

ENERGY HIGH PERFORMANCE COMPUTING CONFERENCE



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FEBRUARY 28 - MARCH 2, 2023
HOUSTON, TEXAS



RICE KEN KENNEDY
INSTITUTE
AI, Data, and Computing for Global Impact

MESSAGE FROM THE KEN KENNEDY INSTITUTE LEADERSHIP

The Ken Kennedy Institute at Rice University is pleased to host the 16th annual Energy High Performance Computing Conference in Houston, TX. The Energy HPC Conference is the premier meeting place for key stakeholders to engage in conversations about challenges, opportunities, and new developments to help advance HPC in the energy industry.

The two-day conference features a remarkable lineup of invited speakers, technical talks, birds of a feather sessions, an exhibit hall, networking receptions, and poster presentations. Thursday is an add-on day with three post-conference workshops to dive deeper into niche topics of interest.

Tuesday's Sponsor Networking Reception will include a specialty wine, cheese, and heavy appetizer selection, with magic and entertainment to complete an evening of connecting with fellow conference attendees and sponsors. Wednesday's Poster Presentation Reception will showcase exciting research happening in the field by the future leaders in high performance computing. Networking breaks during the conference will also feature specialty coffee, a donut wall, and popsicle bar.

We hope that you thoroughly enjoy the conference and use the networking opportunities to initiate collaborations and promote technological innovation that will address computing demands as well as other issues in the energy industry — not just in Houston, but also nationally and internationally.

The Ken Kennedy Institute at Rice University is committed to supporting cutting-edge research, educating innovators, and connecting across industries by bringing together thought leaders from around the world with expertise in artificial intelligence, data, and computing. We are thrilled to host this conference at the service of our regional and global energy and high performance computing communities.

We are grateful to our sponsors, partners, speakers, and attendees who share our enthusiasm and seek the opportunity to support and engage with the community. Finally, we would like to say a special thank you to the exceptional Keith Gray and the Conference Committee for their many contributions to this year's conference — this highly anticipated event exists because of your efforts.

On behalf of the Conference Committee, Rice University, and the Ken Kennedy Institute team, we want to thank you for being here.

Lydia E. Kavraki, PhD

Director, The Ken Kennedy Institute

Angela D. Wilkins, PhD

Executive Director, The Ken Kennedy Institute

Mauricio Araya-Polo, TotalEnergies
Michelle Atkinson, The Ken Kennedy
 Institute, Rice University
David Baldwin, Shell
Jesse Chan, Rice University
Mike Cogan, Equinor
Donny Cooper, TotalEnergies
Erik Engquist, Rice University
Melyssa Fratkin, Texas Advanced
 Computing Center
Esthela Gallardo, Microsoft

Keith Gray, Intel
Elizabeth L'Heureux, bp
Christopher Leader, SLB
Alex Loddock, Chevron
David Martin, Argonne National
 Laboratory
Tom McDonald, Amazon Web Services
Nefeli Moridis, NVIDIA
Samantha Nava, The Ken Kennedy
 Institute, Rice University
Jan Odegard, The Ion

Kelly Peters, The Ken Kennedy
 Institute, Rice University
Jeremy Singer, ExxonMobil
Noella Soares, Shell
Suzy Tichenor, Oak Ridge National
 Laboratory
Mike Townsley, ExxonMobil
Angela Wilkins, The Ken Kennedy
 Institute, Rice University
Muhong Zhou, bp



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The Ken Kennedy Institute is a multidisciplinary group that works collaboratively on groundbreaking research in artificial intelligence, data, and computing. We foster a clear and strategic pathway to real-world impact.

We envision a world where innovation in computing and data improves the human condition - we cannot achieve this without you. Please contact us with your questions and ideas at kenkenney@rice.edu.



