

Computational Frontier Status Update at AF1, Snowmass21

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Nov 22, 2021

Computational Frontier Organization

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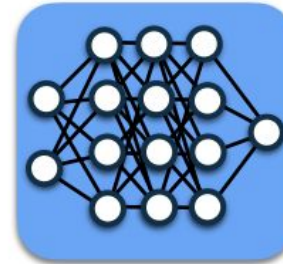
CompF01
Experimental
Algorithm
Parallelization

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



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CompF02
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CompF03
Machine
Learning

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

CompF05
End User
Analysis

vin Davis (U. Mississippi),
Onyisi (U. Texas at Austin),
my Roberts (UC Denver)



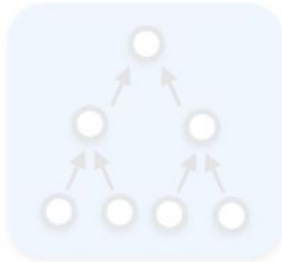
Computing

F07

& Long-term
Data and Code

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

Computational Frontier Organization



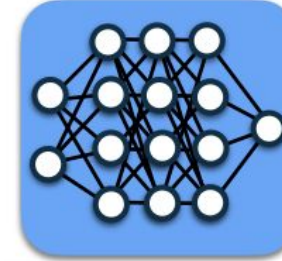
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CompF03
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Physics-specific ML
Simulations
Interpretability & Validations
Community Tools & Standards
Resource Needs & Management
Education & Engagement



CompF05
End User
Analysis

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



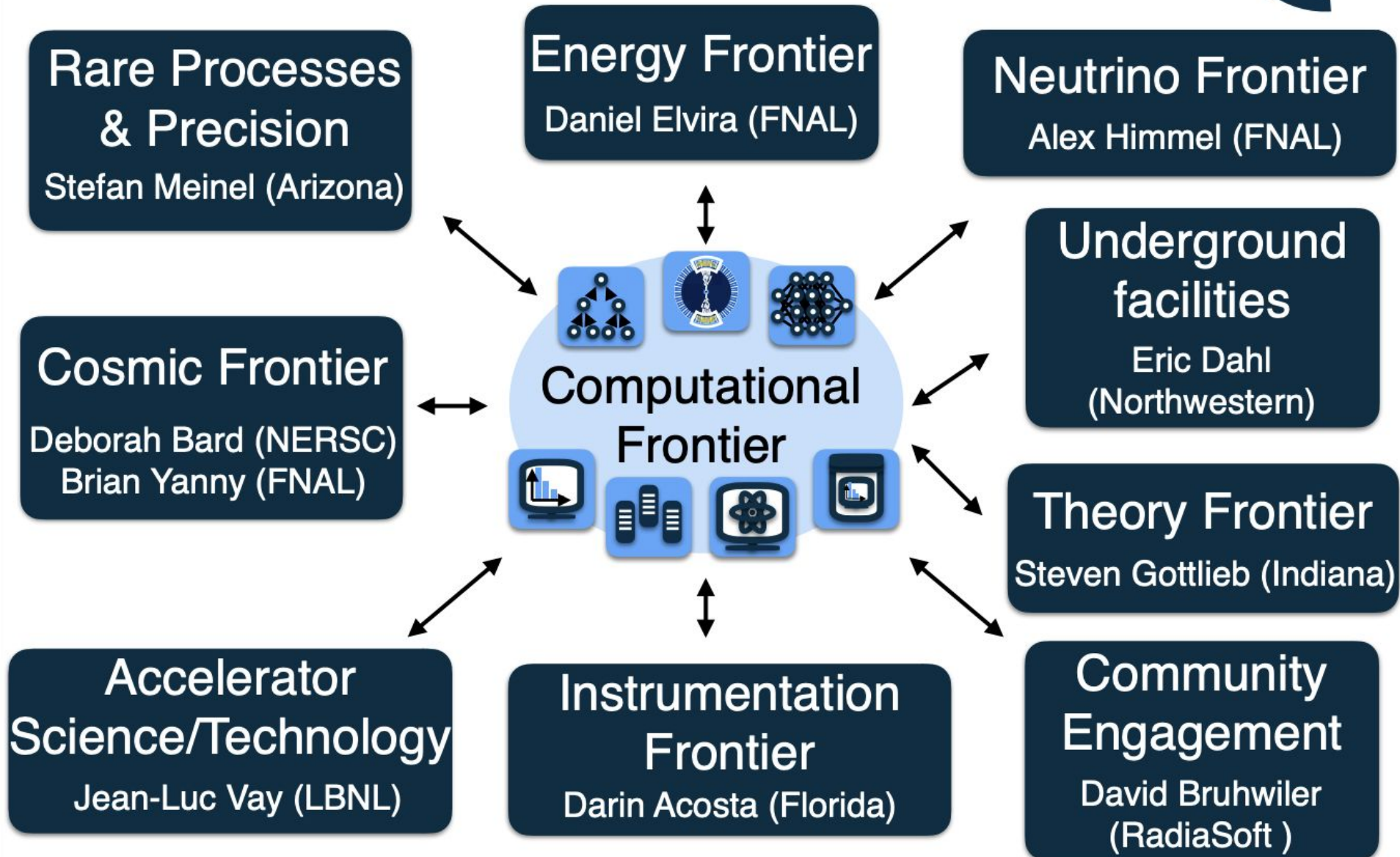
CompF07

Interpretation & Long-term
Preservation of Data and Code

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

Liaisons

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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/ projections 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>

