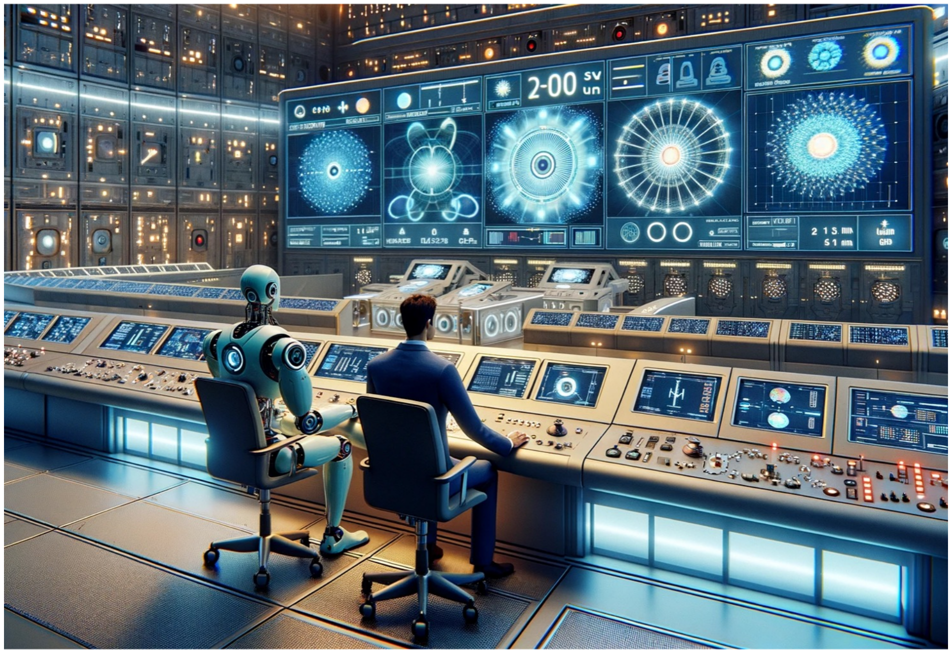
Nuclear Physics and AI

EuCAIFCon 2024



Amber Boehnlein

Jefferson Lab

U.S. DEPARTMENT OF ENERGY | Office of Science

JSA

Context: Long Range Plan

1 | EXECUTIVE SUMMARY

RECOMMENDATION 4

We recommend capitalizing on the unique ways in which nuclear physics can advance discovery science and applications for society by investing in additional projects and new strategic opportunities.

Today's investments enable tomorrow's discoveries, with corresponding benefits to society. We underscore the importance of innovative projects and emerging technologies to extend discovery science, which plays a unique role in supporting national needs.

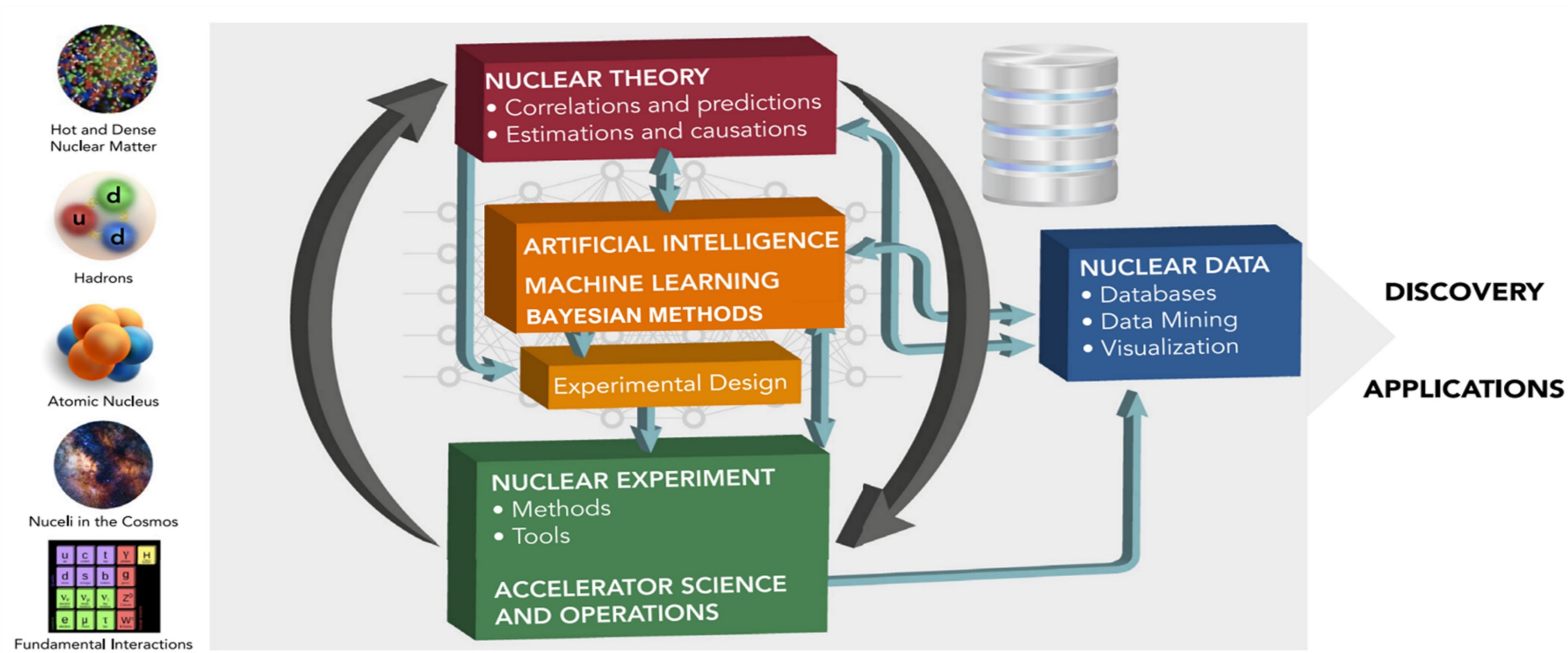
Optimizing scientific discovery from rich experimental and computational data sets produced in nuclear physics research requires utilizing AI and ML technologies. Support for a coordinated effort to integrate AI/ML technologies into the nuclear physics research programs will accelerate discoveries.