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 Houston, TX 77005
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Energy HPC Conference Code of Conduct

The organizers invite all attendees, sponsors/exhibitors, speakers, media, volunteers, and other participants to help us realize a safe and positive conference experience for everyone. The Ken Kennedy Institute works to increase tolerance, opportunity, and diversity in an effort to continually encourage the open exchange of ideas. For these reasons,

the Institute is committed to providing a harassment-free experience at all the events it organizes. If you experience or witness harassment or discriminatory behavior at the conference, report this promptly to kenkenney@rice.edu.

Energy HPC Conference venues are shared with members of the public that

are not attendees of the conference; please be respectful to all patrons of these locations.

Please note that audio recording, videotaping, and/or photography of any portion of the Energy HPC Conference material is strictly prohibited without prior consent of the Energy HPC staff.

2023

ENERGY HIGH PERFORMANCE COMPUTING CONFERENCE

KEYNOTE CONFERENCE SPEAKERS



HENRI CALANDRA

TotalEnergies



JOHN ETGEN

bp



BRONSON MESSER

Oak Ridge National
Laboratory (ORNL)

INVITED CONFERENCE SPEAKERS



WAFIK BEYDOUN

International Association
of Oil & Gas Producers
(IOGP)



GIBBY DUNLEAVY

Constant Impact
LLC



GARY GRIDER

Los Alamos National
Laboratory (ORNL)



SAMIR KHANNA

bp



PARTHA ROUTH

ExxonMobil
Engineering and
Technology Company



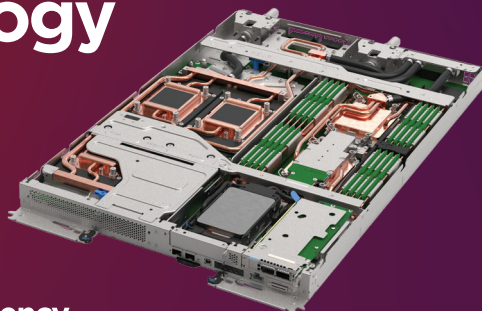
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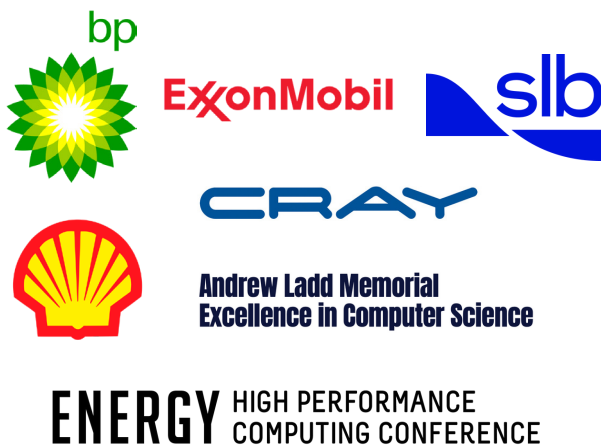
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2022-2023 Ken Kennedy Institute Industry Sponsored Fellowship Recipients



Rice Ken Kennedy Institute Graduate Fellowship Award recipients (top row, from left to right): Fatima Ahsan, Paola Cascante-Bonilla, Chen Chen, Aditya Desai, Victoria Granja, Yumeng Liu, Zichang (Emma) Liu, Nicolae Sapoval, Guanchu Wang



The Ken Kennedy Institute is pleased to recognize the achievements and research of Rice University's graduate students by awarding fellowships to students pursuing research related to high performance computing, computational science and engineering, and data science.

Fellowship awards are made possible with support from bp, ExxonMobil, Shell, SLB, the Energy High Performance Computing Conference, and the Andrew Ladd, Ken Kennedy-Cray, and Scott Morton endowments.

We welcome you to become a partner in sponsoring the Ken Kennedy Institute Fellowship Program at Rice University. For more information, please email kenkennedy@rice.edu.



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Ken Kennedy Institute Computational Science & Engineering Graduate Recruiting Fellowships

Funded by the proceeds from the Energy High Performance Computing Conference, the goal of this fellowship program is to attract exceptional graduate students to Rice University the fields of high performance computing, computational science and engineering, and data science, with special consideration given to students with research interests in areas of relevance to the energy industry.

