Computational Frontier

KITP Snowmass Theory Frontier Conference

Frontier Conveners: *Steven Gottlieb (Indiana University)*, Daniel Elvira (Fermilab), Benjamin Nachman (Berkeley Lab)

Topical Group Conveners: Stephen Bailey (LBL), Wahid Bhimji (LBNL), Peter Boyle (BNL), Giuseppe Cerati (FNAL), Kyle Cranmer (NYU), Gavin Davies (Mississippi), Katrin Heitmann (ANL), Walter Hopkins (ANL), Travis Humble (ORNL), Matias Carrasco Kind (Illinois/NCSA), Meifeng Lin (BNL), Peter Onyisi (Texas), Kevin Pedro (FNAL). Gabe Perdue (FNAL), Ji Qiang (LBNL), Amy Roberts (Denver), Martin Savage (U. Washington), Phiala Shanahan (MIT), Kazuhiro Terao (SLAC), Daniel Whiteson (Irvine), Frank Wuerthwein (UCSD)

Computational Frontier Organization

CompF01
Experimental Algorithm Parallelization

Giuseppe Cerati (FNAL), Katrin Heitmann (ANL), Walter Hopkins (ANL)

CompF02
Theory Calculations & Simulation

Peter Boyle (BNL), Kevin Pedro (FNAL), Ji Qiang (LBNL)

CompF03
Machine Learning

Phiala Shanahan (MIT), Kazu Terao (SLAC), Daniel Whiteson (Irvine)

CompF04
Storage and Processing Resource Access
(Facility and Infrastructure R&D)

Wahid Bhimji (NERSC), Meifeng Lin (BNL), Frank Würthwein (UCSD)

CompF05
End User Analysis

Meeting 2/28

Gavin Davis (U. Mississippi), Peter Onyisi (U. Texas at Austin), Amy Roberts (UC Denver)

CompF06
Quantum Computing

Travis Humble (ORNL), Gabriel Perdue (FNAL), Martin Savage (U. Washington)

CompF07
Reinterpretation & Long-term Preservation of Data and Code

Stephen Bailey (LBNL), Kyle Cranmer (NYU), Matias Carrasco Kind (Illinois/NCSA)

Some facts about LOIs

- 80 LOIs list both Theory Frontier (TF) and Computational Frontier (CompF):
    - For 68 LOIs, TF is listed first
    - For 12 LOIs, CompF is listed first
- Distribution of primary frontier for the 68:
    - Theory (19), Energy (18), Cosmic (11), Rare & Precision (12), Neutrino (7), Accelerator (1), Instrumentation (0), Underground (0), Community (0)
- Distribution of 68, listing both topical groups:

	TF1	TF2	TF3	TF4	TF5	TF6	TF7	TF8	TF9	TF10	TF11
CompF2	8	4	1	1	29	9	7	6	11	2	6
CompF3	1	1	0	0	1	2	7	0	0	0	0
CompF4	0	0	0	0	2	0	0	0	0	0	0
CompF6	6	0	0	0	1	0	0	0	1	6	0

CompF2: Theory Calculations & Simulations

- Six working groups:
  - Cosmic Calculations: Salman Habib, Zarija Lukic. Overlap: TF09
  - Accelerator Simulation
  - Beam and Detector Simulation
  - Physics Generators: Hugh Gallagher, Philip Ilten, StefanHoche, Steve Mrenna, Steven Gardiner, Taylor Childers. Overlap: TF6, TF7, TF8, TF11
  - Perturbative Calculations: Andreas von Manteuffel. Overlap: similar to generators
  - Lattice QCD: Andreas Kronfeld
- 117 LOIs, many cross referenced with a TF topical group.
- Expect at least one white paper from each of the 6 groups above.
- More are welcome!

CompF2: Theory Calculations & Simulations

- Some of white papers expected that are of interest to Theory Frontier
    - Precision Physics Computational Needs: Tobias Neumann, Andreas von Manteuffel, Fernando Cordero
    - USQCD 2019 computing (pre-existing): summary whitepaper page by Andreas Kronfeld + others, with references to USQCD white papers.
    - LQCD Theory forward-looking expansion: Peter Boyle, Chulwoo Jung, USQCD authors
    - Conformal bootstrap: TBD
    - Proposed lattice calculations: cc/cover letter to CompF (not really computing-focused)
    - Cosmology: Salman Habib et al.
    - Vision for generators: Hugh Gallagher, Philip Ilten, Stefan Höche, Steve Mrenna, Steven Gardiner, Taylor Childers
    - Vision for neutrino generators: Hugh Gallagher, Philip Ilten, Stefan Höche, Steve Mrenna, Steven Gardiner, Taylor Childers
    - HSF (HEP Software Foundation) generators (pre-existing): Andreas Valassi

