An Integrated Research Infrastructure framework for digital twins of laser-plasma acceleration experiments

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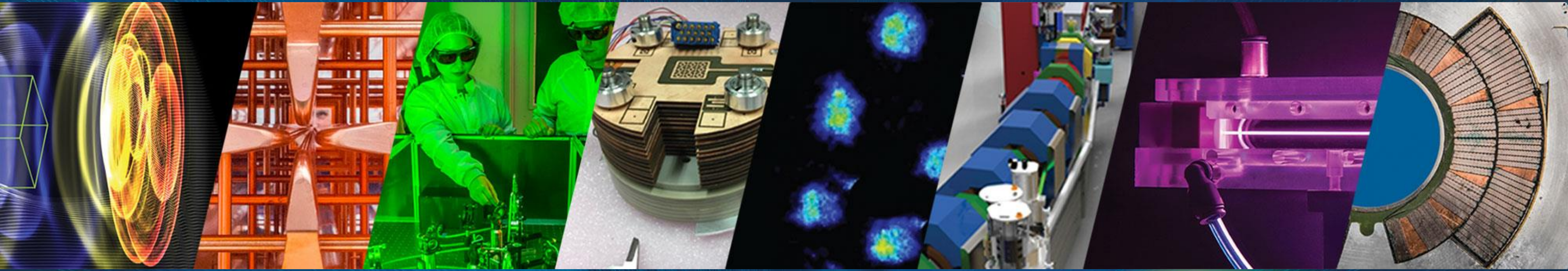

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Context: experiments at LBNL's BELLA facility explore laser-plasma acceleration.

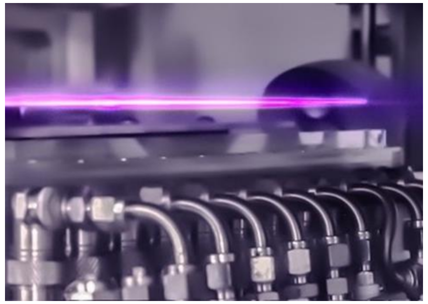
The BELLA facility delivers **ultra-intense, ultra-short laser pulses** to target chambers.

Experiments often consist in **tuning parameters** (e.g., laser focal position, temporal profile, etc.) to achieve **optimal acceleration.** (e.g., maximize accelerated charge)

The objective of this work is to provide **real-time guidance to experiments** when exploring the parameter space.

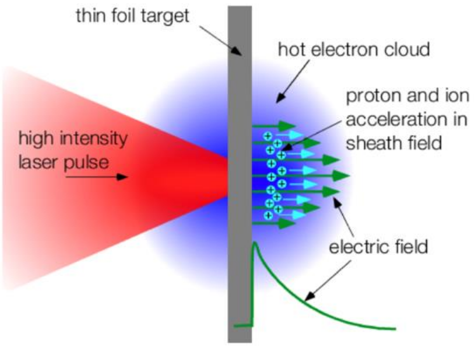
BELLA is used to study **laser-plasma acceleration:**

- Laser interaction with a ~30 cm-long gas target can generate **~10 GeV electron beams**



A. Picksley et al., Phys. Rev. Lett. **133**, 255001 (2024)

- Laser interaction with a solid foil can generate **ions with tens of MeV**



L. Willingale, 2019 CERN accelerator school

Simulations can provide guidance but require HPC resources.

- The outcome (e.g., accelerated charge) for one set of parameters (e.g., laser focal position, temporal profile) can be predicted with **Particle-In-Cell (PIC) simulations**.

