Overview

Gallagher: is there representation from the nuclear theory community? Neutrino generators rely heavily on NP models.

Kronfeld: Nuclear theory is not a P5 activity but the use of NP models in physics generators and detector simulation is very relevant. We should extend invitations but remembering that NP itself is not part of the P5 mandate.

Elvira: We included members of the NP community we know within generators and detector simulation. Those who we reached should invite others they know.

Boyle: We are trying to generate a chain reaction of invitations.

Vay: Detector/beam versus accelerator modeling. What is the difference? Add that detector/beam would not be simulating the accelerator apparatus.

Adelmann/Elvira: beam line in the experiments is within beam simulation versus beam tools that is part of accelerator modeling. Secondary beam lines are in detector/beam, same as decay channels, and anything that simulates particle-matter interactions.

Routes to LOI: Event generators

Mrenna: We should adapt recent HSF notes related to perturbative calculations, HPCs, GPUs into the future. We should self-organize to cover this. Make it specific to LHC. Others? Neutrino, heavy ion, Electron ion? The HSF document should be completed and adapted to the US context.

Ilten: The HSF document is lacking non-LHC and very hard processes.

Boyle: what should we do to cover the areas that are missing?

Mrenna: The question is how we generate rare but important events. These are computationally challenging.

Contact people: Ilten/Mrenna are focusing on LHC and they would volunteer to steer the LOI effort but they need to think of others in communities outside the LHC. Mrenna is volunteering Stefan Hoche and Taylor Childers to also take leadership responsibility. Neutrino generators need to be ready for the DUNE era and this connects with theoretical calculations so there will be a lot of overlap with the neutrino subgroups. Gallagher volunteers to make this connection effective. Gardiner posted a few things on neutrino generators, a few thoughts. He also volunteers to steer the LOI effort.

Gardiner: Several recent workshops related to neutrino generators brought up important issues for the future of the community. Both theoretical and computational topics were discussed at length.

FNAL "Generator Tools Workshop" https://indico.fnal.gov/event/22294/overview in January 2020 (white paper in prep., contact Laura Fields, Minerba Betancourt, or Kevin McFarland for details)

ECT* "Testing and Improving Models of Neutrino Nucleus Interactions in Generators" https://indico.ectstar.eu/event/53/ June 2019

ECT* "Modeling neutrino-nucleus interactions" https://indico.ectstar.eu/event/19/ July 2018

Saori Pastore: here, e.g., you can find NP theorists working on lepton-nucleus interactions

- ECT* “Neutrini and Nuclei: Challenges and Opportunities” http://www.ectstar.eu/node/4439 May 2019

- FNAL “Nuclear and Particle Theory for Accelerator and Neutrino Experiments “ https://indico.fnal.gov/event/20271/overview May 2019

Here are a few other things that might be worth discussing:

- Separate LHC/neutrino/other LOIs or combined?
    - Do individual generators want to express their views in a separate document?
- Overlap and distinctions between the needs/plans for collider versus neutrino generators
    - What can neutrino generator developers learn from their colleagues working on simulations for the LHC?
- Neutrino generator needs/plans outside the "traditional" emphasis on GeV-scale accelerator experiments
    - Very-high-energy astrophysical neutrinos (IceCube)
    - Supernova, solar, and other low-energy (~10 MeV and below) neutrinos (COHERENT, DUNE supernova program, etc.)

Routes to LOI: Accelerator & beam physics modeling

- Laundry list of possible topics (JL Vay):
    - Modeling of
        - rings
        - linacs
        - plasma accelerators
        - beam-beam
        - halo
        - …

- Commonalities in comp. needs
- EVA (End-to-end Virtual Accelerator)
- HPC / Exascale
- Standardization of output data, input scripts
- Data management & data reduction
- AI/ML
- Open Science
- Accelerator stewardship
- Resources, training

A lot is covered in a roadmap for DOE HEP GARD document. Need to coordinate in order not to duplicate effort or have contradictions in documents.

Daniel Elvira: accelerator simulation overlaps with far future as must support accelerators being planned in the 10-15 year time frame and these are further in the future.

Andreas A (PSI) - a few thoughts towards 10 yr's:

- Numerical & Computational Methods for Radiation Generation
    - new numerical schemes (grid/particle noise)
        - higher order methods to make efficient use of GPUs
- computing hardware independent implementation e.g. Trilinos/Kokos
- Theoretical and Numerical Methods for Collisions in High Brightness Electron Beams
- Approaching the Quantum Limits in Novel Accelerator Structures: Quo Vadis with Numerical Simulations
- Surrogate Models and UQ based on Machine and Statistical Learning
    - obtain theoretical understanding why the underlying manifold (accelerator) is so well approximated
    - real time precise surrogate models for integration into the control system
    - fast inverse models & MOO
- Benchmarking Surrogate Models with Real Accelerators

Contact people: Vay volunteers to organize meetings starting soon. David Sagan too. Eric Stern also volunteered. Cho Ng will help with accelerator component simulation.

