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

Accelerator & Beam Physics Modeling interest group

Oct 14, 2020

INTRODUCTION

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 part of topical group **CompF2** and we invite you to *join our *Accelerator & beam physics modeling* mailing list*.

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.

CHAPTER

ONE

INTRODUCTION

1.1 Topics

If you would like to propose changes, additions or comments, please send an e-mail to <mailto:AccBeamModelSnowmass21@lbl.gov>.

As the *Accelerator & beam physics modeling* 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
    - integrable optics accelerators
  - Specific physics/operational topics
    - space charge
    - beam-beam
    - halo formation
    - emittance preservation
    - wake fields
    - impedance
    - electron cloud
    - fast ion instability
    - collisions

        - radiation production and transport
        - spin dynamics
        - coherent synchrotron radiation
        - quantum limit in novel accelerator structures
        - X-ray simulation
        - extreme beams
        - power deposition and resulting radioactivation
        - cooling
        - beam-material interactions (ionization, atomic processes,. . .)
        - dynamic processes during operational scenarios (machine generally has to go through intermediate states with changing optics and fill patterns before it reaches its steady state)
        - injection painting
        - slow extraction
        - slip-stacking
        - . . .
    - Components and realistic beamline elements (fringe fields, high-order effects, etc.)
        - RF cavities
        - Magnets
        - structured plasmas
        - . . .
    - . . .
- **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

- Resources for code support and user support
- Integration of accelerator and detector (for radiation studies) codes
- Mesh refinement
- Synergies with non-HEP science

CHAPTER

TWO

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 August 31, 2020.

For our interest group, we propose to use a simple template to simplify the process:

2.1.1 Proposed Template

We suggest to use the following template for LOIs:

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

We maintain lists of *proposed* and *submitted* LOIs.

Note: We rely on the community (you) to inform us about proposed and submitted LOIs by sending emails to AccBeamModelSnowmass21@lbl.gov.

2.2 Proposed

Proposed topics for LOIs derive from our *topics*.

To propose additions, modifications, provide comments, or if you are interested to participate to the writing - or simply to co-sign - one of the proposed LOIs listed below, send an email to AccBeamModelSnowmass21@lbl.gov or submit a pull request via github.

Many authors shared their LOIs below, prior to submission deadline to Snowmass on Monday, August 31st 2020. For the LOIs that have a link below, contact the first author directly, in order to have your name added, or in order to make other modifications. For all other LOIs, please contact the mailing list for feedback.

- **A modular community ecosystem for multiphysics particle accelerator modeling and design** - view on overleaf - *Jean-Luc Vay, Axel Huebl, David Sagan, David Bruhwiler, Ao Liu, Cho-Kuen Ng, Ji Qiang, Rémi Lehe*.

