Applications of Neural Networks to Modeling and Control of Particle Accelerators

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Fermilab Accelerator Physics and Technology Seminar

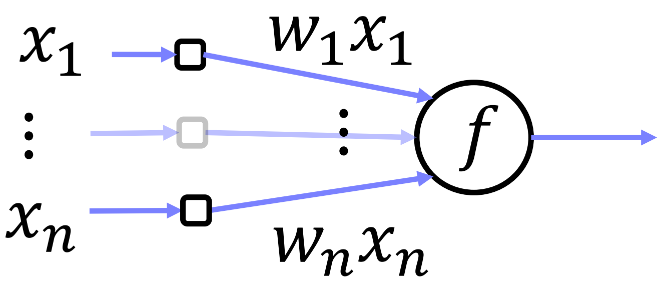
8 June 2017

Overview

- Background on Neural Networks
- Control Challenges in Particle Accelerators
- Overview of Applications *(with some examples)*
  - Online Modeling
  - Model Predictive Control
  - Virtual Diagnostics
  - Failure Prediction, Anomaly Detection, and Machine Protection
  - Reinforcement Learning / Neural Network Control Policies
  - Incorporating Image-based Diagnostics into Control Policies
- Final Notes
  - Practical Challenges
  - Funding Climate
  - Conclusions

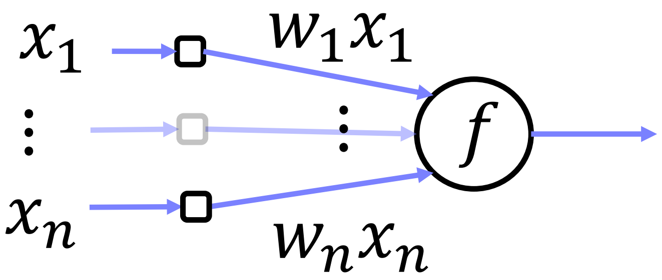
What are neural networks?

Artificial Neural Networks



a neuron or node

Artificial Neural Networks



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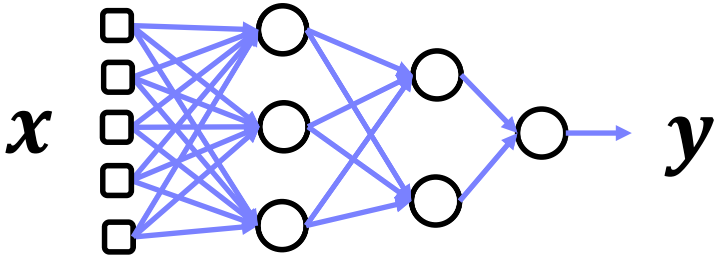
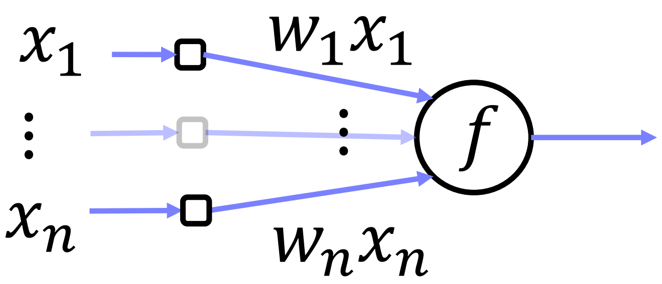


a feed-forward network

Artificial Neural Networks



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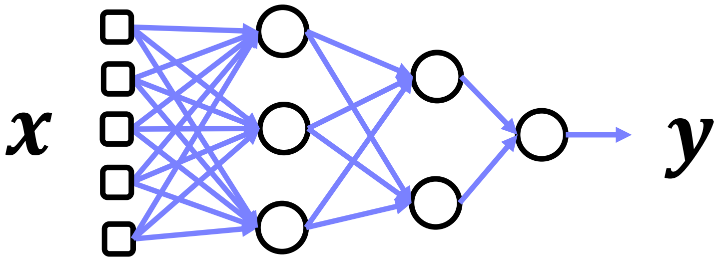

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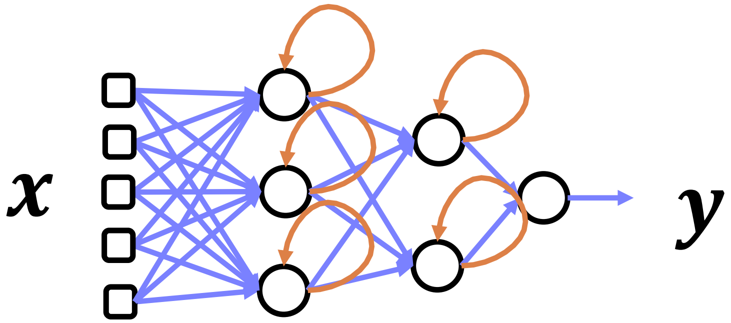
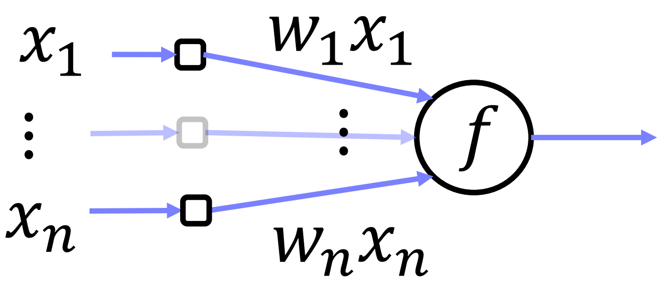


a recurrent network

Artificial Neural Networks



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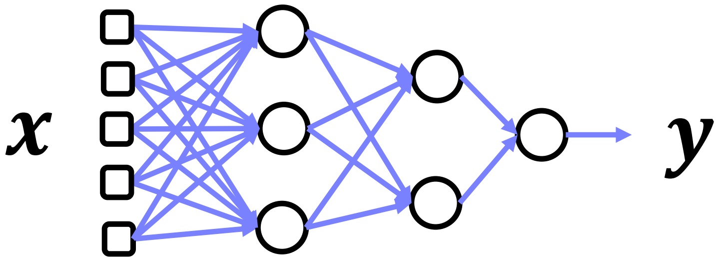

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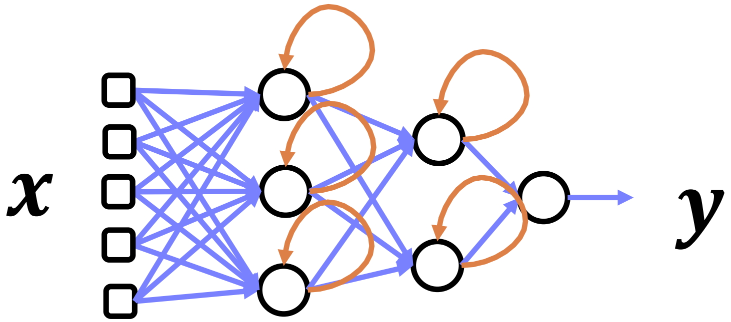
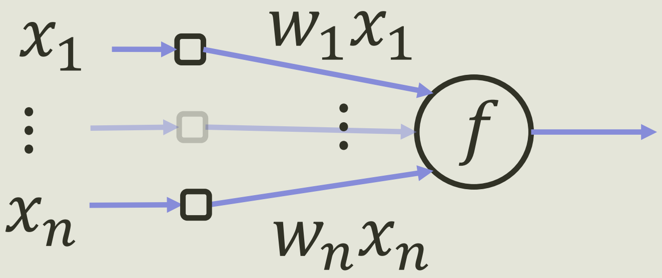


a recurrent network

… many more architectures!

Artificial Neural Networks



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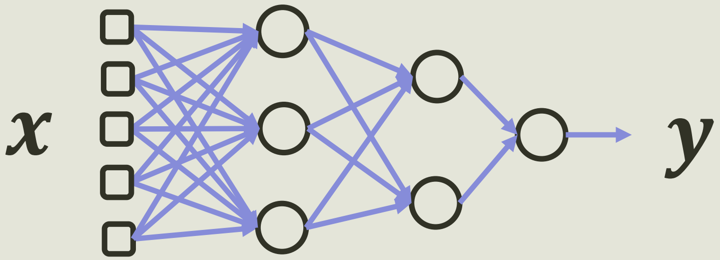

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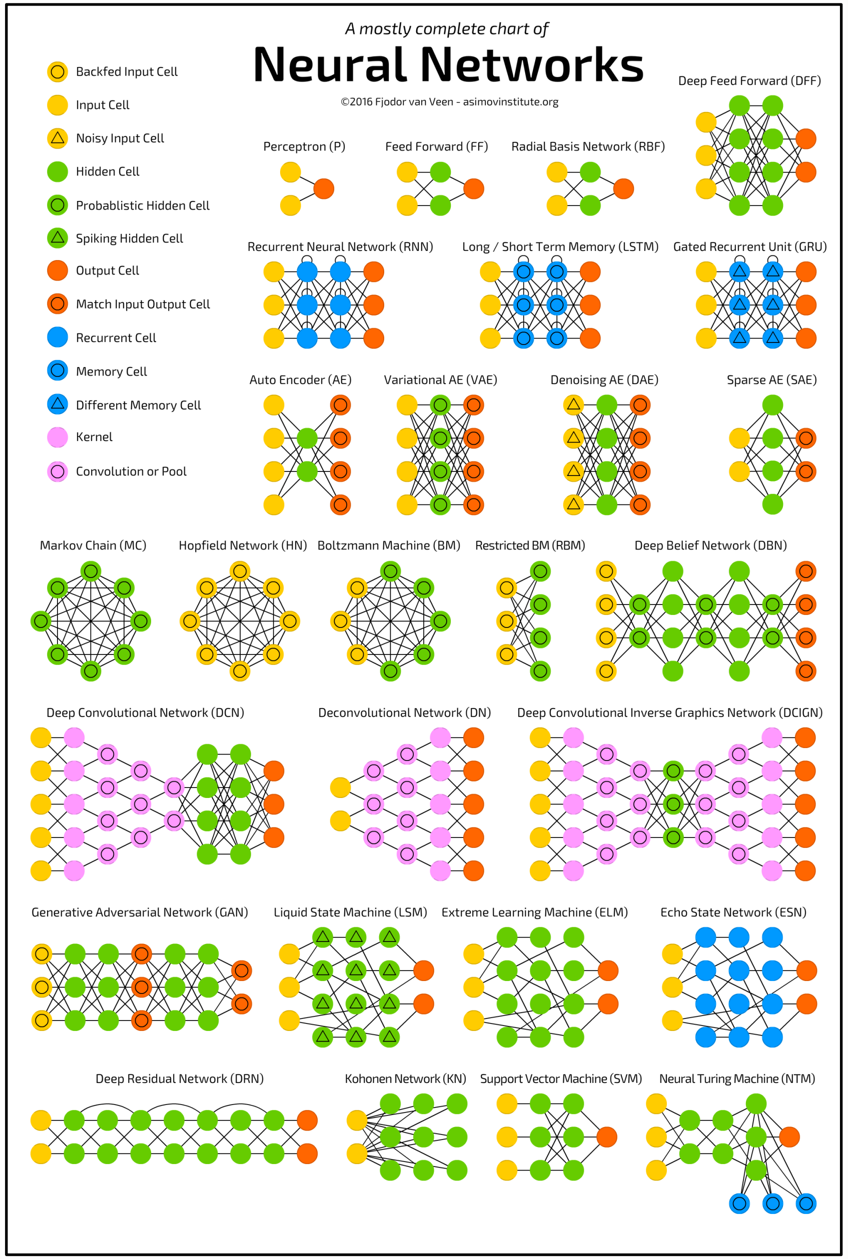


See, for example, the Neural Network Zoo website.

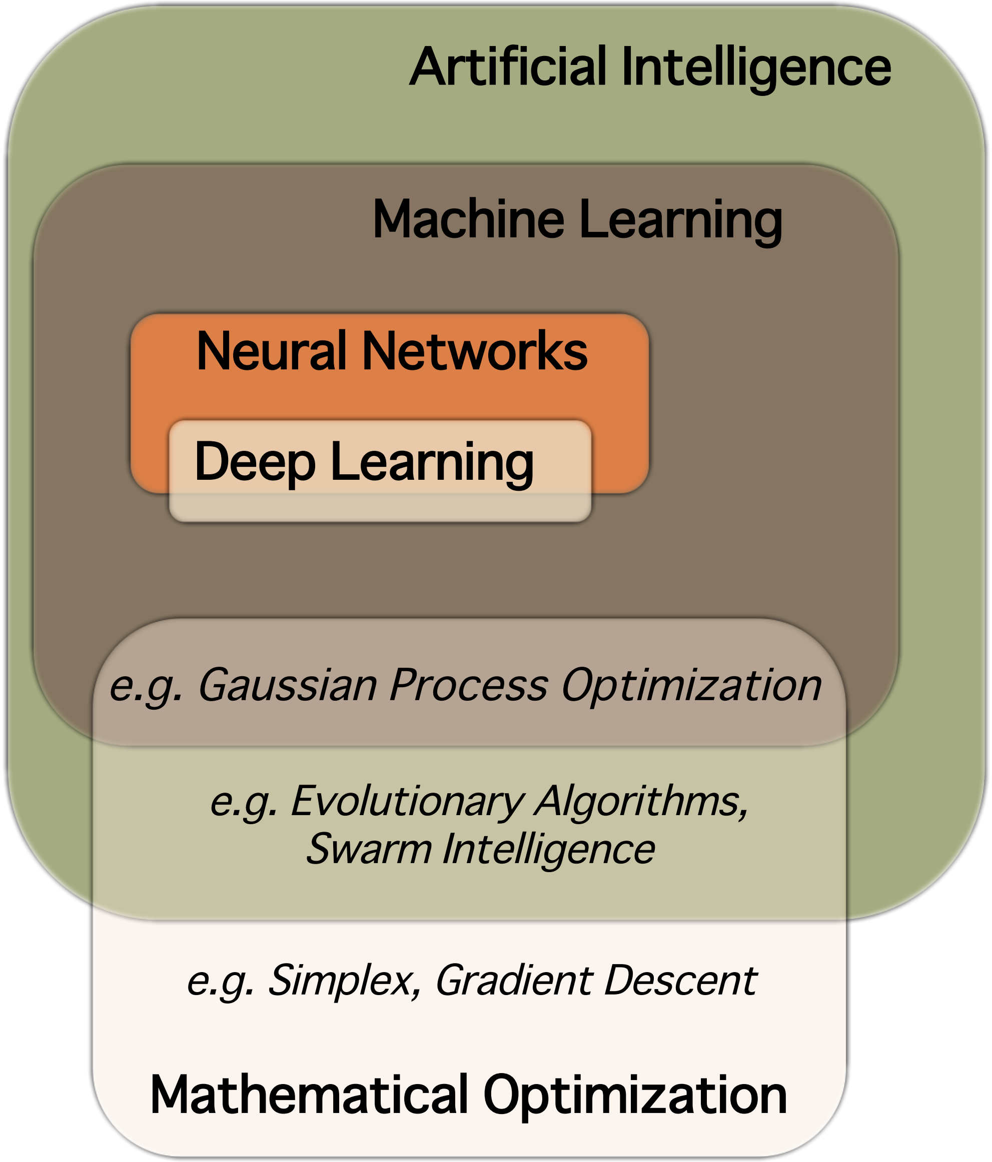
How does this relate to "machine learning," "artificial intelligence," and "deep learning"?

…what do these terms mean anyway?

Field Taxonomy (as of now...)

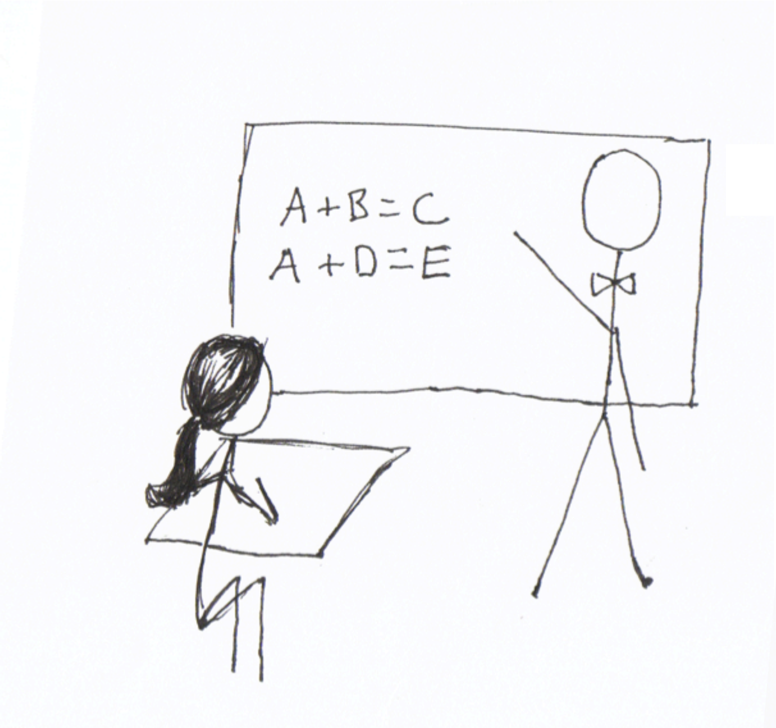
- Artificial Intelligence (AI)
  - *Concerned with enabling machines to exhibit aspects of human intelligence: knowledge, learning, planning, reasoning, perception*
  - Narrow AI: focused on a task or similar set of tasks
  - General AI: human-equivalent or greater performance on any task
- Machine Learning (ML)
  - *Enabling machines to complete tasks without being explicitly programmed*
  - Common tasks: Regression, Classification, Clustering, Dimensionality Reduction
- Neural Networks (NNs)
  - *An approach within ML that uses many connected processing units*
  - Many different architectures and training techniques
- Deep Learning (DL)
  - *Learning hierarchical representations*
  - Right now, largely synonymous with deep (many-layered) NN approaches

Note that these definitions are not rigid: there is a lot of fluidity in the field



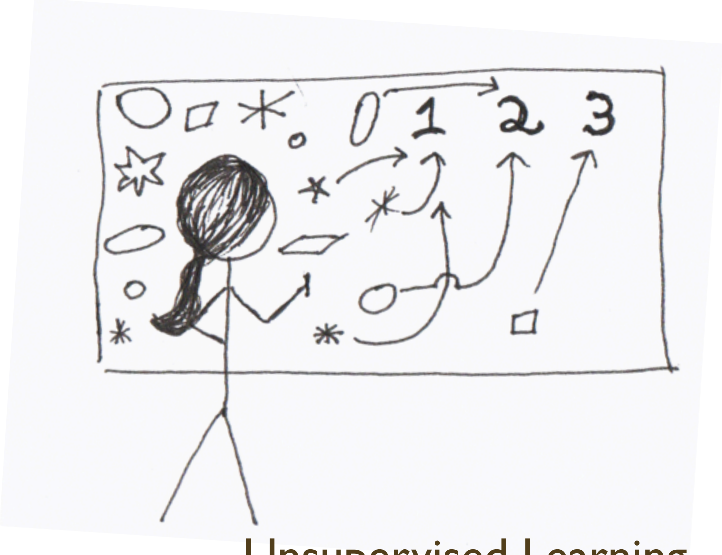
How do neural networks "learn"?

Basic Learning Paradigms



Supervised Learning

learn known input/output pairs



Unsupervised Learning

no labeled data → infer structure

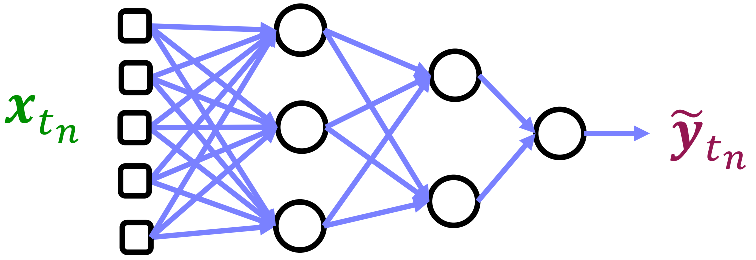
Reinforcement Learning

interact with the environment → adjust behavior based on reaction

Example: multiple-input, single-output process model

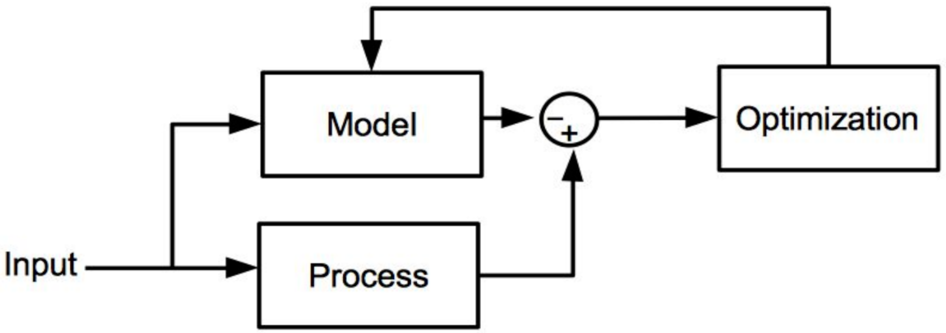
Data set of **input** and **output** pairings:

$$\left.\begin{matrix} x_1 \\ \vdots \\ x_n \end{matrix}\right\} \quad \begin{matrix} \boldsymbol{x}_{t_1} \\ \vdots \\ \boldsymbol{x}_{t_n} \end{matrix} \qquad \begin{matrix} \boldsymbol{y}_{t_1} \\ \vdots \\ \boldsymbol{y}_{t_n} \end{matrix}$$



Want to find approximate map: $\boldsymbol{g}(\boldsymbol{x}) = \boldsymbol{y}$

Model Learning



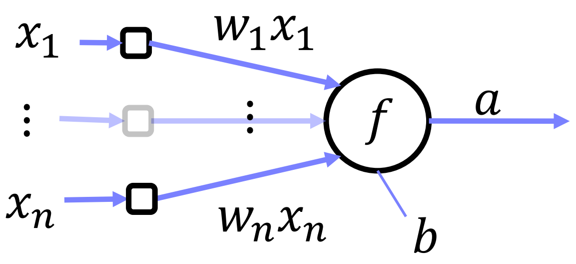
Basic Update Example

$$C(w,b) = \frac{1}{2t_n}\left[\sum_{t_n}(y_{t_n} - \tilde{y}_{t_n})^2\right]$$

$$w_k \longrightarrow w'_k = w_k - \alpha \frac{\partial C}{\partial w_k}$$

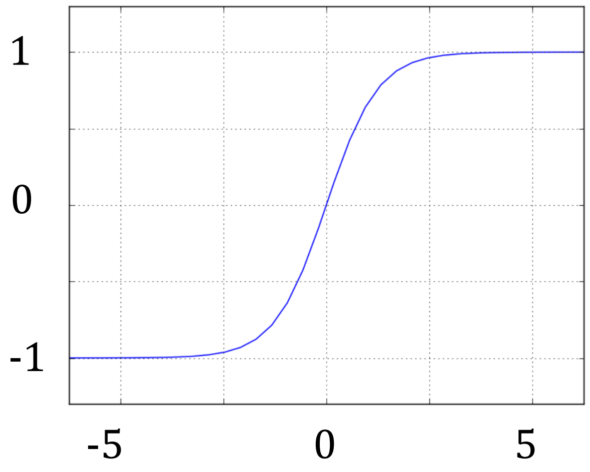
$$b_k \longrightarrow b'_k = b_k - \alpha \frac{\partial C}{\partial b_k}$$

Basic Structures

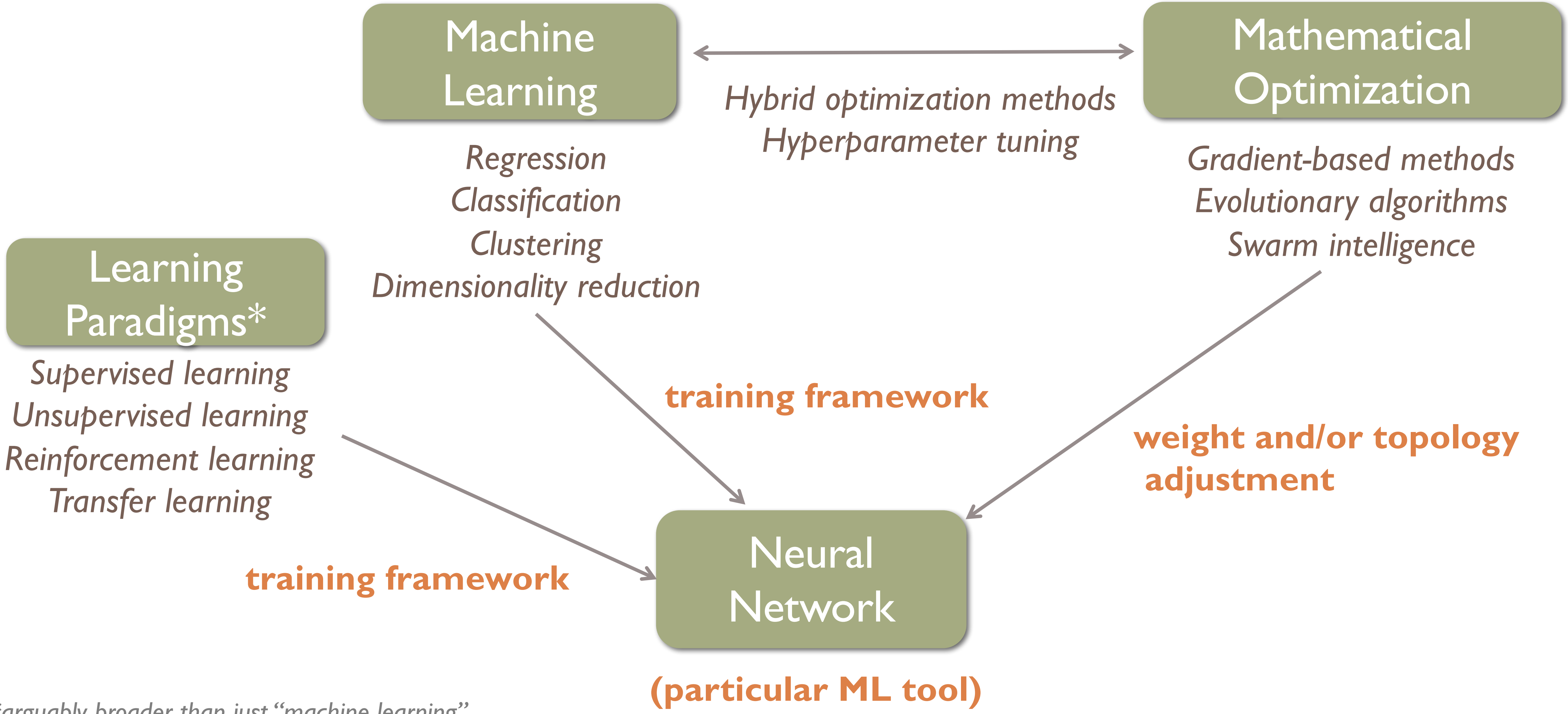


$$f\left(\sum_n w_n x_n + b\right) = a$$

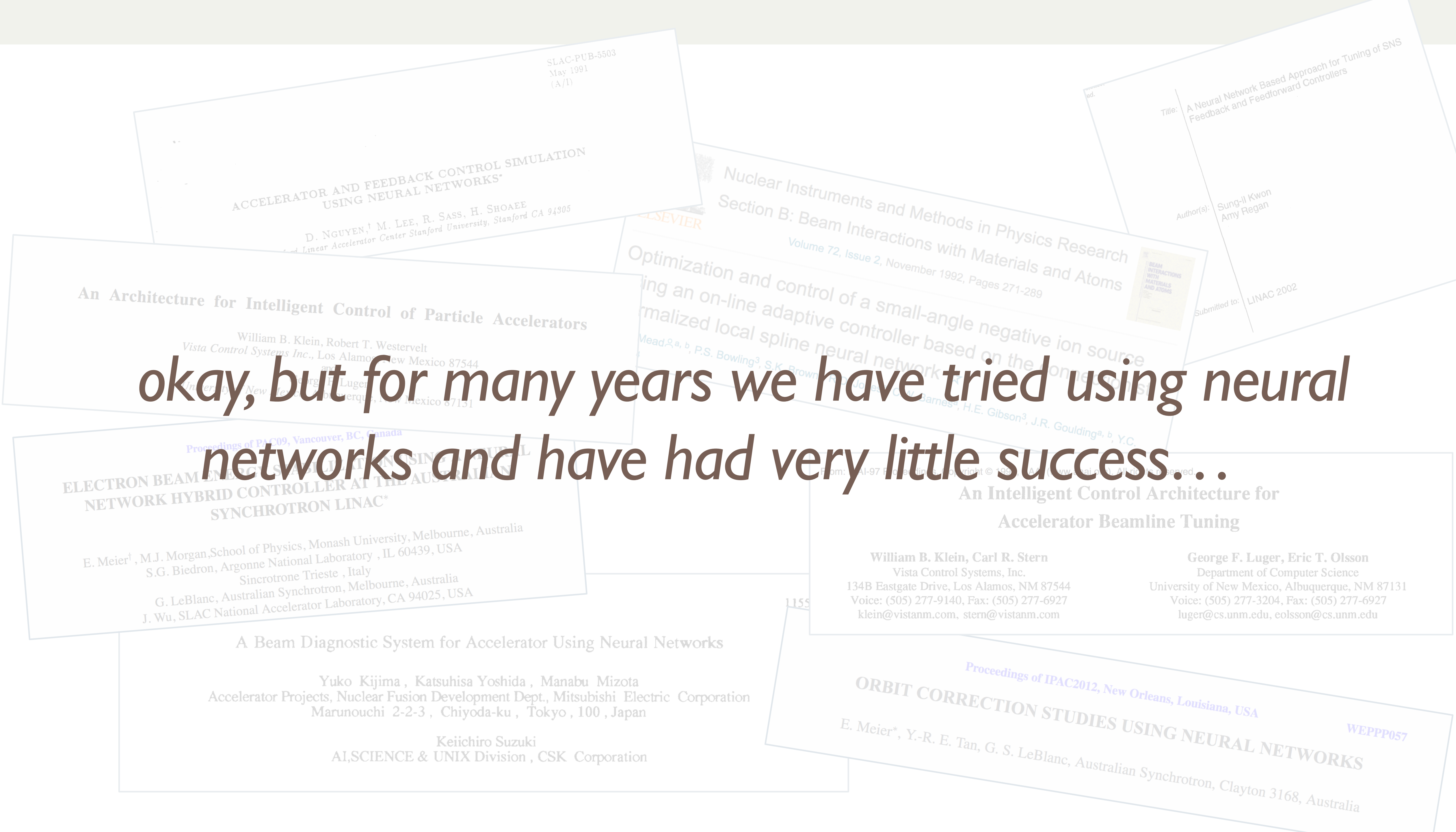
e.g. $f(z) = \frac{2}{(1+e^{-2z})} - 1$



How this all fits together for NNs



*arguably broader than just "machine learning" okay, but for many years we have tried using neural networks and have had very little success…



. . . so, what is different now?

