Snowmass Accelerator Modeling Community Whitepaper

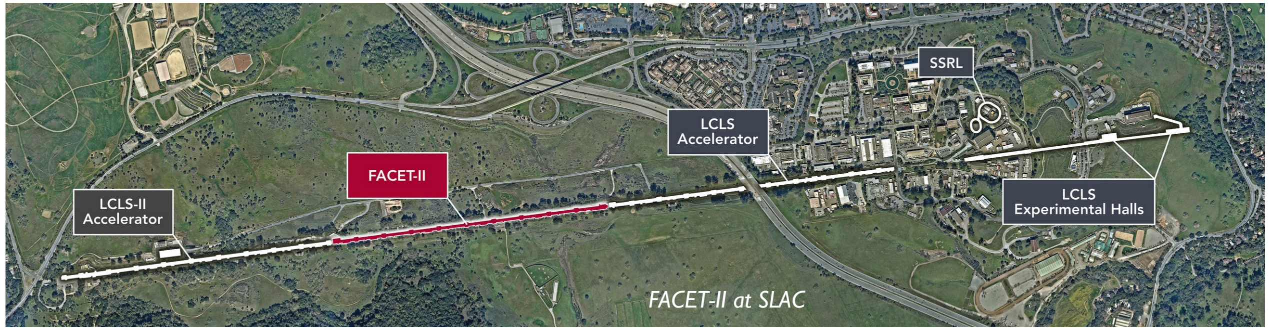
Auralee Edelen, on behalf of the whitepaper authors

SLACmass
May 12, 2022

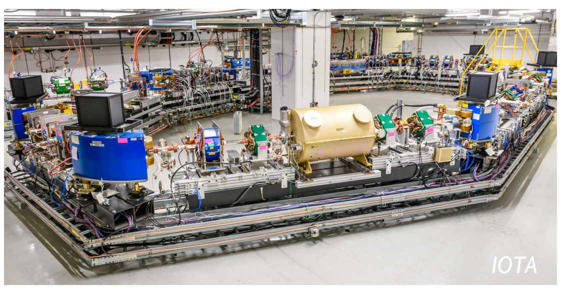
U.S. DEPARTMENT OF ENERGY
Office of Science

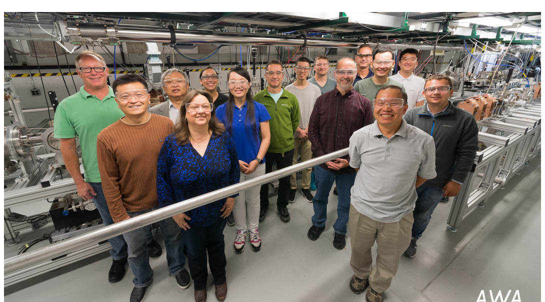
SLAC NATIONAL ACCELERATOR LABORATORY

Large Scientific Facilities

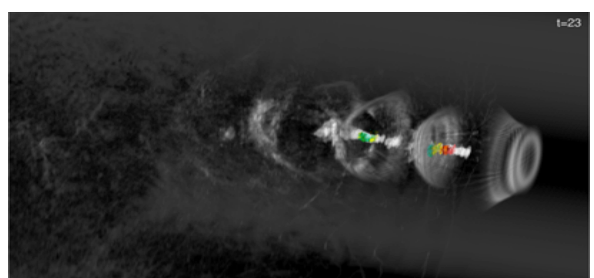


Small Test Facilities





Different Acceleration Schemes



Industrial / Medical

Emory Proton Therapy Center

HEP Grand Challenges for Accelerator and Beam Physics

Grand Challenge #1: Beam Intensity – "How do we increase beam intensities by orders of magnitude?"

Grand Challenge #2: Beam Quality – "How do we increase the beam phase space density by an order of magnitude, towards the quantum degeneracy limit?"

Grand Challenge #3: Beam Control – "How do we measure and control the beam distribution down to the individual particle level?"

Grand Challenge #4: Beam Prediction – "How do we develop predictive 'virtual particle accelerators'?"