- **Beam Dynamics Toolkit** - view on overleaf - *David Sagan, Robert Ryne, Jean-Luc Vay, Georg Hoffstaetter, Ji Qiang, Alex Friedman*.
- **EVA (End-to-end Virtual Accelerators)** - view on overleaf - *Jean-Luc Vay, David Sagan, Axel Huebl*.
- **Develop/integrate data standards & start-to-end workflows for Accelerator Physics** - view on overleaf (submitted) - *Axel Huebl, Jean-Luc Vay, Rémi Lehe, Maxence Thévenet, Christopher Mayes, David Sagan, Yu-Dai Tsai, Juncheng E, Frank Tsung, Henri Vincenti, Angel Ferran Pousa, Nathan M. Cook, Spencer J. Gessner, Franz Poeschel, Michael Bussmann, David P. Grote, Nicholas A. Murphy, Ryan Schmitz, Chun H. Yoon, David L. Bruhwiler, Kyle Cranmer, Samuel R. Yoffe, Brigitte Cros, Auralee L. Edelen, Giordon Stark*.
- **Aspiration for Open Science in Accelerator & Beam Physics Modeling** - view on overleaf (submitted) - *Axel Huebl, Jean-Luc Vay, Rémi Lehe, Christopher Mayes, Yu-Dai Tsai, Alex Friedman, Maxence Thévenet, Henri Vincenti, David L. Bruhwiler, Aaron Sauers, Nathan M. Cook, Spencer J. Gessner, Michael Bussmann, David P. Grote, Ryan Schmitz, Brigitte Cros, David Sagan, Samuel R. Yoffe, Auralee L. Edelen, Angel Ferran Pousa, Giordon Stark*.
- **Machine learning and surrogates models for simulation-based optimization of accelerator design** - view on overleaf - *Remi Lehe, Adi Hanuka, Auralee Edelen, Xiabiao Huang, Christopher Mayes, Nathan Cook, Claudio Emma, Axel Huebl, Ryan Roussel, Maxence Thevenet, Jean-Luc Vay*.
- **Embracing modern software tools and user-friendly practices, when distributing scientific codes** - view on overleaf - *Rémi Lehe, Axel Huebl, Jean-Luc Vay*
- **Center(s) for accelerator and beam modeling** - view on overleaf - *Jean-Luc Vay, David Bruhwiler, David Sagan, Axel Huebl, Rémi Lehe, Cho-Kuen Ng, Ji Qiang*.
- **Plasma acceleration theory and simulation needs** - *Carl Schroeder, Warren Mori, Carlo Benedetti, Eric Esarey, Axel Huebl, Rémi Lehe, Jean-Luc Vay*.
- **Modeling of structured plasmas for next generation accelerators** - *Nathan Cook, Carlo Benedetti, David Bruhwiler, Enrico Brunetti, Stepan Bulanov, Stephen Coleman, Brigitte Cros, Bernhard Ersfeld, Spencer Gessner, Ahmad Fahim Habib, Thomas Heinemann, Bernhard Hidding, George Holt, Dino Jaroszynski, Remi Lehe, Jarrod Leddy, Carl Schroeder, Paul Scherkl, Peter Stoltz, Maxence Thévenet, Petros Tzeferacos, Jean-Luc Vay, Samueal Yoffe, Stephen Webb*.
- **Poisson solver library** - *Ji Qiang*.
- **Physics-based high brightness beam injector modeling** - view on google docs - *Chengkun Huang, Cho Ng, Tom Kwan, Vitaly Pavlenko*.
- **Consortium for PIC modeling in accelerator science** - view on overleaf - *Warren Mori, Frank Tsung*.
- **Cloud computing and use in education** - *David Bruhwiler*.
- **Quantum computing for accelerator and beam physics** - view on overleaf - *He Zhang, Ji Qiang*.
- **Modeling of electron cooling from first princicples** - view on overleaf - *He Zhang*.
- **Numerical Modeling for Superconducting Accelerator Magnets** - *Lucas Brouwer*.
- **Surface Methods for Precision Accelerator Design and Virtual Prototyping of Accelerator Systems** - view on overleaf - *Robert D. Ryne, Dan T. Abell, D.L. Bruhwiler, Alex J. Dragt, Chad Mitchell, Ji Qiang, Jean-Luc Vay, and Peter Walstrom*.

2.3 Submitted

2.3.1 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.*

2.3.2 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.*

2.3.3 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.*

2.3.4 4. Shared Accelerator & Beam Simulation Tools

- **A Parallel Poisson Solver Library for Accelerator Modeling Applications** - download pdf - *Ji Qiang, et al.*
- **Surface Methods for Precision Accelerator Design and Virtual Prototyping of Accelerator Systems** - download pdf - *Robert Ryne, et al.*
- **Beam Dynamics Toolkit** - download pdf - *David Sagan, et al.*
- **A modular community ecosystem for multiphysics particle accelerator modeling and design** - download pdf - *Jean-Luc Vay, et al.*
- **EVA (End-to-end Virtual Accelerators)** - download pdf - *Jean-Luc Vay, et al.*
- **Accelerator and Beam Physics: Grand Challenges and Research Opportunities** download pdf - *Sergei Nagaitsev, et al.*

