## G2S3 on Quantum Computing & Optimization, Week 1 (July 31 - August 4)

8.00	Monday	Tuesday	Wednesday	Thursday	Friday
8:00 am 8:15 am 8:30 am	Registration (MO #355/356)				
8:45 am 9:00 am	Breakfast (MO #355/356)	Breakfast (MO #355/356)	Breakfast (MO #355/356)	Breakfast (MO #355/356)	Breakfast (MO #355/356)
9:15 am 9:30 am	Break Walk to STEPS #101	Quantum Computing Mini Lecture 2 (MO #451) Giacomo Nannicini	Quantum Computing Mini Lecture 3 (MO #451) Giacomo Nannicini	Quantum Computing Mini Lecture 4 (MO #451) Giacomo Nannicini	Quantum Computing Mini Lecture 5 (MO #451) Giacomo Nannicini
9:45 am 10:00 am	Welcome Remarks (STEPS #101)	Giacomo Nannicini	Giacomo Nannicini	Giacomo Nannicini	Giacomo Nannicini
10:15 am 10:30 am	Opening Keynote (STEPS #101) Anna Grassellino, Director				
$^{10:45 am}$ 11:00 am	SQMS Center, Fermilab	Coffee Break	Coffee Break	Coffee Break	Coffee Break
11:15 am 11:30 am	(MO # 355/356)	(MO #355/356)	(MO #355/356)	(MO # 355/356)	(MO #355/356)
11:30 am 11:45 am	Quantum Computing Mini	Optimization Mini	Optimization Mini	Optimization Mini	Research Talk 1 (MO #451)
$12:00 \ noon_{_{12:15 \ pm}}$	Lecture 1 (MO #451) Giacomo Nannicini	Lecture 2 (MO #451) Swati Gupta	Lecture 3 (MO #451) Swati Gupta	Lecture 4 (MO #451) Swati Gupta	Xiu Yang
12:30 pm 12:45 pm					Research Talk 2
1:00 pm					(MO #451) Luis Nunes Vicente
1:15 pm					
1:30 pm 1:45 pm	Lunch	Lunch	Lunch	Lunch	Lunch
$2:\!00\mathrm{pm}_{_{2:15~\mathrm{pm}}}$	(MO #355/356)	(MO #355/356)	(MO #355/356)	(MO #355/356)	(MO #355/356)
2:30 pm	Optimization Mini	Optimization Mini	Quantum Computing Mini	Optimization Mini	Quantum Computing Mini
$3:00 \mathrm{\ pm}$	$\overline{\text{Lecture 1 (MO \#451)}}$	Lab 1 (MO #121)	Lab 1 (MO #121)	Lab 2 (MO # 121)	Lab 2 (MO #121)
3:15 pm	Swati Gupta	Zeguan Wu, Pouya Sampourma- hani	Ramin Fakhimi, Mohammad H. Mohammadi	Zeguan Wu, Pouya Sampourma- hani	Ramin Fakhimi, Mohammad H. Mohammadi
3:30 pm					
$^{3:45 \mathrm{\ pm}}_{4:00 \mathrm{\ pm}}$					
4:15 pm					
4:30 pm 4:45 pm	Break/Remarks	Break/Remarks	Break/Remarks	Break/Remarks	Break/Remarks
5:00 pm			· ·		
5:15 pm	Presentation Round (MO #451)	Quiet/Network Time (MO #451, #453, #375, #355)	Reimbursement Info. Session (MO #451)	Quiet/Network Time (MO #451, #453, #375, #355)	Quiet/Network Time (MO #451, #453, #375, #355)
5:30 pm 5:45 pm	Arielle Carr	(NIO #401, #403, #010, #000)	Christina Stauffer	(110 #401, #400, #010, #000)	(110 #401, #403, #010, #000)
6:00  pm					
6:15 pm	Dinner Banquet (Zoellner Arts Center)	Dinner ( <b>La Lupita</b> , 4 W 4th St Bethle-	Dinner (MO #355/356)	Dinner (MO #355/356)	Dinner (MO #355/356)
6:30 pm 6:45 pm	()	hem, PA)			
7:00  pm					
7:15 pm					
7:30 pm					
$^{7:45 \mathrm{\ pm}}_{8:00 \mathrm{\ pm}}$					
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## G2S3 on Quantum Computing & Optimization, Week 2 (August 7 - August 11)