Routes to LOI: Detector/beam simulation

Genser: NP is important also for interaction of particles with the detector material. Using new computing architectures to do the calculations that we currently do in CPUs.

Boyle: Really interested to capture which algorithms can run efficiently in GPUs and which cannot. Sequential algorithms may be difficult to port. Important to categorize problem-by-problem.

Genser: whole body of work attempting this (moving to GPUs and FPGAs). Rely on papers and work that has been done. There is a 2017 HSF roadmap on detector simulation which we could rely on and update it. We need to focus on LiAr which is another section and the other is hadronic physics because EM is well covered but hadronics is not.

Elvira: Our group should also focus on the physics of detector simulation because there is not any other group that does. So we should focus on physics accuracy in addition to how we do the computation.

Genser: do we have a representative from the dark matter community?
Possible omission of Geant/darkmatter.

Kourlitis: He is from ATLAS and working on accelerating Geant. Focused on geometry acceleration because this is the bottleneck. It is in connection with the ML Snowmass working group. They could use these algorithms in CPUs or GPUs. They are hardware transparent because they will use portability libraries. The point is to accelerate simulation by using ML but not developing novel ML algorithms.

Boyle: High throughput could be the recommendation to close WLCG computing gap ?

Ilten: LHCb focused on fast simulation because they will hit a bottleneck soon.

Marshall: Thinking about various tasks within the ATLAS simulation group. Some of it is in the HSF report but did not get a lot of followup. ML for example replacing modules in G4, making simulation more experiment agnostic. Not a lot of work so far. Also interested in resource gap resolution and how severe this might be for the FCC.

Miha Muskinja [ATLAS, LBL]: Could already get useful information about the resource gap / needed resources for detector simulation from the documents submitted to the European Particle Physics Strategy Update from various experiments (e.g. FCCee, FCChh, CLIC, …).

Boyle: When considering acceleration of something like GEANT some consideration of programming models might help? CUDA, OneAPI/SYCL, OpenMP, HIP etc…. How do you port when they are all different?

Vincent Pascuzzi [ATLAS, LBL]: Also Kokkos/RAJA/Alpaka abstraction layers. There is an ongoing effort (HEP-CCE) evaluating these different “portability solutions.” While these are distinct projects, there is some level of overlap between them, e.g. SYCL/DPC++ (Intel llvm

staging) can target “all” CPUs, CUDA (with some current limitations, e.g. mkl::rng) and in general any SPIR-V-compatible hardware.

Pascuzzi: Currently involved in porting fast simulation of ATLAS calorimeter to run on GPUs (CUDA or SYCL), and working on full MC chain (generator -> analysis data) HPC workflows (in collaboration with other experts).

Contact people: Genser volunteers for coordinating LOI effort. Pascuzzi also volunteers.

Boyle: Different areas can share experience and avoid duplication of efforts. Perhaps we should discuss this during the August 10/11 workshop. How do we learn and share cross cutting computational and software knowledge?

Huebl, Cowan: there is synergetic overlap with methods used to model accelerators (performance portability libraries; ECP project participation). Need to reach out to people working on performance portability libraries (Sandia, Livermore) and get them involved. RAJA, KOKKOS, Alpaka, AMReX.

Routes to LOI: Theoretical calculations (Lattice Field Theory)

- 7 USQCD white papers on archive including computational requirements 2018
- Already pretty good basis but needs some augmentation with additional LOIs plus referring to these
- Some groups planning LOIs. (Riken - Brookhaven - Columbia - UKQCD)?

Andreas Kronfeld USQCD - federation of science collaborations working together for computing resources and software development effort. Don’t really think energy or need to redo these. USQCD plans to submit a LOI as a whole to get the whitepapers included. We might prepare a whitepaper which is a broad summary of how these things are relevant to high energy physics as a whole.
Let the voice of individual science collaborations take over on explaining their special needs independently. E.g. Kaon physics from RBC/Christ./ Similarly Fermilab/MILC will talk about Belle/LHCb physics. USQCD will pitch back to the community. Muon g-2 very timely, but not expected to be on the right time frame for snowmass 21.
Now as FNAL lattice collab. Useful to have some sort of document to describe computing resources for finishing the lattice calculations HVP/HLBL .

Davoudi: coordination for two topics QC, QS, and also ML. Cover theoretical topics important for ML and the era of QC. This is very theory heavy. Lattice computation and theory have to be coordinated. Computational requirements need to be served so they belong to our working group.

Boyle: Staff physicist programmers to support LGT software, ECP took over from SciDAC and argue case for place in roadmap for replacement going forward.