Increased computational capability
enables more complicated NN architectures and faster training + larger data sets

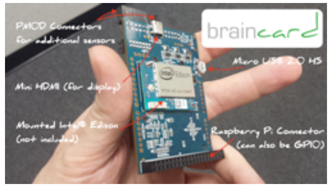
GPUs

IBM, ANL

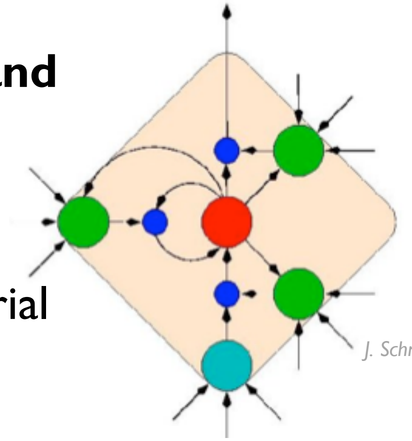
Accessibility of HPC clusters

Can **easily share** large data sets, code, and computing setups (e.g. via cloud computing services)

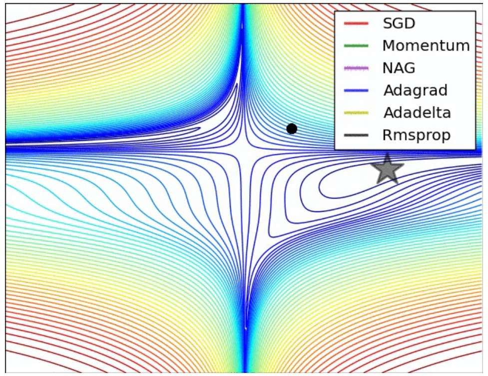
Up-and-coming advancements: neuromorphic hardware



New network architectures and training paradigms,
such as long short term memory (LSTM) networks, neural turing machines, and generative adversarial networks (GANs)



J. Schmidhuber



A. Radford

Better **theoretical understanding** of NNs and improved **optimization methods**

Applications have driven a lot of advancement (both algorithmic and practical/heuristic)

Google

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New network architectures and

Increased com
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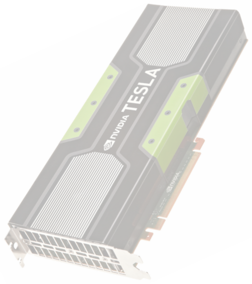
and faster trainin



Learning to Pivot with Adversarial Networks

Gilles Louppe
New York University
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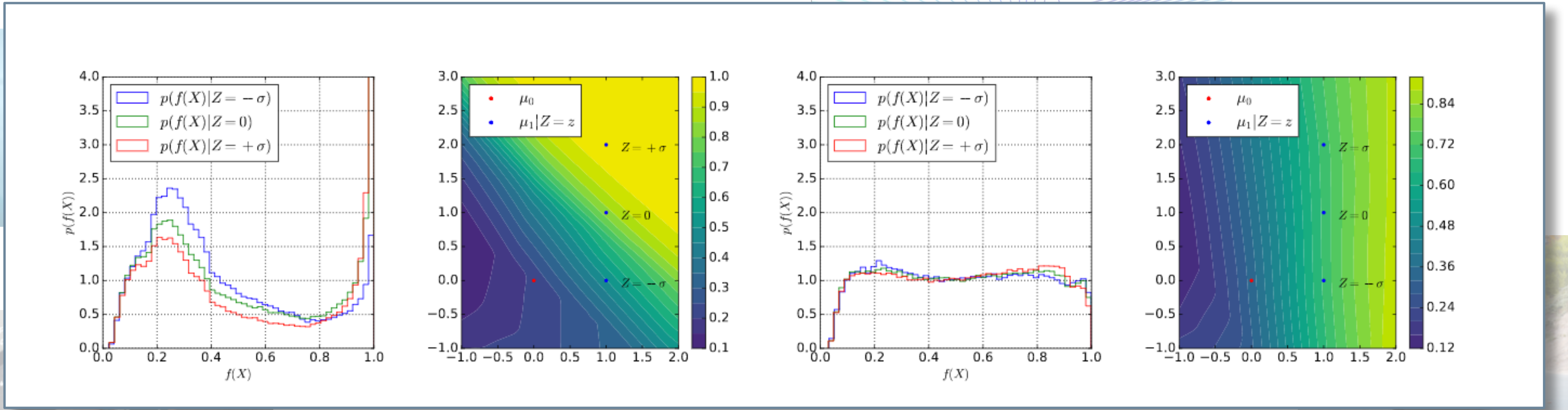
Michael Kagan
SLAC National Accelerator Laboratory
makagan@slac.stanford.edu

Kyle Cranmer
New York University
kyle.cranmer@nyu.edu

r theoretical
rstanding of
NNs and improved



Up-and-coming
advancements:
neuromorphic
hardware

e.g. physics application (HEP) → algorithmic development

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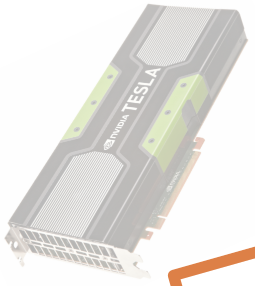
Increased computational capability
enables more complicated NN architectures
and faster training + larger data sets

GPUs



Accessibility

Shutterstock

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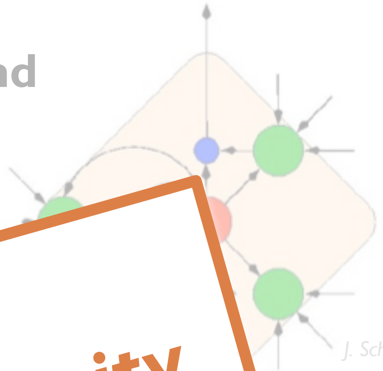

J. Schmidhuber

→ much greater overall technological maturity
→ many advances in the last 3-5 years

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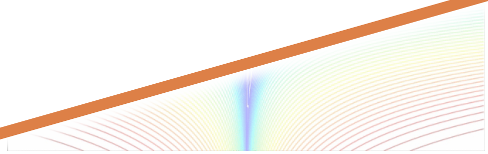
optimization
methods



A. Radford

es)

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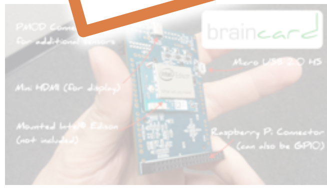


Applications have driven a lot of
advancement (both algorithmic
and practical/heuristic)

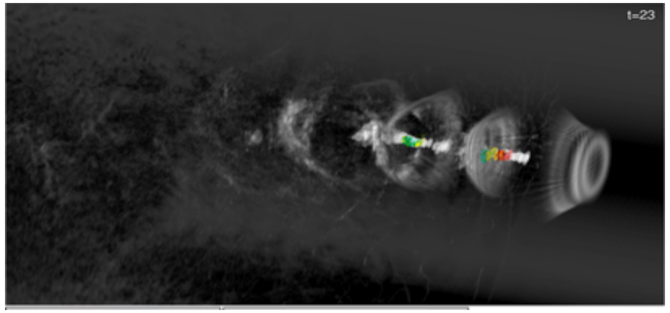
Google

Let's talk about accelerators…

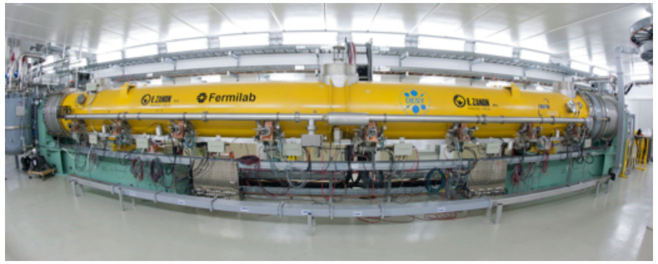
http://fast.fnal.gov/gallery.html

Interesting Technical Challenges

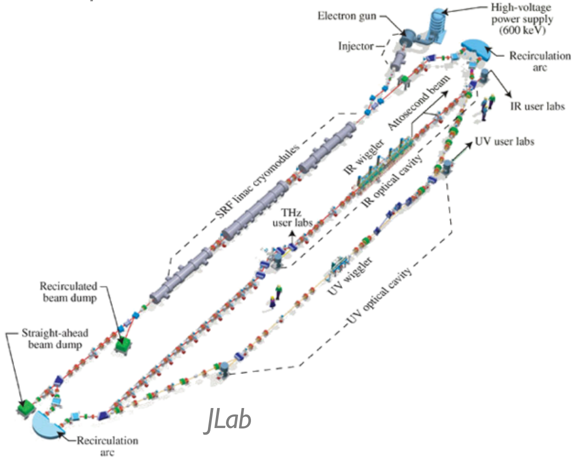
- Complex/nonlinear dynamics
- Many small, compounding errors
- Many parameters to monitor and control
- Interacting sub-systems
- On-demand changes in operational state
- Diagnostics sometimes limited or not put to full use in control (e.g. images)
- Time-varying/ non-stationary behavior



LBNL Visualization Group



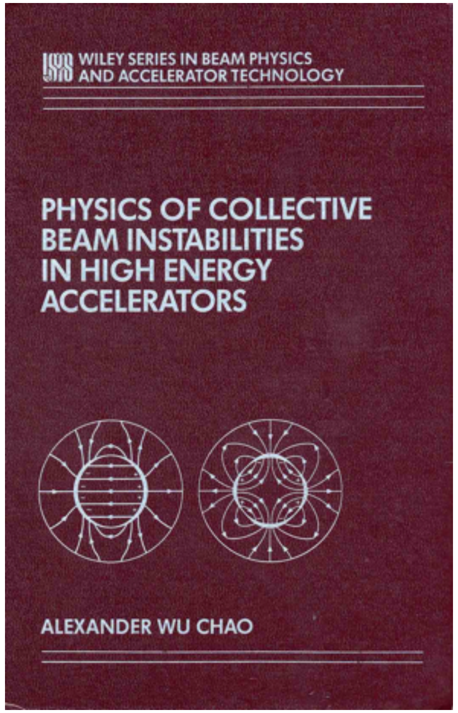
Fermilab



JLab

Strong Incentives for Better Control

- Cost of running → Time/energy efficiency of control
- Cost of unintended down-time → Personnel cost, user time, bulk scientific output
- Achieving performance needed for science goals and other applications
  - *improving accelerator components and control both play a role*



Uncertain, time-varying, nonlinear, many-parameter systems with continuous action spaces:

→ **of great interest for research in control and machine learning**

→ **lots of opportunity to both gain from and contribute to this area**

Global News in 2016:

deepmind.com

https://googleblog.blogspot.com

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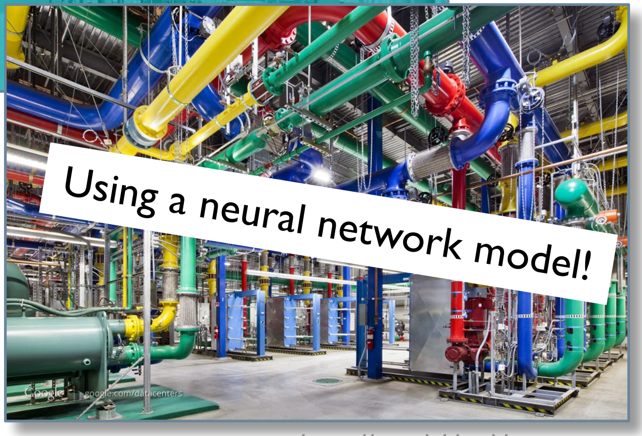
Transport delays, variable heat load
Efficient servers alone not enough



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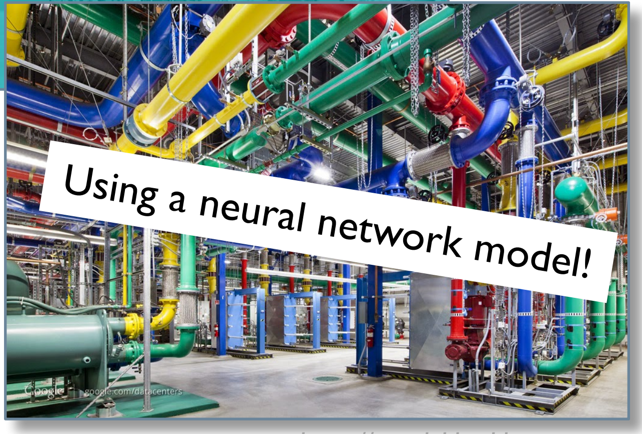

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Work at FNAL during 2014:

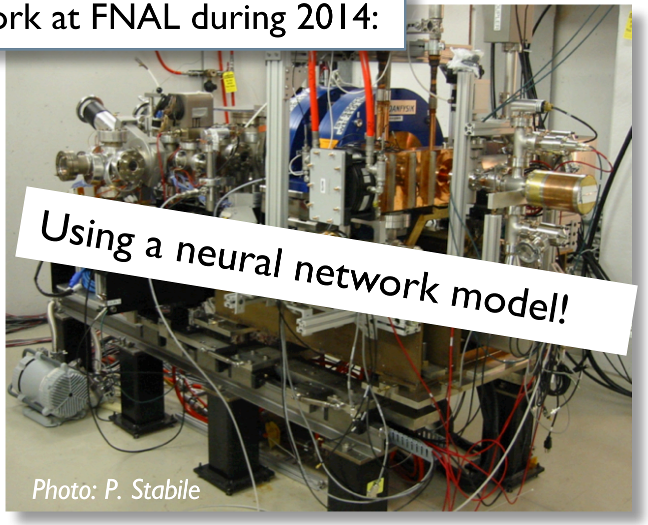

Photo: P. Stabile

A. L. Edelen, et al. IPAC15 ,TUPOA51

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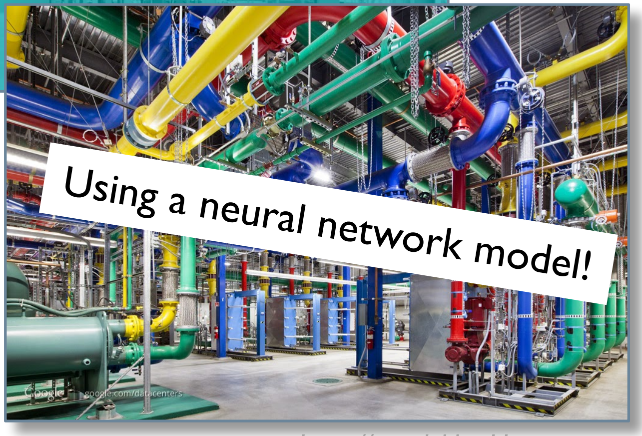

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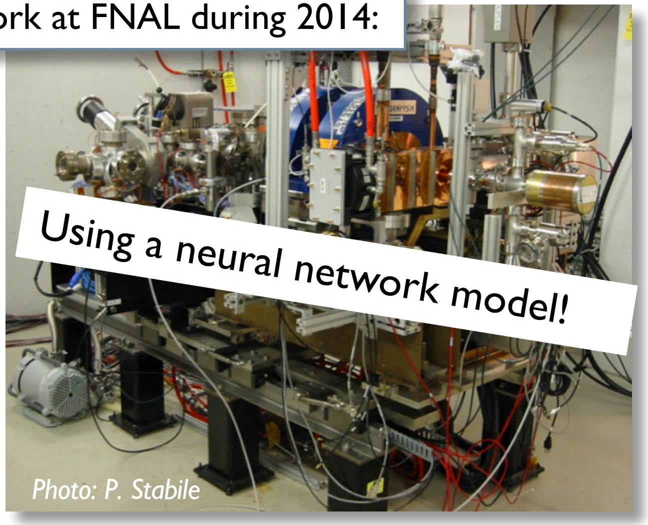

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A. L. Edelen, et al. IPAC15 ,TUPOA51

Looks vaguely familiar…

Transport delays, variable heat load, complex dynamics

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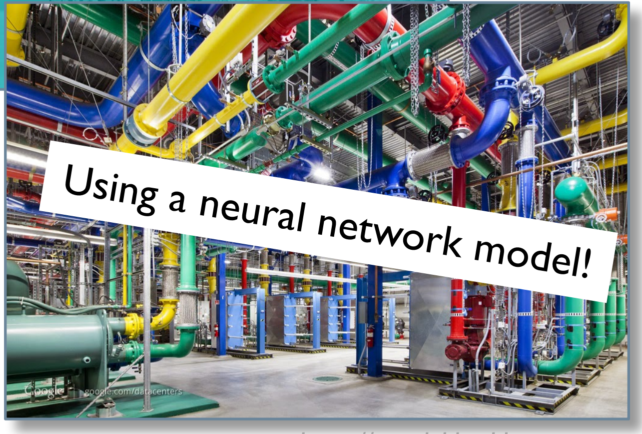

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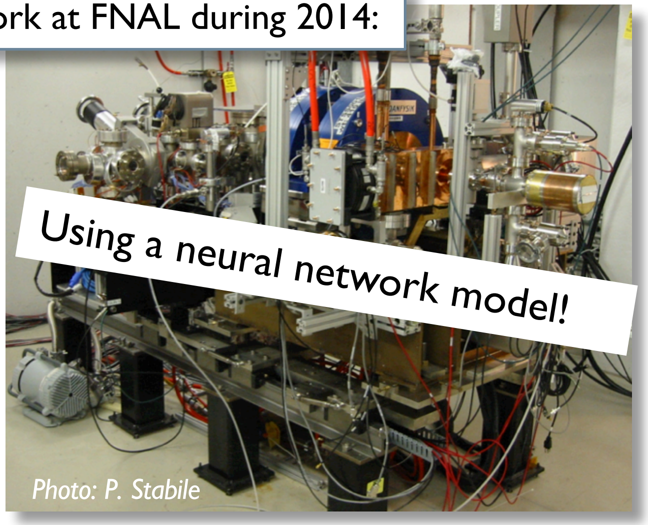

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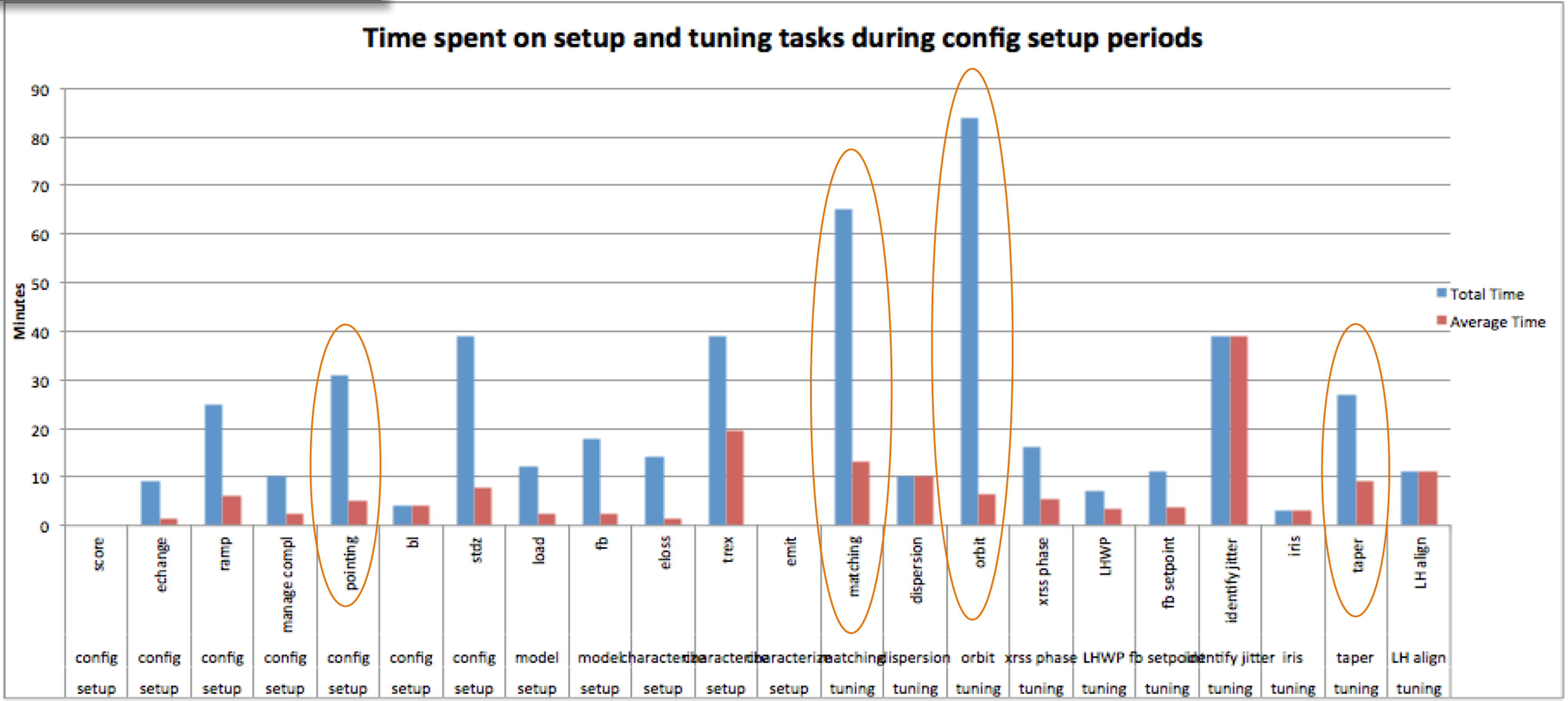
Cryo plant photo: A. Grassellino talk at IPAC '17, (THPPA2)

Example from LCLS



2015: 450 hand tuning hours, 250 dedicated!

⇒ Lots of opportunity to speed operations and relieve operator load

Figure from D. Ratner's presentation at the 8th Hard X-ray FEL Collaboration Meeting, 24-26 October 2016

We rely heavily on operators for day-to-day control tasks . . .

Fermilab Control Room Photo: Reidar Hahn, FNAL

. . . so what can we learn from them,

and what analogous techniques can we use?

Inspiration from Operators

Fermilab Control Room Photo: Reidar Hahn, FNAL

Application Areas for Accelerators

- Online modeling → *NN model*
- Time delays → *model predictive control + NN models*
- Image-based diagnostics → *convolutional or locally-connected NNs*
- Frequent switching between operating conditions → *NN policy*
- Virtual diagnostics → *NN model trained from intercepting diagnostics or simulation*
- Encode an existing policy and/or adapt upon it → *NN policy*
- High-level assessment of machine or device states → *NN process model, classifier*
- Failure prediction / Anomaly detection → *NN process model, classifier*

Online Modeling

- Operators maintain a learned mental machine model: *let's supplement it*

- Ideally:
  - Fast-executing, but accurate enough to be useful
  - Use measured inputs directly from machine
  - Combine *a priori* knowledge + learned parameters

This can be very hard!