Generated by a series of community workshops in 2019-2020 (as suggested by the 2015 HEPAP report), summarized here: https://arxiv.org/ftp/arxiv/papers/2101/2101.04107.pdf

Examples of wide range of physics regimes that needs to be simulated for accelerators…

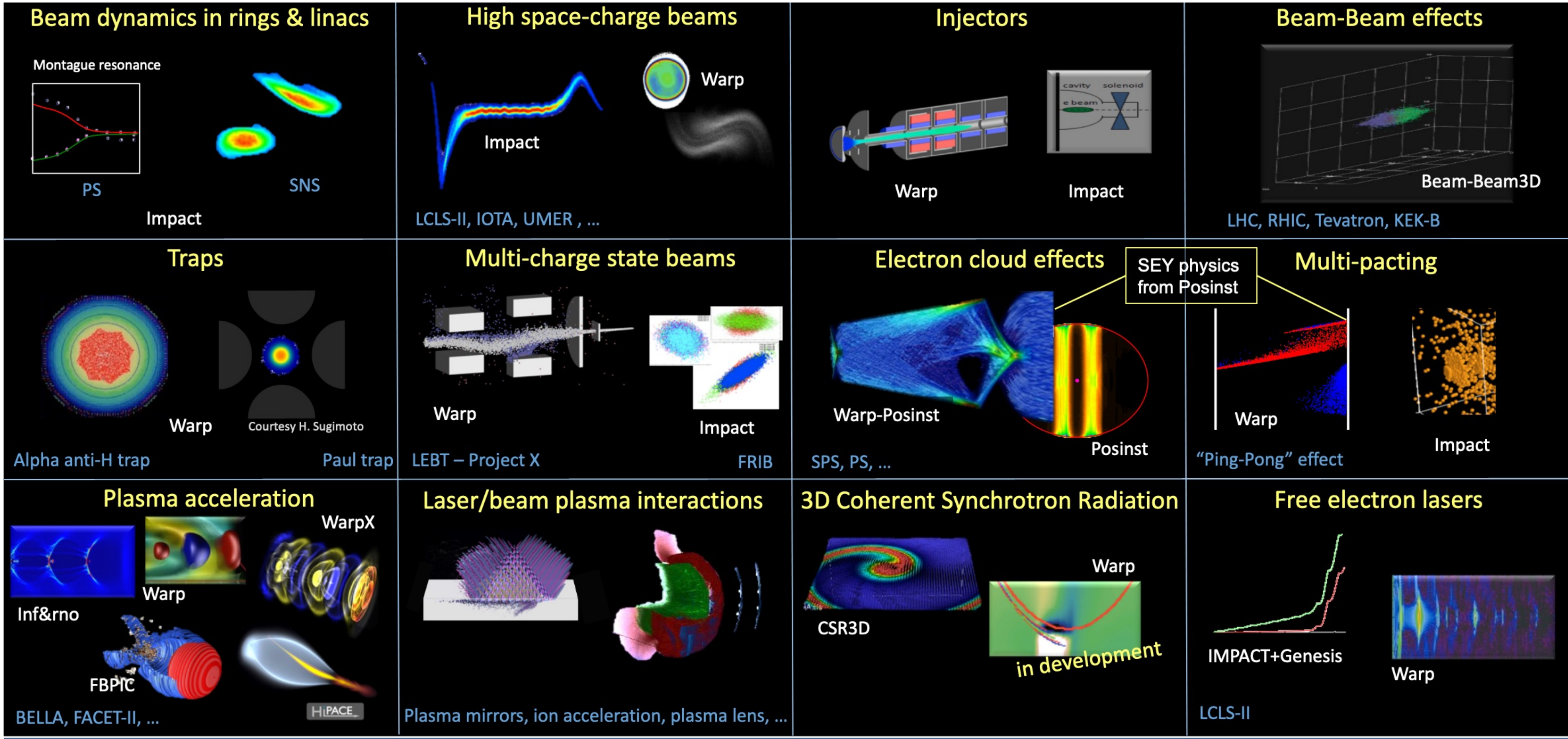


figure courtesy Jean-Luc Vay and the BLAST codes team https://blast.lbl.gov/

→ Accurate physics modeling for future high-intensity, high-charge, high-energy beams is challenging (let alone with novel acceleration schemes)

