Faster, More Accurate Particle Accelerator Models using Machine Learning

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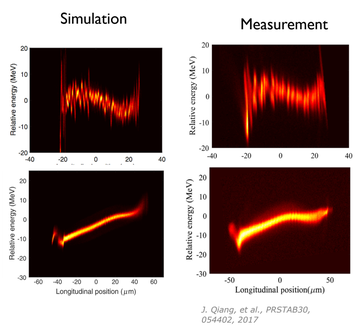
Accelerator simulations can be very computationally intensive and don't always match the machine well

Impedes use in offline start-to-end optimization and control development

Prohibits use as an online model (e.g. diagnostic + control applications)

Often takes much effort to replicate real machine behavior

Start-to-end LCLS simulation
10 hours on thousands of cores at the NERSC

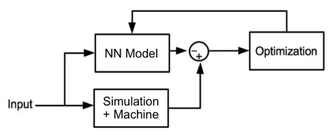


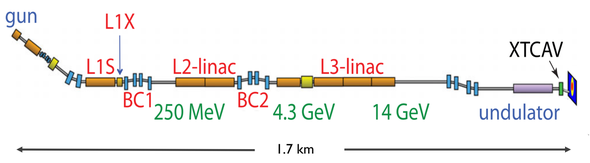
J. Qiang, et al., PRSTAB30, 054402, 2017

Complementary approach: ML model

Once trained, neural networks can execute quickly

Train on sparse sample from high-fidelity simulations
+
Train on measured data





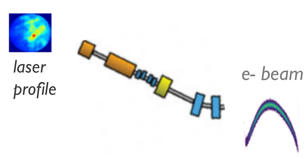
Nonlinear systems with large parameter spaces
Variety of diagnostics, *but limited in number and some not always available*
Time-varying/ non-stationary behavior
On-demand changes in operational state

Dedicated effort in AD to create fast-executing, accurate accelerator models, and use these in control + optimization

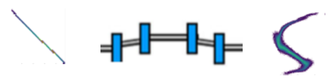
Three Main Approaches for ML Modeling Effort

Modules for slowest simulations

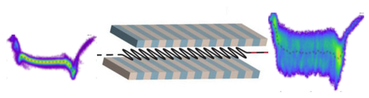
Injector



Bunch Compressors



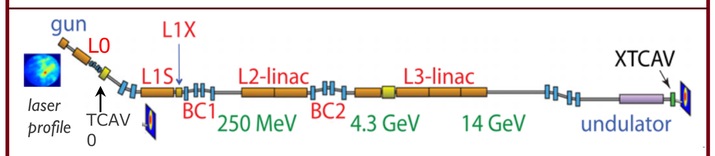
FEL Undulator



Controllable settings
Incoming beam distribution
→ ML Model → Outgoing beam distribution

Beam description:
- *images (beam projections/slices)*
- *6D point clouds (3 spatial, 3 features)*

Start-to-end accelerator models



Controllable settings
Input diagnostics
→ ML Model → Output diagnostics

e.g. beam images
x-ray spectra

e.g. laser spot image

Back-tracking and model inversion

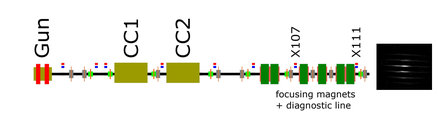
Desired beam output → ML Model → Incoming beam distribution **or** Suggested settings

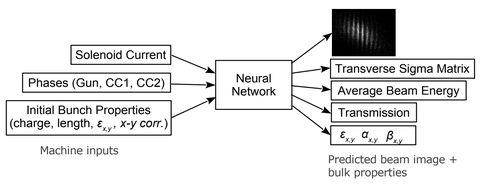
Can we bridge the gap between our simulations and empirical machine behavior?

Poor agreement between physics simulation and measured data
Can't do a full parameter scan on machine (cost / time)

Simulation Data (wide scan) → ML Model ← Measured Data (smaller scan + passive data)

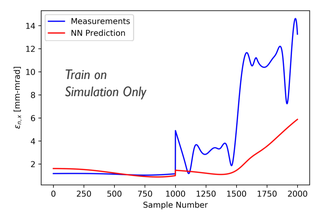
Can we pre-train in simulation and update with measured data?