8:00 am	Monday	Tuesday	Wednesday	Thursday	Friday
8:15 am					
8:30 am 8:45 am	Breakfast (MO #355/356)	Breakfast (MO #355/356)	Breakfast (MO #355/356)	Breakfast (MO #355/356)	Breakfast (MO #355/356)
9:00 am 9:15 am 9:30 am 9:45 am	Optimization Algorithms Lecture 1 (MO #451) Jeffrey M. Larson	Optimization AlgorithmsLecture 2 (MO #451)Jeffrey M. Larson	QA&O Algorithms Lab 2 (MO #121) David E. Bernal	QC&O Algorithms Lecture 2 (MO #451) Ruslan Shaydulin	Quantum Linear Algebra   Lecture 1 (MO #451)   Arielle Carr
10:00 am 10:15 am 10:30 am 10:45 am 11:00 am					
11:15 am	Coffee Break (MO #355/356)	Coffee Break (MO #355/356)	Coffee Break (MO #355/356)	Coffee Break (MO #355/356)	Coffee Break (MO #355/356)
11:30 am 11:45 am 12:00 noon 12:15 pm	QA&O Algorithms Lecture 1 (MO #451) David E. Bernal	QA&O Algorithms Lecture 2 (MO #451) David E. Bernal	QA&O Algorithms Lecture 3 (MO #451) David E. Bernal	Research Talk 4 (MO #451) Brandon Augustino	Quantum Linear Algebra Lecture 2 (MO #451) Arielle Carr
12:30 pm 12:45 pm 1:00 pm 1:15 pm				Research Talk 5 (MO #451) Luis F. Zuluaga	
1:30 pm 1:45 pm 2:00 pm 2:15 pm	Lunch (MO #355/356)	Lunch (MO #355/356)	Lunch (MO #355/356)	Lunch (MO #355/356)	Lunch (MO #355/356)
2:30 pm 2:45 pm	QA&O Algorithms Lab 1 (MO #121)	Optimization Algorithms	QC&O Algorithms	QC&O Algorithms	Walk to STEPS #101
3:00 pm 3:15 pm 3:30 pm 3:45 pm	Lab I (MO #121) David E. Bernal	Lab (MO #451) Jeffrey M. Larson	Lecture 1 (MO #451) Ruslan Shaydulin	Lab (MO #121) Ruslan Shaydulin	Closing Keynote (STEPS #101) Katherine Klymko, NERSC
4:00 pm 4:15 pm					Final Remarks (STEPS #101)
4:30 pm 4:45 pm	Break/Remarks	Break/Remarks	Break/Remarks	Break/Remarks	
5:00 pm 5:15 pm 5:30 pm 5:45 pm 6:00 pm	Research Talk 3 (MO #451) Jefrey M. Larson	Discussion Panel (MO #451) Jeffrey M. Larson, David E. Bernal, Tamás Terlaky	Quiet/Network Time (MO #451, #453, #375, #355)	Research Talk 6 Ruslan Shaydulin (MO #451)	
6:15 pm 6:30 pm 6:45 pm	Dinner (MO #355/356)	Dinner ( <b>La Lupita</b> , 4 W 4th St Bethle- hem, PA)	Dinner (MO #355/356)	Dinner Banquet (Zoellner Arts Center)	Dinner (MO #355/356)
7:00 pm <sup>7:15 pm</sup> 7:30 pm					
$^{7:45 pm} 8:00 pm$					