- Applications
  - A tool for operators + virtual diagnostics
  - Predictive control
  - Help flag aberrant behavior

One approach: faster modeling codes

- Simpler models (tradeoff with accuracy)
- Parallelization and GPU-acceleration of existing codes

  PARMILA *X. Pang, PAC13, MOPMA13*

  elegant *I.V. Pogorelov, et al., IPAC15, MOPMA035*

- Improvements in underlying modeling algorithms

(fractions of a second)

Another approach: machine learning model

- Once trained, neural networks can execute quickly
- Train on slow, high-fidelity simulation results
- Also train on measured results

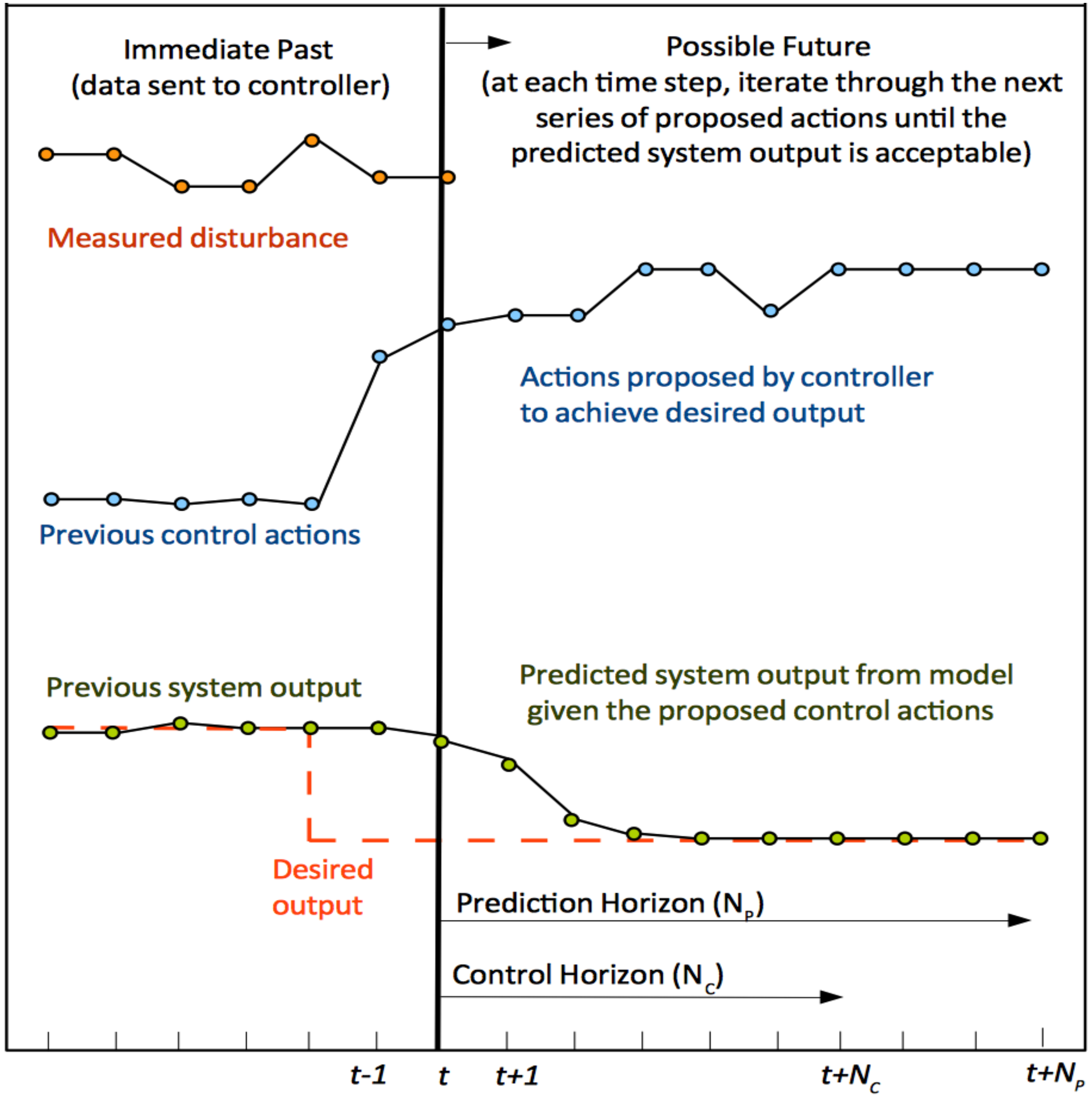
Yields a fast-executing model that can be used operationally, but approximates behavior from high-fidelity simulations (e.g. PIC codes, LPA)

An initial study involving this at FAST:

A. L. Edelen, et al. NAPAC16, TUPOA51

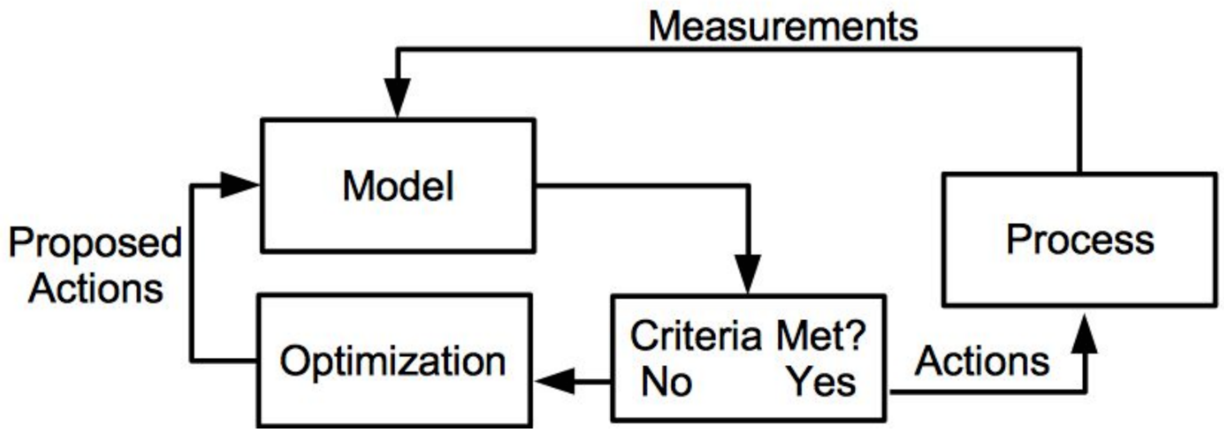
one PARMELA run: ~20 min

Model Predictive Control (Prediction + Planning)

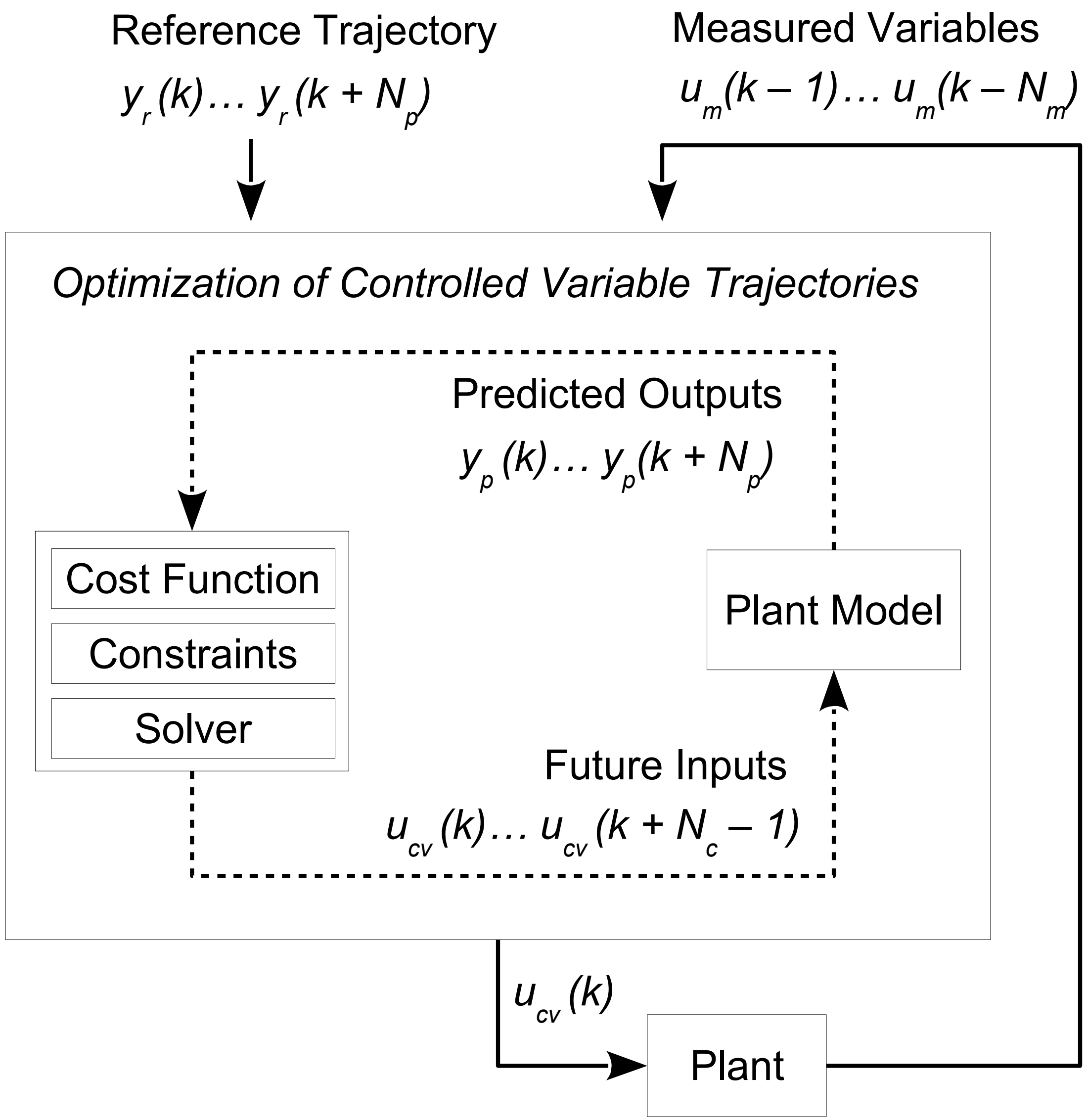


Basic concept:

1. Use a predictive model to assess the outcome of possible future actions
2. Choose the best series of actions
3. Execute the first action
4. Gather next time step of data
5. Repeat



Model Predictive Control (Prediction + Planning)



N_m previous measurements

N_p future time steps predicted

N_c future time steps controlled

$$\sum_{i=1}^{N_p} \{w_y \left[y_r(k+i) - y_p(k+i)\right]\}^2$$
(output variable targets)

$$\sum_{j=1}^{ncv} \sum_{i=0}^{N_p-1} \{w_{u,j} \left[u_j(k+i) - u_{j,ref}(k+i)\right]\}^2$$
(controllable variable targets)

$$\sum_{j=1}^{ncv} \sum_{i=0}^{N_p-1} \{w_{\Delta u,j} \left[u_j(k+i) - u_j(k+i-1)\right]\}^2$$
(movement size)

Temperature Control for the RF Photoinjector at FAST

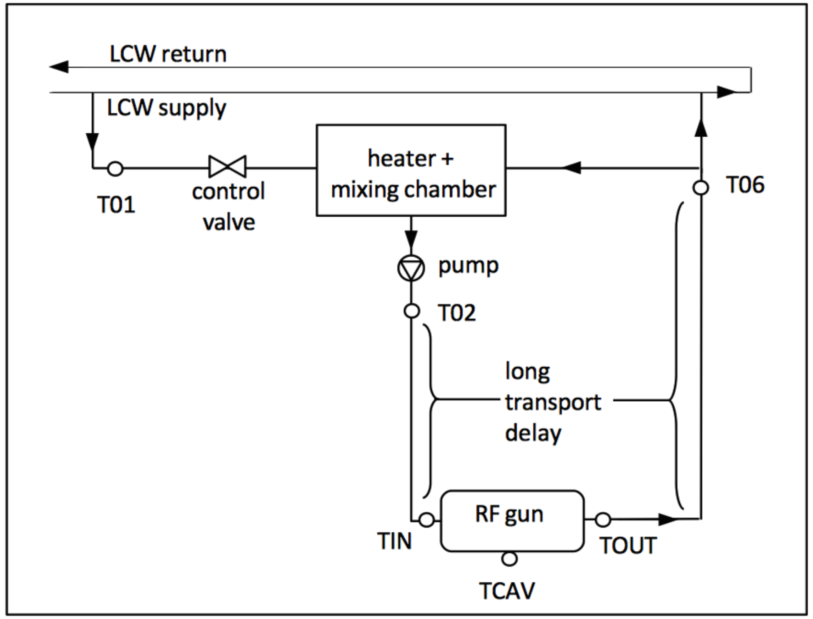
Resonant frequency controlled via temperature

PID control is undesirable in this case:

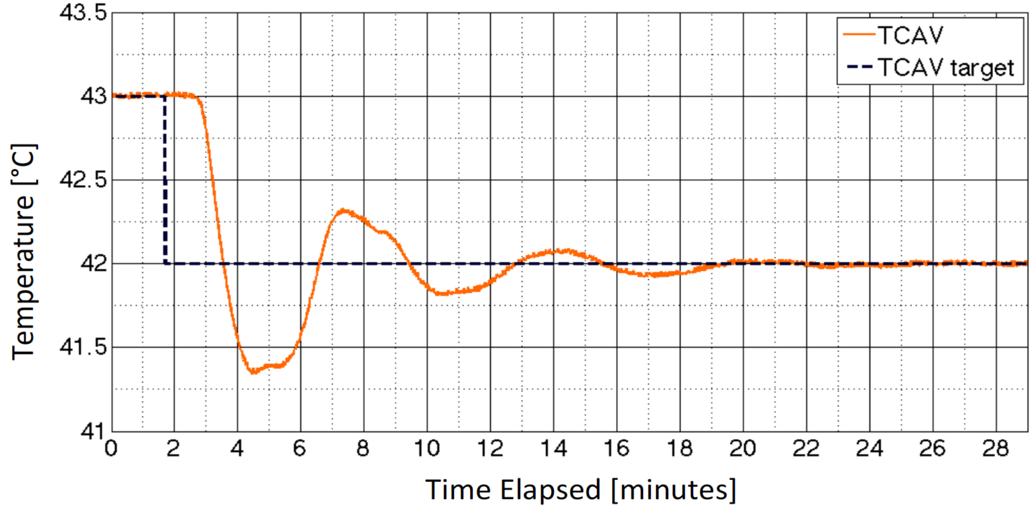
- Long transport delays and thermal responses
- Recirculation leads to secondary impact of disturbances
- Two controllable variables: heater power + valve aperture

Applied model predictive control (MPC) with a neural network model trained on measured data: ~ 5x faster settling time + no large overshoot

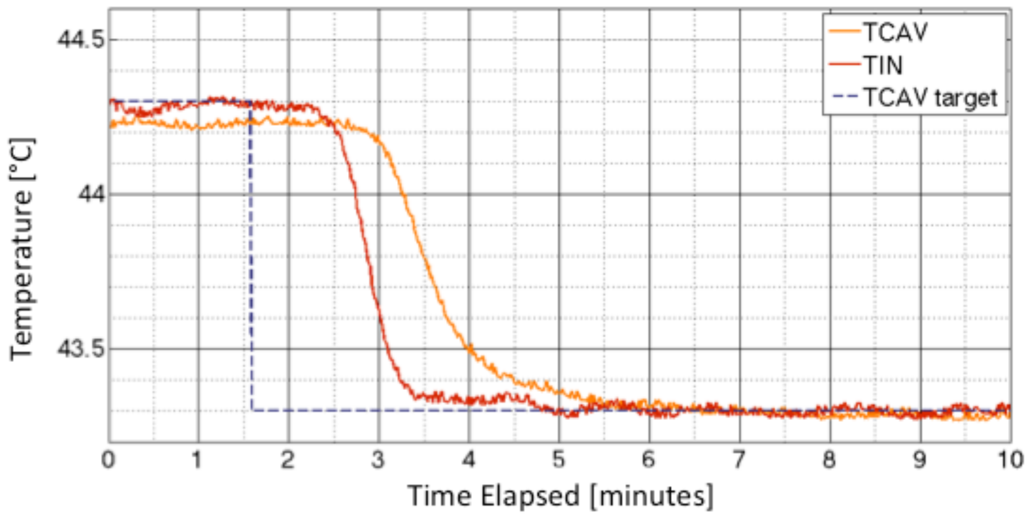
Gun Water System Layout



Existing Feedforward/PID Controller



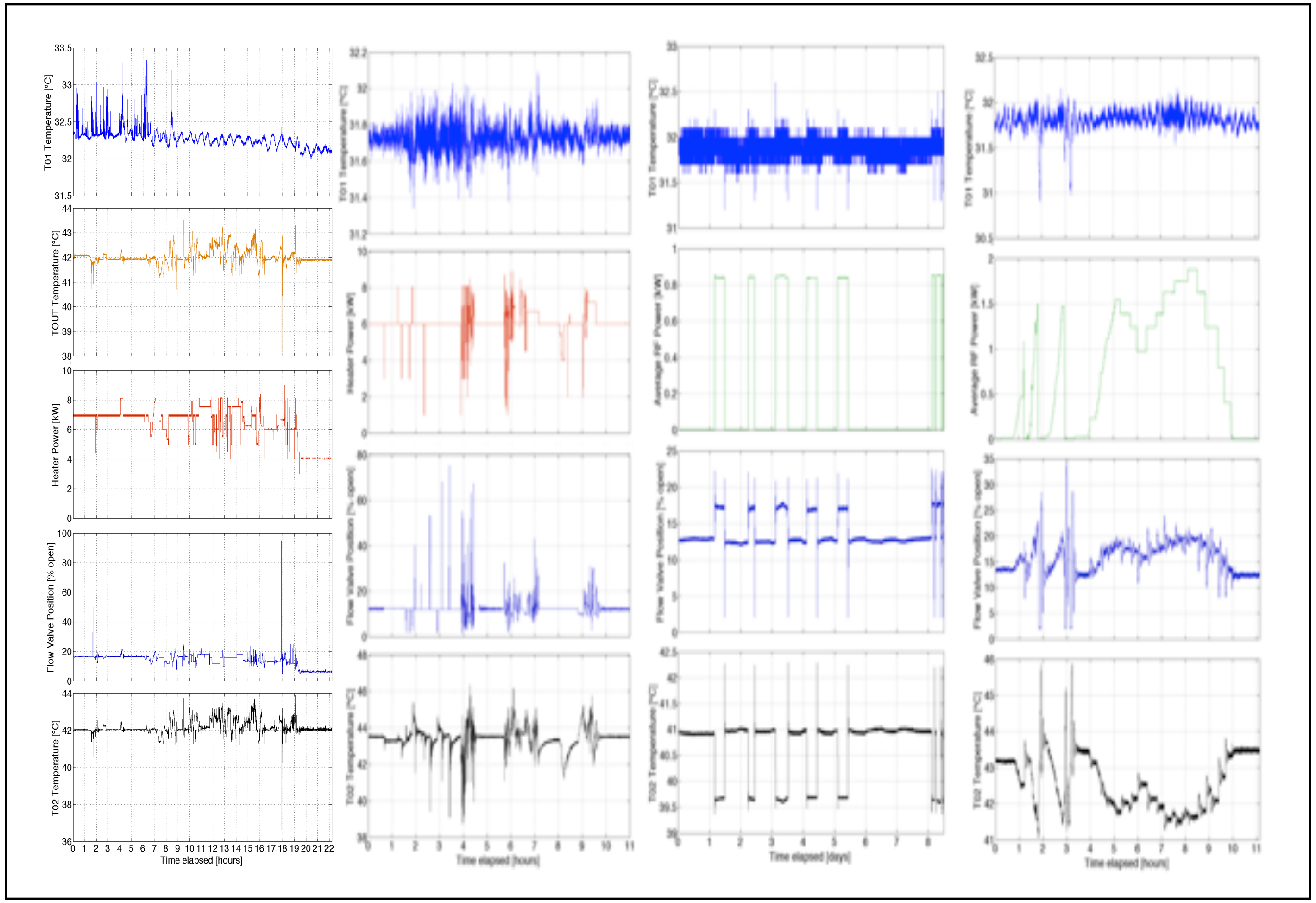
Model Predictive Controller



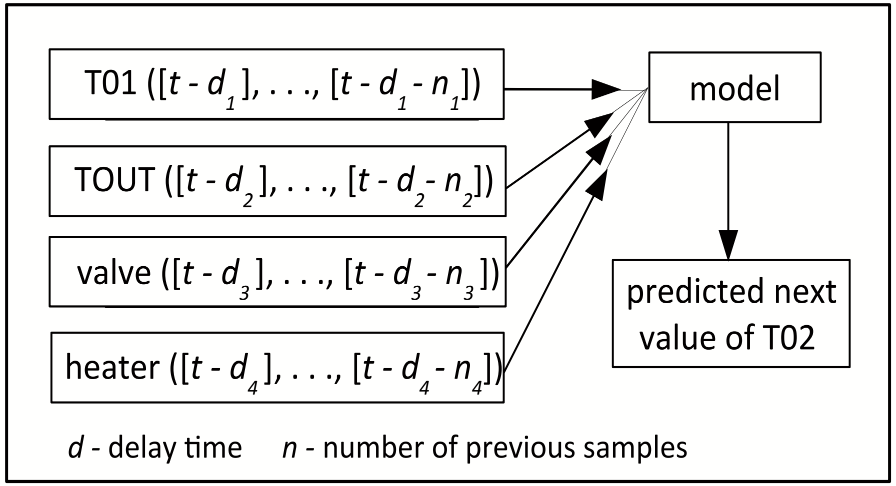
Note that the oscillations are largely due to the transport delays and water recirculation, rather than PID gains

More info: A. L. Edelen. IEEE TNS, vol. 63, no. 2, 2016

Neural Network Model



Training data from machine



NN model

Why does this matter (for resonant frequency control in general)?

LLRF system will compensate for detuning by increasing forward power

But…

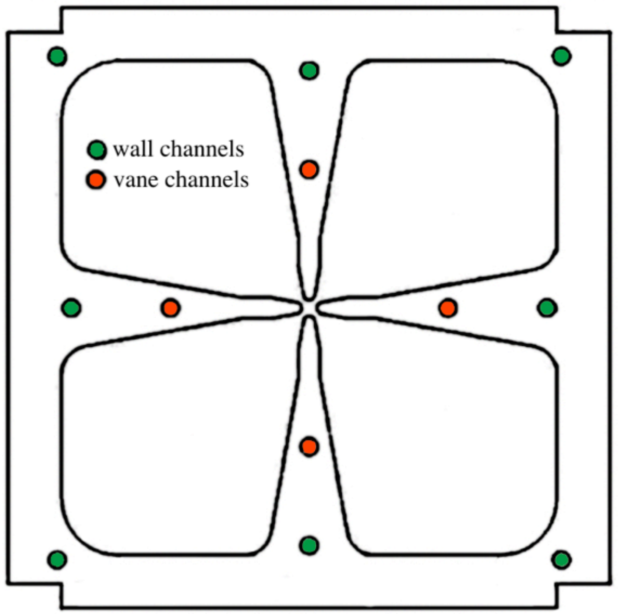
- Ability to do this bounded by the amplifier specs
- RF overhead adds to initial machine cost and footprint
- Using additional RF power → *increasing operational cost*
- Increased waste heat into cooling system → *increasing operational cost*
- If detuned beyond overhead → *interrupt normal operations (beam not properly accelerated or LLRF in frequency-tracking mode)*

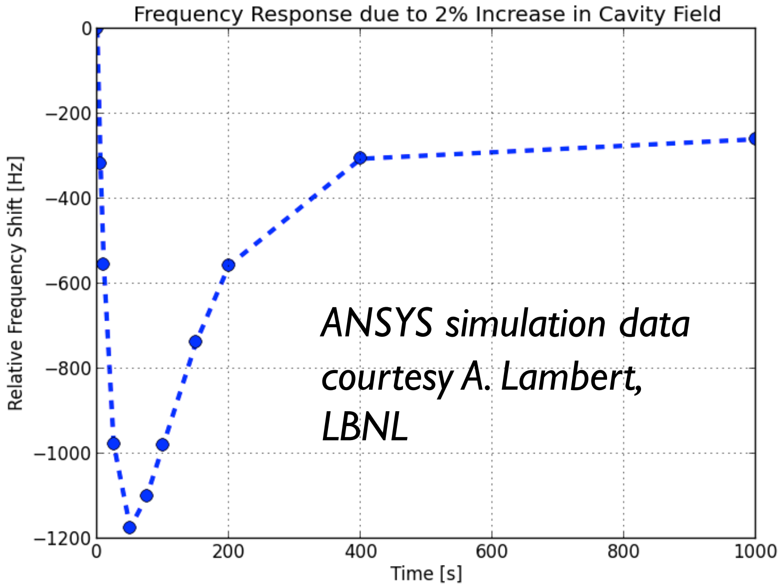
PIP-II Injector Test RFQ

Variable heating

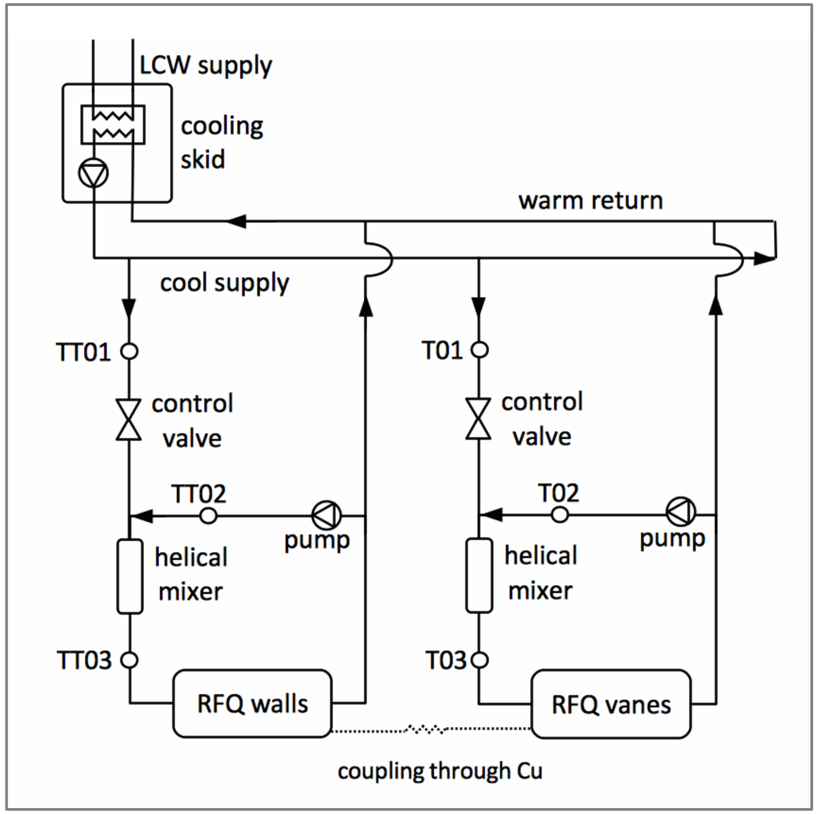
Specification for GDR: 3-kHz maximum frequency shift
Range of RF duty factors and pulse patterns (including up to CW)
-16.7 kHz/°C in the vanes and 13.9 kHz/°C in the walls*