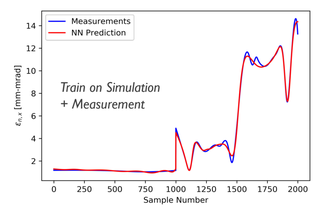




Initial results from study of injector systems look promising

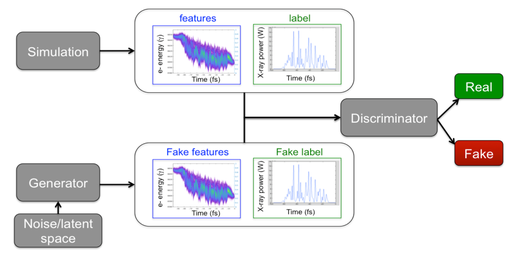
→ need to investigate strategies for doing this routinely and at larger scale

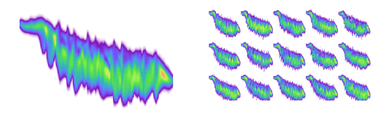




Can we handle statistical fluctuations realistically?

- FEL process has some inherent random behavior
- Want to generate many examples of FEL output with realistic statistical behavior quickly → *e.g. provide data sets for experiment planning*
- Train generative adversarial network (GAN) on simulation data





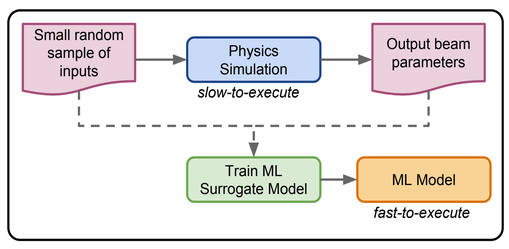
Genesis: ~1000 cpu-sec

GAN (neural net): ~0.001 gpu-sec

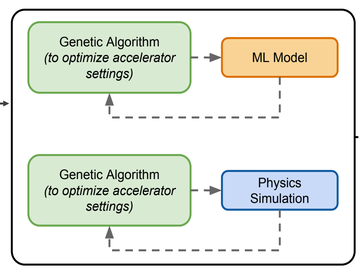
X. Ren

Can We Speed Up Multi-Objective Optimization?

Generate ML Model using Sparse Random Sample



Run Optimizer on ML Model and Physics Simulation

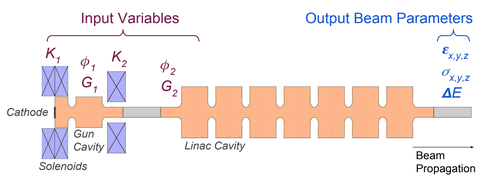


Test Case: Argonne Wakefield Accelerator Injector

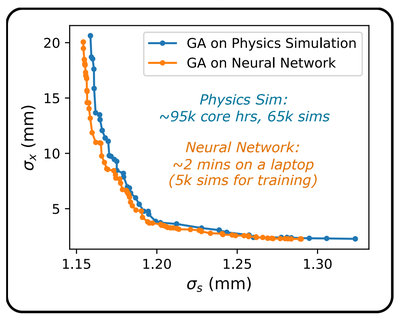
OPAL simulation (PIC) : 3D space charge 3D field maps 10k particles