# Gene Golub SIAM Summer School (G2S3) on Quantum Computing and Optimization

July 31st - August 11th

Quantum Computing and Optimization Laboratory (QCOL) Industrial and Systems Engineering Department Lehigh University Bethlehem, PA





INDUSTRIAL AND SYSTEMS ENGINEERING

#### **Organizing Committee** 1

#### • Co-Chairs





Tamás Terlaky

• PhD students



Sampourmahani



Brandon Augustino



Arielle Carr

Mohammadhossein Mohammadisiahroudi



Xiu Yang

Ramin Fakhimi

• Staff



Joyce L. Gabay



Mark Motsko

### 2 Important Places

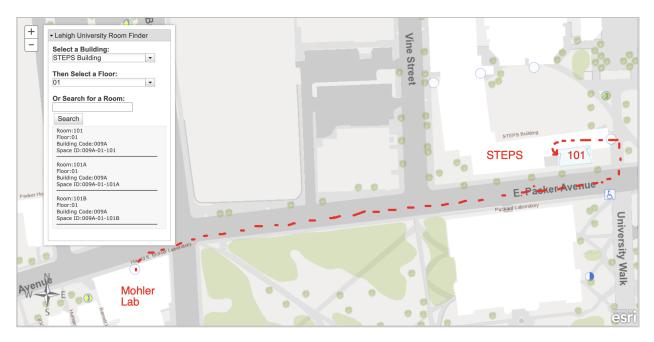
• Lectures: All the lecture sessions will be held in Room #451 of the Mohler Lab building (200 W. Packer Avenue, Bethlehem, PA).



• Labs: All the lab sessions will be held in Room #121 of the Mohler Lab building (200 W. Packer Avenue, Bethlehem, PA).



• Keynote Talks: The Opening and Closing Keynotes (see Schedule) will be held in Room #101 of the STEPS building (1 West Packer Avenue. Bethlehem, PA). The STEPS building is a 3min walk East on Packer Avenue from Mohler Lab.



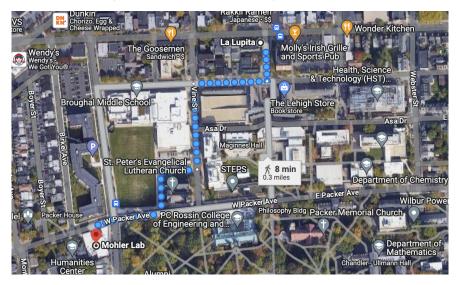
• Breakfast, Lunch and Dinner: Breakfast, Lunch, and (most of the times, see Schedule) will be served in Room #355/356 of the Mohler Lab building (200 W. Packer Avenue, Bethlehem, PA).



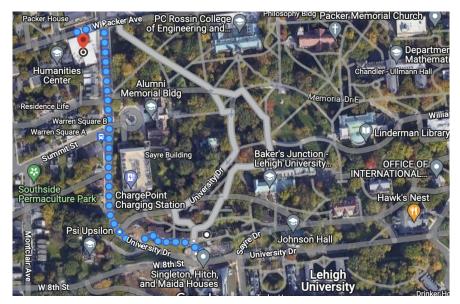
• **Dinner Banquet:** The dinner banquet on Monday, July 31st and on Thursday, August 10th (see Schedule) will be served in the **Zoellner Arts Center** (420 E Packer Ave, Bethlehem, PA). The Zoellner Arts Center is a 9min walk East on Packer Avenue from Mohler Lab.



• Dinner at La Lupita: Dinner banquet on Tuesday, August 1st and on Tuesday, August 8th (see Schedule) will be served in the La Lupita (4 W 4th St Bethlehem, PA). La Lupita is a 8min walk from Mohler Lab.