* A. R. Lambert et al., IPAC'15, WEPTY045

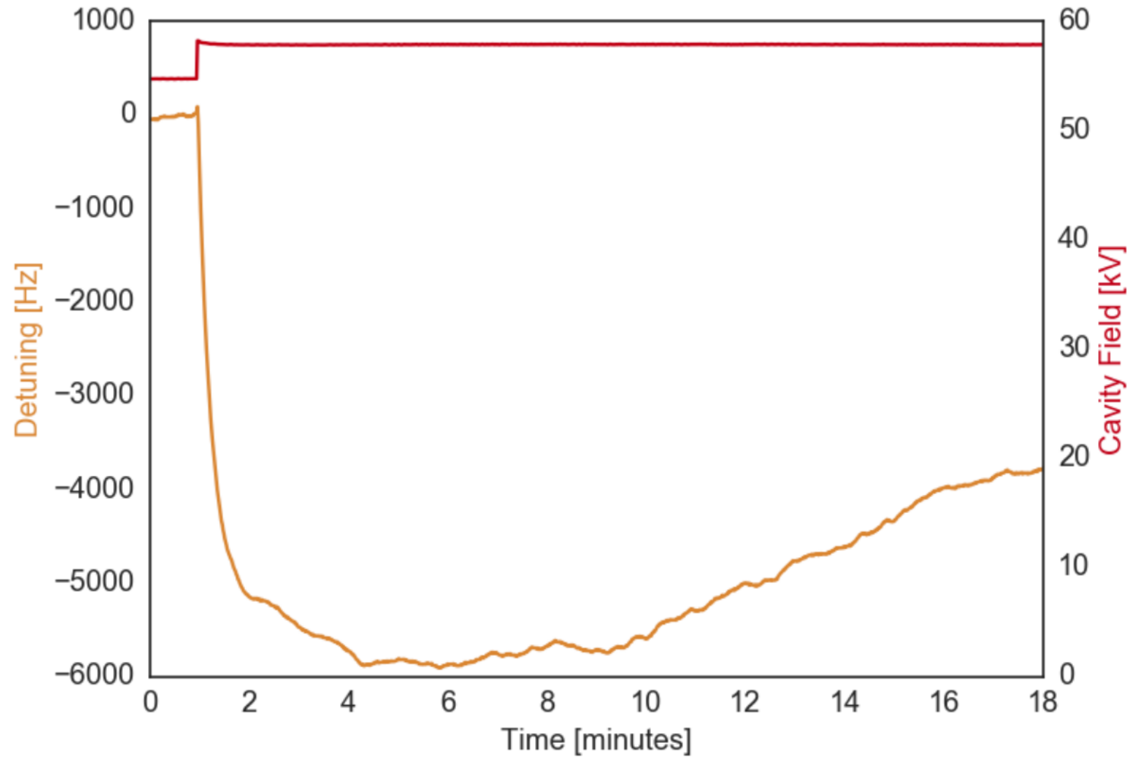




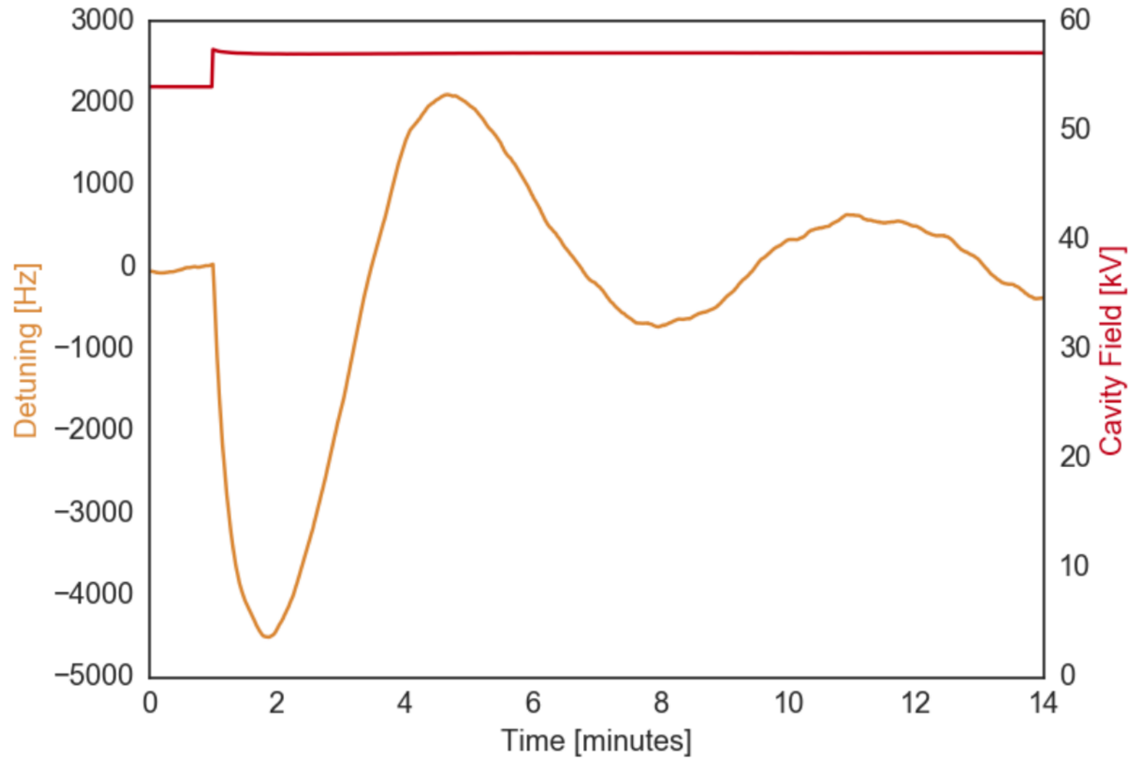
ANSYS simulation data courtesy A. Lambert, LBNL



RFQ Detuning in CW Mode



Example of uncontrolled detuning in CW mode under a small change in cavity field (55 kV to 58 kV)



PI frequency control in CW operation under a small change in cavity field (55 kV to 58 kV)

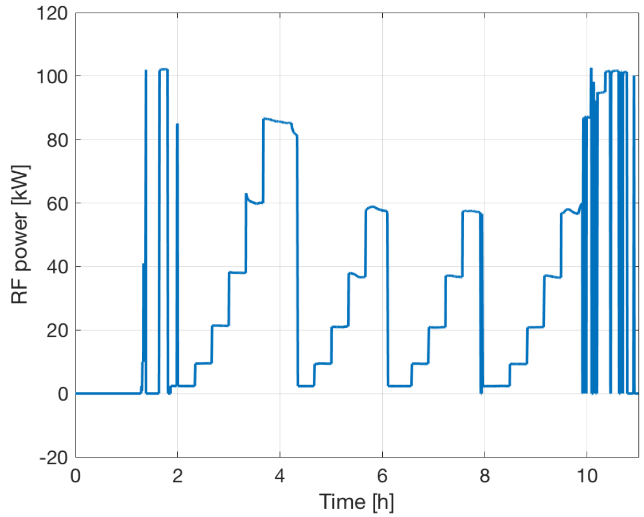
What about a simple first-principles model, or a learned linear model?

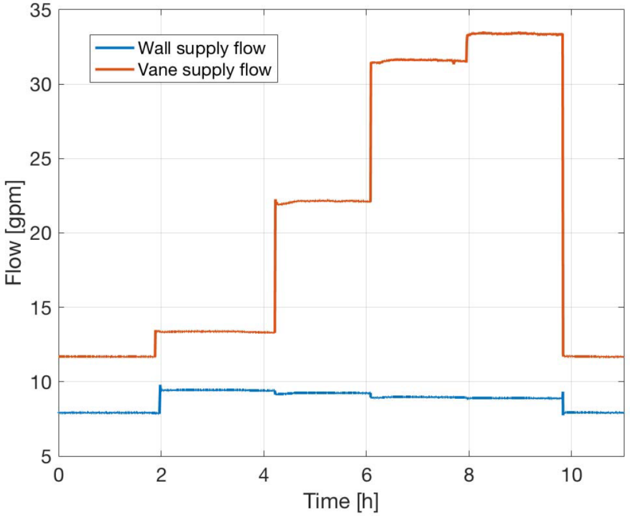
measured input data → first-principles model   4 ms pulse duration, 10 Hz rep rate   variety of valve and power settings

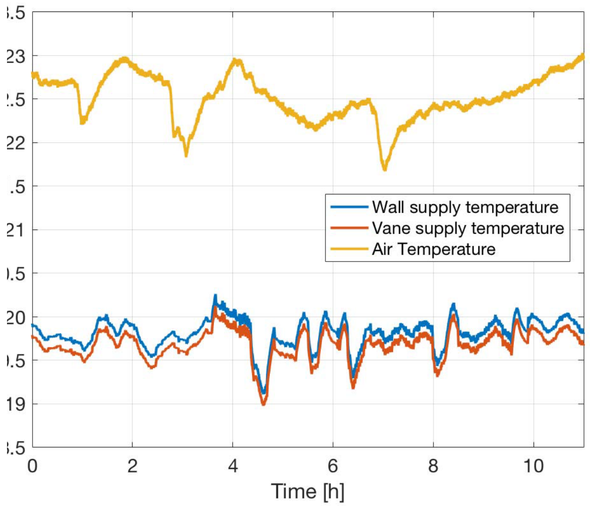
1.67 kHz RMS error

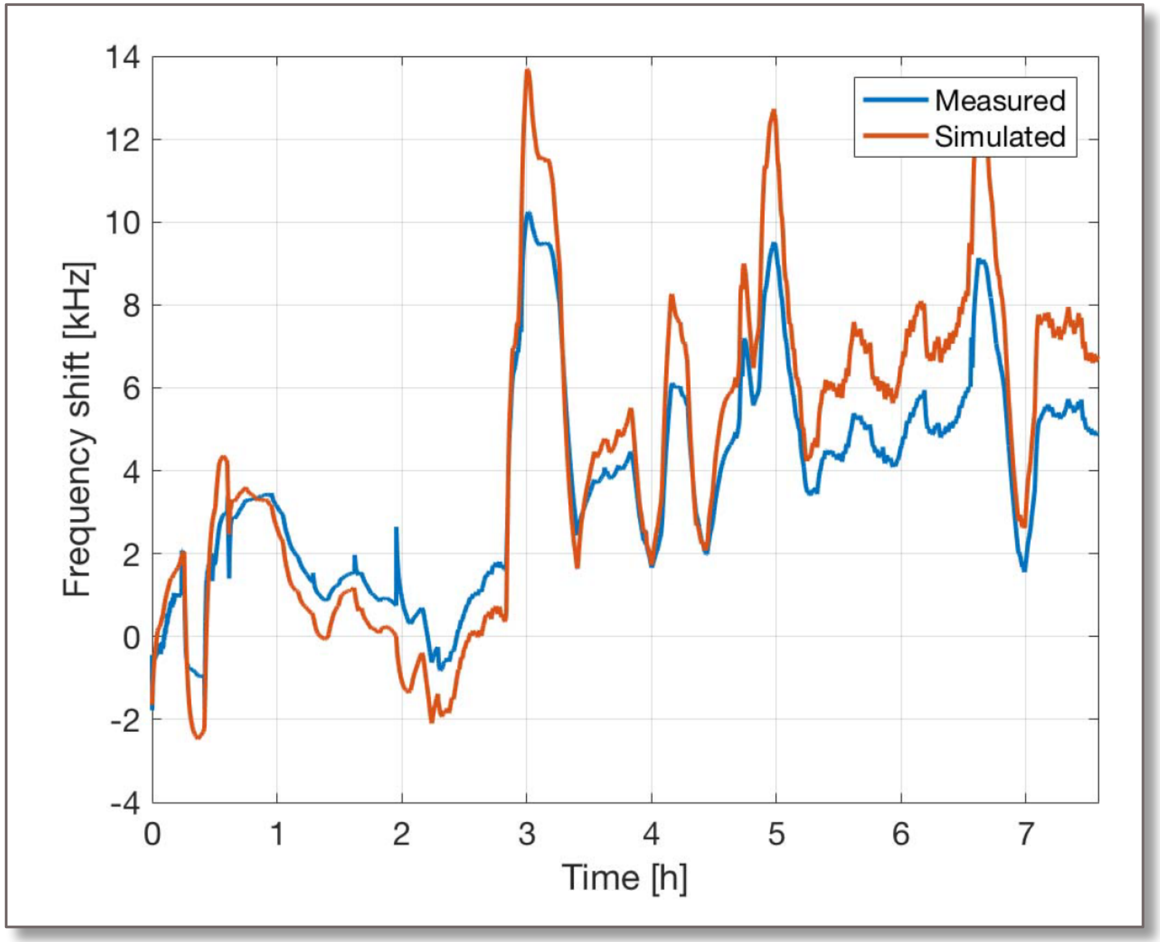
4.01 kHz max error

not good enough!



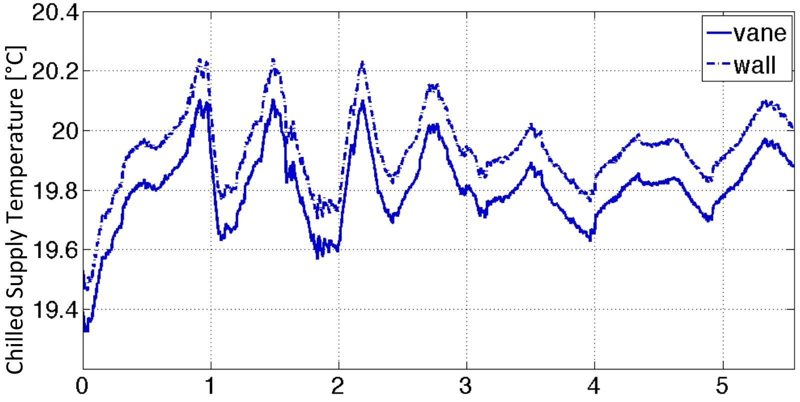


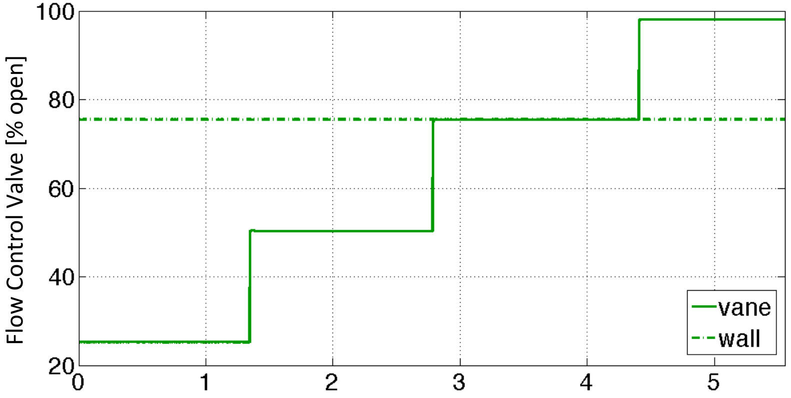


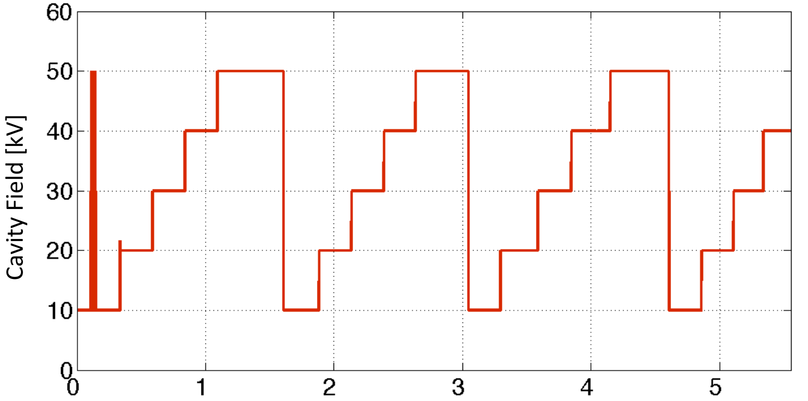


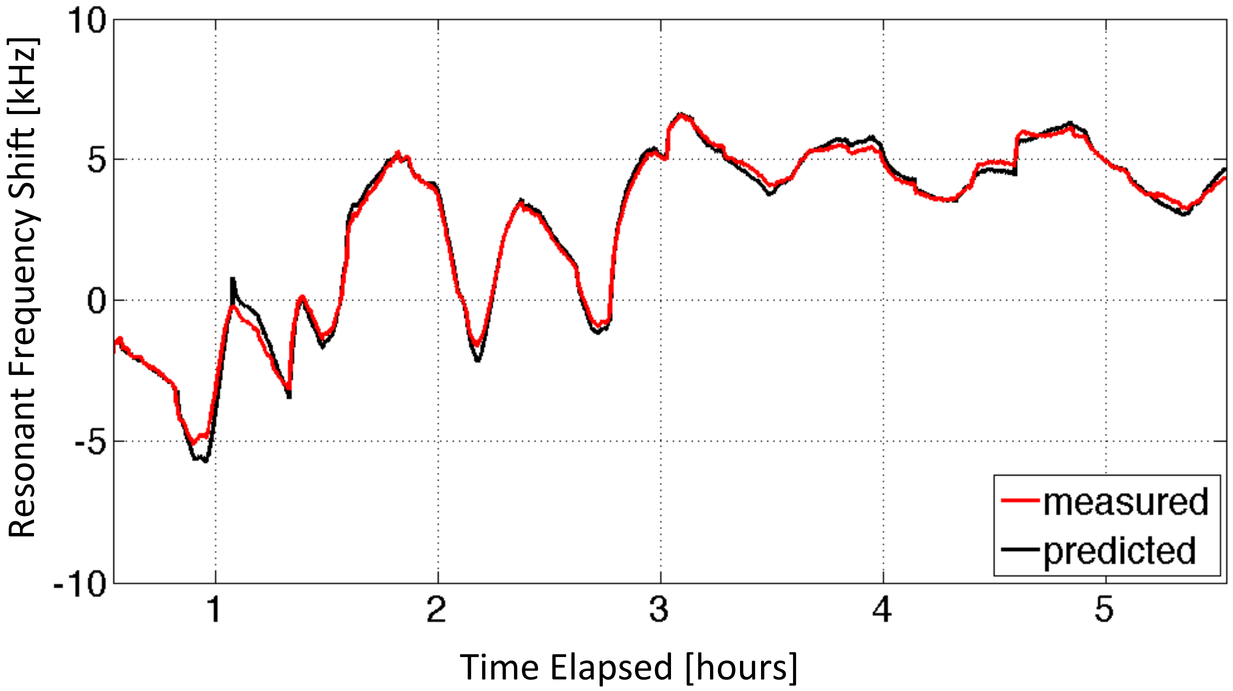
J. Edelen, A. Edelen, et al. TNS 64, vol. 2, (2017)

Neural Network Model









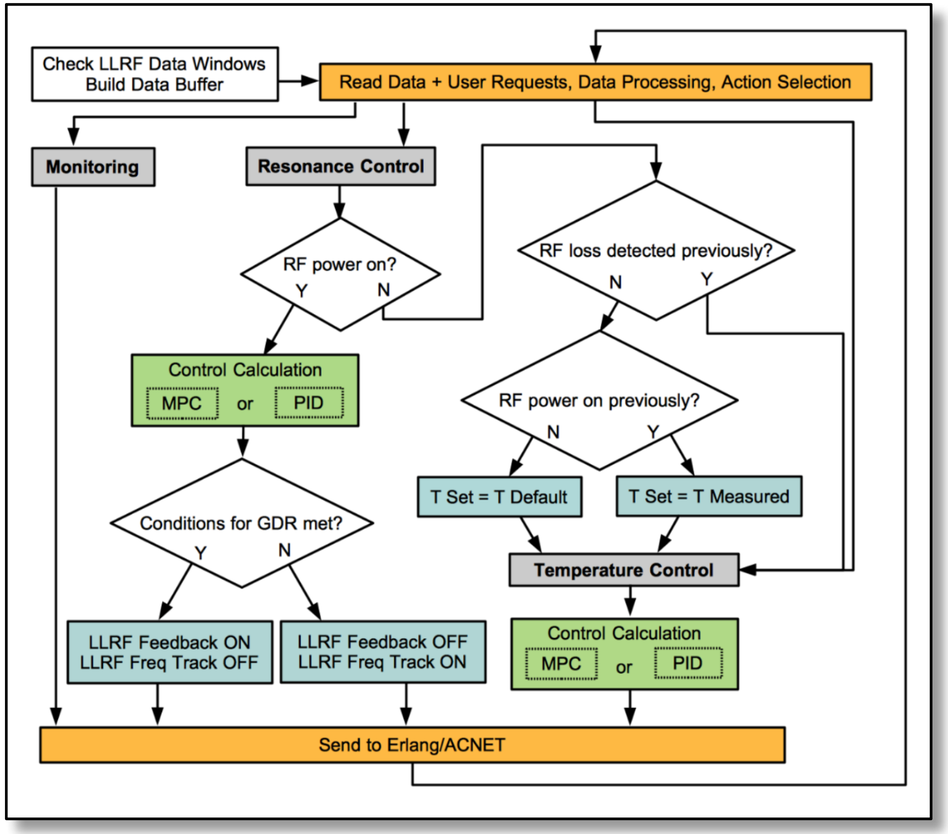
Inputs

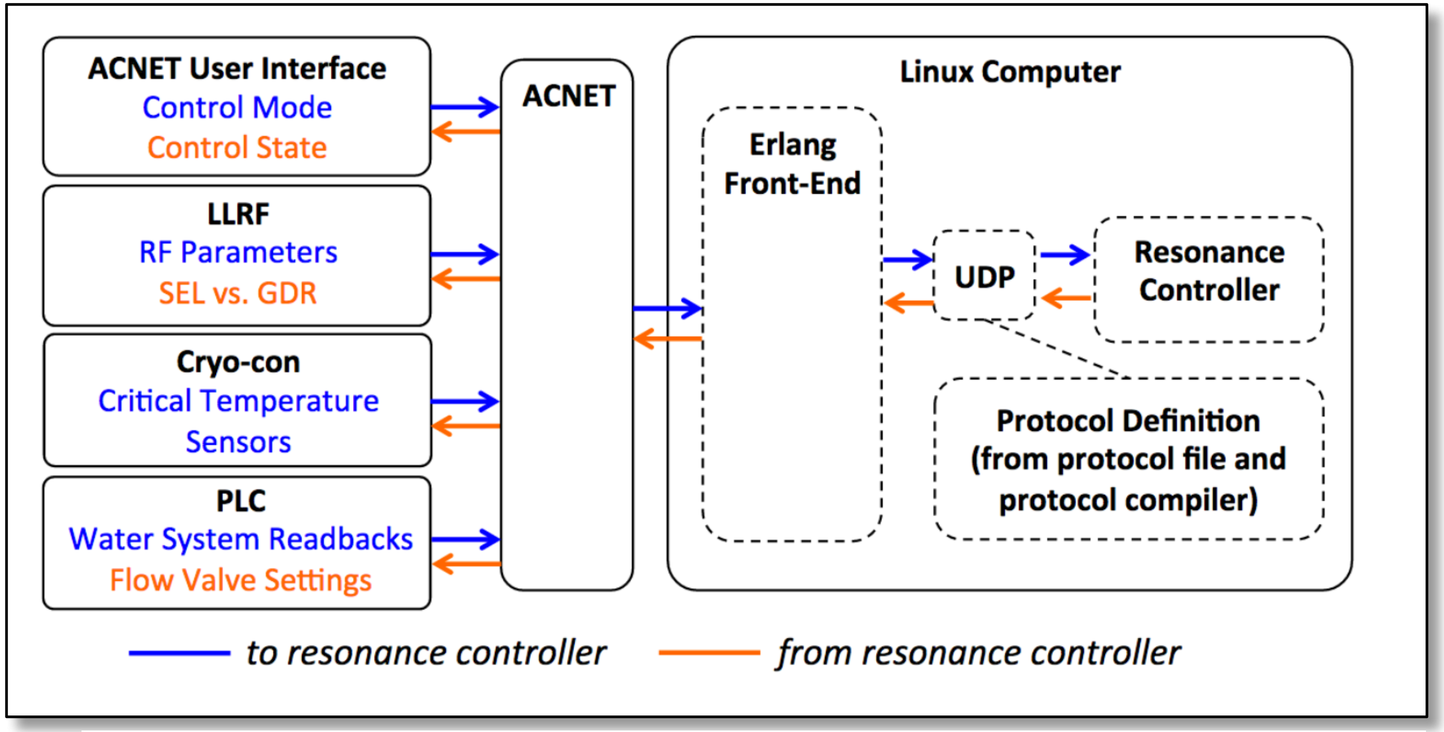
Vane and wall valve settings
Average RF power
Water temperatures
Ambient temperature and humidity

Mean Absolute Prediction Error

346 Hz on the test set
98 Hz on the validation set
115 Hz across all sets

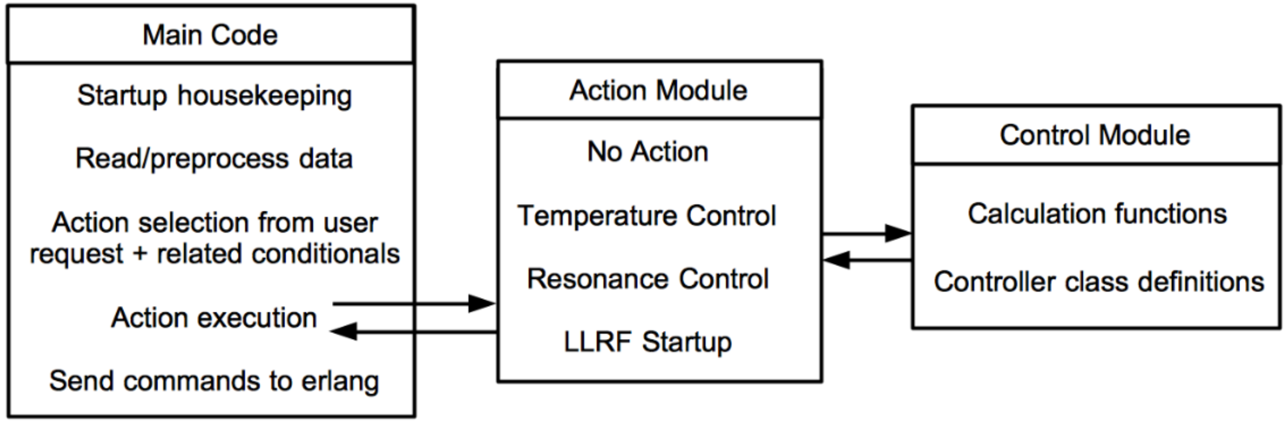
A. Edelen, et al., IPAC '16, THPOY020





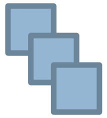
Built a python-based control framework

- *Executes on controls network linux computer*
- *PI control in regular operational use*
- *Preparing for test of MPC*
- *Designed to be portable + modular*



Virtual Diagnostics

Predict what diagnostics might look like when they are unavailable or don't exist

Real values from machine  → **Online Model** → Real-time prediction of beam dynamics at various locations

Virtual Diagnostics

Predict what diagnostics might look like when they are unavailable or don't exist

(fast a priori simulation, or fast ML model trained using simulation data)

Real values from machine → Online Model → Real-time prediction of beam dynamics at various locations

Virtual Diagnostics

Predict what diagnostics might look like when they are unavailable or don't exist