→ Design optimization and advanced phase space manipulation require increasingly high precision

Snowmass21 Accelerator Modeling Community White Paper

by the Beam and Accelerator Modeling Interest Group (BAMIG)*

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Areas of Need Highlighted in the White Paper

Basic Physics Modeling Needs

- Algorithms and modeling tools for current and emerging accelerator types and components *(rf and wakefield acceleration, materials, superconducting magnets etc.), especially to enable higher-precision modeling*

Computational Needs

- Hardware: CPU, GPU, time, memory, archive
- High-throughput computing
- Software performance, portability, and scalability

Emerging Computational Opportunities

- AI/ML, surrogate models, hybrid physics/ML modeling
- Differentiable simulations
- Quantum computing

Sustainability, Reliability, Usability of Code

- Code robustness, validation, benchmarking
- Usability, user support, maintenance
- Training and education

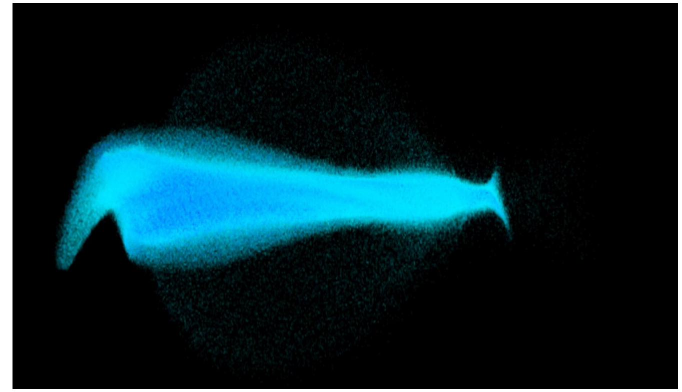
Community Ecosystems and Data Repositories

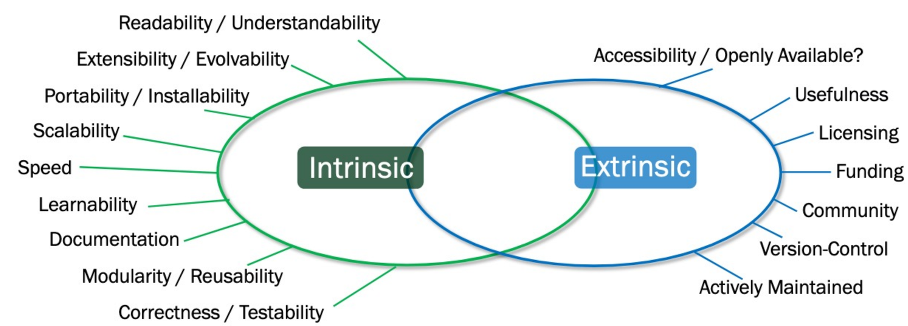
- Integrated workflows and frameworks
- Community standards for data and interfaces
- Open data repositories

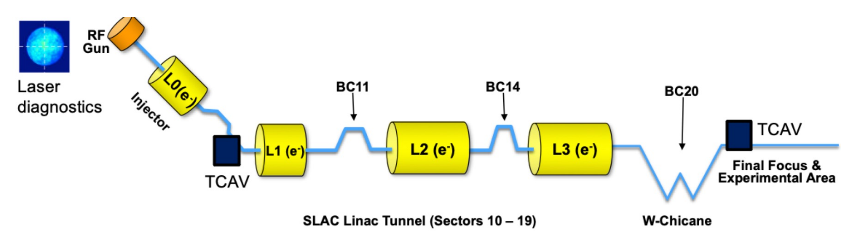
Ultra-precise, ultra-fast "virtual accelerators"