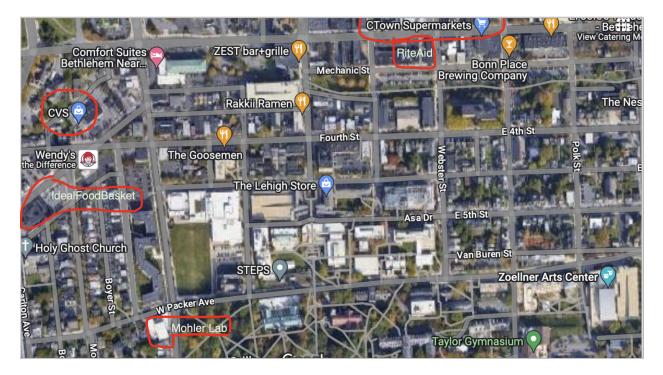


• **Dorms:** Most of the participants will be staying in the **Trembley Park** dorms (71-77 Trembley Drive, Bethlehem, PA). Trembley Park is a 6min walk from Mohler Lab.



• Supermarkets, Drugstores: Supermarkets, Drugstores can be easily found within walking distance of the Mohler Lab building (walk North or North East of Mohler Lab within 3rd and 4th street). Consider for example:

- CVS Pharmacy (Pharmacy/Supermarket): 305 W 4th St., Bethlehem, PA.
- Rite Aid (Pharmacy/Supermarket): 104 E 3rd St., Bethlehem, PA.
- CTown Supermaket: 220/230 E 3rd St., Bethlehem, PA.
- IdealFoodBasket (Supermarket): 410 Montclair Ave, Bethlehem, PA.



#### 3 Program

#### 3.1 Welcome Remarks

Participants will be welcomed to the G2S3 in Quantum Computing & Optimization by remarks from:

- Anand Jagota (Vice Provost for Research, Lehigh University)
- Richard O. Moore (Director of Programs and Services, SIAM)

• Tamás Terlaky (George N. and Soteria Kledaras '87 Endowed Chair Professor, Industrial and Systems Engineering (ISE) Department, Lehigh University)

• Luis N. Vicente (Chair, ISE Department, Lehigh University)

#### 3.2 Opening Keynote



The Opening Keynote will be delivered by Anna Grassellino, Senior Scientist, Fermilab; Center Director, Superconducting Quantum Materials and Systems (SQMS) Center. Her research focuses on radio frequency superconductivity, in particular on understanding and improving SRF cavities performance to enable new applications, spanning from particle accelerators to detectors to quantum information science. Grassellino is a fellow of the American Physical Society and the recipient of numerous awards for her pioneering contributions to SRF technology, including the 2017 Presidential Early Career Award, the 2017 Frank Sacherer Prize of the European Physical Society, the 2016 IEEE PAST Award, the 2016 USPAS prize, a DOE Early Career Award and the New Horizons in Physics Prize by the Breakthrough Foundation. She

holds a Ph.D. in physics from the University of Pennsylvania and a master's of electronic engineering from the University of Pisa, Italy.

**Title:** Enabling Scientific Discovery in Quantum Information Science at the Superconducting Quantum Materials and Systems (SQMS) Center

Abstract: In this talk I will describe the mission, goals and the partnership strengths of the DOE National Quantum Information Science Research Center SQMS. SQMS brings the power of national laboratories, together with industry, academia and other federal entities, to achieve transformational advances in the major cross-cutting challenge of understanding and eliminating the decoherence mechanisms in superconducting 2D and 3D devices, with the final goal of enabling construction and deployment of superior quantum systems for computing and sensing. SQMS combines the strengths of an array of experts and world-class facilities towards these common goals. Materials science experts work in understanding and mitigating the key limiting mechanisms of coherence in the quantum regime. Coherence time is the limit on how long a qubit can retain its quantum state before that state is ruined by noise. It is critical to advancing quantum computing, sensing and communication. SQMS is leading the way in extending coherence time of superconducting quantum systems thanks to world-class materials science and through the world leading expertise in superconducting RF cavities which are integrated with industry-designed and - fabricated computer chips. Leveraging new understanding from the materials development, quantum device and quantum computing researchers will pursue device integration and quantum controls development for 2-D and 3-D superconducting architectures. One of the ambitious goals of SQMS is to build and deploy a beyond-state-of-the-art quantum computer based on superconducting technologies. Its unique high connectivity will provide unprecedented opportunity to explore novel quantum algorithms. SQMS researchers will ultimately build quantum computer prototypes based on 2-D and 3-D architectures, enabling new quantum simulation for science applications. We also employ quantum sensors for several experiments searching for dark matter, gravitational waves and fundamental tests of quantum mechanics.

