

Panel: HPC Challenges in Your Scientific Work

Moderator: Scott Callaghan



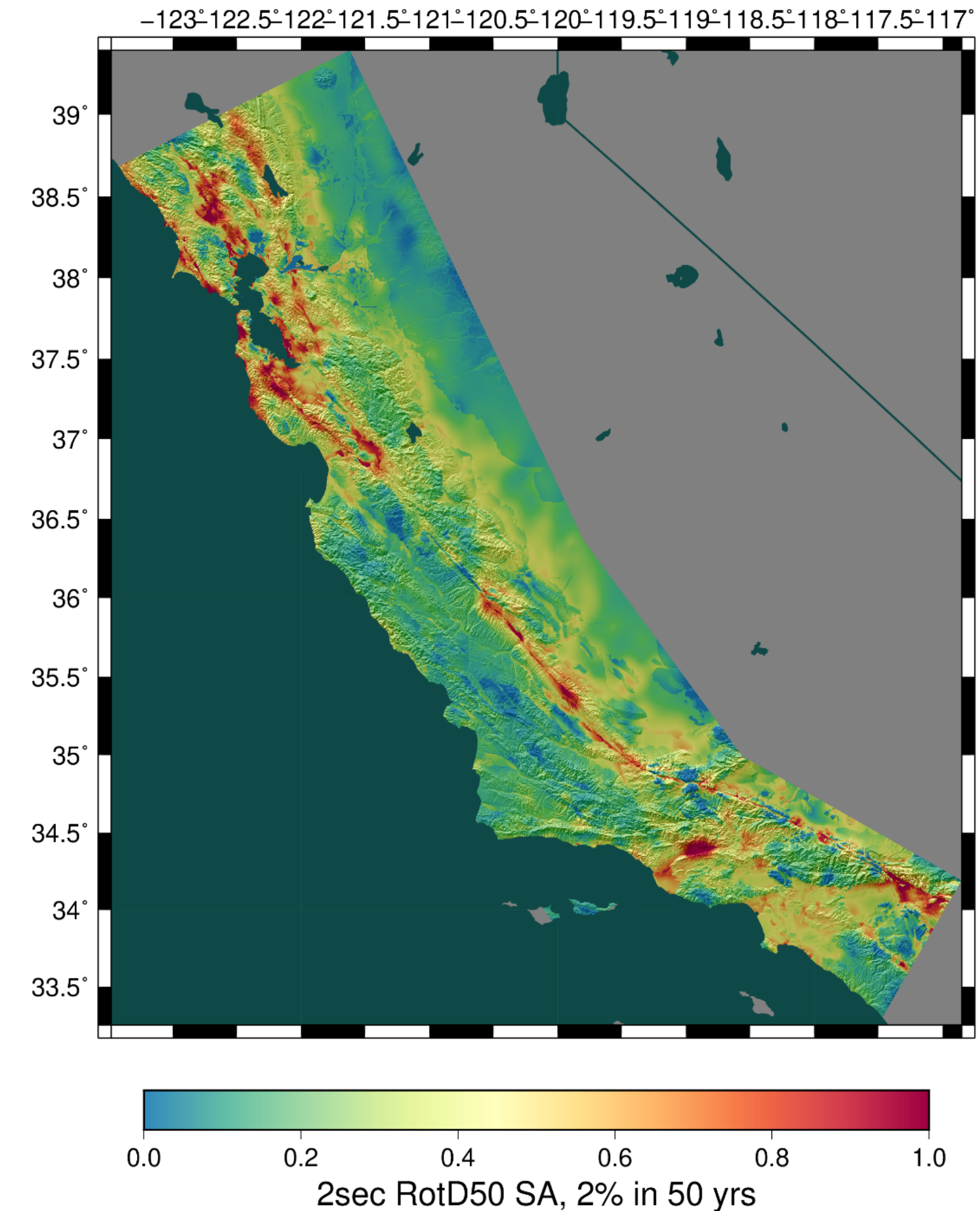
**Join at
slido.com
#2162 914**

**Tom Cheatham
Sarah Beecroft
Samantha Wittke
Michelle Kuchera**

Your Friendly Moderator: Scott Callaghan



- Computer Scientist at the Statewide California Earthquake Center
 - Perform simulations of 600k earthquakes using HPC and HTC for seismic hazard
 - M.S. in CS/HPC
-
- Chair of the ACM Special Interest Group in HPC Education (SIGHPC Education)



Tom: large scale biomolecular simulation, RNA / ligands, force field validation, optimization and assessment

Thomas Cheatham, III

Professor of Medicinal Chemistry, College of Pharmacy, University of Utah, 1/2000-
Director, Center for High Performance Computing, University of Utah 7/1/14-

