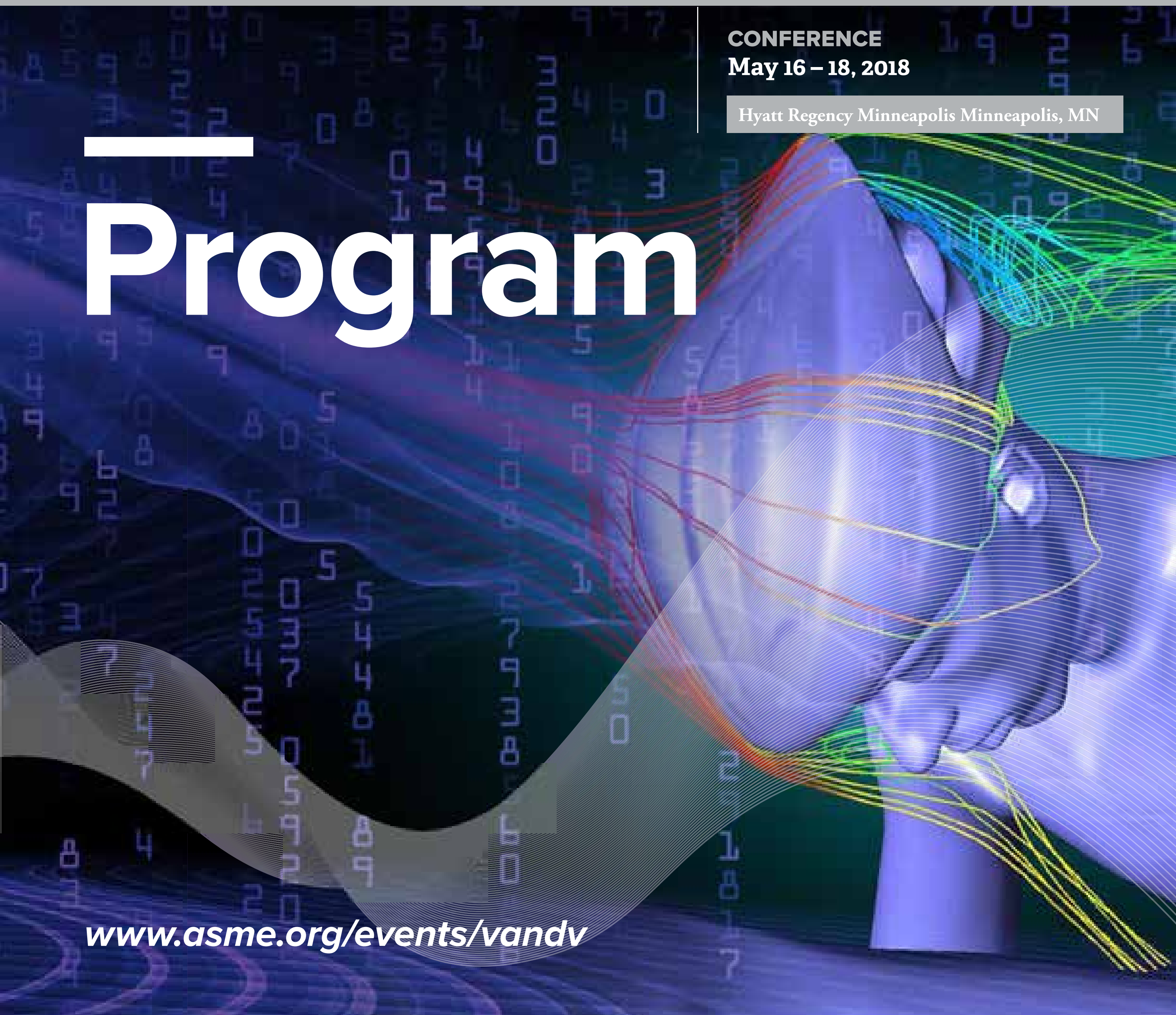
V&V 2018

VERIFICATION AND VALIDATION SYMPOSIUM



CONFERENCE
May 16 – 18, 2018

Hyatt Regency Minneapolis Minneapolis, MN

Program

www.asme.org/events/vandv

The American Society of Mechanical Engineers®
ASME®

ASME
SETTING THE STANDARD

Welcome

Welcome to ASME's 2018 Verification and Validation Symposium!

Dear Colleagues:

Thank you for participating in ASME's annual Verification and Validation Symposium: dedicated entirely to verification, validation and uncertainty quantification of computer simulations. The outstanding response to the call for abstracts has allowed us to create a technical program that has improved each year, bringing 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 Co-Chairs and Organizing Committee

Kate Hyam
ASME

Jeffrey Bodner
Medtronic Corp

Scott Doebling
Los Alamos National Laboratory

Kevin Dowding
Sandia National Laboratories

Luis Eça
IST

Tina Morrison
U.S. Food and Drug Administration

Christopher Roy
Virginia Tech

Ryan Crane
ASME

Marian Heller
ASME

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General Information

REGISTRATION HOURS AND LOCATION

Registration is in the Great Lakes Foyer

Registration Hours:

Monday, May 14:	7:00am – 6:00pm
Tuesday, May 15:	7:00am – 6:00pm
Wednesday, May 16:	7:00am – 6:00pm
Thursday, May 17:	7:00am – 6:00pm
Friday, May 18:	7:00am – 12:00pm

HOTEL BUSINESS SERVICES

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

Business hours are:

Monday – Friday:	7:00am – 5:00pm
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 Hyatt Regency Minneapolis. Please check the schedule for event times and locations.

REGISTRATION FEES

Full Registration Fee includes:

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

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

NAME BADGES

Please wear your name badge at all times; you will need it for admission to all 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 Hyatt Regency Minneapolis. Free Wi-Fi is also available in the lobby of The Hyatt Regency Minneapolis.

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. Advance 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 Hyatt Regency Minneapolis concierge or front desk.

ASME V&V COMMITTEE MEETING SCHEDULE

All meetings are open to the public and Symposium attendees are welcome to attend (except where noted).

MONDAY, MAY 14, 1:00PM-5:00PM

V&V 30 Subcommittee on Verification and Validation in Computational Simulation of Nuclear System Thermal Fluids Behavior, Lake Harriet, 4th Floor

TUESDAY, MAY 15, 8:00AM-5:00PM

V&V 20 Subcommittee on Verification and Validation in Computational Fluid Dynamics and Heat Transfer, Great Lakes A1, 4th Floor

V&V 30 Subcommittee on Verification and Validation in Computational Simulation of Nuclear System Thermal Fluids Behavior, Great Lakes A3, 4th Floor

V&V 60 Computational Modeling in Energy Systems, Lake Harriet, 4th Floor

TUESDAY, MAY 15, 8:30AM-1:00PM

V&V 40 Industry Day (Register at Eventbrite.), Great Lakes C, 4th Floor

TUESDAY, MAY 15 9:00AM-5:00PM

V&V 10 Subcommittee on Verification and Validation in Computational Solid Mechanics, Great Lakes A2, 4th Floor

TUESDAY, MAY 15 2:00PM-4:00PM

ASME V&V 40 – Verification and Validation in Computational Modeling of Medical Devices, Great Lakes C, 4th Floor.

WEDNESDAY, MAY 16, 6:30PM-9:00PM

V&V Standards Committee on Verification and Validation in Computational Modeling and Simulation. Networking Reception will follow and all Symposium attendees are invited, Lake Harriett, 4th Floor

THURSDAY, MAY 17, 6:00PM-9:00PM

V&V 50 Subcommittee on Verification and Validation in Computational Modeling for Advanced Manufacturing, Lake Harriet 4th Floor.

FRIDAY, MAY 18, 1:00PM-5:00PM

V&V 50 Subcommittee on Verification and Validation in Computational Modeling for Advanced Manufacturing, Lake Harriet 4th 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 Kate Hyam, HyamK@asme.org

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

Interested applicants should contact Michelle Pagano, PaganoM@asme.org

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

Interested applicants should contact Kate Hyam, HyamK@asme.org

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

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

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

Interested applicants should contact Kate Hyam hyamk@asme.org

ONE-DAY SEMINAR HELD IN CONJUNCTION WITH THE ASME V&V SYMPOSIUM ON MAY 14-15, 2018

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.

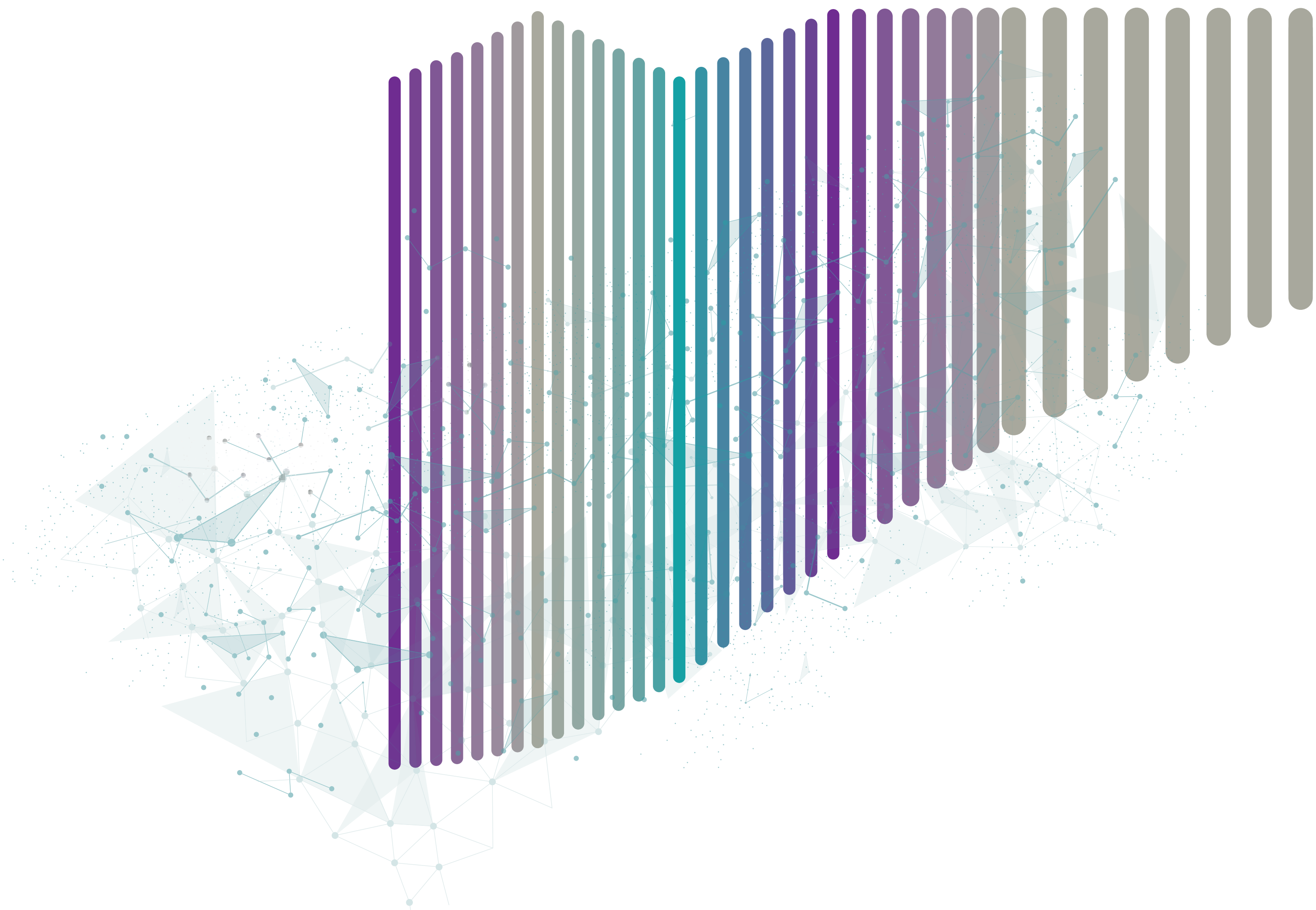
For more information and to register, go to http://go.asme.org/mc133

MONDAY, MAY 14, 9:30AM-600PM

Alliance of Advanced BioMedical Engineering
POWERED BY ASME

AABME CONNECT: WHERE BIOMEDICINE AND ENGINEERING COME TOGETHER

(space is limited – if you are interested in receiving an invitation, please email aabmeconnect@asme.org



PLEASE JOIN US

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

FOLLOWED BY A NETWORKING RECEPTION

WEDNESDAY, MAY 16

HYATT REGENCY

MEETING 6:30PM – 7:30PM

GREAT LAKES B, 4TH FLOOR

RECEPTION 7:30PM – 9:00PM

GREAT LAKES C, 4TH FLOOR

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.

Schedule at a Glance

MONDAY, MAY 14, 2018

TIME	SESSION #	PAGE	SESSION
07:00 AM - 06:00 PM			Registration
07:00 AM - 06:00 PM			Speaker Ready Room
08:00 AM – 05:00 PM			Verification and Validation in Scientific Computing
1:00 PM – 5:00 PM			V&V 30 Subcommittee on Verification and Validation in Computational Simulation of Nuclear System Thermal Fluids Behavior

TUESDAY, MAY 15, 2018

TIME	SESSION #	PAGE	SESSION
07:00 AM - 06:00 PM			Registration
08:00 AM – 05:00 PM			Verification and Validation in Scientific Computing
09:00 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
08:30 AM – 01:00 PM			V&V 40 Subcommittee Industry Day
08:00 AM – 05:00 PM			V&V 60 Subcommittee Computational Modeling in Energy Systems
02:00 AM – 04:00 PM			V&V 40 Subcommittee on Verification and Validation in Computational Modeling of Devices
06:00 PM – 08:00 PM			V&V Standards Committee (Closed Session)

WEDNESDAY, MAY 16, 2018

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	‘(4)		Opening Address and Plenary Presentions
10:00 AM - 10:25 AM			Coffee Break
10:25 AM to 12:30 PM	2-1		Development and Application of Verification and Validation Standards. Session 1
10:25 AM to 12:30 PM	4-1		Uncertainty Quantification, Sensitivity Analysis, and Prediction: Session 1
10:25 AM to 12:30 PM	10-1		Verification and Validation of Nuclear Power Applications
12:30 PM - 01:30 PM			Lunch
01:30 PM to 03:35 PM	2-2		Development and Application of Verification and Validation Standards. Session 2
01:30 PM to 03:35 PM	6-1		Validation Methods
04:00 PM to 06:05 PM	11-1		Verification for Fluid Dynamics and Heat Transfer
03:35 PM - 04:00 PM			Coffee Break
04:00 PM to 06:05 PM	1-4		Code Verification for Applicants in a Regulated Field
04:00 PM to 06:05 PM	3-1		Topics in Verification and Validation
04:00 PM to 06:05 PM	8-1		Verification and Validation for Impact, Blast, and Material Response
06:30 PM to 07:30 PM			V&V Standards Committee Open Session
07:30 PM to 09:00 PM			Networking Reception

TRACK	ROOM
	Registration Desk - Great Lakes (Foyer)
	Lake Nokomis, 4th Fl
MC133	Lake Calhoun, 4th Fl
	Lake Harriett, 4th Fl

TRACK	ROOM
	Registration Desk- Great Lakes Foyer
MC133	Lake Calhoun, 4th Fl
	Great Lakes A2, 4th Fl
	Great Lakes A1, 4th Fl
	Great Lakes A3, 4th Fl
	Great Lakes C, 4th Fl
	Lake Harriett, 4th Fl
	Great Lakes C, 4th Fl
	Great Lakes A3, 4th Fl

TRACK	ROOM
	Registration Desk - Great Lakes (Foyer)
	Great Lakes C, 4th Fl
	Great Lakes B, 4th Fl
	Great Lakes Foyer, 4th Fl
	Great Lakes A1, 4th Fl
	Great Lakes A2, 4th Fl
	Great Lakes A3, 4th Fl
	Great Lakes C, 4th Fl
	Great Lakes A1, 4th Fl
	Great Lakes A2, 4th Fl
	Great Lakes A3, 4th Fl
	Great Lakes Foyer, 4th Fl
	Great Lakes A1, 4th Fl
	Great Lakes A2, 4th Fl
	Great Lakes A3, 4th Fl
	Great Lakes B, 4th Fl
	Great Lakes C, 4th Fl

Schedule at a Glance

THURSDAY, MAY 17, 2018

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	‘(4)		Plenary Session
10:00 AM - 10:25 AM			Coffee Break
10:25 AM to 12:30 PM	1-5		ASME 2018 V&V Verification, Validation, and Uncertainty Quantification: The Unanswered Questions
10:25 AM to 12:30 PM	12-2		Verification Methods
10:25 AM to 12:30 PM	13-2		ASME V&V 40 Subcommittee -- Verification and Validation in Computational Modeling of Medical Devices
12:30 PM - 01:30 PM			Lunch
01:30 PM to 03:35 PM	4-3		Uncertainty Quantification, Sensitivity Analysis, and Prediction: Session 3
01:30 PM to 03:35 PM	5-1		Validation for Fluid Dynamics and Heat Transfer
01:30 PM to 03:35 PM	12-1		Verification Methods
03:35 PM - 04:00 PM			Coffee Break
04:00 PM to 06:05 PM	1-2		V&V BENCHMARK PROBLEM —TWIN JET COMPUTATIONAL FLUID DYNAMICS (CFD) NUMERIC MODEL VALIDATION
04:00 PM to 06:05 PM	9-1		Validation Methods for Solid Mechanics and Structures
04:00 PM to 06:05 PM	13-1		Verification and Validation for Biomedical Engineering
6:00 PM - 9:00 PM			V&V 50 Computational Modeling for Advanced Manufacturing

FRIDAY, MAY 18, 2018

TIME	SESSION #	PAGE	SESSION
07:00 AM - 12:00 PM			Registration
07:00 AM - 08:00 AM			Continental Breakfast
08:00 AM to 10:05 AM	1-1		Unsteady Flow Workshop
08:00 AM to 10:05 AM	17-1		Verification and Validation for Advanced Manufacturing
10:05 AM - 10:30 AM			Coffee Break
10:30 AM to 12:35 PM	1-3		Industry Challenges in Uncertainty Quantification: Bridging the Gap Between Simulation and Test
10:30 AM to 12:35 PM	4-2		Uncertainty Quantification, Sensitivity Analysis, and Prediction: Session 2
1:00 PM - 5:00 PM			V&V 50 Computational Modeling for Advanced Manufacturing

TRACK	ROOM
	Registration Desk- Great Lakes Foyer
	Great Lakes C, 4th Fl
	Great Lakes B, 4th Floor
	Great Lakes , 4th Fl
	Great Lakes B, 4th Fl
	Great Lakes A2, 4th Fl
	Great Lakes A2, 4th Fl
	Great Lakes C, 4th Fl
	Great Lakes A1, 4th Fl
	Great Lakes A2, 4th Fl
	Great Lakes A3, 4th Fl
	Great Lakes Foyer, 4th Fl
	Great Lakes A1, 4th Fl
	Great Lakes A2, 4th Fl
	Great Lakes A3, 4th Fl
	Lake Harriett, 4th Fl

TRACK	ROOM
	Registration Desk- Great Lakes Foyer
	Great Lakes C, 4th Fl
	Great Lakes A1, 4th Fl
	Great Lakes A2, 4th Fl
	Great Lakes Foyer, 4th Fl
	Great Lakes A1, 4th Fl
	Great Lakes A2, 4th Fl
	Lake Harriett, 4th Fl

Session Chairs

TRACK-1 CHALLENGE PROBLEM WORKSHOPS AND PANEL SESSIONS

1-1 Unsteady Flow Workshop

Luis Eca, *IST, Lisbon, Portugal*
Michelle Pagano, *ASME, New York, NY, United States*

1-2 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*

1-3 Industry Challenges in Uncertainty Quantification: Bridging the Gap Between Simulation and Test

Mark Andrews, *SmartUQ, Madison, WI, United States*
Peter Chien, *SmartUQ, Madison, WI, United States*

1-4 Code Verification for Applicants in a Regulated Field

Marc Horner, *ANSYS, Inc., Evanston, IL, United States*
David Moorcroft, *Federal Aviation Administration, Oklahoma City, OK, United States*
Michelle Pagano, *ASME, New York, NY, United States*

1-5 ASME 2018 V&V Verification, Validation, and Uncertainty Quantification: The Unanswered Questions

Scott Doebling, *Los Alamos National Lab, Los Alamos, NM, United States*
Daniel Israel, *Los Alamos National Lab, Los Alamos, NM, United States*

TRACK-2 DEVELOPMENT AND APPLICATION OF VERIFICATION AND VALIDATION STANDARDS

2-1 Development and Application of Verification and Validation Standards. Session 1

William Oberkampf, *W L Oberkampf Consulting, Georgetown, TX, United States*
Ryan Crane, *ASME, New York, NY, United States*

2-2 Development and Application of Verification and Validation Standards. Session 2

Joshua Kaizer, *U.S. Nuclear Regulatory Commission, Abingdon, MD, United States*
Kathryn Hyam, *ASME, New York, NY, United States*

TRACK-3 TOPICS IN VERIFICATION AND VALIDATION

3-1 Topics in Verification and Validation

Donna Guillen, *Idaho National Laboratory, Idaho Falls, ID, United States*
William Oberkampf, *W L Oberkampf Consulting, Georgetown, TX, United States*

TRACK-4 UNCERTAINTY QUANTIFICATION, SENSITIVITY ANALYSIS, AND PREDICTION

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

Kyung Choi, *University Of Iowa, College Of Engineering, Iowa City, IA, United States*
Rafael Ruiz, *Universidad de Chile, Santiago, Chile*

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

Ilias Bilionis, *Purdue University, West Lafayette, IN, United States*
Paul Gardner, *University of Sheffield, Sheffield, United Kingdom*

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

Joseph Beck, *Perceptive Engineering Analytics, LLC, Minneapolis, MN, United States*
Kevin OFlaherty, *SmartUQ, Madison, WI, United States*

TRACK-5 VALIDATION FOR FLUID DYNAMICS AND HEAT TRANSFER

5-1 Validation for Fluid Dynamics and Heat Transfer

V. Gregory Weirs, *Sandia National Laboratories, Albuquerque, NM, United States*
Kenneth Aycock, *US Food and Drug Administration, Silver Springs, MD, United States*

TRACK-6 VALIDATION METHODS

6-1 Validation Methods

William Oberkampf, *W L Oberkampf Consulting, Georgetown, TX, United States*
Mark Andrews, *SmartUQ, Madison, WI, United States*

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

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

Duane Cronin, *University of Waterloo, Waterloo, ON, Canada*
Joanne Budzien, *Los Alamos National Laboratory, Los Alamos, NM, United States*

TRACK-9 VALIDATION METHODS FOR SOLID MECHANICS AND STRUCTURES

9-1 Validation Methods for Solid Mechanics and Structures

Zhong Hu, *South Dakota State University, Brookings, SD, United States*
Duane Cronin, *University of Waterloo, Waterloo, ON, Canada*

TRACK-10 VERIFICATION AND VALIDATION OF NUCLEAR POWER APPLICATIONS

10-1 Verification and Validation of Nuclear Power Applications

Michelle Pagano, *ASME, New York, NY, United States*
Kathryn Hyam, *ASME, New York, NY, United States*

TRACK-11 VERIFICATION FOR FLUID DYNAMICS AND HEAT TRANSFER

11-1 Verification for Fluid Dynamics and Heat Transfer

V. Gregory Weirs, *Sandia National Laboratories, Albuquerque, NM, United States*
Robert Singleton, *Los Alamos National Laboratory, Los Alamos, NM, United States*

TRACK-12 VERIFICATION METHODS

12-1 Verification Methods

Robert Singleton, *Los Alamos National Laboratory, Los Alamos, NM, United States*
Michelle Pagano, *ASME, New York, NY, United States*

12-2 Verification Methods

V. Gregory Weirs, *Sandia National Laboratories, Albuquerque, NM, United States*
Robert Singleton, *Los Alamos National Laboratory, Los Alamos, NM, United States*

TRACK-13 VERIFICATION AND VALIDATION FOR BIOMEDICAL ENGINEERING

13-1 Verification and Validation for Biomedical Engineering

Ali Kiapour, *4WEB Medical Inc., Newton, MA, United States*
Kevin OFlaherty, *SmartUQ, Madison, WI, United States*

13-2 ASME V&V 40 Subcommittee -- Verification and Validation in Computational Modeling of Medical Devices

Tina Morrison, *Food and Drug Administration, Silver Spring, MD, United States*
Marc Horner, *ANSYS, Inc., Evanston, IL, United States*

TRACK-17 VERIFICATION AND VALIDATION FOR ADVANCED MANUFACTURING

17-1 Verification and Validation for Advanced Manufacturing

Marian Heller, *ASME, New York, NY, United States*
Mark Benedict, *AFRL Mantech, WPAFB, OH, United States*

WEDNESDAY, MAY 16 • 8:00AM – 10:00AM • GREAT LAKES B

PLENARY 1: VERIFICATION, VALIDATION, AND UNCERTAINTY QUANTIFICATION – ARE WE MAKING ANY PROGRESS?

