



Particle Accelerators at the Junction of Artificial Intelligence (AI), Optics, Superconducting Magnets (SCM), and Ultrafast Electron Diffraction (UED)

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Abstract

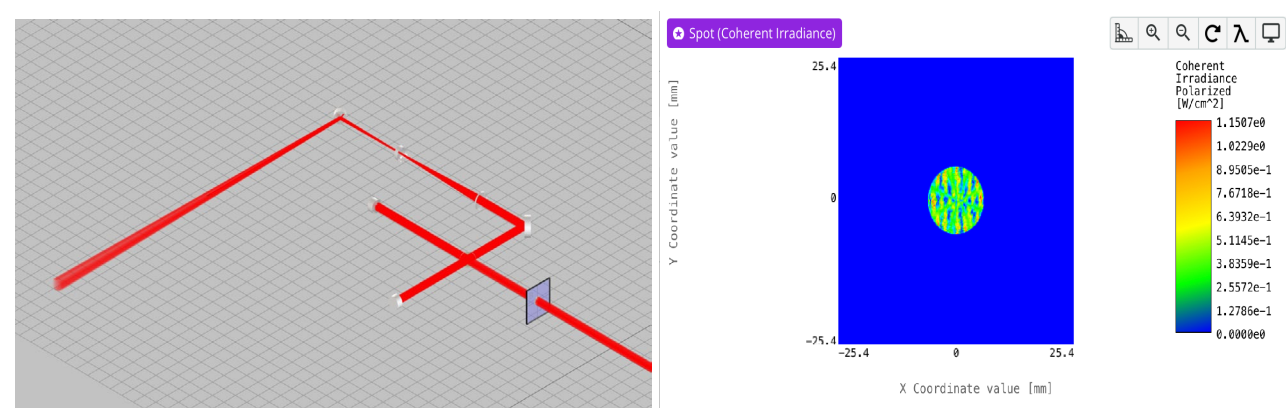
The study of advanced accelerators is essential to the growth of physics and drives technological innovation. This paper explores how automation and artificial intelligence (AI) can improve the performance of accelerator physics at Brookhaven National Laboratory's (BNL) Accelerator Test Facility (ATF). This was done through four modules: AI in materials discovery, optics, superconducting magnets (SCM), and ultrafast electron diffraction (UED). For optics, we examined fiber coupling, timing synchronization, and mirror alignments which the set ups were stimulated in 3D Optix. The SCM module focuses on designing quadrupole magnets in Opera3D and MATLAB to analyze current density scaling effects. UED utilized ImpactX for particle tracking and space-charge simulations to ensure beam integrity. Finally, we used AI in materials discovery by combining feature engineering and embeddings to predict an optical material's refractive index via an ensemble gradient boosting regressor.

Methodology

Optics and Lasers

3DOptix was used to recreate experimental setups and laser propagation through different optical materials and nonlinear crystals.