CompF3: Machine Learning (ML)

- Machine learning is a popular topic in both experiment and theory
- Phiala Shanahan is the topical group convenor working in theory
    - Unfortunately, she was not able to attend this meeting
    - Jesse Thaler spoke on Thursday
- Seven page Google Doc detailing expected white papers and authors
    - https://docs.google.com/document/d/1BFPS7UMFnDPYUVQlSnMkQwvVPgBjz3e1l41iYk_iFL0/edit
    - **Symmetry-group equivariant architectures (David Miller, Mariel Pettee)**
    - **Applications to lattice field theory (Dan Hackett)**
    - **Model-independent searches for New Physics (Charanjit Khosa)**
    - **Opportunities in ML for HEP Researchers (**Savannah Thais)
    - Plus others that might be of less interest to theorists
- There are many opportunities for ML in theory and experiment.

CompF4: Storage and Processing Resource Access

- There were only two LOIs that involved any TF topical group
- Apparently only the lattice field theorists (TF5) are concerned about access!?
- Please consider whether your science will need computing or storage in the next five to ten years (or beyond) that the DOE and NSF need to think about funding.

CompF6: Quantum Computing

- There is a lot of overlap with TF10 Quantum Information Science
  - They have been meeting to coordinate. Topics are not identical
  - Nice talk by Hank Lamm on Quantum Simulations overlaps with CompF interests
- There were also many LOIs with TF1 String Theory, quantum gravity, black holes
- White papers and leads/authors
  - QC for HEP Data Analysis Andrea Delgado and Jean Roch Vlimant
  - Quantum Networks for HEP, Nick Peters
  - Quantum Software Tools and Testbeds for HEP, Travis Humble and Raphael Pooser
  - Quantum Simulation of Field Theories for HEP, Zohreh Davoudi and Christian Bauer
  - Quantum Simulation of Open Systems, Adam Lyon and Jim Kowalkowski
  - Quantum Materials Science Research for HEP, Mattia Chechin and Silvia Zorzetti
  - Tensor Networks for HEP, Yannick Meurice and James Osborn
  - Gravity, Black Holes, and Quantum Computing, Simon Catterall, Veronika Hubeny, and Dan Harlow
  - Machine Learning and Architectural Perspectives for Quantum HEP Applications, Koji Terashi

Key Issues

- Computational Frontier is not like some of the others
  - HEP no longer produces our own custom hardware (for the most part), but DOE has significant influence on industry at high end
  - The hardware we use is not expected to last the life of a large experiment
    - We refresh and change hardware every few years
    - Last decade (or so) has seen multiple disruptive architecture changes
    - Need to continually monitor, engage, and adapt
  - Software may have a much longer lifetime
    - However, it can evolve considerably over the life of an experiment or theoretical collaboration
    - Rapidly evolving programming paradigms & hardware drive radical change in software
    - Languages also have changed over time, Fortran, C, C++, Python, ???
  - Computing skills are in great demand in industry
    - Service to the nation, but we need to sustain our own workforce

Key Questions I

- In view of changing computer architecture, can we parallelize important codes to take advantage of multiple levels of parallelism?
- Can we deal efficiently with multiple levels of memory and storage?
- In a world of distributed computing, do we have sufficient storage with appropriate properties?
    - Can we move the data from storage to compute resources?
- In the longer term, what new experiments might be built and what will be their computing demands?
    - Can those demands be met at reasonable cost?
- Do we need new computing research & engagement in the short term to satisfy future computing challenges?
- HEP may benefit from aggressively accelerated leadership HPC facilities, but how do we cope with multiple custom software environments?

