

NAISE / INQUIRE

QS³: Quantum System Software Stack Workshop Information Booklet

May 23, 2025

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VENUE

NAISE HQ / Northwestern, Evanston Campus

Hogan Building, Suite 1160

2205 Tech Drive, Evanston, IL, 60608

<https://maps.northwestern.edu/facility/88>

PARKING

Northwestern North Parking Garage*

2311 N. campus Drive, Evanston, IL, 60208

<https://maps.northwestern.edu/facility/646>

**once at NAISE, please ask for a validation ticket from Iustitia Ko*

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FINAL AGENDA

QS³: Quantum System Software Stack Workshop

May 23, 2025 @ NAISE, Northwestern - Evanston

All Times CST

08:30AM – 09:00AM Breakfast & Registration

09:00AM – 09:15AM **Welcome & Workshop Charge**

Kate Smith & Nikos Hardavellas, *Northwestern*

09:15AM – 09:45AM **Open Software Ecosystem For Large Scale Quantum-Classical Computational Environments**

Iskandar Sitdikov, *IBM Quantum*

09:45AM – 10:15AM **Quantum System Designs in Transition: Evolving from NISQ to FTQC**

Yufei Ding, *University of California, San Diego (Virtual)*

10:15AM – 10:30AM Break

10:30AM – 10:50AM **Accelerated Quantum Supercomputing**

Yuri Alexeev, *NVIDIA (Virtual)*

10:50AM – 11:40AM **Panel Discussion**

Yufei Ding, *University of California, San Diego (Virtual)*

Yuri Alexeev, *NVIDIA (Virtual)*

Nikos Hardavellas, *Northwestern University*

Swamit Tannu, *University of Wisconsin (Virtual)*

Kate Smith, *Northwestern (Chair)*

11:40AM – 12:20PM Group Photo & Lunch

12:20PM – 12:30PM **NAISE & INQUIRE Welcome**

Neelesh Patankar & Michael Wasielewski, *Northwestern*

12:30PM – 12:50PM **NU-ANL Collaboration Focus Talk**

Ji Liu, *Argonne National Laboratory*

12:50PM – 01:10PM **Quantum-HPC Integration in the Munich Quantum Valley and Europe**

Laura Schulz, *Argonne National Laboratory*

01:10PM – 01:25M Breakout Charge & Transition Time

01:25PM – 02:05PM Breakout Discussions

Group 1: Quantum algorithm design and quantum error correction

Group 2: Quantum compilation and programming languages

Group 3: Technology mapping, hybrid quantum-classical systems, quantum HW/SW co-design, and classical emulation of quantum computation and technology, system calibration and benchmarking

02:05PM – 02:20PM Restructuring Notes & Break

02:20PM – 02:50PM Report Outs

02:50PM – 03:00PM Wrap up & Reflections

03:00PM Adjourn

FINAL (EXTENDED) AGENDA

QS³: Quantum System Software Stack Workshop

May 23, 2025 @ NAISE, Northwestern - Evanston

SCOPE While quantum computing has vast potential, current implementations are constrained by the number of qubits (essential for algorithms with many variables), coherence times (vital for running long algorithms), and gate fidelities (crucial for achieving accurate results). Quantum hardware needs to improve by several orders of magnitude along all these dimensions before it can become truly useful for a wide range of applications. Even though quantum hardware advances toward that goal, waiting for it alone to close the gap between the capabilities it offers, and the needs of applications, may take decades. A more balanced approach would be to complement the hardware with a software stack that utilizes the available limited hardware resources in the most efficient manner possible. This full-stack approach improves quantum performance from the user's viewpoint by collaboratively fine-tuning hardware and software layers, integrating them tightly among them and with classical computing resources, with the aim to make quantum computing practical at an accelerated time scale.