B.A. Chemistry, B.A. Mathematics & Computer Science, Middlebury, ~1988

1988-1990	1990-1997	1997-2000	2000-present
programmer/analyst	graduate school	NIH postdoc	Res Asst Prof → Professor
Harvard U (DAS)	NSF centers	NIH only	CHPC+AAB→TG→XSEDE→BW
CM-2, CM-5, MasPar	T3D, T3E, Crays	beowulf, IBM SP-2	(many + GPUs)



DOE Summer Institute @ Los Alamos (vector)
PSC Summer Institute in parallel computing
PSC Workshop on Heterogeneous Computing
PSC AMBER Workshop (Teacher)

Allocations committee, chair
TeraGrid Science Advisory Board, chair
XSEDE User Advisory Committee, chair
XSEDE SMT, SAB
Blue Waters SETAC
ACI-REF PI Chair, Co-PI
CaRCC Council Chair
RMACC, Vice-Chair / Board
CCES, UNICAMP, Brazil, Intl Adv Board
E-CAS Advisory Board
Frontera @ TACC, Delta @ NCSA
CI CoE – RCD Nexus
ACCESS Research Advisory



Sarah Beecroft



Pawsey

- BSc (Hons) Human Biology
- PhD in human neurogenetics
- Life Science Supercomputing Applications Specialist





Samantha Wittke

CSC - IT Center for Science
CodeRefinery



Application specialist at CSC, Finland

→ User support (e-mail, weekly virtual support sessions), training, documentation, research infrastructure

CodeRefinery

→ From participant to helper, expert helper to co-organizer and instructor; now community manager

Nordic-RSE board member

Background in **Geoecology** and **Geoinformatics** (PhD in progress)

