Computational Frontier

SLACmass retreat, May 12th, 2022
Convener: Tina Cartaro

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SLAC Contributions to Computational Frontier

Computational Frontier (CompF)	Links	SLAC Authors
Small HEP Experiments, Dance, CF computing & modeling	https://arxiv.org/abs/2203.07645 https://arxiv.org/abs/2203.07700 https://arxiv.org/abs/2203.08338	- Monzani, Fan - Monzani, Anderson, Buuck, Cartaro, Fan, Wright - Anderson, Buuck, Cartaro, Fan, Monzani, Wright
Snowmass 2021 Computational Frontier White Paper: Cosmological Simulations and Modeling	https://arxiv.org/abs/2203.07347	Birrer, Omori
Snowmass 2021 Accelerator Modeling Community White Paper	https://arxiv.org/abs/2203.08335	Edelen, Ng, Roussel
Adaptive Machine Learning for Time-Varying Systems: Towards 6D Phase Space Diagnostics of Short Intense Charged Particle Beams	https://arxiv.org/abs/2203.04391	Gessner
Solving Simulation Systematics in and with AI/ML	https://arxiv.org/abs/2203.06112	Terao
The LHC Olympics 2020: A Community Challenge for Anomaly Detection in High Energy Physics	https://arxiv.org/abs/2101.08320	Collins
New directions for surrogate models and differentiable programming for High Energy Physics detector simulation	https://arxiv.org/abs/2203.08806	Kagan
Machine Learning and LHC Event Generation	https://arxiv.org/abs/2203.07460	Kagan
Graph Neural Networks in Particle Physics: Implementations, Innovations, and Challenges	https://arxiv.org/abs/2203.12852	Kagan, Terao
Jas4pp -- a Data-Analysis Framework for Physics and Detector Studies	https://arxiv.org/abs/2011.05329	Graf

Computational Frontier Session

- SLACmass retreat agenda:
  - https://indico.slac.stanford.edu/event/7218/
- Shared drive with slide decks:
  - https://drive.google.com/drive/folders/1x_MzwX97aJ5TiVMAltoyJC_Lxr064XkY
- Computational Frontier contributions are below.

Topic	Contribution	Speaker	Time
Machine Learning and LHC Event Generation - New directions for surrogate models and differentiable programming for High Energy Physics detector simulation	https://arxiv.org/abs/2203.08806 https://arxiv.org/abs/2203.07460	Kagan	6 (5+1)
Computational Frontier White Paper: Cosmological Simulations and Modeling	https://arxiv.org/abs/2203.07347	Birrer	6 (5+1)
Accelerator Modeling Community White Paper	https://arxiv.org/abs/2203.08335	Edelen	6 (5+1)
Small HEP Experiments, Dance, CF computing & modeling	https://arxiv.org/abs/2203.07645 https://arxiv.org/abs/2203.07700 https://arxiv.org/abs/2203.08338	Monzani	12 (10+2)

Cosmological Simulations and Modeling

S. Birrer

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Cosmological Simulations and Modeling

https://arxiv.org/abs/2203.07347

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- Need for simulations:
  - Success of the observational programs require actively pairing with a well-matched state-of-the-art simulation and modeling effort
  - Simulations must deliver guaranteed high-fidelity results for individual surveys as well as for the cross-correlations across different surveys

Cosmological Simulations and Modeling

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- The needed advances are as follows:
  - Development of scientifically rich and broadly-scoped simulations, which capture the relevant physics and correlations between probes
  - Accurate translation of simulation results into realistic image or spectral data to be directly compared with observations
  - Improved emulators and/or data-driven methods serving as surrogates for expensive simulations, constructed from a finite set of full-physics simulations
  - Detailed and transparent verification and validation programs for both simulations and analysis tools

Small HEP Experiments, DANCE, Dark Matter

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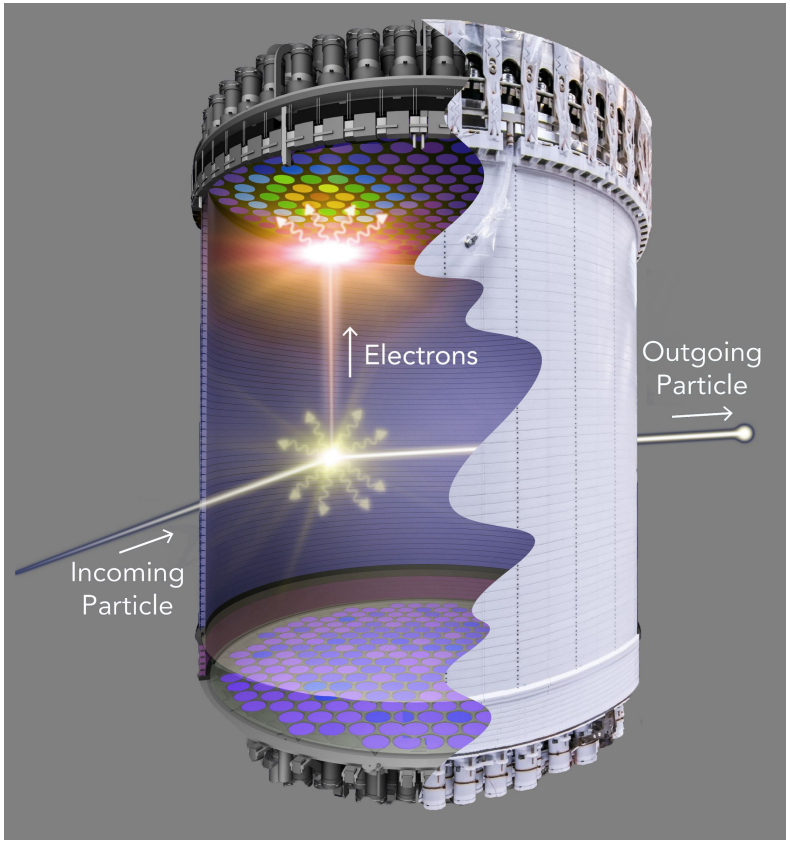
Small HEP Experiments, DANCE, Dark Matter