3DOptix: Michelson Interferometer



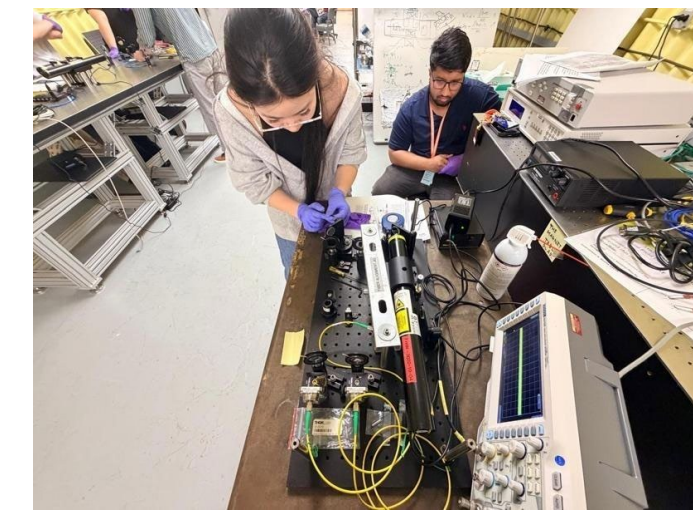
Off-Axis Parabolic Mirror Alignment



Signal Time Delay Measurements



Fiber Optics Alignment

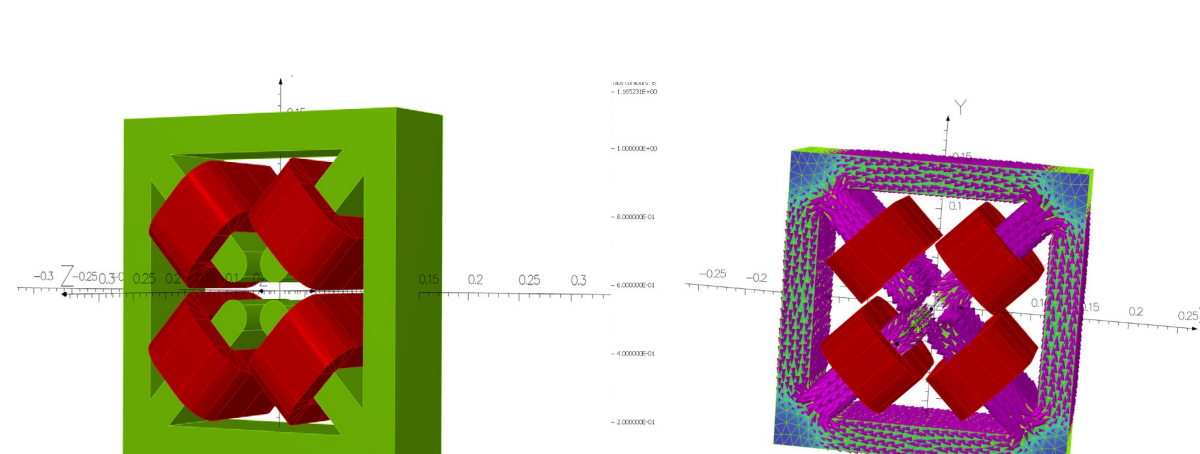


Synchronization of the beam required both precise fiber-optic alignment and accurate signal time delay measurements to ensure simultaneous arrival of the optical and RF signals.

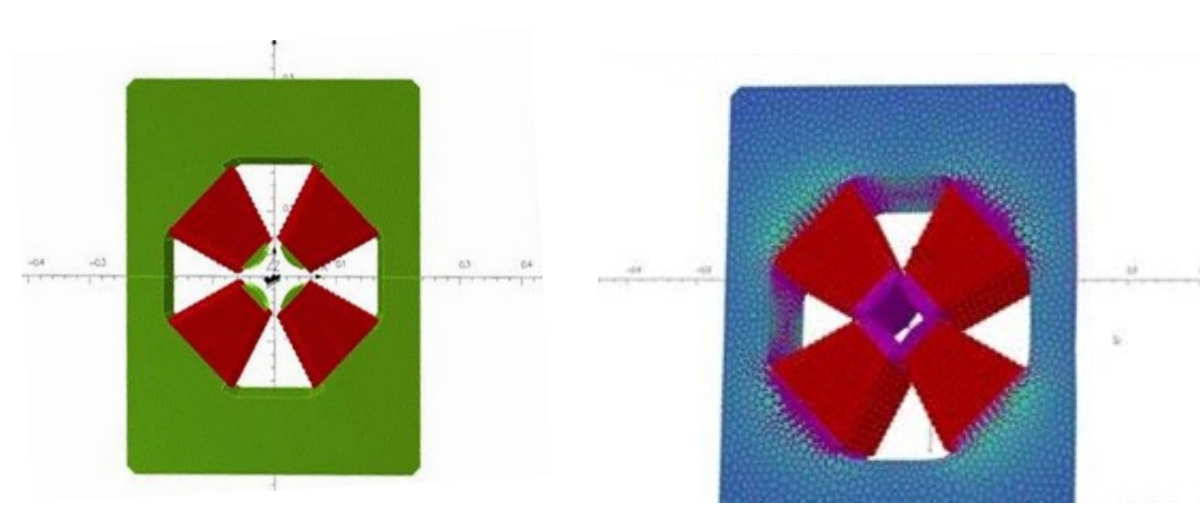
Superconducting Magnets (SCM)

The software Opera3D was used to model two quadrupole magnets for beam focusing. Through a variety of parametric studies by changing the current densities, we assessed the magnetic field strength which was calculated through MATLAB.