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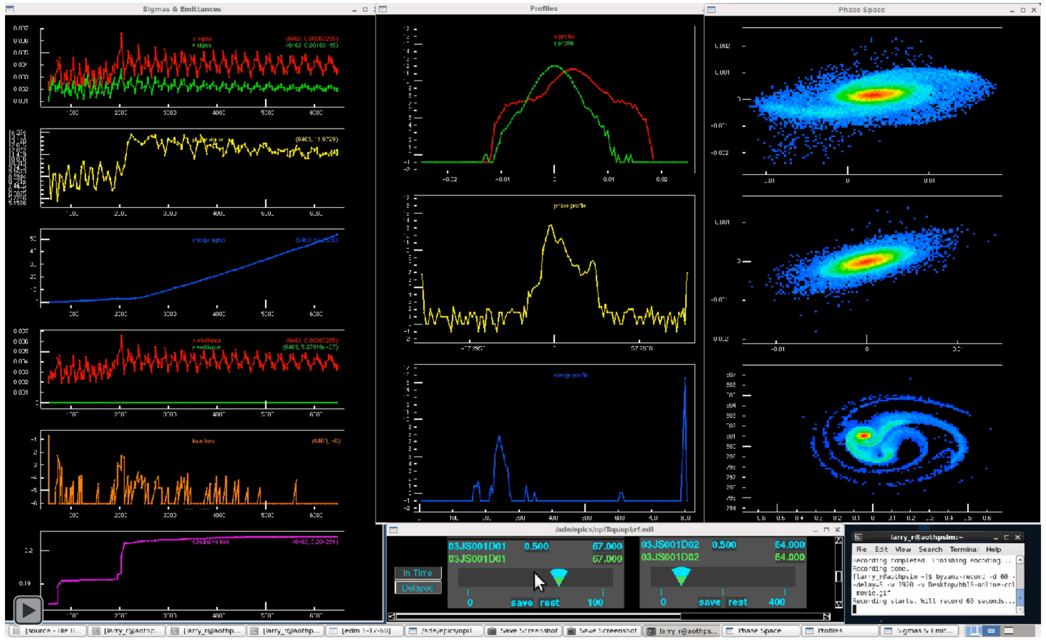


e.g. GPU-accelerated PARMILA at LANSCE

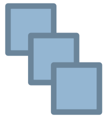
X. Pang, et al., PAC13, MOPMA13
X. Pang, IPAC15, WEXC2
X. Pang and L. Rybarcyk, CPC185, is. 3 (2014)
L. Rybarcyk, et al., IPAC15, MOPWI033
L. Rybarcyk, HB2016, WEPM4Y01

Virtual Diagnostics

Predict what diagnostics might look like when they are unavailable or don't exist

(fast a priori simulation, or fast ML model trained using simulation data)

Real values from machine



→ Online Model → Real-time prediction of beam dynamics at various locations

Virtual Diagnostics

Predict what diagnostics might look like when they are unavailable or don't exist

(fast a priori simulation, or fast ML model trained using simulation data)

Real values from machine → Online Model → Real-time prediction of beam dynamics at various locations

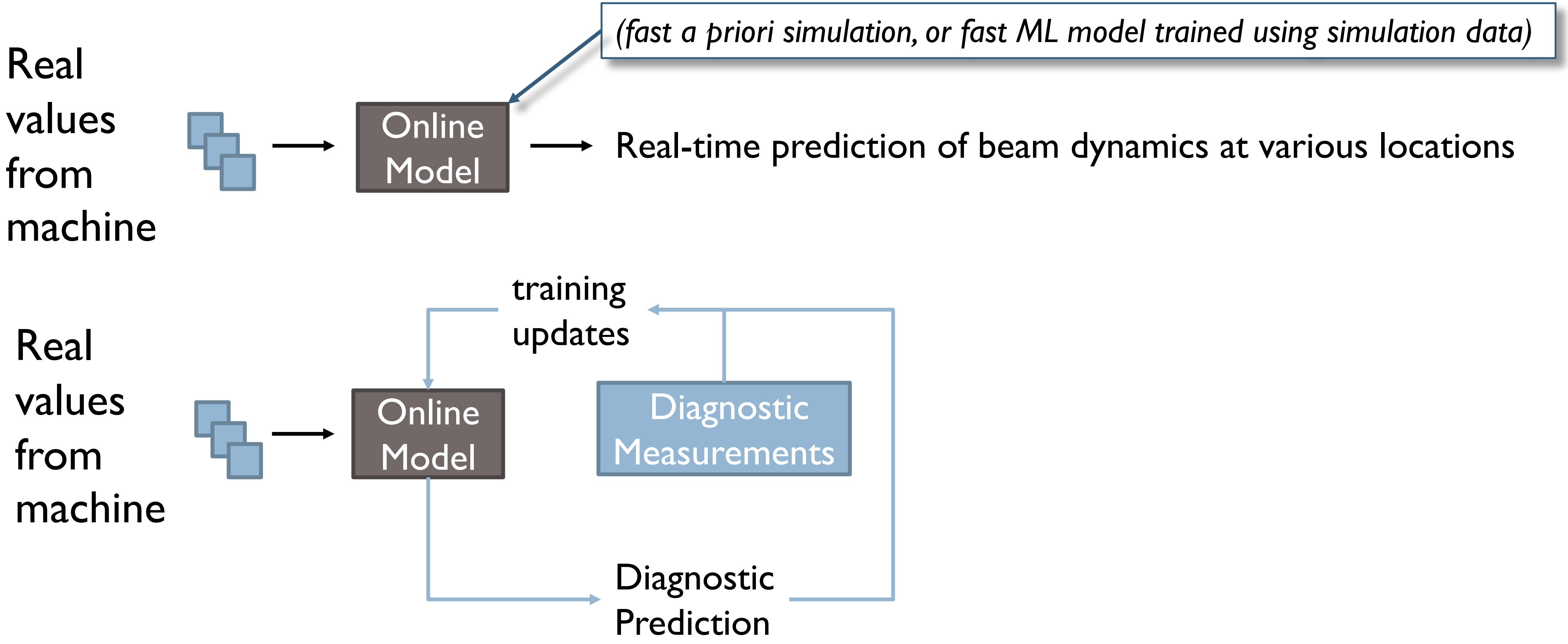
(ML model)

Real values from machine → Online Model

Diagnostic Measurements

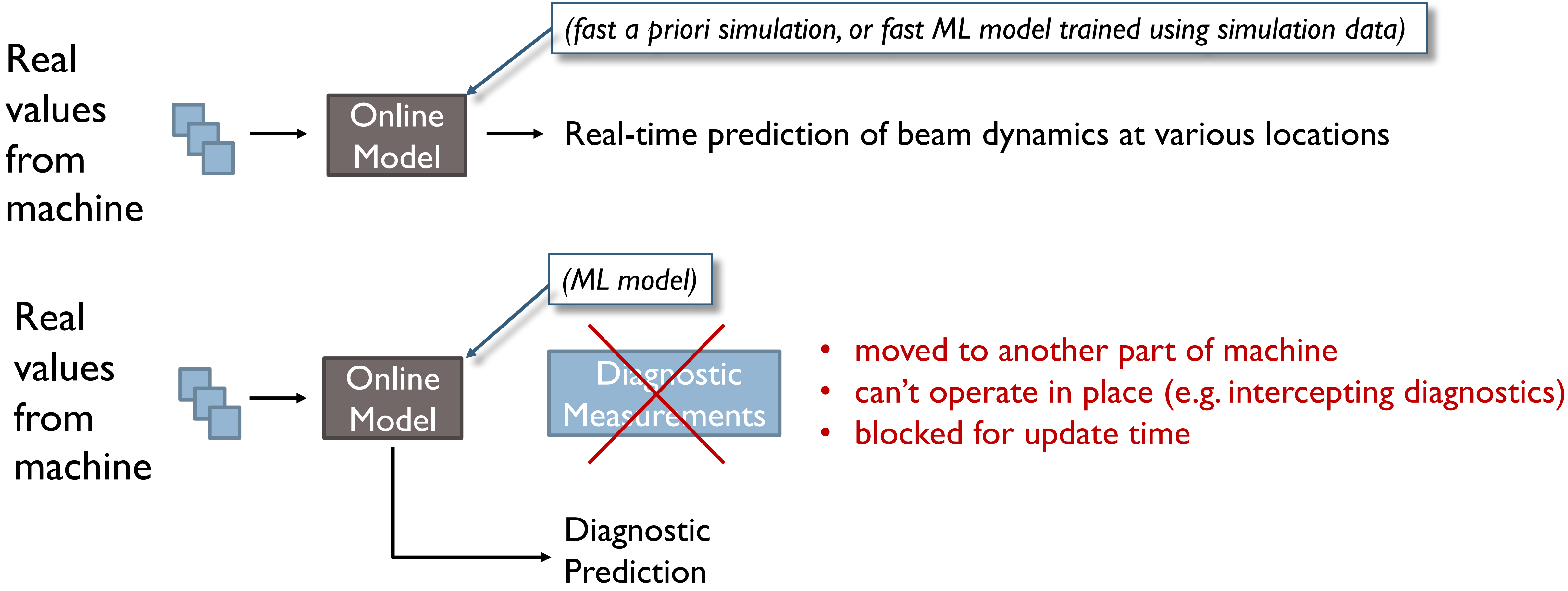
Virtual Diagnostics

Predict what diagnostics might look like when they are unavailable or don’t exist



Virtual Diagnostics

Predict what diagnostics might look like when they are unavailable or don't exist

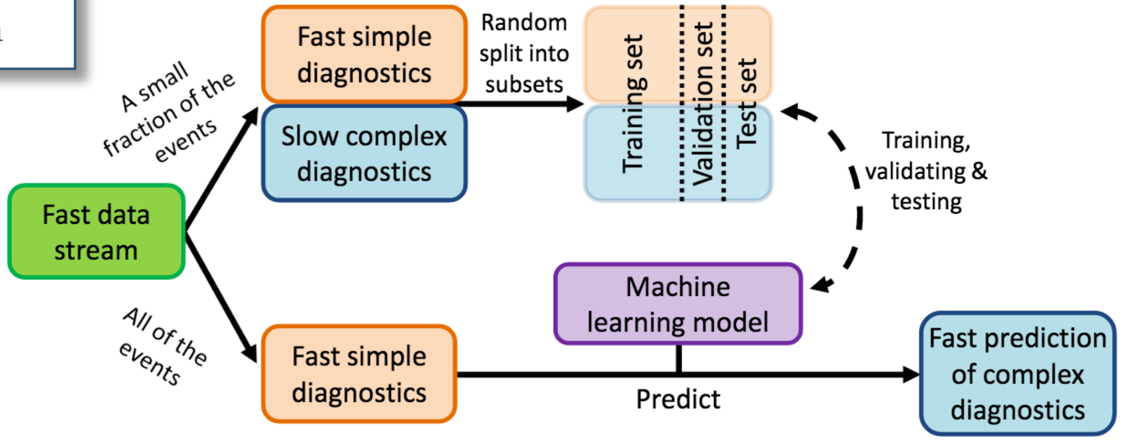


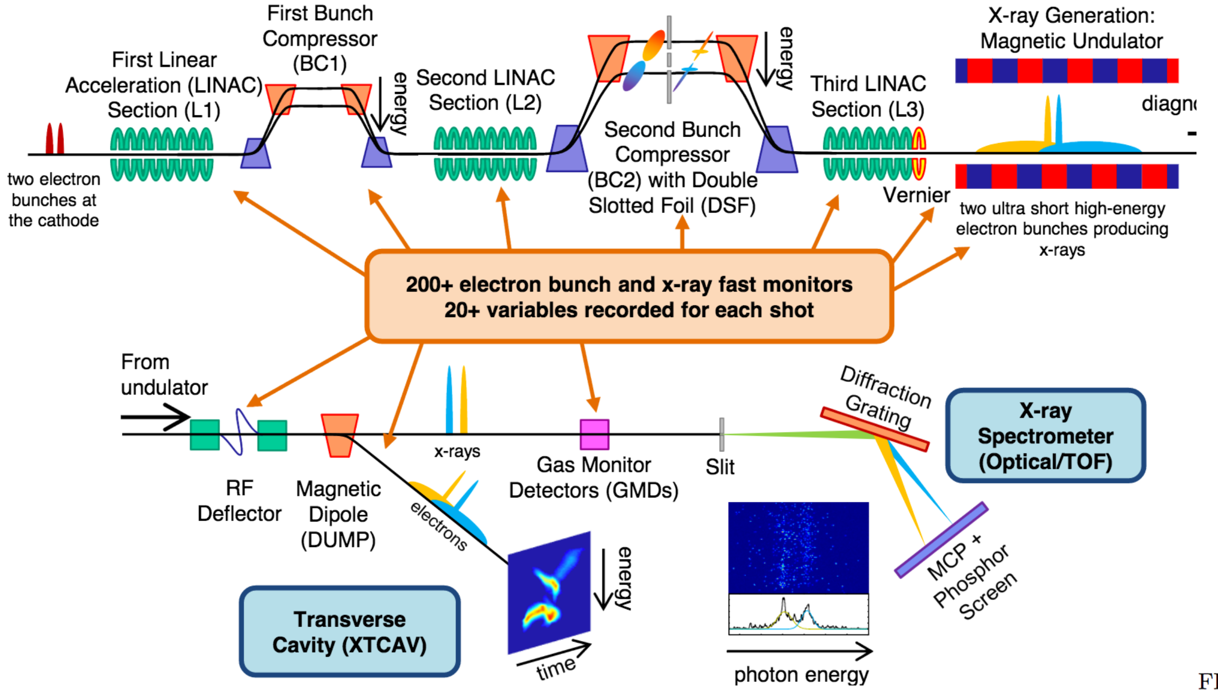
Machine learning applied to single-shot x-ray diagnostics in an XFEL

A. Sanchez-Gonzalez,[1] P. Micaelli,[1] C. Olivier,[1] T. R. Barillot,[1] M. Ilchen,[2,3] A. A. Lutman,[4] A. Marinelli,[4] T. Maxwell,[4] A. Achner,[3] M. Agåker,[5] N. Berrah,[6] C. Bostedt,[4,7] J. Buck,[8] P. H. Bucksbaum,[2,9] S. Carron Montero,[4,10] B. Cooper,[1] J. P. Cryan,[2] M. Dong,[5] R. Feifel,[11] L. J. Frasinski,[1] H. Fukuzawa,[12] A. Galler,[3] G. Hartmann,[8,13] N. Hartmann,[4] W. Helml,[4,14] A. S. Johnson,[1] A. Knie,[13] A. O. Lindahl,[2,11] J. Liu,[3] K. Motomura,[12] M. Mucke,[5] C. O'Grady,[4] J-E. Rubensson,[5] E. R. Simpson,[1] R. J. Squibb,[11] C. Såthe,[15] K. Ueda,[12] M. Vacher,[16,17] D. J. Walke,[1] V. Zhaunerchyk,[11] R. N. Coffee,[4] and J. P. Marangos[1]

A. Sanchez-Gonzalez, et al. https://arxiv.org/pdf/1610.03378.pdf

- Used archived data to learn correlation between fast and slow diagnostics
- Looked at a variety of ML methods and different diagnostics





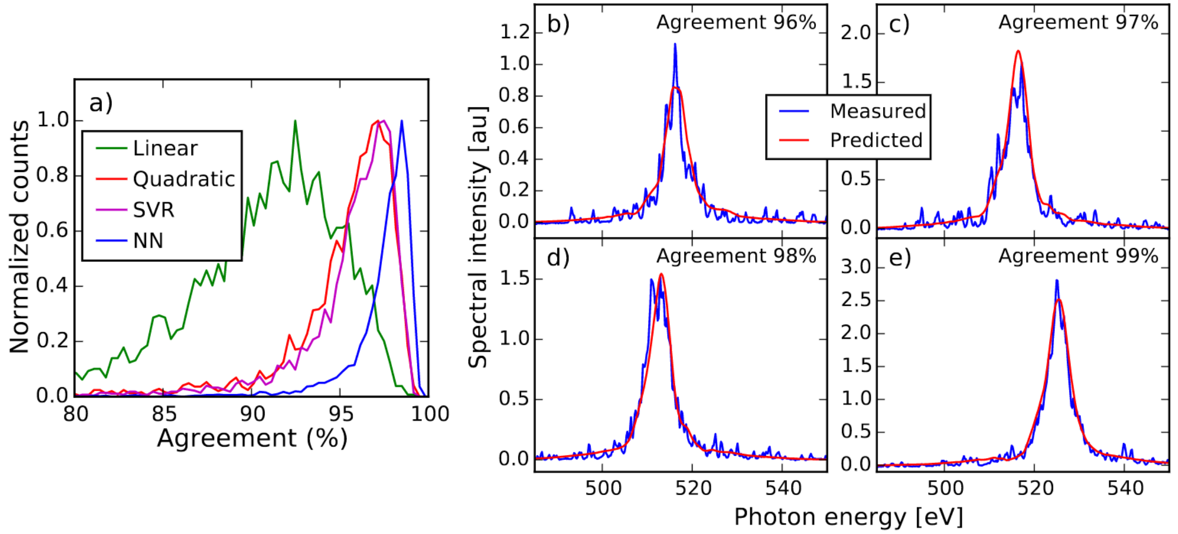


FIG. 4. Spectral shape prediction for a single pulse. (a) Histogram of agreements between the predicted and the measured spectra for the test set using the 4 different models. (b-e) Examples of the measured and the predicted spectra using a neural network to illustrate the accuracy for different agreement values.

Fault Prediction (Prognostics) + Anomaly Detection

Operations:

- Identify aberrant behavior that is correlated with faults, failures, or poor machine states
- Detect deviations from normal operating conditions that may otherwise go noticed

Machine Protection:

catastrophic failures and faults sometimes preceded by tell-tale signs

Replacement Cycles:

predict time-to-failure based on real-time and archived data

Using LSTM recurrent neural networks for detecting anomalous behavior of LHC superconducting magnets

Maciej Wielgosz[a], Andrzej Skoczeń[b], Matej Mertik[c]

[a] Faculty of Computer Science, Electronics and Telecommunications, AGH University of Science and Technology, Kraków, Poland
[b] Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Kraków, Poland
[c] The European Organization for Nuclear Research - CERN, CH-1211 Geneva 23 Switzerland

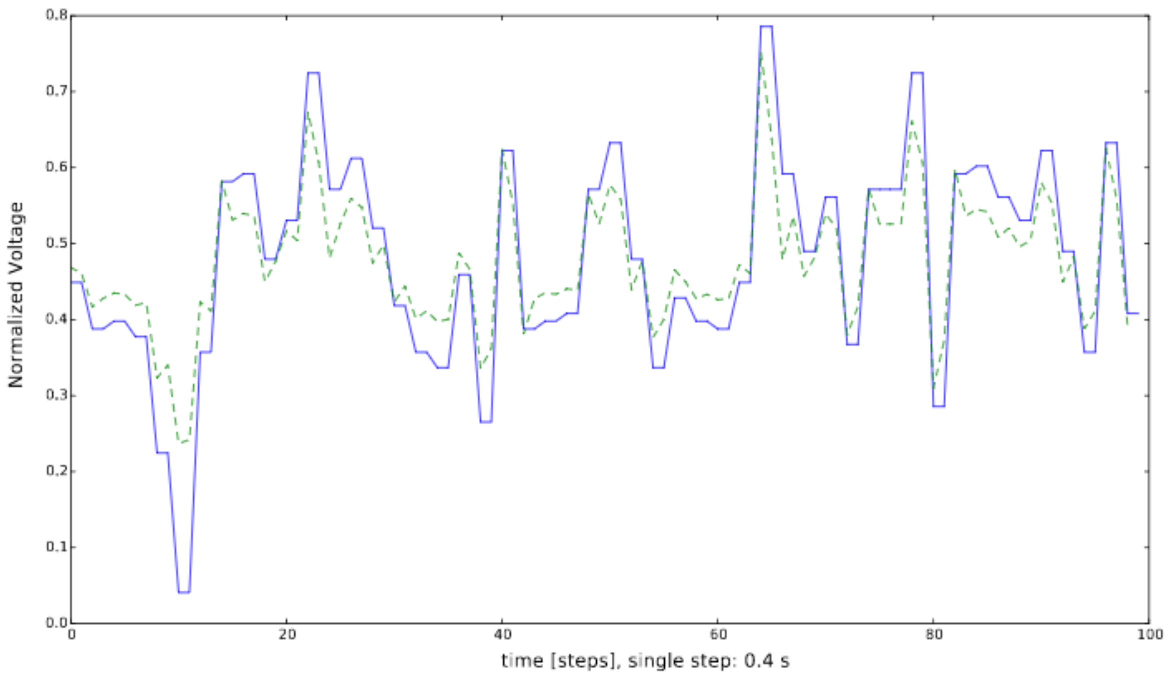
"Some of the most dangerous malfunctions of the magnets are quenches which occur when a part of the superconducting cable becomes normally-conducting."

Aim: use a recurrent NN to identify quench precursors in voltage time series.

→ ***Predict future behavior, then classify it***

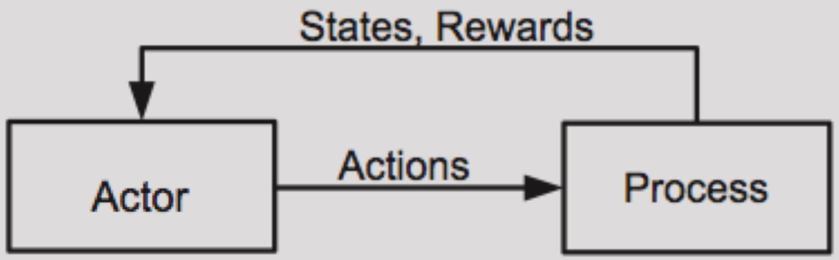
Initial study with small data set:

- 425 quenches for 600 A magnets
- Used archived data from 2008 to 2016
- 16-32 previous values → predict a few time steps ahead



Neural Network Policies and Reinforcement Learning

Actor-only Methods

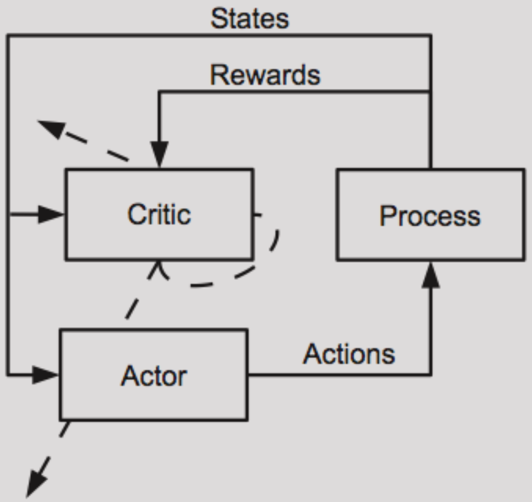


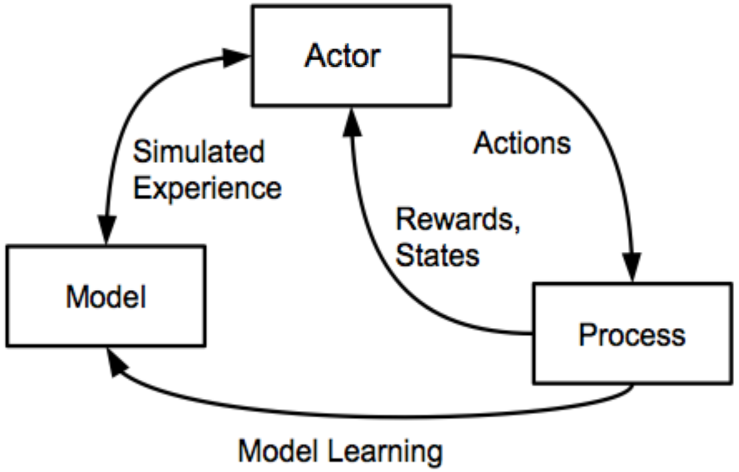
- Actor is a control policy
- Maps states to actions
- Reward provides training signal

Actor-Critic Methods

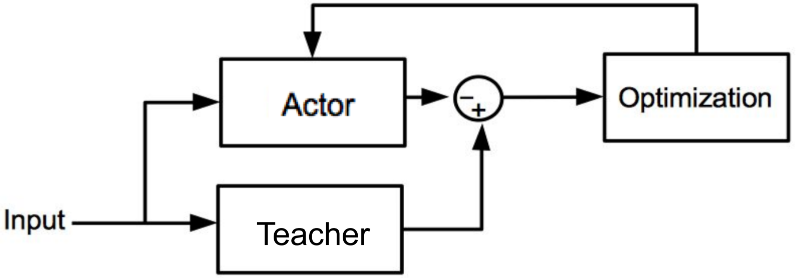
- Critic maps states or state/action pairs to an estimate of long-term reward
- Could be a NN, tabular, etc.
- Critic provides training signal to actor

Without actor: use an optimization algorithm with the critic





Can train on models first to get a good initial solution before deployment

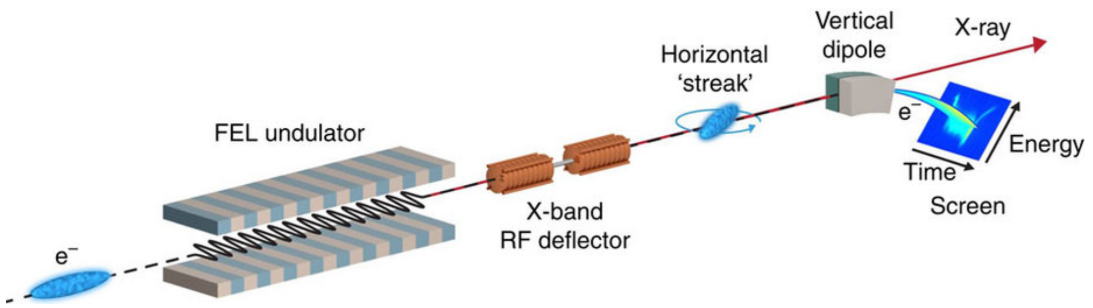


Can use supervised learning to first approximate the behavior of a different control policy

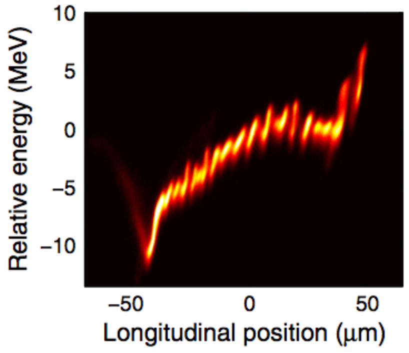
Computer Vision + Neural Network-based RL

- **Image diagnostics** → would be nice to use directly, and some yield relatively complicated information

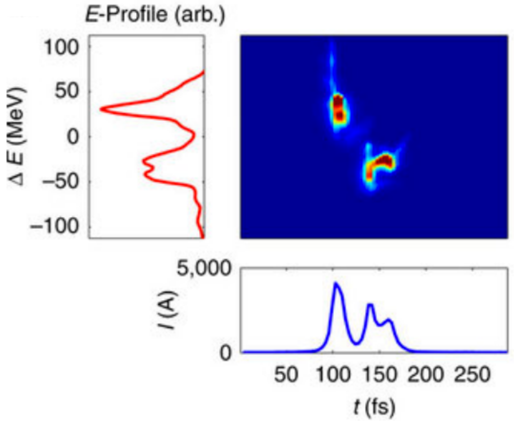
  e.g. XTCAV at SLAC



C. Behrens, et al., Nat. Commun. **5**, 3762 (2014)



D. Ratner, et al., PRSTAB18, 030704 (2015)



A. Marinelli, et al., Nat. Commun. **6**, 6369 (2015)

- **Convolutional Neural Networks (CNNs)** → very good at image processing

- **Reinforcement Learning (RL)** → can learn control policies from data

Why not try using image based diagnostics directly in learned control policies?