- Workshop discussing the computing needs of the “Small” HEP Experiments: https://indico.physics.lbl.gov/event/1756/overview
- Workshop discussing the computational needs of the Dark Matter and Neutrino Community: https://indico.cern.ch/event/82491

Paper Title	Link	SLAC staff
Software and Computing for Small HEP Experiments	https://arxiv.org/abs/2203.07645	Monzani
Snowmass 2021 Cosmic Frontier: Modeling, statistics, simulations, and computing needs for direct dark matter detection	https://arxiv.org/abs/2203.07700	Monzani, Anderson, Buuck, Cartaro, Fan
Dark-matter And Neutrino Computation Explored (DANCE) Community Input to Snowmass	https://arxiv.org/abs/2203.08338	Anderson, Buuck, Cartaro, Fan, Monzani, Wright

“Small” experiments ≠ small datasets/computing problems



Example: LZ is a 10-ton Liquid Xenon TPC

- Combined engineering/science run ongoing
- LZ data is stored and processed at NERSC

Approximate data throughputs:

- Fermi-LAT (>2008): 0.3 PB/year
- LZ (2021-2026): 1-1.5 PB/year, 5 years
- ATLAS (>2010): 3.2 PB/year (raw)

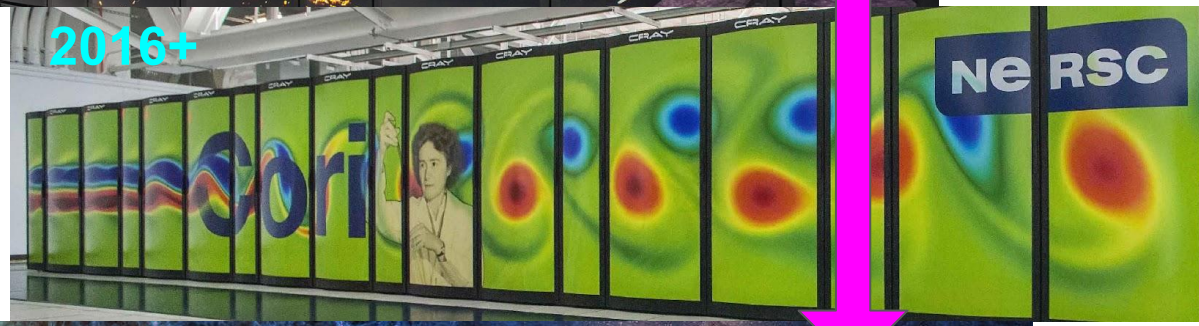
Data volumes for “small” experiments are approaching the LHC scale. Resources are orders of magnitude below LHC/DUNE

How do we deal with this massive amount of data?

The “small experiment” community does not have a culture of large-scale software development. DOE/HEP is not keen on funding a large-scale software effort.

1. Use standard HEP tools as much as possible (Geant4, ROOT, Gaudi, etc.)
   - ↦ Challenge: it is not obvious that “standard HEP tools” are going to be supported for the long run (example: DOE does not fund Geant4 anymore)
2. Pool resources with DM and neutrino experiments with similar needs
   - ↦ Challenge: competition. Few experiments believe in public data/software
3. Use infrastructure at DOE’s supercomputing centers (NERSC, ANL, etc.)
   - ↦ Challenge: no control over architecture. Little to no resources to adapt existing software framework(s) to a constantly evolving paradigm

NERSC: Computing Model Evolution



Common needs identified by the community

Experiment-independent support for “common frameworks”

- Leverage “standard” HEP tools for event simulation/reconstruction, data handling, etc.
- Crucial to (re-)build a “critical mass” of computing experts, supporting bread-and-butter HEP frameworks, to complement growing support for advanced Machine Learning
- DOE terminated its “common” support of Geant4 in 2019. Without G4 or a well-validated replacement, we will not be able to design a new HEP experiment ever again 😱

Mitigate current challenges in training/recruiting/retention:

- Extreme challenges in recruiting, training and retention of people with dual physics and computing expertise. This seems to be getting worse, and not “just” in the Bay Area
- Create a new career trajectory for permanent software and computing experts (RSE). Provide experiment-agnostic funding to support these careers. Joint appointments?