2.3.5 5. Cross-Cutting Standardization and Practice

- **Develop/integrate data standards & start-to-end workflows for Accelerator Physics** - download pdf - *Axel Huebl, et al.*
- **Aspiration for Open Science in Accelerator & Beam Physics Modeling** - download pdf - *Axel Huebl, et al.*
- **Embracing modern software tools and user-friendly practices, when distributing scientific codes** - download pdf - *Remi Lehe, et al.*

2.3.6 6. Community Organization

- **Center(s) for accelerator and beam modeling** - download pdf - *Jean-Luc Vay, et al.*
- **Consortium for PIC Software in Accelerator Science** - download pdf - *Warren Mori, et al.*
- **Collaboration between industry and the HEP community** - download pdf - *David Bruhwiler, et al.*

2.3.7 7. Quantum Computing

- **Getting Ready in Algorithm and Software Development for the Arrival of the Quantum Computing Age** - download pdf - *He Zhang, et al.*

We rely on the community (you) to inform us about proposed and submitted LOIs by sending emails to AccBeamModelSnowmass21@lbl.gov.

CHAPTER

THREE

COMMUNITY

3.1 Mailing list

If you want to be included, removed or suggest additional names, please send an e-mail to AccBeamModelSnowmass21@lbl.gov.

3.1.1 Current people in the list:

(* indicates individuals who have been invited to the mailing list but have yet to accept)

- Andreas Adelmann*
- Eduardo Alves
- James Amundson*
- Thomas Antonsen*
- Mei Bai
- Gabriele Bassi
- Carlo Benedetti
- Martin Berz
- Oleksii Beznosov
- Sandra Biedron
- Michael Borland*
- Lucas Brouwer
- David Bruhwiler
- Yunhai Cai
- John R Cary
- Nathan Cook
- Ben Cowan
- Alexander Debus
- Blagoje Djordjevic
- Zhe Duan*
- Auralee Edelen*
- Jim Ellison*
- Claudio Emma

- Eric Esarey*
- Ricardo Fonseca
- Guiliano Franchetti*
- Alex Friedman
- Cameron Geddes
- Spencer Gessner
- David Grote
- Claire Hansel
- Adi Hanuka
- Yue Hao*
- Klaus Heinemann*
- Georg Hoffstaetter
- Mark Hogan
- Chenkung Huang
- Xiaobiao Huang
- Zhirong Huang
- Axel Huebl
- Andreas Kemp
- Remi Lehe
- Ao Liu
- Steve Lund*
- Chris Mayes*
- Chad Mitchell
- Nikolai Mokhov
- Warren Mori
- Cho-Kuen Ng
- Greg Penn
- Ji Qiang
- Daniel Ratner
- yves roblin
- Kiersten Ruisard
- Robert Ryne
- David Sagan
- Alex Scheinker
- Carl Schroeder
- Brad Shadwick
- Luis Silva
- Kiran Sonnad
- Eric G. Stern

- Reed Teyber
- Maxence Thevenet
- Alec Thomas
- Jean-Luc Vay
- Jorge Vieira
- Robert Warnock
- Stephen Webb
- Scott Wilks*
- Daniel Winklehner
- He Zhang

3.2 Snowmass

3.2.1 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.

3.2.2 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:** `AccBeamModelSnowmass21@lbl.gov`

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

3.2.3 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`
    - 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.

3.3 Meetings

3.3.1 Calendars

Accelerator & beam physics modeling interest group

Calendar

Accelerator Frontier

Meetings and Calendar

Computational Frontier

Indico events (.ical link)

Topical Group: Theoretical Calculations and Simulation (CompF2)

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

3.4 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 group 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.