylinder is located in the center of the channel both horizontally and vertically and is perpendicular to the flow direction. The cylinder has a diameter of 0.64 inches (0.16 meters). Grid-convergence index (GCI) study will be performed to quantify the numerical uncertainty. The ASME Verification and Validation (V&V) 20 Standard is followed to estimate the validation comparison error and the validation uncertainty. The simulations of water flow over the cylinder are verified with the laser Doppler anemometry (LDA) experiments conducted in-house. Additionally, the dominant factor in influencing the accuracy of numerical solutions will be determined among the effects of grid resolution and turbulence models on numerical simulations. ANSYS FLUENT uses a finite-volume technique to integrate the time-dependent equations of motion that govern fluid flows over a finite volume defined a grid element. The pressure-correction technique such as the semi-implicit method for pressure linked equations (SIMPLE) is employed in FLUENT. The geometries are made and meshed in ANSYS Workbench. The absolute convergence criterion is set to 1E-07 for all dependent variables. Second order upwind discretization is used to discretize the convective terms of Navier-Stokes equations.

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#### Recent Advances in Discretization Error Estimation Using Error Transport Equations

Technical Presentation. VVS2017-4106

11:15am - 11:40am

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

Discretization Error Transport Equations (ETE) offer a number of advantages for error estimation relative to existing techniques such as Richardson extrapolation and adjoint methods. Richardson extrapolation requires between two and three systematically-refined grids, all of which need to be in the asymptotic range. When refinement by a factor of two in each direction is used, this typically requires an order of magnitude increase in computational cost with each successive level of mesh refinement. For example, if a mesh size of 1 million cells is required to obtain an asymptotic solution, then two additional solutions on meshes of 8 million and 64 million cells must also be computed. ETE, on the other hand, requires a solution (called the primal solution) on a single grid followed by an (inexpensive) linear solution on the same grid. For the prior example, this would require one solution on a mesh of 1 million cells, followed by a linear solution (at a fraction of the cost of the primal solution) on the same mesh.

While adjoint methods have become the method of choice for estimating discretization error in global solution functionals (such as lift and drag for an aerodynamics simulation), the linearized version of ETE has been shown to be mathematically equivalent to adjoint methods under certain conditions [1] and offers a number of advantages compared to adjoints.

- ETE provides error estimates in all solution functionals simultaneously (whereas one would need to solve a separate adjoint problem for each functional) [2].
- ETE provides error estimates in local field quantities as well as velocities and pressures (whereas one would need to solve a separate adjoint problem for each quantity in each computational cell) [1].
- The discretization error estimates from ETE, when applied as corrections to the primal solution, have been shown to increase the order of accuracy of the corrected solution for all global and local quantities (adjoint methods can only correct a single global quantity to higher order with each adjoint solve).
- 4. ETE can provide reasonable error estimates (both local and global) for cases where the linearization is approximate, e.g., when a linearized Jacobian for a second order discretization is approximated by the linearized Jacobian of a first-order discretization (it is unclear if this would be the case for adjoint methods).

This talk will demonstrate the advantages of ETE versus both adjoints and Richardson extrapolation for the case of inviscid, isentropic flow in a quasi-1D nozzle.

References:

- W. C. Tyson and C. J. Roy, "A Hybrid Adjoint/Error Transport Approach to Error Estimation, Adaptation, and Higher-Order Solutions for Computational Fluid Dynamics"? AIAA Paper 2017-0741, 55th AIAA Aerospace Sciences Meeting, 9-13 January 2017, Grapevine, TX.
- 2. W. C. Tyson, K. Swirydowicz, J. M. Derlaga, C. J. Roy, and E. de Sturler,

"Improved Functional-Based Error Estimation and Adaptation for CFD Applications"? AIAA Paper 2016-3809, 46th AIAA Fluid Dynamics Conference, 13-17 June 2016, Washington, D.C.

### Thermal-Hydraulic Performance of Aluminum Foam Heat Exchangers with Varying Cellular Lattice Structures

Technical Presentation. VVS2017-4138

11:40am - 12:05pm

Edward Kraft, Texas A&M University, College Station, TX, United States

Due to their large surface area to volume ratio, low density, and high strength structure, aluminum metal foams offer a promising application for heat exchangers. One significant design challenge of aluminum foam heat exchangers is optimizing the trade-off between heat transfer performance and pressure drop (i.e., pumping power). Previous experimental investigations successfully quantified the thermal hydraulic behavior of such heat exchangers based on foam porosity, but provide limited insight on the effects of varying cellular lattice structures within their samples. As a result, a CFD analysis using Star CCM+ is carried out for the thermal hydraulic behavior of aluminum foam heat exchangers made of 8 x 8 x 8 lattices based on relative density, unit cell geometry, and unit cell orientation. The k-? model is utilized with applied boundary conditions taken from experiment data to describe the turbulent flow through the heat exchanger. A Grid Convergence Index (GCI) method is used for all models to estimate the discretization error for verification. Numerical results are compared to the experimental data for validation, and the samples are quantified and ranked based on thermal hydraulic performance.

#### Validation and Verification of Simulation Results of an Ultra-Low NOx Burner

Technical Presentation. VVS2017-4124

12:05pm - 12:30pm

Sandeep Alavandi, David Cygan, Gas Technology Institute, Des Plaines, IL, United States, Anchal Jatale, Ansys, Houston, TX, United States, Muhammad Sami, Ansys Inc., Katy, TX, United States

Performing testing for each burner design change requires significant resources. Hence, design changes were made to the Computational Fluid Dynamics (CFD) model and simulations were performed to evaluate and predict the performance of the burner. However, it is necessary to

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quantitatively evaluate the degree of productivity (the measure of accuracy) and quantification of the numerical error. In general, there is a lack of formal scientific verification and validation with uncertainty quantification standards in all industrial sectors and addressing the level of confidence in the prediction extracted from the simulation is extremely beneficial to the industry.

This paper will present the quantitative verification and validation of the numerical error balanced by the need to conserve computational resources. A method to perform verification, validation and uncertainty estimation was applied and results indicated how the uncertainties from the input parameters transferred to the outputs of the CFD simulations. This method includes performing a grid resolution study for solution verification followed by creation of design of experiments. Reduced order models were then created from the Design of Experiments (DOE) results for the use in sampling methods like Monte Carlo in order to estimate the uncertainties. These simulation results and their uncertainties were then compared with experimental data and its uncertainties.

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

#### 4-2 UNCERTAINTY QUANTIFICATION: THEORY PART 2 2ND FLOOR, PALO VERDE B 1:30PM - 3:35PM

Computational Uncertainty Quantification for Predicting the Reproducibility of Experiments in Fluid Dynamics

Technical Presentation. VVS2017-4068

1:30pm - 1:55pm

Denis F. Hinz, Alouette van Hove, Kamstrup A/S, Skanderborg, Denmark

Achieving good reproducibility in fluid flow experiments can be challenging, in particular in scenarios where the experimental boundary conditions are obscure. We use computational uncertainty quantification to predict the repeatability and reproducibility of such experiments. Swirl disturbance generators are commonly used to test the robustness of flow sensors. The characteristics of the disturbed inflow at the sensor are dependent on the type of disturber, the distance between the disturber and sensor, as well as the flow conditions upstream from the disturber. The exact inlet velocity profile at the disturber, however, is often difficult to assess and reproduce, which might reduce the overall reproducibility of the experiment. We investigate the spatial development of velocity profiles downstream from a symmetric and asymmetric swirl disturbance generator subject to arbitrary inlet profiles. The variation in the flow patterns as a consequence of the arbitrary inflow conditions is considered a measure for the repeatability and reproducibility of the swirling flow. Using a non-intrusive polynomial chaos method in combination with OpenFOAM, we obtain the expected value and variance of the crosssectional velocities downstream from the symmetric and asymmetric swirl disturbance generators. Our results suggest that swirling flow downstream from the symmetric swirl disturber is more reproducible at distances smaller than 5 pipe diameters from the disturber. In contrast, at distances

larger than 50 pipe diameters, the flow downstream from the asymmetric swirl disturber is more reproducible. In general, the variance of the axial velocity shows a minimum around the pipe center.

We discuss how this application of computational uncertainty quantification can be used to achieve a better design of experiments for the systematic investigation of flow sensors.

#### A Verification Process for Surrogate Models: Applications to Stress Intensity Factors

Technical Presentation. VVS2017-4085

1:55pm - 2:20pm

*James Sobotka*, R. C. McClung, Southwest Research Institute, San Antonio, TX, United States

This presentation provides an overview of a developing process to establish credibility for surrogate models that cover multi-dimensional, continuous solution spaces. These surrogate models abstract away underlying complexity from users who only provide limited input. However, the abstraction leads to a disagreement between the surrogate model's results and results from precise computational benchmark solutions. In our verification process, this disagreement is quantified using descriptive statistics to support uncertainty quantification, sensitivity analysis, and surrogate model assessments.

Our focus is stress intensity factor (SIF) solutions. SIFs can be evaluated from simulations (e.g., finite element analyses), but these simulations require significant pre-processing, computational resources, and expertise to produce a credible result. It is not tractable (or necessary) to directly simulate a SIF for every crack front. Instead, most analyses of fatigue crack growth employ surrogate SIF solutions based on some combination of mechanics, interpolation, and SIF solutions extracted from earlier analyses.

SIF values from surrogate solutions vary with crack-front stress profiles and several non-dimensional degrees-of-freedom that define the geometry. The verification process treats these inputs (stress profiles and geometry) differently. Stress profiles are selected to exercise principal components of possible gradients (e.g., linear variation over a distance). Hundreds of geometries are selected by Latin Hypercube Sampling to limit redundancy, to fill the design space, and to cover both realistic geometries and extreme configurations. The verification process evaluates the selected stress profiles and the sampled geometries using the surrogate model and a benchmark code (Abaqus).

This presentation shows relevant comparisons between the benchmark code with available exact solutions and legacy solutions to build credibility. The benchmark code employs a Python scripting interface to automate model development, execution, and extraction of key results. The benchmark solution's quality has been extensively checked by visual inspection and numerical metrics.

The ratio of the test code SIF to the benchmark code SIF quantifies agreement for one geometry and loading. Descriptive statistics of these ratios provide convenient measures of relative surrogate quality: mean,

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median, standard deviation, and 5/95% values. Thousands of analyses support visualization of the surrogate model's credibility: predicted vs. actual plots, histograms, and rank-ordering of the agreement ratios, i.e., cumulative distributions functions. Consequently, the verification process results in statistical measures that describe uncertainty of the surrogate model (relative to benchmark solutions). These statistical measures may then be propagated into subsequent analyses and evaluations.

#### Prediction Confidence Estimation in System Output using a Roll-up Methodology

Technical Presentation. VVS2017-4119

2:20pm - 2:45pm

Kyle D. Neal, Chenzhao Li, Zhen Hu, Sankaran Mahadevan, Vanderbilt University, Nashville, TN, United States

Model calibration can be used to infer unknown parameters of a complicated system using observation data of the system response. The calibration results can then be propagated through the system computational model to predict the uncertainty in the system response. However, experimental data may not be available for the quantity of interest thus the calibration of model parameters can only rely on available data from other quantities. Often, experimental data may only be available for a subsystem or lower level which is less complex than the full-scale system of interest. When the subsystem shares the same model parameters with the system, the calibrated model parameters from the subsystem can be extrapolated across levels and used in predicting the quantity of interest. If validation tests are also performed at the lower levels, these can be incorporated in the integration of model calibration and validation results, and propagation of the resultant uncertainty to system-level response (the roll-up concept). The model reliability metric is used to assess the validity of the model used for calibration, based on validation test data. The roll-up distributions are compared against system level calibration posteriors; this comparison is done through global sensitivity analysis. The extrapolation confidence is guantified based on the global sensitivity analysis results. In addition to the forward problem of prediction confidence estimation, this work also addresses the inverse problem of test selection and test design. An optimization procedure is

formulated to maximize roll-up confidence by selecting the most valuable calibration and validation tests at the lower levels. Then the selected lower level tests are designed to maximize the information gain.

The proposed method is applied to the multi-level Sandia dynamics challenge problem (Red-Horse and Paez 2008) which is composed of a system level and two lower levels of lesser complexity. Both forward and inverse UQ problems are investigated - confidence in the system-level prediction is quantified in the forward problem, and lower-level tests are selected and designed in the inverse problem to maximize the systemlevel prediction confidence.

This work is funded by Sandia National Laboratories (Technical Monitor: Joshua Mullins).

References:

Red-Horse, J. R., and T. L. Paez. "Sandia national laboratories validation workshop: structural dynamics application." Computer Methods in Applied Mechanics and Engineering 197, no. 29 (2008): 2578-2584.

#### Gradient-enhanced Gaussian Process Surrogate Models, with Application to Model Validation

Technical Presentation. VVS2017-4135

2:45pm - 3:10pm

*Peter Qian*, University of Wisconsin-Madison, Madison, WI, United States, *Xu He*, Chinese Academy of Science, Beijing, China

How to incorporate gradient info of a computer code is an important problem in verification and validation of computer models. Since such a computer model is expensive to run, the model is often run with a carefully chosen design of experiments and then the data are used for building a surrogate model or called emulator for the computer model. The emulator can then serve as a proxy in conducting detailed model verification and validation that involves prediction, optimization, inverse analysis, sensitivity analysis and uncertainty propagation. The gradient-enhanced Gaussian process emulator is widely used to jointly model the output and its gradients from a computer model. Often there is a trade-off between the statistical and numeric accuracy of an emulator. Indeed, the more data that are available, the better the statistical accuracy that the emulator will typically possess; on the other hand, the emulator can encounter greater numerical problems as the sample size grows, which adversely affects its accuracy. The gradient-enhanced Gaussian process emulator has more numeric problems than in many multivariate cases because of the dependence of the model output and each gradient output. We derive a statistical theory to understand why this problem happens. Our theoretical analysis compares the smallest eigenvalue of the covariance matrix of the ordinary Gaussian process emulator and its counterpart of the gradientenhanced Gaussian process emulator. These results show that the latter will decay much faster as the distance of points approaches to zero. Examples are provided to illustrate the derived results and how to overcome the challenges in using Gradient-enhanced Gaussian process emulators for model verification and validation.

### Evaluation of Uncertainty Treatments for Sparse Samples of Random Variables and Functions

Technical Presentation. VVS2017-4070

3:10pm - 3:35pm

Matthew Bonney , Nicole Breivik, James F. Dempsey, John R. Lewis, George Orient, Vicente Romero, Benjamin Schroeder, , Justin Winokur, Sandia National Laboratories, Albuquerque, NM, United States, Bonnie Antoun, Sandia National Laboratories, Livermore, CA, United States

This talk examines the variability of predicted responses when multiple stress-strain curves (reflecting random variability from replicate material

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tests) are propagated through a finite element model of a ductile steel can being slowly crushed. Over 140 response quantities of interest (including displacements, stresses, strains, and calculated measures of material damage) are tracked in the simulations. Highly nonlinear input-to-output response mappings and non-standard response distributions are involved. Each response quantity's behavior varies according to the particular stress-strain curves used for the materials in the model. We desire to estimate response variability when only a few stress-strain curve samples are available from material testing. Propagation of just a few samples will usually result in significantly underestimated response uncertainty relative to propagation of a much larger population that adequately samples the presiding random-function source. Several statistical methods are tested for effectively treating the sparse data. A multi-attribute weighted performance metric is used to assess the methods? Cost-accuracy-risk performance in estimating various statistics of response over thousands of random trials for each of the 140 response quantities. Performance trends of the various methods are presented. Because of the breadth and depth of this survey, the methods' performance trends may largely apply for other sparsely sampled random variable or function data, whether from experiments or models.

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

### 5-1 VALIDATION FOR FLUID DYNAMICS AND HEAT TRANSFER 2ND FLOOR, PALO VERDE A 1:30PM - 3:35PM

Validation of Continuum Modeling for the Molecular-level Transport Phenomena

Technical Presentation. VVS2017-4026

1:30pm - 1:55pm

#### Yechan Noh, Bohung Kim, University of Ulsan, Ulsan, Korea (Republic)

The validity and limitations of continuous variation of thermodynamic properties in molecular-scale fluid flow and heat transfer are key to providing extended predictions in computational modeling and simulation. In molecular-level momentum/heat transport, the behavior of the molecular system still be predicted through the continuum description based on the differential equation and conservation law, if the system locally satisfy the ergodic hypothesis and the scale of the average is enough to recover the classical thermodynamic properties. However, even in this case, most of governing equations based on continuum prediction (differential form) can cause serious errors due to inaccuracies of boundary conditions in many respects. In short, molecular-level momentum/heat transfer presents significant different responses from continuum modeling because of the interfacial phenomena, and with the boundary definition of line. Therefore, in this study, we present the result of our investigations using molecular dynamics (MD) simulations with modified continuum-based modeling to confirm the validity of the continuum hypothesis. When continuum modeling is given an accurate definition of the interface line to the boundary conditions of continuum modeling, the analytical solution shows that nanometer-sized momentum / heat transport can be properly predicted. The approach of this study has an important impact on overcoming the current limitations in modeling / predicting the behavior a molecular scale system.

#### CFD-DEM and Experimental Investigation of Horizontal Jets in Fluidized Bed of Geldart Group D Particles: Preliminary Activity

Technical Presentation. VVS2017-4038

1:55pm - 2:20pm

Peiyuan Liu, William Fullmer, Casey Q. LaMarche, Christine M. Hrenya, University of Colorado, Boulder, Boulder, CO, United States, Rasa Kales, Allan Issangya, Ray Cocco, PSRI, Chicago, IL, United States

Experiments were undertaken at PSRI with the intent to provide a validation benchmark problem with characterized uncertainties for the coupled computational fluid dynamics-discrete element method (CFD-DEM) modeling approach. This talk will: i) introduce the horizontal jet fluidized bed problem, ii) discuss the methods used to measure the uncertainty in the particle property variables, iii) overview the CFD-DEM numerical method, and iv) report preliminary sensitivity analysis of the model to the measured uncertainties.

A semi-circular bed approximately 1 foot in diameter is used to fluidize solid particles in ambient air passed through a porous plate-wire mesh distributor. Of the several different particles considered, we focus here on studies of 6 mm plastic beads, falling into the Geldart Group D classification. The bed is operated at 10% above and below minimum fluidization. Two opposing high speed air jets operate near the flat face of the unit at two different elevations: approximately 2 and 6 inches above the distributor plate. The column is made of acrylic which allows for the use of a high speed video camera to capture the dynamics of the particles. The bed pressure drop is measured with pressure taps in and above the fluidized bed region (roughly 12 inches of static bed height).

The particle properties needed for CFD-DEM analysis are characterized largely with image/video analysis. The particle size and shape are measured with a series of static images of particles. The restitution coefficient (which characterizes the degree of kinetic energy dissipated during collisions) is measured by analyzing the height of the bounce of a

falling particle. Similarly, the static coefficient of friction is determined by recording and tracking the sliding motion of four-particle sleds down an inclined plane.

The primary feature of the CFD-DEM modeling strategy is that the motion and contact of each individual particle is exactly resolved by solving Newton's equations of motion. The linear spring dashpot, a soft-sphere model, is applied for collisions. A coarse fluid grid is applied, typically on the order of 2 particle diameters. This makes the CFD-DEM method much more computationally efficient than full direct numerical simulation, but also necessitates the use of closure laws, specifically a mean drag law. Preliminary results for the jet penetration distance, the SRQ of interest, will be presented. Further, we hope to report on a systematic sensitivity analysis of the SRQ to the input parameters, which is currently work in progress.

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#### Discharge Coefficient Prediction through an Orifice Plate in a Round Pipe: Experimental and Numerical Investigation

Technical Presentation. VVS2017-4046

2:20pm - 2:45pm

#### Nicolas Lancial, Herve Gamel, Emmanuel Thibert, Nicolas Dessachy, Jose Veau, Arnaud Barthet, EDF R&D, Chatou, France

A square-edged orifice is a pressure differential device commonly used for flow measurements in EDF's nuclear power plants. The present study presents experimental data obtained on EDF R&D test bench for an orifice plate and computational fluid dynamics calculations (CFD) using the k-e turbulence model to predict velocity fields, pressure loss and discharge coefficient around this device. Investigations focus on flow rate through the circular square-edged orifice in a round pipe at a Reynolds number close to 8.69E+05. Two pipe configurations have been tested: one with 44D upstream straight length and the second with 9.4D upstream straight length. Velocity profiles are obtained from Laser Doppler Velocimetry measurement (LDV). Simulations presented are only performed for 44D configuration with an open source CFD package developed by EDF (Code\_Saturne). Numerical sensitivity studies are carried out using different mesh refinements of the k-? turbulence model. Discharge coefficient prediction from CFD are compared with ISO 5167 value for 44D upstream straight length. The percentage change in CD is near 2%. Comparison between experimental and numerical velocity fields is promising, with a maximum relative error close to 2.5% upstream and 3.4% downstream of the orifice plate in the center of the pipe.

#### Comparison of k-Omega and k-Epsilon Turbulence Models and Model Parameters for Low-Reynolds Number Turbulent Flows through an Axisymmetric Constriction in a Circular Pipe

Technical Presentation. VVS2017-4072

2:45pm - 3:10pm

#### Christopher Basciano, Caleb Triece, Siva Balasubramanian, Patrick Downie, BD, Research Triangle Park, NC, United States

Most turbulence models in commercial computational fluid dynamics (CFD) software codes are designed to operate at Reynolds numbers above 10,000. However, many laminar-flow solvers are not able to attain accurate, converged solutions at Reynolds numbers (Re) between 2,500 and 10,000. To provide insight on appropriate model selection and to analyze the impact of individual model parameters, the current study compared the calculated flow fields of multiple well-known, two-equation turbulence models (e.g., k-Omega and k-Epsilon) implemented in the commercial CFD code ANSYS Fluent v17.2. Constant inlet volumetric flow rates at Reynolds numbers less than 10,000 through an axisymmetric constriction in a circular pipe were used as the comparator case between the different turbulence models. The flow regime varied from steady, laminar flow to low Reynolds number turbulent flow that can be treated as statistically steady, such that the time-averaged flow field is constant over time. Experimental data previously published for the same geometry in scientific literature for two of the analyzed Reynolds numbers was used to inform baseline comparisons between the different models and model parameters. Turbulence model comparisons maintained consistent numerical settings (e.g., domain discretization, convergence thresholds, and boundary conditions) but the numerical settings' potential impact on a model's calculations were also investigated. More than ten different permutations of popular two-equation turbulence models were compared against the experimental data, which included equation modifications for low Reynolds Number settings. The study revealed the SST k-Omega and the Realizable k-Epsilon models calculated velocity profiles (at specific locations downstream of the constriction) that were closest to the experimental data. In addition, the model parameter sensitivity of each model was shown to have a varying impact on the calculated velocity profiles at different Reynolds numbers. The previously described simulation work aimed to establish a solid foundation for assessing the capability of common two-equation turbulence models to accurately calculate steady, internal flow fields within circular conduits at Reynolds numbers between 2,000 and 10,000.