High-performance computing (HPC) has led to remarkable scientific progress for nuclear physics, enabled in part by collaboration with computational scientists and applied mathematicians through the DOE Scientific Discovery through Advanced Computing (SciDAC) and NSF Cyberinfrastructure for Sustained Scientific Innovation programs. As we enter the era of exascale computing, with increasing numbers of communities within nuclear physics poised to take advantage of HPC, enhanced support will maximize scientific progress.

LRP is decadal US Community Driven prioritization activity

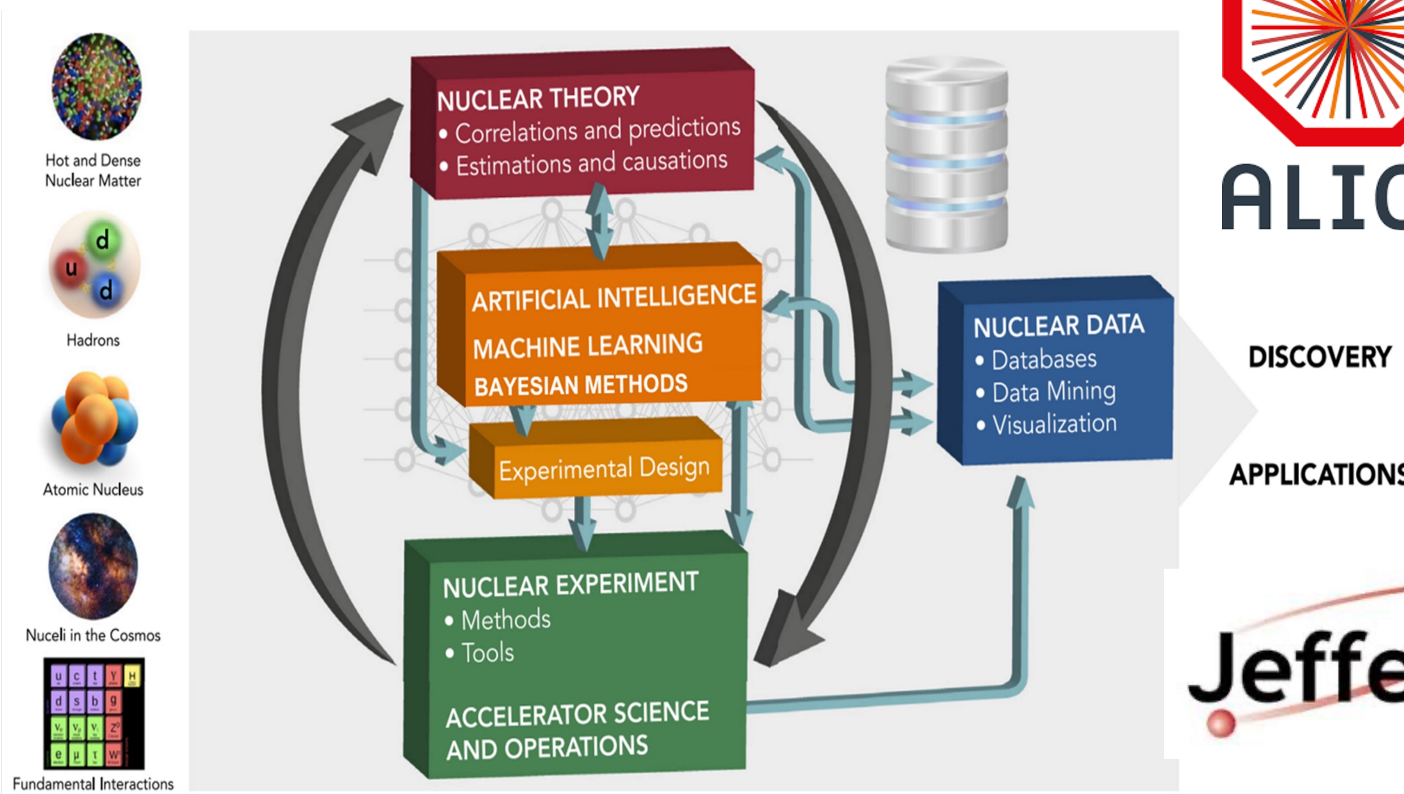
Nuclear Physics AI vision

Speeding-up *the cycle of the scientific method*



Nuclear Physics: Select Experimental facilities

Speeding-up *the cycle of the scientific method*



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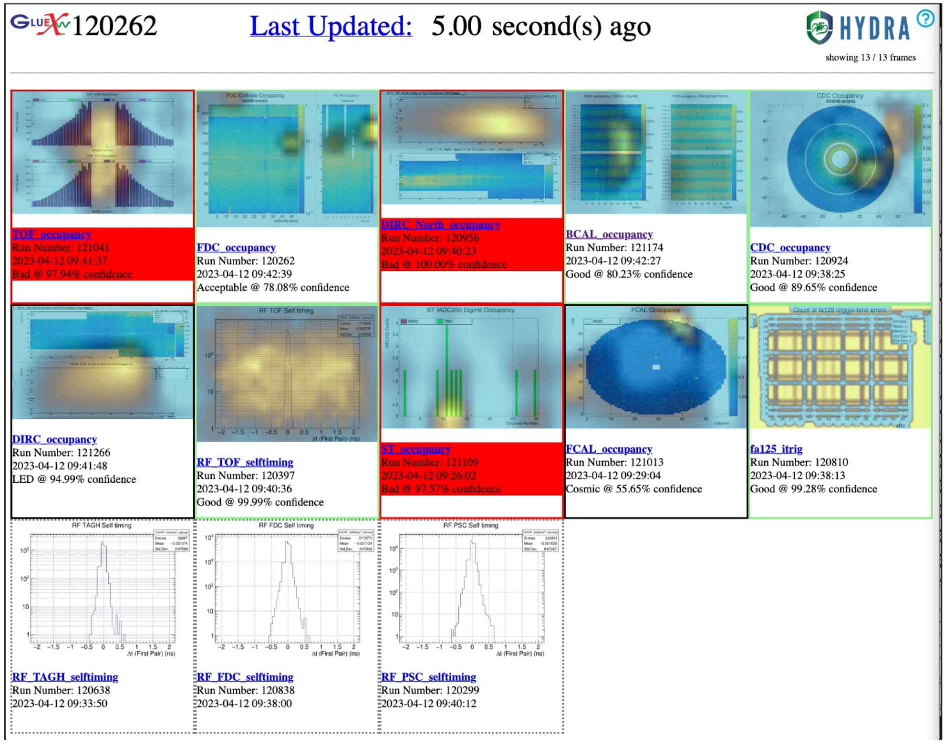
AI applications in NP

- Currently deployed ML applications
  - Detector Operations
  - Reconstruction
  - Lessons (learned)
- Future ambitions
  - Detector Design for the Electron-Ion Collider
  - Theory/experiment integration

Detector Operations: Monitoring at Jefferson Lab

- Hydra: near real-time predictions of detector issues
  - Used in all Halls for monitoring
  - Requires human intervention to fix problems.
- Grad-CAM technique to highlight specific detector areas with issues.
- Data Labeler to efficiently label images
- Library with thresholds and active model designation
- Grafana Dashboard to display prediction over time.