2022-2026



Brianna Barrow
Computer Science



Alyssa Cantu
Computer Science



Rose Graves
Statistics



Kevin McCoy
Statistics



John Steinman
CMOR



Ria Stevens
Computer Science



Xiaoyu (Rosie) Zhu
EEPS

2021-2025

Kelsey Murphy
*Earth, Environmental,
and Planetary Sciences*

Jose Palacio
Statistics

Xinyu (Xin) Yao
Computer Science

2020-2024

Kristen Curry
Computer Science

Raul Garcia
*Computational and
Applied Mathematics*

Bryant Jerome
Applied Physics

Mirae (Sunny) Kim
Computer Science

Camille Little
ECE

Catherine Tuppen
ECE

Cameron Wolfe
Computer Science

Tiancheng Xu
Computer Science

Naiming (Lucy) Liu
ECE

2019-2023

Alejandro Nicolas Diaz
*Computational and
Applied Mathematics*

Yilei Fu
Computer Science

Christina G Taylor
*Computational and
Applied Mathematics*

John Zito
Statistics

2023 PROGRAM | TUESDAY, FEBRUARY 28

B Birds of a Feather (BOF)

I Invited Speaker

K Keynote

N Networking

A Technical Talk: Algorithms

M Technical Talk: Machine Learning

O Technical Talk: Optimization

S Technical Talk: Systems

W Workshop

8:00 a.m. – 8:30 a.m.

N Check-in + Breakfast  Exhibit Hall

8:30 a.m. – 9:30 a.m.

B BOF: Data Management for Huge Data Volumes for HPC  Room 280

Moderator(s): **Esthela Gallardo**, Microsoft; **Stuart Bonnington**

Panelist(s): **John Zinck**, ExxonMobil; **Michael Gujral**, Shell; TBA

8:30 a.m. – 9:30 a.m.

B BOF: Encouraging and Supporting Better Collaboration in Energy HPC  Auditorium

Moderator(s): **Alex Loddock**, Chevron; **Jeremy Singer**, ExxonMobil

Panelist(s): **Gerard Gorman**, Devito Codes/Imperial College London; **Sam Kaplan**, Chevron; **Altay Sansal**, TGS; **Dan Stanzione**, TACC, UT Austin

9:30 a.m. – 10:00 a.m.

N Morning Break  Exhibit Hall

10:00 a.m. – 10:10 a.m.

K Welcome + Recognizing Scott Morton  Auditorium

Speaker(s): **Lydia Kavradi**, The Ken Kennedy Institute, Rice University; **Angela Wilkins**, The Ken Kennedy Institute, Rice University

Speaker(s): **Conference Founders and Colleagues**

10:10 a.m. – 10:50 a.m.

K Session 1: What Really Matters to our Industry in the Area of HPC and the Era of Exascale  Auditorium

Speaker(s): **Henri Calandra**, TotalEnergies; **John Etgen**, bp

10:50 a.m. – 11:30 a.m.

I Session 2: HPC in 2023: The View from TACC on HPC, AI, and People  Auditorium

Speaker(s): **Dan Stanzione**, Texas Advanced Computing Center (TACC), The University of Texas at Austin


11:30 a.m. – 12:30 p.m.

N Lunch  Exhibit Hall

12:30 p.m. – 1:45 p.m.

M Technical Talks: Machine Learning  Auditorium

12:30 p.m. – 1:45 p.m.

S Technical Talks: Systems  Room 280

1:45 p.m. – 2:30 p.m.

N Afternoon Break  Exhibit Hall

2:30 p.m. – 3:10 p.m.

I Session 3: The Road Not Taken, a Data Science Fallacy  Auditorium

Speaker(s): **Gibby Dunleavy**, Constant Impact LLC

3:10 p.m. – 3:50 p.m.

I Session 4: LANL Platform Planning and Update  Auditorium

Speaker(s): **Gary Grider**, Los Alamos National Laboratory (LANL)

3:50 p.m. – 5:30 p.m.

