Computational Frontier Status Update at AF1, Snowmass21

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Computational Frontier Organization

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), 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), Matias Carrasco Kind (Illinois/NCSA)

Computational Frontier Organization

CompF02
Theory
Calculations
& Simulation

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

Cosmic Calculations
Accelerator Simulation
Beam and Detector Simulation
Physics Generators
Perturbative Calculations
Lattice QCD

(other groups also have sub-topics - this is just for illustration)

Computational Frontier Organization

CompF03

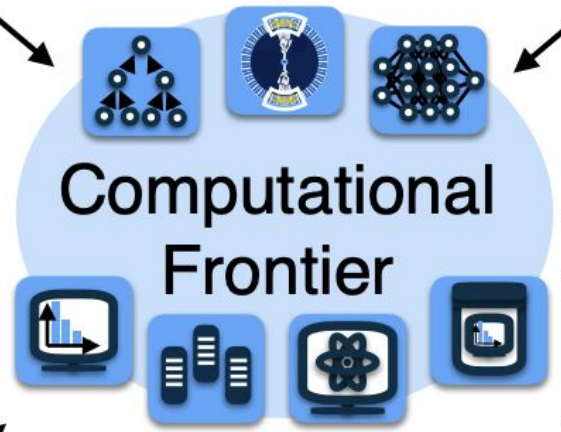
Machine Learning

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

Physics-specific ML
Simulations
Interpretability & Validations
Community Tools & Standards
Resource Needs & Management
Education & Engagement

(other groups also have sub-topics - this is just for illustration)

Liaisons



Rare Processes & Precision
Stefan Meinel (Arizona)

Energy Frontier
Daniel Elvira (FNAL)

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)

Joint CF-AF Discussions from Snowmass Day (9/24)

Asked the question and collected feedback to:

- What are your concerns about software and computing, what keeps you up at night?
- What do we (the Computational Frontier) need to be aware of so that it ends up in our report?
- What are your (the other frontiers) requirements/ project-ions related to software and computing that we should be aware of? Is there existing documentation for them?
- Are there new developments on the horizon that would drive software and computing challenges? New physics, new instrumentation, new simulations?

Feedback & results were channeled into topical groups.

a. Accelerator Modeling
   I. List particle accelerator problems being modelled and to be modelled in your field
   II. Describe the current modeling capabilities to address these problems
      A. Computer hardware used (CPU, GPU, cloud computing, etc)
      B. Software/program paradigm used (serial, parallel, MPI, OpenMP, Hybrid, etc)
      C. Numerical methods used
      D. Current staff/funding level
      E. Education level
      F. Other modeling capabilities
   III. List future needs to address these problems
      A. Computer hardware needs
      B. Software development and maintenance needs
      C. Numerical algorithm/applied math needs
      D. Staff/funding needs
      E. Education needs
      F. Other needs (ML, quantum computing, etc)

Joint CF-AF Discussions from Snowmass Day (9/24)

Feedback & results were channeled into topical groups, excerpts:

Dmitri: EIC, discussions on AI/ML to optimise accelerators. Did not hear about needs for large scale needs, like data analysis for EIC, but likely the area we should ask for scale of needs.

Dmitri: Many facets of computing: simulations, running the experiment in production, design questions.

SG. Are there reports on level of need? JLV Simulation side particularly acute for beam simulation.
Plasma accelerator side ; large space need for large scale simulation, and not just AI/ML. ECP report.

Is Edge relevant for operations/quality/control:
DD - some review of future modern accelerators require would be needed but probably smaller than experiments requirements.
Perhaps 10%, in future might change. Type of computing might be different.

VS: enormous numbers of code, diverse, supported by many groups and benchmarking is not finished.
Not really community standards. Some (madx supported by big labs).

VS: Machines are complex and different parts cannot be viewed/simulated in isolation, need code that can encompass the full system simulation, not there yet but community is thinking about it.

