NIMH VIRTUAL WORKSHOP:
SOLVING COMPUTATIONAL CHALLENGES IN GENOMICS AND NEUROSCIENCE VIA PARALLEL & QUANTUM COMPUTING

March 28, 2018

9:00 am – 1:00 pm EDT

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 (1.15 hour)
- Topic 2: AI, machine learning and parallel computing (1 hour)
- Topic 3: Quantum Algorithms for Accelerated Computation: Opportunities and Challenges (1 hour)
- Roundtable Discussion & Summary (30 mins)
- Summary/closing remarks (10 mins)

9:00 – 9:10 am: **Opening Remarks** – Thomas Lehner, Ph.D., M.P.H., Geetha Senthil, Ph.D., Susan Wright, Ph.D., 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) – Michael Halassa, M.D., Ph.D., Massachusetts Institute of Technology

9:40 – 9:55 am: **Presentation 3:** Neuroimaging – Alan Anticevic, Ph.D., Yale University

9:55 – 10:10 am: **Presentation 4**: Quantitative deep phenotypic analysis – Justin Baker, M.D., Ph.D., Massachusetts General Hospital

10:10 – 10:25 am: **Presentation 5**: Computational modeling (spiking, neural models and ion channel modeling - spiking network simulation) – 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 – Guillermo Sapiro, M.Sc., Ph.D., Duke University

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

11:00 – 11:15 am: **Presentation 3**: Parallel processing & GPUs (Nvidia parallel processing & GPU capabilities for efficient high-performance applications) – Fernanda Foertter, M.S., 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? – Alán Aspuru-Guzik, Ph.D., Harvard University

11:35 – 11:50 am: **Presentation 2**: Status and Prospects for Quantum Hardware – Denise Ruffner, IBM

11:50 am – 12:05 pm: **Presentation 3:** Promising Quantum Computing Algorithms on the Horizon – Ashley Montanaro, Ph.D., University of Bristol

12:05 – 12:20 pm: **Presentation 4**: Quantum Machine Learning and Optimization – Seth Lloyd, Ph.D., Massachusetts Institute of Technology

12:20 – 12:30 pm: **Break**

12:30 – 12:50 pm: **Roundtable Discussion & Summary**
Moderators: Stefan Bekiranov, Ph.D., University of Virginia & John Murray, Ph.D., 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** – Alán Aspuru-Guzik, Ph.D., Harvard University, Alan Anticevic, Ph.D., Yale University

1:00 pm: **Adjourn**