### Validation of the Multi-Mesh and Multi-Solver Rotorcraft Simulation Code

Technical Presentation. VVS2017-4091

3:10pm - 3:35pm

Buvana Jayaraman, Science & Technology Corp., Moffett Filed, CA, United States, Andrew Wissink, Mark Potsdam, Rohit Jain, Joshua Leffell, Joon Lim, US Army ADD, Moffett Field, CA, United States, Beatrice Roget, Vinod Lakshminarayan, Science & Technology Corp., Moffett Field, U S Minor Island, Jayanarayan Sitaraman, Parallel Geometric Algorithms, Sunnyvale, CA, United States

The Helios (Helicopter Overset Simulation) software is the rotary-wing product of the HPCMP CREATETM-AV program, providing high-fidelity Computational Fluid Dynamics (CFD) and Computational Structural Dynamics (CSD) simulation capability for modern rotary-wing aircraft. Helicopters experience a significantly complex flow field due to a variety of complex flow phenomena such as the unsteady interactional aerodynamics between the rotor blades and the fuselage, blade tip vortices, and stall on the retreating side. The high-fidelity multi-disciplinary capabilities in Helios makes it a unique and powerful tool for simulating the complex physics experienced by helicopters and is increasingly being used in conjunction with model and flight test as a DoD acquisition tool for the procurement of new rotary-wing aircrafts.

Helios uses a multi-mesh paradigm that enables the use of structured, unstructured, or strand meshes in the near-body region to accurately capture the viscous turbulent flow and a higher-order Cartesian off-body solver with adaptive mesh refinement (AMR) to accurately resolve the rotor wakes. Fully automatic and parallel domain connectivity solver PUNDIT handles the overset region between the near-body and off-body solvers. MELODI handles the fluid structure interaction, mesh motion and deformation. The comprehensive analysis tools RCAS and CAMRAD are used for solving the structural dynamics and trim. A flexible python software integration framework enables the communication between the various modules in Helios. A body-hierarchy based Graphical User Interface (GUI) is used to support the geometry and input setup for Helios.

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Extensive validation of the complex physics and the different solvers in Helios is routinely carried out for a range of conditions such as hover, forward, and maneuvering flights experienced by the rotorcraft. In this presentation we will present the results from this validation study by comparing the aerodynamic loads and rotor wake predictions with the experimental data for the UH60A and HARTII rotors.

#### References:

- Wissink, A.M., Sitaraman, J., Jayaraman, B., Roget, B., Lakshminarayan, L., Potsdam, M., Jain, R., Leffell, J., Forsythe, J., Bauer, A.,?Recent Advancements in the Helios High-Fidelity Rotorcraft Simulation Code," AIAA-2016-0563, 54th AIAA Aerospace Sciences Meeting, San Diego, Jan 2016.
- Wissink, A.M, Jayaraman, B., and Sitaraman, J., "An Assessment of the Dual Mesh Paradigm Using Different Near-Body Solvers In Helios," AIAA-2017, 55th AIAA Aerospace Sciences Meeting, Grapevine, TX, Jan 2017.

#### TRACK 13 VERIFICATION AND VALIDATION OF MEDICAL DEVICES

### 13-1 VERIFICATION AND VALIDATION OF MEDICAL DEVICES 2ND FLOOR, ACACIA D 1:30PM - 3:35PM

Sensitivity of Aortic Hemodynamics to Uncertainty in Aortic Valve Prosthesis Placement

Technical Presentation. VVS2017-4040

#### 1:30pm - 1:55pm

Kay Brosien, Jens Schaller, Jan Bruening, Florian Hellmeier, Charité - Universitätsmedizin Berlin, Germany, Sarah Nordmeyer, Marcus Kelm, Titus Kuehne, German Heart Institute, Berlin, Germany, Leonid Goubergrits, Charité, Berlin, Germany

Hemodynamic outcome of the surgical replacement of the aortic valve as well as predictive modelling of hemodynamics after the virtual valve replacement are affected by the 3D orientation of the valve prosthesis. The aim of this study was to quantify the variability of post-treatment hemodynamics due to uncertainty in the positioning of a mechanical bi-leaflet aortic valve prosthesis using MRI based CFD analysis. Prior to this study, five clinicians and five biomedical engineers were asked to identify the valve prosthesis annulus plane in a patient-specific geometry. The angular deviation of these planes from the mean plane was 7.5°±7.0°, indicating uncertainty in the positioning of valve prostheses.

A CAD model of the 23 mm On-X (CryoLife, USA) bi-leaflet valve was virtually inserted into the patient-specific geometry. The rotation and the tilting angle of the prosthesis were varied. According surgical information, valve leaflets were oriented parallel to the ventricle septum wall, this was the rotation angle of 0°. The rotation angle was increased in 30° steps to 150°. Additionally, tilting angles of 0°,  $\pm$ 5° and  $\pm$ 10° were varied at a rotation of 0° and 90°, resulting in 14 different valve orientations. The valve placement procedure and flow simulations were performed using

STAR-CCM+ (v.11.04, CD-adapco, USA) and relevant hemodynamic parameters were compared. The virtual placement procedure used the Overset Mesh method.

The transvalvular pressure drop varied between 4.0 and 8.0 mmHg depending on the rotation and tilting angle. Furthermore, the flow profile downstream of the prosthesis was altered by the valve position, resulting in variation of the aortic pressure drop between 2.3 and 4.5 mmHg. The surface averaged wall shear stress varied between 7.5 and 10 Pa, which could be considered neglectable. However, different valve positions caused large variations of the secondary flow degree (SFD) between 0.13 and 0.5. SFD is a measure characterizing secondary flow features defined as the ratio of the in-plane velocity and the through-plane velocity.

While the degree of freedom of the valve orientation during the implantation may be small, even minor changes could cause remarkable differences in hemodynamic parameters. Knowledge of this sensitivity of hemodynamics to the valve position could support development of novel valve prostheses as well as an optimization of valve treatment itself. The results presented here are limited to one patient-specific case and one valve type. Future studies should include a larger cohort of patient-specific cases as well other valve prostheses.

#### Best Practice Guidelines for Patient Specific CFD Simulations Involving Virtual Deployment of Device

Technical Presentation. VVS2017-4078

1:55pm - 2:20pm

#### Santhosh Seshadhri, Medtronic, Hyderabad, Telangana, India

Computational flow dynamics (CFD) is being increasingly used for patient specific studies and its corresponding scientific publications has shown a significant raise in the past decade. With the availability of powerful computational resources, CFD modelling is efficient in creating device designs that can decrease the need for expensive prototyping and laboratory testing. However there are no standardized methods available for using CFD techniques to assess safety of the final medical device designs. Also there is no general agreement on the quantities that should be computed and the most adequate one for interventional support. As an effort to provide best practice guidance the accurate representation of the patient geometry is first addressed. Computational mesh plays a critical role in the outcome of the CFD results and is specially challenging for devices as small as stent. Another challenge is the description of fluid properties. Finally the quantitative outcome of the simulation results is necessary to support interventional decision. In the present work an effort has been made to analyze the most important steps of CFD simulation for patient specific geometries involving virtual stent implantation. From the

outcome of this work best practice guidelines are proposed for the quality evaluation of CFD simulations and not on their medical aspect. The results from this work could be used as a reference for further patient specific CFD analysis.

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#### **Pallet Temperature Model Validation**

Technical Presentation. VVS2017-4110

2:20pm - 2:45pm

*Eugen Nisipeanu, Carlos Corrales, Baxter Healthcare Corporation, Round Lake, IL, United States* 

Good distribution practices of medical intravenous solutions require specification of storage, transportation and distribution temperature conditions. A homogenized heat conduction model was developed to predict product temperature based on ambient temperatures corresponding to various geographical regions and during all seasons.

Various input parameters of the model were calibrated with experimental (training) data at similar locations between experiment and model. A parameter optimization technique was used to determine key input parameters. Finally, the calibrated model was verified and validated following ASME VV20. Uncertainty of the simulation results as well as the experimental data used in the validation was quantified. The levels of verification and validation were driven by risk, per a draft of ASME VV40.

The predictions from this model are intended to be utilized in Baxter investigation efforts where decisions are made to release or discard product that might have reached temperatures outside its allowed limits.

#### Validation Evidence and Regulatory Context of Use: The Need for a Validation Framework for Applications in Evaluation of Automated Fluid Resuscitation Systems

Technical Presentation. VVS2017-4115

#### 2:45pm - 3:10pm

Bahram Parvinian, FDA, Silver Spring, MD, United States, Ramin Bighamian, UMD, College Park, MD, United States, George Kramer, UTMB, Galveston, TX, United States, Richard Gray, FDA, White Oak, MD, United States, Farid Yaghoubi, FDA, White Oak, MD, United States, Tina Morrison, Food and Drug Administration, Silver Spring, MD, United States, Sandy Weininger, FDA, White Oak, MD, United States, Jin Oh Hahn, University of Maryland, College Park, MD, United States, Christopher Scully, FDA, White Oak, MD, United States

Fluid resuscitation is a lifesaving treatment for patients with critical conditions such as hypovolemia, burn injuries, and septic shock. This type of critical care therapy may benefit from increased automation due to its labor intensive nature and ever increasing physical and cognitive workload of clinicians in intensive care units. Use of fluid resuscitation models for design and evaluation of automated fluid delivery systems provides an opportunity for systematic design and evaluation of such systems in challenging clinical scenarios. While there is an abundance of modeling strategies and approaches giving rise to models with wide spectrum of complexity and clinical utility, the validation aspect of these models has not been rigorously investigated. In this presentation, we present a model of physiological response to fluid infusion and hemorrhage consisting of three sub-models associated with blood volume, cardiac output and blood pressure. We then present the

validation activities and types of evidence that may be used to build confidence in the validity of the model thus rendering it credible for design and evaluation of automated fluid resuscitation systems. First, we discuss the calibration step in which the model's ability to be tuned to the observed data is assessed. Second, we discuss the internal validation step1 in which the model's ability to predict unpresented data similar to the calibration data is assessed. Finally, information presented on model structure, properties, and its validation steps will be combined in a framework based on the V&V40 subcommittee draft standard2. We propose modifications to this framework which would render it applicable to the model of fluid resuscitation proposed in this study. We also discuss the future directions on validation steps including potential use of an independent study results for external validation1.

References:

- Guidance for Industry "Population Pharmacokinetics" Food and Drug Administration Center for Drug Evaluation and Research 1999.
- http://www.fda.gov/downloads/MedicalDevices/NewsEvents/ WorkshopsConferences/UCM358733.pdf

#### Disclosure Statements:

Ramin Bighamian and Jin-Oh Hahn have a pending patent related to the blood volume model presented in this study. This material is based on work supported by the Office of Naval Research (ONR) under Grant No. N000141410591, N000141512018, N0001412C0556, and the Food and Drug Administration (FDA) under the Medical Countermeasures Initiative. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the ONR.

#### CFD Optimization and Verification of a Novel, Implantable Rotary Blood Pump Using PIV

Technical Presentation. VVS2017-4120

3:10pm - 3:35pm

J. Ryan Stanfield, University of Utah, Salt Lake City, UT, United States, James Stewart, VADovations, Oklahoma City, OK, United States, Jingchun Wu, Advanced Design Optimization, Irvine, CA, United States

The use of Ventricular Assist Devices (VADs) becomes more commonplace in heart failure patients. The extended use of these devices requires improved hemocompatibility to ensure minimal blood damage. Computational Fluid Dynamics (CFD) is employed to predict blood damage by way of Normalized Index of Hemolysis (NIH), thrombogenicity models, and others. The basis of these models requires an accurate prediction of the flow field and the forces the blood is exposed to during transit through the pump. Here, we report comparisons and validations of CFD predictions via Particle Image Velocimetry (PIV) for a novel, implantable VAD.

Blood flow through the VAD is bounded by a 7mm hydraulic diameter and driven by a rotating impeller. A unique radial inlet geometry and vaned diffuser guide blood into and out of the pump, respectively. For this study

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we primarily use the two-equation Shear Stress Transport (SST) eddyviscosity turbulence model, employing the k-w model in the inner region with the k-e model in the free shear flow region. Optically transparent models and blood analog fluids are created for use in PIV measurements. The velocity vectors of the flow field are obtained and used to derive areas of high shear, stagnation, recirculation, dwell time, etc. The particle exposure history is computationally analyzed by Lagrangian method. The parameters captured in PIV are compared to CFD predictions and used to validate the results. Pressure and averaged volume flow rate are also obtained external to PIV to confirm accuracy of operating conditions.

Direct comparisons are made for a variety of flow conditions, including a typical 3 L/min volume flow rate and 40 mmHg differential pressure at a pump speed of 16000 rpm. Experimental and numerical uncertainties are obtained from experimental data and estimated from grid-refinement studies, respectively. CFD over predicts the results by way of velocity vectors taken at the meridional section.

### TRACK 1 CHALLENGE PROBLEM WORKSHOPS AND PANEL SESSIONS

## 1-1 V&V BENCHMARK PROBLEM - TWIN JET COMPUTATIONAL FLUID DYNAMICS (CFD) NUMERIC MODEL VALIDATION 2ND FLOOR, ACACIA D 4:00PM - 6:05PM

Application of Verification and Validation Techniques in Computational Fluid Dynamics Modeling of Turbulent Twin Jet Flow

Technical Presentation. VVS2017-4033

**Thomas Acker, Seth Lawrence**, Northern Arizona University, Engineering Department, Flagstaff, AZ, United States, **Earl P.N. Duque**, Intelligent Light, Rutherford, NJ, United States

Ubiguitous application of CFD motivate the need to verify and validate CFD models and quantify uncertainty in the results. The objective of this paper is to present results from a verification and validation study of the ASME benchmark turbulent twinjet problem using the commercial CFD code ANSYS Fluent. The twinjet is modeled in two- and three-dimensions, and results are compared with experimental data. Depending upon the solver set-up, the 2-D model converges to a non-physical solution, a result not found in the 3-D simulation. However, choosing the SIMPLEC algorithm in the 2-D model led to a realistic solution and was subsequently applied in both the 2-D and 3-D models. A grid refinement study was performed to estimate the numerical uncertainty via Richardson Extrapolation and the Grid Convergence Index method. The model sensitivity to input parameters was addressed by ranking the importance factors associated with the inputs to the k-epsilon turbulence model, nozzle geometry, and mass-flow-rate at the inlet. In the near jet region, results of this study suggest the turbulent length scale implemented by the turbulence model will influence the re-circulation region and merge point of the two jet flows, associated with this complex turbulent flow regime.

#### **RANS CFD Analysis of the Twin Jet Challenge Problem**

Technical Presentation. VVS2017-4039

#### Jonathan Adams, Adam Jones, Sam Treasure, Rolls-Royce PLC, Derby, United Kingdom

Rolls-Royce is responsible for the design and manufacture of the pressurised water reactors (PWRs) that power the United Kingdom's fleet of nuclear submarines. As part of the design process, extensive numerical analysis of the reactor is carried out. However, the need to provide bounding safety justifications means that some aspects of the analysis are subject to pessimism factors, with larger pessimisms associated with physical phenomena that are less well represented by the model.

Jets are formed when coolant exits the heated core of a PWR. These jets mix in the upper plenum of the reactor before being pumped around the plant. The mixing behaviour of these jets varies in different operating

conditions and accident scenarios. Understanding the behaviour of the jets is therefore essential in order to fully understand the temperature of the fluid entering the plant pipework.

Jet mixing can be analysed with one-dimensional systems codes, however, to ensure that they are bounding the predictions are subject to large pessimisms. In contrast, CFD has the potential to provide more realistic representations of the flow that can be used to reduce the pessimisms applied to systems codes and increase performance. However, to make acceptable safety arguments, CFD must be supported by a broad validation library for all physical phenomena present in a flow. Experimental measurements of realistic plant conditions for all situations of interest are prohibitively expensive. Instead, confidence is built in CFD by validating specific phenomena before modelling larger plant components and systems.

This paper considers the Challenge Problem of the 2017 ASME V&V Symposium, which concerns isothermal mixing of two, parallel, rectangular water jets. The situation can be considered as a simplified representation of the hydraulic behaviour of coolant in the upper plenum of a PWR core, as it leaves the fueled region.

The problem has been simulated using the code CFX with a RANS approach that includes the upstream section of the inlet channels and compared to experimental PIV and LDV measurements. The rectangular nature of the geometry is exploited to create a 2D model, in order to facilitate a range of sensitivity studies on the mesh size, boundary conditions, turbulence model and advection scheme. After completing these sensitivity studies, a 3D model is created and a mesh sensitivity study performed before comparing the results of the finest calculation to the experimental data. The results of these sensitivity studies will be presented at the Symposium.

### Technical Program Wednesday

Validation of URANS and Stress-Blended Eddy Simulations (SBES) in ANSYS CFD for the Turbulent Mixing of Two Parallel Planar Water Jets Impinging on a Stationary Pool

Technical Presentation. VVS2017-4047

*Thomas Frank, Florian Menter,* ANSYS Germany GmbH, Otterfing, Bavaria, Germany

Rectangular jets are encountered in many types of engineering applications and provide a challenge in nuclear reactor systems. In the present study the turbulent mixing and penetration of two parallel planar jets is investigated at Reynolds numbers, which are typical for twin jet behavior in the upper plenums of both a liquid-metal cooled reactor and the very high temperature gas-cooled reactor. The investigation follows the ASME V&V 30 Committee, Benchmark Problem 1 specification for the corresponding experiment carried out by H. Wang & Y. Hassan, Texas A&M University (2015/2016) at the Twin Jet Water Facility (TJWF) designed and built at the University of Tennessee, Knoxville and applies standard best practices and required investigations of experimental and boundary condition uncertainties as far as applicable. The applied high-fidelity measurement techniques like LDA and PIV as well as the broad set of measured local fluid flow quantities like mean velocities, 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 mixing and penetration of two parallel planar jets impinging on a stationary water pool has been investigated for nozzle exit Reynolds number Re=9100 using three ANSYS CFD solvers (ANSYS Fluent, ANSYS CFX and AIM Fluids) and by applying steady-state as well as transient, time-averaged Shear-Stress Transport (SST) and Stress-Blended Eddy Simulation (SBES) turbulence models. In a first investigation the provided stationary inlet boundary conditions at the two nozzle exits for mean axial velocity and turbulence intensity were compared to results of a flow simulation, where mass flow and turbulence intensity boundary conditions were applied to the inlet pipes to the two stagnation boxes upstream the nozzle exits. In this study it was found, that despite the flow development in the narrow nozzle channels over a length of L/a~48 the irregular turbulent flow in these stagnation boxes lead to a transient and irregular fluid flow profile at the planar channel nozzle exits and that the provided experimental boundary condition can only be matched in a statistical time-averaged sense. For this reason, further investigations have been carried out as transient and time-averaged URANS SST or SBES simulations.

Further best practices oriented investigations have been carried out to determine the proper time resolution and flow averaging time to achieve appropriate resolution of all relevant flow phenomena as well as statistical reliability of time-averaged fluid flow quantities for the comparison to the experimental data. A mesh independency study has been carried out on two hexahedral meshes with 6.5 Mill. and 54 Mill. mesh elements as well. Both the time-averaged URANS SST and the time-averaged, scale-resolving SBES model simulations have led to a very good agreement for mean streamwise jet velocities, turbulent kinetic energy and individual Reynolds stress tensor components in comparison to the LDA and PIV data, showing only some minor deviations at intermediate elevations between z/a=5 and z/a=10. In addition, the SBES simulation provides detailed insights into the turbulent jet breakup and mixing by fully

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resolving different turbulent scales on the fine mesh and leading to a slightly more accurate prediction of the jet mixing point in comparison to URANS SST. Furthermore, the transient flow recirculation on top of the nozzle pedestal is resolved by the SBES simulations. The simulation results are highlighting the need to accurately quantify upstream flow conditions when downstream mixing is the phenomenon of interest.

#### Computational Studies of Turbulent Flow Interaction between Twin Rectangular Jets with OpenFOAM

Technical Presentation. VVS2017-4084

Han Li, N.K. Anand, Texas A&M University, College Station, TX, United States, Yassin Hassan, Texas A&M University Nuclear Engineering Department, College Station, TX, United States

Two or multiple parallel jets system is an important flow structure which could accomplish rapid mixing. The mixing feature of parallel jets can be found in many engineering applications. For example, in Very-High-Temperature Reactor (VHTR), the coolants merge in upper or lower plenum after passing through the reactor core, in Sodium Fast Reactor (SFR), the jets mixing of different temperature can cause thermal stresses and flow induced vibration in rod bundle. Computational Fluid Dynamics (CFD) simulations are extensively incorporated when it comes to studying parallel jets mixing phenomenon. Therefore, validation of various turbulent models is of importance to make sure that the numerical results could be trusted and serve as a guide for the future design. In this study, an open source CFD library, OpenFOAM was utilized to perform the numerical simulation. This validation work will consist of two parts. The first part, using design toolkit Dakota [1] interfacing with OpenFOAM, the steady state Reynolds Averaged Navier-Stokes Equations (RANS) simulations will be performed to analyze uncertainty and sensitivity of boundary conditions with mixing characteristics of the twin-jets flow. For the first part, the realizable k-epsilon model was selected for steady-state RANS simulation, and boundary condition sensitivity study was performed to test with the following variables at twin-jet inlets, velocity profiles, turbulence intensity, turbulence dissipation rate. An uncertainty range of merging point and combining point was established based on a series of simulations.

In the second part, Partially-Averaged Navier Stoke Equation (PANS) models were used to perform transient simulations compared to Unsteady Reynolds Averaged Navier-Stokes Equations (URANS) using fluctuating inlet boundary conditions. In transient simulations, k-epsilon PANS was used to compare with k-epsilon URANS. Power spectral density analysis was performed base on velocity probe to compare resolved frequencies of two simulations. It was observed that PANS model could reveal more information and resolved higher frequency in turbulence flow compared to URANS.