Quadrupole Magnet 1



Quadrupole Magnet 2

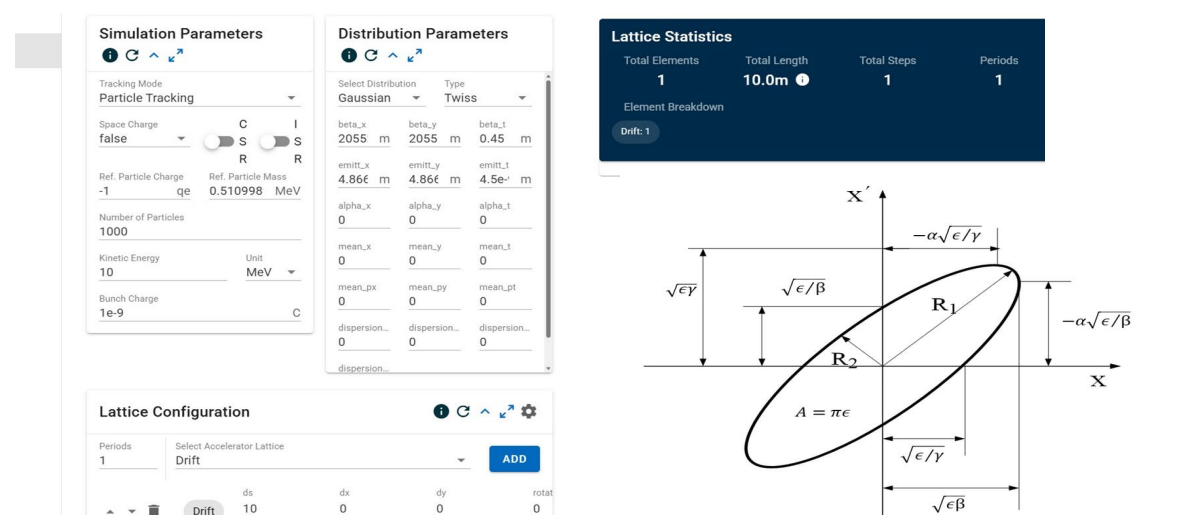


These two quadrupole magnets had electromagnetic modeling performed to evaluate the relationship between current density and magnetic field strength. This helps visualize the optimization of beam transport and focusing of quadrupoles.

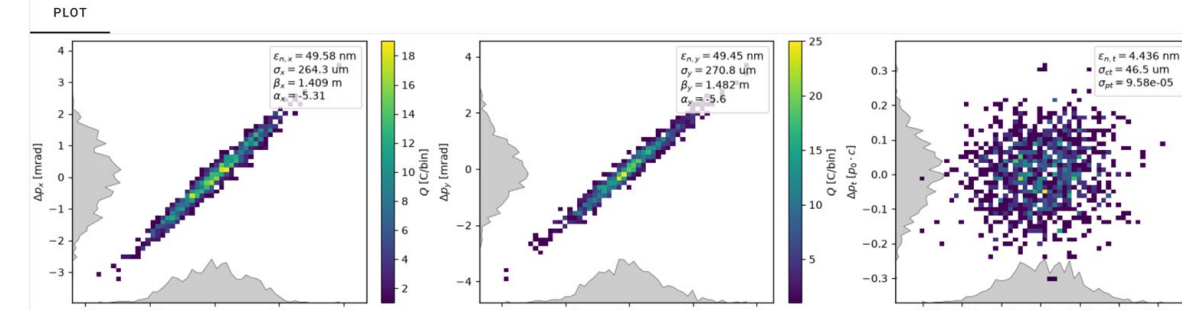
Electron Beam (UED)

The package ImpactX was utilized to simulate electron beam generation, focusing, and propagation.

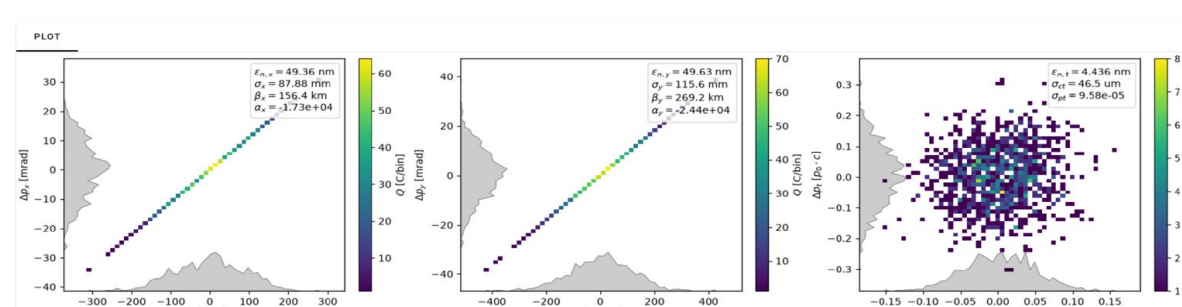
Initial Electron Beam (Normalized Emittance = 1 mm·mrad)