Dr. Ben H. Thacker
Director of the Materials Engineering Department
Southwest Research Institute

Dr. Ben H. Thacker is the Director of the Materials Engineering Department at Southwest Research Institute. The department is quite diverse with many active applied R&D projects in surface engineering, materials development, failure analysis, computational materials, additive manufacturing, environmental effects, biomechanics, life prediction, energy storage, mechanical performance, and uncertainty quantification. His technical contributions have primarily been in the development and implementation of advanced probabilistic methods, application of probabilistic methods to high-consequence engineering problems, and model verification and validation (V&V). He has over 130 publications in these general areas. He is a Registered Professional Engineer in the State of Texas, a Fellow of AIAA, and a founding member of the ASME Subcommittee for V&V of Computational Solid Mechanics. He currently serves as Vice Chair of the ASME V&V Standards Committee for V&V. Dr. Thacker obtained his B.S. from Iowa State University, his M.S. from the University of Connecticut, and his Ph.D. from the University of Texas at Austin.

Abstract: A huge amount of R&D has been and continues to be focused on reducing the time and cost required to develop new materials, products and systems. Augmenting testing with modeling and simulation clearly enables this; however, that is the easy part. The much harder part is trusting model predictions. This is precisely what motivated the development of formal standards for model VVUQ. In addition to our ASME standards, NASA, AIAA, FAA, and USAF have all produced similar or complementary documents. We collectively should be proud of this progress because the body of knowledge represents a high-level of understanding and consensus of VVUQ, but what impact has it had? Quantifying the confidence and predictive accuracy of a model is clearly important, but does it establish trust or credibility in the predictions? Are we making any progress? This presentation will review a few of the more salient points associated with UQ in V&V, and conclude with several real-world examples that utilized VVUQ concepts during the model development process.

PLENARY 2: VALIDATION AND PREDICTIVE CAPABILITY OF IMPERFECT MODELS WITH IMPRECISE DATA

Dr. Scott Ferson
Professor, University of Liverpool
Director of Institute of Risk and Uncertainty

Scott Ferson is director of the Institute for Risk and Uncertainty at the University of Liverpool in the UK. For many years he was senior scientist at Applied Biomathematics and an adjunct professor at the School of Marine and Atmospheric Sciences at Stony Brook University. He was recently a visiting fellow at the Université de Technologie de Compiègne in France. He holds a Ph.D. in Ecology and Evolution from the State University of New York (SUNY) and an A.B. in biology from Wabash College. His professional interests include statistics when empirical information is very sparse, medical risks and population biology, and risk analysis. Ferson has five published books, ten commercially distributed software packages, and over a hundred scholarly publications, mostly in environmental risk analysis, uncertainty propagation, and conservation biology. He is a fellow of the Society for Risk Analysis and was recently named Distinguished Educator by the Society. Ferson has been the central figure in the development of probability bounds analysis, an approach to reliably computing with imprecisely specified probabilistic models. His research over the last decade, funded primarily by the National Institutes of Health, NASA, and Sandia National Laboratories, has focused on developing reliable mathematical and statistical tools for risk assessments and uncertainty analysis when empirical information is very sparse, including methods for quality assurance for Monte Carlo assessments, exact methods for detecting clusters in very small data sets, backcalculation methods for use in remediation planning, and distribution-free methods of risk analysis. He serves on editorial boards for several journals, and he has served on many expert panels in the United States and internationally.

Abstract: Many sophisticated models in engineering today incorporate randomness or stochasticity and make predictions in the form of probability distributions or other structures that express predictive uncertainty. Validation of such models must contend with observations that are often sparse or imprecise, or both. The predictive capability of these models, which determines what we can reliably infer from them, is assessed by whether and how closely the model can be shown to yield predictions conforming with available empirical observations beyond those data used in the model calibration process. Interestingly, a validation match between the model and data can be easier to establish when the predictions or observations are uncertain, but the model's predictive capability is degraded by either uncertainty. It is critical that measures used for validation and estimating predictive capability not confuse variability with lack of knowledge, but rather integrate these two kinds of uncertainties (sometimes denoted 'aleatory' and 'epistemic') in a way that leads to meaningful statements about the fit of the model to data and the reliability of predictions it generates.

THURSDAY, MAY 17 • 8:00AM – 10:00AM • GREAT LAKES B

PLENARY 3: STRATEGIC UTILIZATION OF MODELING TO IMPACT BD

Anita Bestelmeyer
Director, Corporate Computer-Aided Engineering (CAE)
BD Technologies and Innovation (BDTI)

Anita Bestelmeyer currently serves as the Director of BD's Corporate Computer-Aided Engineering (CAE) group in Research Triangle Park, NC at BD Technologies and Innovation (BDTI) and has been in this role since June 2012. The Corporate CAE group is the center-of-expertise in simulation, optimization, advanced prototyping, CT scanning, material testing coordination, web-enabled tools and exponential technologies. The group's mission is to deliver innovative, optimized and robust products to market faster.

Anita started her career at BD in 1991 and has taken on increasing levels of responsibility within the company the last 26 years. Anita has been a champion in deploying CAE technologies to impact the company and successfully built a BDX network across businesses, regions and functions to leverage these tools successfully. She is actively involved in cross-company initiatives such as the Technology Leadership Development Program Steering (TLDP) Committee, "Build Pipeline" - Diversity Action Team, Product Lifecycle Management (PLM) initiative, BDU teacher for Manager Essentials, etc. She was the recipient of the BD Becton Quality Award in 2014 and the BD Howe Technology Award in 2017.

Anita is recognized externally for her in-depth expertise and leadership through invited keynote and panel presentations at industry conferences such as the Society of Women Engineers, Design of Medical Devices, and the Dassault Systemes Simulia Customer Conference. She is also on the Medical Device Innovation Consortium Modeling and Simulation Steering Committee, ASME V&V 40 Committee setting guidelines for computational modeling used in regulatory submission and the BMES/FDA Frontiers in Medical Devices: Innovations in Modeling and Simulation conference leadership. This participation is important to staying on the forefront of the industry in advancing translational and regulatory science.

Prior to BD, Anita worked in the aerospace industry at TRW Inc. Space and Technology group in Redondo Beach, CA from 1984 to 1991. Anita received a B.S. in Civil Engineering from the University of Illinois, Urbana-Champaign in 1983 and a M.S. from the University of California, Berkeley in Civil Engineering, Structural Mechanics in 1984.

Abstract: BD is one of the largest global medical technology companies in the world and is advancing the world of health by improving medical discovery, diagnostics and the delivery of care. BD's Corporate Computer-Aided Engineering (CAE) group is the center-of-expertise for simulation, optimization, advanced prototyping, CT scanning, material testing coordination, web-enabled tools and exponential technologies. The group's mission is to deliver innovative, optimized and robust products to market faster.

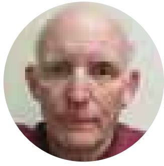
BD's Corporate CAE group in Research Triangle Park, NC has been utilizing simulation for over 30 years to impact the company. The three primary modeling areas include injection molding simulation, structural analysis and computational fluid dynamics. Historically, the use of modeling for BD's high-volume disposable medical devices started with injection molding simulation to ensure design for manufacturability, part quality and manufacturing robustness. The group then implemented structural analyses due to the need to include the effects of nonlinear materials, large deformations, fracture and damage and contact between multiple components. Finally, the use of computational fluid dynamics has been essential to predicting fluid flow effectiveness through BD's products and the human body. Each of these modeling areas are leveraged on a day-to-day basis by the Corporate CAE group and successful case studies and the approach to verification and validation will be shared.

BD has been at the forefront of promoting the acceptance and use of simulation in the medical industry. The Corporate CAE group has been an active participant and voting member on the Verification and Validation (V&V) 40 committee in Computational Modeling of Medical Devices. The goal of this committee is to coordinate, promote, and foster the development of standards that provide procedures for assessing and quantifying the accuracy and credibility of computational models and simulations by device manufacturers and regulatory agencies. BD has also been strong partners in the Medical Device Innovation Consortium (MDIC) since its foundation in 2012. This first-ever public-private partnership was created with the sole objective of advancing medical device regulatory science for patient benefit.

Over the years, BD has effectively leveraged simulation for medical device development throughout the various stages of product development. Simulation is generally used to evaluate new design concepts, identify optimal solutions and realistically predict potential outcomes. This simulation-based approach enables BD to drive informed-based decisions in order to mitigate risk and minimize the number of physical design iterations required. Ultimately, the final selected designs are tested experimentally and simulation results are not generally submitted as regulatory-grade evidence during the regulatory submission process.

In the future, BD's Corporate CAE group plans to grow how simulation-based evidence is used to impact the translational science process, regulatory submissions and ultimately patient outcomes. With BD's recently expanded product portfolio, the opportunities to tap into the benefits of modeling and simulation are quite significant. The group is excited about driving change in the industry and revolutionizing how modeling and simulation can play a role in advancing the world of health.

PLENARY 4: VALIDATING A MODAL OF INTEGRATIVE HUMAN PHYSIOLOGY – DIFICULT OR IMPOSSIBLE?



Dr. Tom Coleman
Professor Emeritus
Department of Physiology and Biophysics
University of Mississippi Medical Center

Tom Coleman was trained in engineering and physiology at the University of Rochester, Mississippi State University, the University of Mississippi Medical Center, and the London Hospital Medical College.

Early work with Dr. Arthur Guyton characterized the interaction of renal function, body fluids and hemodynamics in the genesis of chronic hypertension. The lead publication became a Citation Classic in 1986.

Drs. Coleman and Guyton were among the first to analyze complex physiological systems using mathematical models and computer simulation. In his American Physiological Society Bowditch Lecture in 1975. Dr. Coleman described the role of these methods in modern scientific method.

Subsequently, Dr. Coleman has developed large mathematical models of human physiology, pathophysiology and clinical intervention. This work has led to a variety of books and papers in the areas of experimental and clinical physiology and computer modeling.

Abstract: Modeling integrative human physiological function is not easy.

Here are five considerations relevant to validation.

(1) Our knowledge of human physiological function is continuously changing (for the better, I hope). If we freeze model development in order to formalize validation, the model is immediately outdated. If we support continual model modification in an attempt to improve the model, validation remains a moving target.

(2) Karl Popper has argued that a scientific theory can never be proven to be unquestionably true. But it can easily be proven to be unquestionably false. If we consider a mathematical model to be only a theory, then this argument can be applied modeling. A mathematical model can never be fully validated, but it can readily be invalidated.

Human nature doesn't like this concept.

(3) The evolutionary endpoint appears to be that an organism must live long enough to reproduce (and maybe nurture a bit). There are many different, well-documented physiological pathways that will get the job done. So, data collected from non-human species should be used only with very great caution in human modeling.

(4) Is hearsay admissible data? Some very important insights don't make it all the way to refereed, published literature. But the formal literature is often not physiologically relevant and can simply be wrong. So hearsay data may not be attractive but it can be important.

(5) What about important physiological processes that are just not visible? The model builder can use his or her imagination in building the invisible component, but validation can involve no more than the visible (potential) implications of the invisible.

So the takeaway is: validation is very difficult at best in this setting.

Technical Program
Wednesday, May 16, 2018

TRACK 2 DEVELOPMENT AND APPLICATION OF VERIFICATION AND VALIDATION STANDARDS

2-1 DEVELOPMENT AND APPLICATION OF VERIFICATION AND VALIDATION STANDARDS. SESSION 1
4TH FLOOR, GREAT LAKES A1 10:25AM - 12:30PM

Process Evaluation for Certification by Analysis

Oral Presentation. VVS2018-9379 **10:25AM - 10:50AM**

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

The Federal Aviation Administration (FAA) has standards and regulations that are designed to protect aircraft occupants in the event of a crash. For many components, compliance is demonstrated via physical testing; however, the FAA permits numerical modeling results to also be used to show compliance. While these data fall under existing process controls for certification data, new challenges are arising that require additional guidance. In general, there are two approvals required: approval to manufacture and approval to install. The evaluation for approval to manufacture involves both an evaluation of the design and the materials, to include material variability and factors of safety. For physical testing, there are evaluations of the laboratory that generate the data. This includes an evaluation of the technical capabilities (hardware/software), human capabilities, and the documented processes. For modeling data, similar evaluations are necessary to build confidence in the results. This process evaluation of the modeling capabilities is a corollary to the testing capability evaluation. The applicant should have a developed quality procedure that controls how models will be built, sources of data, verification and validation activities, quality control, acceptability requirements, and how the build process is documented. Of particular interest to regulators is the internal decision making process, for example, what happens if the model doesn't meet an accuracy requirement. The question that the FAA is asking applicants is does your analytical process result in a similar decision to your physical process. As with other regulatory agencies, the FAA is also considering how applicants can demonstrate their abilities, with site inspections, challenge problems, and pilot projects. Overall, the FAA wants to know that a company has a quality procedure and that they follow it leading to the design of safe systems.

Simulation Governance across the Product Lifecycle

Oral Presentation. VVS2018-9407 **10:50AM - 11:15AM**

William Oberkampf, *W L Oberkampf Consulting, Georgetown, TX, United States,* ***Jean Francois Imbert***, *SIMconcept Consulting, Toulouse, France*

Computer simulations are increasingly relied upon to inform business management, project managers, and product designers regarding the quality of engineering products produced by their organization. Here we take a broad view of product quality by including whether the product meets specifications for performance, reliability, safety, and productibility, as well as meeting delivery schedules and cost objectives. To achieve these quality objectives, an organization must integrate a wide range of disparate capabilities and resources across the enterprise, for example, computer aided design, simulation software capability, simulation data management, technical staff competencies, computer resources, experimental characterization of materials, testing of subsystems and products, supplier and manufacturing capabilities, meeting regulatory requirements, and product delivery, support and maintenance capabilities. As simulation takes more responsibility for product quality, organizations must learn how to incorporate and adapt to the specialized needs and data integration needed for simulation. The concept of simulation governance as discussed in this presentation addresses how simulation must be integrated over a wide range of existing business operations so it can yield the benefits trumpeted by marketing phrases such as "virtual product development" and "digital twins". A key success factor is the development by the top management of their strategic vision of the simulation role for future and legacy products. We will discuss the integration of diverse elements of simulation, for example, conceptual and mathematical model formulations, code and solution verification, model validation, uncertainty quantification, risk assessment, and the integration of experimental testing and model parameter calibration. Finally, simulation governance includes the estimation of model predictive uncertainty, including both aleatoric and epistemic uncertainties, and an assessment of the attributes of model predictive capability.

An Agile Verification and Validation Process for Generating Regulatory-Grade Evidence

Oral Presentation. VVS2018-9377 **11:15AM - 11:40AM**

Paulina Rodriguez, Seyed Ahmad Reza Dibaji, Matthew Myers and Tina Morrison *U.S. Food and Drug Administration, Silver Spring, MD, United States,* ***Bruce Murray***, *SUNY At Binghamton, Binghamton, NY, United States*

Computational modeling is a promising tool for advancing medicine and healthcare. One key aspect to ensuring its adoption by regulators is trust in the predictive capability of the modeling, as outlined in the new ASME V&V40 standard. Credibility is established through verification and validation (V&V); demonstrating that the computational model is solved correctly and accurately and that it correctly represents the reality of interest. In many cases, demonstrating these aspects is one "obligatory" step before using the computational model the way the developer intended. V&V is typically performed as a linear, step-by-step process near project completion. Iterative V&V can be more efficient, but a framework is lacking. Therefore, we gathered methods from the software arena called "Agile" and established a truly iterative V&V process in accordance with the FDA's guidance on computational modeling. Our team developed and applied an agile management approach to the V&V process on a single-phase flow and heat transfer computational model of an electronic drug delivery system using commercial software; using agile will ensure a truly iterative model development and V&V. Our modified agile approach includes four key components: Adaptive Software Development (ASD) methods to manage the project through consecutive iteration cycles; Scrum to manage the team; a modified Phenomenological Identification and Ranking Table (PIRT) that monitors the flux in knowledge through the iteration cycles, guides model development and experimental design, and drives project decisions; lastly, Trello a web-based management tool which enables flexible organization and project tracking. We integrated critical elements of the ASME V&V 40 framework into the agile V&V process to enhance decision-making and develop credibility for the context-of-use (COU) of the model, especially as the COU evolves with the addition of credible evidence. While the agile V&V process required continuous planning, it reduced the overall time and resources spent. The time spent on model development, experimental design, troubleshooting, and documentation was reduced due to frequent interactive communication by the team. Additionally, unnecessary simulations and experiments were avoided by iterative decision-making driven by our modified PIRT. The integration of the new V&V 40 standard with agile methods has increased the quality of communication amongst the team, improved knowledge management with PIRT and Trello, supported smart decision-making about limited resources, and is leading us toward an iterative end-to-end regulatory-grade computational model.

Development of V2UP (Verification & Validation plus Uncertainty Quantification and Prediction) Procedure - Implementation of Quality Management Process for Modeling and Simulation V&V

Oral Presentation. VVS2018-9405 **11:40AM - 12:05PM**

Masaaki Tanaka, *Japan Atomic Energy Agency, O-Arai, Ibaraki, Japan*

In order to enhance the simulation credibility, implementation of verification and validation (V&V) including the uncertainty quantification is indispensable process in development of numerical simulation codes. A procedure named V2UP (Verification and Validation plus Uncertainty quantification and Prediction) by referring to existing guidelines on the V&V (ASME V&V-10 and 20) and the methodologies of the safety assessment (CSAU, ISTIR, EMDAP) has been developed at the Japan Atomic Energy Agency. On July 2016, Guideline for Credibility Assessment of Nuclear Simulations (AESJ-SC-A008:2015) was published by the Atomic Energy Society of Japan (AESJ). The guideline of AESJ describes a fundamental concept of the V&V for Modeling and Simulation in four elements: (1) development of conceptual model, (2) mathematical modeling, (3) physical modeling, and (4) assessing predictability of simulation model. In addition, the fundamental concept of the prediction process after the V&V, and the implementation of the quality management (QM) based on ISO9001 are prescribed. Previously, methodology for the uncertainty quantification in the V&V process of the V2UP has been investigated. In this study, implementation of the QM process for the activities in the V&V of the V2UP was investigated. The standards of the V&V for the QM published by the Japan Society for Computational Engineering and Science (JSCES) and the guideline of a model procedure of the QM in the safety assessment of nuclear power plant published by the Japan Nuclear Safety Institute (JANSI) were referred. In order to maintain high quality in the implementation of the V&V by the outsourcing, a consecutive process for the QM consisting of the activities from the order to the delivery in the purchasing process is defined in these documents. In the V2UP, the QM process in the verification and that in the validation has to be separately defined because the verification and the validation are independently carried out. The definitions of the verification and the validation for the QM were reconsidered and the verification of the simulation process and the validation of the simulation process for the QM were defined in addition to the code verification, the solution verification, and the validation of the simulation for the M&S. By using these definitions, the procedures for the QM in the verification and that in the validation were successfully defined in the V2UP in accordance with the requirements in the guideline of the AESJ and the standards of the QM.

It is Too Complex to Validate!

Oral Presentation. VVS2018-9419 **12:05PM - 12:30PM**

Chris Rogers*, Crea Consultants Ltd., Buxton Sk176ay, United Kingdom,* ***William Oberkampf****, W L Oberkampf Consulting, Georgetown, TX, United States, J***oshua Kaizer***, U.S. Nuclear Regulatory Commission, Abingdon, MD, United States,* ***Ryan Crane****, ASME, New York, NY, United States*

This is the response that has been given to many regulatory, safety and licensing assessors when asking for validation of simulation.

Validation is a process which has significant importance with respect to measuring how correct a simulation is; setting bounds of applicability; and predicting potential applicable variances. Validation is an end user requirement as it is impossible for the software developer to know how the user is going to use software. That is, the software developer does not have the insight to prescribe when valid results are obtained for specific applications of the software.

The applicable international quality standard is ISO 9001:2015 Quality management systems - Requirements. For a simulation to be ISO 9001 compliant, Clause 8.3.4 is mandatory, namely:

8.3.4 Design and development controls

The organization shall apply controls to the design and development process to ensure that:

d) Validation activities are conducted to ensure that the resulting products and services meet the requirements for the specified application or intended use.

This presentation will provide the results of work carried out by the NAFEMS Analysis Management Working Group, supported by ASME V&V committee members, to demonstrate that all engineering simulation can be satisfactorily validated to the satisfaction of ISO 9001.

It recognizes that any engineering calculation, however simple it might be, is a simulation. The results of this work therefore apply to all physical engineering simulations ranging from pencil and paper hand calculation through to multi-physics, multi-processor supercomputing. This work also covers extreme conditions such as space vehicles where solid evidence of pre-flight conditions is not available.

TRACK 4 UNCERTAINTY QUANTIFICATION, SENSITIVITY ANALYSIS, AND PREDICTION

4-1 UNCERTAINTY QUANTIFICATION, SENSITIVITY ANALYSIS, AND PREDICTION: SESSION 1
4TH FLOOR, GREAT LAKES A2 10:25AM - 12:30PM

Global Sensitivity Analysis as a Basis for Parameter Prioritization and Enhanced Model Transparency

Oral Presentation. VVS2018-9344 **10:25AM - 10:50AM**

***Sarah Baxter**, Univ of St. Thomas, Saint Paul, MN, United States,*
***Rebecca Bourn**, University of Wisconsin - Milwaukee, Milwaukee, WI, United States*

While mathematical models in engineering generally have a theoretical foundation, often their form is empirical or semi-empirical. Such models are based on experimental observations that suggest a mathematical form, e.g. a linear trend or monotonicity, and parameters are established through curve fitting and optimization. Thus, there can be multiple models of the same event. Uncertainty in model parameters contributes to uncertainty in the validity of model prediction and also makes model selection more difficult.

The focus of this work is a set of mathematical models that have been proposed to predict the dynamic force response of a magnetorheological (MR) damper. MR dampers are semi-active devices designed to mitigate the effects of large forces on structures. They are mechanically simple, can be used over large temperature ranges and have relatively low power requirements. The behavior of the MR damper is intrinsically nonlinear and a challenging aspect of applying this technology has been the development of accurate models to describe the behavior of MR dampers for control design and evaluation purposes.

Recent work compared four mathematical models that predict the dynamic damper force. For each model, the parameters were fit to experimental data through the minimization of an objective function measuring the error between numerical and experimental observations. While all 4 models performed well, those with simple equations and the fewest parameters tended to be faster; the more complex models performed slightly better with respect to accuracy and were less sensitive with respect to time step sizes.

In this work a Global Sensitivity Analysis (GSA) was used to prioritize model parameters in two of the proposed MR damper models, the Algebraic model and the Viscous plus Dahl model, with 6 and 5 parameters respectively. This analysis was based on an output of the global root-mean square error over a period of time. In a second analysis, GSA was performed based on force outputs at singular, characteristic times along the force time curve.

Results of the first analysis prioritize the impacts of parameters on the RMS error and suggest parameters that could be fixed, potentially resulting in simplifications in applying the model. The sensitivity analysis for single point outputs and quantifies the impact of individual parameters on specific characteristics of the force profile, e.g., frequency and amplitude. These results illustrate relative levels of model transparency, i.e., specific connections between individual inputs and outputs, of the two models.

CONFIDENCE-BASED RELIABILITY ASSESSMENT AND TARGET OUTPUT DISTRIBUTION FOR V&V WITH LIMITED NUMBERS OF INPUT & OUTPUT DATA

Oral Presentation. VVS2018-9334 **10:50AM - 11:15AM**

***Kyung Choi, Min-Yeong Moon**, University Of Iowa, College Of Engineering, Iowa City, IA, United States, **Nicholas Gaul**, RAMDO Solutions, LLC, Iowa City, IA, United States, **David Lamb**, U.S. Army TARDEC, Warren, MI, United States*

To be useful, the simulation tools used by industry and defense agencies must be validated for correctly predicting outputs of engineered systems. Furthermore, since real-world phenomena are not deterministic, statistical methods that can quantify uncertainty will be needed. At the same time, the development of verification and validation (V&V) of simulation models entails the acquisition of physical test data of extraordinary detail. However, it is extremely expensive to generate test data of extraordinary detail and practicing engineers can afford only very limited number of test data. It is proposed to use the simulation model specifically output probability density function (PDF) of the simulation model and limited numbers of input and output test data to generate a target output PDF that can be used to measure biasness of the simulation model. To have the target output PDF effective for V&V, it is desirable that the obtained target output PDF is minimally variant when biasness of the simulation model changes.