 Adams, B.M., Bauman, L.E., Bohnhoff, W.J., Dalbey, K.R., Ebeida, M.S., Eddy, J.P., Eldred, M.S., Hough, P.D., Hu, K.T., Jakeman, J.D., Stephens, J.A., Swiler, L.P., Vigil, D.M., and Wildey, T.M., "Dakota, A Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.0 User's Manual," Sandia Technical Report SAND2014-4633, July 2014. Updated November 2015 (Version 6.3)

### Wednesday Technical Program

#### Twin Jet Benchmark Simulations Using a Spectral Element Method Code - Nek5000

#### Technical Presentation. VVS2017-4108

Lane Carasik, Texas A&M University, College Station, TX, United States, Elia Merzari, Argonne National Laboratory, Lemont, IL, United States, Yassin Hassan, Texas A&M University Nuclear Engineering Department, College Station, TX, United States

The benchmark activity involving the twin turbulent rectangular jets of the Twin Jet Water Facility (TJWF) allow for various types of CFD solver methodologies to be tested. Previous efforts has included but is not limited to Reynolds Averaged Navier Stokes (RANS), Partial Averaging Navier Stokes (PANS), and Large Eddy Simulations (LES) using the finite volume method framework. The current work discussed involves the usage of LES based on a Spectral Element Method (SEM) framework to simulate the twin jet behavior. The CFD code package being utilized is Nek5000, an open source code, being developed by Argonne National Laboratory. The twin jet challenge problem benchmark data acquired using laser Doppler velocimetry and particle image velocimetry for merge and combined points, velocity profiles, Reynolds Stress profiles were compared to the Nek5000 predictions.

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

### 4-3 UNCERTAINTY QUANTIFICATION: APPLICATION PART 1 1ST FLOOR, MESQUITE 2 4:00PM - 6:05PM

#### Uncertainty Quantification Of MRI-based Pressure Drop Analysis Using CFD in Patients with Aortic Coarctation

Technical Presentation. VVS2017-4041

4:00pm - 4:25pm

Leonid Goubergrits, Charité-Berlin, Berlin, Germany, Pavlo Yevtushenko, Charité, Berlin, Germany, Jan Bruening, Charité - Universitätsmedizin Berlin, Germany, Marcus Kelm, Titus Kuehne, German Heart Institute Berlin, Germany

Patient-specific CFD analysis using MRI data is proposed to replace invasive pressure drop measurements by catheter in patients with congenital narrowing of the aorta. According to clinical guidelines, the maximal pressure drop is one of the major clinical measures for the medical treatment decision, with a 20 mmHg threshold being commonly used. CFD analysis uses MRI data to set boundary conditions including the reconstructed geometry of the aorta and measured flow rates in order to calculate the maximal pressure drop. However, these boundary conditions are affected by the temporal and spatial resolution of the imaging technique. The aim of this study was to analyze the uncertainty of the CFD-based pressure drop assessment caused by MRI data uncertainty. Data of n=10 patients were acquired using a 1.5 T Achieva device (Philips). The voxel resolution of the anatomical data was approximately 1 mm<sup>3</sup> and the uncertainty of the maximal flow rate was approximately 10%. Reconstruction of the stenosed aorta as well as a modification of the geometry generating 1 mm smaller and 1 mm larger stenosis were done using ZIBAmira software. Simulations with measured, 10% decreased and 10% increased flow rate through the stenosis were performed using commercial software ANSYS-Fluent. The pressure drops PD from nine simulations performed for each patient were used to calculate a second order polynomial describing the pressure drop as a function of the stenosis diameter D [mm] and the flow rate Q [ml/s]: PD=c0+c1\*D+c2\*Q+c3\*D\*Q+c4\*D\*D+c5\*Q\*Q. The resulting patientspecific polynomial allows calculating mean and standard deviation of the pressure drop in the uncertainty region of the measured flow rate and reconstructed stenosis. Furthermore, the polynomial allows calculating diameter and flow rate sensitivities of the pressure drop, i.e. dPD/dD and dPD/dQ, and thus characterizing the stenosis.

The averaged difference between the pressure drop calculated for the reconstructed geometry with the measured flow rate and the mean pressure drop for the uncertainty region was 2 mmHg. The averaged uncertainty of the pressure drop was 5.6 mmHg that is of the same order as the measurement accuracy of catheter-based pressure drop assessment at approximately 6 mmHg. The dPD/dD sensitivity varied between 7 and 25 mmHg/mm, whereas the dPD/dQ sensitivity varied between 0.1 and 0.6 mmHg\*s/ml. Thus, the impact of the uncertainty in diameter is more relevant than the impact of the uncertainty in flow rate. The presented results are of great significance for the translation of CFD analysis into clinical use.

#### Effects of the Depth of Field on Particle Shadow Velocimetry Measurements

Technical Presentation. VVS2017-4045

4:25pm - 4:50pm

Jeff Harris, Pennsylvania State University, Bellefonte, PA, United States, Christine Truong, Michael McPhail, Pennsylvania State University, State College, PA, United States

The uncertainty in particle shadow velocimetry (PSV) measurements due to the finite depth of field of the imaging hardware is presented. PSV is an optical flow measurement technique, akin to planar PIV, that uses cross-correlation of precisely timed images of a seeded flow field to estimate two-dimensional velocity fields. PIV and PSV mainly differ in their illumination source; PIV images light side-scattered from particles by a laser, whereas PSV images particle shadows generated by pulsed LED backlighting. The camera's optics control the depth of the measurement region in PSV, instead of the laser sheet thickness as in PIV. This work aims to quantify the depth of the measurement region in PSV and the dependence of measured displacement uncertainty on this parameter.

Depth of field is typically defined as the distance between near and far objects that are (subjectively) deemed in-focus. However, in PSV and PIV the depth of correlation is what defines the measurement region depth. With volumetric imaging, the depth of correlation is an estimate of the

### Technical Program Wednesday

depth along the optical axis in which particles are significantly influencing the displacement correlations in the PIV algorithms. For example, if there is a velocity gradient through the depth of correlation, the measured velocity will be biased by the particles that are not on the focal plane (i.e. particles that have a different velocity magnitude but are still "visible" to the correlation). Expressions derived for micro-PIV suggest the depth of correlation for a typical PSV setup is roughly an order of magnitude less than the depth of field. We compare this analysis to a simple experiment to estimate the depth of correlation and its contributions to measured velocity statistics. Randomly distributed dots were printed onto clear plastic sheets to serve as an artificial flow field. Two of these sheets were traversed in an in-plane direction, but separated by a distance along the optical axis. The first sheet remained along the focal plane while the second was set at fixed intervals from the first sheet. A series of in-plane displacements were imaged and the images correlated to estimate displacement fields. Depth of correlation is estimated from the statistics of these displacement fields, as a function of the separation between both planes along the optical axis.

#### Cantilever Beam End-to-End UQ Test Problem and Evaluation Criteria for UQ Methods Performance Assessment

Technical Presentation. VVS2017-4071

4:50pm - 5:15pm

#### Vicente Romero, Benjamin Schroeder, Matthew Glickman, Justin Winokur, Sandia National Laboratories, Albuquerque, NM, United States,

A substantial End-to-End UQ test-problem has been developed at Sandia Labs that involves many difficult paradigm and strategy questions and research challenges in uncertainty characterization and roll up in the end-to-end workflow from experiments/experimental data - model development/calibration - validation - extrapolative prediction - margin analysis. The test problem involves uncertainty quantification for stochastic physical systems (populations of cantilever beams having small physical variations from each other). The problem is divided into three parts.

Part I. Experimental Data UQ. This section involves sparse experimental data where a small number of beams are randomly drawn from a large population and then deflection-tested. The tests involve typical experimental circumstances of small load-control variations and systematic and randomly varying measurement errors/uncertainties on experimental input and output quantities. Uncertainty of deflection response and the probability of exceeding a specified threshold deflection are desired for: A) a random beam selected from the large population; and B) ensemble results for the whole (large) population of beams.

Part II. Model material property parameter estimation/calibration. This part involves load-deflection data from Part I; beam geometry measurement data involving random and systematic errors/uncertainties; and several different prediction scenarios for which the model is to be calibrated. Additional sources of uncertainty come from error/uncertainty from model discretization effects and from construction and use of surrogate models if the analyst chooses to employ them to reduce the number of physics model runs to reduce cost. The calibrated parameters are to be used in the prediction models to estimate uncertainty of deflection response and exceedance probability for cases A and B above, and compare results to the data-based estimates in Part I.

Part III. Model validation; potential associated adjustment of prediction model; and extrapolative prediction and margin analysis. Experimental data sets from three load-deflection tests with associated experimental uncertainties and different beam dimensions are supplied in this part for potential model validation assessments at two different scenario conditions. Any or all of the experimental data and validation results, along with the information given and developed in Parts I and II, can be used to inform the physics model and analysis procedure for extrapolative predictions at other sets of conditions (including beam dimension and loading changes) where model predictions are needed because no experimental data is available. Again, uncertainty estimates are sought for beam deflection thresholds at the new conditions.

This End-to-End UQ test problem will be released to other UQ communities as well, such as AIAA Non-Deterministic Approaches, SAE, and SIAM-UQ. A multi-attribute weighted performance metric and evaluation procedure will be suggested for common assessment methodology for UQ method cost-accuracy-risk performance over thousands of random trials of the sparse data and uncertainties involved. To enable this, the uncertainty "truth" models in the problem will be released in approximately one year so researchers and analysts can assess and compare the performance and effectiveness of various UQ approaches and methods.

#### **Uncertainties in Structural Collapse Mitigation**

Technical Presentation. VVS2017-4083

5:15pm - 5:40pm

### **Shalva Marjanishvili**, Hinman Consulting Engineers, Inc., San Francisco, CA, United States

The possibility of a local structural failure to propagate into a global collapse of the structural system has fueled the continued development of improved computational methods to model building behavior, as well as "best practices" engineering standards. In spite of these efforts, recent events are bringing the issue of collapse mitigation to the forefront and highlighting the shortcomings of existing design practices. The catastrophic nature of structural collapse dictates the need for more reliable methodologies to quantify the likelihood of structural failures and strategies to minimize potential consequences. This study presents an evidence that at the point of incipient failure the uncertainties in the results propagate to the level that it is impossible to verify yet validate calculated results. This is especially important when structural engineers are facing ever increasing pressure to design more economical structures thus arriving at a structure that is very close to failure limit.

To substantiate our conclusions, we have performed a series of nonlinear dynamic stochastic analyses of a simple two dimensional one story portal frame structure. The structure is so simple that it can be computationally

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reduced to a dingle-degree-of-freedom model without losing the fidelity of the results. This simple structure is chosen to effectively reduce number of input variables allowing us to concentrating on a computational results. This structure, then is subjected to incrementally higher loads pushing it towards the collapse. The results are represented as a series of deflections for each load. The uncertainty is measured as a variation of the deflections (ie COV or standard deviation). As the structure is "pushed" towards the collapse, uncertainties in the computed deflection become increasingly large. Consequently, it may not be possible to accurately predict when (and if) failure may occur.

Recognizing the need to understand uncertainties associated with risk and probabilities of unlikely events (low probability and high consequence events), this paper sets the stage to better understand the limitations of current numerical analysis methods and discuss innovative alternatives.

Computational solver is based on standard Matlab ODE solver and will be presented at the conference for anyone to be able to replicate the findings of this study.

#### State-of-the-Art Reactor Consequence Analyses Project: Uncertainty Analysis of a Potential Unmitigated Short-Term Station Blackout of the Surry Nuclear Power Station

Technical Presentation. VVS2017-4092

5:40pm - 6:05pm

Suchandra Ghosh, U.S. Nuclear Regulatory Commission, Rockville, MD, United States, Nathan Bixler, Dusty Brooks, Kyle Ross, Sandia National Laboratories, Albuquerque, NM, United States

The evaluation of accident phenomena and the potential offsite consequences of severe nuclear reactor accidents has been the subject of considerable research by the U.S. Nuclear Regulatory Commission (NRC) over the last several decades. As a result of this research, capability exists to conduct more detailed, integrated, and realistic analyses of potential severe accidents at nuclear power plants. Through the application of modern analysis tools and techniques, two State-of-the-Art Reactor Consequence Analyses (SOARCA) project pilot studies were completed in 2012. This project developed a body of knowledge regarding the realistic outcomes of postulated severe nuclear reactor accidents with best-estimate analyses of selected accident scenarios at the Peach Bottom Atomic Power Station (Peach Bottom), a boiling-water reactor (BWR), and the Surry Power Station (Surry), a pressurized-water reactor (PWR). The SOARCA project continued with an integrated uncertainty analysis (UA) of a potential unmitigated long term station blackout (LTSBO) accident at Peach Bottom completed in 2013. This Peach Bottom UA provided important insights regarding how uncertainties in selected severe accident progression and consequence parameters affect the results of the BWR LTSBO analysis. A Surry integrated UA is in progress to provide similar insights for a potential short-term station blackout (STSBO) accident in a PWR.

The focus of the Surry UA was on epistemic (state-of-knowledge) uncertainty in model input parameter values, and limited aleatory uncertainty. The aleatory (random) uncertainty due to weather is handled in the same way as the SOARCA study. In addition, the time-at-cycle (burn-up) and stochastic nature of safety relief valve failure was investigated, which represented aleatory aspects of some input parameters. Key uncertain input parameters were identified in both the MELCOR model for analysis of accident progression and radionuclide release, and the MACCS model for off-site consequence analysis. Distributions of values with their technical bases were developed for each of the uncertain parameters. Uncertainty in these parameters was then propagated in a two-step Monte Carlo simulation. Figures of merit investigated included cesium and iodine release and off-site health risk. The Monte Carlo results were analyzed with statistical regression based methods, scatter plots, and phenomenological investigation of selected individual realizations.

The Surry UA provides insights into which parameter uncertainties are most influential to variations in potential accident progression, source term, and off-site health consequence results. In analyzing the steamgenerator tube rupture (SGTR) variation of the STSBO, this study also provides useful insights into the conditions that lead to SGTR, and the potential consequences of such accident variations.

#### **TRACK 6 VALIDATION METHODS**

#### 6-1 VALIDATION METHODS 2ND FLOOR, PALO VERDE B

4:00PM - 6:05PM

Quality Assurance and Validation of Human Anatomical Models: Anatomy, Tissue Parameters and Model Processing

Technical Presentation. VVS2017-4088

4:00pm - 4:25pm

#### Silvia Farcito, Bryn Lloyd, Esra Neufeld, Niels Kuster, IT'IS Foundation, Zurich, Switzerland

Computational evaluations of medical devices and diagnostic tools, as well as treatment planning and safety evaluations, strongly rely on the usage of accurate models of human anatomy and physiology. The Virtual Population (ViP), developed by the IT'IS Foundation, together with the US Food and Drug Administration (FDA), is a set of highly detailed whole-body models based on magnetic resonance images (MRI) data from healthy volunteers (Gosselin et al., 2014; www.itis.ethz.ch/vip). The ViP models are provided together with a continuously updated and curated database of tissue-specific material properties www.itis.ethz.ch/database).

Several customizations are possible. The posture of these models can be changed, thus expanding the range of applications. Moreover, by applying a new morphing approach that allows for parameterization of BMI and of the size of individual organs, the population coverage of the existing models can be greatly extended. Specifically, a standard model can be morphed to correspond to known variations within the population or to match gross anatomical characteristics of an individual, without introducing artifacts.

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Validation and verification of these computational phantoms is an important and challenging problem. We discuss existing efforts towards verification and validation of the ViP models, both in terms of anatomical correctness and fitness for specific applications. The accuracy and consistency of the ViP v3.1 models is ensured by a set of quality assurance procedures and quality verification checkpoints that take place at various milestones during model generation. We explain these processes, which include clear guidelines how to segment certain tissues and involve systematic internal reviews. External audits carried out by anatomists from the University of Zurich are also included to certify morphological accurateness of the models. For traceability, model and database versions are maintained and linked via a digital object identifier (DOI). While the model generation steps have been improved and systematized, final validation is still completed via experimental evaluation of applicationspecific scenarios. Several validations against measurements and literature data have been performed and will be discussed, including thermal modeling due to MR exposure.

Verification and validation of the new physics-based poser will be discussed in terms of tissue-volume preservation in different postures and by showing how the ViP v3.1 models can be posed without loss of anatomical detail and correctness, even in extreme anatomical positions that represent realistic exposure scenarios.

Acknowledgements: The research leading to these results has received funding from the Swiss Commission for Technology and Innovation (S4L-CAPITALIS CTI 14930.1 PFLS-LS).

#### Validation of Product Life Prediction Models

Technical Presentation. VVS2017-4118

4:25pm - 4:50pm

Dan Ao, Zhen Hu, Sankaran Mahadevan, Vanderbilt University, Nashville, TN, United States

In the development process of engineering products and systems, computational models are usually used to emulate the physics of the system and predict the product life distribution by considering uncertainty of the inputs. However, the life prediction model needs to be validated to make sure it can well represent the actual physical system, before it is applied to product development. In many cases, products may be designed to perform satisfactorily for a very long time, and directly collecting life data for model validation at the operating stress level is usually time-consuming and expensive. In order to overcome this challenge, accelerated life testing (ALT) is employed in the proposed method to collect data for model validation. Based on the prior information extracted from computer simulation models and the collected ALT testing data, stress-life relationship is built to map the life distribution from higher stress levels to nominal stress level. Model validation is then performed based on the comparison between life distribution obtained from the ALT statistical model (empirical distribution) and its counterpart obtained from the computer simulation model. Weak prior information from simulation model and limited testing data due to budget constraints cause uncertainty in the model validation result. Therefore a validation test design optimization model is formulated and solved to obtain the optimal

number of tests and testing stress levels within the testing budget and available testing chamber constraints, in order to minimize the uncertainty in the validation result. A composite helicopter rotor hub component is used to demonstrate the effectiveness of the proposed validation and test design methodology.

#### Validation Assessment of a Coupled Dynamics Model

Technical Presentation. VVS2017-4117

4:50pm - 5:15pm

*Kyle D. Neal, Zhen Hu, Sankaran Mahadevan*, Vanderbilt University, Nashville, TN, United States, *Jon Zumberge*, AFRL, Wright-Patterson Air Force Base, OH, United States, *Thierry Pamphile*, AFRL, Fairborn, OH, United States

This research investigates bias prediction of coupled system models with time series inputs. Bias, or discrepancy, is defined here as the error between a physics model output and experimental observation. This work aims to inform the user under what conditions the physics model is capable of predicting the output of the system within a given tolerance (i.e., for what input time histories the model is useful). A predictor corrector method is investigated to predict the model bias for untested input histories. A surrogate model is built for the bias term, which is then used to correct the simulation model prediction at each time step. Alternatively, the bias term is combined with the simulation model, and a single surrogate model is built for the experimental output. The bias term for untested input histories is then estimated by comparing the experimental output predicted from the surrogate model with the output obtained from the simulation model. The Kriging surrogate modeling method is employed to implement the proposed methodology. From the experiments, high volume data are available for the surrogate model training. To achieve balance between accuracy and efficiency in the proposed methodology, a QR factorization-based method is proposed to optimally select the training points from available data. We also develop an error tracking method to guantify the effect of surrogate model uncertainty at each time step on the uncertainty of bias prediction. Based on the error tracking, we control the error in the model bias prediction to be under a specified level by adaptively adding training points to improve the surrogate model when necessary. The proposed methodology is illustrated for a system with coupling between fluid dynamics and heat transfer models.

This work is funded by the Air Force Research Lab (AFRL).

### Wednesday Technical Program

#### Research on a New Bayesian Validation Method for Multivariate Dynamic Systems under Uncertainty

Technical Presentation. VVS2017-4112

5:15pm - 5:40pm

Yudong Fang, Chongqing University, Shapingba, China, Zhenfei Zhan, Junqi Yang, Chongqing University, Chongqing, China

Computer modeling and simulations are playing an increasingly important role in complex engineering system applications such as reducing vehicle prototype tests and shortening product development time. Increasing computer models are developed to simulate vehicle crashworthiness, dynamic, and fuel efficiency. Before applying these models for product development, model validation needs to be conducted to assess the validity of the models. Model validation is a process to assess the validity and predictive capabilities of computer models in its potential usage by comparing the computer output with test data. In the virtual prototype environment, validation of computational models with multiple and correlated functional responses under uncertainty needs to solve some tough issues: the nonlinear correlation between different functional responses, the uncertainty quantification and propagation, the decisionmaking with conflict validation results for multivariate responses and objective robust metrics.

Aiming to solve the aforementioned problems-based on Bayesian interval hypothesis testing theory, statistic error analysis, probabilistic kernel principal component analysis, and subjective matter experts' based threshold definition and transformation, this paper proposes an integrated validation method for multivariate dynamic systems under uncertainty. The statistic error analysis is used to quantify the errors from the repeated test data and computational simulation results. The probabilistic kernel principal component analysis is employed to handle multivariate nonlinear correlation and to reduce the dimension of the multivariate functional responses. And it also improves the efficiency for the subsequent decision-making of the model validation at the same time. The subjective matter experts' based threshold definition and transformation is used to decide the threshold interval in the reduced data space. The Bayesian interval hypothesis testing is used to quantitatively assess the quality of a multivariate dynamic system. The differences between the average test data and computer simulation results are extracted for dimension reduction, and then Bayesian interval hypothesis testing is performed on the reduced difference data to make an objective decision with considering the conflicting validation results between the different principle components and assess the model validity. In addition, physicsbased threshold is defined and transformed to the reduced space for Bayesian interval hypothesis testing. The proposed method resolves some critical drawbacks of the previous methods and adds some desirable properties of a model validation metric for uncertain dynamic systems, such as symmetry. A real-world dynamic system with multiple,

repeated functional responses is used to demonstrate this new approach, and shows its potential in promoting the continual improvement of virtual prototype testing.

#### Experimental and Numerical Analysis of Injury Risk in Side Impacted Cutaway Bus

Technical Presentation. VVS2017-4055

5:40pm - 6:05pm

Mohammad Reza Seyedi, Grzegorz Dolzyk, Sungmoon Jung, Jerzy Wekezer, Florida State University, Tallahassee, FL, United States

This paper presents the validation process of injury parameters those are extracted from a numerical and experimental model of Anthropomorphic Test Devices (ATD) in side impact crashworthiness analysis (SICA) of cutaway bus. Using ATD in crashworthiness analysis provide a link between a dynamic structural performance of the bus and its occupant's injury. The passenger model allows for the crash analysis by modeling kinetic effects of occupants and their interaction with the vehicle's structure. Injury criteria have been validated and used in this study to address the mechanical responses of passengers in terms of severity of injury and risk of life during the crash.