Solenoid Focusing, 10 MeV



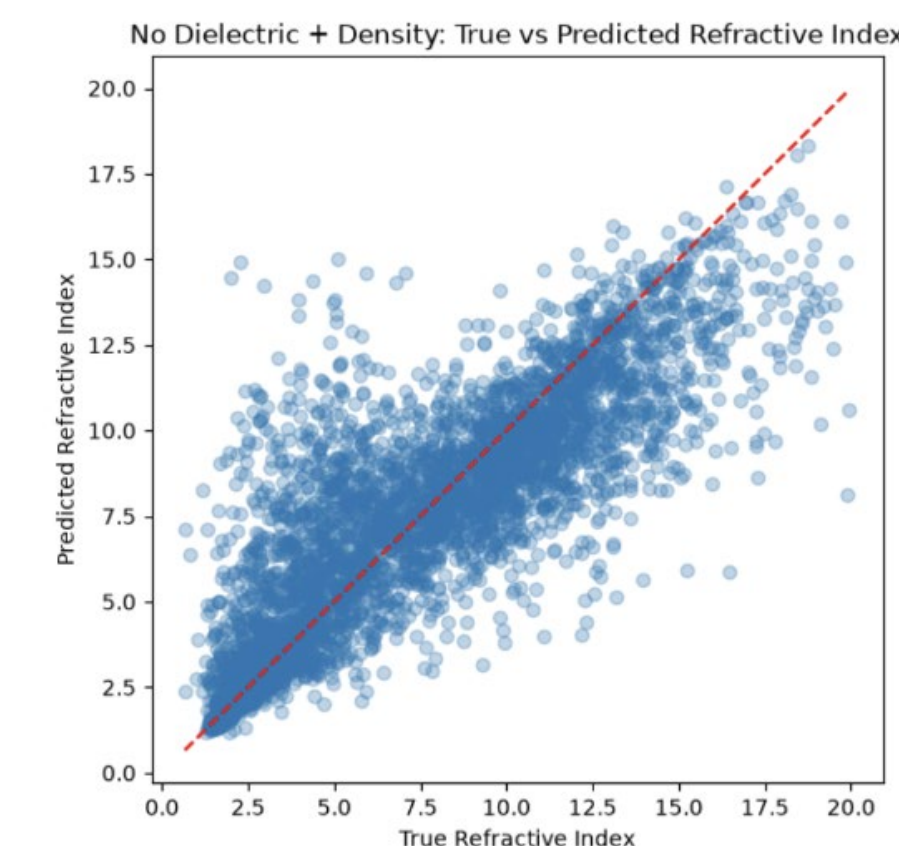
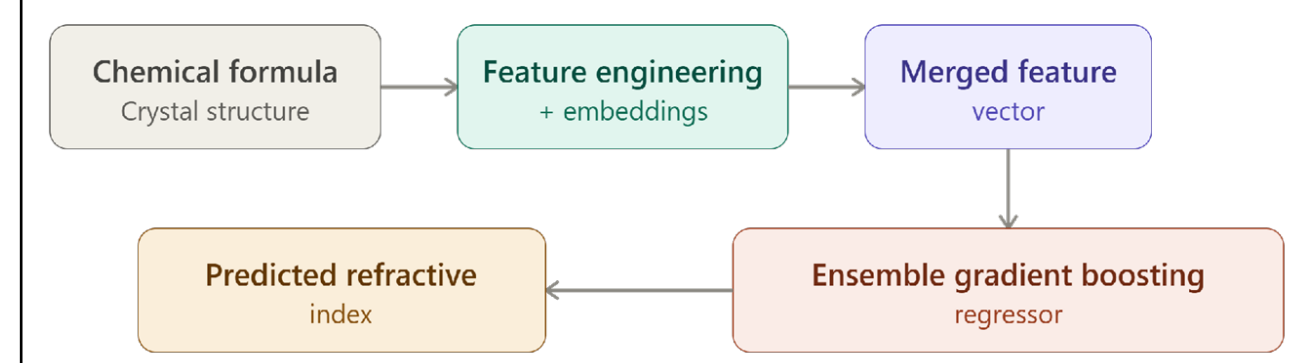
Quadrupole Focusing, 10 MeV



RF cavities were utilized to see energy gain and longitudinal bunching, while space charge simulations, were conducted to evaluate Coulomb repulsion effects on beam size and emittance growth across a range of beam energies (1 MeV–1 GeV).