This workshop will explore the open questions and challenges in developing this quantum software system stack, including complementary hybrid quantum-classical systems. Topics of interest include, but are not limited to, quantum algorithm design, quantum programming languages, compilation (e.g., mapping, gate synthesis, gate scheduling, routing, error mitigation, error detection), quantum error correction (e.g., optimal QEC strategies, resource requirements, noise tolerance, decoding), technology mapping (e.g. quantum/classical partitioning, circuit cutting, backend selection), quantum hardware and software co-design, hybrid quantum-classical systems, optimal quantum control and calibration, and classical emulation of quantum computation and technology (e.g., quantum circuit and device simulation). By defining key challenges and open problems in these areas, this workshop aims to drive progress toward more robust and scalable quantum systems.

All Times CST

08:30AM – 09:00AM Breakfast & Registration

09:00AM – 09:15AM **Welcome & Workshop Charge**

Kate Smith & Nikos Hardavellas, *Northwestern*

09:15AM – 09:45AM **Open Software Ecosystem For Large Scale Quantum-Classical Computational Environments**

Iskandar Sitdikov, *IBM Quantum*

ABSTRACT

We are seeing realization of quantum-centric supercomputing (QCSC) - integrated quantum and classical computing resources working together in parallelized workloads to run computations beyond what was possible before. Advancements in modular hardware architectures, coupled with mature software, provide the foundations for advancing scientific research and industrial applications in this integrated environment. This talk aims to explore open software ecosystem for large scale quantum-classical computing environments. We will talk about existing tools and integration models of bringing Quantum and HPC together. We will look at ongoing efforts and future

development plans for these new heterogeneous systems. Finally, we will post open questions and summarize existing gaps and challenges in QCSC.

BIO *Iskandar Sitdikov is a software architect at IBM Quantum, responsible for an open software ecosystem for large-scale quantum-classical systems. He has a background in distributed computing and machine learning and holds degrees in mathematics and computer science.*

09:45AM – 10:15AM Quantum System Designs in Transition: Evolving from NISQ to FTQC
Yufei Ding, *University of California, San Diego (Virtual)*

ABSTRACT Quantum computing is undergoing a transformative phase, advancing from the noisy intermediate-scale quantum (NISQ) era towards fault-tolerant quantum computing (FTQC). This progress has been fueled by remarkable experimental breakthroughs in recent years, signaling the feasibility of FTQC. This talk will follow this trend, exploring how quantum computing systems, particularly compilers, must adapt to meet the demands of FTQC. We will discuss key challenges, including implementing quantum error correction (QEC) codes on hardware with limited and sparse qubit-to-qubit connectivity, transitioning QEC protection strategies from static error profiling to dynamic error adaptation (e.g., handling error drift and cosmic ray-induced defects), and designing efficient decoders for increasingly complex qLDPC codes. By addressing these issues, we aim to identify the innovations required to bridge the gap between experimental advancements and practical FTQC systems.

BIO *Yufei Ding is an Associate Professor in the Computer Science & Engineering Department at UCSD and the founder of the PICASSO Lab. She holds a Ph.D. in Computer Science from North Carolina State University and a B.S. in Physics from the University of Science and Technology of China. Her research spans domain-specific language design, architecture and compiler optimization, and hardware acceleration. Currently, her work focuses on developing high-performance, energy-efficient, and high-fidelity programming frameworks for emerging technologies, including quantum computing and machine learning. Dr. Ding is a recipient of prestigious honors such as the NSF CAREER Award (2020) and the IEEE Computer Society TCHPC Early Career Researchers Award for Excellence in High-Performance Computing (2019).*

10:15AM – 10:30AM Break

10:30AM – 10:50AM Accelerated Quantum Supercomputing
Yuri Alexeev, *NVIDIA (Virtual)*

ABSTRACT Quantum computing is undergoing a transformative phase, advancing from the noisy intermediate-scale quantum (NISQ) era towards fault-tolerant quantum computing

(FTQC). This progress has been fueled by remarkable experimental breakthroughs in recent years, signaling the feasibility of FTQC. This talk will follow this trend, exploring how quantum computing systems, particularly compilers, must adapt to meet the demands of FTQC. We will discuss key challenges, including implementing quantum error correction (QEC) codes on hardware with limited and sparse qubit-to-qubit connectivity, transitioning QEC protection strategies from static error profiling to dynamic error adaptation (e.g., handling error drift and cosmic ray-induced defects), and designing efficient decoders for increasingly complex qLDPC codes. By addressing these issues, we aim to identify the innovations required to bridge the gap between experimental advancements and practical FTQC systems.