The analysis presented in the paper includes two well-established techniques: 1) full experimental side impact test which was conducted by the Center for Advanced Product Evaluation (CAPE). The procedure of the test was based on the Insurance Institute of Highway Safety (IIHS) side impact crashworthiness protocol. In this test, an impactor accelerated into a stationary bus in which an ATD was belted and placed near the point of impact. The dynamic response of the head, neck, chest and pelvic was recorded. 2) Finite element model (FEM) analysis of the SICA which was conducted by using the verified FE models of: the belted 50th percentile Hybrid III ATD, the cutaway bus, and the impactor. Numerical analysis was carried out by using the nonlinear finite element code Ls-Dyna.

Most of the experimental and FE crashworthiness analyses of buses and their validation processes were focused thus far on the evaluation of structural response. However, to achieve the reliable and reasonable assessment, the passenger responses should be considered. Injury measures for the vehicle occupants should be added as an ultimate and important evaluation criterion for the validation analysis and assessment of the safety of buses. This study presents the assessment of injury risk by using the validated injury parameters of ATD during the side impact test. Injury parameters included: head, chest, pelvic acceleration, upper neck forces and moments, which were extracted from FE analysis and compared with those obtained from experimental data. Comparison of results from the FE analysis and the test shows that simulation results agree well with the experimental side-impact test.

Correlation between simulation and test shows the applicability of using FE model of ATD in vehicle safety analysis of bus and prediction of injury risk for occupants. Although there are no specific regulations and tolerances for bio fidelity of ATDs and the SICA protocols for cutaway buses, but injury parameters could be compared with those set up for side-impact passenger cars. Initial results confirmed that bus' occupants would survive from sustaining fatal injuries during real-world side-impact by vehicles not heavier than pickup trucks. Finally, considering injury criteria in FE crashworthiness parameters and validation process are crucial for assessing a vehicle's crash response. This approach is able to predict the potential injury risk during the side impact and reduces the duration of research and design cycles, and cuts experimental costs, which are crucial for future development of passenger safety technologies.

## Technical Program Thursday, May 4, 2017

### Thursday Technical Program

#### TRACK 3 TOPICS IN VERIFICATION AND VALIDATION

### 3-2 TOPICS IN VERIFICATION AND VALIDATION: PART 1 2ND FLOOR, ACACIA AB 10:25AM - 12:30PM

V&V for Computational Fluid Dynamics of Multiple Parallel Jets Using a Hybrid RANS-LES Method in Fluent

Technical Presentation. VVS2017-4059

#### 10:25am - 10:50am

Jean-Philippe Heliot, CEA, LE BARP, France, Ludovic Chatelier, Institut P', UPR CNRS, Futuroscope Cédex, France, Clément Caplier, Institut P', UPR CNRS 3346, Poitiers, France, Stephane Pecault, CEA, LE BARP, France

Multiple parallel jets are examples of shear flow phenomena widely existing in many industrial applications. The interaction between turbulence jets and the wall of the structure produces mixing phenomena that must be thoroughly understood.

Computational Fluid Dynamics (CFD) simulations are often used to design parts of complex systems. Therefore, validation of turbulence models is of importance to make sure that the numerical results can be trusted. This way, validation against analogous experimental data must be conducted to ensure the accuracy of these numerical models.

The objective of this study focuses on comparing the simulation data with the experiments by quantifying their disparities. The experiments used in this study were performed in the hydraulic facility of the P' Institute (CNRS-University of Poitiers-ISAE/ENSMA, France). This facility features multiple horizontal parallel cylindrical jets injecting fluid into a large transparent tank to study the mixing. The velocity, turbulence intensity, Reynolds stresses and other acquired parameters enable a thorough comparison with the CFD simulations. All experimental quantities are measured using particle image velocimetry (PIV), featuring specifically adapted multi-zone calibrations and image reconstruction procedures.

The purpose of this work is to validate a hybrid RANS-LES model using the industrial code Fluent.

Comprehensive Verification of a CFD model have been conducted by studying mesh convergence, turbulence model and numerical parameters for one drill hole. The best numerical model is then applied to study the fluid flows for the multiple jet case.

For the Validation step, an optimized mesh is generated, with a blockmesh of hexahedrons in the neighborhood of diaphragm and a blockmesh of tetrahedrons in the tank, to ensure that velocity gradients are properly evaluated. SST-k-omega model is selected to perform simulations in the RANS zone and the LES model in the LES zone. An interface between these two zones allows to transfer information for turbulences quantities.

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. A detailed assessment of the possible sources of numerical uncertainty is conducted to ensure valid comparisons between the computational data and the corresponding experimental results.

#### IMPipeline: An Integrated STOP Modeling Pipeline for the WFIRST Coronagraph

Technical Presentation. VVS2017-4037

10:50am - 11:15am

Navtej Saini, Kevin Anderson, Zensheu Chang, Gary Gutt, Bijan Nemati, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, United States

This paper presents an automated software pipeline to perform Structural-Thermal-Optical Performance (STOP) analysis of the WFIRST coronagraph. The Coronagraph Instrument on the Wide Field InfraRed Survey Telescope (WFIRST) will search for exoplanets by controlling the diffraction of the host star light in order to suppress it and allow the planet light to become observable. Since the planet light is billions of times dimmer than the star light, precise control of the light is challenging and susceptible to even minute imperfections such as thermally induced deformations of the optics. The observatory STOP analysis is used to assess the impact of such perturbations. The pipeline integrates the thermal, structural, and optical analysis software to run a STOP analysis in a seamless manner, with each software element running as a task with the final output being optical wavefront errors for an input observational scenario. Use of the IMPipeline allows the users (thermal, mechanical, optical) to verify the observatory model using various test cases. The database which is built from using the IMPipeline allows validation of the observatory model and lends itself for various what-if scenarios to be exercised on an automated basis.

The pipeline is written in the Python high level language and uses the Luigi framework for dependency resolution, workload management, and visualization. The initial version uses Thermal Desktop for thermal analysis, NX NASTRAN for structural analysis, SigFit for optical surface fitting, and CODE V for optical analysis. The pipeline provides flexibility to easily integrate other STOP analysis software as needed. It also features job checkpoint and restart capability (i.e., the user can restart the job from the task where it failed rather than restarting from the beginning). To speed up execution, it utilizes multiprocessing capabilities wherever feasible. Lastly, the pipeline can be easily customized using configuration files and provides users with a web interface to monitor the submitted job. The pipeline will be used to exercise the Coronagraph Instrument performance and serve as a verification tool for analysis and scientific teams.

#### Statistics and Risk-Based VV&A

Technical Presentation. VVS2017-4057

11:15am - 11:40am

James N. Elele, Naval Air Warfare Center Aircraft Division (NAWCAD), Patuxent River, MD, United States, **David Hall**, SURVICE Engineering Co., Carlsbad, CA, United States

Within the US Department of Defense there is a concerted push to base model and simulation (M&S) accreditation decisions on statistical comparisons between M&S predictions and real-world test data. For

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example, recent guidance issued by the Director for Operational Test and Evaluation (DOT&E) has emphasized the need for Design of Experiment (DOE) and statistical analysis techniques to support Verification, Validation and Accreditation (VV&A) of M&S used in support of operational test and evaluation.

Risk-based VV&A is based on the principal that the extent and type of credibility information needed to support an M&S accreditation is a function of the level of risk associated with use of M&S results to support decision-making by the program using those M&S results. How much "V&V" you need to do should be a function of how much harm might be caused by using M&S results that are wrong. The guestion: "Is your model validated"? leads inevitably either to never-ending validation, since there is no definition of what's good enough correlation with test data to decide you can quit doing it, or it ends with the user deciding that validation is too hard (or too expensive) so he or she avoids it altogether. Validation really only has meaning in the context of an application: the user wants to know if the model is demonstrated to be good enough for his purpose. This means that the user has to analyze his application, determine what "good enough" means for him, and only does enough validation to determine if the model meets his needs. In other words, the user must search for "analytical significance" in comparisons with test data, as opposed to simply "statistical significance".

In this paper we explore the ramifications and uses of hypothesis testing, statistical analyses, and review some of the discussions in the literature on confidence intervals, testing for intervals, and other statistical tests for significance as they relate to M&S validation, and ultimately how they do (or do not) relate to analytical significance. Ultimately, VV&A provides the accepted practical method for reducing the risk associated with using M&S and establishing confidence in M&S. The consequences if the model is wrong, and the level of risk one can accept, drive the amount of effort required to establish an acceptable credibility level for the M&S: statistical analysis is only one part of that process.

#### Verification of Coupled Codes (Fluid/Structure and Thermal/ Mechanical)

#### Technical Presentation. VVS2017-4146

11:40am - 12:05pm

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

Code verification for single physics code is now widely employed using exact or manufactured solutions. Verification of coupled codes is less mature and requires verification problems which adequately exercise the appropriate coupling mechanisms. We present two studies on verification of fluid/structure and thermal/mechanical computational codes.

A number of lessons were learned from the development of the verification tests. For example, the test problems were fully coupled but it was possible to pose single physics versions for verification of individual codes, which allowed issues to be found and resolved within each code. Additionally the problems needed adjustment to meet limitations of each

code, such as appropriate initial conditions and linearity assumptions of the exact solutions. The final coupled examples showed approximate second order convergence under fully two-way coupling.

#### Progressively Informed Calibration of BISON Nuclear Fuel Models

12:05 pm - 12:30 pm

#### Garrison Stevens, Los Alamos National Laboratory, Los Alamos, NM, United States

Metallic fuels are gaining interest in the nuclear energy community due to their high thermal conductivities and fuel densities resulting in favorable performance characteristics. Irradiation-induced effects in metallic fuels, such as fission product generation as well as chemical interactions, change the material properties of the fuel. Thermal conductivity becomes a particularly interesting behavior, as fuel burn-up increases porosity, in turn degrading thermal conductivity which is known to be influential in fuel modeling. In addition to neutronic and thermal-mechanical concerns, the behavior and the phase properties of the fuel are not well understood, particularly for U-Pu-Zr fuel.

BISON is a suite of nuclear fuel codes developed to predict the behavior of new metallic fuels. The physics principles embodied in these models include simplifying assumptions and omissions due to incomplete knowledge of underlying relationships. Further information gaps are introduced when experimental data is limited to a handful of tests with no quantification of experimental error. Such gaps in knowledge pose a risk for model calibration, as assumptions regarding the uncertain parameters, experimental error, and inherent model errors affect calibration results.

Herein, we present a progressive approach to calibration of BISON constitutive models. Experimental data are available from two U-Pu-Zr metallic fuel rods tested in the Experimental Breeder Reactor-II; T179 exposed for 92 days to ~2% burnup and DP16 exposed for 485 days to ~10% burnup. Beginning with a nominal calibration, parameters are assumed constant throughout the domain and experimental data points are taken to be an absolute representation of the true process. Experimental uncertainty and model bias are then considered by expert-opinion smoothing and weighting of the experimental curves. Degrading effects of missing physics in the model are demonstrated by phase-dependent weighting of the high burnup DP16 test. Finally, parameterization of the zirconium flux and diffusion is increased to expose implications of missing parameters in the calibration and further illustrate the need for increased model physics to account for burnup dependence.

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

### 4-4 UNCERTAINTY QUANTIFICATION: APPLICATION PART 2 2ND FLOOR, PALO VERDE A 10:25AM - 12:30PM

### Fatigue Damage as a Modal Quantity: Implications for Model Validation and Calibration

Technical Presentation. VVS2017-4011

10:25am - 10:50am

#### Jeffry Sundermeyer, Caterpillar, Inc., Mossville, IL, United States

Test events for large guasi-static earthmoving machine structures often exhibit significant variability in fatigue damage rate during their execution at the proving ground. This variability is the reason that it often takes 20-30 minutes of testing for the fatigue life (the reciprocal of the average damage rate) to stabilize at all measured locations on the structure. Previous attempts to match the average damage rate at all locations via simulation have involved the propagation of variability in inputs through the event simulation, which in turn gives rise to the question of what input distributions ought to be propagated through these simulations. Ordinarily, such inverse problems might be addressed through Bayesian techniques. In this work, however, a different approach is proposed. Particular simulations (called characteristic simulations) will be identified which project believably (as judged by a multivariate hypothesis test on the candidate simulated damage rates vs the test distribution) and usefully onto the eigenvectors of the test damage rate covariance matrix. Coefficients on these characteristic simulations will be calculated in a well-conditioned manner via a least-squares pseudo-inverse so that the best possible agreement between a linear combination of the chosen simulations and the test average damage rates can be obtained. If a next generation design for the machine is to be tested, then the characteristic simulations can be re-run with the new machine, but with all other input parameters unchanged. The results of these characteristic simulations, along with their associated coefficients, can be used to predict the fatigue performance of the new machine design for this particular test event.

#### Approach to Quantification of Uncertainties Due to Imbalances in Model-Basis Data Sets in Statistical Models Involved in Probabilistic Assessments of Leak-Before-Break

Technical Presentation. VVS2017-4022

10:50am - 11:15am

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

Statistical models are widely used in engineering probabilistic assessments. The uncertainty in a response variable predicted using a statistical model is typically represented by a single random variable ("error term") in an otherwise deterministic formulation accounting for the effects of relevant explanatory variables. The estimates of this residual uncertainty will vary with the variations in the model-basis data set used to develop the statistical model. Such variations in the model-basis data set may originate from a number of different sources, but will inevitably result in additional epistemic uncertainty in the model response. This additional uncertainty is not classified as the uncertainty due to the model form because it is not related to the variations in the functional forms used to represent the effects of explanatory variables on the model response.

One common source of this additional data-based uncertainty are imbalances in the model-basis data. The data sets tend to be more balanced when generated from experiments that are planned using the methodology of statistical experimental design. In a perfectly balanced model-basis data set, all relevant explanatory variables in the model formulation, as well as other factors considered to be important but not incorporated into the model formulation explicitly, would be weighted equally. In practice, this is rarely the case, and unequally weighted model-basis data points will result in biased estimates of the model parameters and therefore in additional uncertainty in the model response. This presentation outlines an approach to quantification of such uncertainties for two multi-variable probabilistic models relevant to the scope of leak-before-break assessments performed for CANDU reactors in accordance with the Canadian Nuclear Standard CSA N285.8.

Leak-before-break is demonstrated when the actual length of a postulated growing crack remains smaller than the critical length for crack instability over the entire duration of the process required to bring an operating nuclear reactor to a cold and depressurized state. In CANDU reactors, the influential variables in the probabilistic leak-before-break assessments include the axial growth rate of delayed hydride cracking and fracture toughness of Zr-2.5Nb pressure tubes. Statistical models with associated residual uncertainties had been developed for both variables using non-balanced multi-variable data sets. An approach to quantify the additional uncertainties due to imbalances in the model-basis data sets is discussed in this presentation, and the estimated magnitudes of these uncertainties obtained using this approach are compared with those of the residual uncertainties.

#### Noise Quantification in the Optimization Metric Used to Study Particle Jets during Explosive Dispersal of Solid Particles

Technical Presentation. VVS2017-4094

11:15am - 11:40am

#### M. Giselle Fernández-Godino, Frederick Ouellet, S. Balachandar, Raphael T. Haftka, University of Florida, Gainesville, FL, United States

It is known that dense layers of solid particles surrounding a high energy explosive generate jet-like structures at later times after detonation. Conjectures as to the cause and subsequent development of these jet structures include: (i) imperfections in the casing containing the particles, (ii) inhomogeneities in the initial distribution of particles, (iii) stress chains within the particle bed during shock propagation and (iv) non-classical Rayleigh-Taylor and Richtmyer-Meshkov instabilities.

In this work, we hypothesize that (i), (ii) and (iii) above produce initial variations within the bed of particles that develop into jets. We characterize the variation in particle volume fraction (PVF) in space, as the

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fractional volume locally occupied by particles due to linear and nonlinear growth of these instabilities. Without the inclusion of the right physics it is hard to capture these instabilities in simulations, and as a result, the objective of this work is to explore if the right initial PVF variation would lead to jet formation.

Our goal is to validate that our model leads to the kind of instabilities that are observed in experiments. Hereby, we are seeking the kind of initial disturbances that are most unstable. We expect that the difference between the instabilities that we find in simulations and the instabilities observed in experiments will allow us to improve our particle and fluid models to bring them together.

An optimization process will be carried out to determine the parameters of the initial PVF distribution that would lead to the strongest jet formation. An initial hurdle was to select an objective function that would represent the strength of such jets. After substantial analysis and numerical experimentation, we divide the space into angular sectors and measure the ratio of the number of particles between the sector with most particles and the one with fewest particles. The design variables considered are the amplitude, wavelength, and phase angle between the modes. Preliminary results showed that we can start with an initial perturbation with a ratio of 1.3, and grow it to a ratio of 3.9.

Initial experiments indicated substantial noise of roughly 30% and led to focused noise handling efforts. The cause of the noise was determined to be a combination of randomness in the initial position of the particles and a transition from Cartesian to polar grids. The proposed paper will include both the measures taken to deal with the noise and the results of the optimization.

State-of-the-Art Reactor Consequence Analyses Project: Limited Uncertainty Analysis of a Potential Early Containment Failure at the Sequoyah Nuclear Power Plant

Technical Presentation. VVS2017-4099

11:40am - 12:05pm

Alfred G. (Trey) Hathaway III, Suchandra Ghosh, Hossein Esmaili, U.S. Nuclear Regulatory Commission, Rockville, MD, United States, Kyle Ross, Dusty Brooks, Sandia National Laboratories, Albuquerque, NM, United States

The evaluation of accident phenomena and the potential offsite consequences of severe nuclear reactor accidents has been the subject of considerable research by the U.S. Nuclear Regulatory Commission (NRC) over the last several decades. As a result of this research, capability exists to conduct more detailed, integrated, and realistic analyses of potential severe accidents at nuclear power plants. Through the application of modern analysis tools and techniques, the State-of-the-Art Reactor Consequence Analyses (SOARCA) project was undertaken. This project developed a body of knowledge regarding the realistic outcomes of postulated severe nuclear reactor accidents with best-estimate analyses of selected accident scenarios at the Peach Bottom Atomic Power Station (Peach Bottom), a boiling-water reactor (BWR), and the Surry Power Station (Surry), a pressurized-water reactor (PWR). The SOARCA project continued with an integrated uncertainty analysis (UA) of a potential unmitigated long term station blackout (LTSBO) accident at Peach Bottom completed in 2013.

In addition to an integrated UA performed on the Surry plant, which is underway, a follow-on study was performed on the Sequoyah plant, a PWR, to extend the knowledge base to include an ice condenser style containment. This study examined epistemic uncertainty in model parameters, focusing on parameters which would influence the performance of the containment. Some of the parameters of interest included the number of cycles to failure for the safety valves and the associated open area fraction at failure, containment fragility, and failure open area fraction of the ice condenser doors.

During the course of performing the integrated UA for the Sequoyah plant, a region of safety valve performance was identified which yielded a potential for early containment failure, where containment failure occurs within 24 hours of the initiating event. Due to the limited number of realizations with potential for early containment failure in the integrated UA, a mini-UA was performed to further explore this region to better determine the probability of early containment failure and what uncertainties contribute to early containment failure. As was done for the integrated UA, a Monte Carlo technique was used to perform numerous calculations with uncertain variables sampled from pre-defined probability distributions. For the mini-UA, sampling from the distributions defining the number of cycles to safety valve failure and the open area fraction at failure was limited to the region with increased potential for early containment failure. The Sequoyah mini-UA provides insights into parameter uncertainties which influence the possibility of early containment failure and thereby help us understand conditions that can lead to early failure.

### Uncertainty Quantification of Peristaltic Pump using Sparse Grid Collocations

Technical Presentation. VVS2017-4103

12:05pm - 12:30pm

Bahram Notghi, Baxter Healthcare, Round lake, IL, United States

Rotary peristaltic pumps (RPP) are widely used in pumping blood in extra corporeal therapies like hemodialysis. Typical RPP consists of a rotor, a stator and a tubing in between them. One of the design parameters of the rotor and stator is the maximum displacement induced in the stator by the dynamic motion of the rotor. An explicit dynamic numerical model was constructed which capture the dynamic motion of the rotor. Deterministic numerical simulations provide an accurate approximation of the maximum displacement induced in the stator based on nominal values of model parameters/inputs, however, the inherent uncertainties in some of the model parameters could lead the model to under/overestimate the results. These uncertainties can be the results of variability in manufacturing processes, variation in density of the fluid inside the tube, angular velocity of rotor during different phases of therapy. In this study we chose three uncertain parameters: tube and stator material properties and spring (used in the pump rotor) stiffness. A sparse grid collocation method was selected to create the system response surrogate model for the present

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work due to its capabilities to provide accurate approximations of smooth functions in high dimensions based on a relatively small number of function evaluations. Utilizing a sparse grid approximation allows for construction of the surrogate model with orders of magnitude reduction in the number of higher-order analyses required compared to a standard tensor product implementation with approximately the same level of accuracy. The results indicate that the spring stiffness doesn't have significant effect on the maximum displacement in the stator, but the material properties of the tube and stator have significant effect on the maximum displacement of the stator with respect to uncertain parameters which can provide a better metric for design purposes and establish bounds on the prediction obtained from the model.

In addition, the obtained response surface can identify where additional model calibration can be useful in the validation process.

#### **TRACK 12 VERIFICATION METHODS**

12-1 DISCRETIZATION ERROR ESTIMATION	
2ND FLOOR, PALO VERDE B	10:25AM - 12:30PM

Are We Doing Numerical Error Bars Correctly?

Technical Presentation. VVS2017-4029

10:25am - 10:50am

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

The proper estimation of numerical error in modeling and simulation is difficult to achieve. A big part of the problem is outright laziness, inattention, and acceptance of poor standards. A secondary issue is the mismatch between theory and practice. If we maintain reasonable pressure on the modeling and simulation community we can overcome the first problem, but it does require not accepting substandard work. The second problem requires some focused research, along with a more pragmatic approach to practical problems. Today, we can deal with a simpler problem, where to put the error bars on simulations.