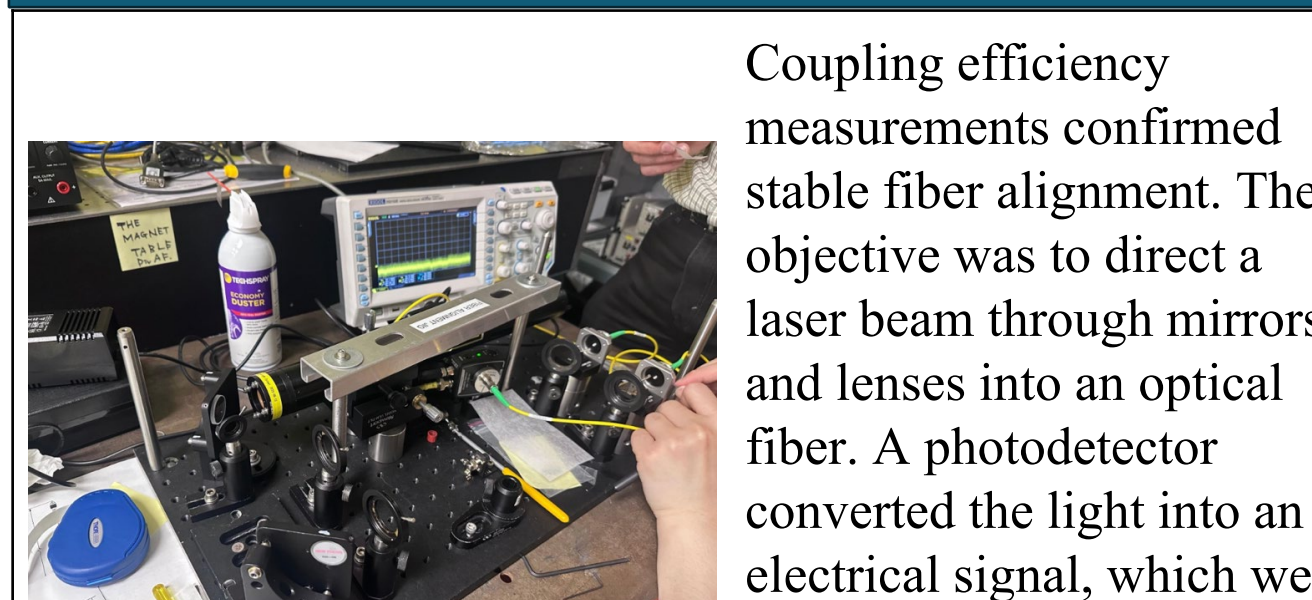
AI in Materials Discovery

ML was used to predict the refractive index of optical materials from their chemical formula and crystal structure. We merged engineered descriptors with embeddings into a unified set, which feeds into an ensemble gradient boosting regressor.



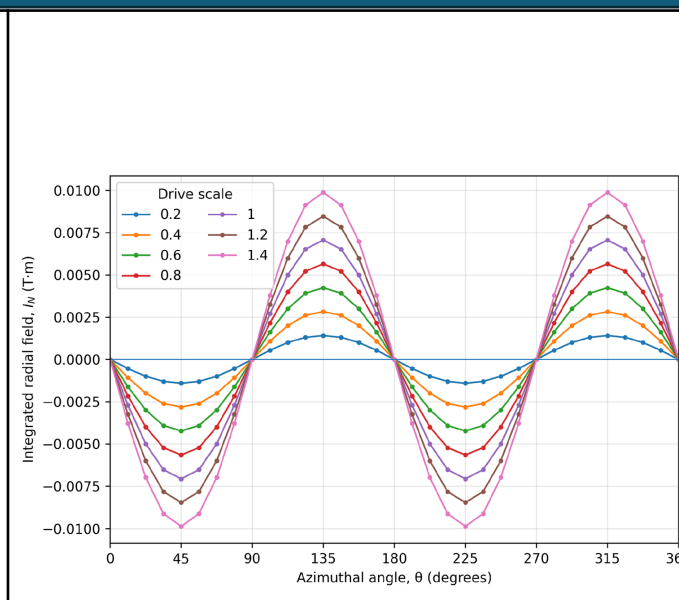
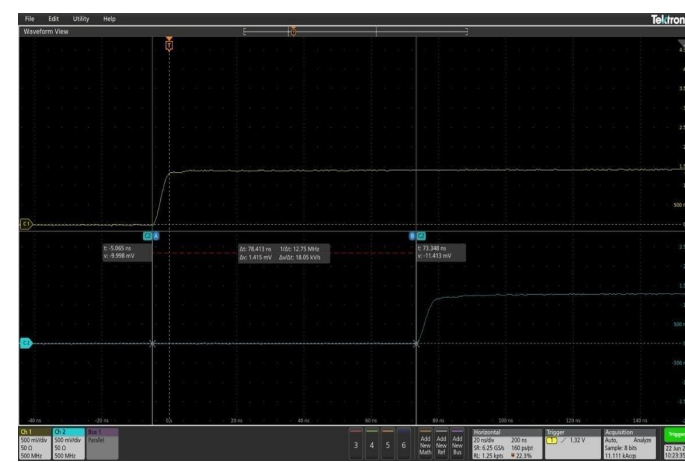
The XGBoost model was trained on engineered descriptors and hidden embeddings to predict refractive index from material composition and crystal structure. XGBoost builds an ensemble of decision trees sequentially, with each tree learning to reduce the remaining prediction error from the previous trees.