What's a relatively simple test case to start with?

Initial Study at FAST/IOTA

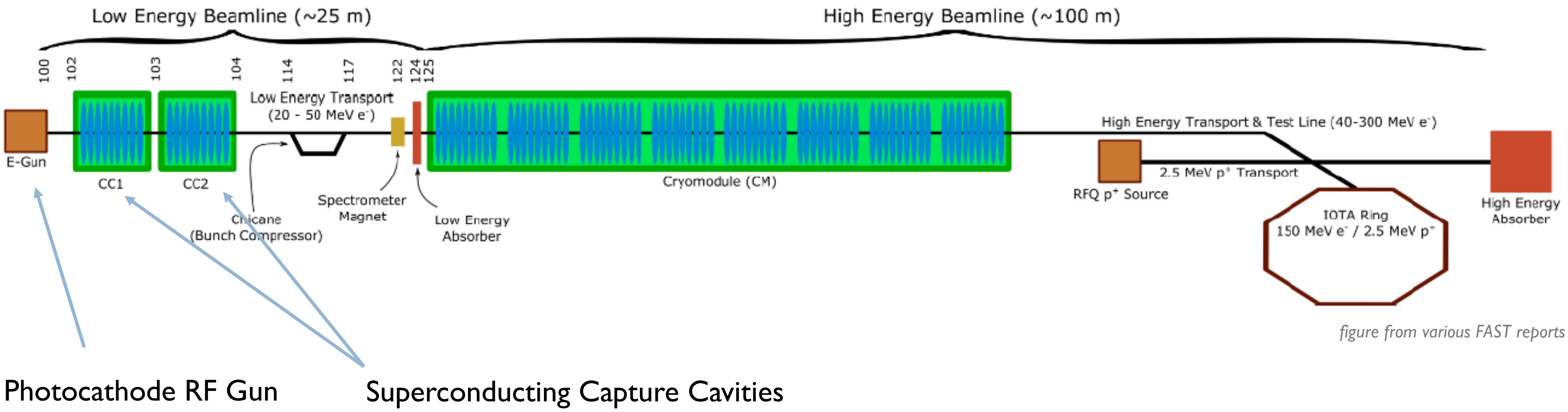


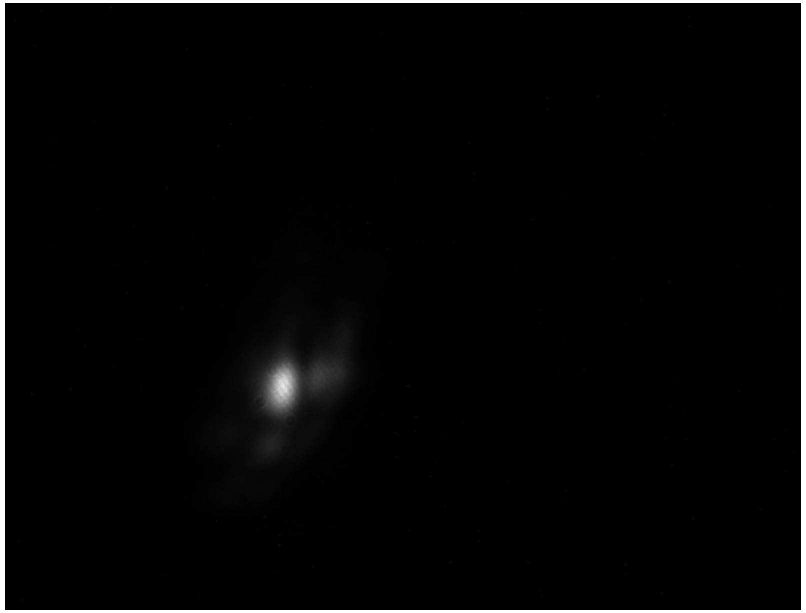
figure from various FAST reports

Initial work with J. Edelen and D. Edstrom, FNAL

Initial Study: Choose Gun Parameters Based on Laser Spot

Motivation:

- Gun phase and solenoid strength tuned daily
- Asymmetries in initial laser distribution result in emittance asymmetries downstream
- Would be nice to obtain optimal gun phase and solenoid strength for a given initial laser distribution automatically (and perhaps prioritize x or y emittance to minimize)



Example virtual cathode image (10 Aug. 2016)

Other perks:

- PARMELA simulation based on survey data already in existence (J. Edelen)
- Try out creating a fast NN modeling tool from slower-executing simulations

Initial Study: Choose Gun Parameters Based on Laser Spo

Motivation:

- Gun phase and sole
- A
- V
  s
  di
  x

Othe

- PAR ... already in existence (J. Edelen)
- Try c ... NN modeling tool from slower-executing simulations

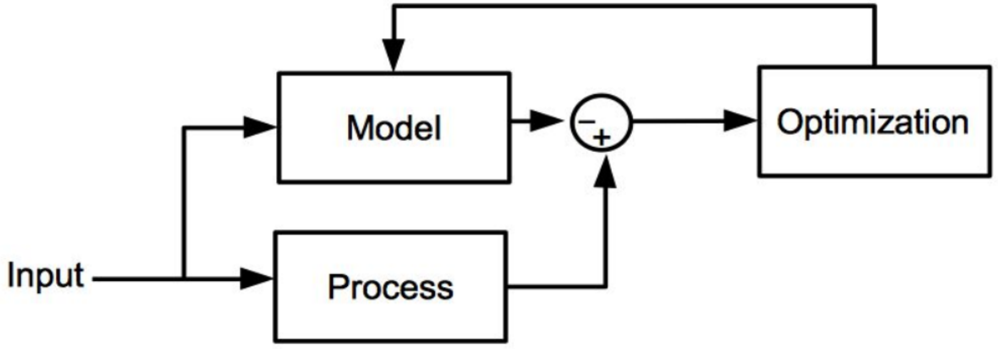
Why not just use online optimization?

Why not just fit a Gaussian to the laser spot to get the information instead of using images directly?

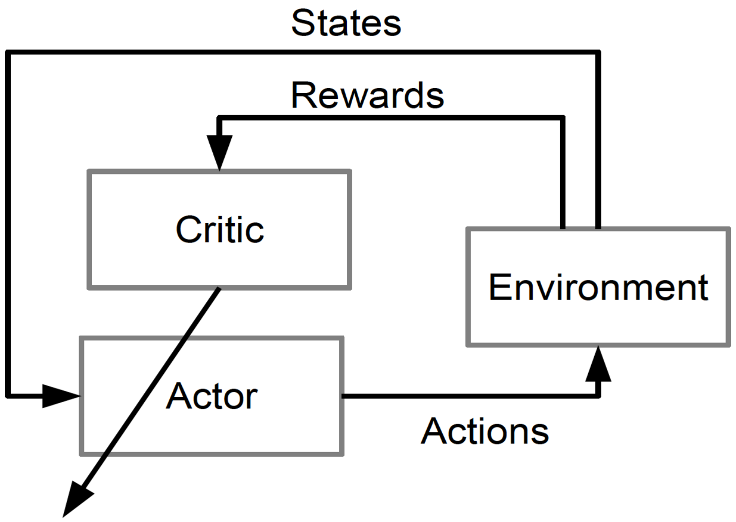
The point of this study: explore this approach on a simple system (it's a stepping stone)

Initial Study: Steps

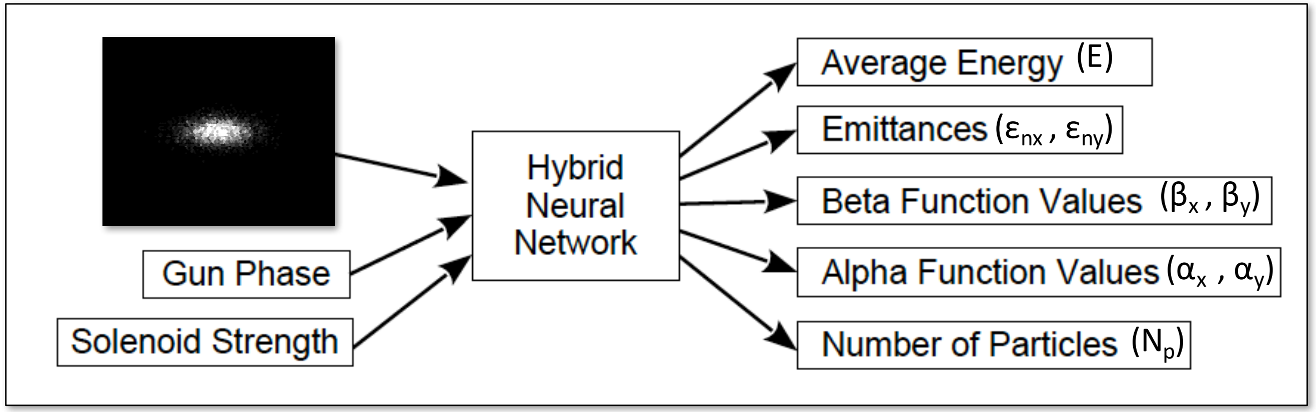
- Gather simulation data from PARMELA scans
- Create a NN model
  - Be certain that the necessary information can be extracted from the image, gun phase, and solenoid strength
- Train a RL controller using that model
- Extension beyond simulation (tentative):
  - Incorporate measured data into model and update controller
  - Carefully test on machine



Model Learning



Policy Learning



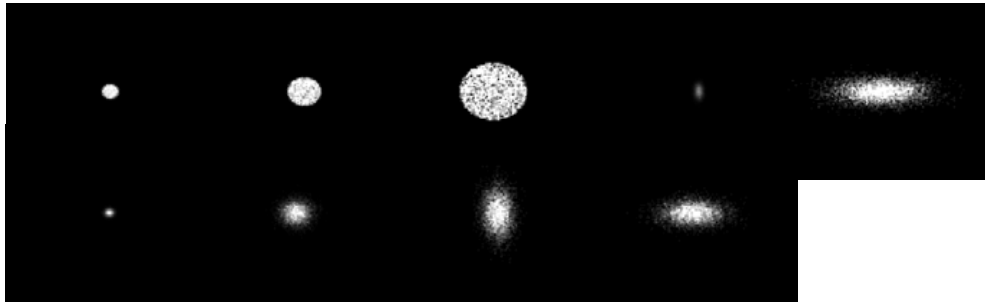
model inputs and outputs

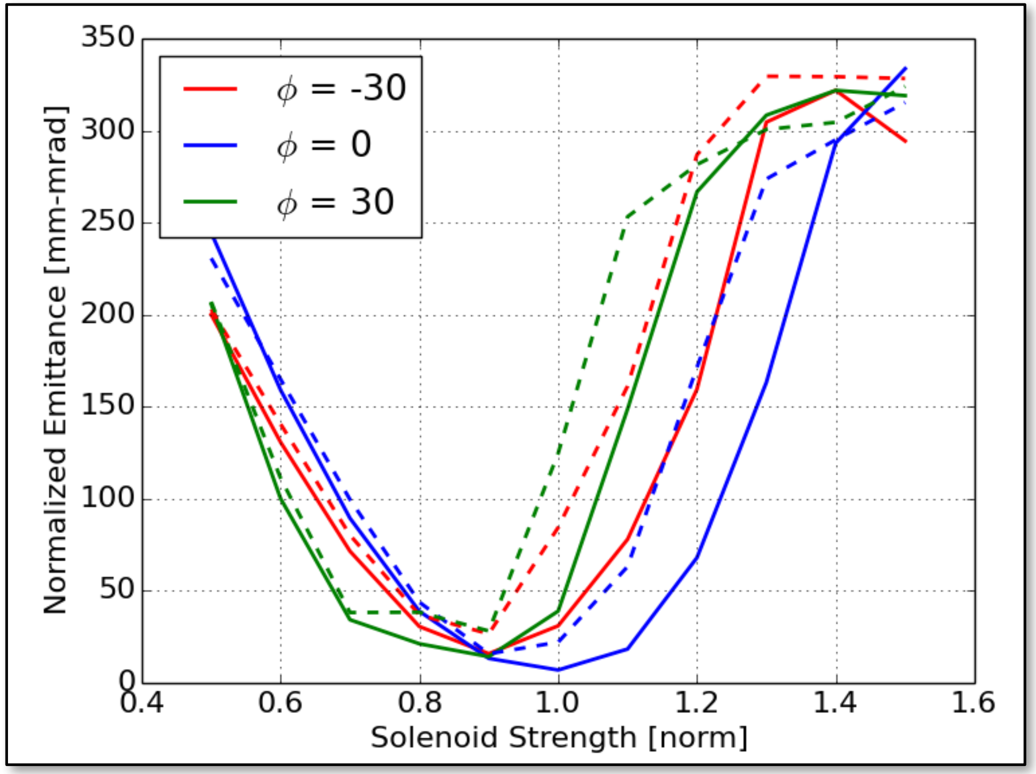
CNN Model: Simulation Data

- PARMELA simulations from the gun up to the exit of CC2
  - 2-D space charge routine
  - Scanned gun phase, solenoid strength, initial beam distribution

- Two sets of data:
  - Fine scans (steps of 5° phase, 5% sol. str.) for sims just past the gun
  - Coarse scans (steps of 10° phase, 10% sol. str.) for sims up through CC2

- Simulated "virtual cathode images"
  - Going from VCI → initial beam distribution ok from prior work
  - Initial beam distribution → simulated VCI probably ok
  - Obviously very "well-behaved" examples





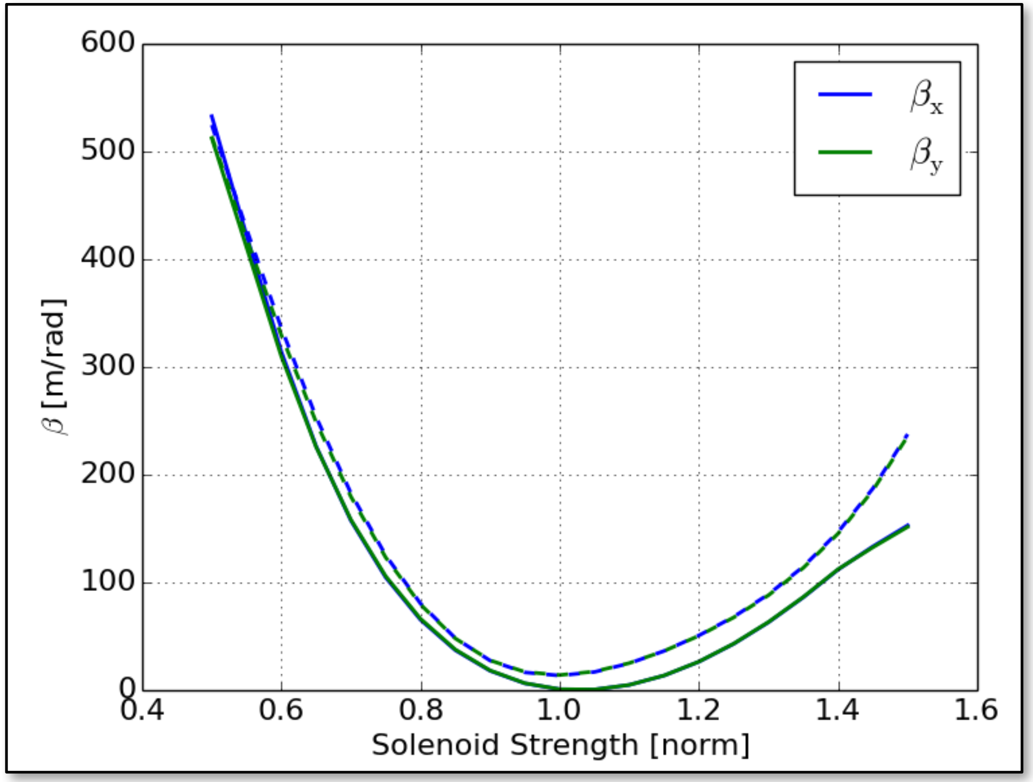
Simulation predictions after CC2. Dashed lines are x-emittance, solid lines are y-emittance.

Caveat: doesn't take into account coupling…later changed NN setup to predict sigma matrix, and also used a 3D space charge routine.

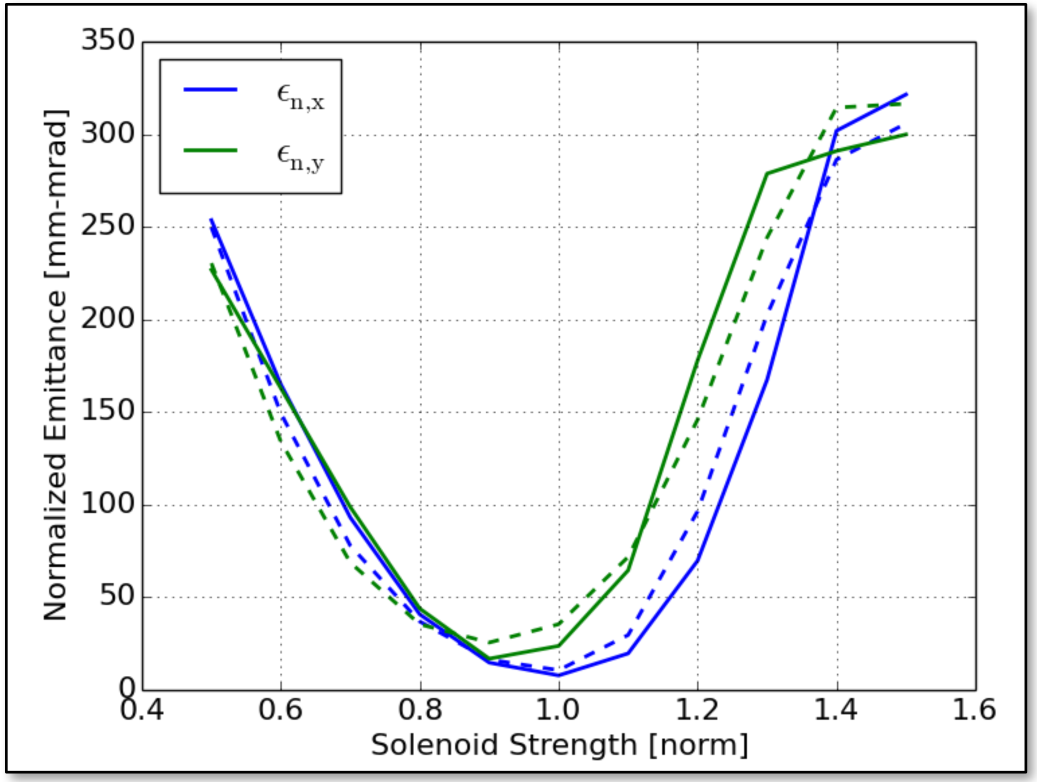
For normalized sol strength, 1 is the setting that produces a peak axial field of 1.8 kG

CNN Model: Two Representative Plots

Dashed lines are NN predictions and solid lines are simulation results



Top-hat initial beam, 0° RF phase, after gun



Asymmetric Gaussian initial beam, 0° RF phase, after CC2

For the gun data, all MAEs are between 0.4% and 1.8% of the parameter ranges.
For the CC2 data, all MAEs are between 0.9% and 3.1% of the parameter ranges.

→ *Not bad for such a small training set*

Fast Switching Between Trajectories

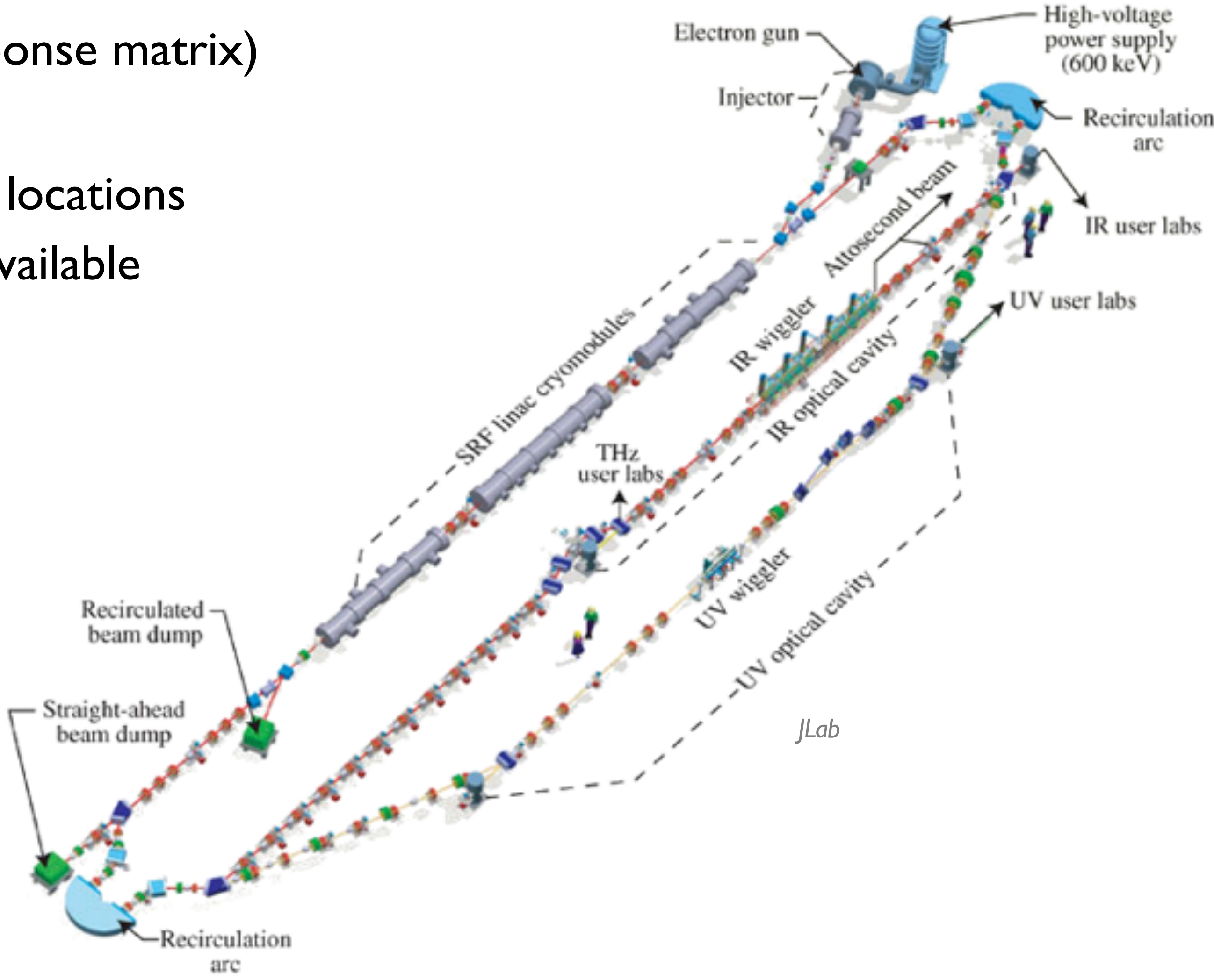
Work with C. Tennant and D. Douglas, JLab

- 76 BPMs, 57 dipoles, 53 quadrupoles
- Traditional approach has never worked (linear response matrix)
- Rely on one expert for steering tune-up
- Want to specify small offsets in trajectory at some locations
- Didn't initially have an up-to-date machine model available

Learn responses (NN model) from tune-up data and dedicated study time:
dipole + quadrupole settings → predict BPMs

Train controller (NN policy) offline using NN model:
desired trajectory → dipole settings
(and penalize losses + large magnet settings)

Test on machine: check to make sure model prediction still accurate and try static controller (non-adaptive)



JLab

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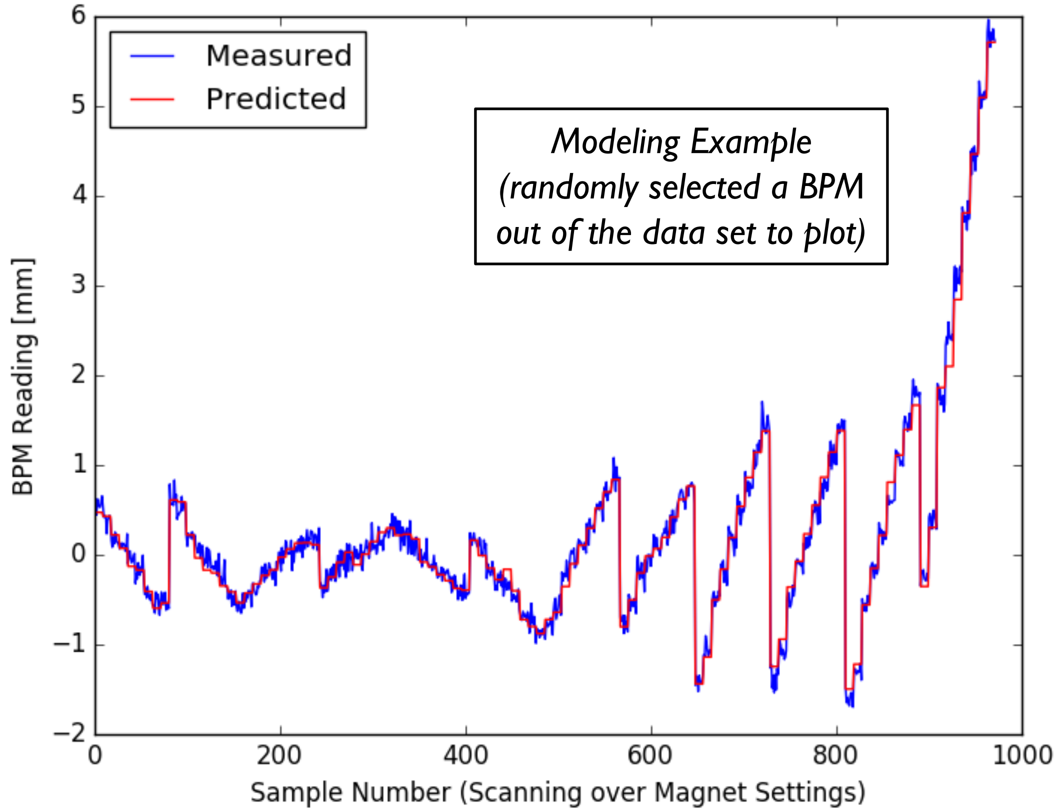
(Very) Preliminary Results:

Model Errors for BPMs:

Training Set:	0.07 mm MAE	0.09 mm STD
Validation Set:	0.08 mm MAE	0.07 mm STD
Test Set:	0.08 mm MAE	0.03 mm STD

Controller: random initial states → on average within 0.2 mm of center immediately



Fast Switching Between Trajectories

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- Want
- Didn

Learn
dedica
dipole

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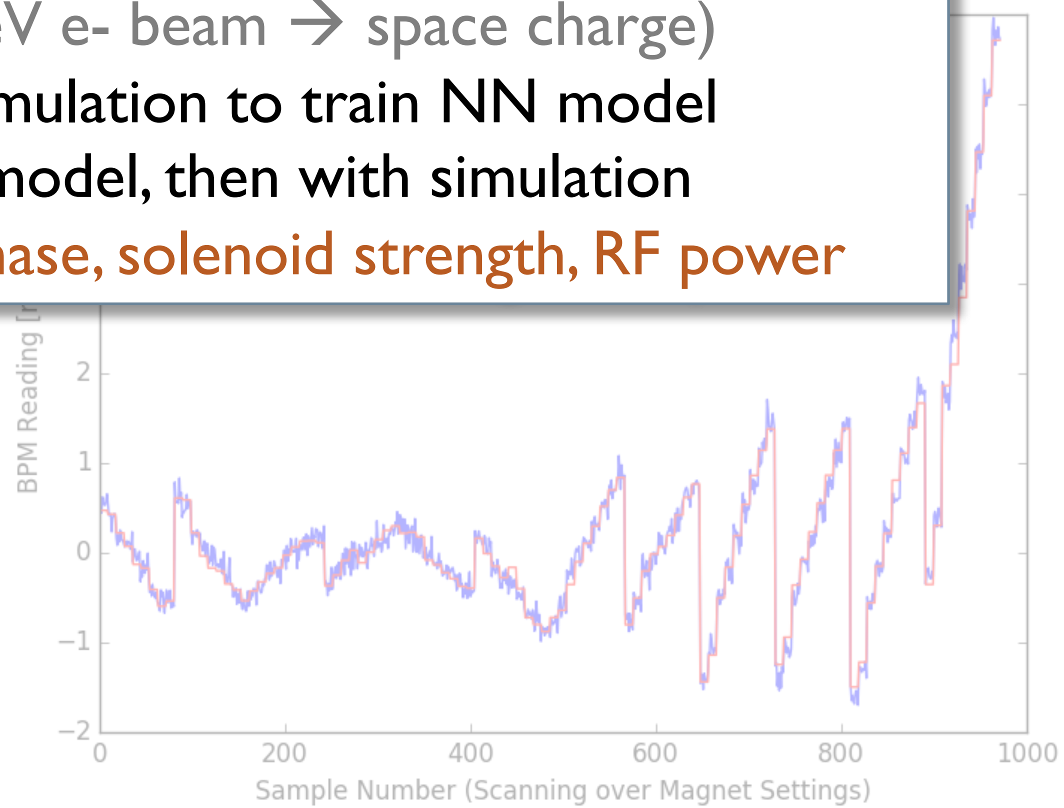


Similar Kind of Task: switching between FEL frequencies (in progress)
→ simulation study with CSU FEL (3 – 6 MeV e- beam → space charge)
→ use optimization iteration output from simulation to train NN model
→ train controller via interaction with NN model, then with simulation
→ given target wavelength: set quads, gun phase, solenoid strength, RF power

Final Notes: Some Practical Challenges

*large enough parameter range and set of examples to generalize well and complete the task

*you can trust it

Need a sufficient amount of reliable* data*

(but not as much as is sometimes claimed in DL)

Training on Measured Data

Undocumented manual changes (e.g. rotating a BPM)

Relevant-but-unlogged parameters

Availability of diagnostics

Observed parameter range in archived data

Time on machine for characterization studies (schedule + expense)

Ideal case:
- *comprehensive, high-resolution data archive*
- *excellent log of manual changes*

Training on Simulation Data

How representative of the real machine behavior?