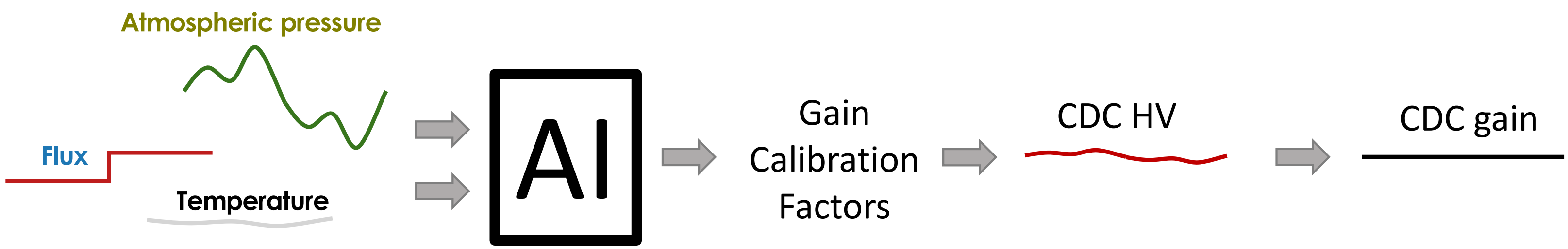


AIEC - AI for Experimental Controls

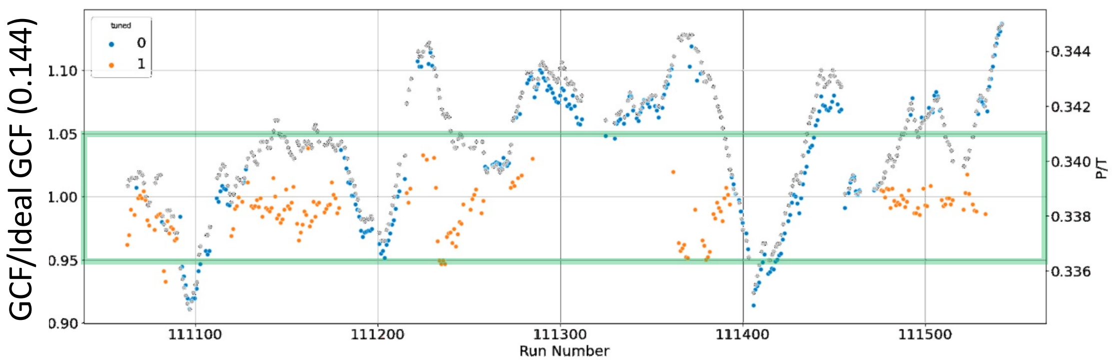
Experimental Physics Software and Computing Infrastructure

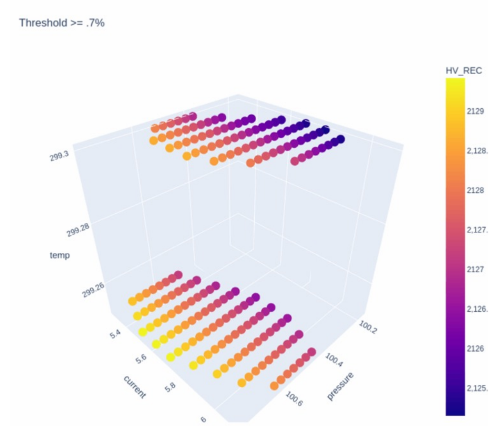
Developed system that uses AI/ML to determine control settings that are automatically applied during production data taking to stabilize gains of drift chambers.

AI trained on existing calibrations derived from data, correlating predicting them from environmental values known prior to data taking



Deployment 3 – PrimEx-η June-Dec 2022





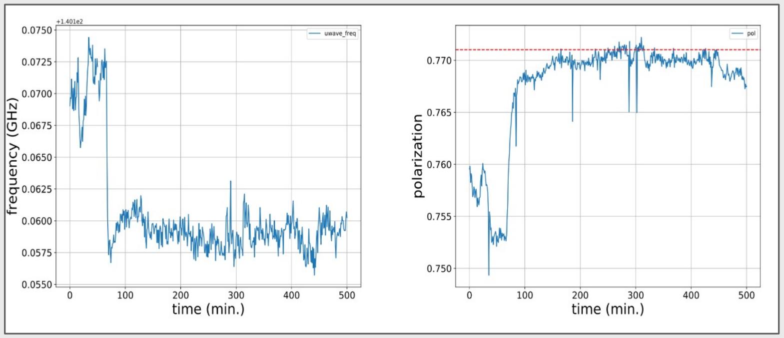
final policy: *when outside the volume of confidence revert to observation mode in order to gather more training data*

