Accelerator & Beam Physics Modeling in the Computational Frontier (CompF2: Theoretical Calculations and Simulation) in Snowmass 2021

Accelerator & Beam Physics Modeling interest group

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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 its own mailing list and slack channel, the interest group herein is part of CompF2.

On **August 10-11, 2020**, we are pleased to invite the community to our virtual kick-off Computational Frontier meeting (indico link). At the meeting, each topical group will present its charge and plans for gathering input from the community. We hope you will attend.

Please join us in planning the future of high energy physics, in the broadest sense. Also note that although this planning exercise is organized for the US, high energy physics is an international activity and we strongly encourage physicists based outside of the US to participate.

INTRODUCTION 1

2 INTRODUCTION

ONE

INTRODUCTION

1.1 Topics

As interest group in the Theoretical Calculations and Simulation (CompF2) topical group in the Computational Frontier our topics of interest include:

· Modeling of

- Specific types of accelerators (leptons, hadrons, gamma, mix)
 - * Injectors
 - * High power targets
 - * Linacs
 - * Rings (multi-bunch injection, etc.)
 - * Recirculating systems
 - * Energy recovery systems
 - * Fixed field accelerators (FFAGs, etc.)
 - * Colliders
- Advanced Concepts
 - * plasma accelerators (LWFA, PWFA)
 - * dielectric
 - * muon accelerators
 - * integral optics accelerators
- Specific physics topics
 - * beam-beam
 - * halo formation
 - * emittance preservation
 - * electron cloud
 - * collisions
 - * radiation production and transport
 - * spin dynamics
 - * space charge
 - * coherent synchrotron radiation
 - * wake fields
 - * quantum limit in novel accelerator structures

- * X-ray simulation
- * extreme beams
- * power deposition and resulting radioactivation
- * cooling
- * beam-material interactions (ionization, atomic processes,...)
- * ...
- Components and realistic beamline elements (fringe fields, high-order effects, etc.)
 - * RF cavities
 - * Magnets
 - * . . .
- _ ...

• Crosscutting topics

- Commonalities in comp. needs
- EVA (End-to-end Virtual Accelerator)
- Design optimization
- HPC / Exascale / programming
 - * GPUs; future hardware
 - * higher order methods/numerical linear algebra to make efficient use of GPUs
 - * computing hardware independent implementation e.g. Kokkos/RAJA/Alpaka/AMReX
 - * Mixed precision: half (various), single and double
 - * Tensor cores
- Standardization of output data, input scripts (openPMD, ...)
- Data management & data reduction
- Online modeling
- AI/ML
- Open Science
- Resources, training
- Cloud computing
- Software sustainability
- Integration of accelerator and detector (for radiation studies) codes

LETTERS OF INTEREST

2.1 Contribute

Snowmass 2021 Letters of Interest (LOI) are informal documents intended to be useful in the first stages of the Snowmass study. They will help Snowmass conveners to prepare the Snowmass Community Planning Meeting that will take place early November 2020 virtually. LoIs could include opinions, interests and proposals that could further be studied. They should contain a maximum of 2 pages of text, plus relevant bibliography. Please make these as simple and easy to read as possible. Authors of the letters are welcome to make a full writeup for their work as a contributed paper and submit it to the Snowmass proceedings. However, a contributed paper is not required.

LoIs should be contributed until ... (Snowmass upload close-out: August 31, 2020).

For our interest group, we propose to use a simple template to simplify the process. They can be contributed in the following ways:

- TODO: pull request example (pdf)
- TODO: or just sent per e-mail to ...

2.1.1 Tentative Plan

(Might be still too prescriptive?)

- Encourage community building via co-authorship by as many authors as possible. One lead starts with an initial skeleton or draft, then augments and crystallizes writing with an increasing number of authors.
- Organizational structure for LOIs/paper:
 - 1 lead.
 - 1st tier co-writers: a few people.
 - 2nd tier co-authors: more people.
 - third tier co-authors: everyone.
- Timeline:
 - Until July 10: organize ourselves, agree on topics, LOIs, structure and timeline.
 - July 10-August 21: one to two weeks per writing step (lead, 1st tier, 2nd tier, 3rd tier).
 - August 22-31: wrap-up and submit.

2.1.2 Templates

We suggest to use the following (tentative) template for LOIs...

- Topic and status.
- Current and future challenges.
- · Advances needed to meet challenges.

Note: Do we collect contributions or do we advise authors to upload for themselves at https://snowmass21.org/loi?

2.2 Proposed

Proposed topics for LOIs derive from our topics.

- Develop accelerator toolkit.
- Integration, interfaces, tooling, continuous testing
- Develop/integrate data standards & start-to-end workflows.
- Compatibility and extensibility of large, complex simulation software? (Similar to ECP xSDK but for acc. modeling) or . . .
- (Re-iterate) Aspiration for Open Science (why and how; demystify misunderstandings)
- . . .

2.3 Submitted

- real letter 1
- real letter 2
- · example rst
- example PDF

COMMUNITY

3.1 Contact

3.1.1 Snowmass 2021

These are the central resources of the Snowmass 2021 process.

- homepage: https://snowmass21.org
- Indico page: https://indico.fnal.gov/category/1098/ (Computational Frontier, Early Career)

All communication types are explained here.

3.1.2 Mailing Lists

Our interest group and community organizes in the following ways:

- Snowmass e-mail server: listserv@fnal.gov(help)
- Snowmass e-mail list: snowmass@fnal.gov(SNOWMASS)
 - snowmass early career (SEC) e-mail list: snowmass-young@fnal.gov (SNOWMASS-YOUNG)
 - computational frontier (CompF) e-mail list: ... there is none yet? ...
 - * CompF conveners: https://snowmass21.org/computational/start
 - · CompF early career point of contact: sec-compf@googlegroups.com
 - * topical group CompF2: Theoretical Calculations and Simulation e-mail list: snowmass-compf02-theorycalcsim@fnal.gov (SNOWMASS-COMPF02-THEORYCALCSIM)
 - · interest group Accelerator & Beam Physics Modeling mailing list: not yet set up, will reach out soon

Please follow the instructions outlined here to join these mailing lists.

3.1.3 Slack Channels

Snowmass 2021 also communicates actively via Slack, which is an online chat service.

- Slack Server: https://snowmass2021.slack.com
- general planning channel: #snowmass-2021-planning #general
 - snowmass early career (SEC) channel (organizers/point of contact): #early-career-snowmass #early-career-rep
 - computational frontier (CompF) channel: #comp_frontier_topics

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- * CompF early career point channel (organizers/point of contact): #early-career-computational-coordination
- * topical group CompF2: Theoretical Calculations and Simulation channel: #compf02-theorycalcsim

Please follow the instructions outlined here to join the Slack server.

3.2 Meetings

3.2.1 Calendars

Computational Frontier

Indico events (.ical link)

Topical Group: Theoretical Calculations and Simulation (CompF2)

... (please see above events by title for now) ...

3.3 Code of Conduct

Please see the Snowmass 2021 code of conduct. As an APS-sponsored process, we will abide by the APS code of conduct for all meetings.

This interest grou[is also part of the process, so in our conversations here we pledge to conduct ourselves in a professional manner that is welcoming to all participants and free from any form of discrimination, harassment, or retaliation. Participants will treat each other with respect and consideration.

In addition, APS DPF has drafted a set of Core Principles and Community Guidelines to which members pledge to adhere. Please see the Snowmass page for more information.