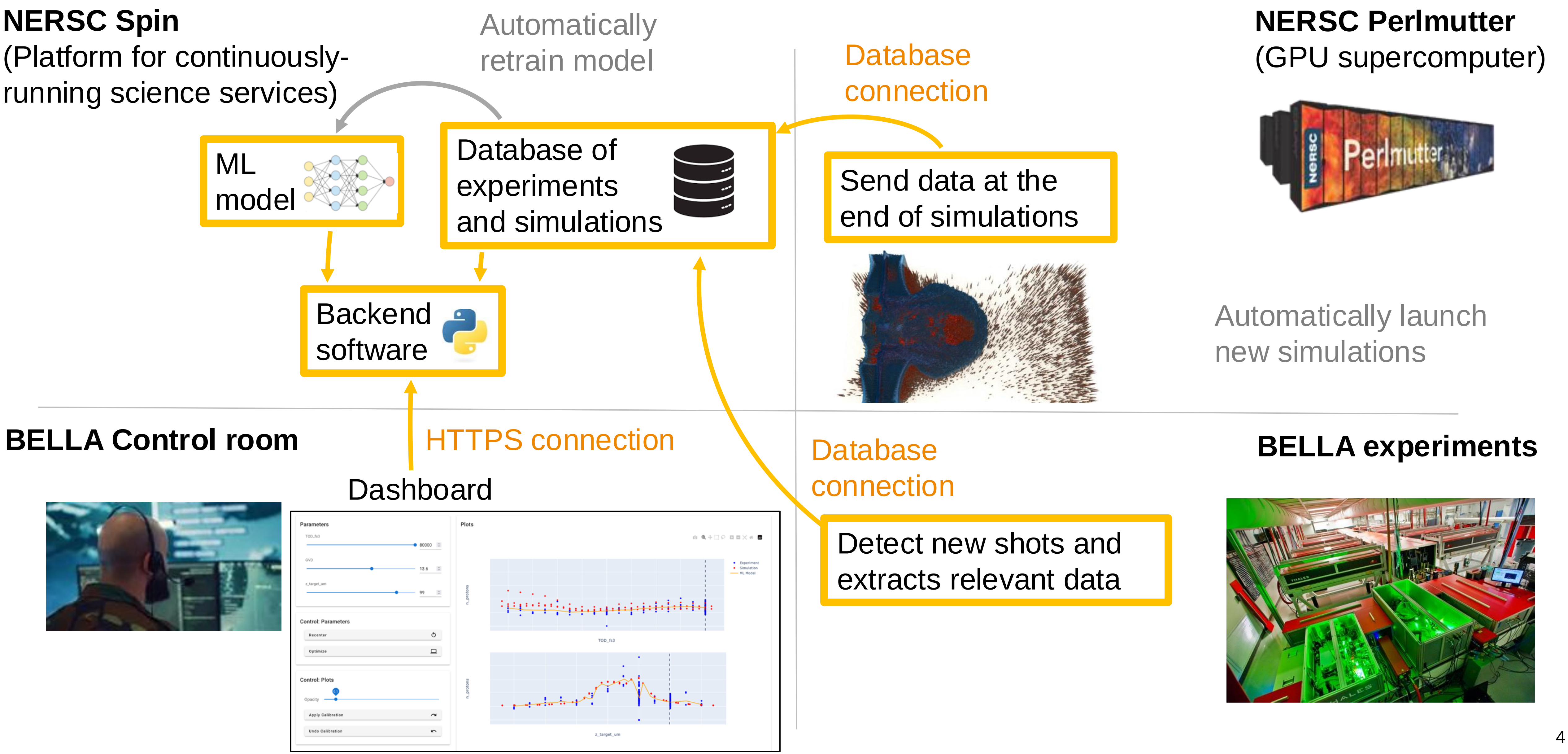
PIC simulation of a solid foil interacting with a laser pulse.

- However, a single PIC simulation can take **tens of minutes**, using **tens of GPUs**, and thus requires a computing facility (e.g., NERSC at LBNL)

- “Real-time” guidance for experiments requires **integration** between the **experimental facility** and the **computing facility**.

NERSC’s GPU supercomputer

We are developing a framework for integration between BELLA and NERSC.



This framework leverages different open-source components.

NERSC Spin

Standardization:
SLAC LUME-model

ML model

Backend software

MongoDB

Database of experiments and simulations

trame

NERSC Perlmutter

pymongo

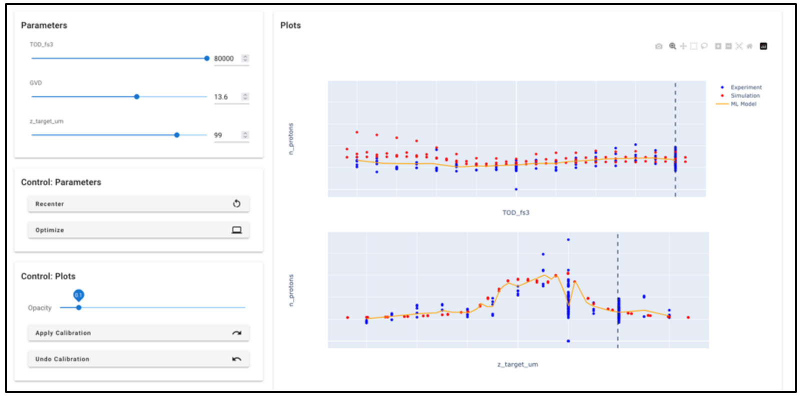
Send data at the end of simulations

Simulations:
BLAST (BEAM PLASMA & ACCELERATOR SIMULATION TOOLKIT) WarpX LASY

Orchestration:
optimas

BELLA Control room

Dashboard



BELLA experiments

pymongo

Detect new shots and extracts relevant data

Note: BELLA does not use EPICS

Tools developed at NERSC facilitate this framework.