In production

DOE NP LAB-20-2261
PI: David Lawrence
Co-PIs: Thomas Britton, Naomi Jarvis

Detector Operations: AI Optimized Polarization

Left: microwave frequency vs. time. Right: corresponding polarization

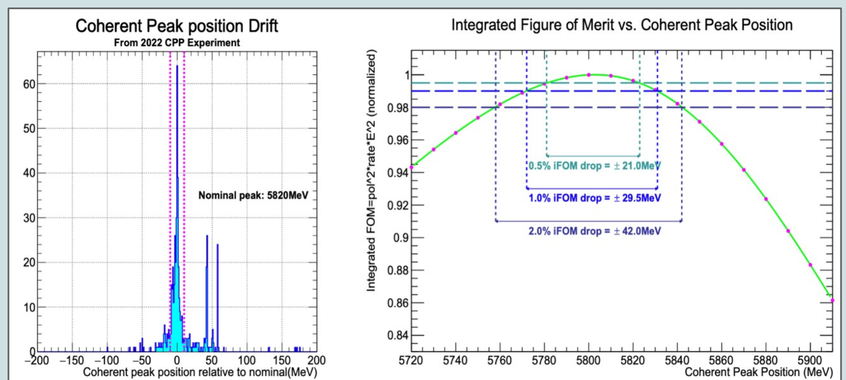


Polarized targets use microwave drivers to maintain polarization (alignment of the magnetic spins) and Nuclear Magnetic Resonance Spectroscopy to measure it. We will use AI/ML to:

- cleanly extract NMR signal from changing background
- adjust μ-wave frequency periodically to maintain optimal polarization

Polarized photon beam uses thin diamond radiator with precise angle adjustment to align edge of coherent bremsstrahlung peak. We will use AI/ML to:

- determine angular shifts needed to maintain coherent peak of polarized bremsstrahlung photons within +/-10MeV its nominal position in real time
- digital-twin of diamond to map degradation as function of position in order to predict location of optimal polarization

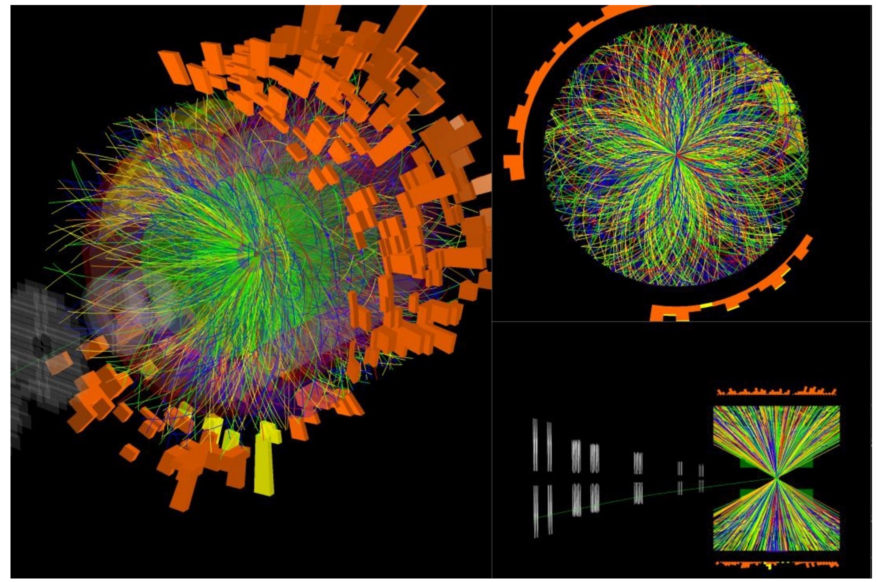


Work begun

Funded through DOE NP FOA SC-0002875
PI: David Lawrence

Applications of Machine Learning in Heavy-Ion Physics Experiments

- Thousands of tracks produced pro Pb-Pb Collision (few Pbytes/run)
- How to identify a rarely produced signal among all these tracks
- How to effectively suppress contamination from wrongly-combined pairs ?



Option 1: "Standard" cut-based selection:

- Compare distributions of signal and background in each variable of interest
- Apply some set of rectangular cuts, usually per momentum interval

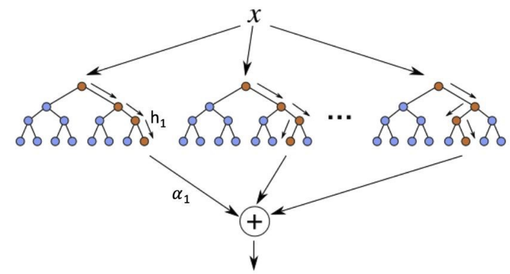
Option 2: Shift toward multivariate techniques:

- Instead of tuning single cuts on individual variables, we want to exploit correlations in feature space to distinguish signal from background
- multidimensional cut space

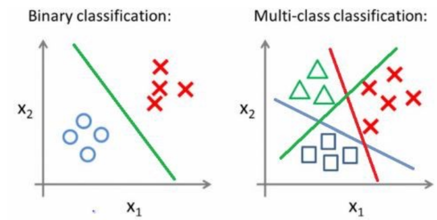
How best to optimise this?

J. Wilkinson, GSI-Darmstadt

Move towards machine learning



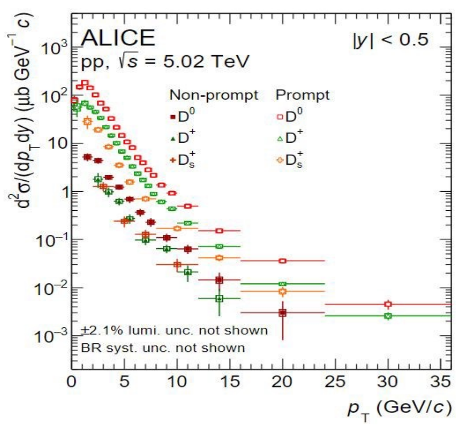
- Simplify a multivariate problem down to a single, “probability-like” parameter to cut on.



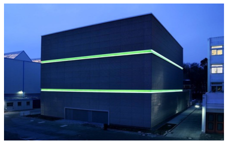
- Each candidate assigned a weight based on final node of each of a series of decision trees (Option of binary classification (signal vs background), or multi-class (signal originating from different sources - a charm decay vs a beauty decay))

- Typical training sample: Monte Carlo enriched with desired sample, background from “sidebands” in data (mass far from particle of interest)