High-fidelity (e.g. PIC) → time-consuming to run

Input/output parameters need to translate directly to what's on the machine (quantitatively)

Retention + availability of prior results: (*optimize and throw the iterations away!*)

Deployment

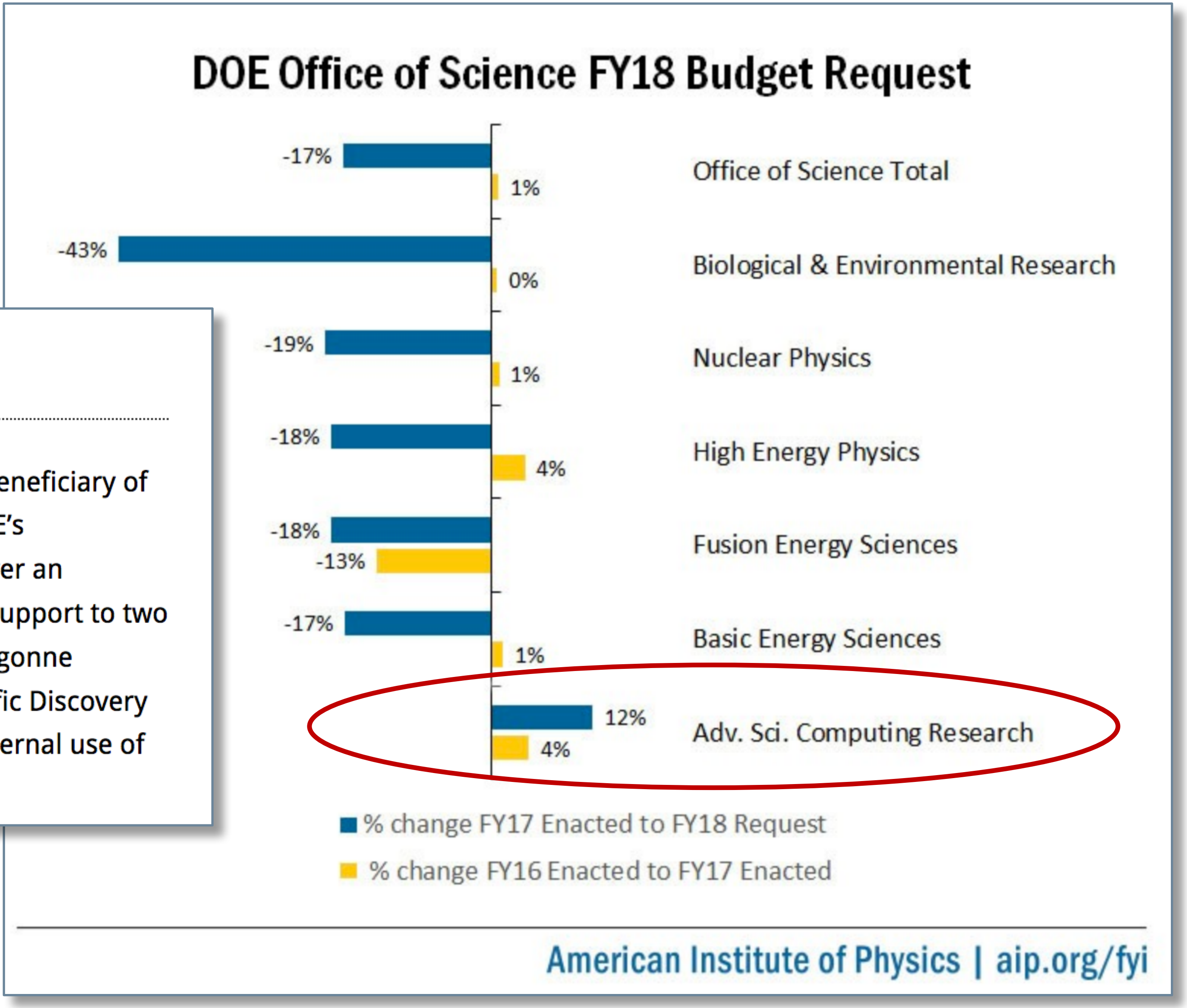
Initial training is on HPC systems → deployment is typically not*
- Execution on front-end: necessary speed + memory?
- Subsequent training: on front-end or transfer to HPC?

Software compatibility for older systems: interface with machine + make use of modern ML software libraries

I/O for large amounts of data

* for now…

Final Notes: Funding Climate



Advanced Scientific Computing Research

Advanced Scientific Computing Research stands out as the primary beneficiary of the Office of Science budget. Its budget includes $347 million for DOE's contribution to the interagency Exascale Computing Initiative to deliver an exascale-capable computing system by 2021. It would also increase support to two of DOE's three Leadership Computing Facilities – at Oak Ridge and Argonne National Laboratories. An additional increase would grow the Scientific Discovery through Advanced Computing (SciDAC) program, which facilitates external use of DOE supercomputers.

Final Notes

- Neural networks are very flexible tools → far more powerful in recent years
- Mostly preliminary results so far, but making progress (+ more infrastructure in place)
- Lots of opportunities to use neural networks (and ML more broadly) to improve accelerator performance on both existing and future machines

Fermilab has a strong presence in machine learning (especially for neural networks/HEP)

Lots of potential for fruitful collaborations on the accelerator side

→ *LBNL, SLAC, LANL, CERN all interested in applying ML to accelerator modeling/controls*

Some possible experiments at Fermilab:

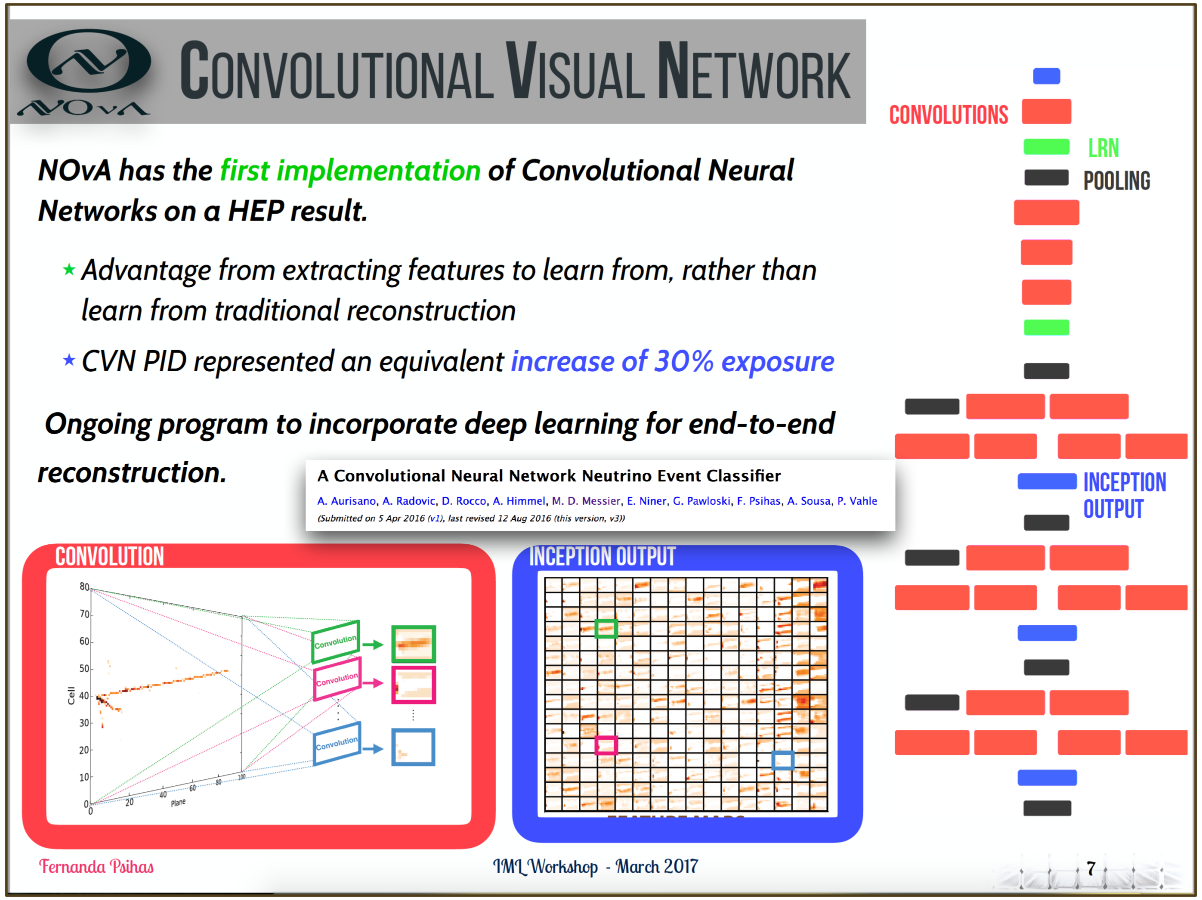
- Ion sources (MPC/RL)
- Cryogenic system control (MPC/RL)
- Fermi Test Beam Facility (fast switching)
- Muon Campus (virtual diagnostics, online modeling)
- Phase space manipulations at FAST (fast switching)

Thanks for your attention!

Final Notes: Fermilab has a strong presence in machine learning (especially for DL/HEP)

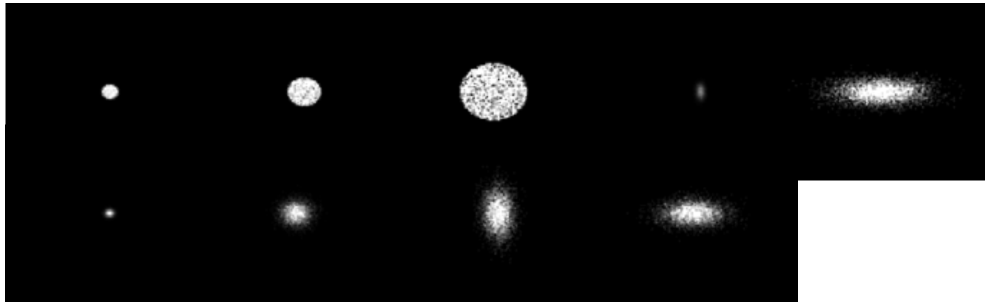
- See Fernanda Psihas New Perspectives 2017 talk
- Ramping up HPC resources
- Slack channel: https://hepmachinelearning.slack.com
- Journal Club meetings
- Monthly Intro meetings
- Website: http://machinelearning.fnal.gov/

CNN Applications for HEP
June 9th
10:30 AM, One West



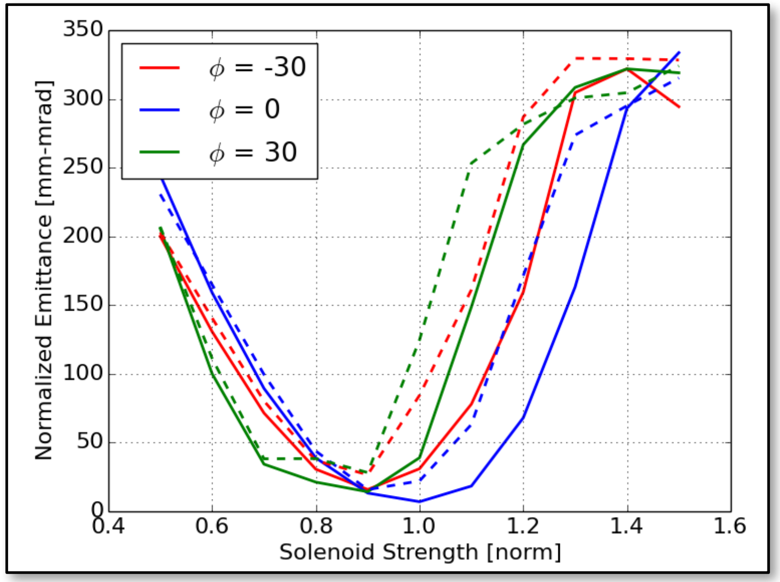
CNN Model: Simulation Data

- PARMELA simulations from the gun up to the exit of CC2
  - 2-D space charge routine
  - Scanned gun phase, solenoid strength, initial beam distribution
- Two sets of data:
  - Fine scans (steps of 5° phase, 5% sol. str.) for sims just past the gun
  - Coarse scans (steps of 10° phase, 10% sol. str.) for sims up through CC2
- Simulated "virtual cathode images"
  - Going from VCI → initial beam distribution ok from prior work
  - Initial beam distribution → simulated VCI probably ok
  - Obviously very "well-behaved" examples



Parameter Ranges used for Model Training

Parameter	Gun Data		CC2 Data	
	Max Value	Min Value	Max Value	Min Value
N_p	5001	1015	5001	1004
ε_{nx} [m-rad]	2.50E-04	1.60E-06	4.00E-04	9.10E-07
ε_{ny} [m-rad]	2.40E-04	1.60E-06	4.00E-04	8.50E-07
α_x [rad]	14.1	-775.1	0.8	-149.8
α_y [rad]	14.5	-797	0.7	-154.5
β_x [m/rad]	950.4	7.90E-02	820.2	0.7
β_y [m/rad]	896.8	8.40E-02	845.7	0.81
E [MeV]	4.6	3.2	47.2	42.8



Simulation predictions after CC2. Dashed lines are x-emittance, solid lines are y-emittance.

Caveat: doesn't take into account coupling…later changed NN setup to predict sigma matrix, and also used a 3D space charge routine.

For normalized sol strength, 1 is the setting that produces a peak axial field of 1.8 kG

CNN Model: Performance

Parameter	Train. MAE	Train. STD	Val. MAE	Val. STD
N_p	69.5	79.8	70.7	75.7
ε_{nx}	2.30E-06	3.50E-06	2.40E-06	3.20E-06
ε_{ny}	2.30E-06	3.40E-06	2.40E-06	3.20E-06
α_x	9	14.9	10.9	16
α_y	8.8	15.3	10.8	16.1
β_x	12.1	17.6	14.8	18.9
β_y	11.7	16.7	14.3	17.9
E	4.90E-03	4.90E-03	5.50E-03	6.00E-03

Performance for the predictions after the gun

Parameter	Train. MAE	Train. STD	Val. MAE	Val. STD
N_p	103.7	141.2	123.3	176.8
ε_{nx}	1.00E-05	1.20E-05	1.20E-05	1.60E-05
ε_{ny}	1.00E-05	1.30E-05	1.20E-05	1.50E-05
α_x	3.4	6.6	3.1	5.9
α_y	3.4	6.6	3.1	5.9
β_x	16.3	33.5	14.7	27.8
β_y	16.4	33.6	14.8	27.5
E	4.00E-02	3.90E-02	4.60E-02	6.20E-02

Performance for the predictions after CC2

For the gun data, all MAEs are between 0.4% and 1.8% of the parameter ranges.
For the CC2 data, all MAEs are between 0.9% and 3.1% of the parameter ranges.

→ Not bad for such a small training set

Present Status and Next Steps

- **Improving the quality of the setup:**
  - Predicting the full sigma matrix
  - More realistic initial distributions
  - Using 3D space charge routine
  - Using locally-connected layers
  - Switching to ASTRA

    (greater execution speed → more training data)

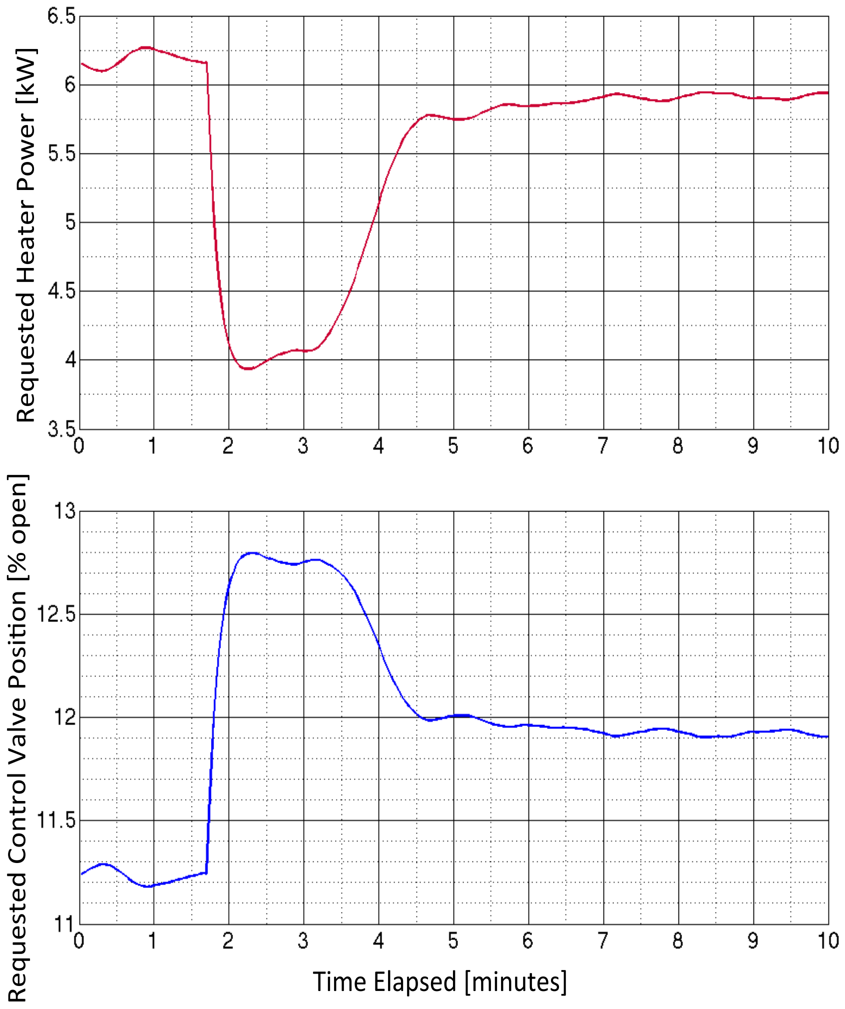
- **Expanding scope to phase space manipulations:**
  - Specify a target sigma matrix
  - Include quads after CC2, capture cavity phases, etc.
  - Collaborating with NIU:
    - RTFB transform is a possible application
    - Alex Halavanau running simulation scans with NIU's newer model → more training data

- **Next steps (in tandem):**
  - Finish simulation study with present setup
  - Extend to phase space manipulation simulation study
  - Solidify plans for incorporating measured data and testing controller
    - Need to align available inputs/controllable variables (e.g. sigma matrix vs. info from emittance monitors, rotation of quads, etc.)
    - Also depends on run schedule, status of new emittance monitors, solid time with consistent setup, etc.

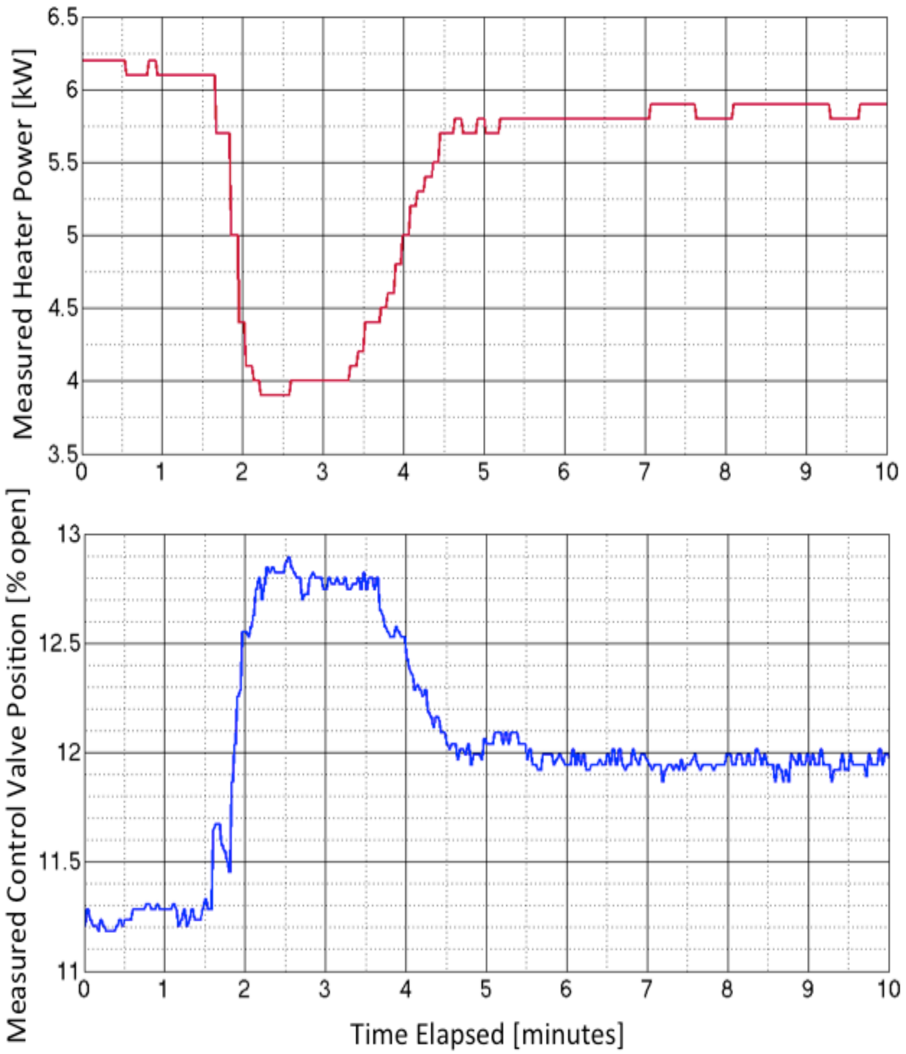
Also, if you have some other possible application and have or can easily obtain training data: don't hesitate to get in touch!