To obtain the proposed target output PDF, a confidence-based reliability assessment method and uncertainty quantification (UQ) are developed given limited input and output test data. To do that, two types of uncertainties need to be considered: (1) aleatory (i.e., irreducible) uncertainty, which refers to the inherent heterogeneity or diversity of data in an assessment, and (2) epistemic (reducible) uncertainty, which refers to imperfections in both simulation & surrogate models as well as input distribution models due to limited numbers of input data. Reliability is a function of aleatory uncertainty, whereas epistemic uncertainty hinders us from accurately assessing reliability. To account for the epistemic uncertainty, we are introducing a confidence measure.

In this presentation, surrogate modeling and computational methods are used to obtain confidence-based reliability assessment and UQ for limited numbers of input and output test data. As the surrogate model induces epistemic uncertainty, it is desirable to minimize this uncertainty by developing accurate surrogate models. Thus, the dynamic Kriging (DKG) modeling method with a local window concept, developed by RAMDO Solutions, is used.

For confidence-based reliability assessment and UQ, in the first step, a bootstrapping method is used to approximate uncertain input distribution models given limited numbers of input data. In the second step, epistemic uncertainty of the output PDF induced by insufficient output test data is quantified using a Bayesian model. In this Bayesian model, output PDF of the simulation model, obtained using bootstrapping selection of input distribution models and the DKG, is used as a prior information. Then candidates of target output PDFs modeled by adaptive kernel density estimation (AKDE) are obtained by considering limited output test data. As a result, reliability becomes uncertain and thus follows certain probability distribution. This distribution will provide quantitative bounds on reliability, i.e., the assessed reliability as a function of confidence level. Once the epistemic uncertainty distribution of the reliability is obtained, the user can select a target confidence level. At the target confidence level, the confidence-based target output PDF and reliability can be obtained, which are confidence-based estimations of the true output PDF and reliability. Finally, the target output PDF (i.e., UQ) is used to measure the biasness of the simulation and surrogate models.

Sensitivity Analysis of a Nuclear Reactor System Finite Element Model

Technical Publication. VVS2018-9306 **11:15AM - 11:40AM**

Gregory Banyay, Jason Young, Stephen Smith, *Westinghouse Electric Company*

The structures associated with the nuclear steam supply system (NSSS) of a pressurized water reactor (PWR) warrant evaluation of various non-stationary loading conditions which could occur over the life of a nuclear power plant. These loading conditions include that associated with a loss of coolant accident and seismic event. The dynamic structural system is represented by a finite element model consisting of significant epistemic and aleatory uncertainties in the physical parameters. To provide an enhanced understanding of the influence of these uncertainties on model results, a sensitivity analysis is performed. This work demonstrates the construction of a computational design of experiment which runs the finite element model a sufficient number of times to train and verify a unique aggregate surrogate model. Adaptive sampling is employed in order to reduce the overall computational burden. The surrogate model is then used to perform both global and local sensitivity analyses.

Bayesian Framework to Quantify Uncertainties in Piezoelectric Energy Harvesters

Technical Presentation. VVS2018-9318 **11:40AM - 12:05PM**

Patricio Peralta, Viviana Meruane and Rafael Ruiz*, Univerisdad de Chile, Santiago, Chile*

The dynamic description of piezoelectric energy harvesters (PEHs) has been widely studied in the last decade. Different deterministic modelling techniques and simplifications have been adopted to describe their electro-mechanical coupling effect in order to increase the accuracy on the output power estimation. Although it is a common practice to use deterministic models to predict the input-output behavior of PEHs, perfect predictions are not expected since these devices are not exempt of uncertainties. The accuracy of the output estimation is affected mainly by three factors: (1) the mathematical model used, (2) the uncertainties on the mathematical model parameters and (3) the uncertainties related to the excitation. These uncertainties should be taken into account in order to generate robust and more plausible predictions. Nevertheless, only a limited attention has been paid in the uncertainty quantification related to model parameters in piezoelectric energy harvesters. The interest of this work is to describe a framework that allows the use of the well-known dynamic estimators in piezoelectric harvester (deterministic performance estimators) but taking into account the random error associated to the mathematical model and the uncertainties on the model parameters. The framework presented could be employed to perform Posterior Robust Stochastic Analysis, which is the case when the harvester can be tested or it is already installed and the experimental data is available. In particular, it is introduced a procedure to update the electromechanical properties of PEHs based on Bayesian updating techniques. The mean of the updated electromechanical properties are identified adopting a Maximum a Posteriori estimate while the probability density function associated is obtained by applying a Laplace?s asymptotic approximation (updated properties could be expressed as a mean value together a band of confidence). The procedure is exemplified using the experimental characterization of 20 PEHs, all of them with same nominal characteristics. Results show the capability of the procedure to update not only the electromechanical properties of each PEH (mandatory information for the prediction of a particular PEH) but also the characteristics of the whole sample of harvesters (mandatory information for design purposes).The results reveal the importance to include the model parameter uncertainties in order to generate robust predictive tools in energy harvesting. In that sense, the present framework constitutes a powerful tool in the robust design and prediction of piezoelectric energy harvester's performance.

Separability of Mesh Bias and Parametric Uncertainty for a Full System Thermal Analysis

Technical Presentation. VVS2018-9339 **12:05PM - 12:30PM**

Benjamin Schroeder, Humberto Silva III *and* ***Kyle D. Smith****, Sandia National Laboratories, Albuquerque, NM, United States*

When making computational simulation predictions of multi-physics engineering systems, sources of uncertainty in the prediction need to be acknowledged and included in the analysis within the current paradigm of striving for simulation credibility. A thermal analysis of an aerospace geometry was performed at Sandia National Laboratories. For this analysis a verification, validation and uncertainty quantification workflow provided structure for the analysis, resulting in the quantification of significant uncertainty sources including spatial numerical error and material property parametric uncertainty. It was hypothesized that the parametric uncertainty and numerical errors were independent and separable for this application. This hypothesis was supported by performing uncertainty quantification simulations at multiple mesh resolutions, while being limited by resources to minimize the number of medium and high resolution simulations. Based on this supported hypothesis, a prediction including parametric uncertainty and a systematic mesh bias are used to make a margin assessment that avoids unnecessary uncertainty obscuring the results and optimizes computing resources.

TRACK 10 VERIFICATION AND VALIDATION OF NUCLEAR POWER APPLICATIONS

10-1 VERIFICATION AND VALIDATION OF NUCLEAR POWER
4TH FLOOR, GREAT LAKES A3 10:25AM - 12:30PM

Introducing V&V&C In Nuclear Thermal-Hydraulics
Technical Presentation. VVS2018-9321 **10:25AM - 10:50AM**

Francesco D'Auria**, University of Pisa, Pisa, Italy,* ***Marco Lanfredini, *GRNSPG-UNIPI, San Piero a Grado (PI), Italy*

V&V constitutes a powerful framework to demonstrate the capability of computational tools in several technological areas. Passing V&V requirements is a needed step before applications. Let's focus hereafter to the area of (transient) Nuclear Thermal-hydraulic (NTH) and let's identify V1 and V2 as acronyms for Verification and Validation, respectively.

Now, V1 is performed within NTH according to the best available techniques and may not suffer of important deficiencies if compared with other technological areas. This is not the case of V2. Three inherent limitations shall be mentioned in the case of Validation in NTH:

1. Validation implies comparison with experimental data: available experimental data cover a (very) small fraction of the parameter range space expected in applications of the codes; this can be easily seen if one considers data in large diameter pipe, high velocity and high pressure or high power and power density. Noticeably, the scaling issue must be addressed in the framework of V2 which may result in controversial findings.

2. Water is at the center of the attention: the physical properties of water are known to a reasonable extent as well as large variations in values of quantities like density or various derivatives are expected within the range of variation of pressure inside application fields. Although not needed for current validation purposes (e.g. validation ranges may not include a situation of critical pressure and large heat flux) physically inconsistent values predicted by empirical correlations outside validation ranges, shall not be tolerated.

3. Occurrence of complex situations like transition from two-phase critical flow to 'Bernoulli-flow' (e.g. towards the end of blow-down) and from film boiling to nucleate boiling, possibly crossing the minimum film boiling temperature (e.g. during reflood).

Therefore, whatever can be mentioned as classical V2 is not or cannot be performed in NTH. So, the idea of the present paper is to add a component to the V&V. This component, or step in the process, is called 'Consistency with Reality', or with the expected phenomenological evidence. The new component may need to be characterized in some cases and is indicated by the letter 'C'. Then, the V&V becomes V&V&C. V&V&C aims at increasing the robustness and the capabilities of concerned models addressing topics like those mentioned above.

The purpose of the paper is to clarify the motivations at the bases of the V&V&C

Estimation of Threshold Parameter and Its Uncertainty Using Multi-Variable Modeling Framework for Response Variable with Binary Experimental Outcomes

Oral Presentation. VVS2018-9353 **10:50AM - 11:15AM**

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

A number of different approaches are used in computational modeling to estimate the model parameters and their uncertainties. In some cases, direct statistical assessment of relevant experimental data obtained for the parameter of interest may be possible. In other cases, it may be necessary to estimate the model parameter and its uncertainty from the response variable of another model containing the parameter of interest and developed for this purpose. An example of the latter approach is discussed in this presentation, which outlines the recently developed framework for estimation of a threshold parameter and its uncertainty in probabilistic evaluations of crack initiation from in-service flaws in CANDU nuclear reactors.

Each one of several hundred fuel channels in the core of a CANDU reactor includes a Zr-2.5%Nb pressure tube, containing nuclear fuel and pressurized heavy water coolant. During operation, the pressure tubes may become susceptible to delayed hydride cracking (DHC) due to the increasing content of hydrogen, in the form of deuterium, generated by the corrosion reaction of the Zr-based material with the heavy water. Therefore, the in-service flaws in pressure tubes are evaluated for DHC initiation. The threshold stress for DHC initiation at the flaw tip depends on the flaw geometry and the material resistance to DHC initiation, and is predicted using models based on the process-zone approach. One of the material parameters required to apply the process-zone predictive models is the threshold stress for DHC initiation at planar surfaces.

In DHC initiation experiments, a surface flaw is required to produce local stress concentration and ensure predictable and reproducible precipitation of hydrides. Therefore, obtaining reliable experimental data for DHC initiation at planar surfaces is extremely challenging. This problem has been addressed by means of developing a multi-variable modeling framework based on the closed-form process-zone representation of the threshold stress for DHC initiation. The developed modeling framework predicts a higher probability of DHC initiation for more severe flaws and for lower material resistance to DHC initiation, and it can be applied to statistically assess the binary outcomes of DHC initiation experiments performed on specimens containing flaws of varying severity. Using this framework, the threshold stress for DHC initiation at planar surfaces can be derived as a distributed parameter for the probabilistic evaluations of crack initiation. The developed framework also allows for potential correlation between the threshold stress for DHC initiation at planar surfaces and the threshold stress intensity factor for DHC initiation from a crack.

Validation of MARS-KS Code for the Analysis of Pressure Transition in Passive Safety Injection System Using Pressure Balancing Line

Oral Presentation. VVS2018-9367 **11:15AM - 11:40AM**

Yu-na Kim, ***Sunil Lee***, ***Sung-Jae Yi*** *and* ***Sung Uk Ryu*** *Korea Atomic Energy Research Institute, DAEJEON, Korea (Republic)*

Recently, a lot of research on inherent safety and passive safety systems of nuclear power plant has been conducted in the nuclear society. H-SIT (Hybrid-Safety Injection Tank), which is being developed for APR+ and IPOWER, has been enhanced to allow passive safety injection without significantly changing the design of the APR1400 by adding PBL (Pressure Balancing Line).It is important to predict and verify the system pressure tendency through the PBL, since the performance of passive safety injection depends on the pressure balance between the primary side and the upper side of H-SIT. Therefore, this study is to confirm that the MARS-KS code, a validation code commonly used in nuclear society, well predicts the pressure balance in this system with appropriate models. When the accident scenario is assumed to be SBLOCA (Small Break Loss Of Coolant Accident), the code predicts that the pressure balance will occur through the following processes. As soon as the accident starts, hot water extracted from the cold leg is injected into H-SIT through the PBL. In the deginning, flashing phenomenon occurs shortly due to the sudden pressure difference, so H-SIT is rapidly pressurized. However, after the pressure is almost equalized, only hot water, which is ineffective to pressurize, is supplied through the PBL, so that the upper pressure of H-SIT could not achieve pressure equilibrium with the primary side. In order to represent this complex pressure balance mechanism, all models should accurately reflect pressure drop, phase change, flashing phenomena and direct condensation. For validation of the MARS-KS, we conducted the validation test and produced experimental data to compare with the analytic results. The experimental facility was established by adding the PBL design to ATLAS (Advanced Thermal-hydraulic Test Loop for Accident Simulation) facility simulating APR1400. The various main parameters such as local pressure, temperature and water level were measured. As a result of the comparison, the MARS-KS code predicts the pressure tendency measured in the experiment, and it is expected that it can be used for H-SIT performance validation if the heat loss and the break flow prediction are supplemented.

Verification and Validation of Simulation Models for Residual Radioactive Contamination from Decommissioning Nuclear Power Plants

Oral Presentation. VVS2018-9348 **11:40AM - 12:05PM**

Huai-En Hsieh, *College of Energy, Xiamen University, Xiamen, China,* ***Yen-Cheng Liu***, *Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan,* ***Mei-Shiue Chen***, *Institute of Nuclear Engineering and Science, National Tsing Hua University, Hsinchu, Taiwan*

Residual radioactive contamination from decommissioning nuclear power plants is a part of important issues in radiological safety. There are lots of international nuclear power plants using the RESRAD computer code for evaluating the potential radiation dose incurred by an individual who works in the building contaminated with radioactive material during the decommissioning process. The purpose of this study attempts using RESRAD computer code to research in the verification and validation of simulation models for residual radioactive contamination from decommissioning nuclear power plants. The results of this study can provide the actual experiment techniques and simulation methodologies with using RESRAD computer code designed in the protectiveness of the human health and environmental impact on radiological safety during the decommissioning process.

In this study, there is a characterization survey in the actual building contaminated with radioactive material first. The characterization survey includes the dimensions of the building, density of the structures, distribution of the radioactive contamination, radiation dose of the workers and backgrounds. The result of characterization survey in a room of the building shows that the east and south walls of the room contaminated, west and north walls of the room uncontaminated, ceiling and floor of the room uncontaminated. This study aims to investigate the east and south contaminated walls with analysis of radionuclide source terms, analysis of radioactive source strength impact, analysis of core samples from the contaminated walls, analysis of radionuclide activity and concentration.

The result of the analysis of radioactive source strength impact shows that there is non-uniform distribution of radioactive contamination on the surfaces of walls. The result of the analysis of core samples from the contaminated walls shows that there is non-uniform distribution of radioactive contamination in the structures of walls. Furthermore, we have the decontamination work inside the building in order to decrease the radiation dose incurred by an individual who works in the building. We also design the radiation shielding outside the building in order to avoid the radiation leakage to environment. In this study, we use the RESRAD computer code for designing the simulation models of an actual building with radioactive contamination, and then we use the results of actual experiments for verifying and validating the computer simulation models. We also compare the radiation doses of computer simulation results with the radiation doses of actual measurement results, and the minimum relative error of verification result is 10.10 %.

TRACK 2 DEVELOPMENT AND APPLICATION OF VERIFICATION AND VALIDATION STANDARDS

2-2 DEVELOPMENT AND APPLICATION OF VERIFICATION AND VALIDATION STANDARDS. SESSION 2

4TH FLOOR, GREAT LAKES A1 1:30PM - 3:35PM

Review of the AP1000 Comprehensive Vibration Assessment Program

Oral Presentation. VVS2018-9329 **1:30PM - 1:55PM**

Gregory Banyay, *Westinghouse Electric Company, Cranberry Township, PA, United States*

The effects of flow-induced vibration (FIV) is a major design consideration for the newer generations of commercial nuclear power plants that are currently coming on line, as well as for operating plant life extensions analyses and next generation plant designs in development. FIV effects are particularly important relative to reactor vessel internals (RVI) and steam system component low-cycle and high-cycle fatigue design and analyses. The U.S. Nuclear Regulatory Commission (NRC) Regulatory Guide (RG) 1.20 outlines specific guidance to conduct a Comprehensive Vibration Assessment Program (CVAP), which is used to confirm the fatigue performance of the RVI, and with recent revisions to the RG, the fatigue performance of the steam system. The RG outlines four primary aspects of the CVAP: vibration and fatigue analyses, vibration measurement, component inspections, and the correlation of all results. While full RVI CVAPs have been completed in the past, along with a few smaller CVAPs for specific RVI components, the last full RVI design CVAP was completed over 20 years ago in both engineering and nuclear regulatory environments that were notably different than that of today's restrictive environments.

This presentation reviews these four primary aspects of a CVAP from both a practical engineering perspective as well as a regulatory perspective, in light of changes over the past two decades. While differences between historical and current CVAPs are discussed, the emphasis of the discussion is on the current engineering methods used for both the analytical/numerical and measurement portions of the work needed for a successful program. Of particular interest for discussion is the need to analyze and correlate numerical predictions and measurement data from a system perspective, as well as consider interactions between major component subsystems.

Much of this review is based on the successful experience with the CVAP for the new Westinghouse AP1000® PWR RVI. However, the review is equally applicable generically to other reactor internals design type CVAPs (e.g., BWR, SMR).

Development of the xRage Inertial Confinement Fusion Validation Suite using Omega Direct-Drive Implosion Experiments

Oral Presentation. VVS2018-9355 **1:55PM - 2:20PM**

Brandon Wilson, Aaron C. Koskelo, *Los Alamos National Laboratory, Los Alamos, NM, United States*

Prediction of inertial confinement fusion (ICF) applications, such as that demonstrated at the National Ignition Facility and Omega laser facility, requires coupling of complex multiphysics models, including plasma transport, radiation-diffusion, opacity, ion physics, and laser physics. LANL is developing an ICF validation suite (ICFVS) to provide the necessary tools and experiments to assess predictability of LANL's multiphysics hydrodynamics code, xRage, over a broad spectrum of ICF-relevant metrics, validation experiments, and physics.

xRage was recently updated to include the laser ray-tracing package Draco from the Laboratory for Laser Energetics (LLE). In this work, we assess the current implementation of the laser package via validation of laser-driven, direct-drive experiments from the Omega laser facility. We follow the ASME V&V Standard for Computational Fluid Dynamics and Heat Transfer (ASME V&V 20) to quantify the laser package validation uncertainty.

The default implementation of the laser package is unable to predict the experimental validation metrics (i.e. absorbed and scattered laser energies from the capsule surface and ablation front position and velocity with time) and validation uncertainty is dominated by experimental uncertainties. However, the validation comparison error is consistently larger than the validation uncertainty, indicating a systematic model form error (i.e. missing physics). We argue cross-beam energy transfer (CBET), one of many un-modeled laser-plasma interactions from the laser system, is a significant source of the missing physics. High priority should be placed on updating the laser package to include CBET predictive capability.

The ICF community commonly employs nonphysical calibration methods to account for the effects of CBET through tuning the thermal flux limiter, tuning the incident laser energy, or both. Although validation is at odds with calibration, we assess both methods to inform the community of strengths, weaknesses, and modeling subtleties. Both methods show increased model accuracy and support CBET as a source of missing physics. However, the incident laser energy tuning method more accurately overcomes CBET deficiencies.

Sensitivities to other model physics are also assessed. Preliminary results show insignificant sensitivity to most code setup parameters, including calculation setup, mesh resolution, material LTE opacities, ionization models, laser configuration, and material EoS.

The usefulness of credibility assessment frameworks

Oral Presentation. VVS2018-9347 **2:20PM - 2:45PM**

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

Credibility assessment frameworks provides a means to assess whether models and simulations can be trusted for their intended purpose. Popular example of such frameworks are the Predictive Capability Maturity Model and NASA-STD-7009. Recently, the U.S. Nuclear Regulatory Commission has further developed these frameworks by adapting their key concepts and combining them with Goal-Structure-Notation. The result is a credibility assessment framework that provides a detailed and organized safety case which captures why a specific model or simulation should be trusted.

This presentation will focus on the U.S. NRC's development of the credibility assessment framework for criterial heat flux and critical power models. First, it will provide a brief introduction to criterial heat flux and critical power. Second, it will provide an overview of credibility assessment frameworks and goal structure notation. Third, it will describe the specific framework developed by the U.S. NRC. Finally, it will discuss the many advantages which have already been seen in applying the framework and suggest future frameworks which may benefit the modeling and simulation community.

Proposing a mathematical V&V taxonomy

Oral Presentation. VVS2018-9346 **2:45PM - 3:10PM**

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

There are certain words in the modeling and simulation community that everyone uses such as modeling, simulation, verification, validation, uncertainty quantification. While there is broad agreement on the overall meaning of these terms, there is often disagreement on the finer details. Further, that disagreement is magnified as those finer details become more important and the terms are used in professional standards and adopted in business practices. While there are numerous proposed definitions for these concepts, there doesn't seem to be a clear reason to choose any set of definitions over any other except due to a democratic process. It was a wise man who once pointed out that applied mathematics is not an exercise in democracy which raises the question, is there a more mathematical approach to these terms?

This presentation will focus on a mathematical approach for defining concepts in M&S and VVUQ. First, it will review a brief history of current definitions, focusing not only on the definitions themselves, but how the definitions were generated. Second, it will then provide a brief summary of set theory and how it can be used to define terms. Third, it will demonstrate how formally defining key concepts as sets (e.g., model, simulation) result in natural definitions for other concepts (e.g., verification, validation). Finally, it will discuss insights into these concepts which are become obvious using the suggested definitions. It is hoped that through the presentation, the audience will gain deeper insight into the key concepts of M&S and VVUQ.

LANL-MMS — A Software Package for the Method of Manufactured Solutions

Oral Presentation. VVS2018-9372 **3:10PM - 3:35PM**

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

The method of manufactured solutions (MMS) is currently considered to be the gold standard for verification of computational physics codes, but it can be challenging to implement. We have developed LANL-MMS, a software package that simplifies the implementation of MMS by automatically generating manufactured source terms for a given mathematical model and test solution. The user may select these from among a variety of pre-defined options or define new ones as needed. We describe the structure and capabilities of LANL-MMS, and we demonstrate how it is used.

TRACK 6 VALIDATION METHODS

6-1 VALIDATION METHODS
4TH FLOOR, GREAT LAKES A2 **1:30PM - 3:35PM**

Systematic Comparison of Experimental and Simulation Data Fields using Compressive Alpert Multiwavelets for Model Validation and Calibration

Oral Presentation. VVS2018-9380 **1:30PM - 1:55PM**

Maher Salloum, Kyle Karlson, *Sandia National Laboratories, Livermore, CA, United States*

Engineering simulations are challenged by the existence of many unknown model parameters. Measured quantities of interest, e.g. stress-strain curves, are usually available from experiments in order to estimate the unknown parameters. This is performed by solving an inverse problem that runs an iterative optimization solver. Measured data fields, e.g. displacement fields, are also needed in many engineering models especially the ones involving heterogeneous materials such as welds. Measured fields should be compared to the simulated fields in order to compute the objective function. While simulated fields are smooth and defined on a given computational mesh, experimental data is often noisy and incomplete due to artifacts in measurement devices. Moreover, experimental and simulation data fields are often defined on unstructured meshes instead of a regular grid. Comparing such data fields is not straightforward. We propose Alpert multiwavelets (AMW) to effectively transform any data field into a spectral space. This allows a systematic modal comparison of the fields instead of a point-to-point spatial comparison. Unlike traditional wavelets, AMW adapt to any mesh and accommodate missing data points by construction. They also filter noise and compress data fields resulting in orders of magnitude of data reduction when computing the objective function. While general, we have applied this technique to tensile simulations of welded materials where plasticity material parameters are estimated from Digital Image Correlation measurements data. Our results indicate that optimal solutions can be obtained systematically at a reasonable computational cost by using AMW to compute the objective function from data fields.