- Interdisciplinary, "end-to-end" simulations
- Tighter integration of simulations with real accelerators

lower-level to higher-level







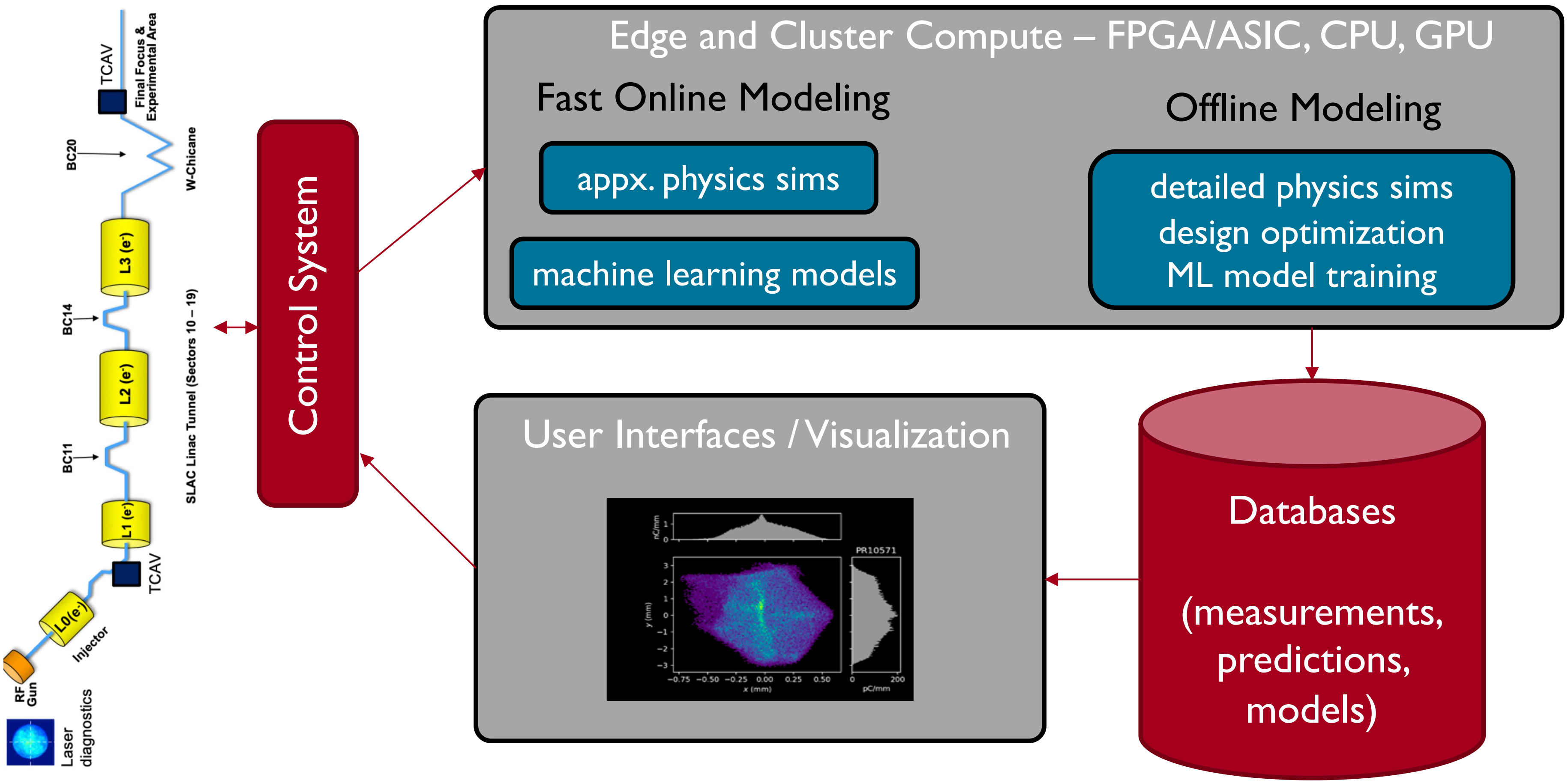
These areas each need support to meet current and future needs of HEP
New capabilities in each area will aid the others