N Sponsor Networking Reception  Exhibit Hall

Technical Talks: Machine Learning 🌈 Auditorium

Moderator(s): *Donny Cooper, TotalEnergies*

- | | |
|--------------------------------|--|
| 12:30 p.m. – 12:55 p.m. | Inversion of Time-Lapse Surface Gravity Data for Detection of 3D CO₂ Plumes via Deep Learning
Author(s): Adrian Celaya , Rice University; Yen Sun , TotalEnergies EP Research & Technology US; Bertrand Denel , TotalEnergies; Antony Price , TotalEnergies; and Mauricio Araya-Polo , TotalEnergies EP Research & Technology US |
| 12:55 p.m. – 1:20 p.m. | Adsorptive CO₂ Removal from Dilute Sources (AC02RDS)
Author(s): Donny Cooper , TotalEnergies; Jake Burner , University of Ottawa; and Santanu Chaudhuri , Argonne National Laboratory |
| 1:20 p.m. – 1:45 p.m. | On Signal Processing Flaws in Convolutional Neural Networks
Author(s): Janis Keuper , Fraunhofer Center HPC |

Technical Talks: Systems 🌈 Room 280

Moderator(s): *David Baldwin, Shell; Tom McDonald, AWS*

- | | |
|--------------------------------|--|
| 12:30 p.m. – 12:55 p.m. | Petrobras HPC Infrastructure
Author(s): Luiz Monnerat , Petrobras |
| 12:55 p.m. – 1:20 p.m. | ExxonMobil's CPU to GPU Transition
Author(s): Steven Mariani , ExxonMobil; Jonathan Phillips , ExxonMobil; Mike Townsley , ExxonMobil; and Rahul Sampath , ExxonMobil |
| 1:20 p.m. – 1:45 p.m. | Is Hybrid Cloud the Way to Unlock Seismic HPC at Scale in the Public Cloud?
Author(s): Tim Roden , Shell; Michael Gujral , Shell; Francesco Menapace , Shell; Michele Isernia , AWS; Chee Choon-Cheng , AWS; and Stephen Whitley , AWS |

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2023 PROGRAM | WEDNESDAY, MARCH 1

B Birds of a Feather (BOF)

I Invited Speaker

K Keynote

N Networking

A Technical Talk: Algorithms

M Technical Talk: Machine Learning

O Technical Talk: Optimization

S Technical Talk: Systems

W Workshop

8:00 a.m. – 8:30 a.m.

N Check-in + Breakfast **>>** Exhibit Hall

8:30 a.m. – 9:30 a.m.

B **BOF: Communicating the Value of HPC and the Case for Growth** **>>** Auditorium
Moderator(s): David Baldwin, Shell; Jeremy Singer, ExxonMobil
Panelist(s): Bronson Messer, ORNL; Gary Grider, LANL; Diego Klahr, TotalEnergies; Elizabeth L'heureux, bp; Charlie Fazzino, ExxonMobil

8:30 a.m. – 9:30 a.m.

B **BOF: Women in Energy/HPC – Leveling the Playing Field** **>>** Room 280
Moderator(s): Melyssa Fratkin, Texas Women in HPC, TACC
Panelist(s): Cristina Beldica, Intel; Esthela Gallardo, Microsoft; Arianna Martin, bp/NAG; Rosalinda Mendez, NOA Research, LLC; Marlo Nordt, Chevron; Noella Soares, Shell

9:30 a.m. – 10:00 a.m.

N Morning Break **>>** Exhibit Hall

10:00 a.m. – 10:05 a.m.

K **Welcome** **>>** Auditorium
Speaker(s): Samantha Nava, The Ken Kennedy Institute, Rice University

10:05 a.m. – 10:45 a.m.

K **Session 5: Frontier: The World's First Exascale Supercomputer** **>>** Auditorium
Speaker(s): Bronson Messer, Oak Ridge National Laboratory (ORNL)

10:45 a.m. – 11:25 a.m.