Results & Analysis



Coupling efficiency measurements confirmed stable fiber alignment. The objective was to direct a laser beam through mirrors and lenses into an optical fiber. A photodetector converted the light into an electrical signal, which we then saw on an oscilloscope.

Using an oscilloscope, we measured the propagation delay of a pulse through a 50-foot coaxial cable to be 77.874 ns, a signal velocity of 1.957×10^8 m/s and a velocity factor of 0.65. This is consistent with an RG-58 cable and confirms accurate signal timing measurement.



The integrated radial field shows a $\cos(2\theta)$ pattern, repeating every 180 degrees. Field amplitude scales proportionally with drive scale from 0.2 to 1.4, confirming a linear relationship between excitation current and field strength.

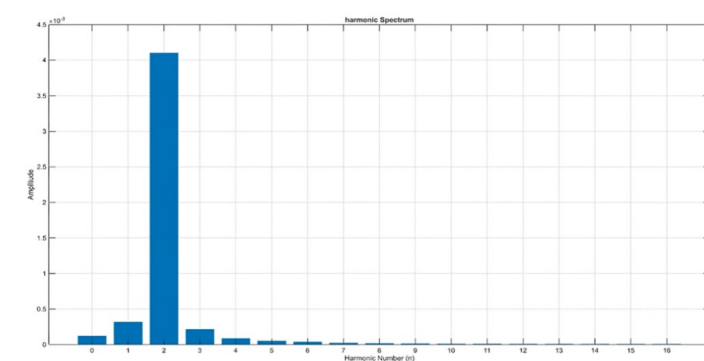
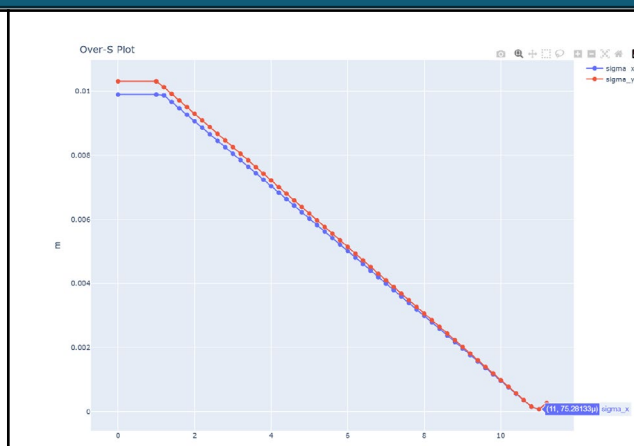


Fig. 1: 0.2 current density scale factor

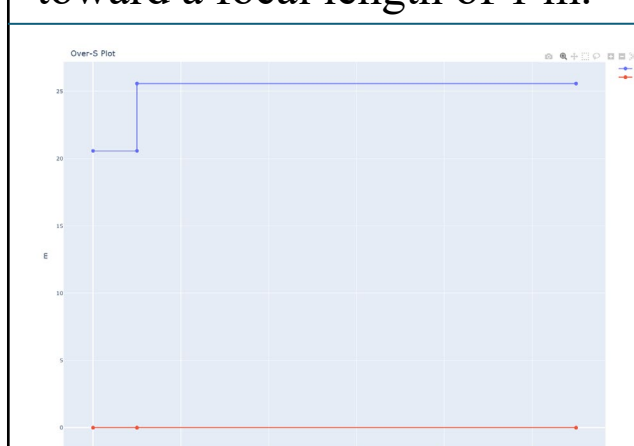
Harmonic decomposition at each drive scale shows a dominant quadrupole ($n = 2$) component, with higher-order harmonics contributing marginally. This distribution remains this way across all ten drive scales, indicating stable field purity throughout the operating range.



