**NIMH VIRTUAL WORKSHOP:**

 **SOLVING COMPUTATIONAL CHALLENGES IN GENOMICS AND NEUROSCIENCE VIA PARALLEL & QUANTUM COMPUTING**

**March 28, 2018**

**9:00 am – 1:00 pm EST**

**Goal of the workshop**

This virtual workshop aims to highlight core computational problems faced by genetics and the subdomains of neuroscience that parallel or quantum computing can address. By bringing together experts in quantum and parallel computing with experts in genetics and neuroscience, we hope to start a dialogue between academic and industry partners working in this area with the focus on algorithm optimization and development. This virtual workshop will be the forum and the nexus to find convergence between cross-disciplinary fields that are operating mostly independently – 1) genomics and neuroscience, and 2) AI/machine learning and 3) quantum computing. The goal is to identify key avenues for computation optimization via parallel and quantum algorithms. This workshop will facilitate the use of state-of-art computational technologies for addressing core bottlenecks in genomics and neuroscience.

**Overview**

This workshop will cover the following topics with 5 minutes break following each topic discussion:

* Opening Remarks (10 min)
* Topic 1: Computational Challenges in Genetics and Neuroscience (1.5 hour)
* Topic 2: AI, machine learning and parallel computing (45 min)
* Topic 3: Quantum Algorithms for Accelerated Computation: Opportunities and Challenges (1 hour)
* Roundtable Discussion & Summary (30 mins)

***\*NOTE****: Some speakers are yet to be confirmed and/or subject to change.*

9:00 – 9:10 am: **Opening Remarks** – Thomas Lehner, Geetha Senthil, Susan

Wright, National Institute of Mental Health, Office of Genomics Research Coordination

**Morning Session**

**Chairs:** Alan Anticevic, Ph.D., Yale University and Alan Aspuru-Guzik, Ph.D., Harvard University

**Topic 1: Computational Challenges in Genetics and Neuroscience**

This session is to highlight where computational challenges/bottlenecks exist at the level of scaling (data and computational features) and computational speedup.

9:10 – 9:25 am: **Presentation 1**: Genetics and functional genomics

Michael McConnell, Ph.D., University of Virginia, Michael Gandal, M.D., Ph.D., University of California, Los Angeles

9:25 – 9:40 am: **Presentation 2**: Neurophysiology (processing data, extracting, analysis)

**Potential speakers:** Mike Halassa, M.D., Ph.D., Massachusetts Institute of Technology

9:40 – 9:55 am: **Presentation 3:** Neuroimaging

**Potential speakers:** Alan Anticevic, Ph.D., Yale University, Stephen Smith, Oxford

9:55 – 10:10 am: **Presentation 4**: Quantitative deep phenotypic analysis

**Potential speakers:** Andrey Rzhetsky, Ph.D., University of Chicago, Justin Baker, M.D., Ph.D., Massachusetts General Hospital, Jukka-Pekka Onnela, M.Sc., Ph.D., Harvard University

10:10 – 10:25 am: **Presentation 5**: Computational modeling

**Suggested topic:** Spiking and neural models and ion channel modelling - spiking network simulation

**Speakers:** John Murray, Ph.D., Yale University, Michael Hines, Ph.D., Yale University

10:25 – 10:30 am: **Break**

**Topic 2: AI, machine deep learning and parallel computing**

This session is to discuss application of state-of-the-art classical parallel computing algorithm applications for machine learning, simulation, & optimization of analysis with ‘big’ data.

10:30 – 10:45 am: **Presentation 1**: Overview of machine learning via classical and parallel computing technologies

 **Potential speakers:** Guillermo Sapiro, M.Sc., Ph.D., Duke University

10:45 – 11:00 am: **Presentation 2**: Deep Learning for AI applications - e.g. DeepMind

**Potential speakers:** Tim Lillicrap, Ph.D., DeepMind

11:00 – 11:15 am: **Presentation 3**: Parallel processing & GPUs

**Suggested topic:** Nvidia parallel processing & GPU capabilities for efficient high-performance applications

**Potential speakers:** Alan will reach out to his contact at Nvidia

11:15 – 11:20 am: **Break**

**Afternoon Session:**

**Chairs**: Aram Harrow, Ph.D., Massachusetts Institute of Technology, and John Murray, Ph.D.,

Yale University

**Topic 3: Quantum Algorithms for Accelerated Computation: Opportunities and Challenges**

This session will discuss the current state of quantum hardware and algorithms.  What kind of advantages (either in terms of speed or solution quality) can be obtained by using quantum machine learning?  How close are existing or proposed near-term hardware platforms to being able to implement these algorithms?

11:20 – 11:35 am: **Presentation 1:** Overview and primer: what is quantum computing good for?

**Potential speakers:**  Alán Aspuru-Guzik, Ph.D., Harvard University

11:35 – 11:50 am: **Presentation 2**: Status and Prospects for Quantum Hardware

**Potential speaker:** Nicole Barberis, IBM

11:50 am – 12:05 pm: **Presentation 3:** Promising Quantum Computing Algorithms on the

Horizon

**Potential speakers:** Ashley Montanaro, Ph.D., University of Bristol

12:05 – 12:20 pm: **Presentation 4**: Quantum Machine Learning and Optimization

Seth Lloyd, Massachusetts Institute of Technology

12:20 – 12:30 pm: **Break**

12:30 – 12:50 pm:  **Roundtable Discussion & Summary**

**Moderators:** Stefan Bekiranov, University of Virginia & John Murray, Yale University

* What are the immediate avenues for computation optimization via parallel computing?
* Which problems are suitable for parallel vs. quantum computing?
* What are the distinct challenges facing parallel vs quantum computing platforms?
* Which are the most impactful avenues for quantum algorithm development from the standpoint of neuroscience and genomics?
* Opportunities for public private partnership?

12:50 – 1:00 pm: **Summary/Closing Remarks**

**Potential speakers:** Alán Aspuru-Guzik, Harvard University, Alan Anticevic, Yale University

1:00 pm:  **Adjourn**