samantha.wittke@csc.fi

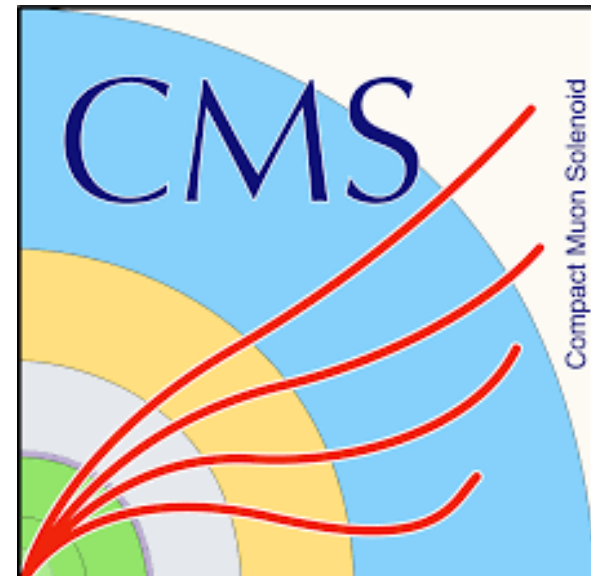
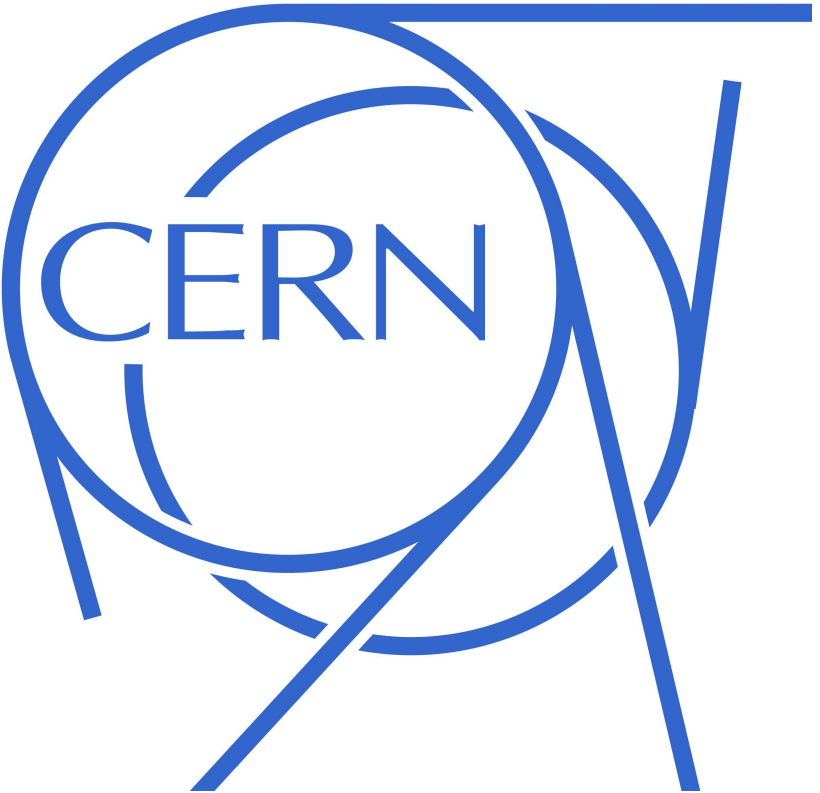
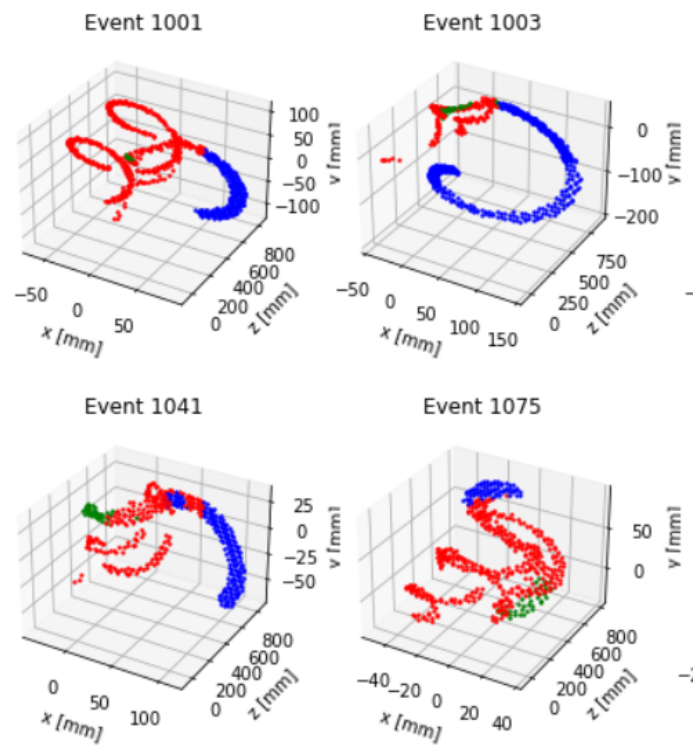
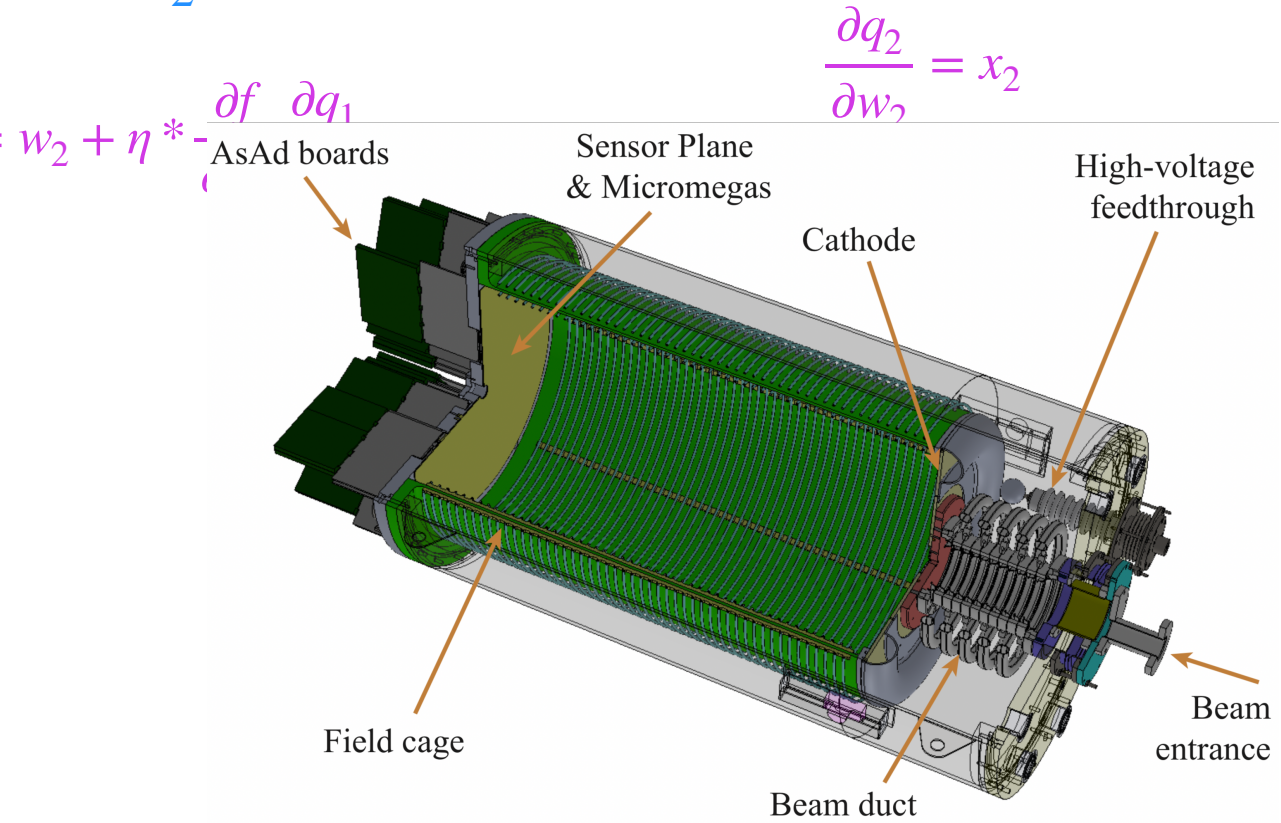
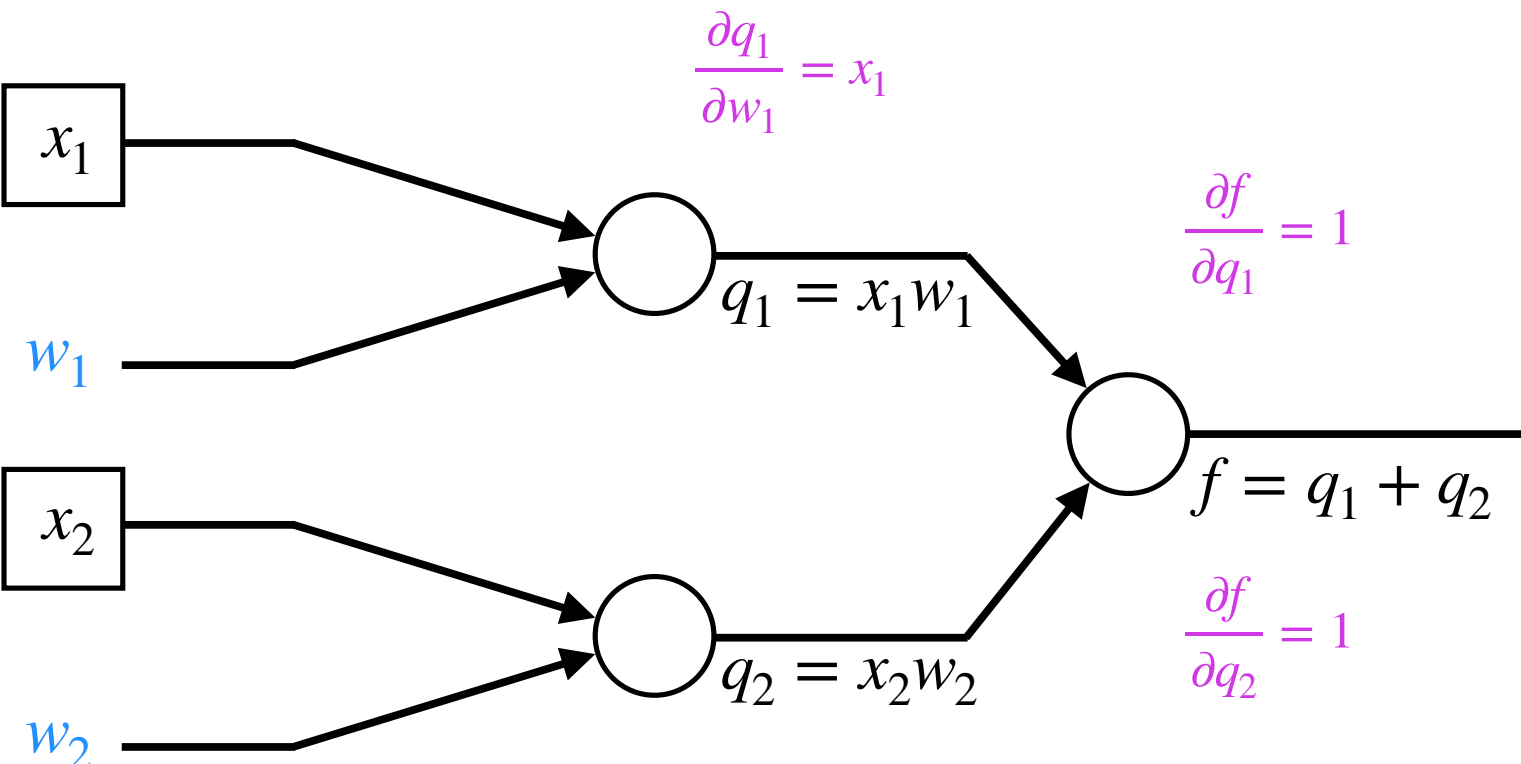
MICHELLE KUCHERA

B.S., M.S. PHYSICS

M.S., PH.D. COMPUTATIONAL SCIENCE



$$w_1 = w_1 + \eta * \frac{\partial f}{\partial q_1} \frac{\partial q_1}{\partial w_1}$$



PhD: GPUs for Bayesian Neural Networks (🙄)



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