I **Session 6: Full Wave-field Inversion: Journey Towards Practical Applications** **>>** Auditorium
Speaker(s): Partha Routh, ExxonMobil Engineering and Technology Company

11:25 a.m. – 12:30 p.m.

N Lunch **>>** Exhibit Hall

12:30 p.m. – 1:50 p.m.

A **Technical Talks: Algorithms** **>** Auditorium

12:30 p.m. – 1:50 p.m.

O **Technical Talks: Optimization** **>** Room 280

1:50 p.m. – 2:30 p.m.

N Afternoon Break **>>** Exhibit Hall

2:30 p.m. – 3:10 p.m.

I **Session 7: Role of HPC in the Energy Transition** **>>** Auditorium
Speaker(s): Samir Khanna, bp

3:10 p.m. – 3:50 p.m.

I **Session 8: A Conversation with Wafik Beydoun** **>>** Auditorium
Moderator(s): Melyssa Fratkin, TACC
Speaker(s): Wafik Beydoun, International Association of Oil & Gas Producers (IOGP)

3:50 p.m. – 5:30 p.m.

N Poster Presentation Reception **>>** Exhibit Hall

Technical Talks: Algorithms Auditorium

Moderator(s): *Mike Townsley, ExxonMobil*

12:30 p.m. – 12:50 p.m.	OpenMP Device Offloading for Seismic Modeling Author(s): Baodi Shan , SUNY Stony Brook; and Mauricio Araya-Polo , TotalEnergies EP Research & Technology US
12:50 p.m. – 1:10 p.m.	3D Finite Difference Elastic Wave Simulation on Nonuniform Grids Author(s): Longfei Gao , University of Texas at Austin; Omar Ghattas , University of Texas at Austin; and David Keyes , KAUST
1:10 p.m. – 1:30 p.m.	How Digital Approach Accelerated Velocity Model Building While Addressing the Data Scarcity Barrier to Leveraging Deep Learning Author(s): Apurva Gala , Shell; Pandu Devarakota , Shell; Engin Alkan , Shell; John Kimbro , Shell; and Gislain Madiba , Shell
1:30 p.m. – 1:50 p.m.	Solving Combinatorial Optimization Problem of Oil and Gas Supply Chain Optimization Using Simulated/Vector Annealing on Vector Engine Accelerator Author(s): Deepak Pathania , NEC Corporation India Private Limited and Shintaro Momose , NEC Corporation (Raghunandan Mathur present for Deepak)

Technical Talks: Optimization Room 280

Moderator(s): *Alex Loddoch, Chevron*

12:30 p.m. – 12:50 p.m.	Efficient Asynchronous Data Storage for FWI Workflows in GEOSX Author(s): Xavier Lacoste , TotalEnergies
12:50 p.m. – 1:10 p.m.	Accelerating I/O Intensive GPU Applications (eg. Seismic Imaging) by Providing a Direct Pathway for the GPU to Access Storage Author(s): Anand Manian , Oracle; Fatmir Hoxha , NVIDIA
1:10 p.m. – 1:30 p.m.	JavaSeis Cloud: A Micro-Service Framework for Seismic Processing Author(s): Chuck Mosher , MoMacMo Limited; Sanjay Sood , MoMacMo Limited; and Robert Ferguson , University of Calgary
1:30 p.m. – 1:50 p.m.	Optimizing a Multi-Dimensional Convolution Operator on GPUs for 3D Marchenko Imaging Author(s): Victor Koehne , SENAI CIMATEC HPC Center; Matheu Santos , SENAI CIMATEC HPC Center; Rodrigo Santos , SENAI CIMATEC HPC Center; Guillaume Barnier , NVIDIA; Fatmir Hoxha , NVIDIA; and Pedro Cruz , NVIDIA

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If you decide to add-on a Thursday workshop after you have already registered, please reach out to conference staff to update your registration.

MARCH 2 • THURSDAY

8:00 a.m. – 3:30 p.m.