Ultra-precise and Ultra-fast "Virtual Accelerators"

- Traditionally accelerator simulations have been partitioned by the required physics (nonlinear collective effects, plasma stages) → *need interdisciplinary, end-to-end simulations; can extend to experiment/detector*

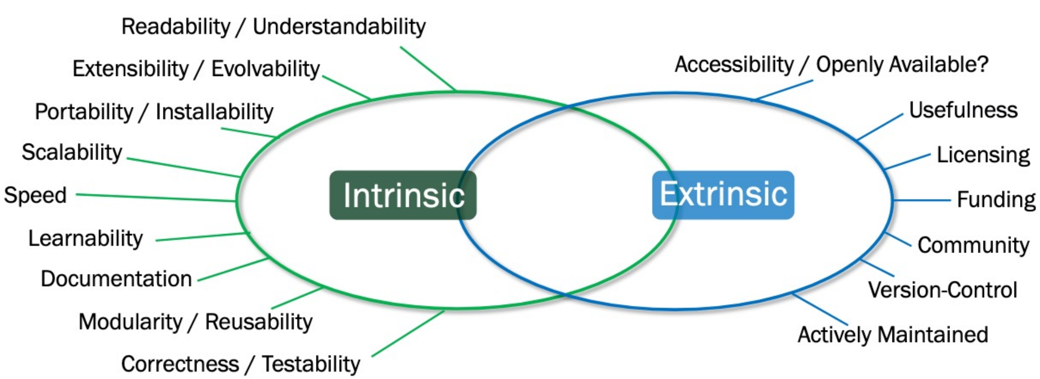
- Traditionally, detailed simulations have been "offline"; adjustments to match measured data have been limited or done by hand → *now looking to have tighter integration with the real accelerator (virtual/digital twin)*

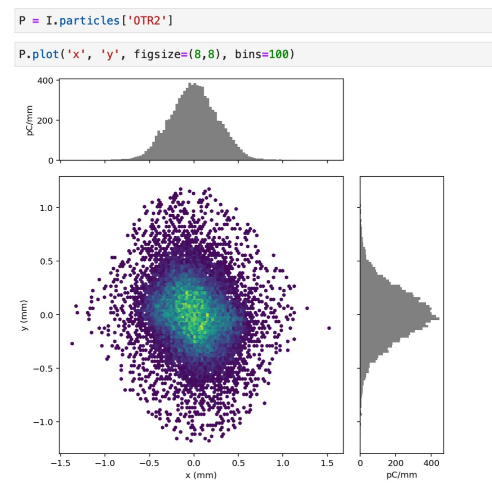
- Want tunability from ultra-precise and ultra-fast → *need incorporation of new algorithmic approaches for enhanced speed and/or precision (GPU acceleration, machine learning based surrogates, new computational physics algorithms)*



Community Ecosystems and User Training/Support

- Codes are very heterogeneous, often require expertise to run, and user-friendliness is highly variable
- Need **integrated workflows and frameworks,** interoperability between different simulation codes
- Need **shared standards** for data descriptions and code interfacing
- Need **shared data** repositories to help facilitate benchmarking, algorithm development, conserving resources, etc.
- Need dedicated resources for **user support, training, improvements to usability**





Code Performance and Computational Needs

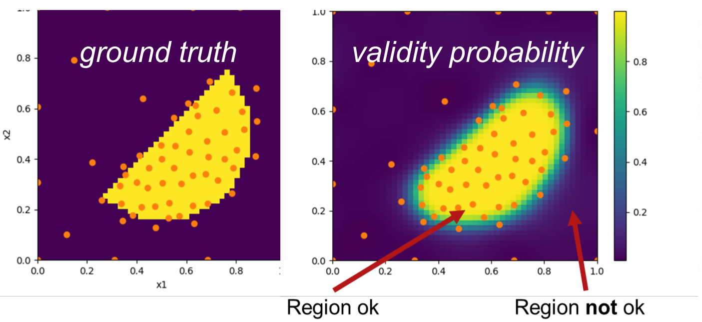
- Need more support for increasing **code robustness, validation, benchmarking, and software maintenance**
- Need more support for **streamlining code performance**
  - Heterogeneous compute (CPU, GPU, mix of traditional physics simulations and ML-based modeling)
  - High-throughput computing
  - Portability and scalability of codes
- Hardware resources: CPU, GPU, time, memory