NERSC Spin

Platform for **continuously-running** science services

- Scientists **upload a Docker container** that defines the science service (e.g., web-based application)
- NERSC Spin **handles the rest:** deploys the Docker container on NERSC infrastructure, using Kubernetes
  - managed infrastructure: monitoring, load-balancing, security, …
  - high uptime / availability
  - access to NERSC databases and filesystem

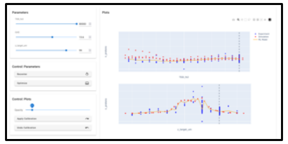
NERSC Superfacility API

Python API to submit/monitor jobs on Perlmutter

- Can be used on remote servers (including Spin) No need to SSH to Perlmutter
- Example usage:
  - Automate retraining of the model
  - Launch simulations from the dashboard

NERSC Spin

Backend software



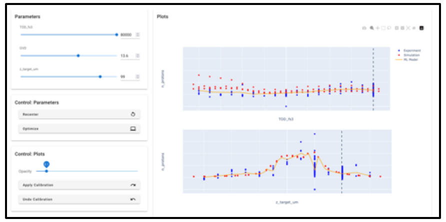
submit

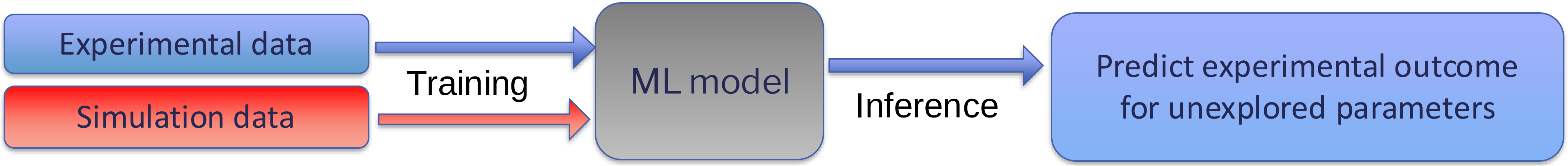
NERSC Perlmutter

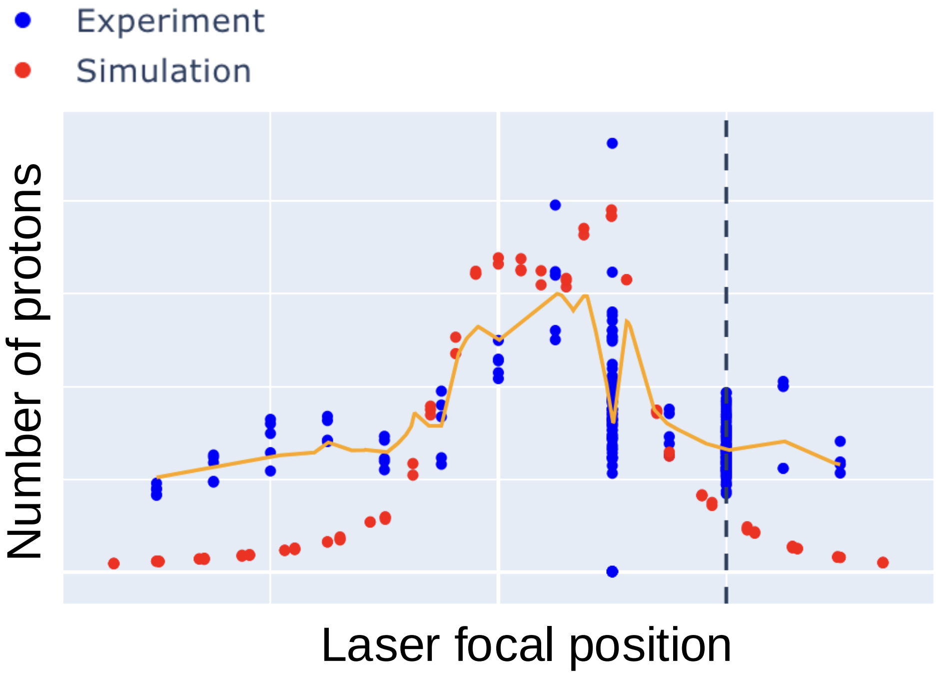
- retraining
- simulations

Challenge: experiments and simulations do not always match quantitatively.