Implicit in this discussion is an assumption of convergence for a local sequence of calculations. One of the key realities is the relative rarity of calculations in the asymptotic range of convergence. Current approach centers the error bar on the finite grid solution of interest, usually the finest mesh used. This has the effect of giving the impression that this solution is the most likely answer, and the true answer could be either direction from that answer. Neither of these suggestions is supported by the data used to construct the error bar. The current error bars suggest incorrectly that the most likely error is zero.

Part of the problem is the origin of error bars in common practice, and a serious technical difference in their derivation. A common setting for error

bars is measurement error. Here a number of measurements are taken and then analyzed to provide a single value. In the most common use the mean value is presented as the measurement. Scientists then assume that the error bar is centered about the mean through assuming normal statistics. This point of view is the standard way of viewing an error bar and implicitly plays in the mind of those viewing numerical error. This implicit view is dangerous because it imposes a technical perspective that does not fit numerical error.

The evidence is pointing to the extrapolated solution as the most likely answer, and the difference between that solution and the mesh of interest is the most likely error. For this reason the error bar should be centered on the extrapolated solution. Thus most likely error is non-zero. There is a secondary impact of this bias that is no less important. The current standard approach also discounts the potential for the numerical error to be larger than the best estimate.

### Convergence Checks and Error Estimates for Finite Element Analysis in Fracture Mechanics

Technical Presentation. VVS2017-4069

10:50am - 11:15am

Ajay Kardak, Openso Engineering, Edwardsville, IL, United States, Glenn Sinclair, Louisiana State University, Baton Rouge, LA, United States

Fracture mechanics is the technology used today to estimate crack growth in components and so control it. The key parameter used to this end in fracture mechanics is the stress intensity factor, the coefficient of the participating, crack-tip, stress singularity. While there are now extensive compendia of stress intensity factors in handbooks for a wide variety of cracked configurations, frequently configurations are encountered in practice that are not included in these handbooks. Finite element analysis (FEA) has become the method of choice for determining stress intensity factors under these circumstances. Such FEA faces two challenges: resolving the crack-tip fields sufficiently accurately and, thereafter, extracting stress intensity factors correctly. The principal means of meeting the first of these challenges with FEA is via guarterpoint elements. The principal means of meeting the second of these challenges is via either path-independent integrals or crack-flank displacement fitting. While these approaches have become accepted in the fracture mechanics community, there is a question re how does the finite element engineer practicing them know how accurately the FEA has determined a stress intensity factor. Our intent is to address this verification issue.

Here, then, we seek to apply the convergence checks and error estimates for the FEA of stresses reported in earlier symposia and now available in [1]. We apply these checks to cracked configurations with varying crack lengths subjected to both tensile and shear loading. The ten test problems so treated have exact solutions so that there is no ambiguity as to what actual error is present in their FEA, thereby enabling a true assessment of the effectiveness or otherwise of the error estimates obtained. The FEA of these test problems employs a sequence of up to five successively, fairly-systematically, refined meshes. Obtaining error estimates from this FEA using the approach in [1] is straightforward. These error estimates

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consistently confirm the actual error present when path-independent integrals are used, either with quarter-point elements or without. On the other hand, they fail to correctly assess the error present with displacement fitting because the fitting procedure itself has error that is not accounted for in [1] which only tracks discretization error. Accordingly the convergence checks and error estimates of [1] are effective when FEA for stress intensity factors employs path-independent integrals, ineffective when this FEA uses displacement fitting.

#### References:

 Sinclair, G.B., Beisheim, J.R., and Roache, P.J., "Effective Convergence Checks for Verifying Finite Element Stresses at Two-Dimensional Stress Concentrations," ASME J. Verification, Validation and Uncertainty Quantification, Vol. 1, pp. 041003-1-9 (2016).

#### Solution Verification Using the Robust Multi-Regression Approach

Technical Presentation. VVS2017-4096

11:15am - 11:40am

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

Solution verification has traditionally been based on Richardson extrapolation and used to estimate the either the infinite-resolution value or the numerical error of a quantity of interest (QoI). The QoI is usually a scalar value chosen by the analyst - a quantity integrated over all or part of the domain, the value at a particular location and time - in general, a functional of the numerical solution. Richardson extrapolation relies on a number of assumptions. In practice, violations of these assumptions are common, resulting in a lack of robustness of the method and poor error estimates. Ultimately, these issues undermine the analyst's confidence in the approach even when it produces reasonable results.

In this talk we explore the Robust Multi-Regression (RMR) approach of Rider et al. to address many of the shortcomings of Richardson extrapolation. RMR generates a number of error estimates, and can incorporate subject matter expertise, to provide an error estimate and a measure of that estimate's uncertainty. RMR's improved robustness allows us to apply it to field variables (nodal values across the whole computational domain), which provides richer information about simulations to the analyst.

#### Verification of Code Convergence Order in the Presence of Numerical Error

Technical Presentation. VVS2017-4100

11:40am - 12:05pm

Gowri Srinivasan, Diane E Vaughan, Scott Doebling, Los Alamos National Lab, Los Alamos, NM, United States

Numerical error is often present in the code output due to a variety of reasons including truncation of infinite series, approximations of integrals, gradients etc. In such cases where the numerical error is comparable to the discretization error, the generalized Richardson extrapolation fails to provide reliable estimates of the order of code convergence. We illustrate the advantages of using optimization and linear regression methods to estimate the order of code convergence in the presence of large numerical error. In this study we use several examples including datasets from V&V20-2009 and physics problems that use ExactPack solvers in order to demonstrate the efficacy of our methods and present our recommendations for determining whether the numerical solution has converged to exact solution.

#### TRACK 3 TOPICS IN VERIFICATION AND VALIDATION

### 3-1 V&V WORKFLOW DEVELOPMENT AND APPLICATIONS 2ND FLOOR, ACACIA AB 1:30PM - 3:35PM

Verification and Validation Analysis and Visualization Tools using MBSE

Technical Presentation. VVS2017-4042

1:30pm - 1:55pm

*Kimberly Simpson, Marc Sarrel,* Caltech/Jet Propulsion Laboratory, Pasadena, CA, United States, *Tim Brady*, Johnson Space Center, Houston, *TX*, United States

Documents have typically been main conveyers of information and the authoritative source for system verification and validation (V&V) plans and activities. Difficulties lie in the management of a document-based V&V process because there are inherent interdependencies between integration and test schedules, test environments, requirements and verification activities. Additionally, as systems complexity increases, system-level (V&V) is often no longer performed using dedicated, localized test environments. Emulators, simulators, test harnesses, and/or software required may be widely distributed and involve a variety of test engineers and equipment distributed around the country. Each facility may have test equipment and software of varying degrees of fidelity. No single facility may exist that brings together the highest fidelity equipment. Distributed facilities may have only loose network connections between them, if any.

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To more effectively manage the growing complexity of system-level V&V, NASA/JPL has developed a rigorous and repeatable model based systems engineering (MBSE) methodology to assist with managing system-level V&V activities. The MBSE methodology facilitates the understanding of the system under test and its inherent interdependencies. The process of assimilating and integrating V&Vrelated products into a series of phased, cohesive system test configuration views provides a more comprehensive understanding of: 1) usage of the test facility, 2) the schedule and fidelity of simulators, flight hardware and software to be delivered by phase and 3) the test activities, written procedures and system capabilities to be verified and validated.

The MBSE methodology is adaptable to change and enables accurate, reliable and automated V&V analysis. The verification requirements, testbed schematics, version of hardware and software elements are transferred into the SysML model to enable integration and interrogation of information within the model. System "views", defined by stakeholder needs, are generated by querying the SysML model using scripts and visualization software. The re-projected technical views are then used to clearly communicate to management and engineering teams the phased test configurations, verification activities to be performed and requirements to be closed using each of these configurations, planned hardware/software deliveries required for testing and overall progress of V&V closure activities.

This paper will provide an overview of the general MBSE engineering methodology, the details of the SysML approach developed, its benefits, and how the capability may be more broadly applied to other system V&V efforts.

#### Applying Model-Based Systems Engineering in Verification and Validation of an Emergency Department Simulation Model

Technical Presentation. VVS2017-4077

1:55pm - 2:20pm

Mohamed Elshal, Hazim El-Mounayri, Indiana University - Purdue University of Indianapolis, Indianapolis, IN, United States

Healthcare system in the United States has multiple issues regarding quality, cost and outcome of patient care process. Several initiatives have been led regarding the need for systems engineering methodologies and tools to address healthcare delivery challenges for patients and healthcare organizations, one of which is a collaboration between Eskenazi Health Hospital and Indiana University to address resource allocation, cost estimation and crowding inside Eskenazi Emergency Department (ED) using a group of verified, validated and tested models. Discrete-Event Simulation is commonly employed for that purpose; however, simulation as a tool does not allow all system's stakeholders: Clinicians, Engineers, and Managers to understand their system and be engaged in the verification and validation process to overcome uncertainty in simulation results. A systems level approach is followed to evaluate crowding measures, optimize resource allocation and estimate the cost of emergency care. ED domain model is constructed based on process documents, interviews and real-time observation. Data requirements are identified, and data is collected and analyzed from

various sources to build statistical models. Stakeholder requirements are gathered based on interviews with key stakeholders involved to capture human resource information and interactions. Model-based systems engineering framework is developed using OMG Systems Modeling Language (SysML); which enables model reuse, supports multiple system views, and enhance system's verification and validation processes. Systems tools such as Cameo Systems Modeler from NoMAgic' and Microsoft Visio are used to design multiple system views of the ED. Those system views provide a formal approach and inherent rigor to capture and communicate system behavior. Validation is conducted through continuous cycles using SysML framework; where requirements, system diagrams and outcome measures are validated directly with system's stakeholders; as well as systems engineers and simulation experts. ED performance outcomes are evaluated by mapping the activity views of the system into an executable model using a powerful discrete-event simulation tool: Tecnomatix from Siemens- This executable model is used to replicate the current "As-Is" state of the system and estimate the measures of effectiveness (MOEs) used to assess ED's crowding condition. In conclusion, systems level approach provides a deeper and a clearer understanding of the internal and external entities that form the ED system. The comprehensive system views provide an on-going and early validation process that is supported by simulation and analysis. Results from simulation of the executable process models will be presented. The results will focus on the replication of the observed ED behavior.

#### An Approach Integrating PCMM, UQ and Evidence Theory for System Requirements Verification by Analysis with Solid Mechanics Models

Technical Presentation. VVS2017-4082

2:20pm - 2:45pm

#### George Orient, Vit Babuska, Chi Lo, John Mersch, Sandia National Laboratories, Albuquerque, NM, United States

A case study highlighting the computational steps of establishing credibility of a solid mechanics impact problem model and use of the compiled evidence to support quantitative program decisions is presented. An integrated modeling and testing strategy at the commencement of the CompSim (Computational Simulation) activity establishes the intended use of the model and documents the modeling and test integration plan. A PIRT (Phenomena Identification and Ranking Table) is used to identify and prioritize physical phenomena and perform gap analysis in terms of necessary capabilities and production-level code feature implementations required to construct the model. At significant stages of the project PCMM (Predictive Capability Maturity Model) assessment, a qualitative expert elicitation based process is performed to establish rigor of the CompSim modeling effort. These activities are necessary conditions for establishing model credibility, but they are not sufficient because they provide no quantifiable guidance or insight about how to use and interpret the modeling results for decision making.

The case study describes a project to determine the critical impact velocity beyond which the modeled device is no longer guaranteed to function. Acceleration and weld failure metrics of an internal structure are defined as Qols (Quantities of Interest). A solid mechanics model is constructed observing program resource limitations and analysis

### Technical Program Thursday

governance principles. An inventory of aleatory, computational and model form uncertainties is assembled, and strategies for their characterization is established. Formal UQ over the aleatory random variables is performed. Validation metrics are used to evaluate discrepancies between model and test data. At this point, the customers and the CompSim team agree that the model is generally useful for qualitative decisions such as design trades but its utility for quantitative conclusions including demonstration of compliance with requirements is not established. Expert judgment from CompSim SMEs is collected to bound the effect of known uncertainties not currently modeled such as the effect of tolerances as well as to anticipate unknown uncertainties. Elicitation of the integrated team consisting of system engineering and CompSim practitioners results in quantified requirements expressed as ranges on acceptance threshold levels of the Qols. Evidence theory is applied to convolve quantitative and qualitative uncertainties (aleatory UQ, numerical, model form uncertainties and SME judgement) resulting in belief and plausibility cumulative distributions at several impact velocities.

The processes outlined in this work illustrates a structured transparent and quantitative approach to establishing model credibility and supporting decisions by an integrated multi-disciplinary project team.

#### Curation of Code Verification Studies with Lightweight Simulation Process and Data Management

Technical Presentation. VVS2017-4064

2:45pm - 3:10pm

*Kyle Hickmann, Daniel Israel,* Los Alamos National Laboratory, Los Alamos, NM, United States

Large-scale verification and validation (V&V) studies for physics codes used by the national laboratories have been hindered by the lack of a natural way to track changes in V&V performance throughout the code's evolution. As new physics models or processes are added to existing codes it may happen that performance on one verification test problem improves while performance on a second test problem degrades. For this reason the ability to observe a code's V&V performance over its entire life cycle is desirable for steering resource allocation during development. To provide this functionality in the Verification Test Suite (VTS) at Los Alamos National Laboratory we have developed lightweight simulation process and data management (LSPDM), a command-line tool for creating and managing a repository of verification studies. LSPDM is capable of tracking computational processes, data, and analysis results in a versioncontrol-like repository organized by the flow of information between process execution, data generation, and test analysis. In this presentation we will provide an overview of LSPDM's organization, functionality, and demonstrate verification studies tracked by LSPDM.

#### How to Manage the Model V&V in Engineer Application

Technical Presentation. VVS2017-4086

3:10pm - 3:35pm

Qiang Yu, Huan Li, Junyong Yang, ANWISE Technology Ltd., Beijing, China

Model Verification and Validation is very complicated. It may refer to many activities including simulation model discrete error control, algorithm convergence study, model simplification reasonableness study, simulation and test result comparison, model parameter sensitivity analysis, model update, etc.

In fact, model V&V is also an expensive investment. We have to build a V&V team, develop V&V tools, and prepare some hierarchical test and simulation database for Validation. In the product development process, model V&V research will definitely cost a lot. So how to make model V&V more practical, efficient, are the problems we should care about in practical use.

In this presentation, a Model Validation management platform C-SDM will be scheduled. In C-SDM, V&V participants can build and save the hierarchical simulation models which are to be validated, and can also define a V&V process which can guide people how to conduct the V&V activities with specified V&V tools. More important, C-SDM can help people to capture the knowledge get from the model V&V application, build the high credibility validated hierarchical models, which can be saved as the intelligence asset for the R&D department. C-SDM illustrates a method how to make model V&V more practical and fruitful.

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

## 10-1 VERIFICATION AND VALIDATION OF NUCLEAR POWER APPLICATIONS: PART 1 2ND FLOOR, ACACIA D 1:30PM - 3:35PM

Validation Analysis for Computational Fluid Dynamics Simulations of Wire-Wrapped Nuclear Fuel Assemblies

Technical Presentation. VVS2017-4139

#### 1:30pm - 1:55pm

#### 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

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include both unheated assemblies that measured velocities with Particle Image Velocimetry and Particle Tracking Velocimetry, and heated assemblies that measured temperatures with thermocouples. Both classes of experiments also measured pressure drops with pressure transducers. The numerical component involves high-fidelity Large-Eddy Simulation modeling and industrial-level Reynolds Averaged Navier-Stokes (RANS) modeling of the experiments. At the previous ASME V&V meeting (2016), code and solution verification results were presented for the RANS simulations. For the current presentation, results of the industrial-level CFD solutions are validated with experiments. The CFD simulation results are obtained without guidance from experimental results, but use "as-built" geometry and "as-tested" conditions.

CFD simulations of helically wire-wrapped fuel assemblies employ meshes of bare pins without wire-wrap in the bundle, where the effect of wirewrapping 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 validation is accomplished by comparing pressure drops on duct faces, mean temperatures at specific axial heights, local temperatures on the external surfaces of unheated tubes and on duct faces, and both average and local velocities in various regions of the bundles.

The CFD pressure drops compare adequately to the experiments across lengths corresponding to integer multiples of wire-pitches although across lengths corresponding to non-integer multiples of wire-pitch increased error is evident. This slightly increased error seems to be due to an over-prediction of the magnitude of a Transverse Pressure Gradient that forms due to the bulk swirl that develops from the wire-wrapping. Mean temperatures, determined from averaging local temperature values at locations corresponding to experimental thermocouple locations, match well with the experimental results. The vast majority of the local temperatures on pin surfaces and duct walls are within the +/- 2'C uncertainty of the experimental values. The CFD velocity fields display satisfactory qualitative agreement with the time-averaged fields from the experiments.

#### Knowledgebase Structure Formulation and Requirements Development in a Data-Sparse Reality

Technical Presentation. VVS2017-4019

1:55pm - 2:20pm

Weiju Ren, Lianshan Lin, Oak Ridge National Laboratory, Oak Ridge, TN, United States

It is a commonplace in developing verification and validation (V&V) of advanced modeling and simulation codes that the incapability of acquiring satisfactory validation data becomes a showstopper and must first be tackled before any confident V&V developments can be conducted. Desired validation data are often found scattered in different places with the data interrelationships not well documented, incomplete with information for some parameters missing, nonexistent, or unrealistic to experimentally generate. Furthermore, with very different technical backgrounds, the modeler, the experimentalist, and the knowledgebase developer that must be involved in the desired validation data development often cannot communicate effectively without a data package template that is representative of the data structure for the information domain of interest to the intended code validation.

In a pilot project planning for development of the Nuclear Energy - Knowledgebase for Advanced Modeling and Simulation (NE-KAMS), the legendary TREAT Experiments Database is adopted to provide core elements for creating an ideal validation data package. Data gaps and missing data interrelationships will be identified from these core elements. All the identified missing elements will then be filled in with experimental data if available from other existing sources or with dummy data if nonexistent. The resulting hybrid validation data package (composed of experimental and dummy data) will provide a clear and complete instance delineating the structure of the desired validation data and enabling effective communication among the modeler, the experimentalist, and the knowledgebase developer. With a good common understanding of the desired data structure by the three parties of subject matter experts, further existing data hunting will be effectively conducted, new experimental data generation will be realistically pursued, knowledgebase schema will be practically designed; and code validation will be confidently planned.

The hybrid data package will first be uploaded into NE-KAMS with some as-needed structural expansion and functionality development to establish a common base for communications among the three parties of subject matter experts including the modeler, the experimentalist, and the knowledgebase developer. The uploaded hybrid data package will also provide a blueprint for creating a complete validation data package of experimental data, and further, facilitate networking scattered existing datasets preserved in different sources for the complete package. The network will allow new experimental data to be generated and preserved in databases at different locations for cost and time efficiency. Meanwhile, a duplicate will be uploaded into NE-KAMS for backup and enhanced accessibility.

This approach will establish requirements for a networked transient fuel database, formulate the structure of transient fuel information domain, deliver a tangible framework along with operation protocols for transient fuel validation data accumulation and management, provide a visual instance of a complete validation data package to facilitate future experimental data generation and validation development planning, and retain unique expertise required for long-term nuclear energy knowledge and code validation development and operation. It will also set a precedent for networking international databases and facilitate planning for collaborating with the Organization for Economic Co-operation and Development (OECD)/Nuclear Energy Agency (NEA) efforts in nuclear knowledge management.

### Technical Program Thursday

#### An Exercise in Multiphysics V&V of a Research Reactor Fuel Plate Model

Technical Presentation. VVS2017-4061

2:20pm - 2:45pm

Michael Richards, Arthur Ruggles, Kivanc Ekici, University of Tennessee, Knoxville, TN, United States, James D. Freels, Oak Ridge National Laboratory, Oak Ridge, TN, United States

The ongoing effort to convert nuclear research reactors from high to low enriched uranium fuels requires information about the potential consequences of manufacturing defects in fuel plates. Of particular concern are non-bonds, areas where the cladding fails to mechanically bond to the fuel meat, and fuel segregations, concentrations of uranium that produce energy at higher rates than the surrounding fuel. Each of these defects can cause localized areas of increased temperature known as hotspots. This study presents the development of a multiphysics model of a fuel plate for the high flux isotope reactor at Oak Ridge National Laboratory. This model incorporates both of the mentioned fuel defects and enlists a new approach for modeling non-bonds. Code and solution verification and validation, as an approach to quantifying the trustworthiness of a simulation, are discussed. Code verification is performed on relevant portions of COMSOL Multiphysics heat transfer and computational fluid dynamics modules. The heat transfer module performs as expected while the CFD module produces decreasing orders of convergence under grid refinement. When different domains and multiple physics are coupled, additional difficulties arise leading again to inconsistent convergence under grid refinement. Due to the lack of experimental data available for the fuel plate hotspots, solution verification and validation are performed on a narrow channel model with features similar to the fuel plates under consideration. Numerical errors are estimated based on grid convergence testing. Validation of that same model, as a surrogate for the fuel plate model being developed, is accomplished with the use of experimental data from the Advanced Neutron Source Reactor Thermal Hydraulic Test Loop. Final estimates of the model error along with uncertainty in that error are presented. A sensitivity analysis is performed on the hotspot model. The most influential parameters are identified for further study.

#### Verification and Validation of Thermal-Hydraulic Codes for the Analysis of Superconducting Magnets in Nuclear Fusion Reactors

Technical Presentation. VVS2017-4080

2:45pm - 3:10pm

**Roberto Zanino, Laura Savoldi**, Dipartimento Energia, Politecnico Di Torino, Torino, Italy

The main line of development for nuclear fusion reactors today (e.g. ITER) is based on the magnetic confinement of the plasma in a tokamak (i.e. toroidal axisymmetric) configuration. The magnets to be used for this purpose will be superconducting (SC), in order to reduce the needed cooling power to an acceptable fraction of the power produced by the plant. The superconductors chosen for these magnets might be in the

future characterized by high critical temperatures, but so far both ITER, under construction in Cadarache, France, and the EU proposal for a demonstration reactor (DEMO), are using low-critical-temperature superconductors, cooled by supercritical He in forced convection at ~ 4.5 K inlet temperature.