Discrepancy Estimation for Dynamics Model Prediction

Oral Presentation. VVS2018-9394 **1:55PM - 2:20PM**

Sankaran Mahadevan, *Prof., Nashville, TN, United States*, ***Kyle Neal***, *Vanderbilt University, Nashville, TN, United States*, ***Zhen Hu***, *University of Michigan Dearborn, Dearborn, MI, United States*, ***Jon Zumberge***, *U.S. Air Force Research Labratory, Dayton, 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. Two surrogate modeling-based methods are developed to predict the bias in a simulation output for some untested input time history: bias surrogate and observation surrogate. The first method constructs a surrogate model for the bias in terms of model inputs, whereas the second method constructs a surrogate model for the observed outputs in terms of the model inputs; both methods use data collected from a set of previously conducted experiments. The bias surrogate method implements a predictor-corrector approach where a surrogate model is built for the bias term, which is then used to correct the simulation model prediction at each time step. Alternatively, in the observation surrogate method, the bias term is combined with the simulation model, and a single surrogate model is built for the experimental output. A neural network-based surrogate modeling technique is employed to implement the proposed methodology. From the experiments, high volume data are available for the surrogate model training. The neural network trains on the entire dataset to produce either a static or dynamic surrogate model depending on whether training is performed in a batch manner or not. The proposed methodology is illustrated for an air cycle machine (ACM), which is a refrigeration unit commonly on board aircraft.

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

Research on a Functional Validation Method for Multivariate Dynamic Systems from the Perspective of Function

Oral Presentation. VVS2018-9401 **2:20PM - 2:45PM**

***Yudong Fang**, **Jun Lu, Junqi Yang** and **Zhenfei Zhan,** 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, noise vibration and harshness, and fuel efficiency. As a process to assess the validity and predictive capabilities of computer models in its potential usage by comparing the computer output with test data, the model validation needs to be conducted before applying these computer models for product development. In the virtual prototype environment, validation of computational models with multiple and correlated functional responses needs to solve some tough issues: the nonlinear correlation between different functional responses, the decision-making with conflict validation results for multivariate responses and objective robust metrics. In addition the responses of complex dynamic system is continuous in a continuous time domain the existing validation methods based on discrete method may lead to the regardless of the functional data features. Aiming to solve the aforementioned problems based on Bayesian interval hypothesis testing theory, functional data analysis method, functional kernel principal component analysis, and subjective matter experts' based threshold definition and transformation, this paper proposes an integrated validation method for multivariate dynamic system under virtual prototype environment. In the proposed method, all of the time history responses of the computer simulation model and physical test are firstly represented by functions. These functional representations are transformed to a lower dimensional feature space using functional kernel principal components analysis. The employment of the functional kernel principal components analysis handles multivariate nonlinear correlation 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. Three independent error measures that associated with physically meaningful characteristics (phase, magnitude, and slope) are extracted for the dimension reduced function, 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. The proposed method resolves some critical drawbacks of the previous methods and adds some desirable properties of a model validation metric for multivariable dynamic systems, such as symmetry and functionality. A real-world dynamic system with multiple, functional responses is used to demonstrate this new approach, and shows its potential in promoting the continual improvement of virtual prototype testing.

Assessment of Model Validation and Calibration Approaches in the Presence of Uncertainty

Oral Presentation. VVS2018-9412 **2:45PM - 3:10PM**

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

Model validation is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. The results of a model validation study can be used to either quantify the model form uncertainty or to improve/calibrate the model. However, the model validation process can become complicated if there is uncertainty in the simulation and/or experimental outcomes. These uncertainties can be in the form of aleatory uncertainties due to randomness or epistemic uncertainties due to lack of knowledge. We will use three different approaches for addressing model validation: 1) the area validation metric, 2) a modified area validation metric with confidence intervals, and 3) the standard validation uncertainty from ASME V&V 20. To provide an unambiguous assessment of these different approaches, synthetic experimental values were generated from computational fluid dynamics simulations of a multi-element aircraft wing. A simplified model was then developed using a combination of thin airfoil theory and lifting line theory. This simplified model was then assessed using the synthetic experimental data. The quantities examined include the lift and moment coefficients for the wing with varying angles of attack and flap deflection angles.

An Evaluation of Validation Metrics for Probabilistic Model Outputs

Technical Publication. VVS2018-9327 **3:10PM - 3:35PM**

***Paul Gardner**, **Charles Lord, Robert**, **J. Barthorpe**, University of Sheffield, Sheffield, United Kingdom*

Probabilistic modelling methods are increasingly being employed in engineering applications. These approaches make inferences about the distribution, or summary statistical moments, for output quantities. A challenge in applying probabilistic models is validating the output distributions. This is of particular importance when using uncertainty quantification (UQ) methods that incorporate a method for determining model discrepancy. This term defines the difference between a physical model with true parameters and the observed physical process. Methods for learning model discrepancy are often formulated as non-parametric regression. This results from the assumption that the functional form of the model discrepancy is unknown a priori; otherwise it would be included in the physical model. The inferred model discrepancy distribution will affect the predictive output distribution and can be a good indicator of model form errors within the physical model. Additionally, approaches to UQ often assume a distribution for output predictions, e.g. that the output distribution is Gaussian. Hence, validation of the predictive distributions is important in determining the limitation of these assumptions, and whether an alternative method with different assumptions is required. For these reasons an ideal validation metric is one that intuitively provides information on key divergences between the output and validation distributions. Furthermore, it should be interpretable across different problems in order to informatively select the ideal UQ method. A difficulty in validating probabilistic models is that the number of validation samples obtained must be sufficient to accurately understand the underlying distribution of the physical process. Consequently, validation metrics that require density estimation prior to calculation may be more susceptible to errors caused by limited validation data. In this paper, two families of metrics for quantifying differences between distributions are compared: f-divergence and integral probability metrics (IPM). Traditionally, f-divergence metrics have been more widely used, most notably the Kullback-Leibler divergence, whilst IPMs have been mainly confined to kernel machine methods. In order to compare these families of metrics a case study on a representative five story building structure is presented. This case study applies Bayesian history matching, a UQ method with model discrepancy, to identify the distribution of natural frequencies under different pseudo-damage scenarios. The output from this approach is validated against specific metrics from each of the two families of metrics. Discussions and evaluation of these metrics are performed with comments on ease of computation, interpretability and quantity of information provided.

TRACK 11 VERIFICATION FOR FLUID DYNAMICS AND HEAT TRANSFER

11-1 VERIFICATION FOR FLUID DYNAMICS AND HEAT TRANSFER
4TH FLOOR, GREAT LAKES A3 — 1:30PM - 3:35PM

Uncertainty Study Of Flow Over Plate And Around Hydrofoil with OpenFOAM

Oral Presentation. VVS2018-9333 **1:30PM - 1:55PM**

Shanqin Jin, *Memorial University of Newfoundland, St. John's, NL, Canada*

Computational Fluid Dynamics (CFD) has developed into an important engineering tool that is currently applied to make project decisions. The popularity of OpenFOAM for various CFD applications is rapidly growing in recent years. As consequence, reliability and credibility of numerical simulations with OpenFOAM is an unavoidable issue, a logical step forward is then to pay due attention to the assessment of numerical uncertainties (Verification). This paper presents solution verification exercise for the flow over a flat plate and around the NACA 0012 hydrofoil with OpenFOAM. In the present work, six cases (flow over a flat plate for Reynolds numbers of 10000000, 100000000 and 1000000000; flow around the NACA 0012 hydrofoil at Reynolds number of 6×1000000 and angles of attack of 0º, 4º and 10º) are simulated by using OpenFOAM. All numerical cases are statistically steady flows of an incompressible fluid that were simulated in several geometrically similar grid sets. For flow over a plate, 10 set grids and each set has 13 levels of grid refinement are simulated with three eddy-viscosity turbulence models: Spalart & Allmaras one-equation model; Shear-stress transport (SST) k-w two-equation and k-kl-w three-equation, based on SIMPLE algorithm. In terms of flow around NACA 0012 hydrofoil, 4 set grids and each set has 9 levels of grid refinement are applied with Spalart & Allmaras one-equation model based on same algorithm.

For solution verification, the uncertainty estimators which are Grid Convergence Index (GCI) method, Factor of Safety method (FS) and Least Squared Root methods (LSR) are applied to evaluate the uncertainty of the results. This paper contains five sections. The first section is introduction and then the mathematical formations of RANS equations and uncertainty verification methods are shown in the second section. The third part is numerical model, the simulation models and the detail information of these grid groups are introduced in this section. The fourth section is result, the iterative error and uncertainty analysis results from above three uncertainty estimators are shown in this section. Furthermore, the estimation of discretization errors and discretization error bars are figured out. Finally, the conclusion and discussion are drawn in last section.

ASSESSMENT OF DISCRETIZATION UNCERTAINTY ESTIMATORS BASED ON GRID REFINEMENT STUDIES

Oral Presentation. VVS2018-9340 **1:55PM - 2:20PM**

Luis Eca, *IST, Lisbon, Portugal,* ***Guilherme Vaz***, *MARIN, Wageningen, Netherlands,* ***Martin Hoekstra***, *Maritime Research Institute Netherlands, Wageningen, Netherlands,* ***Scott Doebling***, *Los Alamos National Lab, Los Alamos, NM, United States,* ***V. Gregory Weirs***, *Sandia National Laboratories, Albuquerque, NM, United States,* ***Tyrone Phillips***, *University of British Columbia, Blacksburg, VA, United States,* ***Christopher Roy***, *Virginia Tech, Blacksburg, VA, United States*

Recently, a set of data from the calculation of the flow over a flat plate and around the NACA 0012 airfoil has been proposed for the assessment of the discretization uncertainty estimators based on grid refinement studies [1].

In this paper, we assess the performance of 8 discretization uncertainty estimates: the method proposed by Xing and Stern in [2]; a revised version of the previous method [3]; the implementation of the GCI method of Roache [4] of the Workshop organizers; the GCI as described in the ASME V&V Standard of 2009 [5]; a generalization of the GCI method proposed in [6] and its most recent version that incorporates weighted fits taken from robust statistics; the method proposed in [7] and the Robust Verification Analysis proposed in [8].

The performance of the different methods is evaluated determining the number of cases where the uncertainty cannot be estimated and the ratio R between the estimated uncertainty and the error E, which is based on an estimate of the exact solution presented in [1, 9].

Keywords: Discretization uncertainty, Grid refinement.

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4C code solution verification

Oral Presentation. VVS2018-9390 **2:20PM - 2:45PM**

***Roberto Zanino, Roberto Bonifetto, Laura Savoldi**, Dipartimento Energia, Politecnico Di Torino, Torino, Italy, **Andrea Zappatore**, Politecnico di Torino, Torino, Torino, Italy*

The worldwide research on nuclear fusion reactors is currently relying on several experimental devices and computational tools that should help in the design and realization of the first demonstrator power plant, like, e.g., the European DEMO. The 4C code is the state-of-the-art tool for the thermal-hydraulic simulation of tokamak superconducting magnet systems based on Low Critical Temperature Cable-in-Conduit Conductors (CICC) cooled by forced-flow supercritical helium. It was developed at Politecnico di Torino over the last ~10 years and it includes three different modules: 1) the multi-conductor module solves the 1D transient non-linear Euler-like set of partial differential equations in each cooling channel of the winding pack (WP), coupled with the 1D transient heat conduction equation for the solids; 2) the structure module solves with the open-source Freefem++ code a set of 2D transient heat conduction problems approximating the 3D problem in the casing, which encloses the WP; 3) the cryogenic circuit module provides self-consistent boundary conditions to the WP: it solves transient non-linear Euler-like equations in the 1D components (pipes) and mass and energy balance in the 0D components (manifolds, etc.), using OpenModelica. Although the 4C code has already been successfully validated against experimental data covering a wide range of transients and time-scales, a systematic verification exercise has never been pursued so far.

In this work, we apply the method of the manufactured solutions to 4C, to achieve its first solution verification. We adopt a systematic procedure, verifying first every single module and then the coupling between them. In particular, we begin verifying the multi-conductor module starting from a single conductor under isothermal conditions: we show that the computed solution agrees with the analytical (manufactured) solution. Then, the verification of the energy equation is performed, still for a single conductor. The multi-conductor module verification is achieved considering the inter-conductors thermal coupling. The method is applied separately to the stand-alone circuit module, and then to the conductor and circuit modules coupled together. Finally, after the verification of the structure module, the coupling between the WP and the structures is verified, completing the 4C solution verification journey.

Beyond our interest in applying the method of manufactured solutions for the 4C code verification, this work also aims at raising awareness in developers and analysts in our field about the feasibility of and need for such verification exercise, being it an indispensable step for confirming the reliability of any code.

Verification for Hypersonic, Reacting Turbulent Flow

Oral Presentation. VVS2018-9406 **2:45PM - 3:10PM**

***Brian Carnes, Brian Freno, Tom Smith, V. Gregory Weirs** Sandia National Laboratories, Albuquerque, NM, United States, **Marco Arienti**, Sandia Labs, Livermore, U S Minor Island, **Erin Mussoni**, Sandia Labs, Livermore, CA, United States*

A new simulation code for hypersonic, reacting turbulent flow (SPARC) is being developed at Sandia National Laboratories. This talk discusses recent work to verify the correctness of the implementation of physics and algorithms in SPARC in the context of significant validation efforts. We discuss several code verification activities designed to support the validation work. These include tests with exact solutions for inviscid flow features such as shocks and expansion regions, and tests using manufactured solutions to verify design order accuracy. Of particular interest are verification of boundary conditions, reacting flow, and laminar and turbulent boundary layers. For turbulent flow, some verification problems are based on benchmark problems from the NASA Turbulence Modeling Resource website. We also provide examples of solution verification applied to simulations of validation experiments with hypersonic laminar flow over a double cone. Here careful consideration is given to iterative convergence, mesh design for 2D axisymmetric flow in a 3D code, and extrapolation of surface quantities such as heat flux and pressure.

Contact Discontinuities in xRage

Oral Presentation. VVS2018-9410 **3:10PM - 3:35PM**

Robert Singleton, *Los Alamos National Laboratory, Los Alamos, NM, United States*

Banks, Aslam, and Rider (2008) have shown that contact discontinuities have a convergence rate of p/(p+1) for a p-th order accurate code. The Los Alamos code xRage is 2nd order accurate, and we therefore expect to see a convergence rate of 2/3 for the contact. However, in simulations of the Sod problem, one must run at extremely fine resolutions before this theoretical convergence rate is observed. This resolution is much smaller than one would typically use in a numerical simulation of an engineering or physics problem, which leads to the conclusion that one almost always runs far outside the range of convergence in most simulations of interest. This also seems to hold true for shocks and rarefactions, both of which have a theoretical convergence rate of 1. However, by choosing a small window about the contact over which to perform the convergence analysis, rather than the entire domain of the problem, the density variable reaches the theoretical limit of 2/3 almost immediately at quite coarse resolutions. This windowing method, therefore, might be useful for observing the theoretical rates for discontinuities in other problems as well, although there is a catch. While the density appears to converge as expected, the velocity and pressure show anomalous convergence behavior at all resolutions. Application of the windowing method will be shown for density, velocity, and pressure with hypotheses for the anomalous convergence behavior tested.

TRACK 1 CHALLENGE PROBLEM WORKSHOPS AND PANEL SESSIONS

1-4 CODE VERIFICATION FOR APPLICANTS IN A REGULATED FIELD
4TH FLOOR, GREAT LAKES A1 4:00PM - 6:05PM

Code Verification for Applicants in a Regulated Field [Panel]

Oral Presentation. VVS2018-9395 **4:00PM - 6:05PM**

Marc Horner, *ANSYS, Inc., Evanston, IL, United States,* ***David Moorcroft***, *Federal Aviation Administration, Oklahoma City, OK, United States*

This panel will discuss the challenges of completing and documenting code verification for modeling and simulation users working in regulated fields. The intent is to initiate a conversation on:

1. What is code verification?

2. What needs to be done if using Commercial-off-the-Shelf software?

   How much is enough? Who?s responsible (developer vs applicant)? Does it need to be evaluated on the applicant?s system?

3. What documentation should be provide to a regulatory body for acceptance? How much documentation?

The panel will include members of regulatory agencies providing research opinions and published agency policy, code developers discussing the challenges they face, members of research organizations providing guidance based on their experience, and commercial organizations providing their experience/challenges with code verification.

Panel Participants:
Prasanna Hariharan, US Food and Drug Administration
Josh Kaizer, US Nuclear Regulatory Commission
David Moorcroft, US Federal Aviation Administration
Marc Horner, Ansys
Kristian Debus, Siemens PLM Software
Ashley Peterson, Medtronics
John Dong, The Boeing Company

TRACK 3 TOPICS IN VERIFICATION AND VALIDATION

3-1 TOPICS IN VERIFICATION AND VALIDATION
4TH FLOOR, GREAT LAKES A2 4:00PM - 6:05PM

Models, Uncertainty, and the Sandia V&V Challenge Problem

Technical Publication. VVS2018-9308 **4:00PM - 4:25PM**

George Hazelrigg, *Independent Author, Vienna, VA, United States,* ***Georgia-Ann Klutke***, *National Science Foundation, Alexandria, VA, United States*

In this paper, we argue that the Sandia V&V Challenge Problem is ill-posed in that the answers sought do not, mathematically, exist. This effectively discredits both the methodologies applied to the problem and the results, regardless of the approach taken. We apply our arguments to show the types of mistakes present in the papers presented in J. of VVUQ along with the Challenge Problem. Further, we show that, when the problem is properly posed, both the applicable methodology and the solution techniques are easily drawn from the well-developed mathematics of probability and decision theory. The unfortunate aspect of the Challenge Problem as currently stated is that it leads to incorrect and inappropriate mathematical approaches that should be avoided and corrected in the current literature.

Virtually-Guided Certification with Uncertainty Quantification Applied to Die Casting

Technical Publication. VVS2018-9323 **4:25PM - 4:50PM**

Shantanu Shahane, ***Soham Mujumdar***, ***Namjung Kim***, ***Pikee Priya***, ***Narayana Aluru***, ***Shiv G Kapoor***, ***Placid Ferreira***, ***Surya Vanka*** *University of Illinois at Urbana Champaign, Urbana, IL, United States*

Die casting is a type of metal casting in which liquid metal is solidified in a reusable die. Automotive and housing industries are main consumers of die cast products. Simulations and experiments are used to understand the physics and improve product quality in manufacturing. Computer simulations are convenient and financially viable compared to full scale experiments. Alloy material properties, interface conditions at the mold, thermal boundary conditions etc. affect product quality in die casting. Hence all these are used as inputs to simulations. However, in such a complex process, measuring and controlling these process parameters is difficult. Conventional deterministic simulations are insufficient to completely estimate the effect of stochastic variation in the process parameters on product quality. In this research, a framework to simulate the effect of stochastic variation together with verification, validation, sensitivity analysis and uncertainty quantification is proposed. This framework includes high speed numerical simulations, micro-structure and mechanical properties predication models along with experimental inputs for calibration and validation.

Three-dimensional finite volume based software to solve Navier-Stokes and energy equations is developed. Fluid flow, natural convection, heat transfer and solidification physics is modeled. Since complex geometries can be meshed with smaller number of unstructured elements and lesser stair-casing error compared to Cartesian orthogonal structured mesh, an unstructured mesh is used in this software. Algebraic multigrid method is used to accelerate convergence. Parallelization is done on multiple CPU cores using MPI. Temperature gradients and cooling rates thus estimated are used as input to empirical models of micro-structure parameters including dendrite arm spacing and grain size. Experimental data helps to calibrate these empirical models for a given alloy. Published numerical and experimental results are used to verify and validate respectively the entire framework. Practical engineering problems have hundreds of process parameters and performing simulations or experiments to quantify the effect of stochastic variation of each process parameter on the product quality is difficult. Hence sensitivity analysis is performed to identify critical process parameters which affect the product quality significantly and thus control them within desired tolerance.

This framework employs both experimental data and stochastic variation in process parameters with numerical modeling and thus enhances the utility of traditional numerical simulations used in die casting to have a better prediction of product quality. Although the framework is being developed and applied to die casting, it can be easily generalized to any manufacturing process or other engineering problems as well.

Experimental Calibration Of A Biohydrogen Production Estimation Model

Technical Publication. VVS2018-9341 **4:50PM - 5:15PM**

***Fernando Gallego Dias**, **José Viriato Coelho Vargas**, **Vanessa M Kava**, **Wellington Balmant**, **André B Mariano**, UFPR, Curitiba, Parana, Brazil, **Sam Yang**, **Juan C Ordonez** Florida State University, Tallahassee, FL, United States*

In this work, a dynamic physics-based model developed for the prediction of biohydrogen production in a compact tubular photobioreactor was calibrated experimentally. The spatial domain in the model was discretized with lumped control volumes, and the principles of classical thermodynamics, mass, species and heat transfer were combined to derive a system of ordinary differential equations whose solution was the temperature and mass fraction distributions across the entire system. Two microalgae species, namely, Acutodesmus obliquus and Chlamydomonas reinhardtii strain cc125 were cultured in triplicate with different culture media via indirect biophotolysis. Experimental biomass and hydrogen concentrations were then used to adjust the specific microalgae growth and hydrogen production coefficients based on residual sum of squares and the direct search method.

Thermal Response of Open-Cell Porous Materials: A Numerical Study and Model Assessment

Technical Publication. VVS2018-9317 **5:15PM - 5:40PM**

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

The evaluation of effective material properties in heterogeneous materials (e.g., composites or multicomponent structures) has direct relevance to a vast number of applications, including nuclear fuel assembly, electronic packaging, municipal solid waste, and others. The work described in this paper is devoted to the numerical verification assessment of the thermal behavior of porous materials obtained from thermal modeling and simulation. Two-dimensional, steady state analyses were conducted on unit cell nano-porous media models using the finite element method (FEM). The effective thermal conductivity of the structures was simulated, encompassing a range of porosity. The geometries of the models were generated based on ordered cylindrical pores in four different porosities. The dimensionless effective thermal conductivity was compared in all simulated cases. In this investigation, the method of manufactured solutions (MMS) is used to perform code verification, and the grid convergence index (GCI) is employed to estimate discretization uncertainty (solution verification). The system response quantity (SRQ) under investigation is the dimensionless effective thermal conductivity across the unit cell. Code verification concludes a roughly second order accurate solver. It was found that the introduction of porosity to the material reduces effective thermal conductivity, as anticipated. The approach can be readily generalized to study a wide variety of porous solids from nano-structured materials to geological structures.

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

8-1 VERIFICATION &VALIDATION FOR IMPACT, BLAST, AND MATERIAL RESPONSE
4TH FLOOR, GREAT LAKES A3 4:00PM - 6:05PM

Laboratory system testing uncertainty of a twelve accelerometer channel (“12a”) impact monitoring mouthguard to quantify head impacts for athletes and soldiers

Oral Presentation. VVS2018-9330 **4:00PM - 4:25PM**

Adam Bartsch, ***Rajiv Dama*** *Prevent Biometrics, Minneapolis, MN, United States*, ***Sergey Samorezov***, *Cleveland Clinic, Cleveland, OH, United States*

As frontline caregivers continue to have difficulty identifying concussed athletes and soldiers, there is an unmet need for a trustworthy real-time impact monitoring system to identify risky head impacts. And in finite element modeling, a dearth of accurate and precise single head impact kinematic data sets has held back the identification of brain tissue level failure mechanisms. The first step toward providing computational modelers with sufficiently certain input kinematics data sets is to quantify laboratory uncertainty of devices that estimate head impact kinematics.

In this study we conducted n=265 laboratory calibration tests of a wireless impact monitoring mouthguard equipped with twelve accelerometer channels (“12a”).

Tests were done with Industry standard impactors (linear pneumatic, pendulum) as well as Reference headforms (Hybrid III, NOCSAE) equipped with kinematics data acquisition.

Spatial and scalar peak data correlations of the 12a impact monitoring mouthguard vs. Reference fit a linear model for all tested impact locations and directions, with maximum 1-sigma uncertainty of +/-7g up to 113g linear acceleration and +/-800rad/s2 up to 8300rad/s2 angular acceleration.

Non-trivial processing algorithm, mouthguard customization, knowledge of accelerometer positions and orientations, and linearization of individual accelerometer outputs were required to achieve this level of certainty.

The 12a impact monitor is currently optimized for computation of skull kinematics during the primary acceleration-deceleration phase of impact in helmeted sports where nominal frequency content is 20-80Hz. Higher measurement uncertainty, especially in unpadded testing, was due to high frequency signals above 100Hz.

The 12a Impact Monitoring Mouthguard scalar outputs are suitable for low uncertainty measurement and computational modeling of single head impact scalar PLA and PAA in American football and bare head activities so long as human on-field impact conditions are within laboratory calibration ranges.

If on-field impacts occur outside the ranges of laboratory calibrations then the 12a impact monitoring mouthguard must have accuracy calibration expanded to include the true on-field range(s).

Ongoing work involves collecting user-specific head impact doses with 12a impact monitoring mouthguard, verifying these doses fall within the laboratory calibration ranges, understanding the athlete’s individual dose-response profile and creating a data analysis firmware that more accurately computes skull kinematics from high frequency (100Hz+) bare head impacts. The ultimate goal of our work is to correlate trustworthy spatial and temporal estimates of single and cumulative head impact doses with computational models of tissue level brain damage mechanisms.