BIO

Dr. Yuri Alexeev is a senior quantum algorithm engineer at NVIDIA Corporation and a senior member of the IEEE Society. He works on the development of quantum computing algorithms, error correction/mitigation techniques, and numerical simulations of quantum systems using CUDA-Q, AI techniques, and accelerated quantum supercomputing. Dr. Alexeev received his Ph.D. in Physical Chemistry from Iowa State University while a graduate student in Mark Gordon's quantum chemistry group. After graduation, Dr. Alexeev became a postdoctoral fellow at Pacific Northwest National Laboratory; later, he joined the Nobel Prize winner Dr. Martin Karplus' group at Harvard University and Université de Strasbourg. Later, he joined Argonne National Laboratory and worked as a principal project specialist at Argonne Leadership Computing Facility in the area of quantum and HPC integration.

10:50AM – 11:40AM Panel Discussion

Yufei Ding, *University of California, San Diego (Virtual)*
Yuri Alexeev, *NVIDIA (Virtual)*
Nikos Hardavellas, *Northwestern University*
Swamit Tannu, *University of Wisconsin (Virtual)*
Kate Smith, *Northwestern (Chair)*

BIOS

Yufei Ding & Yuri Alexeev – *see bios in morning talks.*
Nikos Hardavellas & Kate Smith – *see organizer bios.*

Swamit Tannu is an Assistant Professor in the Computer Sciences department at the University of Wisconsin-Madison, where he leads the QUEST Research Group. His research focuses on developing architectural and systems abstractions for quantum computers. Swamit's work has been recognized with the NSF CAREER Award, the Stamatis Vassiliadis Best Paper Award at Computing Frontiers, and also been inducted into the MICRO Hall of Fame. Swamit earned his Ph.D. from Georgia Tech in Dec. 2020 before joining the University of Wisconsin-Madison.

11:40AM – 12:20PM Group Photo & Lunch

12:20PM – 12:30PM NAISE & INQUIRE Welcome
Neelesh Patankar & Michael Wasielewski, *Northwestern*

BIOS *Neelesh Patankar – see organizer bios.*

Michael Wasilewski is the Clare Hamilton Hall Professor of Chemistry, Northwestern University, Director of the Institute for Quantum Information Research and Engineering (INQUIRE), and Director of the Center for Molecular Quantum Transduction, a US-DOE Energy Frontier Research Center. He received his Ph.D. from the University of Chicago and was a postdoctoral fellow at Columbia University. He began his career at Argonne National Laboratory, where he advanced to Senior Scientist and Group Leader. In 1994, he joined the faculty of Northwestern University. From 2001-2004 he served as Chair of the Department of Chemistry at Northwestern. His research has resulted in over 830 publications and focuses on light-driven processes in molecules and materials, artificial photosynthesis, molecular electronics, and quantum information science. He is a member of the National Academy of Sciences and the American Academy of Arts and Sciences.

12:30PM – 12:50PM Toward Reliable Quantum Systems: Collaborative Research from Argonne and Northwestern
Ji Liu, *Argonne National Laboratory*

ABSTRACT As quantum computing scales toward practical applications, improving reliability under noisy conditions remains a central challenge. In this talk, I will present recent collaborative research between Argonne National Laboratory and Northwestern University focused on enhancing quantum reliability. The first part introduces Pauli Check Extrapolation (PCE), a scalable error mitigation method that leverages lightweight detection to estimate ideal outcomes. Next, I will discuss a resource allocation framework that guides the quantum program outcomes toward regions that produce higher-fidelity final distributions based on error detection data. Finally, I will share ongoing software efforts at Argonne that support benchmarking, circuit synthesis and optimization. Together, these efforts aim to provide practical pathways for building reliable quantum systems.