The design temperature margin before a normal zone is initiated in the magnet is of only 0.7 K. If the temperature increases above the margin, the initial normal zone may be propagated by hot He advection, i.e. evolve into a quench. In case of malfunction or inadequacy of the protection system, the quench may damage the magnet because of overheating and/ or pressurization. Since the magnets must essentially survive for the entire lifetime of the plant, the development, verification and validation (V&V) of codes, able to reliably predict the evolution of thermal-hydraulic (TH) transients in the magnets, with particular reference to the quench propagation, is essential for the safe and reliable operation of the fusion reactor.

In the paper we first review the status of V&V of the most important TH codes currently used for the analysis of SC magnets in fusion applications. Different time scales will be considered, ranging from the ms characteristic of the thermal stability of the magnet (i.e. the time needed for a thermal disturbance to evolve into a quench, or to recover the SC state) until the week-long cooldown transients needed to bring a large magnet from room temperature till operating temperature. Since it will be shown that this status is far from satisfactory, a possible strategy to reach an acceptable level of V&V will be proposed. The strategy is based 1) on the identification of a limited set of benchmark cases, one for each relevant time scale, to test and compare the candidate codes (verification step), and 2) on the identification of an experimental database for a limited set of transients (stability, quench initiation and propagation, cooldown) and, if needed, on the proposal of additional tests to complete it (validation step).

#### Metamodel-based Inverse Uncertainty Quantification of TRACE Physical Model Parameters

Technical Presentation. VVS2017-4081

3:10pm - 3:35pm

*Xu Wu, Tomasz Kozlowski, Hadi Meidani*, University of Illinois Urbana-Champaign, Urbana, IL, United States

Within the BEPU (Best Estimate plus Uncertainty) methodology uncertainties must be quantified in order to prove that the investigated design remains within acceptance criteria. For best-estimate system thermal-hydraulics codes like TRACE and RELAP5, significant uncertainties come from the closure laws which are used to describe transfer terms in the balance equations. The accuracy and uncertainty information of these correlations are usually unknown to the code users, which results in the user simply ignoring or describing them using expert opinion or personal judgment during uncertainty and sensitivity analysis. The purpose of this paper is to replace such ad-hoc expert judgment of the uncertainty information of TRACE physical model parameters with inverse Uncertainty Quantification (UQ) based on OECD/NRC BWR Full-size Fine-Mesh Bundle Tests (BFBT) benchmark steady-state void fraction data.

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Inverse UQ seeks statistical descriptions of the physical model random input parameters that are consistent with the experimental data. Inverse UQ always captures the uncertainty of its estimates rather than merely determining point estimates of the best-fit input parameters. Bayesian analysis is used to establish the inverse UQ problems based on experimental data, with systematic and rigorously derived surrogate models based on Sparse Gird Stochastic Collocation. Global sensitivity analysis including Sobol' indices and correlation coefficients are used to identify the important TRACE input parameters. Several adaptive Markov Chain Monte Carlo sampling techniques are investigated and implemented to explore the posterior probability density functions. This research solves the problem of lack of uncertainty information for TRACE physical model parameters for the closure relations. The quantified uncertainties are necessary for future uncertainty and sensitivity study of TRACE code in nuclear reactor system design and safety analysis.

#### **TRACK 12 VERIFICATION METHODS**

2ND FLOOR, PALO VERDE A	1:30PM - 3:35PM
12-2 VERIFICATION TEST SUITES	

#### The LANL Code Verification Test Suite

Technical Presentation. VVS2017-4049

1:30pm - 1:55pm

Scott Doebling, Los Alamos National Lab, Los Alamos, NM, United States

The Los Alamos National Laboratory (LANL) Code Verification Test Suite (VTS) is a repository of tools and test problems to enable standardized code verification testing for computational physics simulation codes. Such testing provides an objective evaluation of code accuracy and spatial convergence, as well as an objective basis for comparing test problem results across codes. The standardization and configuration management of the suite ensures consistency and repeatability in the verification analysis, and a traceable pedigree for the results. The tools and test problems are formulated such that they are usable, maintainable, customizable, and extendable by the code end-user community at LANL. The VTS has six fundamental components:

(1) Standardized test problem definitions, representing the same test problem across different computational physics codes; (2) Test problem "exact" (analytic and semi-analytic) solutions

generated via the LANL open-source software package ExactPack, ensuring that consistent and pedigreed test problem solutions are used for all code verification analyses; (3) Tools and standards for generating and managing code input decks and executing simulations; (4) Code verification analysis tools (also part of ExactPack) to perform tasks such as loading data, computing error norms, performing convergence analyses, and creating plots; (5) Automated documentation capabilities, for consistent, customizable, and archive-quality reporting; and (6) Simulation process and data management using the LANL software package LSPDM to manage the pedigree of VTS contents and results. The presentation will also cover a description of the suite of tests currently in the VTS, as well as some sample results and demonstrations of the customizable analysis capabilities.

#### Highlights from the LANL Verification Test Suite

Technical Presentation. VVS2017-4062

1:55pm - 2:20pm

Daniel Israel, Scott Doebling, Kyle Hickmann, Los Alamos National Laboratory, Los Alamos, NM, United States, Robert Singleton, Los Alamos National Laboratory, Santa Fe, NM, United States

The Los Alamos Verification Test Suite (VTS) is a collection of common test cases setup in LANL codes and designed to give a comprehensive picture of state of the codes at any given time. The cases are defined in a standards document which is publicly available (LA-UR-14-20418). Simulation process and data management software is used to simplify repeating the tests and tracking the pedigree of the results. In this presentation, we will present selected highlights from the latest version of VTS. The primary focus will be on code performance in capturing shock physics.

#### Heat Flow Verification Problems in ExactPack

Technical Presentation. VVS2017-4063

2:20pm - 2:45pm

Robert Singleton, Los Alamos National Laboratory, Santa Fe, NM, United States

This presentation includes several 1D and 2D heat conduction test problems, in Planar and Cylindrical geometries, that have recently been put into the verification tool, ExactPack, for this purpose. Multimaterial heat diffusion is a challenge for codes when the grid is misaligned between materials, as the code either over counts or under counts the energy at the material interfaces. While boundaries may start off aligned, they can easily become misaligned through hydrodynamic motion. Methods for treating these problems usually involve a surrogate mesh of some kind, such as the Thin Mesh in FLAG. Rigorous verification methods are therefore needed to assess these methods.

### Technical Program Thursday

#### **Radiative-shock Solutions for Code Verification**

Technical Presentation. VVS2017-4105

2:45pm - 3:10pm

Jim Ferguson, Los Alamos National Laboratory, Los Alamos, NM, United States

Code verification of radiation hydrodynamic algorithms is difficult because of the multi-physics, multi-scale nature of the physical environment being modeled. Radiative-shock solutions provide one type of problem that have been used as a code-verification tool for this coupled-physics environment. We present examples of how these solutions have been used recently to verify new algorithms, and also how new physics is currently being added to generate solutions of a more complex nature. We also show how metrics from these solutions can be used for code verification in ways other than the standard time- and spatial-convergence analyses.

#### EOSlib: A Reference Implementation for Thermodynamic Models

#### Technical Presentation. VVS2017-4065

3:10pm - 3:35pm

**C. Nathan Woods, Ralph Menikoff**, Los Alamos National Laboratory, Los Alamos, NM, United States

Verification of computational physics codes, whether using test problems or manufactured solutions, necessarily requires the use of an appropriate thermodynamic model. These models are themselves complex and can be challenging to implement. These challenges have greatly impeded the development of verification test problems using complex thermodynamic models, which makes it difficult to establish confidence in physics codes that implement these models. We have developed EOSlib, a stand-alone software package that includes a variety of thermodynamic models. This software library may be used directly or as a reference benchmark against which other implementations of thermodynamic models may be compared. We describe the overall structure and design of the code, and highlight several useful features, including a unified model API, segregated data files, and simple extensibility. We demonstrate these capabilities with a number of examples and discuss plans for incorporating this functionality into ExactPack and the LANL Verification Test Suite.

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

#### 2-2 APPLICATION OF STANDARDS 2ND FLOOR, PALO VERDE A

4:00PM - 6:05PM

#### Lab Accreditation – Assuring Verification When Testing is Right

Technical Presentation. VVS2017-4009

4:00pm - 4:25pm

Dr. George Anastasopoulos, International Accreditation Service, Brea, CA, United States

Richard J. Peppin, P.E., Senior Consultant, RION Co., Ltd.

Testing (and calibration) laboratories, to be good, must provide consistent accurate and precise measurements of the test objects based on their well-defined procedures. Lab accreditation is one way to assure the engineers, scientists, and technicians in the lab AND the lab customers and the public have confidence in the skills, facilities, and results of the lab's work. There is an international standard, ISO/IEC 17025-2005 "General requirements for the competence of testing and calibration laboratories." This standard is for use by laboratories in developing their management system, for quality, administrative, and technical operations. Following this standard will help labs assure quality in their work. To assure the public (and the lab's customers) that the lab does follow this, an objective agency evaluates the lab's quality program. This process is called "accreditation." Accreditation is done under strict quality control by accrediting agencies, of which there are several available for worldwide labs.

Most of the presentation will emphasize what is required and involved in the accreditation process This presentation will also discuss 1) why accreditation is useful, 2) who does the accreditation, 3) how are they qualified to do accreditation, 4) how costs are determined and, 5) how fast can it be accomplished.

(i) ISO/IEC 17025:2005 specifies the general requirements for the competence to carry out tests and/or calibrations, including sampling. It covers testing and calibration performed using standard methods, non-standard methods, and laboratory-developed methods. It is applicable to all organizations performing tests and/or calibrations. These include, for example, first-, second- and third-party laboratories, and laboratories where testing and/or calibration forms part of inspection and product certification. The standard is applicable to all laboratories regardless of the number of personnel or the extent of the scope of testing and/or calibration activities. When a laboratory does not undertake one or more of the activities covered by the standard, such as sampling and the design/development of new methods, the requirements of those clauses do not apply.

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#### **Practical Challenges of Implementing Certification by Virtual Testing**

Technical Presentation. VVS2017-4098

4:25pm - 4:50pm

Mahmood Tabaddor, UL LLC, Northbrook, IL, United States

As a safety science organization that provides certification related services based on physical testing, we have for several years been providing our customers an opportunity to allow for certification decisions to be made based on data from predictive modeling. These models may be physics-based or machine learning based, however, all must submit to a rigorous yet flexible V&V type process. In this presentation, we will discuss some of the challenges in implementing a practical process for Certification by Virtual Testing where the maturity for the process is affected by many parameters, such as understanding of key physics to sophistication of modeling tool to technical judgments to quality of datasets, etc. and yet it is important to deliver value to the customer without being unnecessarily burdensome.

It is important to understand that by moving towards a Certification by Virtual Testing offering, there is some risk that is introduced and we discuss how this risk can be mitigated and how some of this risk is actually less than what might be thought to exist when making decisions based on data from physical testing. At UL we are committed to leading Certification by Virtual Testing for consumer products and other product categories but in a more holistic approach, one that isn?t simply focused on a single V&V activity but a range of activities that feed into each other and ensure integrity and transparency to the entire process.

Development of Verification, Validation and Uncertainty Quantification Roadmap with Systematic Set of Validation Experiments and Simulation Campaign

Technical Presentation. VVS2017-4007

4:50pm - 5:15pm

Jordan Musser, Mehrdad Shahnam, Avinash Vaidheeswaran, National Energy Technology Laboratory, Morgantown, WV, United States, Aytekin Gel, ALPEMI Consulting LLC / NETL, Phoenix, AZ, United States, William Rogers, National Energy Technology Laboratory, Moatsville, WV, United States

A roadmap for validation and uncertainty quantification of multiphase flows is proposed. This work builds upon the ASME standards (ASME Guide for Verification and Validation in Computational Solid Mechanics, V&V10-2006), to address the lack of a systematic validation process for multiphase flows. The procedure being developed takes into account both experimentation and computational models. The experiments are specifically designed for validation of the multiphase computational fluid dynamics (CFD) suite, Multiphase Flow with Interphase Exchanges, MFIX. A bench top hopper for granular bulk-solid discharge is used to demonstrate the proposed procedure. Control variables, response variables, and physical constraints are identified for both experiments and simulations through surveying subject matter experts. Statistical design of experiment techniques are employed to specify rigorous experimental and simulation campaigns. The material properties are held-constant factors, hence all experiments are performed with high density polyethylene (HDPE) particles. The experimental control variables, orifice diameter and apex angle, largely influence the discharge flow rate. The measured angle of repose is constant since all the experiments are performed with the same material. Preliminary MFIX simulation results are in good agreement with the data on discharge flow rate, but the angle of repose is under-predicted.

#### Monitoring, Diagnostic, and Prognostic Research and Standards Development to Promote Health and Control Management of Manufacturing Systems

Technical Presentation. VVS2017-4123

5:15pm - 5:40pm

**Brian Weiss**, 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 decisionmakers 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, component, and sub-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 standard 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 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.

NIST is working with ASME to form a new Standards Committee on Advanced Manufacturing. Advanced monitoring, diagnostic, and prognostic technologies for manufacturing has been identified as a key area to be addressed by the new Committee. Initial efforts are underway to gather requirements from industry as to the specific elements this standard should focus. As such, ASME is planning a requirements gathering workshop to be held at the conclusion of the ASME Manufacturing Science and Engineering Conference (MSEC) in June 2017 in Los Angeles. It is expected that NIST's research efforts will support the development and output of the PHMC-relevant standards within the Advanced Manufacturing Committee.

### Technical Program Thursday

This presentation will highlight NIST's research to 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. This will include discussion of three key research thrusts: Machine Tool Linear Axes Diagnostics and Prognostics (at the component level), Health and Control Management 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. This research will also support the Standards to be formed under the new Advanced Manufacturing Committee.

#### Experimental and Analytical Studies of Rollover Test of Cutaway Bus

Technical Presentation. VVS2017-4056

5:40pm - 6:05pm

*Grzegorz Dolzyk, MohammadReza Seyedi, Jerzy Wekezer,* Florida State University, Tallahassee, FL, United States, *Sungmoon Jung,* FAMU-FSU College of Engineering, Tallahassee, FL

Anthropomorphic test devices (ATDs) are the common tools used for evaluation of safety in automotive research and industry. In this study, the dummy Hybrid III 50th male was used in rollover test and numerical analyses. Validation data was obtained from the rollover test which was conducted in accordance to the UN-ECE R66 Regulation. Numerical analyses were carried by the LS-Dyna FE code. The purpose of this study was threefold. The first was validation of the numerical model of cutaway bus for the crash simulations with ATDs. The second was to evaluate the injury criteria and safety assessment. The third to check the sensitivity of the computational model to bus geometry and material property changes. The validation was quantitatively assessed by the comparing acceleration time histories of the head and chest and upper neck forces with the corresponding data from the experiment.

Representativeness of the UN-ECE R66 Regulation is still questionable for some researchers, when bus or passenger performance is considered. The injury criteria values obtained from the test confirmed this hypothesis. Numerical analysis revealed that potential damage might be severe when partial ejection takes place resulting in a direct contact between the head and the ground. Partial ejection occurrence depends on the window's size and location, likewise the initial arm position above the window's bottom rail enables bigger excursion out of the bus structure.

The experimental data and video documentation alone were insufficient to fully explain the character of the dummy impact during the test. The numerical tests revealed that there was no direct contact between the head and the ground through the shattered window, which was indicated by the insignificant value of the Head Injury Criteria (HIC). We found that slightly higher response of torso was caused by the straight impact of dummy's shoulder with ground.

Several sources of errors were identified. They included modeling of the entire bus with its seats, ATD, seatbelts, window glass, experimental errors and others, yet verification and validation process demonstrated

reasonable correlation for the head, chest and pelvic accelerations. A comparison of neck forces and moments is less satisfactory due to higher sensitivity to the angle of the impact, which is affected by the nature of rollover test. During the free fall phase, ATD slightly changed its position, which was challenging to replicate in analysis.

### 2-3 NAFEMS STANDARDS DEVELOPMENT ACTIVITIES 2ND FLOOR, PALO VERDE B 4:00PM - 6:05PM

#### The NAFEMS Engineering Simulation Quality Standard

Technical Presentation. VVS2017-4122

*Chris Rogers*, Crea Consultants Ltd., Buxton, United Kingdom, *Ian Symington*, NAFEMS, Knutsford, Cheshire, United Kingdom

The presentation will cover the NAFEMS Analysis Management Working Group and the current key activities which include:

- 1. The Engineering Simulation Quality Management Standard
- 2. The work of AMWG in general and the close links with ASME V&V.
- 3. The NAFEMS VVUQ publication tree.

TRACK 10 VERIFICATION AND VALIDATION OF NUCLEAR POWER APPLICATIONS

#### 10-2 VERIFICATION AND VALIDATION OF NUCLEAR POWER APPLICATIONS: PART 2 2ND FLOOR, ACACIA D 4:00PM - 6:05PM

#### **Considerations for Advanced Modeling and Simulation Review**

Technical Presentation. VVS2017-4097

4:00pm - 4:25pm

### Joshua Kaizer, U.S. Nuclear Regulatory Commission, Germantown, MD, United States

Recently, there has been increased interest in the use of advanced simulations in supporting commercial nuclear power plants. This interest seems to be spurred on by programs such as the Consortium for the Advanced Simulation of Light water Reactors (CASL), Nuclear Energy Advanced Modeling and Simulation (NEAMS), the potential for advanced reactors, and the desire for accident tolerant fuel. This has resulted in many questions to the U.S. Nuclear Regulatory Commission (NRC) on how such advanced simulations would be reviewed. The NRC has a very long and successful history of reviewing the models and simulations currently used to support the nuclear fleet, however, it is not clear how much of the current review methods would be applicable to advanced simulations.

Therefore, this presentation will provide a background on the modeling and simulation reviewed by the NRC, will detail some of the challenges

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confronted during a review, and will provide some considerations for reviewing advanced simulations in the future. The background begins by categorizing the many different types of analyses which are used to support a nuclear power plant and the level of NRC review for each type. This leads to the clarification of safety analysis (i.e., the analysis of greatest interest) and introduces the concept of an Evaluation Framework.

With the concept of the evaluation framework introduced, the presentation next focuses on the challenges confronted during a review of such a framework. This includes answering questions such as "how much is enough" (e.g., has enough data been provided? are the uncertainties well-understood? is the impact of compensating errors acceptably low?). The current guidance for the review of frameworks will be briefly summarized and discussed. Further clarification is provided by describing this review process view framework in terms of activities related to Verification, Validation, and Uncertainty Quantification.

Finally, the presentation will focus on advanced simulations. First, a clear definition for advanced simulation will be provided. Then the methods for review of these simulations will be discussed in light of the current review methods. This discussion will provide a number of considerations for the review of advanced simulations including the possibility of a tandem simulation approach (i.e., a high maturity with low fidelity simulation supporting a high fidelity but low maturity simulation), continuous simulation (i.e., running simulations as the plant parameters change), continuous validation (i.e., ongoing validation experiments used to confirm / update key models), and the potential for a more inspection based approach for VVUQ. It is hoped that through the presentation, the audience will gain a sense of how the NRC currently reviews modeling and simulation, some of the challenges which will be a faced in the future, and some considerations which may help with those challenges.

#### An SBO analysis for Maanshan PWR using MELCOR 2.1/SNAP

Technical Presentation. VVS2017-4121

4:25pm - 4:50pm

Jason Chang, Yu Chiang, Jung-Hua Yang, Shao-Wen Chen, Jong-rong Wang, National Tsing Hua University, Hsinchu City, Taiwan

Severe accident researches at nuclear power plants (NPPs) have been intensively concerned since the Fukushima event. Because of the similarity of natural conditions, Taiwan researchers spent huge effort on safety analysis and procedure improvement of the NPPs. In this study, a hypothetical Station Blackout (SBO) transient of the Maanshan NPP was established by MELCOR2.1/SNAP code. A real happened SBO event of Maanshan plant was also simulated in this study.

The MELCOR model of Maanshan NPP, which coupled with SNAP code for graphical interface, was constructed to analyze the Maanshan SBO transient. Our aim was to analyze the severe accident process from SBO transient to RPV failure, hydrogen burn and the release of radionuclides. Before the transient simulation, a 300 sec steady state test for the MELCOR model was performed.

Maanshan NPP is a Westinghouse three-loop PWR design with rated core thermal power of 2822MWt. The MELCOR model for Maanshan NPP includes Reactor Pressure Vessel (RPV), cavity, and pressurizer, reactor cooling system (RCS), steam generator (SG), containment and containment spray. In 2001, a real 2hrs SBO event happened in unit 1 of Maanshan NPP. In this research, the MELCOR SBO case was verified with TRACE model to simulate the SBO event happened in 2001.

The study is divided into forth sections. In the first part, the capability of thermal-hydraulic analysis for MELCOR SBO model of Maanshan NPP was verified by comparing the results with the TRACE SBO model. Remarkable parameters from the results such as reactor power, vessel pressure, and PCT and core water level were discussed. The MELCOR case of the real event in 2001 is also constructed and compared with TRACE in this section. Second, the SBO case simulation would continue with no safety injection considered. The MELCOR results after core damage were discussed to evaluate the plant safety. Parameters were discussed in detail, such as hydrogen explosion, containment overpressure, debris relocation, radionuclides movement, etc. Finally, Sensitivity studies of Auxiliary Feed Water (AFW) supply were done by MELCOR, which could provide a reference standard for water injection to keep the nuclear fuels covered with water and prevent fuel cladding from damage.

The thermal hydraulic behavior of Maanshan NPP RCS during the transient was considered in this research. Parameters such as peak cladding temperature (PCT), RPV pressure, core water level of the MELCOR model were compared with another code named TRACE which is value to the thermal-hydraulic safety studies. By the comparison between parameters from MELCOR and TRACE, we found a similar tendency which implies that MELCOR has the capability to deal with thermal-hydraulic calculations. Similar conclusions can be obtained from other studies compared with MAAP or RELAP5 code.

In conclusion, this study showed the important phenomena during an SBO accident of Maanshan NPP. The results could help NPP safety analysis and emergency procedure improvement in a beyond design basis accident.