Best Practices in HPC Systems Management >> Auditorium

Speaker(s): Practitioners and Experts from Industry, Academia, and National Labs

8:00 a.m. – 4:00 p.m.



Introduction to Physics-Informed Machine Learning with Modulus >> 10th Floor
Conference Room 1003

Speaker(s): Pavel Dimitrov, NVIDIA; Ken Hester, NVIDIA; Fatmir Hoxha, NVIDIA;
Guillaume Barnier, NVIDIA; Guillaume Thomas Collignon, NVIDIA; Igor Terentyev, NVIDIA;
Kashif Chauhan, NVIDIA

8:00 a.m. – 4:00 p.m.



Devito Training >> Room 280 + Exhibit Hall

Speaker(s): Gerard Gorman, Devito Codes; Fabio Luporini, Devito Codes; Rhodri Nelson,
Imperial College London; Ed Caunt, Imperial College London; Zoe Leibowitz, Imperial
College London

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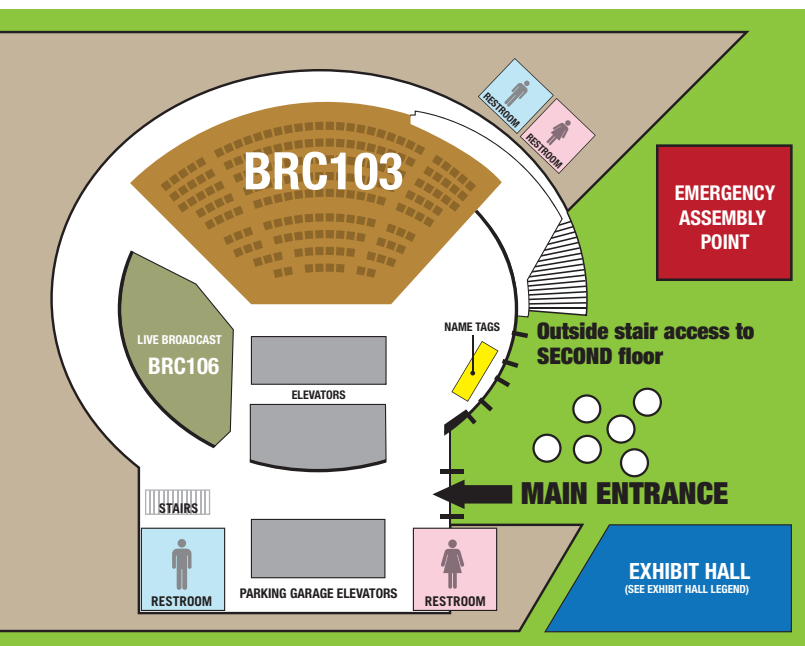
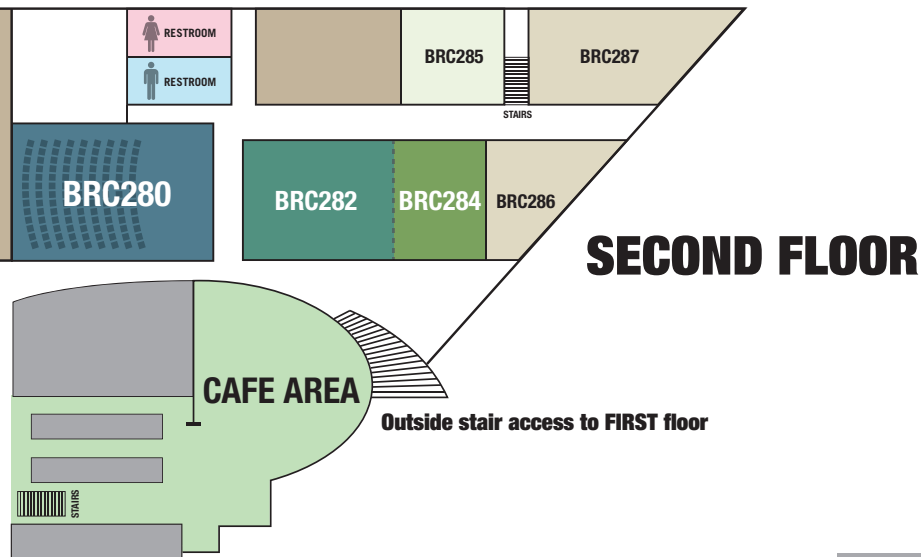
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PARKING** →