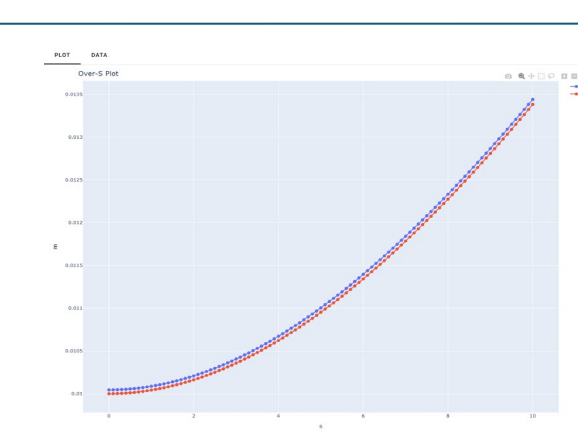
Beam size decreases sharply from an initial 1 cm as the solenoid focuses the beam toward a focal length of 1 m.



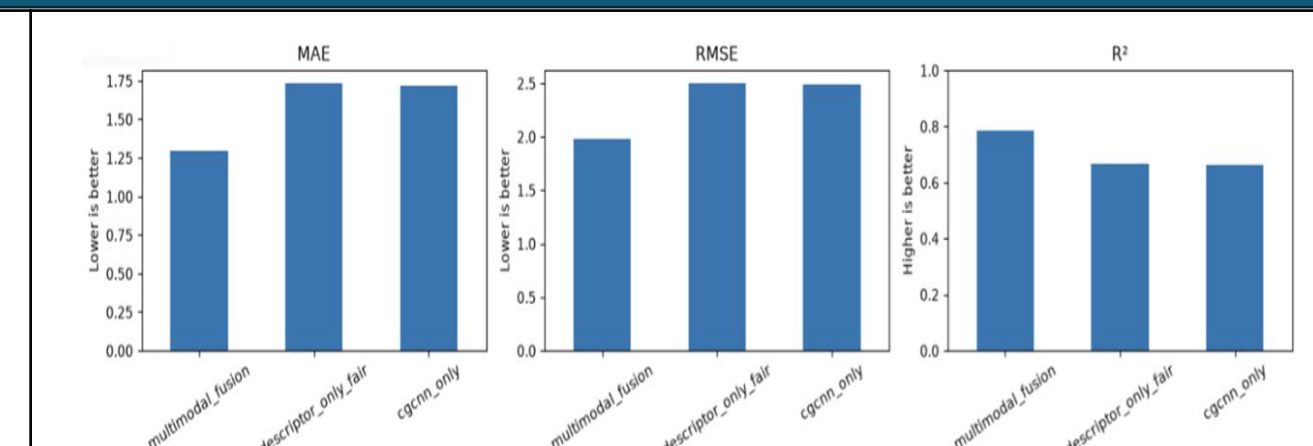
The quadrupole focuses the beam in one transverse plane while defocusing the other.