BIO *Ji Liu is an Assistant Computer Scientist at Argonne National Laboratory. His research focuses on developing open-source software stacks for quantum computing, systematic approaches for optimizing quantum simulations, and advanced noise mitigation techniques. His work has been recognized with the 2022 HPCA Distinguished Artifact Award and as a 2024 ISCA Best Paper Finalist.*

12:50PM – 01:10PM Quantum-HPC Integration in the Munich Quantum Valley and Europe

Laura Schulz, *Argonne National Laboratory*

ABSTRACT

The unique nature of quantum-based computation opens the possibility for new discovery in important classes of applications. Now on a (long, rocky) path towards maturation and scaling, the integration of quantum acceleration into high-performance computing (HPC) comes into focus and reinforces the overall trend towards next-generation heterogeneous supercomputing to tackle highly complex, composite scientific and engineering challenges in order to achieve useable and useful quantum-accelerated HPC, integration at all layers must happen, from brick-and-mortar infrastructure through best-fit applications to multidisciplinary mindsets. In this talk, I discuss efforts I led within the Munich Quantum Valley and through EuroHPC to address these challenges and to offer some lessons learned and insight for next steps on the path.

BIO

Laura Schulz is the Project Lead for Innovation at the Argonne Leadership Computing Facility at Argonne National Laboratory. Her focus is on future heterogeneous systems, integration and workflows. Before ANL, she was the head of Quantum Computing and Technologies at the Leibniz Supercomputing Centre (LRZ) of the Munich Quantum Valley. In this role, she led several quantum-HPC integration efforts at the regional and European levels, was the lead author of LRZ's Strategic Plan for Quantum Computing, and the PI for Germany's EuroHPC Joint Undertaking project Euro-Q-Exa,. She led multiple efforts toward integrating emerging quantum accelerators into several layers of the HPC ecosystem: from placement and residency in HPC centers, through hardware and software hybridization to user-centric adoption of HPCQC workflows and applications. Prior to moving to Germany, she was part of the Computation directorate at Lawrence Livermore National Laboratory (LLNL) as well as LLNL's High Performance Computing Innovation Center (HPCIC), which connected industry with the lab's novel technologies in HPC. Laura was named an HPCWire 2023 Person to Watch.

01:10PM – 01:25M Breakout Charge & Transition Time

Kate Smith, *Northwestern*

01:25PM – 02:05PM Breakout Session:

Group 1: Quantum algorithm design and quantum error correction (e.g., optimal QEC strategies, resource requirements, noise tolerance, decoding)

Discussion Lead: Alvin Gonzales, Scribe: Kabir Dubey

Group 2: Quantum compilation (e.g., mapping, gate synthesis, gate scheduling, routing, error mitigation, error detection) and programming languages

Discussion Lead: Nikos Hardavellas, Scribe: Quinn Langfitt

Group 3: Technology mapping (e.g. quantum/classical partitioning, circuit cutting, backend selection), hybrid quantum-classical systems, quantum HW/SW co-design, and

classical emulation of quantum computation and technology (e.g., quantum circuit and device simulation), system calibration and benchmarking