#### Verification of Predicted Powers and Shim Positions for Advanced Test Reactor Cycle 159-1

Technical Presentation. VVS2017-4130

4:50pm - 5:15pm

#### Nathan Manwaring, Nathan Manwaring, Thomas Eiden, Rose Holtz, Idaho National Laboratory, Idaho Falls, ID, United States

This work summarizes information obtained during Cycle 159A-1 of the Advanced Test Reactor (ATR). Safety-related analyses prior to Cycle 159A-1 required predicting localized reactor powers at various times during operation and predicting positions of various control shims. These predictions are compared to measured data obtained over the course of Cycle 159A-1, to include indicated powers and shim positions. The correctness of predictions for this cycle is one verification of the computer code used to make them. Additionally, the effects of various experiments irradiated during Cycle 159A-1 are compared in the predictive model and in the measured data. Thus models of the cycle-specific experiments are

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validated, in addition to models of shims and other elements in the ATR base model. Further validation is provided by entering indicated shim positions and extracting calculated powers, which are compared with indicated powers. Requested irradiation services were successfully provided.

#### Validation of Thermalhydraulic Computer Codes Used in Safety Analysis: Regulatory Perspective

Technical Presentation. VVS2017-4141

5:15pm - 5:40pm

Janusz E Kowalski, Canadian Nuclear Safety Commission, Ottawa, ON, Canada

The Canadian Nuclear Safety Commission (CNSC) and the Canadian Standards Association (CSA) frameworks specify the requirements for validation activities applicable to the computer codes used in the design and safety analyses of nuclear power plants [1, 2]. The regulatory framework requires that thermal hydraulic codes' capabilities and limits, as well as the quantification of code accuracy, must be assessed during the validation process.

During the past three decades, considerable resources have been devoted in Canada to establish and conduct validation of the computer codes used in safety analysis. The validation effort was primarily phenomena-based and did not fully quantify the code prediction accuracy of key safety parameters.

Recently, CNSC staff have indicated the need to change the validation approach and conduct future validation using key parameters such as trip parameters and Figure of Merit (FOM). In this new approach, the identification of important phenomena and parameters is directly linked to the acceptance criteria and FOM, forming an essential step of the parameter-based validation process.

This paper describes the regulatory approach used in the review of code validation submissions, including the assessment approach and the review acceptance criteria. CNSC expectations on the code validation process are discussed, with a focus on the data qualification and methodology used for determining the code accuracy.

The scope of the review performed by the CNSC staff may be different from case to case. It may consist either of a comprehensive evaluation of the validation program or a more detailed assessment of specific validation activities (e.g. qualification of the data used for validation exercises).

#### References:

- Deterministic Safety Analysis, Regulatory document REGDOC-2.4.1, Canadian Nuclear Safety Commission, May 2014.
- Quality Assurance of Analytical, Scientific, and Design Computer Programs, Canadian Standard Association, N286.7-16, January 2016.

#### **Benchmark of Transient Nuclear Fuel Performance Codes**

Technical Presentation. VVS2017-4152

5:40pm - 6:05pm

Heng Ban, Utah State University, Logan, UT, United States

Nuclear fuel performance under transient conditions, such as reactivity insertion accidents, is essential for the development of advanced accident tolerant fuels for light water reactors. The knowledge also provides the foundation for regulatory requirements in design-based accident analysis. Currently, multi-physics and multiscale computational codes are developed to provide a fundamental understanding of the complex fuel failure phenomena. However, the validation of those models proved to be a significant challenge. This paper summarizes our efforts to benchmark the multi-physics, three-dimensional finite element fuel performance code BISON, which is developed by the Idaho National Laboratory of the US Department of Energy. The results were compared with similar codes used in the world and showed significant need for V&V. Our overall effort in V&V for coupled neutron physics, thermal hydraulics, and transient fuel performance is also introduced to provide a general framework of our research.

## Technical Program Friday, May 5, 2017

### Technical Program Friday

### TRACK 1 CHALLENGE PROBLEM WORKSHOPS AND PANEL SESSIONS

## 1-2 WORKSHOP ON ITERATIVE ERRORS IN UNSTEADY FLOW SIMULATIONS 2ND FLOOR, PALO VERDE A 8:00AM - 10:05AM

#### **Presentation of Submitted Results Iterative Errors Workshop**

Technical Presentation. VVS2017-4073

Luis Eca, IST, Lisbon, Portugal, Guilherme Vaz, MARIN, Wageningen, Netherlands, Martin Hoekstra, Consultant Netherlands

The V&V 20 subcommittee on Verification and Validation in Computational Fluid Dynamics and Heat Transfer is sponsoring a workshop organized by Luís Eça, Martin Hoekstra and Guilherme Vaz, to address the effect of iterative errors on Unsteady Flow Simulations.

The focus of this Workshop is on flow solvers that use implicit time integration techniques, which have to solve a system of non-linear equations at each time step. If the contribution of the iterative error becomes dominant, it may spoil the results without being noticed; grid/ time refinement becomes useless and is sure to give a misleading result for the discretization error of the simulations. Therefore, it is important to estimate iterative errors in unsteady flow simulations, however difficult that may be in practice.

The proposed exercise is the calculation of the two-dimensional (laminar) flow around a circular cylinder at Reynolds numbers based on the incoming velocity and cylinder diameter of 100 and/or 150. Participants are requested to determine the selected quantities of interest using at least three different levels of the iterative convergence criteria used at each time step. Grids, suggested boundary conditions, selected flow quantities and instructions for the submission of results are available at http://web.tecnico.ulisboa.pt/ist12278/Workshop\_iterative\_2017.htm.

The data obtained from these calculations will allow the comparison of results obtained with different flow solvers and iterative convergence criteria. Furthermore, the existence of three data points per submission will allow us to check the consistency of iterative error estimators for unsteady flow simulations.

The WEB page mentioned above will also be used to report the results and conclusions of the Workshop.

#### Impact of Iterative Errors in Unsteady Flow Simulations

Technical Presentation. VVS2017-4127

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

This is a contribution to the Workshop on Iterative Errors in Unsteady Flow Simulations.

#### Discussion of submitted results to the Workshop on Iteration Errors on Unsteady Flow Simulations

Technical Presentation. VVS2017-4076

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

Overview of the results presented by the different participants. Discussion of the main trends observed in the data. Open floor discussion. Conclusions of the Workshop.

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

#### 9-1 VALIDATION METHODS FOR SOLID MECHANICS AND STRUCTURES 2ND FLOOR, PALO VERDE B 8:00AM - 10:05AM

Model Validation for Transportation Accident Investigations: Challenges and Strategies

Technical Presentation. VVS2017-4025

8:00am - 8:25am

Xiaohu Liu, National Transportation Safety Board, Washington, DC, United States

Finite element (FE) modeling in the area of accident investigation has many challenges: the structures involved may not have been manufactured according to spec, the actual material used may be unknown, age of the structure and the environment may have caused degradation, the uncertainty of the loads sustained during the accident, and so on. On top of all these challenges, FE modeling in this area is often a reverse engineering problem where there could be many possibilities that lead to the same end result. For these reasons, model validation is crucial yet a difficult task for FE modeling to be legit and successful for accident investigations. This paper will describe challenges and strategies for FE model validation from the angle of transportation accident investigations performed by the National Transportation Safety Board (NTSB). The NTSB is an independent U.S. federal agency charged with determining the probable cause of transportation accidents and promoting transportation safety. This paper will discuss examples from past NTSB accident investigations of different modes of transportation where FE modeling was extensively used. Specifically, the following examples will be discussed: 1. The fracture of a freight train axle from a railroad accident; 2. The failure of a tee connection from a pipe line accident; 3. The fracture of an amphibious vehicle front axle from a highway accident; and 4. The failure of a helicopter blade from an aviation accident. In each example, the FE modeling work performed will be described and focus will be on model validation. The topics that will be touched upon include obtaining accurate part geometry, material characterization, loading specification and sensitivity analysis. As an important part of model validation, the failure analysis work performed by the NTSB Material Laboratory will also be discussed.

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#### Validation of Structural Dynamic Models

Technical Presentation. VVS2017-4050

8:25am - 8:50am

**Thomas Paez**, Thomas Paez Consulting, Albuquerque, NM, United States, **Timothy Hasselman**, Timothy Hasselman Consulting, Palos Verdes Estates, CA, United States

It is becoming customary, in many fields, to require that system models be validated prior to their use in system response prediction, particularly in consequential scenarios. The activities required to perform a model validation have been developed and are well documented. A critical step leading to validation comparisons, at least, for structural dynamic models, is calibration of model parameters. The manner of calibration and tolerances used to judge acceptability of a calibration relate to the potential accuracy that is achievable during validation.

This talk extends some work commenced one year ago. That work developed a Bayesian approach for the identification of model component parameters, and a general, statistical technique for judging whether or not the parameters identified for the model are acceptable according to some T-squared distribution-based criteria. The talk to be presented at this meeting, first, considers how the process of model validation relates to the model calibration process. It seems logical that when stringent criteria are applied during the calibration process, then the potential for accuracy of model predictions is enhanced during model validation comparisons. This issue is explored in the framework of an experimental/numerical example. The second topic to be covered involves measures of structural dynamic response and validation metrics. Several measures of response appropriate to structural dynamic systems are discussed, as well as validation metrics appropriate to those measures.

The example in this talk involves dynamic observations from a stochastic, substantially nonlinear mechanical joint used in an aerospace structure. A stochastic model has been calibrated using excitation and response data from swept sine experiments at multiple levels and using multiple hardware assemblies. The objective now is to attempt to validate the model for its predictive capability in random vibration environments. Multiple validation metrics are considered, and it is shown that some metrics are more difficult to satisfy than others.

#### Uncertainty Quantification Approach for As-Manufactured Turbine Engine Rotor Dynamic Response

Technical Presentation. VVS2017-4054

8:50am - 9:15am

Jeff Brown, US Air Force Research Laboratory, Wright Patterson AFB, OH, United States, Alex Kaszynski, AAS, Dayton, OH, United States, Joseph Beck, AFRL/RQTI, Wright Patterson AFB, OH, United States, Emily Henry, Daniel Gillaugh, US Air Force Research Laboratory, Wright Patterson AFB, OH, United States

Turbine engines rely on stationary vanes and rotating bladed disks to generate propulsive power. As the rotating blades pass the vanes they

must endure harmonic aerodynamic loading at frequencies related to the number of vanes and engine RPM. When the natural frequencies of the bladed disks align with harmonic frequencies, resonance increases the dynamic response and can lead to High Cycle Fatigue (HCF) failures. Prediction of rotor dynamic response must consider airfoil manufacturing deviations that lead to mistuned dynamic response, a phenomenon caused by small blade-to-blade deviations in frequency that can cause up to 400% response amplification above an ideal cyclically symmetric response analysis. This presentation describes a set of methods developed to quantify the uncertainty of as-manufacture rotor dynamic response. The process begins with an optical geometry measurement process using a structured light system to generate high fidelity 3D point cloud representations of the entire rotor surface with accuracy of 0.0005" in. Uncertainty in the measurements are assessed through reference geometries, repeated rotor scanning, and a method to propagate measurement uncertainty effects on forced response predictions. The propagation approach leverages a mesh morphing method to update a design intent Finite Element Model (FEM) to the 3D point cloud generated by the structured light system. Methods to optimize element quality are employed to minimized error and both FEM mesh and point cloud density studies are conducted to reduce guantified predictive uncertainty. The as-measured rotor models are validated with an experimental capability called traveling wave excitation which provides a bench-level capability to apply dynamic excitation in harmonic patterns to rotor airfoils to simulate rotating engine loading. Experimental uncertainty is quantified through repeated testing and used with the uncertainty bounded FEM results for model validation. The validated model is used in a probabilistic simulation of fleet response that uses a geometric parameter reduction technique, a Gaussian Stochastic Process emulation of airfoil behavior, and an efficient substructuring reduced order model that couples airfoils for mistuned rotor predictions. These fleet predictions are validated with a large sample of manufactured rotors. When combined, these methodologies produce a comprehensive quantification of the uncertainty of as-manufactured rotor response and are enabling new advances in engine design and fleet sustainment.

#### Verification and Validation of Analysis Results Created during Development of Mine Trucks at Atlas Copco Rock Drills AB

Technical Presentation. VVS2017-4018

9:15am - 9:40am

Jari Hyvarinen, Atlas Copco Rock Drills AB, Örebro, Sweden

During the development of mine trucks at Atlas Copco it is assumed that a quasi-static approximation of the vehicle behavior is adequate. However with growing size of the vehicle this approximation becomes questionable. The finite element models used also assumes that vehicles can be described using a linear finite element (FE) model. For the latest mine truck with a 65 ton capacity these described assumptions were made in the early design phase. Due to a compressed development time schedule some regions with higher than desired stress levels remained when the prototype vehicles were built. Strain gauge and acceleration measurements were made to reveal the severity of the remaining structural issues.

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The driving sequences used during testing of the prototypes were selected based on earlier measurements at customer sites on smaller vehicles. It was found that not only did the measurements show higher than desired quasi-static stress levels, but the stress levels were in many regions much higher than calculated. The quasi-static analysis procedures use so called cubic-mean stress criteria below which the stress levels are required to be to achieve acceptable fatigue life. With the cubic-mean stresses calculated from the experimental data being much higher than anticipated the question was of course, what was the cause of this?

By first extracting the frequency spectrums of the measured acceleration and strain responses it was possible to characterize the signals. To find what was causing the peaks in the response spectrums a combination of modal analysis and PSD spectrum analysis was performed on the FE-model of the vehicle. The PSD spectrum analysis as loads uses the PSD acceleration spectrums that were extracted from the measured data.

The results revealed that dynamic amplifications caused the high stress levels due to that the vehicles characteristic modes had ended up with too low frequencies. The conclusions that were drawn was that the pre-series vehicles would need redesigns in the critical regions and that more attention need to be paid to vehicle dynamics in the future when developing these vehicles.

This paper shows the type of FE- models used and describes the process used during evaluation of the calculated and experimental results. The comparison showed that in regions where quasi-static calculated and experimental evaluation give similar results, the Palmgren-Miner accumulated damage based fatigue-life analysis of the scaled test data demonstrated that acceptable fatigue-life had been achieved. In regions where large differences between quasi-static calculations and corresponding measured data were observed, very short fatigue-life was predicted using a combined experimental and calculated fatigue evaluation approach.

### Model Validation of Multi-layer HDPE Material on Dynamic Analysis with Model Bias Prediction

Technical Presentation. VVS2017-4034

9:40am - 10:05am

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

With the increasing development in automotive industry, finite element (FE) analysis with model bias prediction have been used more and more widely in the fields of chassis design, body weight reduction optimization and some components development, which reduced the development cycles and enhanced analysis accuracy significantly. However, for the development process of plastic materials products, such as fuel tank made of multi-layer high density polyethylene (HDPE), there is few study of model validation or verification, which results in too time-consuming to enhance non-risky design decisions. In this study, to correct the discrepancy and uncertainty of the simulated dynamic model, 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 of dynamic simulations coupled with model bias prediction is increased apparently.

### TRACK 17 VERIFICATION AND VALIDATION FOR ADVANCED MANUFACTURING

## 17-1 ASME V&V 50 VERIFICATION AND VALIDATION OFCOMPUTATIONAL MODELING FOR ADVANCED MANUFACTURING2ND FLOOR, ACACIA D8:00AM - 10:05AM

#### VVUQ Applications in Process Technologies for Advanced Manufacturing

Technical Presentation. VVS2017-4107

8:00am - 8:25am

Huijuan Dai, GE Global Research, Niskayuna, NY, United States,Adegboyega Makinde, General Electric Global Research Center, Austin, TX, United States

The Verification, Validation and Uncertainty Quantification (VVUQ) Application in Process Technologies working group in ASME V&V50 subcommittee is to develop and establish best practice for verification, validation, and uncertainty quantification in computational modeling for advanced manufacturing process. Computational models are playing an ever-increasingly important role in advanced manufacturing, including:

- Physics-based models, which encode the physical principles and mathematical solutions
- Data-driven models, including models of artificial intelligence, which are based on the understanding of the manufacturing process from in-suit or post-manufacturing measurements
- 3. Hybrid models, which combine physics-based models with data assimilation

These models are widely used to optimize process parameters to minimize manufacturing defects, reduce the number of physical trials and consequently reduce cost. However, for manufacturing process modeling, current V&V standards have little guidance on how to establish the model credibility and quantify uncertainties in materials properties and process variables. To help develop VVUQ guidelines for manufacturing process simulation, two user cases are defined:

- 1. Case I: investment casting of a simple rod
- 2. Case II: additive process of a cube

Both simulations and testing will be conducted and compared with analytical solutions for validation and verification. The methodology for quantifying the uncertainties at different stages of manufacturing process will also be developed through the two user cases.

### Friday Technical Program

#### Verification and Validation Interactions with the Model Life Cycle

Technical Presentation. VVS2017-4095

#### 8:25am - 8:50am

Joe Hightower, The Boeing Company, Seattle, WA, United States, Guodong Shao, NIST, Gaithersburg, MD, United States, Eric Sawyer, Honeywell FM & T, Kansas City, MO, United States, Rumi Ghosh, Robert Bosch, LLC, Palo Alto, CA, United States, Aaron Bernreuther, Honeywell FM&T, Kansas City, MO, United States, William Schindel, ICTT System Sciences, Terre Haute, IN, United States, Mark Benedict, AFRL Mantech, WPAFB, OH, United States

Advanced Manufacturing presents many opportunities to employ modeling and simulation. Modeling and simulation can reduce the cost and time to develop new advanced processes. Some processes, such as additive manufacturing, require models to maintain process control. Quality Control can use models to ensure that quality goals are met. All models must be verified and validated to ensure credibility. V&V methods exist for developing some models in certain domains and are included in standards such as the ASME V&V 10 and V&V 20 standards. However, no standards exists for maintaining model credibility throughout its life cycle. Under the ASME V&V 50 subcommittee, a working group on "Verification and Validation Interactions with the Model Life Cycle" is developing generic guidelines and best practices to address this gap.

The model life cycle includes five stages: requirements definition, model development, model deployment, model maintenance, and model retirement. In each stage we identify procedures, methods, and best practices required to ensure that model credibility is maintained. In addition, we will make strategic use of configuration management, methods for revalidation, and existing relevant standards for each stage.

The guidelines and best practices we are developing will apply to three categories of models including data driven, physics based, and hybrid models for advanced manufacturing applications.

This presentation reports the current efforts and progress of the ASME V&V 50 Working Group on Verification and Validation Interactions with the Model Life Cycle. This working group is currently performing the following tasks: (1) investigate the existing model V&V and Uncertainty Quantification (VV-UQ) procedures and methodologies; (2) identify relevant standards for model/software/system lifecycle; (3) study different applications of advanced manufacturing; and (4) generalize the VV-UQ procedures for different model lifecycle stages. The completed guideline and proposed generic methodologies will help users and modelers of manufacturing applications ensure and maintain the validity and quantified uncertainty throughout the lifecycle of the models they generate.

### Terminology, Concepts, Relationships and Taxonomy for VVUQ in Advanced Manufacturing

Technical Presentation. VVS2017-4131

#### 8:50am - 9:15am

Sankaran Mahadevan, Vanderbilt University, Nashville, TN, United States, Yung-Tsun Tina Lee, National Institute of Standards and Technology, Gaithersburg, MD, United States, Gaurav Ameta, Dakota Consulting, Silver Spring, MD, United States, Sanjay Jain, George Washington University, Washington, DC, United States

This presentation summarizes the ongoing work of V&V 50 Subcommittee's task group on terminology, concepts, relationships, and taxonomy for VVUQ in advanced manufacturing applications. The task group is charged with the following activities: (1) survey the definitions in existing V&V standards and guides (e.g., ASME, IEEE, AIAA, ISO, DoD etc.); (2) explore applicability of existing definitions to advanced manufacturing; (3) suggest adaptations/extensions of existing definitions to advanced manufacturing; and (4) suggest definitions of new concepts unique to advanced manufacturing. The terminology being surveyed is divided into four groups: verification, validation, calibration, and uncertainty quantification. Within verification, the focus is on concepts related to code verification, solution verification, error estimation, and accuracy requirements. Within validation, the focus is on concepts related to system response quantities of interest, validation domain vs. application domain, accuracy requirements, validation metrics, and validation hierarchy. Within calibration, the concepts relate to model parameters, model discrepancy, physics-based vs. data-driven vs. hybrid models, calibration data issues, and fusion of heterogeneous data. Within uncertainty guantification, the focus is on both aleatory and epistemic uncertainty sources, uncertainty aggregation and roll-up towards system-level prediction, model predictive capability assessment, and quantification of margins and uncertainty (QMU). This activity will liaison with other task groups within V&V50, as well as build on previous and ongoing work by other V&V subcommittees.

#### Verification-Validation and Uncertainty Quantification Methods for Data-Driven Models in Advanced Manufacturing

Technical Presentation. VVS2017-4137

9:15am - 9:40am

Ronay Ak, Yung-Tsun Tina Lee, Guodong Shao, National Institute of Standards and Technology, Gaithersburg, MD, United States, Rumi Ghosh, Robert Bosch, LLC, Palo Alto, CA, United States, Sagar Kamarthi, Northeastern University, Boston, MA, United States

Application-specific Verification and Validation (V&V) has been the focus of attention for several groups in scientific and engineering communities over the last two decades. The charter of the American Society of Mechanical Engineers (ASME) V&V standards committee is to create best practices and guidelines for V&V Uncertainty Quantification (UQ) in Computational Modeling and Simulation in various domains. The ASME V&V 50 Subcommittee was recently established to address the applications in advanced manufacturing. The Subcommittee consists of

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five working groups of which the VV-Uncertainty Quantification (UQ) methods in data-driven and hybrid models is one.

The mission of the VV-Uncertainty Quantification (UQ) methods in data-driven and hybrid models working group is to provide solutions to the V&V and UQ problems related to data-driven and hybrid models that manufacturing companies tackle. A data-driven model (DDM) in a manufacturing domain is built using data analytics techniques to analyze the data generated by a manufacturing process or system. Data analytics techniques include but are not limited to statistical, data mining and machine learning predictive and descriptive models. The objective of a DDM is to find a mapping between the input and output with or without explicit knowledge of the physical behavior of the process or system. Hybrid models refer to models which combine data-driven models and physically-based models in an optimal way. In order for users to be confident that the model is valid for its intended application, a DDM or a hybrid model has to be verified and validated, and the uncertainties associated with the model and data have to be properly quantified.

Manufacturing has become significantly data-intensive in recent years. Continuous improvements in sensor technologies and data acquisition systems allow manufacturers to effectively and efficiently collect large and diverse volumes of data. Data analytics has demonstrated great potential for transforming raw data into information and knowledge for smart decision making during design, manufacturing, use, and post-use.