SM2021-COMP2-AccBeamModel

Search docs

INTRODUCTION

Topics

LETTERS OF INTEREST

Contribute

Proposed

Submitted

WHITE PAPERS

Contribute

Proposed

Submitted

MEETINGS

Calendars

Snowmass Community Planning Meeting

COMMUNITY

Mailing list

Snowmass

Code of Conduct

Accelerator & Beam Physics Modeling

Edit on GitHub

Accelerator & Beam Physics Modeling

This is the homepage of the *Accelerator & beam physics modeling* interest group in the topical group *Theoretical Calculations and Simulation (CompF2)*. CompF2 is part of the *Computational Frontier (CompF)* in the *Snowmass 2021* process organized by the Division of Particles and Fields (DPF) of the American Physical Society.

Every half-decade or so the *US high energy physics community* engages in a **planning process** that looks ahead five to ten years to prioritize possible future directions and projects. There used to be a meeting lasting several weeks in Snowmass, Colorado for this exercise. Although we no longer have a long meeting there, the name Snowmass has stuck. The previous plan was called Snowmass 2013, and we are now working on **Snowmass 2021**, which will culminate with a large meeting **July 11-20, 2021** in Seattle and a report later that Fall.

The planning is organized by "Frontiers," and we are part of the *Computational Frontier (CompF)*. It is important that experiments and groups doing large scale computations be well represented in the Computational Frontier.

The work within this frontier is organized into **seven topical groups**:

- CompF1: Experimental Algorithm Parallelization
- **CompF2: Theoretical Calculations and Simulation**
- CompF3: Machine Learning
- CompF4: Storage and processing resource access (Facility and Infrastructure R&D)
- CompF5: End user analysis
- CompF6: Quantum computing
- CompF7: Reinterpretation and long-term preservation of data and code

Each **topical group** has an overarching mailing list and slack channel. The interest group herein is

Submitted

INTRODUCTION

Topics

LETTERS OF INTEREST

Contribute

Proposed

Submitted

- 1. Machine Learning
- 2. Physics for Conventional Accelerators
- 3. Physics for Advanced Accelerator Concepts
- 4. Shared Accelerator & Beam Simulation Tools
- 5. Cross-Cutting Standardization and Practice
- 6. Community Organization
- 7. Quantum Computing

WHITE PAPERS

Contribute

Proposed

Submitted

MEETINGS

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Submitted

1. Machine Learning

- Machine Learning Meets the Challenges of HEP Research and Development - [download pdf](#) - *Brendan O'Shea, et al.*
- Machine learning and surrogate models for simulation-based optimization of accelerator design - [download pdf](#) - *Remi Lehe, et al.*
- Application of Machine Learning to Particle Accelerator Simulations - [download pdf](#) - *Daniel Winklehner, et al.*
- Adaptive Machine Learning for Time Varying Systems: Noninvasive Diagnostics and Automatic Control for Short Intense Bunches - [download pdf](#) - *Alexander Scheinker, et al.*

2. Physics for Conventional Accelerators

- Loss prediction through modeling of high dynamic range beam distributions - [download pdf](#) - *Kiersten Ruisard, et al.*
- Electron Cooling Simulation Based on First Principles - [download pdf](#) - *He Zhang, et al.*
- Interdisciplinary simulations: Integrating accelerator RF and particle-matter interaction codes - [download pdf](#) - *Ao Liu, et al.*
- Physics-based high-fidelity modeling of high brightness beam injectors - [download pdf](#) - *Chengkun Huang, et al.*
- Numerical Modeling for Superconducting Accelerator Magnets - [download pdf](#) - *Lucas Brouwer, et al.*

3. Physics for Advanced Accelerator Concepts

- Computational modeling needs of plasma-based accelerators towards future colliders - [download pdf](#) - *Warren Mori, et al.*
- Modeling of structured plasmas for next generation accelerators - [download pdf](#) - *Nathan Cook, et al.*
- Modeling Needs for Structured Wakefield Accelerators - [download pdf](#) - *Nathan Cook, et al.*

4. Shared Accelerator & Beam Simulation Tools

- A Parallel Poisson Solver Library for Accelerator Modeling Applications - [download pdf](#) - *Ji Qiang, et al.*

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 were 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](https://arxiv.org/abs/2108.11027) / [DOI:10.1088/1748-0221/16/10/T10002](https://doi.org/10.1088/1748-0221/16/10/T10002)
- **Modeling of Advanced Accelerator Concepts** - Jean-Luc Vay, et al.
[arXiv:2109.05133](https://arxiv.org/abs/2109.05133) / [DOI:10.1088/1748-0221/16/10/T10003](https://doi.org/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 Lols 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 a¹, Name b², and ...³

¹*Affiliation A*

²*Affiliation B*

³...

November 17, 2021

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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