#### Potential ML/AI Applications for Accelerator Design & Simulation

#### B. Mustapha Physics Division, ANL NP Roundtable on ML/AI for Accelerator Facilities January 30<sup>th</sup>, 2020





# CONTENT

- A Philosophical View of ML / AI in Science / Physics
- Potential Applications to Design Optimization of Accelerator Components
- Potential Applications to Accelerator Design and Simulation
- Potential Applications to Simulate failure scenarios and recovery for existing facilities → Identify critical cases and data requirements for prediction and prevention
- Summary Final Comments





### PHILOSOPHICAL VIEW OF ML/AI IN SCIENCE

- Application of ML / AI in Science is to accelerate discovery Not to replace scientific models
- It can accelerate the path to a solution of a problem within the defined boundary
- Or it can find a new solution in an unexplored space, eventually leading to new discovery
- You will always need verification and validation of the solution using a scientific model or experimental measurements





#### POTENTIAL APPLICATIONS TO DESIGN OPTIMIZATION OF ACCELERATOR COMPONENTS

- Electromagnetic design optimization of accelerator components with complicated geometries. Examples: RFQs, Multi-cell high-gradient structures, Complex magnet designs ...
- These are multi-parameter (geometry details) multi-objective optimization (rf & field parameters: frequency, R/Q, field flatness/uniformity, field harmonics ...)
- Simulations with CST/HFSS/Opera are time consuming, only a coarse parameter grid can be simulated in reasonable time!
- A faster ML model can be trained on the coarse grid results, then be used to "simulate" points on a finer grid, leading a better/absolute optimum that can be later verified with full simulations …



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#### EXAMPLE: MULTI-CELL HIGH-GRADIENT ACCELERATING STRUCTURE - FOR 50 MV/M



- Close to 100 geometric parameters, including rounding of the edges …
- Need to optimize: Frequency, cell coupling, tuning, input coupling, field flatness, ...
- Only a few parameter combinations can be simulated in reasonable time, requiring large memory for sufficient meshing and long computing time!
- A trained ML model can significantly speed-up the path to optimum solution ...

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#### POTENTIAL APPLICATIONS TO ACCELERATOR DESIGN AND SIMULATION

- Large scale simulations of an accelerator design (linac or ring) to check design robustness. Examples: Error and beam loss analysis for a linac, dynamic aperture optimization for a storage ring
- These error simulations of full accelerator systems are usually done by particle tracking to estimate and locate eventual beam losses
- They are time consuming and often limited by either the number of simulated particles or the number of randomly generated lattice error configurations that can be simulated in reasonable time!

 A fast Surrogate ML model can be trained to reproduce the physical model, then be used to "simulate" many more particles and or lattice error configurations → Faster design iteration



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#### EXAMPLE: ERROR SIMULATION & SENSITIVITY ANALYSIS FOR A LINAC DESIGN – RISP LINAC

Start-to-end beam simulations, error sensitivity and beam loss analysis

LEBT RFQ MEBT QWR-I-1 QWR-I-2 QWR-II-1 QWR-II-2 QWR-II-3 QWR-II-4 QWR-II-5 QWR-II-6 QWR-II-7



- Large scale computing required for these simulations, which are time consuming and usually limited in both the number of particles and lattice configurations
- A Surrogate ML model trained using the physics model of the linac can allow the simulation of more beam particles and lattice error configurations ...

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#### POTENTIAL APPLICATIONS TO SIMULATE FAILURE & RECOVERY OF ACCELERATORS

- An accelerator can fail in many different ways, but we can rarely predict when and how it'll fail. Furthermore, we don't have enough data to understand and predict the different failure scenarios!
- Simulations can be used to fill this data gap and help identify the data needed to be able to predict these failures and how to quickly recover from them → Optimization of diagnostics and data requirements!
- Based on this, an optimum set of diagnostics (beam or else) can be added to an existing machine to collect the required data to be used for better prediction of failure modes and help fast recovery.
- A fast ML model, trained on a combination of existing data and simulations, can be used to study different failure modes and identify the required but missing information → Faster machine recovery

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## **SUMMARY – FINAL COMMENTS**

- ML/AI has the potential of accelerating discovery in Science with many possible applications in Accelerator Physics
- Potential Applications in Accelerator Design & Simulation:
  - Design optimization of complex accelerator components
  - Large scale simulation of accelerator lattice for faster design iteration
  - Fill-in the operational data gap with simulations and identify data requirement for future applications. Ex.- Study failure modes & recovery in an existing facility & identify additional diagnostics requirements to acquire the missing data
- An important parameter to consider: Gain vs. cost in time & effort needs to be evaluated!





# THANKS