VS: Feedback and control - none use AI/ML but might in future. Something needs to be done

VS: Many codes are common use between accelerator and detectors. Should work with colleagues, Fluke, Geant, Mars etc.... Community standard codes should be supported on a regular/consistent predictable basis. Has been a big challenge in the past, resources for this are not available at a sufficient level. National Labs would be natural places for some of this.

SG: code support and maintenance

Software and Computing for Small HEP Experiments (11/15-16)

hosted by the Snowmass Computational Frontier (CompF) - centered around software and computing for the "small" experiments in our community. The mandate for this workshop was:

- Identify unique *computational challenges* of the "***small" experiment community***
  In order to be inclusive, no imposed definition of "small" - asked experiments to self-select.
- *Gather input* about what is needed in terms of computation for these experiments to be successful
- *Connect members* of the "small" experiment community to the computational frontier in Snowmass and ***encourage participation in topical groups***
- Foster the ***development and re-use of open-source software***, building on the work of the *HEP Software Foundation* and other *collaborative efforts* within the community.

Brief results (summary by Ben Nachmann)

- "Just because the experiments are small does not mean the needs are small."
- ***A white paper is evolving and anyone is welcome to join.***
- All working groups might be interested in this white paper.
- Challenges are ***more acute*** for small experiments.

See https://indico.physics.lbl.gov/event/1756/ and discussion continues on #computingforsmallexps on Slack.

Activities in beam & accelerator modeling @ Snowmass21

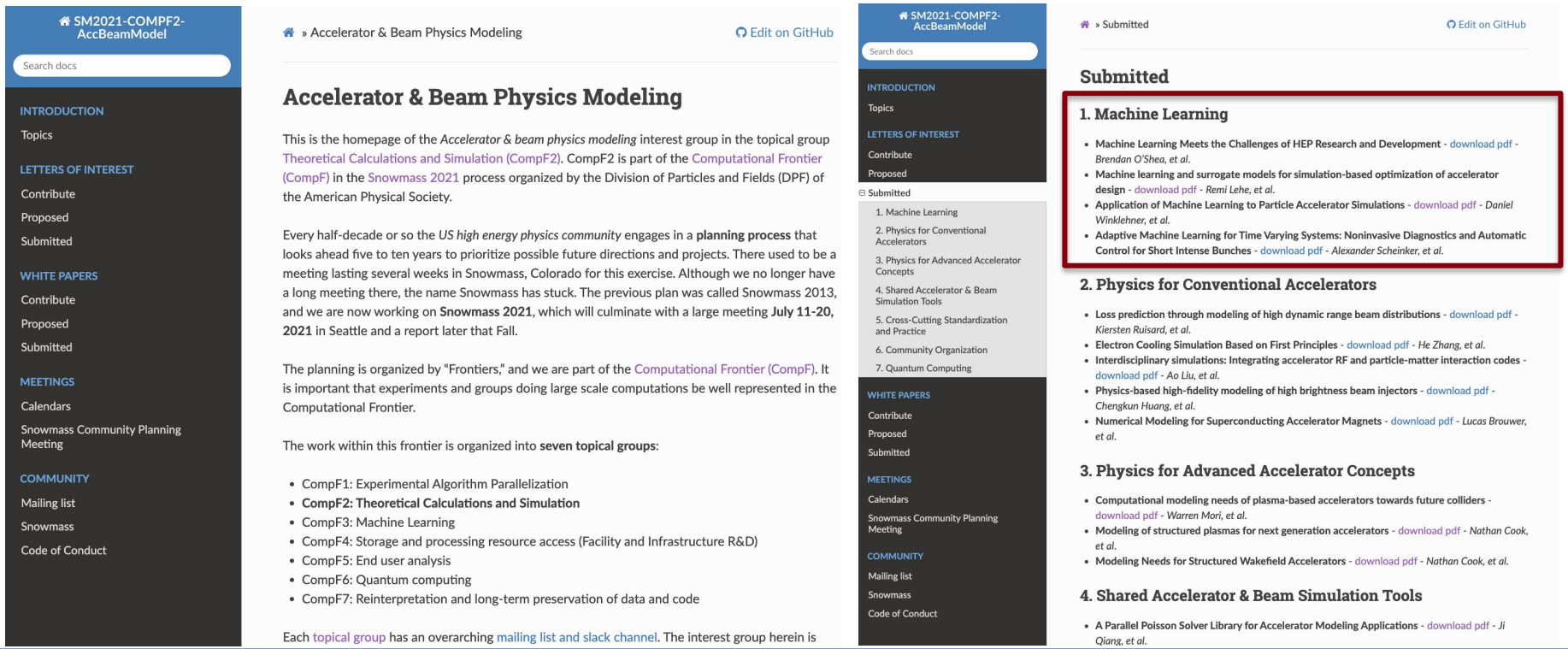
Ji Qiang
CompF2
Theoretical Calculations & Simulation

