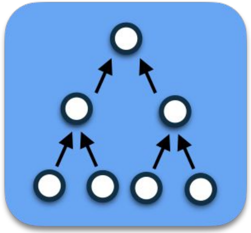
Computational Frontier

Community Planning Meeting Thursday Summary

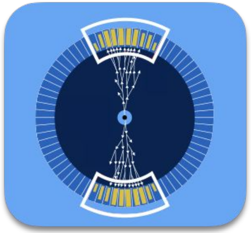
Frontier Conveners: *Steven Gottlieb (Indiana University)*, Oli Gutsche (Fermilab), Benjamin Nachman (Berkeley Lab)

Topical Group Conveners: Wahid Bhimji (LBNL), Peter Boyle (BNL), Giuseppe Cerati (FNAL), Kyle Cranmer (NYU), Gavin Davies (Mississippi), Daniel Elvira (FNAL), Rob Gardner (UChicago), Katrin Heitmann (ANL), Mike Hildreth (Notre Dame), Walter Hopkins (ANL), Travis Humble (ORNL), Matias Carrasco Kind (Illinois/NCSA), Peter Onyisi (Texas), Gabe Perdue (FNAL), Ji Qiang (LBNL), Amy Roberts (Denver), Martin Savage (Washington), Phiala Shanahan (MIT), Kazu Terao (SLAC), Daniel Whiteson (Irvine), Frank Wuerthwein (UCSD)



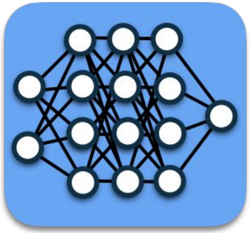
CompF01
Experimental Algorithm Parallelization

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



CompF02
Theory Calculations & Simulation

Peter Boyle (BNL), Daniel Elvira (FNAL), Ji Qiang (LBNL)



CompF03
Machine Learning

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

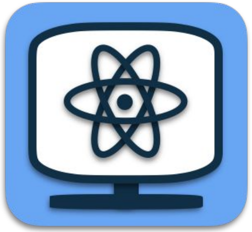
CompF04
Storage and Processing Resource Access

(Facility and Infrastructure R&D)

Wahid Bhimji (NERSC), Rob Gardner (U. Chicago), Frank Würthwein (UCSD)