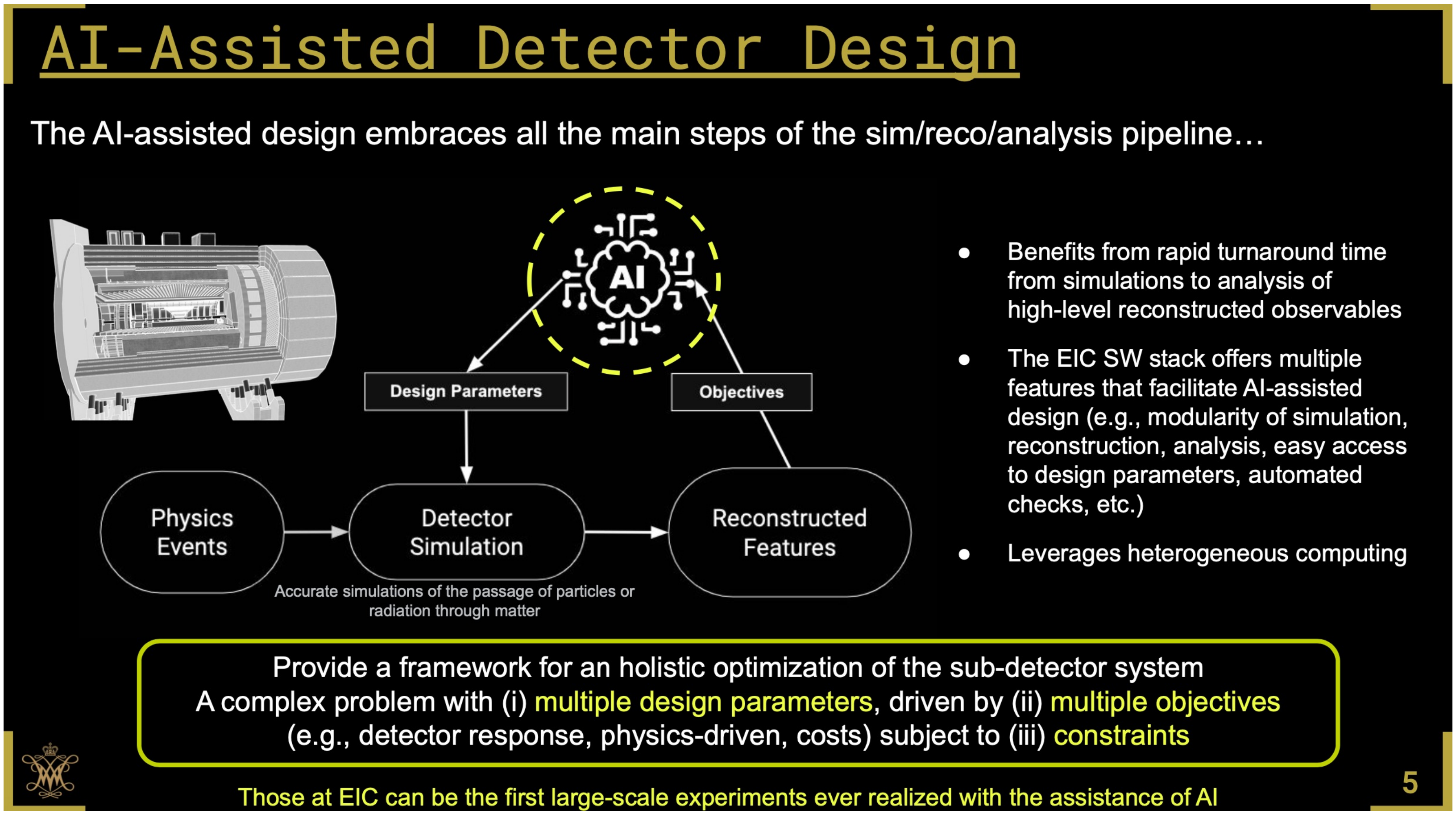
Successfully applied in ALICE for analysis of beauty production in D^0 decays; work ongoing to extend Λ_c analysis to use this



J. Wilkinson, GSI-Darmstadt

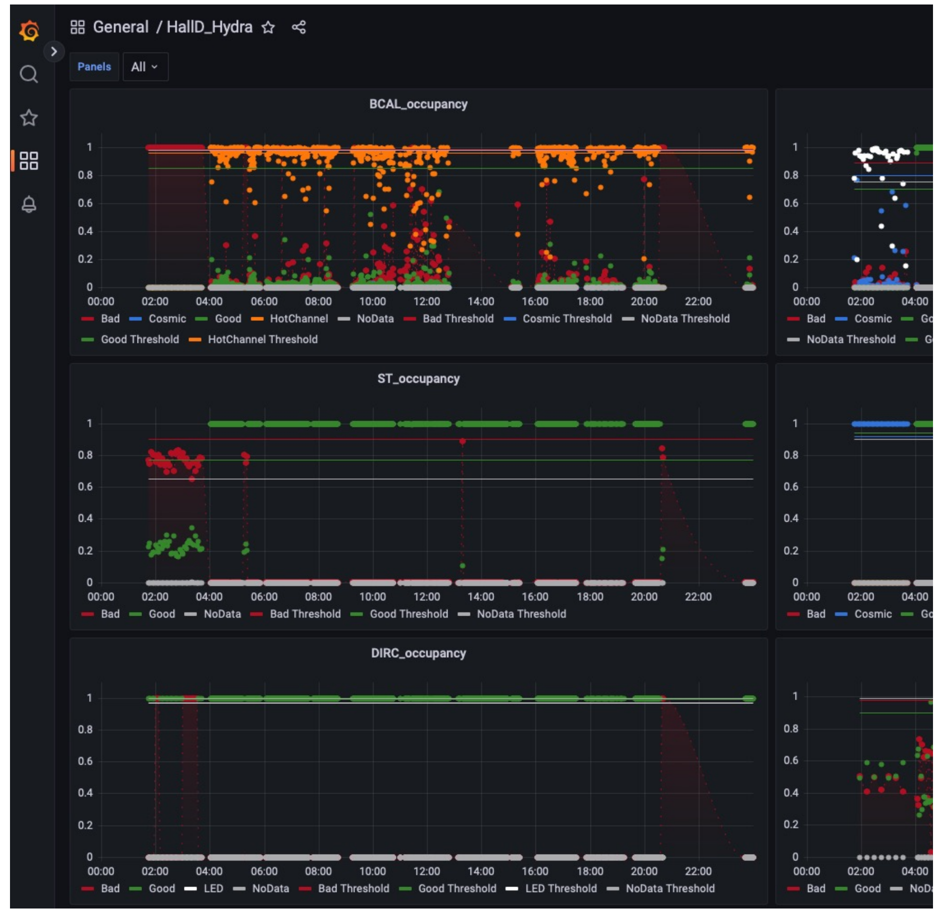


Future Ambitions: Electron Ion Collider



Lessons

- Data Science is about DATA
  - AI/ML prompts different views of much data at what precision should be collected.
  - AI/ML changes our view of what we can accomplish with our data
- Operating Facilities typically have over-constrained and static budgets
  - AI/ML can have significant ‘ROI’
- It’s a Journey to getting buy-in for AI/ML in operations
  - Even when the ML algorithms are demonstrably solving a real problem with integrity
  - At the same time, success does breed more success