The objective of this presentation is to introduce the VV-UQ methods in data-driven and hybrid models working group with the focus predominantly on the VV-UQ aspect of data-driven modeling the working group's initial research area. We will discuss the technical approach and up-to-date progress of the working group. The working group aims at deriving a generic guideline by performing the following tasks: (i) investigate the existing VV-UQ standards/procedures and data-mining process models like CRISP-DM, and adapt them to advance manufacturing (if applicable); (ii) closely study the use cases of DDMs defined by industry and academia; iii) uncover the commonalities in the patterns of VV-UQ for advanced manufacturing and generalize the problems; and iv) provide generic recommendations and resolutions for each type of problems. This generic guideline will enable practitioners of VV-UQ to better assess and enhance the credibility of their data-driven and hybrid models.

#### VVUQ Challenges and Methods in Systems of Models Working Group

Technical Presentation. VVS2017-4140

9:40am - 10:05am

Barron Bichon, Southwest Research Institute, San Antonio, TX, United States

The ASME V&V 10 guide decomposes an engineered system into a model hierarchy and then discusses in detail the process of validating each individual computational model independently. Manufacturing, however, is inherently a process that involves a series of models that do not lend themselves naturally to this decomposition. The goal of this working group is to provide guidelines for validating this series of models - this "system" - as a whole rather than validating each model individually. This creates a

number of challenges that may not be strictly unique to manufacturing, but nevertheless are not directly addressed by the other ASME V&V subcommittees and is thus an area where the V&V 50 Subcommittee can add value to the community.

### TRACK 1 CHALLENGE PROBLEM WORKSHOPS AND PANEL SESSIONS

## 1-3 WORKSHOP ON ESTIMATION OF DISCRETIZATION ERRORS BASED ON GRID REFINEMENT STUDIES 2ND FLOOR, PALO VERDE A 10:30AM - 12:35PM

Presentation of Submitted Results to the Workshop on Discretizaton Errors Estimation

#### Technical Presentation. VVS2017-4074

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

The V&V 20 subcommittee on Verification and Validation in Computational Fluid Dynamics and Heat Transfer is sponsoring a workshop organized by Luís Eça, Martin Hoekstra and Guilherme Vaz to address the estimation of numerical uncertainties based on grid refinement studies. The focus is the estimation of discretization errors of steady flows, i.e. parametric uncertainty is not addressed and iterative and round-off errors are so small that they may be assumed negligible and independent of the discretization error.

Solution Verification based on a grid refinement study requires first of all the solution of one and the same problem on a number of geometrically similar grids. Afterwards, an estimate of the numerical uncertainty of the solution on (usually) the finest grid is made applying some kind of procedure. It is this procedure, of which several have been proposed, that is the key of this workshop. So participants do not have to make their own numerical solutions, but just have to apply their preferred procedure on data provided by the organizers and to report their results.

The data provided are related to six cases: flow over a flat plate for Reynolds numbers of 107, 108 and 109; flow around the NACA 0012 airfoil at Reynolds number of 6×106 and angles of attack of 0°, 4° and 10°. All test cases are statistically steady flows of an incompressible fluid that were simulated in several geometrically similar grid sets with three eddy-viscosity turbulence models: Spalart & Allmaras one-equation model; Shear-stress transport (SST) k-w two-equation model and KSKL two-equation model. For each test case we provide the following information:

A list of functional and local flow quantities to estimate the uncertainties (the quantities of interest).

The numerical solution and the typical cell size of all quantities of interest for at least 9 levels of grid refinement that cover at least a grid refinement ratio of 4.

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The requested information from the participants is:

Estimated numerical uncertainty for the quantities of interest for different levels of grid refinement.

Reference to the procedure applied or description of the procedure adopted (if not available in the open literature).

The goal of this exercise is to check the consistency of the estimated error bars for different levels of grid refinement and/or different grids with the same number of cells and flow conditions. Furthermore, this exercise will also allow us to check the consistency of the estimates obtained by different users applying the same method. Hopefully, such exercise will help us to identify the main difficulties in making reliable error estimates based on grid refinement studies. A complete description of the selected test case, the proposed data and instructions for the submission of results are available at http://web.tecnico.ulisboa.pt/ist12278/Discretization/ Workshop\_discretization\_2017.htm. The same WEB page will be used to report the results and conclusions of the Workshop.

### Global Deviation Uncertainty Estimator Applied to the 2017 Workshop on Estimation of Discretization Errors

#### Technical Presentation. VVS2017-4101

*Tyrone Phillips*, South Dakota School of Mines and Technology, Rapidi City, SD, United States, *Christopher Roy*, Virginia Tech, Blacksburg, VA, United States

This talk will discuss the authors' contributions to the Workshop on Estimation of Discretization Errors Based on Grid Refinement Studies [1]. Data was provided by the organizers for two cases of interest: turbulent flow over a flat plate at three different Reynolds numbers (107, 108, and 109) and turbulent flow over a NACA 0012 airfoil at three different angles of attack (0 deg., 4 deg., and 10 deg.). Each case provided by the organizers was run with three different turbulence models: the Spalart-Allmaras one-equation turbulence model, the Menter SST k-omega two-equation model, and the k-sqrt(k)L two-equation model.

Estimates of numerical uncertainty due to discretization error are made. For local (i.e., surface and field) quantities, numerical uncertainty estimates are made based on the authors' recently developed global deviation uncertainty estimator [2]. The approach requires solutions on at least three systematically-refined [3] grids and involves the computation of a global deviation from the formal order of accuracy [4] that applies to the three solutions. This method was shown to out-perform other local uncertainty estimators over a wide range of 2D and 3D test cases, providing better conservativeness (i.e., percentage of cases where the uncertainty estimate captures the exact solution) while still providing a tight uncertainty estimate. For global quantities such as lift and drag coefficients, the Grid Convergence Index [5] as implemented by Oberkampf and Roy [3] is used.

#### References:

- Workshop on Estimation of Discretization Errors Based on Grid Refinement Studies, http://web.tecnico.ulisboa.pt/ist12278/ Discretization/Workshop\_discretization\_2017.htm, last accessed February 6, 2017.
- T. S. Phillips and C. J. Roy, "A New Extrapolation-Based Uncertainty Estimator for Computational Fluid Dynamics," ASME Journal of Verification, Validation, and Uncertainty Quantification, Vol. 1, No. 4, December 2016.
- W. L. Oberkampf and C. J. Roy, Verification and Validation in Scientific Computing, Cambridge University Press, Cambridge, 2010.
- T. S. Phillips and C. J. Roy, "Richardson Extrapolation-Based Discretization Uncertainty Estimation for Computational Fluid Dynamics," ASME Journal of Fluids Engineering, Vol. 136, No. 12, 2014, pp. 121401-121411.
- P. J. Roache, "Perspective: A Method of Uniform Reporting of Grid Refinement Studies," ASME Journal of Fluids Engineering, Vol. 116, No. 3, 1994, pp. 405-413.

#### **Grid Refinement and Estimation of Discretization Error**

Technical Presentation. VVS2017-4128

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

This is a contribution to the Workshop on Estimation of Discretization Errors based on Grid Refinement Studies.

### Discussion of Submitted Results to the Workshop on Estimation of Discretization Errors based on Grid Refinement Studies

Technical Presentation. VVS2017-4075

Luis Eca, IST, Lisbon, Portugal, Guilherme Vaz, MARIN, Wageningen, Netherlands, Martin Hoekstra, Consultant Netherlands

Overview of the results presented by the different participants. Discussion of the main trends observed in the data. Open floor discussion. Conclusions of the Workshop.

### Technical Program Friday

#### TRACK 3 TOPICS IN VERIFICATION AND VALIDATION

### 3-3 TOPICS IN VERIFICATION AND VALIDATION: PART 22ND FLOOR, ACACIA AB10:30AM - 12:35PM

#### **Reducing Prediction Uncertainty in Random Simulations**

Technical Presentation. VVS2017-4051

10:30am - 10:55am

Kenneth Tanski, Logica LLC, Florence, SC, United States

Random Simulations result in a distribution that represents the outcome of events under various input conditions. The, response distributions produced are comprised of indicators including the mean, dispersion, skewness, and kurtosis.

If the response forms a normal distribution, then the standard deviation is used to determine the dispersion which is part of the prediction of an event under different scenarios, or factors and their levels. The ppm can also be used as an indicator of the event response at various response locations.

If the response distribution is normal but skewed to any degree, which is typically the case, then this creates an error in the calculated standard deviation used for prediction and increases the uncertainty in the event predication capability.

To mitigate the effects of skewness on event prediction, Logica has developed a method that greatly mitigates this effect by incorporating finite mathematics. With this method, the standard deviation can now be calculated with greater accuracy, reducing the uncertainty in the prediction of events.

This method can also be used for non-normal distributions. In this case the ppm is used as the method of determining the improved prediction capability.

The presentation is given in an easy to comprehend user friendly format with no in depth knowledge of Statistics required.

#### **Uncertainty and Response**

Technical Presentation. VVS2017-4053

10:55am - 11:20am

Kenneth Tanski, Logica LLC, Florence, SC, United States

The response typically of interest is a model created from an orthogonal array is the "Y" or mean model. This model in turn creates a response curve. But this response can have various degrees of uncertainty that often lead to errors in predictions.

To better understand the true degree of uncertainty of a response, the "S" or dispersion model needs to be considered as well.

In this paper we will illustrate how a mean model can yield significantly different response curves from its mean + dispersion response curve counterpart, and how to better quantify the effects of uncertainty into a response curve.

This paper is written and presented in an easy to comprehend and user friendly format where little Statistical background is required.

#### Validation of a Thermo-Mechanical Model for a Brake System

Technical Presentation. VVS2017-4044

11:20am - 11:45am

Myeongjae Han, Tae-won Park, Ajou University, Suwon-si, Korea (Republic)

Friction of a brake system decelerates the disc velocity by converting kinetic energy into thermal energy. Friction between the disc and the pad causes a rapid temperature rise in a very short period of time. This heat generation subsequently increases the thermal expansion coefficient and friction coefficient in friction materials, leading to change contact conditions in the frictional contact surface. The thermoelastic instability due to the coupling of such thermal and elastic contact makes numerical analysis difficult.

In this paper, we propose a three-dimensional multiphysics model coupling both thermal and mechanical models to consider these operating conditions. The analysis model is a multibody system composed of one disc, two pads and four pistons. For the reliability of this analysis model, the following experiments were performed. To obtain accurate temperature results, samples of the friction material were fabricated and material property tests were carried out. Mechanical properties such as elastic modulus, shear modulus and Poisson's ratio were measured using ETEK3000 test equipment. Temperature-dependent thermal properties such as thermal conductivity, specific heat and coefficient of thermal expansion were measured by the test method according to ASTM E1461 and ASTM E831. In order to validate the reliability of finite element model and material properties, modal analysis results were then compared with modal test results using an impact hammer. As a result, natural frequencies and mode shapes of the disc and pad were confirmed.

Temperature analysis results were compared with experimental results using a brake dynamometer (Automotive Inertia Brake Dynamometer Model 3000). The results of dynamic characteristics such as disc angular velocity, brake torque variation, pad pressure, and coefficient of friction were also confirmed. The JASO C406\_2000 test specification which was used primarily for brake performance testing was used.

Therefore, the thermal and dynamic behaviors of the brake system due to the heat generation of frictional contact occurring during braking were confirmed by coupled thermo-mechanical analysis using the thermoelastic properties obtained from the experiment. The reliability of the finite element model and material properties was validated through modal test. Finally, experimental results of the temperature and dynamic characteristics were validated by using the brake dynamometer tests.

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Design modification of a brake disk and pad have been performed using the proposed model. Newly designed brake disk and pad have been built and tested. The comparison between the existing and improved designs proves the effectiveness of the design method using the proposed multiphysics model.

#### Use of Wavelet Multiscale Decomposition for Numerical and Experimental Mode Shape Correlation

Technical Presentation. VVS2017-4149

11:45am - 12:10pm

*Walter Ponge-Ferreira*, Escola Politécnica da Universidade de São Paulo, São Paulo, São Paulo, Brazil

An important issue in model updating is the comparison and correlation of experimental and numerical modes of vibration of structures. Many updating approaches target the minimization of the difference in both results, mode shapes, and natural frequencies. To compare experimental and analytical mode shapes, we must use some transformation to expand or reduce the number of degrees of freedom. Unfortunately, experimental results have often only a reduced number of measured degrees of freedom, and though, are not much sensitive to the influence of boundary conditions. Otherwise, experimental boundary conditions are not as reliable as numerical, e.g.; it is very hard to construct a clamped boundary condition for a beamlike structure in the laboratory. However, the influence of boundary conditions on the shape of modes of vibration are usually localized in space and more visible at a particular scale of the model. Therefore, it is convenient not to overemphasize the difference between experimental and numerical mode shapes near boundary locations. Wavelet multiscale analysis can be used to decompose the mode shapes in different scales and locations. Local aspects of the mode shapes obtained numerically, must be filtered out, before comparing experimental and numerical results. Experimental results error are fitted on the wavelet multiscale base of the numerical mode shapes. Finally, it is possible to compare experimental and numerical results taking into account the local and spatial accuracy of the model. This approach was used to investigate simple beamlike structures and plane stress structures to verify its potential to improve model updating and model validation technics.

Summary of presentation: introduction, wavelet multiscale decomposition, comparison and correlation of mode shapes, error multi-scale fitting, correlation of modes in different levels and approximations, uncertainty analysis, and conclusion.

#### Numerical Simulation and Experimental Analysis of Axial - flow Pump System for Bell- type Inlet Passage

Technical Presentation. VVS2017-4010

12:10pm - 12:35pm

Xie Chuanliu, Tang Fangping, Zhou Jiren, Xia Ye, Duan Xiaohui, Zhang Wenpeng, Yangzhou University, Yangzhou, Jiangsu, China

Based on the RNG k-? turbulence model and the Renault time N-S equation, the CFD software was used to simulate the three-dimensional flow of the axial flow pump of the bell-type inlet channel and verified by the model test. The three - dimensional flow simulation of the pump device including the inlet channel, impeller, guide vane and outlet channel is carried out by CFX. The energy performance test and the cavitation performance test were carried out in 5 different blade angles, and the inlet and outlet channel pressure difference test was carried out in one of the selected blade angles, and the test bench error was less than 0.3%. Based on numerical simulation and model test results: the maximum efficiency of the vertical axial pump is 76%, and the efficiency of the pump is 75.74% on the 6.63m of design point. Numerical simulation and model test in the 1.1-1.5 optimal flow condition, the performance curve of the numerical simulation is about 3% higher than that of the experimental results. Under the 0.9-1.1 optimal flow condition, the performance curve of the numerical simulation is about 2% higher than that of experimental results. Under the 0.6-0.9 flow optimal condition, the performance curve of the numerical simulation is about 4% less than that of experimental results. The results show that the numerical simulation is more accurate in predicting the design point of the axial pump of performance curve and the reliability of the numerical simulation can be reduced when deviation from design point. The numerical simulation shows that the hydraulic loss of the inlet channel is about 0.146m and the hydraulic loss of the outlet channel is about 0.561m. It is difficult to measure the circumferential velocity of the test section of the inlet and outlet channel, therefore, the hydraulic loss of the model test and the numerical simulation has some deviation, but the order of magnitude has the same trend. The flow pattern through the numerical simulation of the inlet and outlet channel is obtained under calculated conditions, and the inlet and outlet channels are free of vortex and other bad flow patterns compared to model test. It is shown that numerical simulation is more accurate in predicting flow pattern. It can be seen from the above that the numerical simulation is reliable when predicting the performance of the axial flow pump. The numerical simulation is used to predict the axial flow pump of the bell-type inlet channel, which shortens the test cycle and saves the cost. Numerical simulation can accurately and reliably guide the application of engineering, and provide reference for the design and safe operation of similar pump station.

Key words: axial - flow pump device; numerical simulation; model test; bell- type inlet passage; verification

References: "Numerical Simulation and Experimental Analysis of Axial - flow Pump System for Bell- type Inlet Passage," submitted to the Ninth International Pumping Machinery Symposium, which is being held at FEDSM2017.

### Technical Program Friday

#### TRACK 8 VERIFICATION & VALIDATION FOR IMPACT, BLAST, AND **MATERIAL RESPONSE**

#### 8-1 VERIFICATION & VALIDATION FOR IMPACT. BLAST. AND MATERIAL RESPONSE **2ND FLOOR, PALO VERDE B** 10:30AM - 12:35PM

#### Study on a Surface-surface Comparison-based Validation Metric for **Vehicle Crashworthiness Simulations**

Technical Presentation, VVS2017-4089

10:30am - 10:55am

#### Jungi Yang, Zhenfei Zhan, Yudong Fang, Chongqing University, Chongqing, China

Computer Aided Engineering (CAE) models have proven themselves to be efficient surrogates of real-world systems in automotive industries and academia. To successfully integrate the CAE models into analysis process, model validation is necessarily required to assess the models' predictive capabilities regarding their intended usage. In the context of model validation, quantitative comparison which considers specific measurements in real-world systems and corresponding simulations serves as a principal step in the assessment process. For many engineering applications (e.g. passive safety of vehicle), surface deformation frequently serves as an essential measurement for validation activities to make decision on the quality of a model. However, recent approaches for such application are commonly based on graphical comparison, while error measure for surface in engineering has not been well studied.

To deal with this problem, a validation metric, which combines the discrepancies measurements in magnitude and shape, is proposed to evaluate the inconsistence between two deformed surfaces. The process contains two main parallel assessment procedures for magnitude error and shape error, respectively. A 2-dimentional dynamic time warping (2D-DTW) algorithm is exploited to match the shape features (i.e. peaks and valleys) of surfaces. The pre-processed surfaces are then submitted to the following distance measurement calculation. For shape error, geometric feature, say Gaussian and mean curvatures of surfaces are evaluated for surface characterization, based on which a surface descriptor is extracted. Wavelet theory based multi-resolution analysis framework is developed for discrepancy quantification. With the quantified surface features, wavelet decomposition based multi-resolution analysis is then formulated for shape error evaluation.

A case study about elastic-plastic deformation analysis is utilized to show the validity of the proposed validation method. Three models with different fidelity are designed to simulate the behavior of the plate bending test. Various simulation parameters help to specify the features of the three simulation formulations. According to the assessment results, the errors in magnitude and shape can be separately recognized based on the proposed validation metric. Moreover, the ranking results regarding model fidelity are consistent with the assumptions which are made according to the configurations of the three formulations. Based on the case study, it is suggested that the proposed surface-surface validation

metric has the capability to quantify and differentiate the fidelity of models. The method has then been applied to real-world case in vehicle safety application. The results shows the metric's capability of recognizing the surface features correctly and assessing models fidelity quantitatively, as well as its potential in engineering applications.

#### Verifying FLAG Using Hunter's and Blake's Problems as Implemented in ExactPack

Technical Presentation. VVS2017-4052

10:55am – 11:20am

#### Joanne Budzien, John Walter, Los Alamos National Laboratory, Los Alamos, NM, United States

Hunter's problem has been proposed as an extension to the tri-laboratory suite of verification problems (Kamm et al. LA-14379, 2008). The current work will report on implementing Hunter's problem into an updated Verification Test Suite at Los Alamos National Laboratory as well as comparisons of the analytical solution with the numerical solution produced by the hydrocode FLAG. Comparisons with the results of the Blake problem will also be made.

Hunter's problem (Hunter, Proceedings of the Conference on Properties of Materials at High Rates of Strain, London 1957, pp. 147-155, 1957) is a generalization of the Blake problem (Blake, J. Acoust. Soc. Am. vol. 24, pp. 211-215, 1952). Hunter's problem is an interesting extension to the Blake problem that has substantially less literature devoted to it. Both problems test the small strain dynamic response of a material with an inclusion at the center and tracking a spherically symmetric wave as it propagates through the material. Blake's problem assumes purely linear elastic response by the medium while Hunter's problem also includes an elastic- perfectly plastic response. By applying a particular time-dependent pressure history on the inner wall of the spherical inclusion, the boundary between the elastic (outer) solution region and the plastic (inner) region will move at constant velocity. For verification purposes, this constant velocity condition is important since it allows for a closed-form solution of the inclusion pressure as a function of time. With this constant velocity elastic-plastic boundary assumption, the stress and velocity fields may also be computed in closed form and those fields can then be compared to the output from the code.

#### Method of Manufactured Solution for Large Deformation Problem of Hyper-elasticity

Technical Presentation. VVS2017-4104

11:20am – 11:45am

Takahiro Yamada, Yokohama National University, Yokohama, Kanagawa, Japan

The method of manufactured solution proposed by Roache [1] is widely used to verify numerical codes in fluid dynamics. In this method, second derivatives of given solutions or spatial derivatives of stresses derived

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from given solutions are required to calculate body forces. However such derivatives can hardly be evaluated in nonlinear problems of solid materials and hence it is not popular in solid mechanics. The author developed an alternative technique to calculate equivalent nodal vectors of body forces without calculation of the second order derivative of solutions for the method of nearby problems [2]. 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. We have applied our procedure to the problems of elastoplasticity, which is a typical model of manufactured solution for large deformation problems of hyper-elasticty, which is often used to describe rubbler-like materials.

In our approach, an arbitrary displacement field can be prescribed for manufactured solutions. However solids undergoing the large deformations usually exhibit incompressible or nearly incompressible behaviors and hence displacement fields of manufactured solutions are required to satisfy incompressibility or very small volumetric change. Thus we developed a procedure to construct displacement fields in which volumetric changes are controlled in the large deformation state.

Several representative numerical results are presented to discuss the properties of proposed manufactured solutions.

- P. J. Roache and S. Steinberg, "Symbolic manipulation and computational fluid dynamics," AIAA Journal, Vol. 22, No. 10, 1984, pp. 1390-1394.
- T. Yamada, "Verification Procedure Based on Method of Nearby Problems for Finite Element Analysis of Solid," ASME 2015 Verification and Validation symposium, 2015.



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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

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

Interested applicants should contact Fred Constantino, ConstantinoF@ asme.org

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

Interested applicants should contact Marian Heller, HellerME@asme.org

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

Interested applicants should contact Ryan Crane, CraneR@asme.org

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

Interested applicants should contact Ryan Crane, CraneR@asme.org

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

Interested applicants should contact Marian Heller, HellerME@asme.org

ASME V&V 60 - Verification and Validation of Computational Modeling for Energy Systems

Interested applicants should contact Ryan Crane, CraneR@asme.org

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