Simulation and Assessment of a Novel Sphere-on-Glass Ballistic Impact Experiment

Oral Presentation. VVS2018-9337 **4:25PM - 4:50PM**

Prusodman Sathananthan, ***Dilaver Singh***, ***Duane Cronin*** *University of Waterloo, Waterloo, ON, Canada*, ***Alexandra Sirois***, *Defense Research and Development Canada, Québec, QC, Canada*

Transparent armor provides situational awareness and protection from ballistic threats, making it a critical component in armored vehicles. A disadvantage of transparent armor is its weight relative to its opaque counterparts. Transparent laminates can be optimized for weight, but this requires validated models of ballistic impact on transparent materials. Previous studies have investigated ballistic impact on confined or laminated ceramics. These methods do not allow for measurement of features such as radial crack propagation and back face spall. To address this, a novel test methodology using a steel sphere impacting an unsupported glass tile is proposed. The Sphere-on-Glass (SOG) tests were performed on unconfined soda-lime glass tiles, impacted by steel ball bearings at 100, 200, 300, 500 and 800m/s. The impact events were recorded with high speed video cameras (1 million frames per second). Kinematic data (projectile residual velocity) and damage propagation velocities (crack speeds and comminution front) were measured using image tracking software and used to evaluate numerical models. Post impact analysis of select samples were also performed to further validate model response with respect to fracture.

A finite element model of the experimental tests was created in a commercial explicit finite element code (LS-Dyna). Three formulations including Lagrangian with erosion, Smooth Particle Hydrodynamics (SPH), and Element Free Galerkin (EFG) were investigated with the widely used Johnson-Holmquist 2 constitutive model. The discretization error was quantified using a mesh convergence study at three finite element mesh sizes: 1.00mm, 0.50mm and 0.25mm. The residual projectile velocity was used as the assessment parameter. A Richardson extrapolation was used to estimate the converged solution. It is accepted that discontinuities such as element erosion and shock waves may invalidate the underlying assumptions used in the Richardson extrapolation. To improve interpretation of the results, intermediate mesh sizes were also assessed to confirm the asymptotic behavior of the final solution with respect to mesh size.

The Lagrangian model converged asymptotically, with an observed order of convergence of 1.88. Both the SPH and EFG models did not show asymptotic convergence. Confidence intervals (95%) were computed and compared to the measured residual velocity at 800m/s (129±13 m/s). The Lagrangian model had a larger confidence interval (221± 165 m/s) but contained the measured residual velocity. Both the SPH and EFG models had tighter confidence intervals (219±26 m/s and 444±15m/s respectively), but did not contain the measured residual velocity. The models predicted regions of comminution consistent with test results, but did not accurately predict the radial fracture patterns seen in the experiments, which is a known limitation of the constitutive model. The Sphere-on-Glass tile tests proved to be a novel validation dataset, incorporating real-time visualization and tracking of damage propagation and provided key quantitative data which can be used to improve future ballistic models.

V&V of Under-body Blast Analysis Methodology for Army Ground Vehicles

Oral Presentation. VVS2018-9371 **4:50PM - 5:15PM**

Andrew Drysdale*, *Douglas Howle, *US Army Research Laboratory, Aberdeen Proving Ground, MD, United States*

The US Army Research Laboratory (ARL) has developed, through a multi-year program of dedicated funding, an analysis process for consideration of ground vehicle survivability against buried bare-charge threats. The key, and most innovative, products of ARL's under-body blast methodology (UBM) process are occupant injury predictions along the most relevant injury modes. Additionally, UBM is designed to be multi-stage and modular so that it can be customized to the application as much as possible. Modeling challenges include the complex geometries and failure modes of relevant target vehicles; the violent, impulsive loading of the threat environment; non-linear energy-absorbing components along key load paths; difficulty in characterization of occupant response to known loading; and the high degree of sensitivity of outputs to small changes in input conditions that are difficult to measure. Because of these sources of uncertainties, and in response to regulatory mandates from the Army, a comprehensive V&V of the process is essential. Both verification and validation of the UBM process encountered stubborn challenges. Reliance on commercial finite-element modeling software limited the scope of verification in most stages of the analysis process. The inherent unrepeatability and expense of the phenomena under investigation made the acquisition of robust data sets for validation difficult. The pioneering nature of the model's application meant that a consensus regarding appropriate evaluation metrics and pass/fail thresholds was elusive. The eventual path to accreditation for use in Army live-fire test and evaluation (LFT&E) required creative solutions to each of these issues. This presentation gives an overview of Army LFT&E, how UBM fits into that program, how the UBM process is designed to work, and an example of nominal outputs. It delves into specific challenges faced in the V&V process and how they were addressed in order to satisfy accreditation requirements. Emphasis is placed on its application to evaluation of the Joint Light Tactical Vehicle, the context for which this initial V&V was conducted.

Importance of Finite Element Mesh Resolution and Response Metrics to Model Blunt Thoracic Impact

Oral Presentation. VVS2018-9392 **5:15PM - 5:40PM**

Jeffrey B. Barker*, *Duane Cronin, *University of Waterloo, Waterloo, ON, Canada*

Human body models (HMB) have become increasingly important in the assessment and development of human safety systems. A critical aspect of detailed finite element HBM is verification and validation of the models over a representative range of impact conditions; however, often mesh sensitivity studies are not undertaken due to pragmatic limitations such as computational time. In this study, the effect of the muscle tissue mesh density on blunt thoracic impact kinetics and kinematics were investigated using a previously developed detailed finite element thorax model.

The detailed thorax model (325,065 elements) comprised: the outer muscle tissue, sternum, rib cage, costal cartilage, lungs, heart, mediastinum and spine. Two loading regimes with corresponding PMHS experimental data were applied to the thorax model. The first load case was a frontal pendulum impact (23.4 kg, 150mm diameter) with impact velocities of 4.3 m/s, 6.7 m/s, and 10.0 m/s. In the second case, three baton impacts (140g, 37mm diameter) at 20 m/s and 40m/s; and (30g, 37 mm diameter) at 60 m/s were investigated. The impacts were centered on the sternum at the height of the 8th thoracic vertebrae. The original finite element mesh was reduced in size twice by splitting the elements resulting in three finite element mesh densities for the muscle tissue (Coarse: 26,142 elements; Intermediate: 209,108 elements; Fine: 1,672,836 elements). For each case, the model force and displacement responses were sampled at the same frequency as in the corresponding experimental cases.

The pendulum impacts showed similar responses for the plateau force with varying mesh density, but did have higher initial peak force (20%) for the coarse mesh relative to the fine mesh. The model response was within the experimental response corridors. Changes in response were more pronounced for the smaller diameter baton impacts. The peak force decreased with smaller element size while the responses for the 140g impact at 20 m/s and 40 m/s were within the published response corridors, the responses for the 30g (60 m/s) impact were outside the response corridors. This may indicate a need for improved high deformation rate material properties and further mesh refinement. Refining the muscle tissue element size reduced the response stiffness for all impact cases, with larger differences identified for smaller impact areas and lower mass projectiles. This was attributed to improved mass distribution with a refined mesh, and an improved prediction of local strain rate in the muscle tissue material. Thus, the required finite element size for a given problem depends on the impact scenario and must be evaluated to ensure meaningful numerical results.

Validation of Puncture Simulations of Railroad Tank Cars Using Full-scale Impact Test Data

Technical Publication. VVS2018-9322 **5:40PM - 6:05PM**

Michael Carolan, ***Benjamin Perlman***, *USDOT/Volpe National Transportation Systems Center, Cambridge, MA, United States,* ***Francisco Gonzalez, III***, *USDOT, Federal Railroad Administration, Washington, DC, United States*

The U.S. Department of Transportation's Federal Railroad Administration (FRA) has sponsored a series of full-scale dynamic shell impact tests to railroad tank cars. Currently, there are no required finite element (FE) model validation criteria or procedures in the field of railroad tank car puncture testing and simulation. Within the shell impact testing program sponsored by FRA, comparisons made between test measurements and simulation results have included the overall force-time or force-indentation histories, the puncture/non-puncture outcomes, the rigid body motions of the tank car, the internal pressures within the lading, and the energy absorbed by the tank during the impact. While qualitative comparisons (e.g. the shapes of the indentation) and quantitative comparisons (e.g. peak impact forces) have been made between tests and simulations, there are currently no requirements or guidelines on which specific behaviors should be compared, or what measurable level of agreement would be acceptable demonstration of model validation. It is desirable that a framework for model validation, including well-defined criteria for comparison, be developed or adopted if simulation is to be used without companion shell impact testing for future tank car development. One of the challenges to developing model validation criteria and procedures for tank car shell puncture is the number of complex behaviors encountered in this problem, and the variety of approaches that could be used in simulating these behaviors. The FE models used to simulate tank car shell impacts include several complex behaviors, each of which can introduce uncertainty into the overall response of the model. These behaviors include dynamic impacts, non-linear steel material behavior, including ductile tearing, two-phase (water and air) fluid-structure interaction, and contact between rigid and deformable bodies. Several candidate qualitative and quantitative comparisons of test measurements and simulations results are discussed in this paper. They are applied to two recently-completed shell impact tests of railroad tank cars sponsored by FRA. For each test, companion FE simulation was performed by the Volpe National Transportation Systems Center (Volpe). The process of FE model development, including material characterization, is discussed in detail for each FE model. For each test, the test objectives, procedures, and key instrumentation are summarized. For each set of test and simulations, several corresponding results are compared between the test measurements and the simulation results. Discussion of the qualitative and quantitative similarities and differences between test measurements and simulation results are also discussed. Additionally, this paper includes discussion of approaches to model validation employed in other industries or areas of transportation where similar modeling aspects have been encountered.

Technical Program
Thursday, May 17, 2018

TRACK 1 CHALLENGE PROBLEM WORKSHOPS AND PANEL SESSIONS

1-5 ASME 2018 V&V VERIFICATION, VALIDATION, AND UNCERTAINTY QUANTIFICATION: THE UNANSWERED QUESTIONS
4TH FLOOR, GREAT LAKES A1 10:25AM - 12:30PM

***Paul Deacon**, Siemens PLM Software, **Aaron Koskelo**, Los Alamos National Lab, **Sankaran Mahadevan**, Vanderbilt University, **Chris Roy**, Virginia Tech University, **Daniel Segalman**, Michigan State University*

The purpose of this panel discussion is to provoke a discussion among the Verification, Validation, and Uncertainty Quantification (VVUQ) community as to the great "Unanswered Questions" in the field. Over the past twenty years, the field of VVUQ has emerged as a discipline unto itself, cutting across traditional disciplines and individual technical specialties. In traditional disciplines, there often exist a well-known set of important "Unanswered Questions" in that field. Sometimes these questions are codified into a set of axiomatic statements, and sometimes they are merely oral tradition. Sometimes the field is in consensus that these questions are important, but often there is not consensus, and this often leads to spirited technical interchange between experts in the field adopting opposing viewpoints. The process of discussing and attempting to clearly document these questions will help to inspire and organize research activities in the field to work towards an overall improvement in the state-of-the-art and state-of-the-practice in VVUQ. Format: 3-5 panelists, with some recognized stature in the field. A pre-conference survey is used to collect input from the community on the "Unanswered Questions in VVUQ." The panel discussion will start with a moderator presenting the results of the survey, followed by each panelist take 5-10 minutes to comment on the results and present views of their own. Remaining time will be used for a roundtable discussion with the audience.

TRACK 12 VERIFICATION METHODS

12-2 VERIFICATION METHODS
4TH FLOOR, GREAT LAKES A2 10:25AM - 12:30PM

Verification Of Plasticity Models For Production Finite Element Codes

Oral Presentation. VVS2018-9383 **10:25AM - 10:50AM**

***William Scherzinger**, **Brian Lester**, Sandia National Laboratories, Albuquerque, NM, United States, **Jake Ostien**, Sandia National Laboratories, Livermore, CA, United States*

Constitutive models provide the underlying material behavior for solid mechanics finite element codes. Given this, verification of the constitutive models is important for ensuring the credibility of analyses using these codes. Unfortunately, due to the wide range of material behavior, no simple framework exists for verification of constitutive models. This work presents the verification of a family of plasticity models implemented in the Sierra/SolidMechanics code at Sandia National Laboratories. These models have undergone extensive verification testing that synthesizes an understanding of the models, continuum mechanics, and the finite element formulation in the code to rigorously verify their implementation. Rate independent and rate dependent models, with assorted hardening laws and both isotropic and anisotropic yield surface descriptions, have been implemented and verified through a series of uniaxial tension and pure shear boundary value problems. The verification of the plasticity models is presented in detail, but more importantly techniques and approaches are described that we believe can be extended to other classes of constitutive models.

Method of Nearby Problems for Large Deformation Analyses of Hyperelasticity

Oral Presentation. VVS2018-9402 **10:50AM - 11:15AM**

***Takahiro Yamada**, Yokohama National University, Yokohama, Japan*

The method of nearby problems developed by Roy et al. is a sophisticated verification procedure, in which the problems with exact solutions near the target problem of interest can be generated by a curve fitting of a numerical solution to a continuous function. To apply this method to solid problems in the conventional procedure, spatial derivatives of stresses derived from given displacement solutions, which is hardly calculated for general constitutive laws, are required to calculate body forces in the nearby problem. Therefore they have been not popular in solid mechanics. To circumvent such difficulty, the author developed an alternative procedure to calculate equivalent nodal vectors of body forces without calculation of the spatial derivative of stresses. It is based on the weak formulation of the problems of solid and the actual procedure to calculate equivalent nodal force vectors is similar to the evaluation of internal force, in which the work product of the stress and virtual strain is integrated over the domain. In our previous work, small deformation problems are considered and nearby solutions are constructed by the projection of a finite element solution of displacement onto an approximating function space using the inner product in the Sobolev space H1. The projection is carried out for each component of displacement fields. For the approximating function space, the uniform tensor product B-spline functions are employed and complex geometry is modeled by using the fictitious domain approach. In this work, we apply our approach to large deformation problems of hyperelasticity, which is a material model for rubber-like materials and biomaterials. In such problems, materials exhibit incompressible or nearly incompressible behaviors. If nearby solutions of displacement fields are constructed for each component independently, they cannot satisfy the incompressible or nearly compressible condition and unreasonable body forces need to be applied. In this work, projection with constraint condition of incompressibility is proposed. This procedure is based on the minimization of H1 norm of whole displacement fields with penalty term associated with incompressibility. Several representative numerical results are presented to show the validity of the present approach. Solution verification is also performed by using the present procedure.

Error Quantification for Large-Deformation Solid Mechanics with Adaptive Remeshing

Oral Presentation. VVS2018-9411 **11:15AM - 11:40AM**

Andrew Stershic*, *Lauren Beghini*, *Guy Bergel*, *Alex Hanson*, *Kevin Manktelow, *Sandia National Laboratories, Livermore, CA, United States*

Several manufacturing processes relevant to the aerospace industry, such as forging and welding, consist of high-temperature loading of stock material and result in large local deformation. When such processes are modeled computationally using the finite element method, high mesh distortion reduces the model's accuracy and robustness. Adaptive remeshing capabilities present an attractive solution to address the issue of high mesh distortion without significantly increasing the model's computational cost.

In this work, we verify the simulation process that uses adaptive remeshing to model thermo-mechanical forging and welding in SIERRA, a scalable multi-physics finite element code produced by Sandia National Laboratories.

The enhancement of solution quality is assessed using an error metric; as the manufacturing simulations of interest are geometrically and physically complex, no exact solution is available for comparison. Further, due to the presence of contact singularities, we cannot use fine mesh comparisons in place of exact solutions as a basis of comparison. Consequently, we employ a variant of the classical approach of Zienkiewicz and Zhu [1], wherein an element field (piecewise constant) is projected to the nodes (piecewise bilinear) in place of an exact solution, as the higher-order field better approximates the true solution. The difference between the projected and original solutions estimates the finite element error. Specifically, we employ the Frobenius norm of the Cauchy stress tensor to form the scalar error metric.

The adaptive remeshing capability is primarily evaluated on two examples: (1) a necking tensile-bar problem and (2) a resistance-forge-welding simulation. We assess several different choices of mesh sizing strategies used to remesh the geometry while keeping the mesh size and computational expense constant. We find that the application of adaptive remeshing increases solution robustness and reduces the error estimate for these large-deformation simulations.

Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

References:

[1] O. C. Zienkiewicz and J. Z. Zhu, "A simple error estimator and adaptive procedure for practical engineering analysis," International Journal of Numerical Methods in Engineering, vol. 24, no. 2, pp. 337-357, 1987.

A Case Study in Mesh Verification

Oral Presentation. VVS2018-9409 **11:40AM - 12:05PM**

Adam Johnson, *Honeywell FM&T, Overland Park, KS, United States*

At the Kansas City National Security Campus (KCNSC), simulation analysts are often called upon to provide quick-turn solutions to manufacturing roadblocks. This environment presents challenges in the execution of model verification, such as mesh verification studies. A tool was developed to automate the process of performing Richardson's extrapolation to provide the analyst a discretization error estimate. This tool was designed to balance the underlying pitfalls of Richardson's extrapolation and deliver feedback when certain requirements are not met. This presentation provides an example of how automation has been used to promote model verification in a manufacturing environment while highlighting the inherent challenges involved.

The Kansas City National Security Campus is operated by Honeywell Federal Manufacturing & Technologies, LLC for the United States Department of Energy under Contract No. DE-NA0002839

Code Verification Studies for a Solid Mechanics Code – Triumphs and Trials

Oral Presentation. VVS2018-9364 **12:05PM - 12:30PM**

James Cox, *Sandia National Laboratories, Albuquerque, NM, United States*

High consequence applications for Solid Mechanics codes motivate rigorous code verification to improve the credibility of analysis results used by decision makers. Code verification is foundational to establishing this credibility, since model calibration, solution verification, and validation presume the code is correctly approximating the underlying mathematical models.

Many code verification problems for solid mechanics are based upon classical solutions for linear elasticity problems. While verification of the code with these types of problems provides some evidence of code correctness, simplifying assumptions in the analytical solution process and/or inconsistency of the governing equations between the code and test problem can limit the value of the verification tests. In some cases convergence testing can be applied, but in other cases it is not effective. The method of manufactured solutions, while effective for many classes of problems for overcoming these issues, can be difficult to apply to some solid mechanics problems, particularly those with material history dependence.

In this presentation, we will summarize some code verification studies that address both classical and manufactured solutions for solid mechanics. Problems with hyperelastic material models are often amenable to manufacturing a solution, as the strong form of the boundary-initial-value problem is governed by differential equations. Starting simple, we consider quadratic displacement fields which can be thought of as being one step past a "patch test" for lower order elements. Another approach has been to manufacture a solution starting with the displacement field from a classical solution, and then applying the governing nonlinear differential equations to "manufacture the corresponding problem." The classical stress concentration problem for the stress around a circular hole is examined, for which convergence results using both the classical and a manufactured solution are compared.

When constitutive models include history dependence, (e.g., hypoelastic and elastoplastic models), the governing strong form of the boundary-initial-value problem includes integrodifferential equations, which significantly complicate the manufacturing of solutions. When the problem also includes contact, the corresponding kinematic constraints can render a meaningful manufactured solution practically intractable. We consider a simplification to the manufacturing process (semi-manufactured) to make a hypoelastic problem (without contact) more tractable. For a problem with both contact and plasticity, we take a more pragmatic approach, applying solution verification to examine the convergence tendency of the code. The strength of the test is its closer proximity to the actual application space, but the verification cannot claim convergence to the correct solution, only to "a solution."

TRACK 13 VERIFICATION AND VALIDATION FOR BIOMEDICAL ENGINEERING

13-2 ASME V&V 40 SUBCOMMITTEE — VERIFICATION AND VALIDATION IN COMPUTATIONAL MODELING OF MEDICAL DEVICES

4TH FLOOR, GREAT LAKES A3 10:25AM - 12:30PM

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

Oral Presentation. VVS2018-9426

Tina Morrison*, Food and Drug Administration, Silver Spring, MD, United States,* ***Marc Horner****, ANSYS, Inc., Evanston, IL, United States,* ***Ryan Crane****, ASME, New York, NY, United States*

The ASME V&V40 Subcommittee is hosting this session on regulatory success stories in medical devices with computational modeling. The session will feature seven speakers from the medical device industry and the FDA presenting a variety of case studies in cardiovascular, hospital, surgical, and orthopedic device areas. This session will be chaired by Tina Morrison (FDA), Chair, ASME V&V40 and Marc Horner (ANSYS), Co-Chair, ASME V&V40. All presentations are by subcommittee members of ASME V&V40.

Presentations will be 12-15 minutes, followed by a group Q&A. Speakers are presented in alphabetical order by last name.

Payman Afshari, Depuy Synthes: Application of a computational model to determine the MR conditional Radiofrequency labeling parameters for the Anterior Cervical Plates implanted in patients being scanned in a 1.5T and 3T MRI machines; DePuy Synthes Spine received 510k clearance based on the submitted evidence from the computational model.

Christopher Basciano, BD Technologies and Innovations: An approach that BD Corporate Computer-Aided Engineering (CAE) has leveraged to tackle the challenge of establishing confidence in computational modeling and simulation results is to conduct and present verification studies to various teams within the company. The current presentation will discuss verification case studies in computational fluid dynamics as well as some common terminology used to communicate the significance of the verification work to non-technical audiences.

Jeff Bischoff, Zimmer Biomet: Application of the V&V40 philosophy to evaluate the primary stability of a shoulder prosthesis.

Jeff Bodner, Medtronic Restorative Therapies Group: Simulation and rigorous VVUQ in a regulatory submission that addressed a CAPA related to an implantable drug delivery pump.

Prasanna Hariharan, FDA: Application of computational modeling for a tumor ablation procedure. A computational heat transfer model was used to show that the temperature rise during the ablation will not cause damage to sensitive structures around the ablation site. The risk and credible assessment process as demonstrated by V&V40 showed that the model was not credible enough to answer the question of interest. However, because of the credibility assessment, additional bench tests were conducted to satisfactorily address the question of interest.

Ali Kiapour, 4WEB Medical: Application of a validated FEA model of a lateral truss inter-body spine fixation device for worst case identification and design evaluation/assessment; the computational analysis aimed to show that the lateral cage is not a new worst case compared to a previously FDA cleared truss device, thus not requiring additional mechanical testing for 510k submission. Computational modeling was used as an efficient tool to justify the mechanical performance of the lateral device in the 510k submission, eliminating the need for experimental testing, 4WEB Medical saved time and money and successfully launched the product into the U.S. market.

Tina Zhao & Paul Schmidt, Edwards Lifesciences: Three examples of V&V of structural FEA of cardiovascular medical devices, covering low, medium, and high modeling risk categories.

TRACK 4 UNCERTAINTY QUANTIFICATION, SENSITIVITY ANALYSIS, AND PREDICTION

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

4TH FLOOR, GREAT LAKES A1 1:30PM - 3:35PM

Principled Use of Expert Judgment for Uncertainty Estimation

Oral Presentation. VVS2018-9384 **1:30PM - 1:55PM**

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

To avoid the sort of implicit assumption of ZERO uncertainty one can use (expert) judgment to fill in the information gap. This can be accomplished in a distinctly principled fashion and always works better with a basis in evidence. The key is the recognition that we base our uncertainty on a model (a model that is associated with error too). The models are fairly standard and need a certain minimum amount of information to be solvable, and we are always better off with too much information making it effectively over-determined. Here we look at several forms of models that lead to uncertainty estimation including discretization error, and statistical models applicable to epistemic or experimental uncertainty.

We recently had a method published that discusses how to include expert judgment in the determination of numerical error and uncertainty using models of this type. This model can be solved along with data using minimization techniques including the expert judgment as constraints on the solution for the unknowns. For both the over and the under-determined cases different minimizations one can get multiple solutions to the model and robust statistical techniques may be used to find the "best" answers. This means that one needs to resort to more than simple curve fitting, and least squares procedures; one needs to solve a nonlinear problem associated with minimizing the fitting error (i.e., residuals) with respect to other error representations.

A lot of this information is probably good to include as part of the analysis when you have enough information too. The right way to think about this information is as constraints on the solution. If the constraints are active they have been triggered by the analysis and help determine the solution. In this way the solution can be shown to be consistent with the views of the expertise. A key to this entire discussion is the need to resist the default uncertainty of ZERO as a principle. It would be best if real problem specific work were conducted to estimate uncertainties, the right calculations, right meshes and right experiments. If one doesn't have the time, money or willingness, the answer is to call upon experts to fill in the gap using justifiable assumptions and information while taking an appropriate penalty for the lack of effort. This would go a long way to improving the state of practice in computational science, modeling and simulation.