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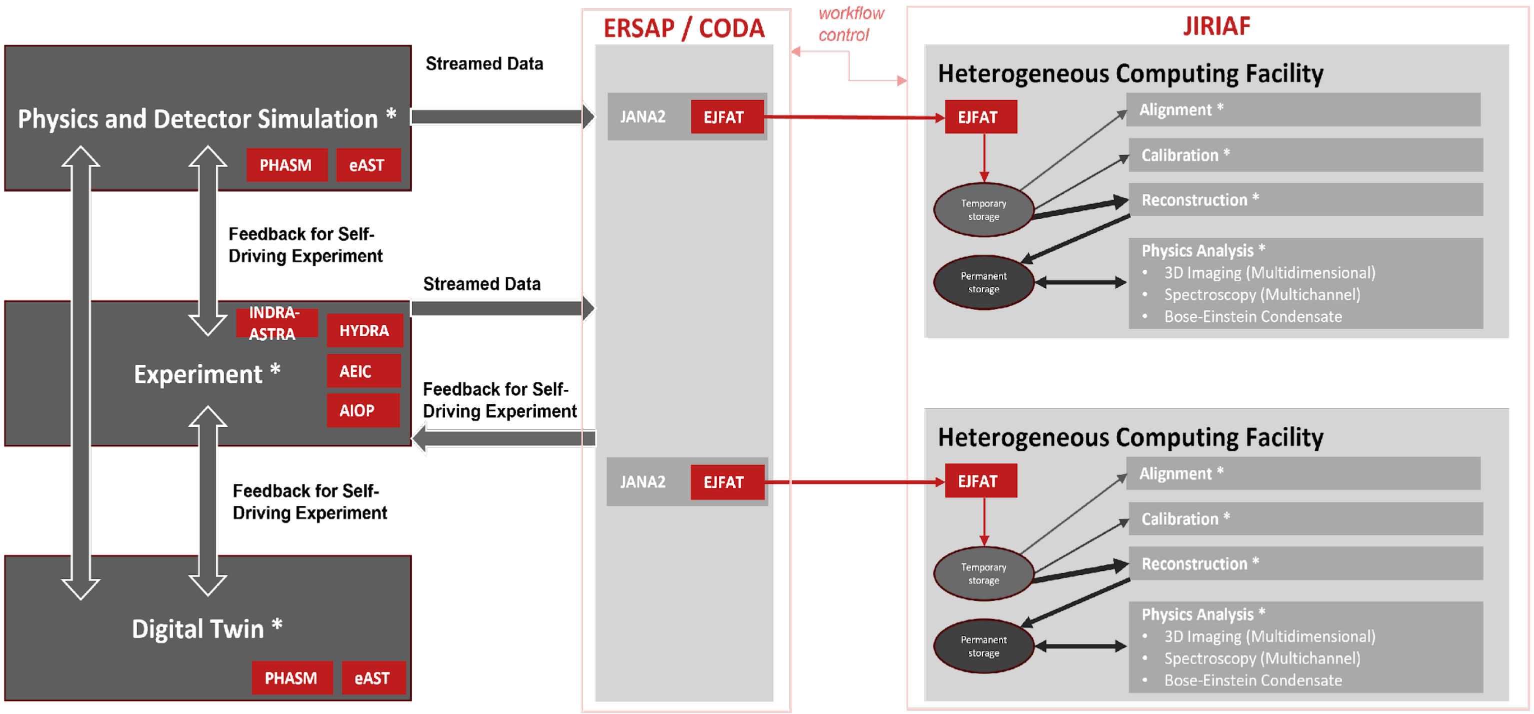
Computing Model Design: EPIC



*** AI/ML**

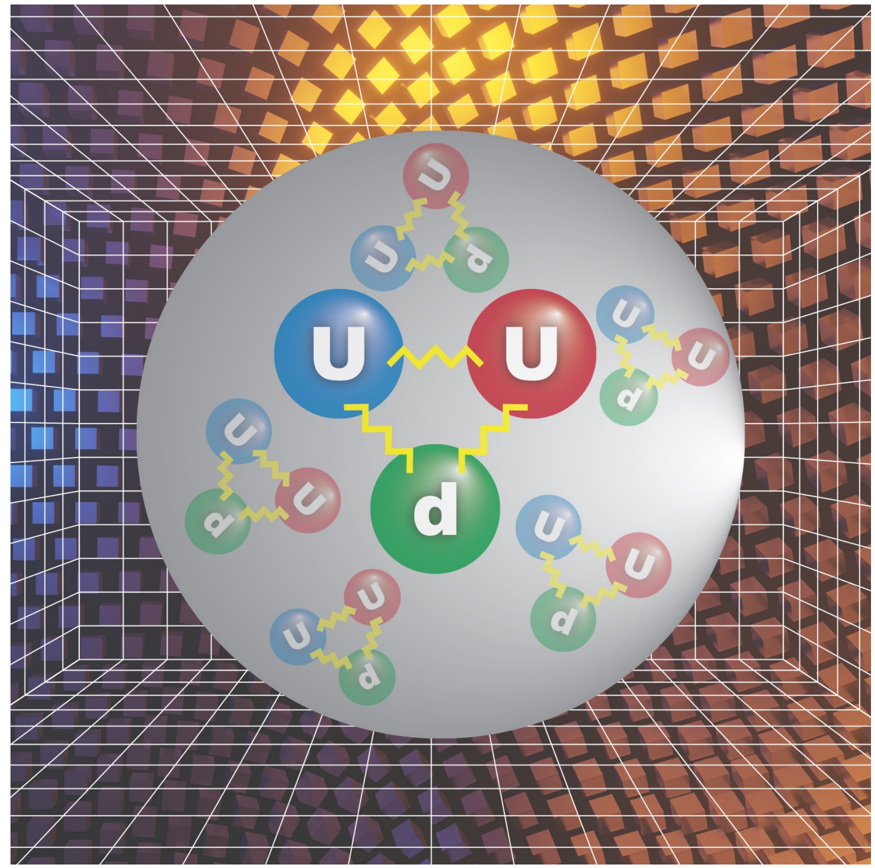
The AI promise:

AI-empowered discovery

- Accelerating understanding of complex theory and data
- Automated research workflows
- Integration of multi-modal data
- Discovery: data mining, visualization, interpretable AI
- Data preservation/future-proofing
- Real-time experimental steering

New developments enabling high-impact AI applications

- Exascale computing
- Large language models
- Foundation Models
- Generative AI/interpretable AI
- AI-driven unbinned analysis



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Nuclear Physics Discovery

3D imaging of the internal structure of protons

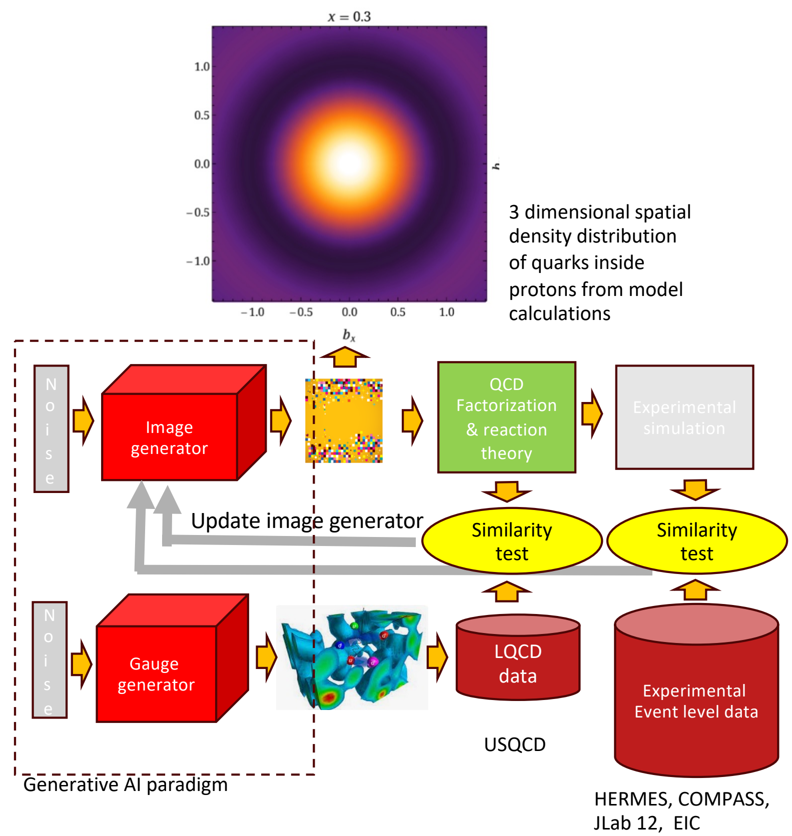
Critical Opportunity: Protons emerge from interactions between quarks and gluons, with the unique feature of confinement making it impossible to observe quarks and gluons directy by any modern detector. With experimental and theoretical progress, the nuclear physics community is poised, for the first time, to achieve real time 3-dimensional imaging of internal structure of protons. To peer into the proton to see quarks and gluons indirectly requires integration of experimental simulations and complex theoretical frameworks for processing large scale data from high luminosity experiments (JLab & EIC) in an unprecedented time scale only accessible by exascale computing. Scalable generative AI for real time analysis addresses fundamental challenges in nuclear theory simulations and provides a robust uncertainty quantification that are necessary for 3-D imaging.

Expected Impacts:
- Fast and AI empowered analysis tools to study the internal quantum structure of basic building blocks of matter. Development of distributed learning in the era of AI and exascale computing for analyzing datasets across DOE complex.
- Solving the proton imaging problem will couple AI driven analysis in nuclear theory with high performance computing to provide data analytic pipeline that will be broadly applicable to other areas of science. A composable AI-driven framework will enable nuclear physicists to discover new physics insights that are not accessible with current techniques.
- The development of AI-driven data analytic ecosystem will make the US a leader in addressing the most complex and challenging problems in fundamental science.

Required R&D:
- Applied Math to derive algorithms to utilize generative AI for computational nuclear simulations and inverse design problems in nuclear quantum theory including lattice QCD.
- Experimental simulation and theory frameworks using differentiable programing paradigm.
- Distributed generative AI-based physics analysis workflows for exascale computing.

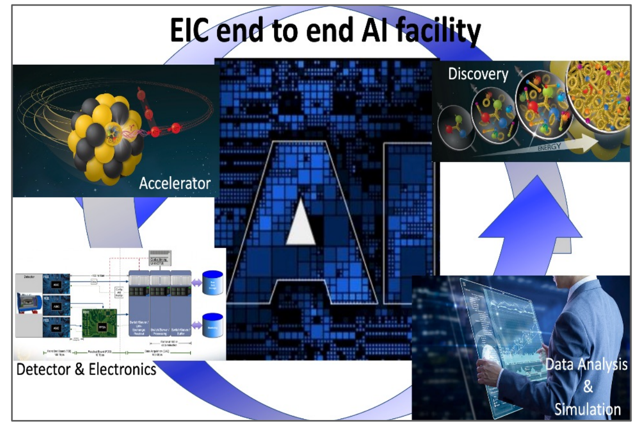
Timeline:
- Near term: 1-3 years: Robust generative AI based inference algorithms. First integrated experimental and theoretical imaging based physics analysis framework.
- Mid term: 3-5 years: Scalable analysis framework for imaging the proton
- Long term: 5-10 years: First images of the proton.