#### 3.3 Quantum Computing Mini



The Quantum Computing Mini will provide a quick but comprehensive introduction to the fundamentals of quantum computing and will be delivered by **Giacomo Nannicini, Associate Professor, University of Southern California (USC)**. Before joining USC, Nannicini was a Research Staff Member in the Quantum Algorithms group at the IBM T. J. Watson Research Center. He was also an assistant professor in Engineering Systems and Design at the Singapore University of Technology and Design. His main research interest is optimization broadly defined and its applications. Giacomo received several awards, including the 2021 Beale–Orchard-Hays prize, the 2015 Robert Faure prize, and the 2012 Glover-Klingman prize. His algorithms and software are used by one of the largest real-time traffic and mobility information groups in

Europe and in IBM Watson Studio

Lecture 1 : Introduction. Model of computation. Qubit states. Gates and measurement.

Lecture 2 : Phase kickback. Amplitude amplification. Quantum search and variants.

Lecture 3 : Quantum Fourier Transform. Phase estimation.

Lecture 4 : Quantum gradient algorithm. Purifications.

Lecture 5 : Block-encodings. Quantum linear system solvers.

The Quantum Computing Mini lectures' will be complemented by two hands-on computer lab sessions designed and delivered by Ramin Fakhimi and Mohammad H. Mohammadi, PhD student members of the Quantum Computing and Optimization Laboratory (QCOL), Lehigh University.

Lab 1 : Basic introductory session. Quantum Fourier transform

Lab 2 : Quantum phase estimation. Quantum gradient algorithm on a simple example.

#### 3.4 Optimization Mini



The Optimization Mini will provide a quick but comprehensive introduction to the fundamentals of optimization and will be delivered by **Swati Gupta**, **Assistant Professor**, **Massachusetts Institute of Technology (MIT)**. Before joining MIT, Gupta served a the Fouts Family Early Career Professor and Assistant Professor in the Stewart School of Industrial & Systems Engineering at Georgia Tech. She serves as the lead of Ethical AI in the NSF AI Institute on Advances in Optimization. She received a Ph.D. in Operations Research from MIT. Her research interests include optimization, machine learning, and algorithmic fairness, spanning various domains such as e-commerce, quantum optimization, and energy. She received the Class of 1934: Student Recognition of Excellence in Teaching in 2021 and 2022 at Georgia Tech, the JP Morgan

Early Career Faculty Award in 2021, and the NSF CISE Research Initiation Initiative Award in 2019, and the Google Women in Engineering Award (India) in 2011. She was also awarded the prestigious Simons-Berkeley Research Fellowship in 2017-2018, where she was selected as the Microsoft Research Fellow in 2018. Her research and students have received recognition at various venues like INFORMS Doing Good with OR 2022 (finalist), MIP Poster 2022 (honorable mention), INFORMS Undergraduate Operations Research 2018 (honorable mention), INFORMS Computing Society 2016 (special recognition), and INFORMS Service Science Student Paper 2016 (finalist). Dr. Gupta's research is partially funded by the NSF and DARPA.

Lecture 1 : Introduction to Math Optimization. Polyhedral Theory. Linear Programming. Simplex.

Lecture 2 : Discrete Optimization. Computational Complexity. Network Flows. Cutting Planes, Branch and Bound.

Lecture 3 : Non-linear Optimization. Convexity. Gradient Methods.

Lecture 4 : Interior Point Methods and Semidefinite Optimization.

The Optimization Mini lectures' will be complemented by two hands-on computer lab sessions designed and delivered by Zeguan Wu and Pouya Sampourmahani, PhD student members of the Quantum Computing and Optimization Laboratory (QCOL), Lehigh University.