Surrogate Modeling Of Blade Mode Shape Spatial Variation Due To Geometric Uncertainties

Oral Presentation. VVS2018-9396 **1:55APM - 2:20PM**

Joseph Beck**,** Perceptive Engineering Analytics, LLC, Minneapolis, MN, United States, ***Jeff Brown***, US Air Force Research Laboratory, Wright Patterson AFB, OH, United States, ***Alex Kaszynski***, Universal Technology Corporation, Dayton, OH, United States

Mistuning due to manufacturing variations and uneven in-service wear of Integrally Bladed Rotors (IBRs) can result in rogue blade failures in the field. Predicting the response of mistuned IBRs requires a probabilistic approach due to the randomness of mistuning. To do this, reduced order models (ROMs) are desired that are capable of running in a fraction of time compared to full finite element models. ROMs often employ sub-structuring approaches that divide the IBR into components. Solving each component can still require significant computational resources for geometric mistuning since the mode shapes and natural frequencies are needed for each component. Therefore, creating surrogate models of component mode shapes and frequencies is desirable in ROM development. This effort focuses on the development of a surrogate model for predicting blade mode shapes for use in an IBR ROM. Surrogate modeling mode shapes is particularly challenging due to the high dimensionality of the output data. Each blade component can still contain thousands of degrees of freedom (DOFs). Furthermore, the inputs to the surrogate are point cloud data of as-manufactured blades that also contain thousands of DOFs. Latent variable models are an attractive choice out of hopes that a few latent variables not directly observed in the original data are capable of an input/output mapping. One such approach is Canonical Correlation Analysis (CCA). This method seeks to identify the linear relationship between N samples of two co-occurring multidimensional, random variables. However, obtaining reliable CCA estimates requires N to be 40-60 times larger than the dimensionality of the mode shape and point cloud data. Since this is infeasible, a Bayesian CCA approach is utilized that augments the small sample size with prior distributions in the model. This approach creates a shared latent variable space between the mode shape and point cloud data and two latent variable spaces specific to each data set. In addition to providing accurate mode shape predictions, the Bayesian formulation allows quantification of the uncertainty in the prediction at each location in the mode shape. Results are presented for two industrial IBR geometries.

Uncertainty Quantification and Digital Engineering Applications in Turbine Engine System Design and Life Cycle Management

Oral Presentation. VVS2018-9400 **2:20PM - 2:45PM**

Kevin OFlaherty, Mark Andrews*, SmartUQ, Madison, WI, United States*

Essentially every government and private engineering group in involved in the US Aerospace and Defense Industry has some form of ongoing digital engineering activity. The vision for full implementation of these digital engineering efforts is to connect research, development, production, operations, and sustainment to improve the efficiencies, effectiveness, and affordability of aerospace systems over the entire life cycle. This presentation discusses the basic capabilities required of a model-based digital engineering approach to successfully achieve this vision:

-An end-to-end system model – ability to transfer knowledge upstream and downstream and from program to program

-Application of reduced order response surfaces and probabilistic analyses to quantify uncertainty and risks in cost and performance at critical decision points

-Single, authoritative digital representation of the system over the life cycle – the authoritative digital surrogate "truth source"

This presentation illustrates both conceptual and practical applications of using Uncertainty Quantification (UQ) techniques to perform probabilistic analyses. The application of UQ techniques to the output from engineering analyses using model-based approaches is essential to providing critical decision-quality information at key decision points in an aerospace system's life cycle. Approaches will be presented for the continued collection and application of UQ knowledge over each stage of a generalized life cycle framework covering system design, manufacture, and sustainment. The use of this approach allows engineers to quantify and reduce uncertainties systematically and provides decision makers with probabilistic assessments of performance, risk, and costs which are essential to critical decisions. As an illustration, a series of probabilistic analyses performed as part of the initial design of a turbine blade will be used to demonstrate the utility of UQ in identifying program risks and improving design quality. The application of UQ concepts to life cycle management will be addressed, highlighting the benefits to decision makers of having actionable engineering information throughout a system's life cycle.

Sensitivity of Global Equation of State Validity to Calibrated Parameter Sets in the Simulation of Energetic Materials

Oral Presentation. VVS2018-9356 **2:45PM - 3:10PM**

Michael Crochet*, Air Force Research Laboratory/University of Dayton Research Institute, Valparaiso, FL, United States*

Engineering hydrodynamic computational codes are commonly used to simulate the behavior of energetic materials, where chemical reaction is initiated by a mechanical stimulus. The underlying continuum models require an algebraic relation among the material state properties, known as an equation of state (EOS). The Mie-Gruneisen EOS is used extensively in energetics modeling to characterize both the reactant and product materials. According to this description, the material mass-specific energy varies linearly with pressure for a fixed specific volume. These quantities are referenced to pressure and specific energy functions that correspond to isentropic expansion curves following a detonation event. The various EOS models employed in energetics modeling (e.g., Jones-Wilkins-Lee, Davis wide-ranging, etc.) therefore differ in the functional forms of the expansion isentropes and the manner in which these are calibrated to experiments.

In addition to the parameterization of the reference curves using experimental data, it is crucial that the square of the material sound speed c^2>0 throughout the relevant domain of phase space for both reactants and products. Otherwise, the calculation of complex sound speeds prevents the propagation of acoustic waves and causes computational codes to fail. However, this requirement is not explicitly considered during the calibration process, instead focusing on ensuring consistency among the respective pressures and densities of the reactants and products under highly compressive, or overdriven, loading conditions. As a result, the domain over which the square of the sound speed is positive is sensitive to the parametrization of both the reactants and products EOS and the uncertainties in these values.

In this work we present an analysis of the domains of validity for the explosive PBX-9502, showing results for two sets of calibrated parameters for the Davis wide-ranging EOS. Here, we define a strong condition for the positivity of c^2 by requiring the pressure and density to be non-negative, ensuring physically meaningful values. The results of the analysis indicate the existence of substantial invalid regions at high densities, consistent with overdriven detonation regimes. Such a result is somewhat expected since the functional forms of the expansion isentropes are extrapolated from experimental data in this domain. However, the size of the invalid region changes significantly with the set of calibrated parameters used. The size of this region can have important numerical stability implications if the path of the post-detonation expansion wave travels through invalid regions of phase space. This work suggests that the positivity of c^2 should be included as an additional constraint in EOS calibration to minimize the risk of invalid phase-space regimes.

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A Bayesian semi-parametric method for inferring physics models and associated uncertainty

Oral Presentation. VVS2018-9378 **3:10PM - 3:35PM**

Stephen A. Andrews*,* ***Andrew M. Fraser,*** *Los Alamos National Laboratory, Los Alamos, NM, United States*

We present a method for inferring functions to represent physics models which best predict the results of multiple independent experiments, as well as their associated uncertainty. As an example, we consider the equation of state for the products of detonation of high explosives. The relationship between pressure and specific volume along an isentrope is represented in a semi-parametric manner where the function is the product of a vector of coefficients and a large set of basic functions. We develop a Bayesian algorithm which determines the best set of coefficients given data from multiple experiments. Our Bayesian analysis also allows us to determine both the total uncertainty in the function given all experimental data as well as the regime in which the data from each experiment most tightly constrain the function.

TRACK 5 VALIDATION FOR FLUID DYNAMICS AND HEAT TRANSFER

5-1 VALIDATION FOR FLUID DYNAMICS AND HEAT TRANSFER
4TH FLOOR, GREAT LAKES A2 1:30PM - 3:35PM

Implementation of Multiphase Particle-in-Cell (MP-PIC) Methodology in MFiX

Oral Presentation. VVS2018-9336 **1:30PM - 1:55PM**

MaryAnn Clarke*,* ***Avinash Vaidheeswaran****, West Virginia University Research Corporation, Morgantown, WV, United States,* ***Jordan Musser,*** *National Energy Technology Laboratory, Morgantown, WV, United States,* ***William Rogers****, NETL, Morgantown, WV, United States*

There is considerable need for efficiency and accuracy when modeling industrial-scale multiphase flows. The Eulerian-only methodologies, where the solids-phase is represented as a secondary continuum, are known to be computationally efficient. However, using a continuum approximation to describe discrete entities can be problematic, leaving solution verification of Eulerian-only codes far from being fully addressed. On the other hand, the discrete element method (DEM) based on an Eulerian-Lagrangian mathematical approach is known for solution accuracy. However, DEM becomes computationally burdened at high particle counts. Consequently, for dense particle configurations, especially in the limit of close-packing, neither of these approaches are considered ideal. A more desirable alternative is the multiphase Particle-in-Cell (MP-PIC) methodology where particles are grouped into computational parcels. Intra-parcel interactions are managed with constitutive relations instead of detailed Newtonian mechanics thereby accelerating computation. Some solution fidelity is lost, but for this concession, considerable computational speed is gained. In this work, the implementation of MP-PIC in MFiX is discussed along with its validation to illustrate computational and predictive performance.

Quantitative Assessment of Pulsatile Flow through a Sudden Contraction Using Computational Fluid Dynamics and Particle Image Velocimetry

Oral Presentation. VVS2018-9391 **1:55PM - 2:20PM**

Stephen Gent, ***Aaron Propst*** *South Dakota State University, Brookings, SD, United States,* ***Tyler Remund***, ***Patrick Kelly***, *Sanford Health, Sioux Falls, SD, United States*

The objective of this study was to assess and compare the velocity profiles of an incompressible fluid traveling through a sudden contracting pipe in a transient, pulsatile flow. In this study, a closed-loop benchtop experiment was constructed with a clear, noncompliant acrylic with a proximal diameter of 46mm and a distal diameter of 20mm. A variable flow rate pump supplied transient waveform to provide a pulsatile flow through the test region. Particle Image Velocimetry (PIV) was used to measure the velocity profiles immediately proximal and distal to the contraction. A comparable CFD model was constructed with the same geometric features as the test section. The fluid properties in the CFD model were assigned to be the same as the test fluid, and the inlet boundary conditions of the test loop were set to replicate the flow rate of the pump. A sensitivity analysis was performed to determine the effects of each variable in affecting the velocity, including the uncertainties in flow rate, proximal and distal diameters, and fluid density and viscosity, to name a few. The velocity profiles of the experiment and the CFD models were compared at multiple locations proximal and distal to the contraction, for several time steps in the pulsatile flow. The results indicate agreement within five percent between the CFD and experimental results. The intention of this study is to validate the results of the CFD model with experimental data to demonstrate the modeling approach employed is suitable for an internal pulsatile flow. The overarching goal of this study is to be able to show the validity of the CFD modeling approach in the simulation of pulsatile flow in both native vessels and implantable cardiovascular devices.

Sensitivity Study of Foaming Behavior of Simulant Tank Waste during Vitrification Tests in a Laboratory-Scale Melter

Oral Presentation. VVS2018-9417 **2:20PM - 2:45PM**

Donna Guillen, ***Alexander Abboud***, *Idaho National Laboratory, Idaho Falls, ID, United States,* ***Richard Pokorny***, *UCT Prague, Prague, Czech Republic*

Laboratory experiments were performed in conjunction with computational fluid dynamic (CFD) simulations to provide insight into the fluid dynamic and heat transfer processes that affect melt rate of waste slurry during vitrification. Large, Joule-heated melters will be used to vitrify radioactive tank waste generated over nearly five decades of nuclear weapons production at the Hanford site into a stable borosilicate glass waste form for disposal. Tank waste is mixed with silica and other glass-forming and glass-modifying additives to form a slurry that is fed to a melter that operates at 1150°C. When the slurry comprised of tank waste (consisting of 40 to 60% water) and glass formers is poured into the melter from above, a cold cap (sometimes referred to as the batch blanket layer) forms, covering ~90-95% of the melt surface. A sensitivity study was performed using a small-scale, Inconel-lined melter to provide insight into the foaming behavior of the slurry during vitrification. Air is injected into the melter using a bubbler inserted from the top down to the base of the melter. Due to the high viscosity of the molten waste glass simulant, large bubbles form that rise and interact with the foam layer at the base of the cold cap. For simplicity, the cold cap is approximated as a rigid solid with a slip boundary condition and a volumetric gas source below the cold cap to simulate foaming. Using the DAKOTA toolkit, Latin hypercube sampling was performed to assess the sensitivity of the foam layer to glass viscosity and thermal conductivity, bubbling flow rate, and foaming rate. Quantities of interest are the horizontal and vertical velocity, temperature gradient beneath the cold cap, and thickness of the foam layer. The computational results are validated by comparison with X-ray tomography images and theoretical calculations based upon boundary layer theory.

A Validation Study for a Hypersonic Flow Model

Oral Presentation. VVS2018-9414 **2:45PM - 3:10PM**

Brian Carnes, ***Derek Dinzl***, ***Micah Howard***, ***Sarah Kieweg***, ***William Rider***, ***Tom Smith***, ***V. Gregory Weirs*** *Sandia National Laboratories, Albuquerque, NM, United States,* ***Jaideep Ray***, *Sandia National Laboratories, Livermore, CA, United States*

A new simulation code for hypersonic, reacting turbulent flow (SPARC) is being developed at Sandia National Laboratories. This presentation focuses on validation efforts for hypersonic reacting laminar flows over a double-cone configuration. This is work in progress and will be presented partly as a case study to highlight how plans are adjusted and objectives rescoped as new information and results are obtained.

Initial verification & validation plans were developed. The verification effort has seen only minor adjustments and is described in a companion talk. However, the evolution of the validation plan has been driven by the available experimental data - free stream conditions as a simulation boundary condition and surface pressure and heat transfer measurements as quantities of interest (QoIs). Validation evidence, through uncertainty characterization and propagation, sensitivity analysis, and validation metrics, is presented via the QoIs.

A naïve attempt to reproduce the measurements via simulation failed and the freestream boundary conditions that modeled the experiment were found to be open to question. The assumption that the solution data should agree with the experimental data, on the forward cone of a double-cone configuration upstream of any separated flow, provided the motivation to infer the freestream conditions from surface measurements via an inverse problem. A sensitivity analysis was undertaken to identify which of the freestream quantities could be estimated from the experimental measurements. Given the sparsity and uncertainty in the experimental data, a Bayesian inverse problem was formulated, and a three-dimensional joint probability density function (PDF) computed for the freestream density, velocity and temperature. Computations involved constructing a polynomial chaos expansion emulator for SPARC and performing Markov chain Monte Carlo sampling to realize the joint PDF. Posterior predictive tests showed a significant narrowing of prediction uncertainty post-calibration; further, the experimental measurements were fully bracketed by the posterior predictive ensemble.

Observations on how the context shapes the validation process and the conclusions that can be drawn from it will be presented.

Uncertainty quantification and sensitivity analysis for the environmental dispersion of contaminants

Oral Presentation. VVS2018-9422 **3:10PM - 3:35PM**

Abhinav Gairola, ***Hitesh Bindra***, *Kansas State University, Manhattan, KS, United States*

Accidental release of hazardous contaminants in the atmosphere, hydrosphere and lithosphere can have serious implications on the interacting biosphere. It is important to accurately account for the distribution of these contaminants. But owing to the multitude of modeling parameters and associated parametric variances it is not possible for a first principle deterministic model to capture the environmental dispersion of these pollutants without certain level of uncertainties. Due to tightly coupled non-linear physics, the uncertainties cannot be quantied using perturbation theory or adjoint based methods. Hence, there is an inherent need of stochastic models which can encompass both the epis-temic and aleatory uncertainties. The two types of uncertainties which effect the system behavior are epistemic and aleatory or ontological in nature, which are intertwined at the microscopic level [1], therefore it is rather imprecise to study the effect of two on the system behavior separately. Owing to its incorporation of randomness at the microscopic or particle level stochastic dierential equation is an attractive tool, which may provide interesting insights to the spatio-temporal movement of the species under consideration. The stochastic models so developed can serve in developing a more pragmatic approach towards validation and impact quantication.

The approach discussed in this talk can be applied to the homogeneous medium or in the other words in the media where there is no memory effect can creep in, and also to the heterogeneous media. In heterogeneous media, there are dangling ends and other attributes which create a sense of memory in the system, by resorting to a fractional Brownian motion approach (fBm) attributed to Mandelbrot & Van Ness. [2]

References

[1] Gowri Srinivasan, Daniel M Tartakovsky, Bruce A Robinson, and Alejandro B Aceves. Quantication of uncertainty in geochemical reactions. Water resources research, 43(12), 2007.

[2] Benoit B Mandelbrot and John W Van Ness. Fractional brownian motions, fractional noises and applications. SIAM review, 10(4):422{437, 1968.

TRACK 12 VERIFICATION METHODS

12-1 VERIFICATION METHODS
4TH FLOOR, GREAT LAKES A3 1:30PM - 3:35PM

Convergence Checks and Error Estimates for Finite Element Stresses at Stress Concentrations: Effects of Different Mesh Refinement Factors

Oral Presentation. VVS2018-9343 **1:30PM - 1:55PM**

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

Convergence checks and companion error estimates for verifying finite element stresses at stress concentrations are developed in [1] following suggestions from ASME's guide [2]. These checks employ mesh refinement that has element extents successively reduced by a constant refinement factor, lambda. To date, the readily implemented value of lambda = 2 has been used with the checks. With lambda = 2, the checks are shown to lead to accurate error estimation on a series of 2D test problems in [1], and we have reported their like effectiveness on 3D test problems at this conference.

For 2D problems, lambda = 2 results in a quadrupling of element numbers with mesh refinement. As of now, this has not prevented the attainment of a good level of accuracy for peak stresses in 2D problems, as well as recognition of this level with the error estimates of [1]. For 3D problems, lambda = 2 results in eightfold increases in element numbers. On occasion, this has prevented the attainment of a good level of accuracy. In such instances, one could employ submodeling to improve accuracy. Alternatively, one could lower lambda and thereby continue refinement somewhat, and so possibly achieve the level of accuracy desired. Here we report some results for this latter approach.

Specifically we report finite element results for peak stresses in nine 3D test problems. These problems have exact solutions for the peak stresses involved, and companion stress concentration factors span a range which is greater than that normally encountered in practice. Complete mesh sequences with lambda = 5/4 and lambda = 3/2 throughout are used in the finite element analysis. For lambda = 5/4, error estimates are erratic initially, but ultimately are in reasonable agreement with actual errors. For lambda = 3/2 error estimates track actual errors well throughout. Both lambda values enable additional meshes to be run with improved accuracy. Moreover, both permit the estimation of errors for these additional meshes to be sufficiently effective so that the improved accuracy is recognized.

References

1. 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. 0410031-8 (2016).

2. ASME, Guide for Verification and Validation in Computational Solid Mechanics, American Society of Mechanical Engineers, New York, Standard No. ASME V&V10 (2006).

Characterization of Solution Verification

Oral Presentation. VVS2018-9354 **1:55PM - 2:20PM**

***Aaron Krueger**, **Yassin Hassan** Texas A&M University, College Station, TX, United States, **Vincent Mousseau**, Sandia National Laboratories, Albuquerque, NM, United States*

The use of solution verification methods has rapidly increased within the past two decades. While these methods, such as GCI and Least Squared GCI, have matured and proven to be useful, the methods rely on solutions that are within the asymptotic range. The asymptotic range is defined as the range of discretization sizes that force the leading truncation error term to be dominant. While this definition might be perceived as straightforward, the practical implementation of determining the asymptotic range is not. This study shows some of the key variables that impact a simulation's ability to be within the asymptotic range. This first part of the study calculates the higher order terms individually using the modified equation analysis. This calculation is important when determining if the leading truncated terms are dominating the higher order terms. The second part of the study assesses different solution verification methods ability to estimate the discretization error outside the asymptotic range, around the start of the asymptotic range, and inside the asymptotic range.

Using Verney's Problem and ExactPack to Verify FLAG

Oral Presentation. VVS2018-9357 **2:20PM - 2:45PM**

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

Verney's problem [1] is description of the dynamics of a rigid, incompressible, perfectly-plastic spherical shell that is collapsing under an applied load. This problem tests the conversion of kinetic energy into plastic work as well as final shell dimension. The mathematical model has a closed form prediction for both those quantities. Verney's problem has been proposed as an extension to the tri-laboratory suite of verification problems [2]. The current work will report on implementing Verney's problem into the code ExactPack for calculating the exact solution as well as in an updated Verification Test Suite at Los Alamos National Laboratory. Comparisons will be presented between the analytical solution and the numerical solution produced by the hydrocode FLAG. In addition, comparisons will be made to experimental work for copper.

References:

[1]. Verney, in Behavior of Dense Media under High Dynamic Pressures, Symposium, H.D.P., IUTAM, Paris 1967, Gordon & Breach, New York, pp. 293-303 (1968).

[2]. Kamm et al. LA-14379, 2008.

EOSlib: Software Reference Implementation for Equations of State

Oral Presentation. VVS2018-9365 **2:45PM - 3:10PM**

***William Magrogan**, **Ralph Menikoff**, **Austin McCartney**, **C. Nathan Woods**, Los Alamos National Laboratory, Los Alamos, NM, United States*

EOSlib is a software library written at Los Alamos National Laboratory to serve as a reference implementation of various analytic equations of state (EOSs). Core utilities include querying basic thermodynamic quantities, such as pressure, temperature, entropy, etc., and the library also provides tools for computing loci at constant entropy and temperature. EOSlib includes a user-extensible database of parameters for many different thermodynamic models, as well as tools for combining these into mixtures. EOSlib can also be used for calculations on nonequilibrium systems containing internal degrees of freedom, such as a reacting mixture governed by a rate law. EOSlib has a long track record of use for thermodynamic calculations involving high explosives. The library is implemented in C++ with both Python and command-line interfaces. We will present the core features of EOSlib and demonstrate examples of how it can be used as part of a verification workflow.

Finite Element Method Solution Uncertainty, Asymptotic Solution, and a New Approach to Accuracy Assessment (*)

Technical Publication. VVS2018-9320 **3:10PM - 3:35PM**

***Jeffrey Fong**, National Institute of Standards & Technology, Montgomery Village, MD, United States, **Pedro V. Marcal**, MPACT, Corp., Oak Park, CA, United States, **Robert Rainsberger**, XYZ Scientific Applications, Pleasant Hill, CA, United States, **Li Ma**, Theiss Research, La Jolla, CA, United States, **N. Alan Heckert**, **James J. Filliben** National Institute of Standards & Technology, Gaithersburg, MD, United States*

Errors and uncertainties in finite element method (FEM) computing can come from the following eight sources, the first four being FEM-method-specific, and the second four, model-specific: (1) Computing platform such as ABAQUS, ANSYS, COMSOL, LS-DYNA, etc.; (2) choice of element types in designing a mesh; (3) choice of mean element density or degrees of freedom (d.o.f.) in the same mesh design; (4) choice of a percent relative error (PRE) or the Rate of PRE per d.o.f. on a log-log plot to assure solution convergence; (5) uncertainty in geometric parameters of the model; (6) uncertainty in physical and material property parameters of the model; (7) uncertainty in loading parameters of the model, and (8) uncertainty in the choice of the model. By considering every FEM solution as the result of a numerical experiment for a fixed model, a purely mathematical problem, i.e., solution verification, can be addressed by first quantifying the errors and uncertainties due to the first four of the eight sources listed above, and then developing numerical algorithms and easy-to-use metrics to assess the solution accuracy of all candidate solutions. In this paper, we present a new approach to FEM verification by applying three mathematical methods and formulating three metrics for solution accuracy assessment. The three methods are: (1) A 4-parameter logistic function to find an asymptotic solution of FEM simulations; (2) the nonlinear least squares method in combination with the logistic function to find an estimate of the 95 % confidence bounds of the asymptotic solution; and (3) the definition of the Jacobian of a single finite element in order to compute the Jacobians of all elements in a FEM mesh. Using those three methods, we develop numerical tools to estimate (a) the uncertainty of a FEM solution at one billion d.o.f., (b) the gain in the rate of PRE per d.o.f. as the asymptotic solution approaches very large d.o.f.'s, and (c) the estimated mean of the Jacobian distribution (mJ) of a given mesh design. Those three quantities are shown to be useful metrics to assess the accuracy of candidate solutions in order to arrive at a so-called "best" estimate with uncertainty quantification. Our results include calibration of those three metrics using problems of known analytical solutions and the application of the metrics to sample problems, of which no theoretical solution is known to exist.

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TRACK 1 CHALLENGE PROBLEM WORKSHOPS AND PANEL SESSIONS

1-2 V&V BENCHMARK PROBLEM – TWIN JET COMPUTATIONAL FLUID DYNAMICS (CFD) NUMERIC MODEL VALIDATION
4TH FLOOR, GREAT LAKES A1 — 4:00PM - 6:05PM

Ubiquitous 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.