ML-based Accelerator Modeling

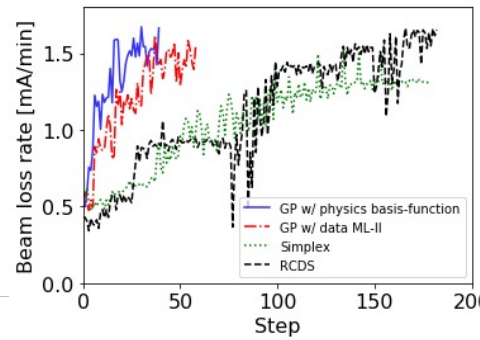
Techniques for combining physics and ML modeling *(more reliable/transferrable, require less data)*, including differentiable simulators

Algorithms for efficient optimization and characterization *(useful for simulation exploration/design, data generation, machine characterization)*

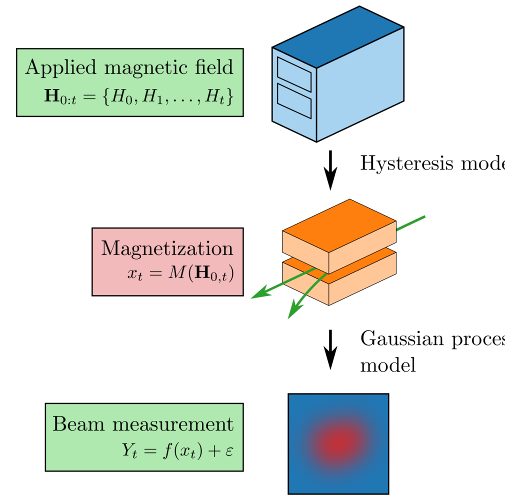
Roussel et. al. *Nat. Comm.* **2021**



Sampling constraints learned on-the-fly