Kronfeld : yes, post 2023 need this to continue.
Kronfeld - mail the whole mailing list to alert people. Computing LOI should be from USQCD and the ECP participants / committees.

Zohreh : approach coordination on at least two topics - Quantum computing and Machine learning. Theoretical developments covered, new and emerging. Emphasize algorithm development as an activity.

Boyle: QCD and ML topical working groups. F02 - need LGT phenomenology turned into computational requirements.

Kronfeld: volunteers to coordinate the effort related to LOI submission, heavily borrowing on existing documentation. Christ hopes to have many LOI from different topics and groups.

Gottlieb: is not worried about LQCD being mentioned in many different fora within the Snowmass process.

Routes to LOI: Theoretical calculations (Perturbative)

Laura Reina: Christian Bauer was on. Involved substantially in this field. Speaks as a convener for EF. Views natural community that should give input CF02 is the theory community working on precision calcs for colliders. This means people working on pert. QCD and EW, multiloop, high multiplicity calcs. Reached a level of computational needs that are OOM greater than 10 years ago. Really be part of discussion.

Laura: worked on previous snowmass - tried to gather the community to convey the idea that they need to be cohesively studying computational needs and develop new techniques. Some success in making aware of the problem. But not complete success. Can't give personal commitment to organise that, but can provide ideas and names of points of contact. Involve EF theory conveners (EW, precision physics etc.. QCD, PDF, GPDFs). Becoming more demanding and promising for the future. Need an LOI. In theory frontier have at least two groups TF06 (theory techniques for precision physics) and TF07 (collider physics). Need computational support for both symbolic calculation and numerical integration, up to even new ideas of machine learning augmentation. Should be part of the discussion. Topics like NNLO and beyond.

Choices within EF is discussing future, future colliders. Baseline is HL LHC. Snow

Laura Reina: It is important to spell out the physics generators requirements and theory calculation computing challenges associated with the far future programs that the physis frontiers are discussing (e.g. EF).

Action: Take up contacting recommended people with Laura (Daniel, Peter to take forward?).

Resummation community? Christian Bauer will help establish contacts.

Routes to LOI: Cosmic Frontier simulation

Salman Habib: ECP project, also develop high performance scalable code for next generations. Multiple levels of engagement. People who run, analyse, etc.. Have a complicated network of people in science exploitation. Hundreds of people in downstream analysis and so on. Lots of overlap in performance, portability, cross cuts. Should establish better relations. Some in beam/acc with cosmo, but should expand. People should worry about hardware changes much more than just accelerators. Driven by commercial interests, such as streaming AI processors. Lot of work on compilers by big companies - can snowmass understand where things are going? E.g. Cloud, HPC.

Pascuzzi: Useful to collaborate and build relationships with big companies to keep up with their future plans, where things are going. ECP doing this well with Intel, NERSC (and others) have good working relationships with NVIDIA, etc.

Boyle - would like to share in cross cutting work thinking.
Steve - is it only going to get harder.
Ji - yeah, but MPI made it easier. [Anecdote - Boyle, yeah used PVM before MPI awful!]
Salman - compilers have always promised to solve it. But never gave performance. But optimising to the wire, you end up doing work.
Peter - history makes it harder over time.
Salman - yeah… problematic
Katrin - theory computing interaction ; seen already groups seeing efforts being established about simulation. She can help start.

Contact people: Salman Habib and Zarija Lukic volunteer to coordinate the LOI effort.

Salman: how to restrict Cosmology to the P5 subset?
Steve: Last time we did this - Andrew Connolly, Julian Borrill, Katrin Heitmann, Brian Nord are people who wrote the report last time. Take them and get their younger colleagues involved. Also look at a topical group from Perturbative from last time, coauthors with Laura Reina.

Areas requiring more engagement

- Theoretical calculations, perturbative.

    - Laura to help with names and contacting
    - Peter, Daniel volunteered to work with her
    - Steve suggested prior conveners as points of contact.
    - White paper on software crisis?
- Cosmological Frontier
    - Katrin: can help start.
    - Steve: Last time we did this - Andrew Connolly, Julian Borel, Katrin Heitmann, Brian Nord are people who wrote the report last time. Take them and get their younger colleagues involved.
- Dark Matter search experiments
    - GEANT4 style simulation for DM experiments needs representation.
- Andreas Adelman - area where we should all have one voice is difficult architectures in future, can we all do this jointly. Suggest a single cross cutting activity.
    - Peter: Organise joint architecture / evolution/ computing calls for CompF02 for cross cutting. How broad should it go? Can we share.
    - Steve: important topic.
    - Salman : also important we can’t be sure of future, but can predict several futures. NERSC - CPU -> GPU etc.. Really important.