Discussion Lead: Kate Smith, Scribe: Ansh Singal

02:05PM – 02:20PM Restructuring Notes & Break

02:20PM – 02:50PM Report Outs

02:50PM – 03:00PM Wrap up & Reflections

03:00PM Adjourn

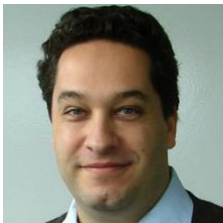
WORKSHOP ORGANIZERS

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Kate Smith is an Assistant Professor of Computer Science at Northwestern. Within the scope of quantum computing, Kate's active areas of research include computer architecture, distributed computing, optimized compilation, error mitigation, simulation, and security. Prior to joining Northwestern CS in January 2024, Kate was at Inflection where she managed the software engineering team responsible for maintaining Superstaq, a physics-aware quantum compiler, and directed the R&D for projects related to optimized compilation, error mitigation, and simulation of quantum programs on a wide range of quantum technology platforms. From January 2020 to September 2022, Kate was a CQE/IBM postdoctoral scholar within the University of Chicago Department of Computer Science where she was a member of the Enabling Practical-Scale Quantum Computing (EPiQC) group. Kate received a B.S. in Mathematics and a B.S. in Electrical Engineering in 2014 and a M.S. in Electrical Engineering in 2015 from Southern Methodist University (SMU). In addition, she earned her Ph.D. in Electrical Engineering at SMU in December 2019.



Nikos Hardavellas is a Professor of Computer Science and Electrical and Computer Engineering at Northwestern. He earned a Ph.D. in Computer Science from Carnegie Mellon University in 2009, an M.S. in Computer Science from Carnegie Mellon University, and an M.S. in Computer Science from the University of Rochester. He works on parallel systems and computer architecture, primarily on techniques to enable extreme-scale multicore processors, novel memory systems, and practical quantum systems. His research aims to pave the way to energy-efficient computing by investigating ideas to combat dark silicon, and to speed up the execution of programs by several factors through parallelism extraction, novel architectures, blending of compilers, runtimes, operating systems and hardware, and the use of emerging technologies such as photonics. His current research focuses primarily on the quantum system software stack, quantum compilation, fault-tolerant quantum computing and error management, memory-centric computing, and programmable memory systems.



Neelesh Patankar is the Director of Northwestern – Argonne Institute for Scientific and Engineering Excellence (NAISE). He received his BS (B.Tech.) in Mechanical Engineering from the Indian Institute of Technology, Bombay (1993) and his doctorate in Mechanical Engineering from the University of Pennsylvania (1997). Following his Ph.D., he was a post-doctoral associate with Prof. Daniel D. Joseph at the University of Minnesota until 2000. He joined the Department of Mechanical Engineering at Northwestern University in 2000 where is currently a Professor. Neelesh is a Fellow of the American Physical Society. He has received the NSF CAREER award, the International Conference on Multiphase Flow's Junior Award, the Prominent Researcher Award from microFIP, and has been selected to the Defense Science Study Group. Neelesh has been on the Editorial Boards of the Journal of Computational Physics, ASME Journal of Fluids Engineering, and

Scientific Reports. He has also received several university-wide teaching awards at Northwestern University including Charles Deering McCormick Teaching Professorship.



Enectali Figueroa-Feliciano is the Associate Vice President for Research for National Laboratories at Northwestern and a Professor at Department of Physics and Astronomy. He is interested in finding physics beyond the standard model and technical applications of our methods to quantum computing. He is a member of the Quantum Science Center, one of five DOE National Quantum Initiative centers, and in collaboration with Fermilab is studying the physics of superconducting qubits and their interactions with the environment. He is interested in transmon qubit design, the physics of coherence and two-level systems, quantum acoustics, and novel quantum sensors.



Begum Gulsoy is the Director of Research for Office for National Laboratories and NAISE at Northwestern, a Research Associate Professor at the Department of Materials Science and Engineering with a joint affiliation with the Materials Science Division of Argonne National Laboratory. She earned a Ph.D. (2010) and a M.S. (2008) in Materials Science and Engineering from Carnegie Mellon University, and a B.S. (2006) in Materials Science and Engineering from Sabanci University. Her research focuses on developing computational tools for automated data processing of large, multi-modal tomographic materials data sets for microstructural characterization as well as development of dynamic and smart image acquisition and sampling technologies.