Lab 1 : Using Linear and Integer Optimization solvers/algorithms.

Lab 2 : Using Non-linear and Semidefinite Optimization solvers/algorithms.

#### 3.5 Optimization Algorithms



The Optimization Algorithms lectures will cover derivative-free and stochastic optimization algorithms, as well as optimization algorithms for quantum information systems (QIS) and will be delivered by **Jeffrey M. Larson, Computational Mathematician, Argonne National Laboratory**. Larson develops, analyzes, and implements algorithms for solving difficult numerical optimization problems. He is especially interested in algorithms for solving problems in quantum information science, simulation optimization, and vehicle routing. Jeff joined Argonne in 2014 as a postdoctoral appointee after a postdoctoral position at the KTH Royal Institute of Technology. He earned his Ph.D. in applied mathematics from the University of Colorado Denver in 2012.

Lecture 1, Lecture 2, and Lab : The lectures and lab will be centered around the following topics:

- Derivative-Free Optimization:
  - Common heuristics
  - Mesh Methods
  - Gaussian Processes
  - Line Search methods
  - Trust Region methods
- Stochastic Optimization
  - Kiefer-Wolfowitz
  - SPSA
  - Model-Based Methods
- Optimization for QIS
  - Concurrence maximization
  - Optimal circuit cutting
  - Optimizing variational parameters
  - Frequency quantum
  - Maximizing Quantum Fisher Information
  - In the Lab we will explore the use of optimization methods and models to address problems up and down the quantum computing "stack".

#### 3.6 Quantum Annealing & Optimization (QA&O) Algorithms



The QA&O Algorithms lectures will cover the fundamentals of quantum annealing and its applications in different areas of quantum computing & optimization and will be delivered by **David E. Bernal, Assistant Professor, Purdue University**. Bernal has a Ph.D. in Chemical Engineering from Carnegie Mellon University, where one of his interests was to study the use of quantum algorithms for nonlinear combinatorial optimization. During his Ph.D., Bernal developed and co-taught the course on Quantum Integer Programming. Bernal is currently an Associate Scientist in Quantum Computing at the Research Institute of Advanced Computer Science (RIACS) of the Universities Space Research Association (USRA) and QuAIL at NASA, developing and benchmarking quantum and physics-inspired optimization methods. This Fall, Bernal will start a tenuretrack position at the Davidson School of Chemical Engineering at Purdue University.

Lecture 1, Lecture 2, Lecture 3, Lab 1 and Lab 2 : The lectures and labs will be centered around the topics covered in:

Bernal, D. E., Tayur, S., & Venturelli, D. (2020). Quantum Integer Programming (QuIP) 47-779: Lecture Notes. arXiv preprint arXiv:2012.11382, https://arxiv.org/abs/2012.11382.

and use material from the repository: https://github.com/pedromxavier/QUBO-notebooks

#### 3.7 Quantum Computing & Optimization (QC&O) Algorithms



The QC&O Algorithms lectures will cover the fundamentals of quantum walks and the quantum approximation optimization algorithm (QAOA) and will be delivered by **Ruslan Shaydulin**, **Vice President - Applied Research Lead at JPMorgan Chase & Co.** Shaydulin received the B.S. degree in applied mathematics and physics from the Moscow Institute of Physics and Technology, Moscow, Russia, in 2016, and the Ph.D. degree in computer science from Clemson University, Clemson, SC, USA, in 2020. Shaydulin's research centers on applying quantum algorithms to classical problems, with a focus on optimization and machine learning. Prior to joining JPMorgan Chase, Ruslan was a Maria Goeppert Mayer fellow at Argonne National Laboratory.

Lecture 1 : Quantum walks. Quantum walks for search and optimization.