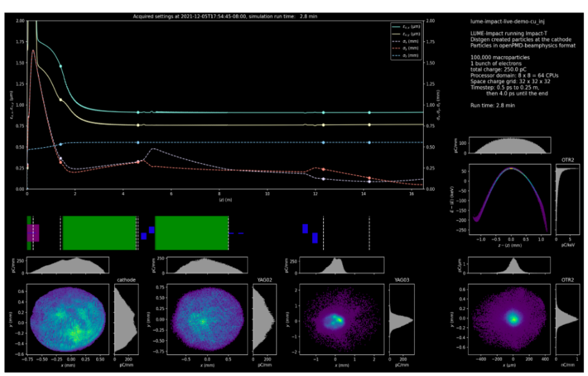


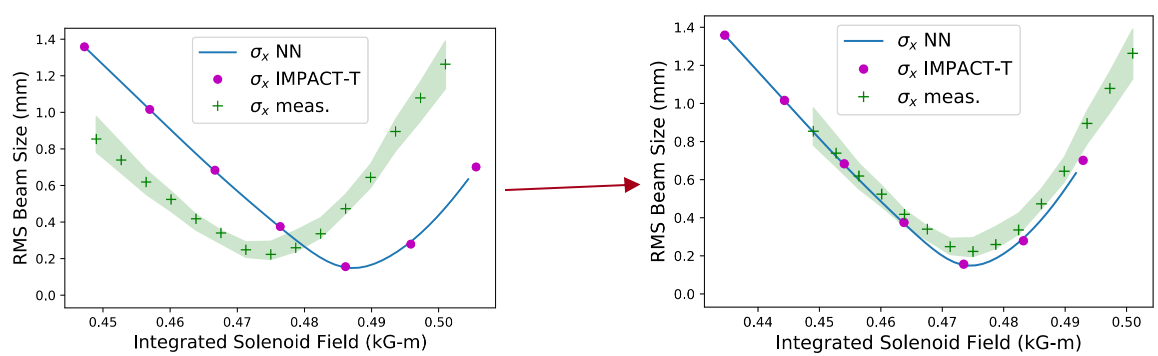
Hanuka et. al. PRAB , **2021**



Roussel et. al. *PRL*. **2022**

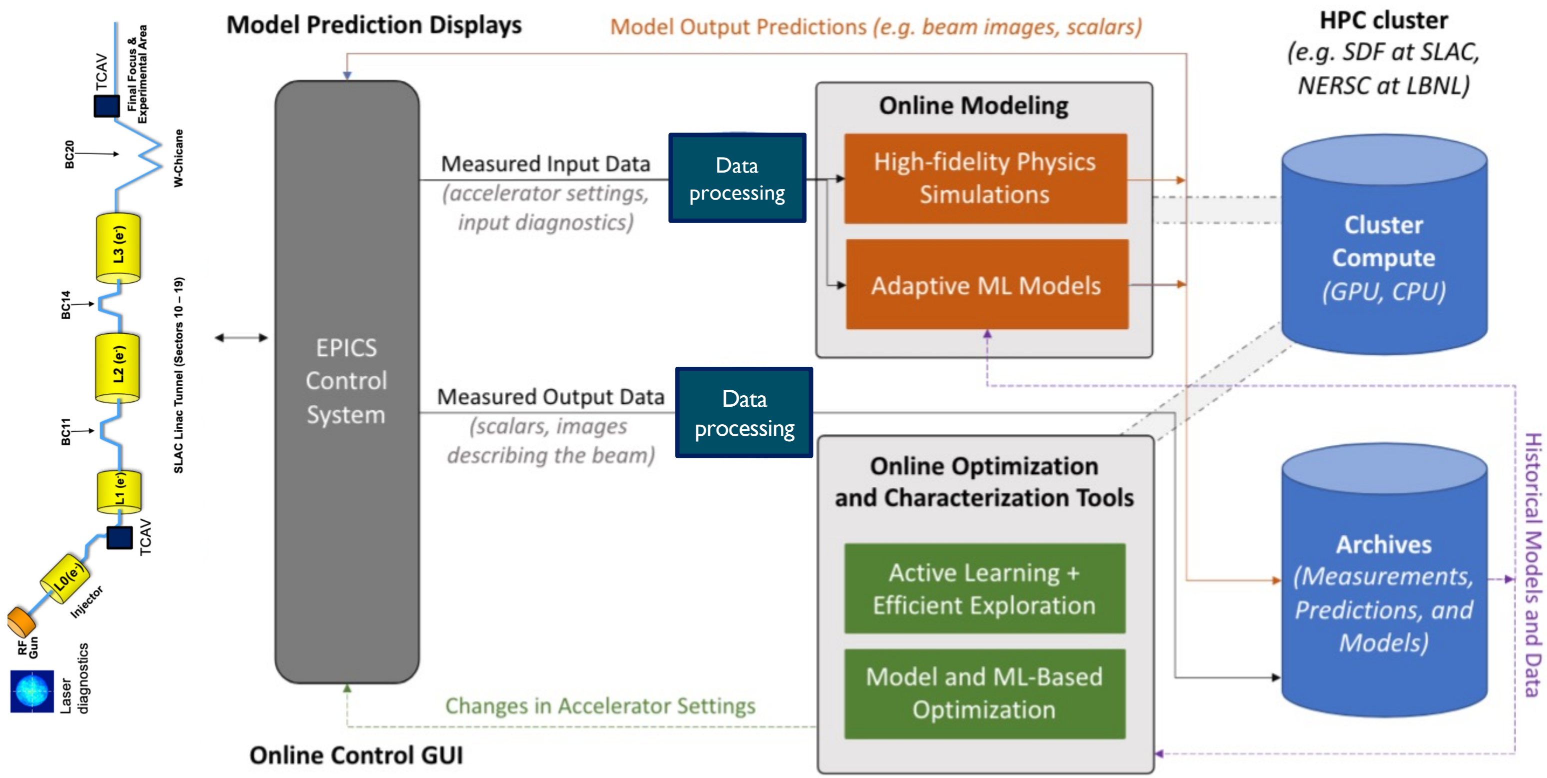
Techniques for fast, accurate, adaptive modeling: use in end-to-end design optimization and control prototyping, deploy models online (< 1Hz rep rate), and enable adaptation to new conditions (new beam params., drift, sim-to-real). Includes considerations of model uncertainty quantification and robustness.