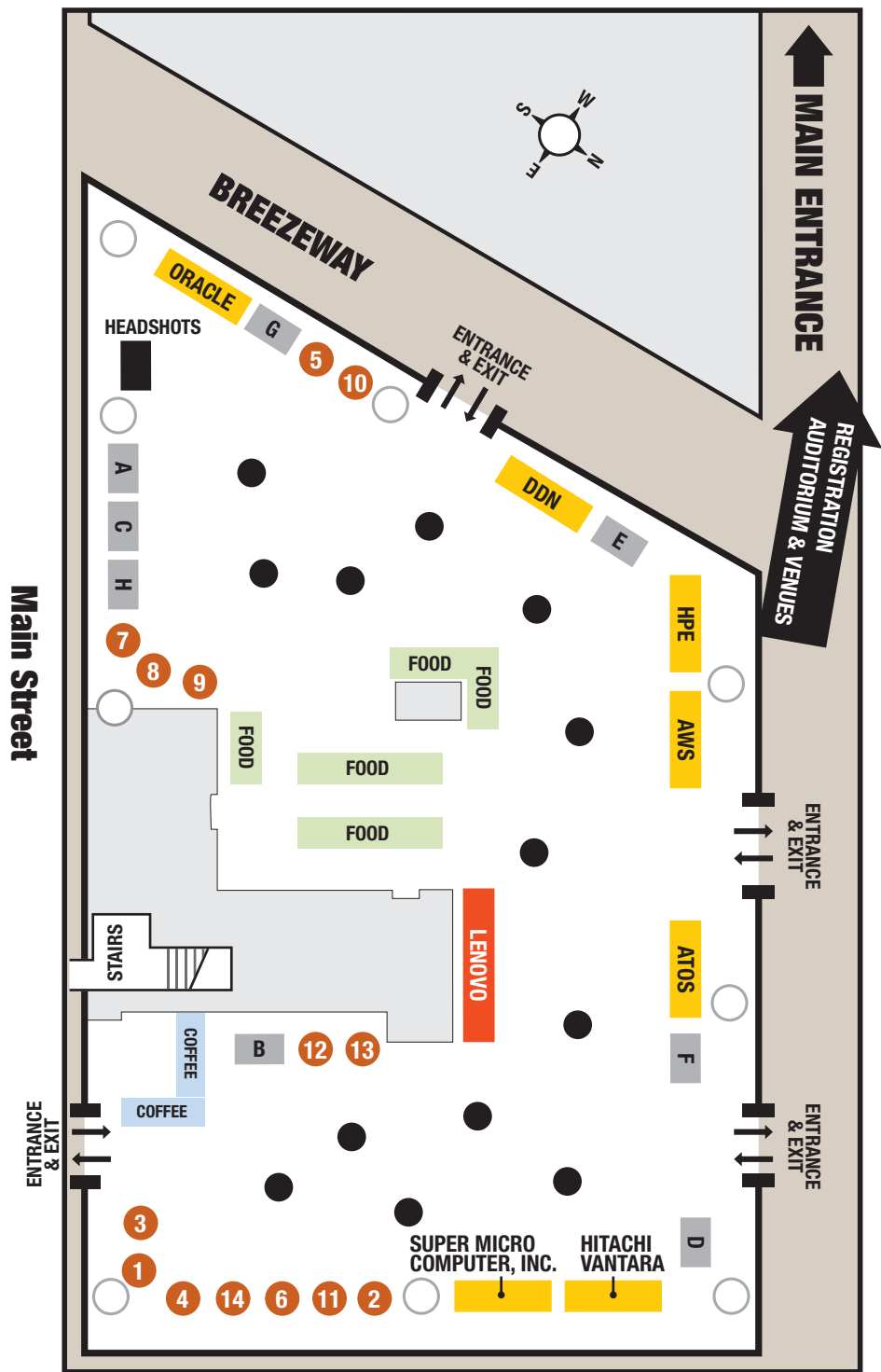
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Dave McDonnell, Chris Maestas, (IBM)