CompF05
End User Analysis

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

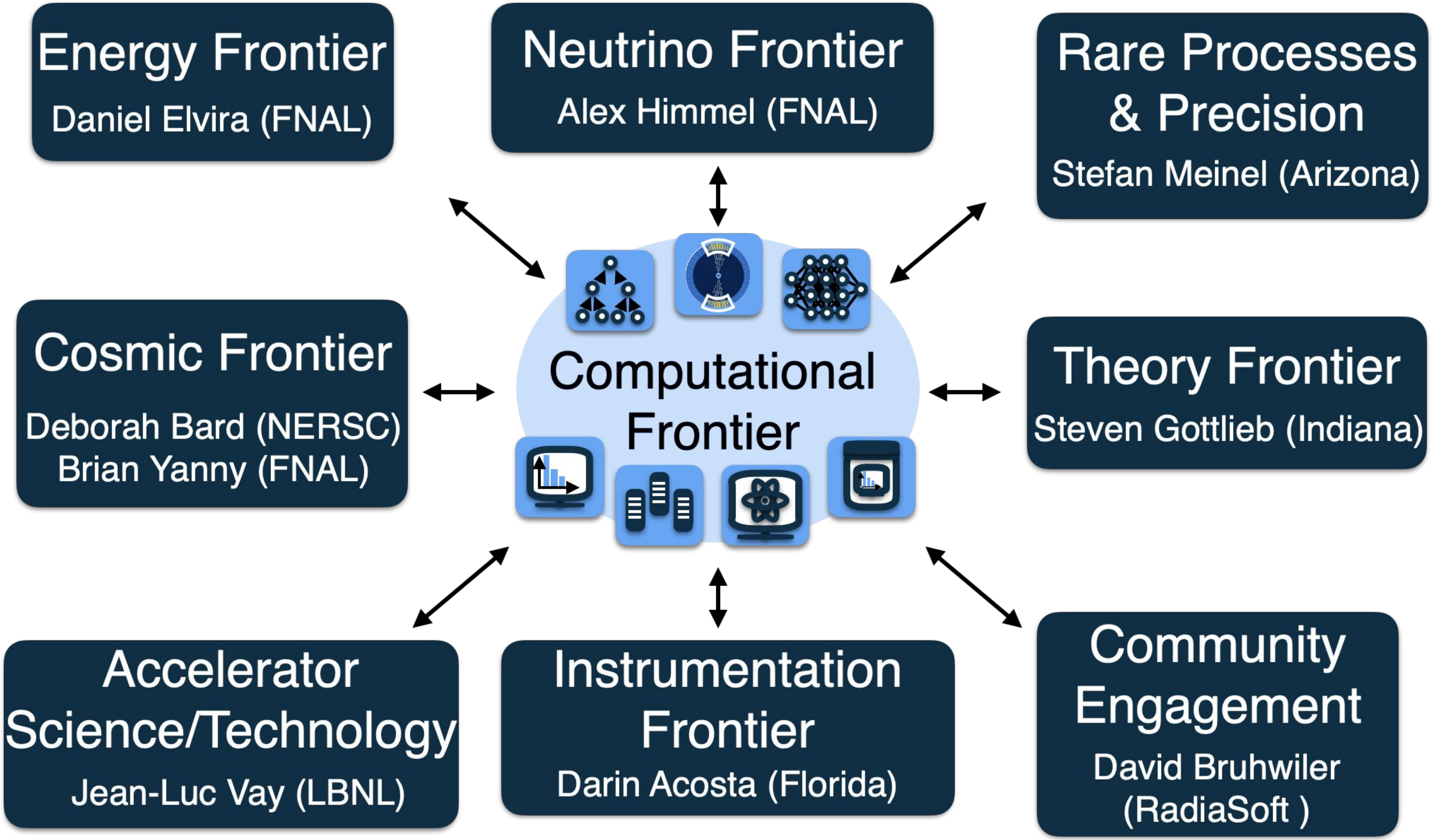


CompF06
Quantum Computing

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

CompF07
Reinterpretation & Long-term Preservation of Data and Code

Kyle Cranmer (NYU), Mike Hildreth (Notre Dame), Matias Carrasco Kind (Illinois/NCSA)


Energy Frontier
Daniel Elvira (FNAL)
Neutrino Frontier
Alex Himmel (FNAL)
Rare Processes & Precision
Stefan Meinel (Arizona)
Cosmic Frontier
Deborah Bard (NERSC)
Brian Yanny (FNAL)
Computational Frontier
Theory Frontier
Steven Gottlieb (Indiana)
Accelerator Science/Technology
Jean-Luc Vay (LBNL)
Instrumentation Frontier
Darin Acosta (Florida)
Community Engagement
David Bruhwiler (RadiaSoft)

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?

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 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?

Outcomes of CPM Breakout Sessions

- We have 130 LOIs in which we are the primary frontier
- We are also listed on 97 additional LOIs
- Computing is needed for all experiments and many theoretical calculations
    - 13 joint sessions held on Tuesday
    - 4 joint sessions on Wednesday
    - It is impossible to adequately summarize ~230 LOIs and 17 joint sessions in a 15 minute presentation.
- We have had many opportunities to work with the topical group conveners in other frontiers in order to learn of their needs and plans
    - We do not yet know what new experiments will be proposed so cannot yet start to anticipate their needs except with the broadest brush

CPM Breakout Sessions (continued)

- Concern about training and workforce development is common across our topical groups and frontiers
- Cosmic frontier would benefit from central data storage that would allow better collaboration among surveys
- Effort for common software used by many experiments needs a new way of common support, e.g., GEANT
- Innovation in machine learning requires public benchmark datasets
- The proliferation of parallel sessions was a challenge:
    - Many relevant sessions. Hard to integrate what has been going on. Almost exclusively attended energy frontier. Need to bring different communities together.
    - Multiple sessions in parallel discussing machine learning
    - We will need to address this challenge, probably through our future interfrontier workshops

Future plans

- We will soon be deciding on the need for meetings with the other Frontiers
- We have biweekly meetings of our topical group conveners and liaisons
- We expect that we will want to do some surveys of large experimental and theoretical collaborations to determine their needs and concerns
- Topical group conveners will work with community to assure a reasonable number of white papers provide adequate information to back up our findings
- 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