Computational Studies of Turbulent Flow Interaction Between Twin Rectangular Jets with OpenFOAM

Oral Presentation. VVS2018-9351

Han Li, Yassin Hassan, N.K. Anand*, Texas A&M University, 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 that 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 the past validation and verification studies, the steady state Reynolds Averaged Navier-Stokes Equations (RANS) simulations were performed and investigated boundary condition sensitivities with the realizable k-epilson model. The results showed the importance of boundary conditions, not only velocity profile but also turbulent quantities such as k and epilson profile that could affect merging point. In this study, an open source CFD library, OpenFOAM was utilized to perform the numerical simulation with a Partially-Averaged Navier Stoke Equations model and a Large Eddy Simulation (LES) model.

Partially-Averaged Navier Stoke Equation (PANS) models were considered as a hybrid model. In present study, with time varying boundary conditions mapped from PIV measurement, k-epilson PANS model were used to perform transient simulations and compared to Unsteady Reynolds Averaged Navier-Stokes Equations (URANS) model. As a result, the PANS results showed a good agreement in terms of the merging point (4.3%). Power spectrum density (PSD) analysis was performed based on the velocity at four sample locations to compare resolved frequencies between the PANS and the URANS models. It was observed that PANS model presented better capabilities in resolving higher turbulence flow frequencies compared with the URANS, based on the PSD analysis.

Large Eddy Simulation (LES) technique was also used on a mesh with 32 Million cells. A fluctuating boundary condition was used. LES simulation showed a good agreement with PIV in merging point. Proper Orthogonal Decomposition (POD) analysis was applied on a sample plane. POD analysis visualized the interaction between two jets and the multi-scale vortical structures. By comparing with the POD analysis from PIV experiment, the POD from LES showed similar structures and spectral frequencies.

TRACK 9 VALIDATION METHODS FOR SOLID MECHANICS AND STRUCTURES

9-1 VALIDATION METHODS FOR SOLID MECHANICS AND STRUCTURES
4TH FLOOR, GREAT LAKES A2 4:00PM - 6:05PM

Modeling and Validating Residual Stresses in Thick-Walled Cylinders

Oral Presentation. VVS2018-9309 **4:00PM - 4:25PM**

Zhong Hu, *South Dakota State University, Brookings, SD, United States*

An ever-increasing industrial demand for pressurized thick-walled cylindrical components drives research and practice to increase their strength-weight ratio, extend their fatigue life, or to increase their pressure-carrying capacity. This can be achieved through an energy-efficient and safe swage autofrettage process by generating a favorable compressive residual hoop stress field in the inner layer of the cylinder prior to use. In this work, the swage autofrettage processes of thick-walled cylinders were numerically investigated based on finite element analysis. An elastic nonlinear strain hardening plastic material model with the Bauschinger effect was adopted. The residual stresses in swage autofrettaged thick-walled cylinders were predicted. The results from computer modeling were compared with the experimental results from Sachs boring technique, a technique for the measurement of axisymmetric residual stresses from the analysis of strain relaxations during the incremental removal of layers of material from an axisymmetric component. Furthermore, in order to comparing the modeling results with the measurements from the neutron diffraction method (a high resolution nondestructive measurements of atomic structure of a material) taken in the disks cutting from the cylinders, the ring-cutting procedures for preparing neutron diffraction testing were virtually realized in the modeling, and the residual stresses and strains were rearranged during the ring-cutting procedure. The modeling results were compared with the neutron diffraction measurements. Finally, the modeling method was validated.

Stress Error Affected Zone of Finite Element Results by Wavelet Multiscale Analysis

Oral Presentation. VVS2018-9312 **4:25PM - 4:50PM**

Walter Ponge-Ferreira, *Escola Politecnica Da Universidade De Sao Paulo, São Paulo, São Paulo, Brazil*

Wavelet multiscale analysis is used to decompose the stress field of structures with stress concentrations and detect the error affected zone on the structure. First, the numerical solution of plane stress structures is decomposed by wavelet multiscale analysis to separate the near field stress concentration from the far field. The wavelet decomposition separates the stress into different scales, weights the stress in different stress paths, and locates the stress concentration position on the structure. This approach was applied to a plate with different stress paths and stress concentration at circular holes. Modeling error is fit to the wavelet multiscale representation of the stress field by least square method. Hence, the modeling error could be associated with different scales and locations, giving a spatial view of the error influenced zone. Causality analysis is used to identify possible causes for the modeling errors. This technique is used for model validation, improves the understanding and confidence of the analysis. Summary of presentation: motivation, wavelet multiscale analysis, wavelet decomposition of stressed structure, modeling error fitting, causality analysis, and conclusion.

The Dynamics of Fluid Conveying Hydraulic Hose

Oral Presentation. VVS2018-9352 **4:50PM - 5:15PM**

Jari Hyvarinen, *Epiroc Rock Drills AB, Orebro, Sweden*

Fatigue failure of hydraulic hose and its connections, caused by violent vibrations, is a large factor creating operational and maintenance cost for the end user of rock drill equipment. Hydraulic hoses are used as a parts of the energy feeding system in rock drills, for mining and civil construction operations, developed by Epiroc Rick Drill AB in Sweden. The work presented here show an approach taken to create an understanding of the dynamic behavior of a selected hydraulic hose. The performed investigation include an evaluation, of if it was sufficient to use bending and torsional rests to evaluate equivalent the stiffness properties of the steel wire reinforced rubber hose. The analysis approach use in the work presented include a numerical analysis using BEM (boundary element method) to describe the interface between the fluid and the structure to evaluating the dynamics of pressurized hose with conveying fluid. Experimental modal analysis was used to validate the numerical model. In addition the damping characteristics, of the pressurized hose with internal fluid flow at different flow rates, was investigated. The validation approach currently used is using small accelerometers together with LMS Test. Lab based experimental modal hammering and evaluation. Pre-tension and pressure induced tension is monitored with an in-house developed strain gauge based load cell. High speed camera and point laser measurements have also been utilized as backup. The analysis and experiments show that a complex coupling, of pure structural bending modes, appear when the hose is subjected to internal flow. Some of the mode shapes show a circular motion of the hose cross sections. As show in this presentation, these coupled modes seem to become increasingly sensitive to external or internal excitation with increasing flow rate.

Code Verification for Solid Mechanics Problems including Superelastic Nitinol

Oral Presentation. VVS2018-9374 **5:15PM - 5:40PM**

Kenneth Aycock, *US Food and Drug Administration, Silver Spring, MD, United States,* ***Nuno Rebelo***, *Dassault Systemes Simulia Corp, Santa Clara, CA, United States,* ***Brent Craven***, *US Food and Drug Administration, Silver Spring, MD, United States*

Although much progress has been made in advancing and standardizing verification, validation, and uncertainty quantification (VVUQ) practices in recent years, examples of rigorous code verification for solid mechanics problems in the literature are sparse - particularly for non-trivial, large-deformation analyses involving nonlinear materials.

We present code verification of the commercial finite element software ABAQUS for elastostatic solid mechanics problems relevant to medical devices. Specifically, method of manufactured solutions (MMS) verification is performed for infinitesimal and finite strain formulations with linear elastic and hyperelastic constitutive models. A separate method of exact solutions (MES) verification is also performed for the superelastic constitutive model in ABAQUS, which is commonly used to simulate nitinol medical devices. The MES is performed in lieu of MMS since the rate-based equations for superelasticity cannot be represented in closed-form.

To perform the MMS verification, a three-dimensional unit cube composed of C3D8I elements is considered. Analytical source terms are generated by substituting a prescribed, three-dimensional displacement field composed of trigonometric functions into the governing equations using a symbolic math package (SymPy/Python or Mathematica). The generated source terms are then implemented in ABAQUS simulations as point loads with appropriate nodal volume weighting, a grid refinement study is performed, and the results are post-processed to extract error norms and the observed orders of convergence.

The MES verification of the superelastic constitutive model is instead carried out on an affine deformation problem using a single C3D8I element. Because the underlying equations for the constitutive model are cast in rate-form and cannot be integrated analytically, numerical results are compared to surrogate analytical solutions for linear transformation behavior at points of theoretically exact equivalence: the initiation, midpoint, and endpoint of austenite-martensite phase transformation.

The linear and hyperelastic MMS results show excellent agreement between the observed and theoretical orders of convergence for both the small and large strain formulations. The MES results also show excellent agreement between analytical and numerical calculations, providing evidence of proper implementation of the superelastic constitutive model. Validation activities can be now performed with greater confidence that coding errors do not influence simulation predictions.

Acknowledgements:

This study was funded by the U.S. FDA Center for Devices and Radiological Health (CDRH) Critical Path program. The mention of commercial products, their sources, or their use in connection with material reported herein is not to be construed as either an actual or implied endorsement of such products by the Department of Health and Human Services.

Validation of Methodology to Evaluate Risk Reduction in Tank Car Derailments

Technical Publication. VVS2018-9331 **5:40PM - 6:05PM**

***Francisco Gonzalez, III**, USDOT, Federal Railroad Administration, Washington, DC, United States, **Anand Prabhakaran**, **Graydon Booth**, **Florentina M. Gantoi**, **Arkaprabha Ghosh**, Sharma & Associates, Inc., Countryside, IL, United States*

Critical derailment incidents associated with crude oil and ethanol transport have led to a renewed focus on improving the performance of tank cars against the potential for puncture under derailment conditions. Proposed strategies for improving accident performance have included design changes to tank cars, as well as, operational considerations such as reduced speeds.

In prior publications, the authors have described the development of a novel methodology for quantifying and characterizing the reductions in risk that result from changes to tank car designs or the tank car operating environment. The methodology considers key elements that are relevant to tank car derailment performance, including variations in derailment scenarios, chaotic derailment dynamics, nominal distributions of impact loads and impactor sizes, operating speed differences, and variations in tank car designs, and combines these elements into a consistent framework to estimate the relative merit of proposed mitigation strategies.

The modeling approach involves detailed computer simulations of derailment events, for which typical validation techniques are difficult to apply. Freight train derailments are uncontrolled chain events, which are prohibitively expensive to stage and instrument; and their chaotic nature makes the unique outcome of each event extremely sensitive to its particular set of initial and bounding conditions. Furthermore, the purpose of the modeling was to estimate the global risk reduction expected in the U.S. from tank car derailments, not to predict the outcome of a specific derailment event.

These challenges call into question which validation techniques are most appropriate, considering both the modeling intent as well the availability and fidelity of the data sets available for validation. This paper provides an overview of the verification and validation efforts that have been used to enhance confidence in this methodology.

TRACK 13 VERIFICATION AND VALIDATION FOR BIOMEDICAL ENGINEERING

13-1 VERIFICATION AND VALIDATION FOR BIOMEDICAL ENGINEERING

4TH FLOOR, GREAT LAKES A3 4:00PM - 6:05PM

A threshold-based approach for determining acceptance criteria during computational model validation

Oral Presentation. VVS2018-9416 **4:00PM - 4:25PM**

***Prasanna Hariharan**, **Richard Malinauskas**, **Tina Morrison**, **Matthew Myers** Food and Drug Administration, Silver Spring, MD, United States **Gavin D'Souza**, University of Cincinnati, Silver Spring, MD, United States, **Marc Horner**, ANSYS, Inc., Evanston, IL*

A credible computational fluid dynamics (CFD) model has the potential to provide a meaningful evaluation of medical device safety. One major challenge in establishing model credibility is to determine the required degree of similarity between the model and experimental results. This study proposes a threshold-based approach for establishing the model acceptability. The approach provides a well-defined acceptance criteria, which is a function of the proximity of the simulation and experimental results to the safety threshold. The acceptance criteria developed following the threshold approach is not only a function of the Error, E (defined as the difference between experiments and simulations), but also considers the risk to patient safety because of E. The method is applicable for scenarios in which a safety threshold can be clearly defined (e.g., the viscous shear-stress threshold for hemolysis in blood contacting devices).

The applicability of this new validation approach was tested using the example of blood flow through the FDA-developed nozzle geometry. The context of use (COU) was to evaluate if the instantaneous viscous shear stresses present during flow though the nozzle at Reynolds numbers (Re) of 3500 and 6500 were below a commonly accepted threshold for hemolysis. The CFD results ("S") for velocity and viscous shear stress were compared with inter-laboratory experimental measurements ("D"). The uncertainties in the CFD and experimental results due to input parameter uncertainties were quantified following the ASME V&V 20 standard.

The credibility of the CFD models for both Re=3500 and 6500 conditions could not be sufficiently established by performing a direct comparison between the CFD and experimental results using a statistical Student's t-test. However, following the threshold-based approach, a Student's t-test comparing |S-D| and |Threshold-S| for Re=3500 showed that the model could be considered sufficiently credible for the COU. For Re=6500, at certain geometrical locations of the flow domain where the shear stress values are near the hemolysis threshold, the CFD model could not be considered sufficiently credible for the COU. Analysis showed that the credibility of the model could be sufficiently established either by reducing the uncertainties in the experiments, the simulations, and the threshold defined value, or by increasing the sample size for the experiments and simulations. Our threshold approach can be applied to all types of computational models and provides an objective method for determining model credibility in the evaluation of medical devices.

Validation and Verification on Interventional Implantable Devices

Oral Presentation. VVS2018-9342 **4:25PM - 4:50PM**

Hui Zuo, ***Chenxi Wang*** *Suzhou Medical Implant Mechanics CO. Ltd., Suzhou, Jiangsu, China,* ***Xiaoyan Gong***, *Suzhou InnoMed Medical Device Co. Ltd., Suzhou, Jiangsu, China*

Two kinds of interventional products, a stent and an occlude are used as examples for verification and validation of non-linear finite element analysis. Mesh density, element type, computational algorithms, implementations of non-linear constitutive laws, and experiment noises are considered during the study to gain confidence on the fatigue safety predictions of the devices.

Quantification of Uncertainties in System Properties for Prediction of Core Temperature During Unplanned Perioperative Hypothermia Using a Three-Dimensional Whole Body Model

Oral Presentation. VVS2018-9386 **4:50PM - 5:15PM**

Anup Paul, ***Mark Burchnall***, ***Robert States***, ***Harbinder Pordal***, ***Clinton Haynes*** *Stress Engineering Services, Inc., Mason, OH, United States*

Introduction: Unplanned hypothermia, i.e. core temperature less than 36 degrees C, in surgical patients receiving anesthesia can cause complications [1]. The physiological thermoregulation response of the body is altered in an anesthetized patient, thus exacerbating heat loss from the extremities. Hypothermia related perioperative complications include wound infections, altered drug metabolism, impaired blood clotting and prolonged recovery time. Maintaining normothermia using active warming devices, especially during the intraoperative period, can help prevent complications and also reduce hospitalization costs. Current warming methods include blankets, fluid warmers, warmed IV fluids and forced-air warming blankets. Although forced-air warming blankets have demonstrated superior clinical performance, its effectiveness may be limited by the size and location of the surgical site. Therefore, it is necessary to continue developing and evaluating devices with improved efficiency in maintaining normal perioperative body temperature. Effective using of credible computational modeling and simulations can enable faster and safer pathways to market while reducing the size of animal and human clinical trials [2]. A key factor in the risk-informed credibility assessment of computational models is the quantification of uncertainties in model outputs due to uncertainties in system properties (input parameters).

Methods: In this study we utilize a computational whole body model [3] to predict the drop in core temperature during the first 60 minutes of the surgical procedure. The model has two components: the Pennes bioheat equation to simulate tissue temperature and an energy balance equation to determine the change in blood temperature. The uncertainty in the predicted core temperature due to variabilities in the tissue parameters, metabolic rate and boundary conditions is calculated using the sensitivity coefficient (local) method for parameter sensitivity propagation. The sensitivity coefficients will be obtained using a second-order finite difference approximation.

Results: The expected results from this study will identify and quantify the uncertainties in the input parameters and the uncertainties propagated to the predicted core temperature drop. The importance factors will also be computed to assess the relative importance of the input parameters on the model uncertainty.

Conclusion: The assessment of model uncertainties is a key component of the verification and validation evidence to support the use of the computational model for medical device development.

References:

1. Wagner DV. Unplanned perioperative hypothermia. AORN J. 2006 Feb

2. FDA.gov. CDRH Regulatory Science and Research. Regulatory Science Priorities. Published 2016.

3. Paul et al. 2015, Predicting Temperature Changes During Cold Water

Immersion and Exercise Scenarios: Application of a Tissue Blood Interactive Whole-Body Model, Numerical. Heat Transfer, Part A, 68(6), pp. 598-618.

A Framework for Generating Mitral Valve Finite Element Models that Match Diseased States

Oral Presentation. VVS2018-9393 **5:15PM - 5:40PM**

***Reza Salari, Sella Yunjie Wang**, **Mahesh Kailasam**, **Yev Kaufman**, Thornton Tomasetti, Cupertino, CA, United States*

Finite element-based evaluation and prediction of the behavior of implanted medical devices by including interactions of the devices with human body organs has emerged as an essential technique in the march towards patient-specific treatments. One of the main challenges in this progress is the ability to create finite element models of organs or parts that match various diseased states, with patient-specific finite element models being the ultimate goal. One approach to creating diseased-state finite element models of an organ or body part is to use imaging data sets with segmentation-based methods to generate corresponding 3D models and meshes. Despite significant improvements in segmentation software, this process can still be time consuming and very importantly may not capture all the details that would be required in a finite element model for the simulated behavior to match the diseased organ or body part behavior, especially when there is motion involved, such as with cardiac motion. An alternative approach, one that can even be used in conjunction with the segmentation approach, is to modify a pre-existing, reasonably representative, finite element model in a manner that would allow the simulated behavior of an organ or body part to match targeted behavior. In this study, we demonstrate that a shape matching, inverse finite element framework can be applied to develop simulations of the mitral valve (MV) that are a closer match to observed behavior, such as diseased states and eventually patient-specific behaviors. We start with the Living Heart Human Model (LHHM) as the baseline finite element model fairly accurately representing a healthy heart, from which we create a submodel of the mitral region, consisting of the mitral annulus, leaflets, and chordae, for efficiency reasons. In the next step, the differences observed between the mitral valve leaflet positions in this baseline submodel and defined targeted leaflet positions is minimized through an optimization process which adjusts chordae lengths as design parameters, although additional parameters such as the material properties of the chordae or locations of attachment points could also be considered. This automated and scalable (additional parameters can be included as needed) framework offers an efficient solution for generating finite element models that more closely match targeted disease states and observed patient-specific behavior.

Interlaboratory Simulations of Compression-Bending Testing of Spinal Rods

Oral Presentation. VVS2018-9418 **5:40PM - 6:05PM**

***Marc Horner**, ANSYS, Inc., Evanston, IL, United States, **Srinidhi Nagaraja**, G.Rau Inc., Santa Clara, CA, United States, **Andrew Baumann**, U.S. Food and Drug Administration, Silver Spring, MD, United States, **Galyna Loughran**, Excelen: Center for Bone & Joint Research and Education, Minneapolis, MN, United States, **Kumar Kartikeya**, ANSYS, Inc., Pune, India, **Jason Inzana**, Zimmer Biomet, Broomfield, CO, United States, **Anup Gandhi**, Zimmer Biomet, Westminster, CO, United States*

ASTM standardized test methods are used extensively to evaluate the mechanical performance of spinal devices, particularly to support their regulatory clearance. By contrast, finite element analysis (FEA) is primarily performed during spinal device development and is infrequently used as part of the regulatory submission. In this study, experimental results for ASTM F1717 (Standard Test Methods for Spinal Implant Constructs in a Vertebrectomy Model) were compared to interlaboratory computational simulations of the F1717 test method. In order to develop best practices for computational modeling of this test method, we investigated the influence of several modeling input parameters on the predicted compression-bending response.

ASTM F1717 testing was performed on generic pedicle screw constructs consisting of monoaxial pedicle screws (Ti-6Al-4V), set screws (Ti-6Al-4V), spinal rods (Ti-6Al-4V), and test blocks (UHMWPE) in compression-bending. An interlaboratory FEA study replicating the experimental testing was performed by FDA, ANSYS, and Excelen. Each lab was blinded to experimental results. Material properties were obtained from the literature for the UHMWPE components. Titanium spinal rods were modeled as an isotropic material using either a multilinear isotropic hardening approach (MISO model) or by fitting the experimental test data to a bilinear elasto-plastic model, the parameters of which were determined from tensile testing per ASTM E8 of dogbone specimens. Initial simulations assumed perfectly-bonded contact at all interfaces in the spinal construct. After comparing initial simulations experimental results, various model parameters (e.g., element type, discretization, interconnection between construct components) were altered to understand the influence of these parameters on the mechanical behavior of the construct.

There was less than 10% difference in the ASTM F1717 force-displacement curves submitted by the three modeling groups. Compared to experimental force-displacement curves, all simulations exhibited slightly stiffer behavior (less than 15% difference) throughout.In conclusion, it is critical to establish a standardized framework for computational stress analysis to increase the use of modeling in orthopedic regulatory submissions. This study is working towards that goal by outlining the influence of various model assumptions and parameters on the mechanical response of pedicle screw-rod constructs, along with their associated uncertainties. This information will further elucidate best practices for conducting FEA for this product area.

Technical Program
Friday, May 18, 2018

TRACK 1 CHALLENGE PROBLEM WORKSHOPS AND PANEL SESSIONS

1-1 UNSTEADY FLOW WORKSHOP
4TH FLOOR, GREAT LAKES A1 8:00AM - 10:05AM

Session Organizer: **Luis Eca**, IST, Libon, Portugal

Introduction to the Workshop on Iterative Error in Unsteady Flow Simulations

Oral Presentation. VVS2018-9310

***Luis Eca**, IST, Lisbon, Portugal, **Guilherme Vaz**, MARIN, Wageningen, Netherlands, **Martin Hoekstra**, Maritime Research Intitute Netherlands, Wageningen, Netherlands*

Presentation of the objectives of the Workshop and of the submissions (codes, discretization techniques, solution procedures). Overview of the submitted data.

Participation in the Workshop on Iterative Errors in Unsteady Flow Simulations

Oral Presentation. VVS2018-9361

***Sophie Porter,** Rolls-Royce PLC, Derby, United Kingdom*

Two-dimensional laminar flow around a circular cylinder is modelled using the general purpose CFD software suite ANSYS CFX version 14.5. The flow domain is resolved using an implicit fully-coupled solver with the specified blend factor? advection scheme with a blend factor of 1. A second order Euler transient scheme is used and each time step is resolved iteratively until convergence criteria are met, with up to 3 iterations per time step allowed.

Solutions are calculated for four grids and four different time steps. Different root-mean-square residual targets and imbalance criteria are used to investigate the impact of these targets on the grid convergence index and predicted lift, draft, separation angle and vortex shedding frequency.

Sources of user error are discussed and it is shown how these can lead to significant differences in the predicted drag and lift coefficients.

Workshop on Iterative errors in Unsteady Flow Simulations: STAR-CCM+ results

Oral Presentation. VVS2018-9368

***Laura Savoldi**, **Andrea Bertinetti**, **Roberto Zanino**, **Andrea Zappatore** Dipartimento Energia, Politecnico Di Torino, Torino, (TO), Italy, **Rosa Difonzo**, NEMO group, Dipartimento Energia, Politecnico di Torino, Torino, Italy*

The simulation of a laminar two-dimensional external flow around a cylinder for an incompressible fluid with Reynolds number Re = 100 is the test case used in the 2nd Workshop on iterative Error in Unsteady Flow Simulation. The Nuclear Engineering Modelling (NEMO) group of the Politecnico di Torino participates to the Workshop using the commercial software STAR-CCM+ v.12.06.010-R8. Different combinations of pre-set grids and time steps have been considered in the simulations, using for each combination four different numbers of inner iteration (i.e. 10, 50, 100 and 200) per time step. Following the requests of the workshop organizers, the drag, the lift and the pressure coefficients are monitored during the transient, up to the point when the solution reaches the periodicity (after ~ 200 s from the initial condition of quiet fluid). The angle of separation of the flow from the cylinder is also evaluated monitoring the surface point where the shear stress becomes zero. The results of the simulations will be made available in due time before the workshop, to contribute to the comparison between different participants.

Participation in the Workshop on Iterative Errors in Unsteady Flow Simulations

Oral Presentation. VVS2018-9408

***Jernej Drofelnik**, **Benjamin Moss**, **Andrea Da Ronch**, University of Southampton, Southampton, Hampshire, United Kingdom*

This work concerns the laminar two-dimensional incompressible flow around a circular cylinder, setting the Reynolds number, based on the incoming velocity and cylinder diameter, to 100. The flow solver employed in this study is the DLR Tau, a finite volume based CFD flow solver used by a number of aerospace industries across Europe. Our numerical setup includes an edge based vertex centered scheme, where the convective terms are computed using second order upwind scheme, and the viscous terms are computed with second order central scheme. Numerical integration is performed with explicit four stage Runge Kutta scheme, and the dual time stepping approach of Jameson is employed for the time accurate computations. We are using four provided multi-block structured grids, and the prescribed physical time steps for each of the four grids. Final results will include the time histories for at least four cycles, which are no longer affected by the initial condition. This will allow the comparison of our results with other flow solvers.