BED: A Real-Time Object Detection System for Edge Devices

Guanchu Wang, Daochen Zha, Alfredo Costilla Reyes, Xia Hu (Rice University), Zaid Pervaiz Bhat, Zhimeng Jiang, Yi-Wei Chen (Texas A&M University), Afshin Niktash, Gorkem Ulkar, Erman Okman (Analog Devices), Xuanting Cai (Meta Platforms, Inc.)

Deep Learning Strategies for Seismic Demultiple

Mario Fernandez (Fraunhofer ITWM, École Normale Supérieure), Norman Ettrich (Fraunhofer ITWM), Matthias Delescluse (École Normale Supérieure), Alain Rabaute (Sorbonne Université), Janis Keuper (Fraunhofer ITWM, Offenburg University)

Devito - From Seismic to Covid

Zoe Leibowitz (Imperial College London)

Efficient Model Compression with Random Operation Access Specific Tile (ROAST) Hashing

Aditya Desai, Keren Zhou, Anshumali Shrivastava (Rice University)

EMvelop Stimulation: Minimally Invasive Deep Brain Stimulation Using Temporally Interfering Electromagnetic Waves

Fatima Ahsan, Taiyun Chi, Behnaam Aazhang (Rice University), Raymond Cho, Sameer Anil Sheth, Wayne Goodman (Baylor College of Medicine)

Evolutionary Power Spectra Estimation of Nonstationary Stochastic Processes by Energy-Based Reckoning

Hanshu Zhang, Pol Spanos (Rice University), Alberto Di Matteo (University of Palermo)

How Extra Dispatchable Energy Could Solve Energy Crisis in Texas

Chen Chen, Daniel Cohan (Rice University)

Independent Physics-Guided Mesh Adaptivity and Finite Element Discretization for High-Performance Multiphysics Modeling

Ahmed Almetwally, Mary Wheeler (University of Texas at Austin)

Learning Closed-Form Equations for Subgrid-Scale Closures from High-Fidelity Data: Promises and Challenges

Karan Jakhar, Yifei Guan, Rambod Mojjani, Ashesh Chattopadhyay, Pedram Hassanzadeh (Rice University)

MLPerf Storage Benchmark Aids Deployment Planning for AI/ML Processing

Curtis Anderson, Jeff Whitaker (Panasas Inc.)

Preparing HPCToolkit for Exascale Supercomputers

Yumeng Liu, Jonathon Anderson, John Mellor-Crummey (Rice University)

QualD: Enabling Earlier Detection of Recently Emerged SARS-CoV-2 Variants of Concern in Wastewater

Nicolae Sapoval, Yunxi Liu, Esther G Lou, Katherine B Ensor, Lauren B Stadler, Todd J Treangen (Rice University), Loren Hopkins, Rebecca Schneider (Houston Health Department)

Robust Synchronization and Policy Adaptation for Networked Heterogeneous Agents

Miguel Felipe Arevalo-Castiblanco, Cesar A. Uribe (Rice University), Eduardo Mojica-Nava (Universidad Nacional de Colombia)

SimVQA: Exploring Simulated Environments for Visual Question Answering

Paola Cascante-Bonilla, Vicente Ordonez (Rice University)

Wave Propagation on the STX Accelerator

Ryuichi Sai, John Mellor-Crummey (Rice University), Marc Andre Heller, Jens Kruger (Fraunhofer ITWM), Mauricio Araya-Polo (TotalEnergies EP Research & Technology US)

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2023 AI IN HEALTH CONFERENCE

OCTOBER 9 – 12, 2023

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