NSGA-II for optimization: 200 generations ~350 individuals

5K random points for training



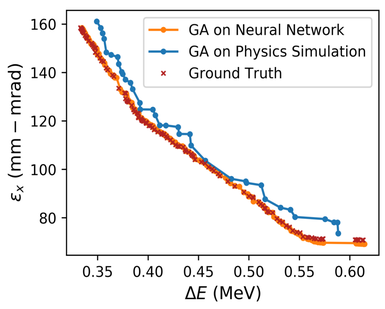
Compare Resulting Pareto Fronts

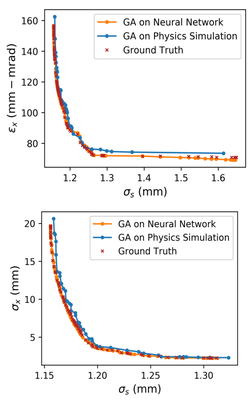


In some cases, optimization over simulation takes too long to converge

→ validate Pareto front from neural network more directly

Get Pareto points from Neural Net → Verify points through Simulation





Neural network gave a ***better* approximation of the true Pareto front** than the naïve GA on the simulation

Required **13x fewer simulations** and had **10^6 faster execution** in the optimization

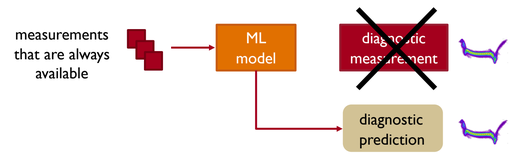
- Promising results on a common problem
- But, small parameter space (6 inputs, 7 outputs)
- Only deterministic processes (e.g. unlike FEL)

→ How will this scale to larger + more complex sections?

Can we use ML-based virtual diagnostics?

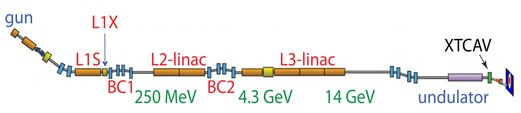
Real diagnostic not always available:
- *destructive, cannot use during user operations*
- *not sensitive in entire operating range*
- *slower update rate than desired*
- *moved to another location (e.g. cost constraints)*

→ *FACET-II XTCAV*
→ *LCLS-II XTCAV*



Still can have diagnostic prediction for user analysis and system control!

FACET-II / LCLS study

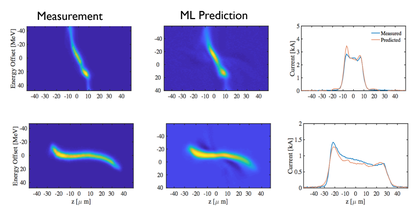


Two machine parameters scanned:

L1s phase: -21 to -27.8 deg

BC2 peak current: 1-7 kA

- 5 inputs to neural network
  - *L1S and L1X amplitude, L1S phase*
  - *BC1&2 peak current*
- Reasonable performance predicting profiles and XTCAV images
- Key is varied data set from scan, and data preparation (e.g. ROI selection)



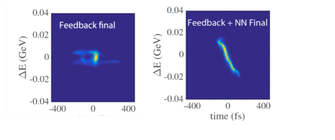
→ Long-term prediction accuracy? (e.g. drift) *→ How best to flag bad shots? (e.g. bad BC2 input)*

→ How best to handle region where detector not sensitive for FACET-II (fill in with simulation)?

Example inverse model: warm start for local optimizer

"ES" optimization algorithm can tune many parameters efficiently
- But can get stuck in local minima + can take awhile to converge *(e.g. hundreds of iterations)*
- *Given target beam parameters, a neural network can provide suggested initial settings*

Preliminary study at LCLS:
- Scanned L1S phase and BC2 peak current
- Trained network to map phase space to settings
- Compared ES with/without warm start for extreme change in phase space



→ ES alone unable to converge, but able to converge from settings suggested by NN

→ Need to extend to wider range of parameters, look at performance over time

Wish List and Challenges

Wish list
- Train on simulation → *orders of magnitude speedup + enable use as online model*
- Train on measurements → *more closely match to real accelerator behavior*
- Use as a virtual diagnostic → *predict what an unavailable diagnostic would show*
- Use for offline for experiment planning, design studies, and prototyping control algorithms
- Use online as an operational aid and in model-based control schemes

Challenges
- Flagging when to trust the model (e.g. bad shots)
- How best to retrain + strategies for deciding when to retrain
- How best to combine simulation and measured data
- Scaling to higher dimension + problem complexity
- Efficiently handling different data types: 6D point clouds, images, scalars