Foam-Extend Computations for the 2nd Workshop on Iterative Errors in Unsteady Flow Simulations Using Time and Under-relaxation Consistent Solution Algorithms

Oral Presentation. VVS2018-9420

***Vuko Vukcevic**, **Zeljko Tukovic**, **Hrvoje Jasak**, Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Zagreb, Croatia (Hrvatska)*

The group from Faculty of Mechanical Engineering and Naval Architecture (University of Zagreb, Croatia) developing and maintaining foam-extend, a community driven fork of the OpenFOAM software will perform unsteady computations for the 2nd Workshop on Iterative Errors in Unsteady Flow Simulations. The simulations will be performed for the 2D laminar flow past a cylinder according to the guidelines. Recently developed time and under-relaxation consistent segregated solution algorithms will be used. The results will be submitted by May 1st, 2018.

Discussion of results of the Workshop on Iterative Errors in Unsteady Flow Simulations

Oral Presentation. VVS2018-9311

Luis Eca, *IST, Lisbon, Portugal,* ***Guilherme Vaz***, *MARIN, Wageningen, Netherlands,* ***Martin Hoekstra***, *Maritime Research Intitute Netherlands, Wageningen, Netherlands*

Discussion of results submitted to the Workshop on Iterative Errors in Unsteady Flow Simulations.

TRACK 17 VERIFICATION AND VALIDATION FOR ADVANCED MANUFACTURING

17-1 VERIFICATION AND VALIDATION FOR ADVANCED MANUFACTURING
4TH FLOOR, GREAT LAKES A2 8:00AM - 10:05AM

VVUQ Applications in Process Technologies for Advanced Manufacturing

Oral Presentation. VVS2018-9421 **8:00AM - 8:25AM**

Huijuan Dai, *GE Global Research, Niskayuna, NY, United States,* ***Gaurav Ameta***, *Dakota Consulting, Silver Spring, MD, United States,* ***Adegboyega Makinde***, *General Electric Global Research Center, Austin, TX, United States,* ***Sudarsan Rachuri***, ***Mahesh Mani***, *Department of Energy, Washington, DC, United States,* ***Nathan Andrews***, *Southwest Research Institute, San Antonio, TX, United States,* ***Mark Benedict***, *AFRL Mantech, Wpafb, OH, United States,* ***Sankaran Mahadevan***, *Prof., Nashville, TN, United States,* ***Sagar Kamarthi***, *Northeastern University, Boston, MA, United States*

Modeling and simulation play increasingly important roles in advanced manufacturing. Both physics-based and data driven models are widely used to optimize process parameters in order to minimize manufacturing defects, reduce the number of physical trials and consequently reduce cost. However, these models are mainly focused on specific problems for specific applications. Advanced manufacturing, as a multi-step, multi-scale and multi-physics process, has a lack of standards/guidelines such that the outcome of a simulation model highly depends on the modeler?s experience and expertise. The current working group is established in the ASME V&V50 subcommittee to help develop and establish best practice for verification, validation, and uncertainty quantification (VVUQ) in computational modeling for advanced manufacturing process. To help develop VVUQ guidelines for advanced manufacturing process simulation, the working group will start with a simple case for additive manufacturing. The main input parameters of the case are laser power and scan speed. The primary output of the models is the melt pool width, given different combinations of power and scan speed. Simulation model and non-linear regression models will be trained on measured training data and then validated using test data. The process of verification and validation of these models will be presented and then generalized in order to aid in developing the VVUQ guidelines.

Verification and Validation Interactions with the Model Life Cycle

Oral Presentation. VVS2018-9423 **8:25AM - 8:50AM**

Joe Hightower, *The Boeing Company, Seattle, WA, United States,* ***Guodong Shao***, *NIST, Gaithersburg, MD, United States,* ***Eric Sawyer***, *Lawrence Livermore National Laboratory, Livermore, CA, United States,* ***Rumi Ghosh***, *Robert Bosch, LLC, Palo Alto, CA, United States,* ***Aaron Bernreuter***, *Honeywell, Morris Plains, NJ, United States,* ***William Schindel***, *ICTT System Sciences, Terre Haute, IN, United States,* ***Mark Benedict***, *AFRL Mantech, Wpafb, OH, United States,* ***Laura Pullum***, *Oak Ridge National Laboratory, Oak Ridge, TN, United States,* ***Mahmood Tabaddor***, *UL LLC, Rochester, MI, 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. Verification and Validation (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 exist 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. 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 and use. This presentation updates the 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 in advanced manufacturing; and (4) generalize the VV-UQ procedures for different model lifecycle stages. We have developed a model-based requirement generation framework based on the VVUQ pattern and finished activity modeling for model development and deployment phases.

Verification-Validation And Uncertainty Quantification Methods For Data-Driven Models In Advanced Manufacturing

Oral Presentation. VVS2018-9424 **8:50AM - 9:15AM**

Ronay Ak*, *Yung-Tsun Lee*, *Guodong Shao *National Institute of Standards and Technology, Gaithersburg, MD, United States,* ***Rumi Ghosh****, Robert Bosch, LLC, Palo Alto, CA, United States,* ***Heather Reed****, Thornton Tomasetti - Weidlinger Applied Science Practice, New York, NY, United States,* ***Laura Pullum****, Oak Ridge National Laboratory, Oak Ridge, TN, United States*

The Verification and Validation of Computational Modeling for Advanced Manufacturing, or V&V 50, is one of the subcommittees under the American Society of Mechanical Engineers (ASME) Verification and Validation standards committee. The charter of the V&V 50 is to provide procedures for verification, validation, and uncertainty quantification in computational models including predictive models and simulations for advanced manufacturing. The Verification, Validation, and-Uncertainty Quantification (VV-UQ) methods in data-driven and hybrid models working group, or VV-UQ WG, under the V&V 50, addresses the applications in advanced manufacturing with focus on VV-UQ methods in data-driven and hybrid models. The mission of the working group is to provide a framework and guidance to the VV-UQ issues/problems related to data-driven and hybrid models that manufacturing industry tackle. The manufacturing industry has become significantly data-intensive in recent years. Continuous improvements in sensor technologies and data acquisition systems allow the manufacturing industry to effectively and efficiently collect large and diverse volumes of data. Data analytics has demonstrated its 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 describe the VV-UQ WG's ongoing activities with the focus predominantly on the VV-UQ aspect of data-driven modeling. A data-driven model (DDM) in the manufacturing domain can be built using data analytics techniques to analyze the data generated by the manufacturing processes or system. Data analytics techniques include, but are not limited to, statistical, data mining, and machine learning descriptive and predictive models. The objective of a DDM is to find an empirical map between the input and output with or without explicit knowledge of the physical behavior of the process or system. For model credibility, the DDM must be verified and validated, and the uncertainties associated with the model should be quantified and their effects propagated to the outcome quantities of interest. In this presentation, we will discuss the technical approach and up-to-date progress of the VV-UQ WG. The working group aims to define the general guideline for VV-UQ by performing the following tasks: (i) investigate existing VV-UQ standards/procedures and data-mining process models like ASME V&V 10 and Cross-Industry Standard Process for Data Mining (CRISP-DM), and adapt them to advanced manufacturing VV-UQ where applicable; (ii) study different use cases of DDMs defined by industry and academia; (iii) uncover the commonalities in the patterns of VV-UQ for advanced manufacturing and generalize issues/problems in advanced manufacturing; and (iv) provide generic recommendations/resolutions to each type of issue/problem. An activity flowchart for DDM based on supervised learning has been developed and its associated documentation, including an example, is being created. The flowchart and document provide a clear VV-UQ process for DDM and provide the foundation for a general guideline, which will enable practitioners of VV-UQ to better assess and enhance the credibility of their data-driven and hybrid models built to solve advanced manufacturing problems.

ACKNOWLEDGMENTS

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Terminology, Concepts, Relationships and Taxonomy for VVUQ in Manufacturing

Oral Presentation. VVS2018-9425 **9:15AM - 9:40AM**

Sankaran Mahadevan*, Prof., Nashville, TN, United States,* ***Yung-Tsun 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 or 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 quantification, 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.

Computational and Experimental Efforts to Quantify Uncertainty of Turbomachinery Components

Oral Presentation. VVS2018-9389 **9:40AM - 10:05AM**

Jeff Brown, *US Air Force Research Laboratory, Wright Patterson AFB, OH, United States*

This presentation reviews recent activities to understand the variation in manufactured turbomachinery components, their structural and aerodynamic models, and the experimental data used for validation. Results from structured light geometry measurements for high pressure turbine and compressor airfoils are reviewed and assessed with principal component analysis. The modes from this analysis are used as variables to emulate the structural frequency, mode shape, steady aerodynamic efficiency, and unsteady surface pressure. These results are compared to structural bench testing and rotating rig aerodynamic testing. A new tetrahedral-element based approach for constructing the as-manufactured components is discussed and a compared with the results from more conventional hexahedral models. Efforts are also shown to improve structural emulator accuracy through inclusion of gradient information gathered from a computationally efficient eigensensitivity solution. New strategies to emulate spatial field responses such as the airfoil structural mode shapes are discussed. To conclude, future directions and challenges are discussed.

TRACK 1 CHALLENGE PROBLEM WORKSHOPS AND PANEL SESSIONS

1-3 INDUSTRY CHALLENGES IN UNCERTAINTY QUANTIFICATION: BRIDGING THE GAP BETWEEN SIMULATION AND TEST
4TH FLOOR, GREAT LAKES A1 10:30AM - 12:35PM

Session Organizer: ***Mark Andrews***, *SmartUQ, Madison, WI, United States*
Session Co-Organizer: ***Peter Chien***, *SmartUQ, Madison, WI, United States*

By applying advanced statistical methods such as Uncertainty Quantification (UQ), simulation models have become a trustworthy source of information for decision analytics. Unfortunately, there are significant cultural and technical challenges which prevent organizations from utilizing UQ methods and techniques in their engineering practice. This tutorial will provide an overview of UQ concepts and methodology and discuss the strategies for addressing these challenges. One of the strategies is performing statistical calibration to understand how well numerical simulation represents reality. Using a case study for illustration, the tutorial will sequentially walk through the statistical calibration process used to quantify uncertainties for simulations and physical experiments. Attendees should leave the tutorial with an understanding of UQ concepts and techniques, how to apply statistical calibration to their combined simulation and testing environments, and the fundamental value that UQ brings. As a purely educational tutorial, SmartUQ software will only be used for illustration of the methods and examples presented.

TRACK 4 UNCERTAINTY QUANTIFICATION, SENSITIVITY ANALYSIS, AND PREDICTION

4-2 UNCERTAINTY QUANTIFICATION, SENSITIVITY ANALYSIS, AND PREDICTION: SESSION 2
4TH FLOOR, GREAT LAKES A2 10:30AM - 12:35PM

Optimal Information Acquisition Algorithms for Inferring the Order of Sensitivity Indices

Oral Presentation. VVS2018-9350 **10:30AM - 10:55AM**

Piyush Pandita, ***Ilias Bilionis***, *Purdue University, West Lafayette, IN, United States,* ***Jesper Kristensen***, *General Electric Co, Niskayuna, NY, United States*

Numerous engineering problems are characterized by objective functions, where the evaluation of the objective via experiment and/or simulation comes at the expense of vast resources. In some problems, running a simple instance of the objective can take days or weeks. The goal of these problems is to identify regions of design space which satisfy a set of criteria defined at the outset (which includes optimization cases). In many engineering applications, it is of key interest to understand which design variables drive changes in the objectives and to compute the relative order of importance. This question is answered via a combination of data-driven modeling and global sensitivity analysis where so-called sensitivity indices are computed. A relative comparison of the size of the indices indicates which variables are more important than others in driving the objective. Towards this, Bayesian global sensitivity analysis (BGSA) constructs a computationally cheap probabilistic surrogate of the expensive objective function(s) using Gaussian Process (GP) regression. The GP surrogate(s) provides approximate samples, requiring relatively few resources, of the underlying function from which the usual variance based sensitivity index is computed for each sample. The Bayesian sensitivity indices are obtained by averaging over all the above samples. In this work, we develop an optimal acquisition strategy for obtaining the most relevant regions of the design space if one mainly cares about obtaining accurate ranking of the sensitivity indices. We propose an algorithm that evaluates the merit of a hypothetical measurement towards the segregation of the individual sensitivity indices. This framework guides the designer towards evaluating the objective function to acquire information about the sensitivities sequentially. We verify and validate the proposed methodology by applying it on synthetic test problems with known solutions. We then demonstrate our approach on a real-world industry engineering problem of optimizing a compressor for oil applications. The problem is characterized by an expensive objective (lab tests; each taking 1-2 days to complete) and a high-dimensional input space with on the order of 30 input variables. This is an important problem since it provides an essential step towards enabling the customer to propose more competitive products in the market by more carefully analyzing and quantifying the compressor capabilities.

Experimental Data UQ and QMU for Stochastic Systems characterized through Sparse Unit Testing involving Variability and Uncertainties in Measurements, Loading, and System Properties

Oral Presentation. VVS2018-9373 **10:55AM - 11:20AM**

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

An extension to the Coleman & Steele [1] and ASME PTC-19.1 [2] experimental data uncertainty methodologies is illustrated for sparse replicate tests involving stochastically varying systems with small random variations in system properties (geometries, material properties, etc.). The tests also involve small load-control variations and measurement errors/uncertainties on experimental inputs and outputs. Some of the uncertainties are described by intervals and others by probability distributions. The methodology is demonstrated on the Data UQ portion of the Sandia Cantilever Beam End-to-End UQ problem [3,4]. A small number of beams are randomly drawn from a large population and then deflection-tested. The tests involve substantial aleatory and epistemic uncertainties from the sources mentioned above. Uncertainty of deflection response and of the probability of exceeding a specified deflection threshold are estimated for: A) the whole population of beams; and B) a random beam selected from the population. Results are compared to the truth quantities for several random trials involving different realizations of the uncertain quantities in the experiments.

[1] Coleman, H.W., and Steele, Jr., W.G., Experimentation and Uncertainty Analysis for Engineers, 2nd Edition, John Wiley & Sons, New York, NY, 1999.

[2] ASME PTC 19.1-2005, Test Uncertainty.

[3] Romero, V., B. Schroeder, M. Glickman, Cantilever Beam End-to-End UQ Test Problem: Handling Experimental and Simulation Uncertainties in Model Calibration, Model Validation, Extrapolative Prediction, and Risk Assessment, Sandia National Laboratories document SAND2017-4689 O, version BeamTestProblem-34.pdf, Jan. 2018.).

[4] Romero, V., Cantilever Beam End-to-End UQ Test Problem and Evaluation Criteria for UQ Methods Performance Assessment, Sandia National Laboratories document SAND2017-4592 C presented at 2017 ASME V&V Symposium, May 3-5, Las Vegas, NV (in ASME V&V Symposium proceedings archive).

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Quantify the Uncertainty: 95% Confidence in Aerodynamic Model Predictions

Oral Presentation. VVS2018-9375 **11:20AM - 11:45AM**

Seth S. Lawrence, ***Earl P.N. Duque***, *Intelligent Light, Rutherford, NJ, United States*, ***Andrew Cary, John A. Schaefer***, *Boeing Research and Technology, St. Louis, MO, United States*

The uncertainty in model results may be quantified through rigorous verification, validation and uncertainty quantification (VVUQ) procedures. This presentation will present the application of the Oberkampf and Roy Uncertainty framework that was applied to several aerodynamics studies. The first UQ study was a NACA0012 airfoil case at zero lift, demonstrating the underlying principles behind a total uncertainty study (numerical, input, and model form uncertainty). Numerical uncertainty was found via grid refinement using the OVERFLOW 2 solver to carry out computations and Dakota was used to perform mixed UQ statistical input analysis of the solver input parameters. A comparative analysis was made using polynomial chaos expansion (PCE) to identify potential differences associated with uncertainty quantification methods. Model form uncertainty was found using validation of the model results via experimental data and the Area Validation Metric methodology techniques. The second UQ study considered the two AIAA High Lift Prediction workshop 3 configurations. Common Research Model and the JAXA standard model. Simulations were performed to compute 95% confidence levels in lift, drag and pitching moment predictions by the OVERFLOW 2 solver. The implementation of VVUQ techniques to complex engineering problems was shown to necessitate the need for new adaptive workflows that can take advantage of the large computational resources required for a thorough UQ analysis.

Discrete-Direct Calibration, Real-Space Validation, and Predictor-Corrector Extrapolation applied to the Cantilever Beam End-to-End UQ Problem

Oral Presentation. VVS2018-9376 **11:45AM - 12:10PM**

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

A novel set of coordinated methods comprising a systems approach to model calibration, validation, and extrapolative prediction will be illustrated on the Sandia Cantilever Beam End-to-End UQ problem [1,2]. The problem involves many challenging uncertainty treatment aspects summarized below. The problem emphasizes difficult paradigm and strategy issues encountered in real end-to-end UQ problems while being computationally trivial so that approaches and methodologies can be focused on. The talk will present a set of practical calibration, validation, and extrapolation approaches that suitably extend end-to-end, demonstrated on the Beam problem with standard EXCEL spreadsheet tools. Other approaches are sought that extend end-to-end in a satisfactory manner. Initial examination of methods in the literature has revealed a lack of other suitable end-to-end UQ frameworks for the Beam problem.

The Beam problem is a simplified prototype problem for stochastic physical systems with scalar inputs and outputs. Responses are to be predicted for a population of nominally identical cantilever beams with small variations in material stiffness and geometry (beam lengths, widths, heights). To estimate material stiffness variability in the population of beams, model calibrations [3] are conducted for a small subset of tested beams selected at random from the larger population. The tests at temperature T1 measure deflection under a prescribed target load. Small control variations exist in the actual applied loads in the four tests. Random and systematic errors/uncertainties exist in the measurements of load magnitude and beam dimensions and deflection. The random measurement errors vary from test to test according to a specified probability distribution. Systematic measurement errors are strongly correlated across the tests and are described by a prescribed interval range of uncertainty. Substantial epistemic uncertainty concerning the aleatory distribution of material stiffness properties exists due to the small number of tests. The material stiffness variability/uncertainty description from the calibrations is used with the differential equation based physics model to predict responses at different circumstances as follows. Model validation is conducted at two configurations: A) a single test at the calibration temperature T1 but different beam dimensions and configurationally different loading; B) two tests at temperature T2 (temperature is suspected to affect material stiffness) with the beam dimensions in A but different loading. Information from the validation assessments may be used in further predictions of beam population responses at the geometry and loading conditions in A and B but temperature extrapolation to T3. Predictions are sought for beam population tip displacements and the proportion of beams that exceed a critical displacement threshold.

[1] Romero, V., B. Schroeder, M. Glickman, Cantilever Beam End-to-End UQ Test Problem: Handling Experimental and Simulation Uncertainties in Model Calibration, Model Validation, Extrapolative Prediction, and Risk Assessment, Sandia National Laboratories document SAND2017-4689 O, version BeamTestProblem-34.pdf, Jan. 2018.

[2] Romero, V., Cantilever Beam End-to-End UQ Test Problem and Evaluation Criteria for UQ Methods Performance Assessment, Sandia National Laboratories document SAND2017-4592 C presented at 2017 ASME V&V Symposium, May 3-5, Las Vegas, NV (in ASME V&V Symposium proceedings archive).

[3] Romero, V.J., Discrete-Direct Model Calibration and Propagation Approach addressing Sparse Replicate Tests and Material, Geometric, and Measurement Uncertainties, Sandia National Laboratories document SAND2017-12524 C, Soc. Auto. Engrs. 2018 World Congress (WCX18) paper 2018-01-1101, April 10-12, Detroit.

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Deep UQ - Learning deep neural network surrogate models for uncertainty quantification

Oral Presentation. VVS2018-9381 **12:10PM - 12:35PM**

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

State-of-the-art computer codes for simulating real physical phenomena are often characterized by vast numbers of input parameters. Often, these input parameters are uncertain, and one needs to rigorously assess the effect of these uncertainties on the outputs from the computer codes. Performing uncertainty quantification (UQ) tasks with Monte Carlo (MC) methods is almost always infeasible because of the need to perform hundreds of thousands or even millions of forward model evaluations in order to obtain convergent statistics. One, thus, tries to construct a cheap-to-evaluate surrogate model to replace the forward model solver. However, for systems with large numbers of input parameters, one has to deal with the curse of dimensionality - the exponential increase in the volume of the input space, as the number of parameters increases linearly. This necessitates the application of suitable dimensionality reduction techniques. A popular class of dimensionality reduction methods are those that attempt to recover a low dimensional representation of the high dimensional feature space. Such methods, however, often tend to overestimate the intrinsic dimensionality of the input feature space. We demonstrate the use of deep neural networks (DNN) to construct surrogate models for numerical simulators. We parameterize the structure of the DNN in a manner that lends the DNN surrogate the interpretation of recovering a low dimensional nonlinear manifold. The model response is a parameterized nonlinear function of the low dimensional projections of the input. We think of this low dimensional manifold as a nonlinear generalization of the notion of the active subspace. Our approach is demonstrated with a problem on uncertainty quantification in two-dimensional, single phase, steady-state flow representing flow in an idealized oil reservoir. The dynamics of porous media flow are governed by Darcy's law, which is parameterized by a permeability tensor. Uncertainties in the soil structure makes this high-dimensional permeability tensor uncertain. Mathematically, the task of performing UQ in this idealized oil reservoir reduces to the task of solving a stochastic elliptic partial differential equation (SPDE) with uncertain diffusion coefficient. We deviate from traditional formulations of the SPDE problem by not imposing a specific covariance structure on the random diffusion coefficient. Instead we attempt to solve a more challenging problem of learning a map between an arbitrary snapshot of the permeability tensor and the pressure field.

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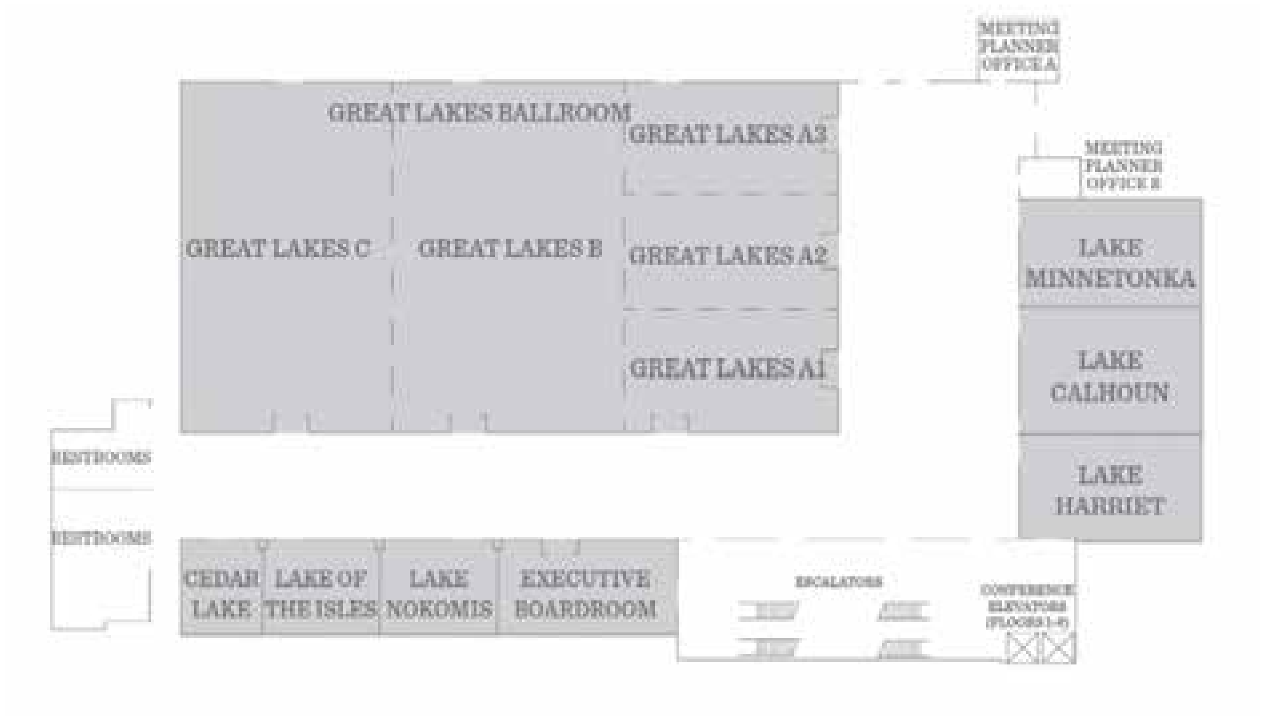

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