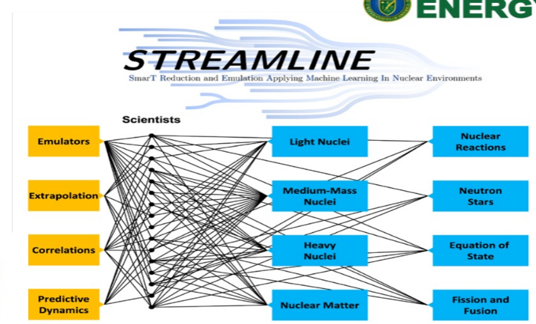
Anl/Jlab



Envisioning the future: Scientific Discovery

- Fertile time for considering new methodologies
- Frequent themes
  - Faster time to solution
    - Real-Time analysis on streamed data
    - Surrogate models
  - Unfolding experimental data and other forms of solving inverse problems
  - Digital twins of physical systems
    - Continual learning
  - Anomaly detection for rare events
  - Unbinned or event-level data sets to expose richer correlations
  - ‘Multi-modal’ data sets
    - Different modes of one data source (LLM)





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Observations/Conclusions

- AI/ML has demonstrated efficiencies in operations
  - To improve time to solution
  - To reduce human labor
  - To improve/facilitate analysis
- AI/ML is a priority for Nuclear Physics as an important tool for discovery science
- The concerns are the same across the scientific domains:
  - Affordability
  - Robustness, reliability, interpretability
  - Data Integrity
  - Workforce
  - Funding mechanisms
  - Interplay with Big Tech (including security concerns)

- Are there opportunities for collaboration? Yes!
  - The NP community is in an envisioning stage which is an ideal time to engage!

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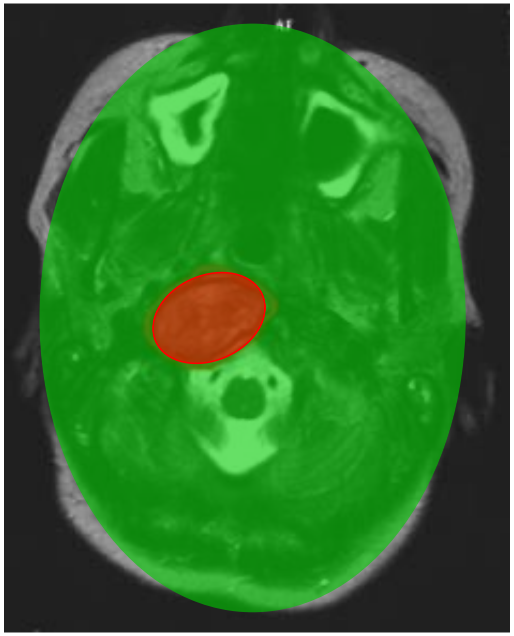
AI applications in radiotherapy

Ion beams

©University Hospital Heidelberg

- AI can predict anatomical deformations over the treatment course
- Enables treatment planning that is robust with respect to these changes
- More streamlined adaptation possible



Aim of the treatment:

Destroy cancer cells with radiation

but also

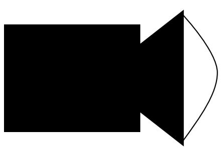
Maximize sparing of surrounding healthy tissue

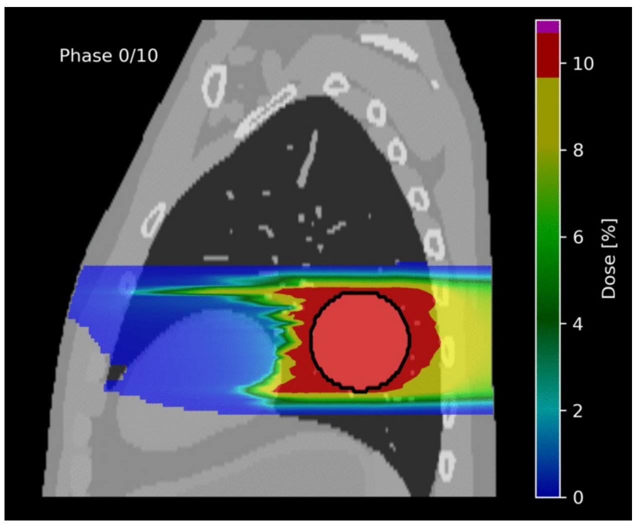
Lennart Volz
Biophysics, GSI

Adaptation: breathing motion and real-time adaptation

Motion Monitoring

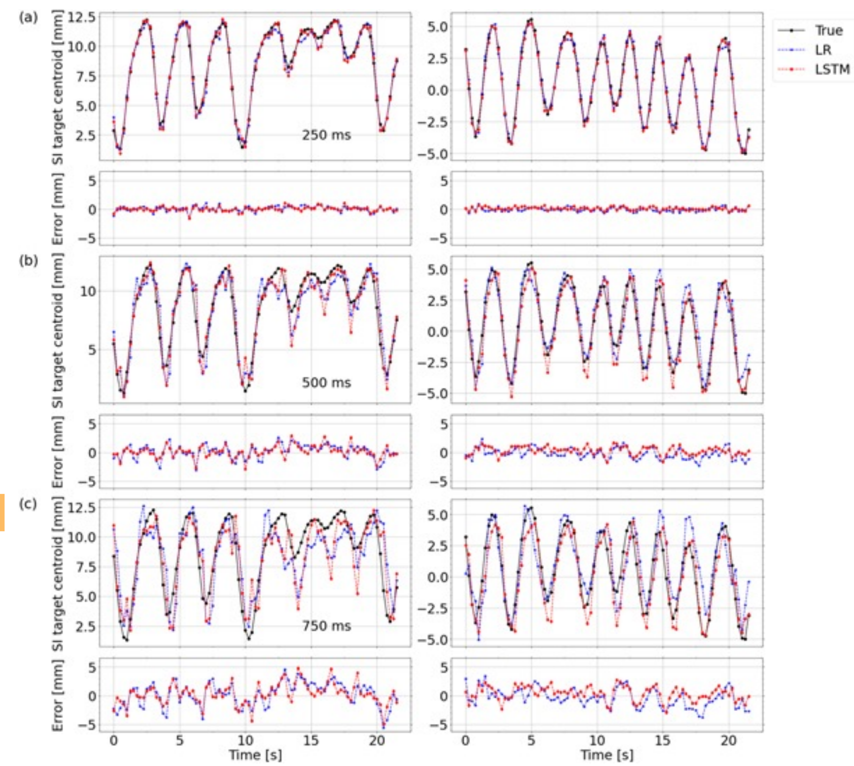
AI based motion prediction





Adapt

Graeff, Phys Med 2014; Lis, … Graeff, Front Oncol 2021; Steinsberger, … , Graeff, IJROBP 2022



Lombardo *et al* 2022 *Phys. Med. Biol.* **67** 095006