Lecture 2 : Quantum Approximate Optimization Algorithm (QAOA). QAOA as a quantum walk and its circuit implementation

Lab : implementing QAOA in Qiskit from scratch

#### 3.8 Quantum Linear Algebra



The Quantum Linear Algebra lectures will cover the fundamentals of how to extend linear algebra techniques that are ubiquitous to optimization to the realm of quantum computing and will be delivered by **Arielle Carr, Assistant Professor, Computer Science and Engineering, Lehigh University**. Carr's research focus is in the fields of applied linear algebra and applied numerical analysis, particularly on analysis and development of parallel algorithms and recycling techniques to improve costs associated with computing the iterative solution of large, sparse linear systems and eigenvalue problems. More recently, she has been exploring the necessary theoretical and practical modifications to effectively translate classical linear algebra to quantum linear algebra. She joined Lehigh as a professor of practice in 2018, and earned her Ph.D. in mathematics

from Virginia Tech in 2021.

Lecture 1, Lecture 2 : From Linear Algebra to Quantum Linear Algebra and applications.

- preconditioning quantum linear systems,
- eigenvalues, and the quantum singular value decomposition.
- Krylov methods

#### 3.9 Research Talks

Talk 1: Quantifying and Mitigating Measurement Errors in Quantum Computing

Speaker: Xiu Yang, Industrial and Systems Engineering, Lehigh University

**Abstract:** Various noise models have been developed in quantum computing study to describe the propagation and effect of the noise from imperfect implementation of hardware. We infer such parameters using Bayesian approaches, and implement this method to study the gate and measurement error. By characterising the device errors in this way, we further improve error filters accordingly. Experiments conducted on IBM's quantum computing devices suggest that our approach provides more accurate error mitigation results than existing error-mitigation techniques, in which error rates are estimated as deterministic values.

Talk 2: Trust-region and direct-search methods for stochastic non-smooth derivative-free optimization

Speaker: Luis Nunes Vicente, Industrial and Systems Engineering, Lehigh University

Abstract: Using tail bounds, we introduce a new probabilistic condition for function estimation in stochastic derivative-free optimization which leads to a reduction in the number of samples and eases algorithmic analyses. Moreover, we develop simple stochastic direct-search and trust-region methods for the optimization of a potentially non-smooth function whose values can only be estimated via stochastic observations. For trial points to be accepted, these algorithms require the estimated function values to yield a sufficient decrease measured in terms of a power larger than 1 of the algorithmic stepsize. Our new tail bound condition is precisely imposed on the reduction estimate used to achieve such a sufficient decrease. This condition allows us to select the stepsize power used for sufficient decrease in such a way to reduce the number of samples needed per iteration. In previous works, the number of samples necessary for global convergence at every iteration k of this type of algorithms was  $O(\Delta k^{-4})$ , where  $\Delta k$  is the stepsize or trust-region radius. However, using the new tail bound condition, and under mild assumptions on the noise, one can prove that such a number of samples is only  $O(\Delta k^{-2-\epsilon})$ , where  $\epsilon > 0$  can be made arbitrarily small by selecting the power of the stepsize in the sufficient decrease test arbitrarily close to 1. The global convergence properties of the stochastic direct-search and trust-region algorithms are established under the new tail bound condition. Numerical results are presented comparing the performance of these methods against StoMADS.

Talk 3: Structure-Aware Methods for Expensive Derivative-Free Composite Optimization

Speaker: Jeffrey M. Larson, Argonne National Laboratory

**Abstract:** We present new methods for solving a broad class of bound-constrained smooth and nonsmooth composite minimization problems. These methods are specially designed for objectives that are some known mapping of outputs from a computationally expensive function. We provide accompanying implementations of these methods: in particular, a novel manifold sampling algorithm with subproblems that are in a sense primal versions of the dual problems solved by previous manifold sampling methods and a method that employs more difficult optimization subproblems. For these two methods, we provide rigorous convergence analysis and guarantees. We demonstrate extensive testing of these methods. Open-source implementations of these methods are available.