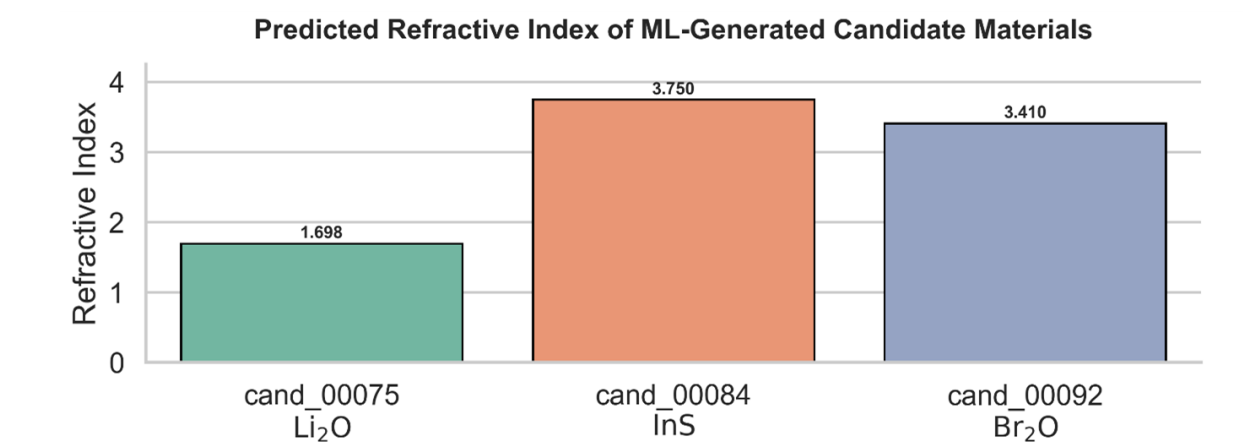
At a phase of 0° with $V = 5$, the ShortRF element produces maximum acceleration, reflected by the flat energy profile.



With space charge on, σ_x and σ_y grow from 1-1.34 cm over the 10 m drift due to electron repulsion-induced defocusing.



The multimodal fusion model achieves the lowest MAE and RMSE alongside the highest R^2 (≈ 0.76), outperforming the descriptor-only and CGCNN-only baselines across all three metrics.



Formula	Band Gap (eV)	Refractive Index	Material Family
Li ₂ O	5.924	1.688	Binary Oxide
InS	1.769	3.750	III-VI Chalcogenide
Br ₂ O	2.182	3.410	Halide Oxide

Conclusions & Future Work

Throughout the four modules, we explored key technologies used in particle accelerators. In the *Optics and Lasers* module, we designed laser setups using 3DOptix while developing hands-on experience with fiber optics, OAPs, and oscilloscopes. In the *SCM* module, we used harmonic analysis of magnetic field profiles to see if our quadrupole designs achieved strong field purity with minimal unwanted components. The *UED* module showed how beam dynamics are affected by parameters like emittance, charge, and energy, with simulations confirming the importance of space charge effects and magnetic focusing for maintaining beam quality. In *AI in Materials Discovery*, our model successfully predicted optical materials' refractive indices from chemical formula and structure. The combination of these experiences deepened our comprehension of how optics, magnets, beam physics, and AI collaborate in confluence to advance accelerator science and technologies. Future work will gear towards integrating these ideas further, such as applying AI-driven predictions to guide optical material selection for real-time beam diagnostics.

References

- [1] Chen, T., & Guestrin, C. (2016). XGBoost: A scalable tree boosting system. Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (pp. 785–794). <https://doi.org/10.1145/2939672.2939785>
- [2] Perry, M. D., & Mourou, G. (1994). Terawatt to petawatt subpicosecond lasers. *Science*, 264(5161), 917–924. <https://doi.org/10.1126/science.264.5161.917>
- [3] Rossi, L. (2023). Particle Accelerators and Cuprate Superconductors. *Physica C: Superconductivity and Its Applications*, 614, 1354360. <https://doi.org/10.1016/j.physc.2023.1354360>
- [4] Shaaban, M., El-Borgi, S., & Krishnamoorthy, A. (2025). Machine learning for experimental design of ultrafast electron diffraction. *Scientific Reports*, 15(1). <https://doi.org/10.1038/s41598-025-06779-z>
- [5] Ward, L., Agrawal, A., Choudhary, A., & Wolverton, C. (2016). A general-purpose machine learning framework for predicting properties of inorganic materials. *npj Computational Materials*, 2, 16028. <https://www.nature.com/articles/npjcompumats201628>

Acknowledgements

Funding for this research is provided by the U.S. Department of Energy under the Reaching a New Energy Sciences Workforce (RENEW) Grant "Science and Engineering Apprenticeship Program in Accelerator Science and Technology", Grant # DE-SC0025742 and the Brookhaven National Laboratory. We sincerely appreciate and thank the help of Jason Becker, Christopher Tamargo, from the SCM Division, Jhair Alzamora, Paul Jacob, Karl Kusche, Spencer Diamond and Miguel Long from the Accelerator Test Facilities (ATF) Division at BNL, as well as the rest of the scientists, engineers, and technicians at the ATF and SCM divisions for the continued support in this work. We would like to express our appreciation to the mentors, researchers and administrators of the SESAPARD/RENEW program for their dedication and guidance during this research project. No export control work done.