Jean-Luc Vay
Liaison
CompF/AF

Axel Huebl
Early Career – CompF

Beam & Accelerator Modeling Interest Group

- Mailing list: AccBeamModelSnowmass21@lbl.gov
- Bi-weekly meeting
- Website: https://snowmass-compf2-accbeammodel.github.io



Including discussions, LOIs, white papers, etc. on Machine Learning for beam physics & accelerators.

LOIs, ICFA Papers and Status Community Whitepaper

Progress in the **CompF2 (Theory Calc. & Sim.)** topical group ***Accelerator & Beam Physics Modeling.***

26 LOIs collected, presented and discussed (see previous slide).

In September 2021, a subset of the above topics where published in two peer reviewed articles in the Journal of Instrumentation (JINST), ICFA Beam Dynamics Newsletters #82: Advanced Accelerator Modeling, 2021:

- ***Simulations of Future Particle Accelerators: Issues and Mitigations*** - David Sagan, et al. arXiv:2108.11027 / DOI:10.1088/1748-0221/16/10/T10002

- ***Modeling of Advanced Accelerator Concepts*** - Jean-Luc Vay, et al. arXiv:2109.05133 / DOI:10.1088/1748-0221/16/10/T10003

Started developing a common white paper (next two slides).

CompF2: Questions to Address in White Paper

Questions & tasks formulated by CompF conveners to shape the scope of white papers.

With the purpose to collect information useful to transform requirements of near-future and far-future physics programs into Software and Computing (S&C) effort and R&D.

Aim to expand on Snowmass LoIs and input to quantify:

- (bespoke) Calculation and simulation software required
- **Size of software R&D effort per project/facility and area**
- **Nature and scale of computational needs**
- **S&C areas of expertise and interest where to focus US effort Questions target near- (10-15 years) and far-future (>20 years) facilities/experiments .**

Please note that far-future physics programs present immediate S&C needs and challenges in the form of tools and resources for designing experimental facilities and making the physics case.

It would be useful to describe the facilities or experiments discussed in your white paper in terms of numbers which are relevant to computing planning (accelerator and detector parameters, trigger, data volumes, etc).

The Acc. & Beam Modeling Interest Group is working on community white paper

Snowmass21 Accelerator Modeling Community White Paper

(White Paper Submitted to Snowmass 2021,
Computational & Accelerator Frontiers)

Beam and Accelerator Modeling Interest Group (BAMIG)*

Name a[1], Name b[2], and ...[3]

[1] *Affiliation A*
[2] *Affiliation B*
[3] ...

November 17, 2021

Contents

Timeline

"To allow topical group conveners sufficient time to consider white papers, we ask all who wish to contribute to submit (via email to topical group conveners) at least a title and abstract by the end of January, 2022. White papers whose title and abstract are submitted later are not guaranteed full consideration. The general Snowmass deadline also applies." - under consideration for CF homepage

- **January 31, 2022:** Title and abstract of white papers
- ~~January 31~~, TBD 2022: White Paper submission to arXiv

- May 31, 2022: Preliminary reports by the Topical Groups
- June 30, 2022: Preliminary reports by the Frontiers
- July, 2022: Snowmass Community Summer Study (CSS) at UW-Seattle

- September 30, 2022: All final reports by TGs and Frontiers
- October 31, 2022: Snowmass Book and the online archive documents