Talk 4: Quantum interior point methods for Semidefinite Optimization

Speaker: Brandon Augustino, Industrial and Systems Engineering, Lehigh University

**Abstract:** Semidefinite optimization problems form a fundamental family of convex programs due to their expressive power, and the fact that they can be solved in polynomial time using interior point methods (IPMs). The dominant operation at each iterate of an IPM is the solution of a linear system of equations, and recent years have seen a considerable interest in attempting to use quantum linear systems algorithms (QLSAs) to accelerate this step, giving rise to a new class of algorithms known as Quantum Interior Point Methods (QIPMs). In this talk, we discuss the QIPM in its application to solving semidefinite problems, and in particular, how to deal with the challenges posed by quantum noise. We then discuss how iterative refinement techniques can be used to improve the worst-case performance of the QIPM.

Talk 5: QUBO Formulations of Combinatorial Optimization Problems for Quantum Computing Devices

Speaker: Luis F. Zuluaga, Industrial and Systems Engineering, Lehigh University

**Abstract:** Quantum devices can be used to solve constrained combinatorial optimization (COPT) problems thanks to the use of penalization methods to embed the COPT problem's constraints in its objective to obtain a quadratic unconstrained binary optimization (QUBO) reformulation of the COPT. However, the particular way in which this penalization is carried out, affects the value of the penalty parameters, as well as the number of additional binary variables that are needed to obtain the desired QUBO reformulation. In turn, these factors substantially affect the ability of quantum computers to efficiently solve these constrained COPT problems. This efficiency is key towards the goal of using quantum computers to solve constrained COPT problems more efficiently than with classical computers. Along these lines, in this talk we consider how to obtain *best* QUBO reformulations for a number of fundamental COPT problems.

Talk 6: Towards practical quantum optimization

Speaker: Ruslan Shaydulin, JPMorgan Chase & Co.

**Abstract:** Quantum computers have the potential to provide computational speedups for a wide range of industry-relevant problems. However, many hurdles have to be overcome before the proposed algorithms like Quantum Approximate Optimization Algorithm (QAOA) and, more broadly, variational quantum algorithms for optimization can be applied to industrial problems. In this talk, I will present a few results towards that goal. First, I will argue for the centrality of constraints to industry problems and discuss our solutions to enforcing them in quantum optimization. Second, I will demonstrate the hardness of parameter optimization in QAOA when applied to problems with non-integer eigenvalues, and present our recent theoretical and numerical results towards establishing a robust parameter setting strategy for QAOA.

#### 3.10 Closing Keynote



The Closing Keynote will be delivered by Katie Klymko, Staff Member, National Energy Research Scientific Computing (NERSC) Center. Katie Klymko received her PhD in 2018 from UC Berkeley where she worked on the statistical mechanics of non-equilibrium systems using computational and analytical techniques. She was a postdoc at LBL from October of 2018 through September of 2021, working on a range of topics including fluctuating hydrodynamics/finite volume methods for modeling mesoscale systems and more recently quantum computing algorithms. Her work in quantum computing has focused on the development of efficient methods for eigenvalue calculations in molecular systems as well as quantum computing algorithms to explore thermodynamic properties. In October of 2021, she became a staff member at NERSC where

she is working to integrate HPC and quantum computing.

**Title:** Quantum Computing from NERSC's Perspective

**Abstract:** The question of how quantum computing will impact and integrate with HPC over the next decade has become increasingly important as quantum hardware matures. In this talk I will discuss the steps NERSC, the primary scientific computing facility for the Office of Science in the U.S. Department of Energy, is taking to address this question. I will describe our collaborative efforts with Berkeley's Advanced Quantum Testbed, aimed at enhancing hybrid quantum-classical algorithms. Additionally, I will highlight our research and development partnership with QuEra, a neutral atom quantum computing company. Moreover, I will showcase our utilization of NERSC's classical resources to accelerate the advancement of quantum algorithms. By sharing these insights, I hope to provide a comprehensive perspective on the anticipated impact of quantum computing on the next era of supercomputing centers.