Database of experiments and simulations







Simulations generally reproduce the **correct trends**, but are not always in **quantitative agreement** with experiments.

Many potential reasons:

- Simplifying physics assumptions in simulations
- Imperfect knowledge of experimental conditions
- Uncalibrated experimental diagnostics

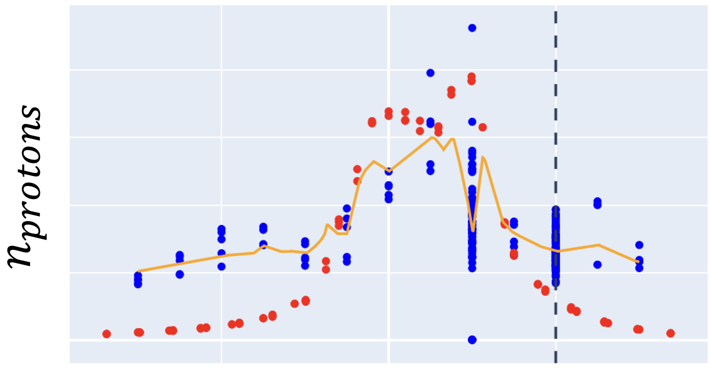
Needs to be addressed, in order to train the ML model on the combined database.

Disagreement between experiments and simulation can be overcome by learning an empirical calibration.

Learn **empirical calibration constants**, that translate simulation data to experimental data.
T. Boltz et al., arXiv:2403.03225 (2024)

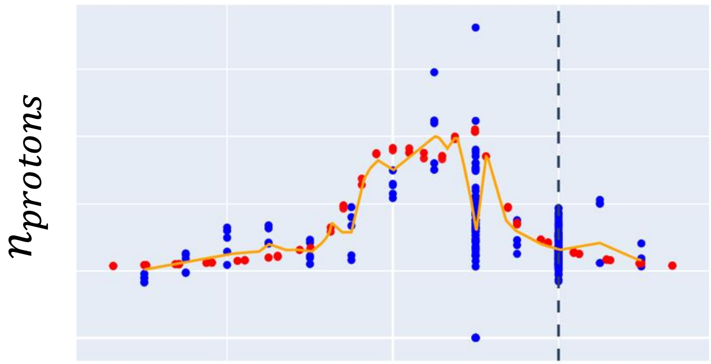
$$n_{protons,exp.} = \alpha \, n_{protons,sim.} + \beta$$

Learned by gradient descent, while training the ML model.

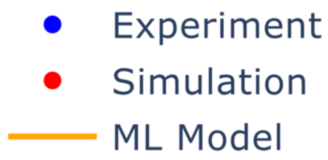


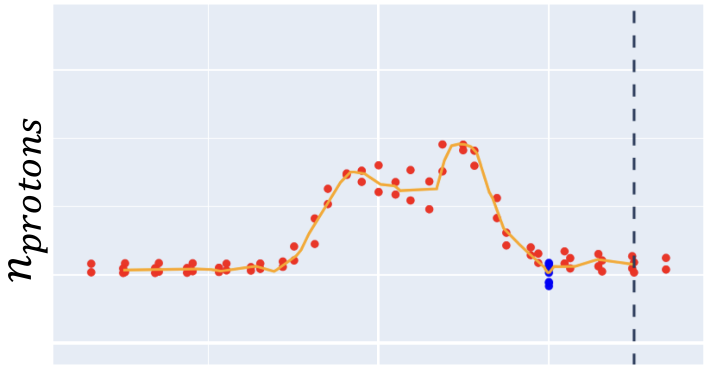
Laser focal position

Calibrate simulations



Laser focal position





Laser focal position

Laser pulse with a different temporal profile.

Once the calibration is learned, it can potentially be used for predictions where experimental data is sparse.

Conclusion

- We are building a framework for **real-time guidance during experiments**, based on **HPC simulations**
- The framework leverages open-source tools to **integrate** the experimental facility and computing facility.
- Real-time guidance is based on **ML models** that learn from both experimental and simulation data, but a key challenge is to manage **discrepancies between these two sources of data.**
- Our framework is to be deployed in real-time in BELLA experiments within the next few weeks…
- Potential **early template** for DOE "Integrated Research Infrastructure" efforts to connect experiments with DOE HPC facilities

This is a team effort! Many thanks to all who made it possible!

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Work supported by the Laboratory Directed Research and Development (LDRD) Program of LBNL.

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Synergistic work supported by the NERSC Science Acceleration Program (NESAP)

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Student contributions supported by the Visiting Faculty Program