Integration of AI/ML and Online Accelerator Modeling / Control

- Many proof-of-principle results for AI/ML modeling and control of accelerators → *usually in limited ranges of operating conditions or addressing isolated problems (e.g. only optimization, only modeling)*
- **Need to address integration into dedicated operation:**
  - Need a comprehensive ***facility-agnostic*** software/hardware ecosystem that can couple HPC, online simulation, and AI/ML
  - Need to assess/address robustness challenges of dedicated operation and coupling different types of AI/ML tasks together
  - Coupling of AI/ML, traditional algorithms, and human-in-the-loop operations *(provide useful/actionable information rather than add to information overload)*



White Paper Recommendations

https://arxiv.org/abs/2203.08335

Recommendation on basic physics modeling needs: Support the development of a comprehensive portfolio of particle accelerator and beam physics modeling tools for all types of particle accelerators (e.g., RF-based, plasma-based, structured-based wakefield, plasmionic), accelerator components (e.g., materials, superconducting magnets, structured plasmas), and which target the Accelerator and Beam Physics Thrust Grand Challenges on intensity, quality, control, and prediction.

Recommendation on computational needs: Support the development of increasingly powerful and specialized High-Performance Computing (HPC) and High-Throughput Computing (HTC) capabilities for accelerator modeling, and maintenance of software to run efficiently on these hardware (e.g., port of codes to GPUs) with efficient and scalable I/O, post-processing and in situ data analysis solutions, which will be needed to support ab initio modeling at increasing fidelity, training of surrogate models and AI/ML guided designs.

Recommendation on sustainability, reliability, user support, training: Provide sufficient resources for code maintenance, automated testing, benchmarking, documentation and code reviews. Convene a community effort to identify topics and teaching teams to deliver academic classes designed to foster sharing and cooperation, to be taught at the U.S. Particle accelerator school.

Recommendation on cutting-edge and emerging computing opportunities: Support the research and development on cutting-edge and emerging computing opportunities, including advanced algorithms, AI/ML methods, quantum computing algorithms for beam and accelerator physics, as well as on the development of storage ring quantum computers. *Support the development of ML modeling techniques and their integration into accelerator simulation and control systems, with an emphasis on fast-executing (up to real-time) and differentiable models, continual learning and adaptive ML for time-varying systems and distribution shifts, uncertainty quantification to assess confidence of model predictions, and physics-informed methods to enable broader model generalization to new conditions and reduced reliance on large training data sets*

Recommendation on community ecosystems & data repositories: Organize the beam and accelerator modeling tools and community through the development of (a) ecosystems of codes, libraries and frameworks that are interoperable via open community data standards, (b) open access data repositories for reuse and community surrogate model training, (c) dedicated centers and distributed consortia with open community governance models and dedicated personnel to engage in cross-organization and -industry development, standardization, application and evaluation of accelerator and beam modeling software and data.

Recommendation on the next frontier - ultraprecise, ultrafast virtual twins of particle accelerators: Support the development of accelerator modeling software that orchestrate interdisciplinary set of tools with standardized data representations to enable end-to-end virtual accelerator modeling and virtual twins of particle accelerators, which combine first-principle models together with machine learning-based surrogate models, for tunability from maximum precision for accurate and realistic accelerator design to maximum speed for online particle accelerator tuning.