Key Questions II

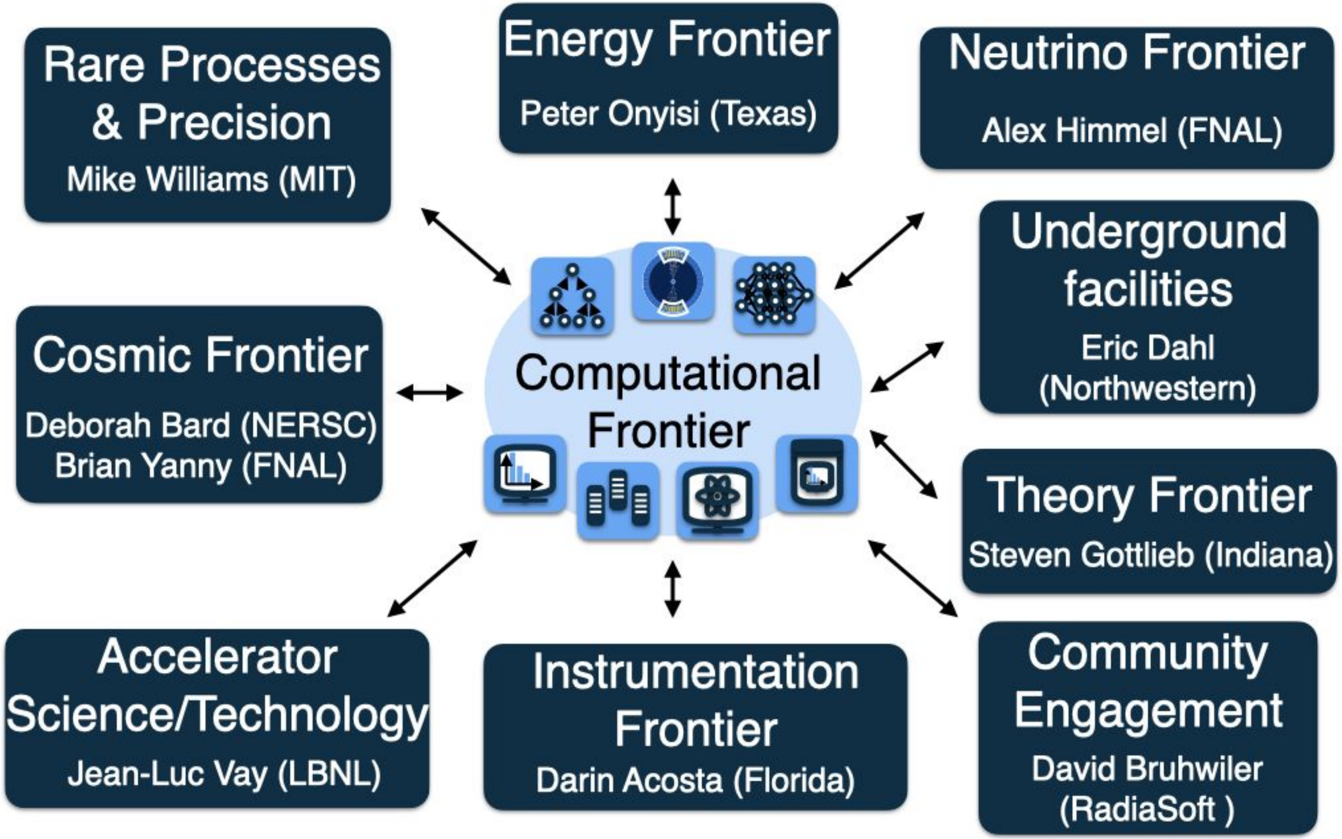
- How can we best take advantage of exciting developments in:
    - machine learning and artificial intelligence?
    - quantum computing?
        - Do we need our own computing center with multiple experimental computers?
        - How can DOE and NSF centers better support ML/AI and QC projects?
- How to sustainably develop, collaborate on, support, and maintain software?
- How to ensure reproducibility, extensibility & reliability?
- Do we have enough physicists with computing skills to develop the software that will be needed?
- How do we train people in computing so that they have the requisite skills?
- Do we need to employ computer scientists, applied mathematicians & engineers to build multidisciplinary teams?
    - Can we afford to do so?
    - Can we afford not to do so?

Future plans

- Hope members of the theory community will continue to be involved or get involved with topical groups of Computation Frontier relevant to their research need.
- Mailing lists and slack channel details can be found on Snowmass wiki
- CompF goal is to identify:
  - Computing needs that must be met to achieve success
  - Opportunities to advance and take advantage of machine learning and quantum computing
  - Research in computing that must be performed to achieve our scientific goals
  - Ways to leverage the large national investments by DOE and NSF in cyberinfrastructure
  - Ways to assure an adequate number of personnel to develop, support, and maintain needed software

Thank You!

Liaisons


Rare Processes & Precision
Mike Williams (MIT)
Energy Frontier
Peter Onyisi (Texas)
Neutrino Frontier
Alex Himmel (FNAL)
Cosmic Frontier
Deborah Bard (NERSC)
Brian Yanny (FNAL)
Computational Frontier
Underground facilities
Eric Dahl (Northwestern)
Theory Frontier
Steven Gottlieb (Indiana)
Accelerator Science/Technology
Jean-Luc Vay (LBNL)
Instrumentation Frontier
Darin Acosta (Florida)
Community Engagement
David Bruhwiler (RadiaSoft)