MPC Benchmark Controller: Actions

Requested by Controller



Actual Read-backs



Could optimize for lower heater power

Backpropagation

Vectorized notation: $a_j = f\left(\sum_k w_{jk} x_k + b_j\right) \rightarrow f(wx + b)$

Layer-by layer: $a^l = f\left(w^l a^{l-1} + b^l\right) = f(z^l)$

a_j j^{th} node activation

b_j j^{th} node bias

w_{jk} j^{th} node in layer l, k^{th} node in $l-1$

f applied element-wise

$$\delta_j^l \equiv \frac{\partial C}{\partial z_j^l}$$

$$\delta_j^{N_l} = \frac{\partial C}{\partial a_j^{N_l}} f'(z_j^{N_l}) \quad \rightarrow \quad \delta^{N_l} = \nabla_a C \odot f'(z^{N_l})$$

$$\delta_j^l = \sum_k \frac{\partial C}{\partial z_k^{l+1}} \frac{\partial z_k^{l+1}}{\partial z_j^l} = \sum_k \delta_k^{l+1} \frac{\partial z_k^{l+1}}{\partial z_j^l}$$

$$= \sum_k w_{kj}^{l+1} \delta_k^{l+1} f'(z_j^l)$$

$$z_k^{l+1} = \sum_j w_{kj}^{l+1} a_j^l + b_k^{l+1}$$

$$= \sum_j w_{kj}^{l+1} f(z_j^l) + b_k^{l+1}$$

$$\frac{\partial z_k^{l+1}}{\partial z_j^l} = w_{kj}^{l+1} f'(z_j^l)$$

For each training instance:

1. **Forward Pass:**

   For l = 1, 2, 3 … N_l

   $$z^l = w^l a^{l-1} + b$$

   $$a^l = f(z^l)$$

2. **'Error':**

   $$\delta^{N_l} = \nabla_a C \odot f'(z^{N_l})$$

3. **Backward Pass:**

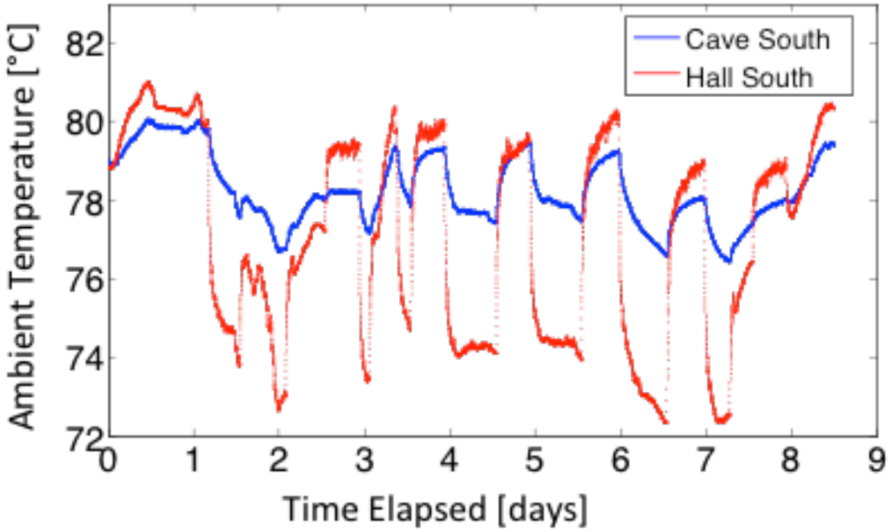
   For l = $N_l - 1, N_l - 2, \ldots 1$

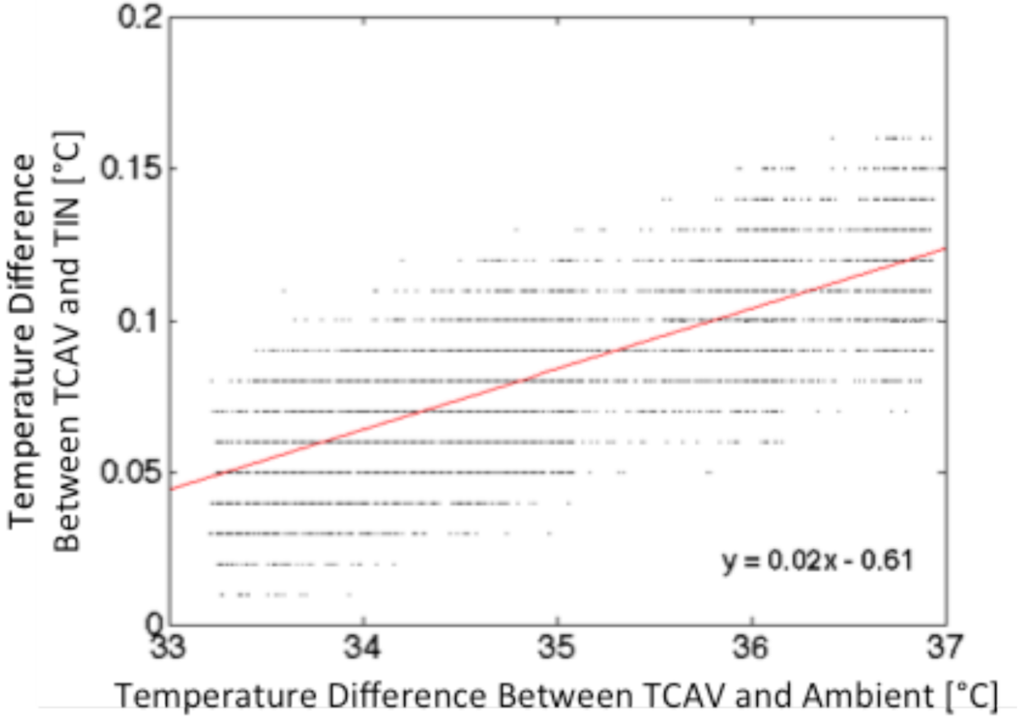
   $$\delta^l = w^{l+1} \delta^{l+1} \odot f'(z^l)$$

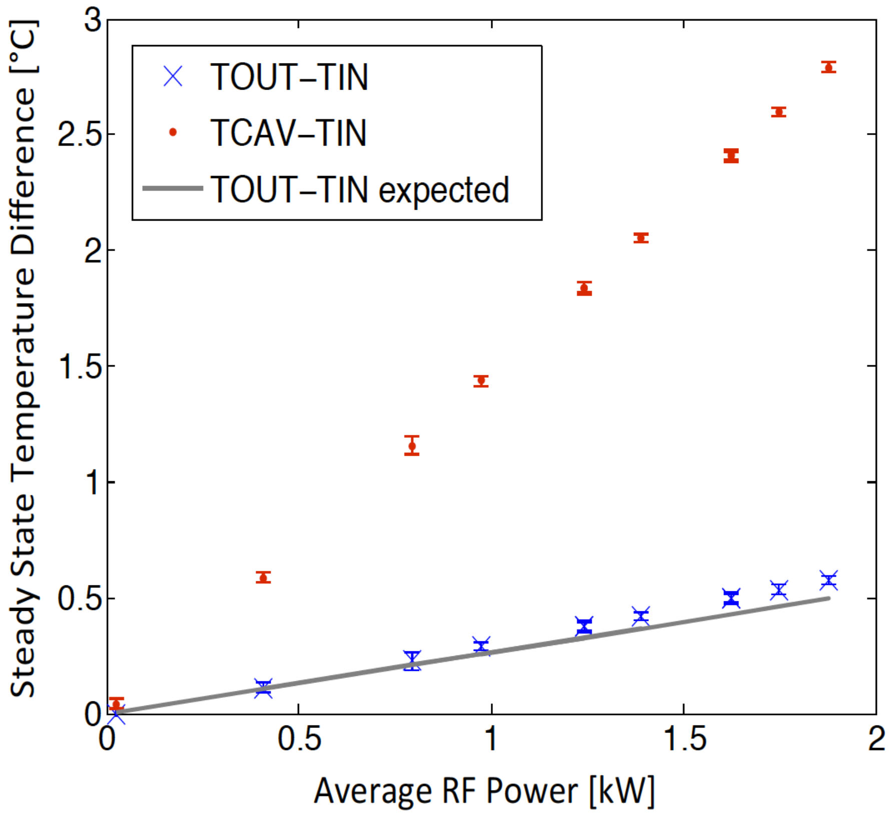
4. **Final Derivatives:**

   $$\frac{\partial C}{\partial w_{jk}^l} = a_k^{l-1} \delta_j^l \qquad \frac{\partial C}{\partial b_j^l} = \delta_j^l$$

FAST Gun Temperature Considerations





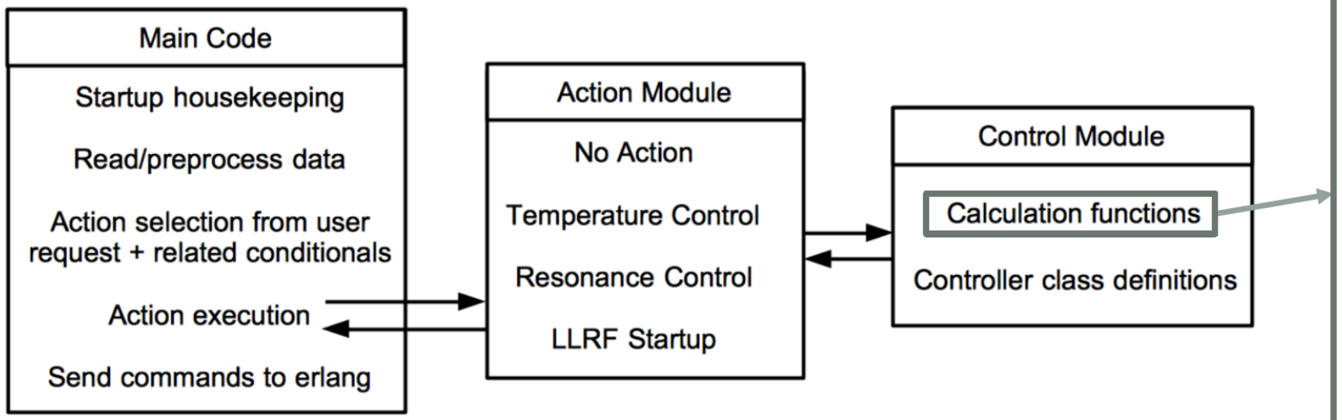


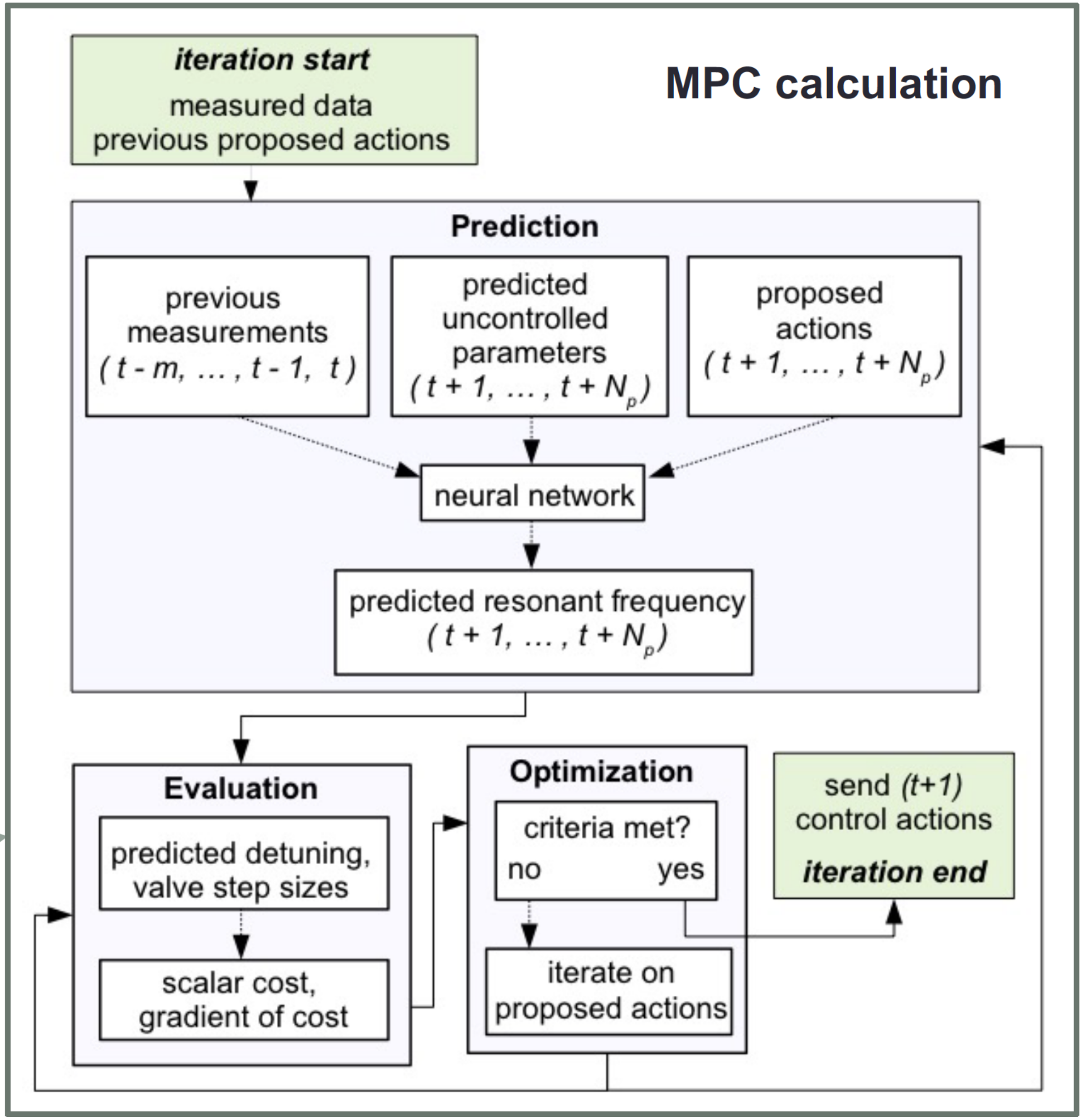
$$P_{cool} = \frac{(T_{OUT}[°C] - T_{IN}[°C]) \times (Flow\ [GPM])}{Water\ Cooling\ Capacity\ \left[\frac{GPM-°C}{kW}\right]}$$

$$P_{cool} = P_{IN} \approx P_{RF_{avg.}}$$

In the resonance control framework

- N_p future time steps
- *m* previous measurements for each input variable
- “actions” are vane and wall flow valve settings

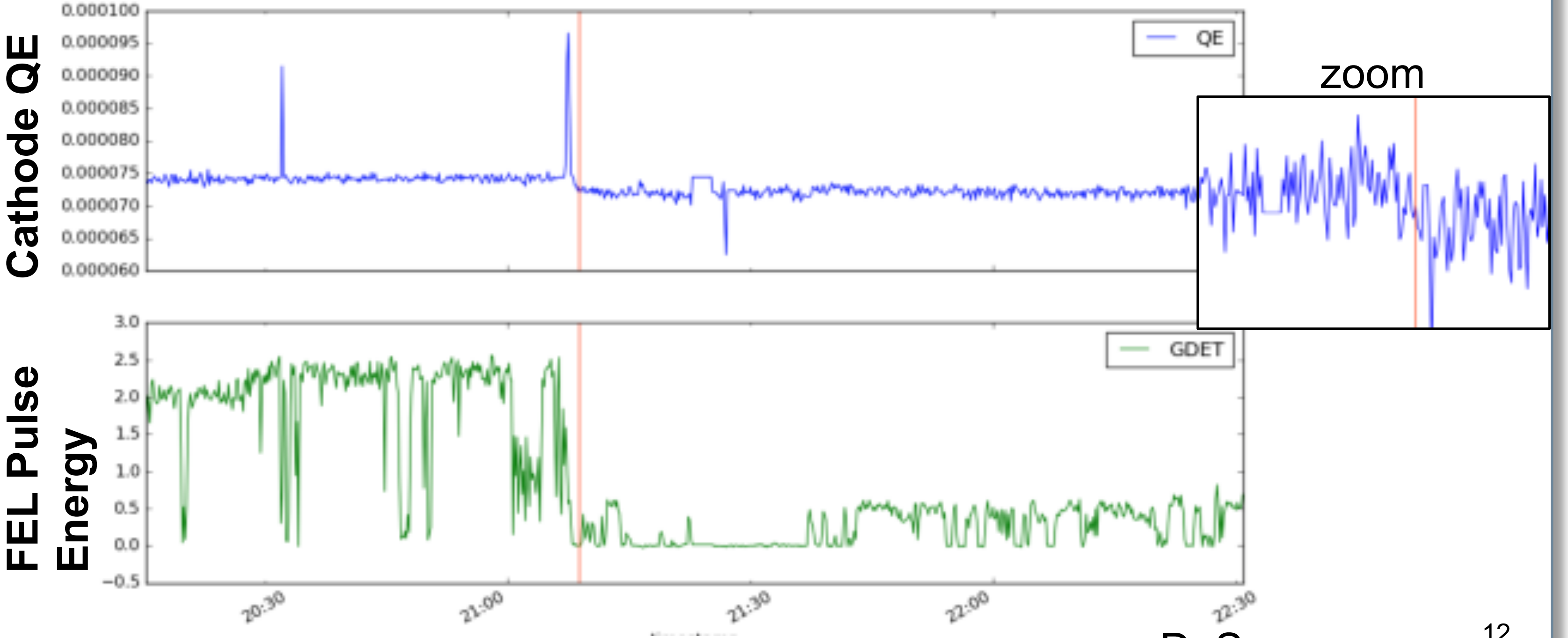




Example from D. Ratner presentation at 2017 DS@HEP:

Cathode QE drop caused hours of downtime.

Breakout detection (Twitter algorithm) would have found change immediately!

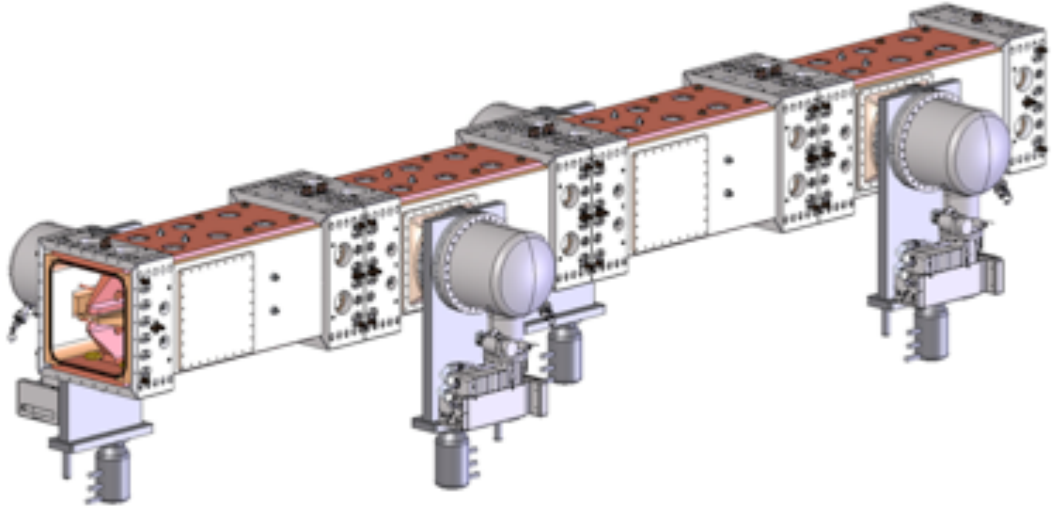


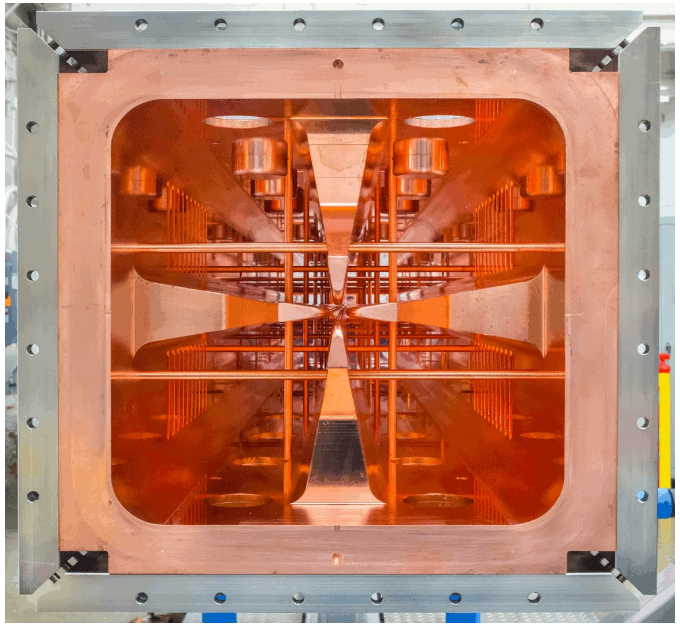
D. Sanzone

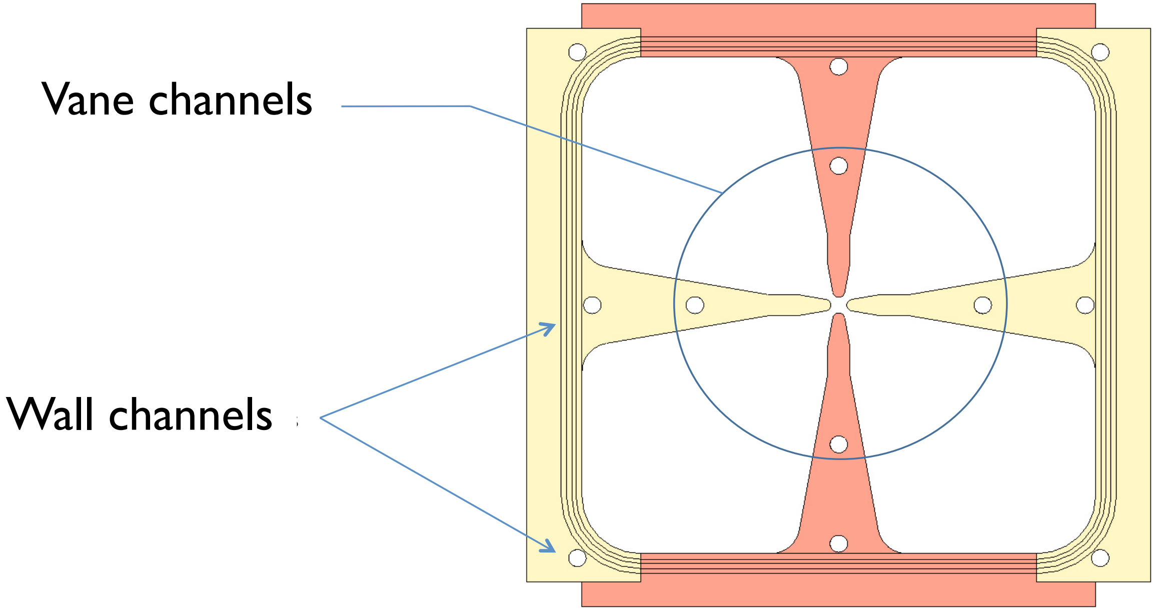
PXIE RFQ

3-kHz max. freq. shift

0.1-°C water stabilization







All images courtesy LBNL, D. Li, A. Lambert

FAST Photoinjector

RF electron gun at the Fermilab Accelerator Science and Technology (FAST) facility

- — Long, variable time delays
- — Tight tolerances
- — Recursive behavior
- — Two controllable parameters

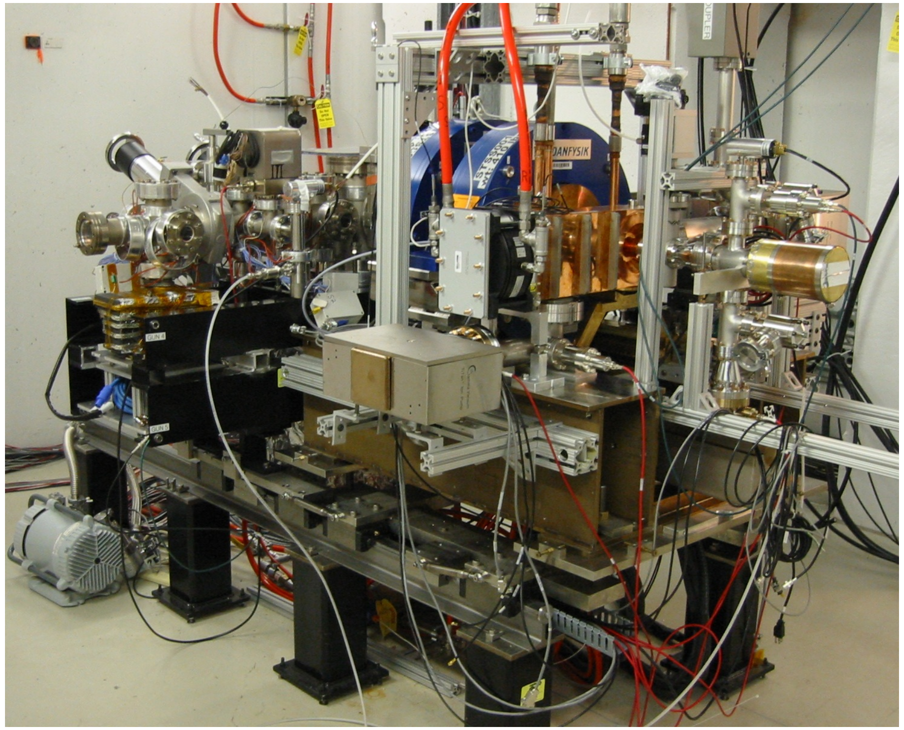


Photo: P. Stabile

FAST RF Gun Parameters	
Gun Parameters	
Type	Photoinjector
Number of cells	1½
RF Mode	$TM_{010,\pi}$
Loaded Q	~11,700
RF Frequency	1.3 GHz
Frequency Shift	23 kHz/°C
Nominal Operating Parameters	
Macropulse Duration	1 ms
Repetition Rate	1–5 Hz
Bunch Frequency	3 MHz
Design Gradient	40–45 MV/m
Power Source	5 MW Klystron

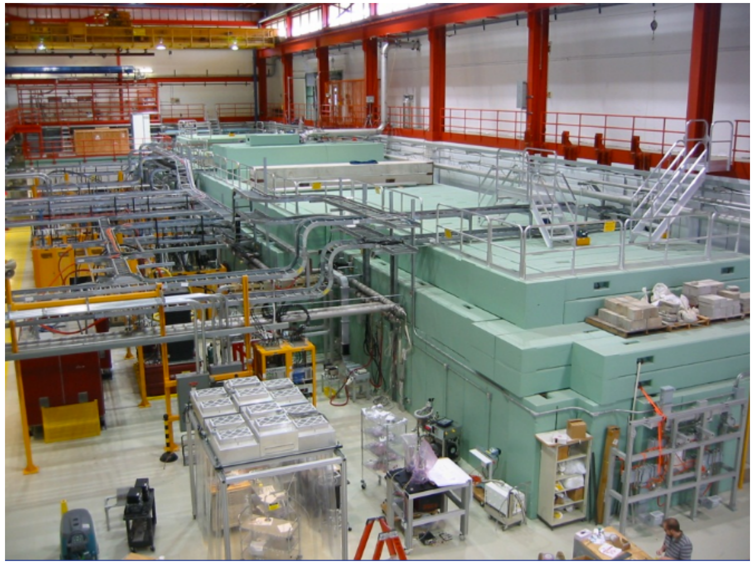


Photo: E. Harms

PIP-II RFQ

Right now: 100s to 5ms pulse at 10 Hz

~100 kW forward RF power

PXIE RFQ Parameters	
RFQ Design Parameters	
RF frequency	162.5 MHz
Q-factor	~13,900
Loaded Q	~7,000
Physical Length	4.45 m (2.4 wavelengths)
Vane-to-Vane Voltage	60 kV
Estimated Power Dissipation	< 100 kW
RF Repetition Rate	pulsed – CW
Beam Parameters	
Current	0.5 – 10 mA (nominal 5 mA)
Input Energy	30 keV
Output Energy	2.1 MeV

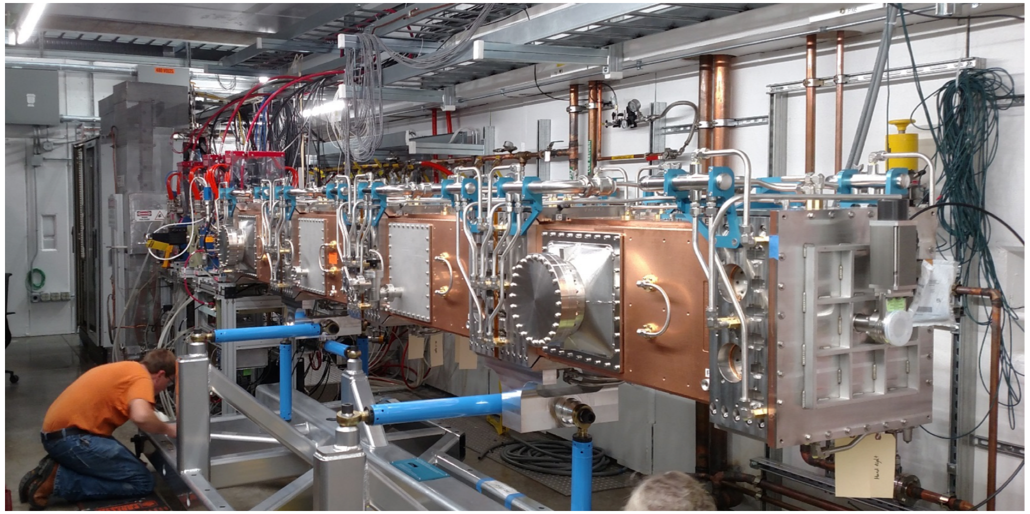
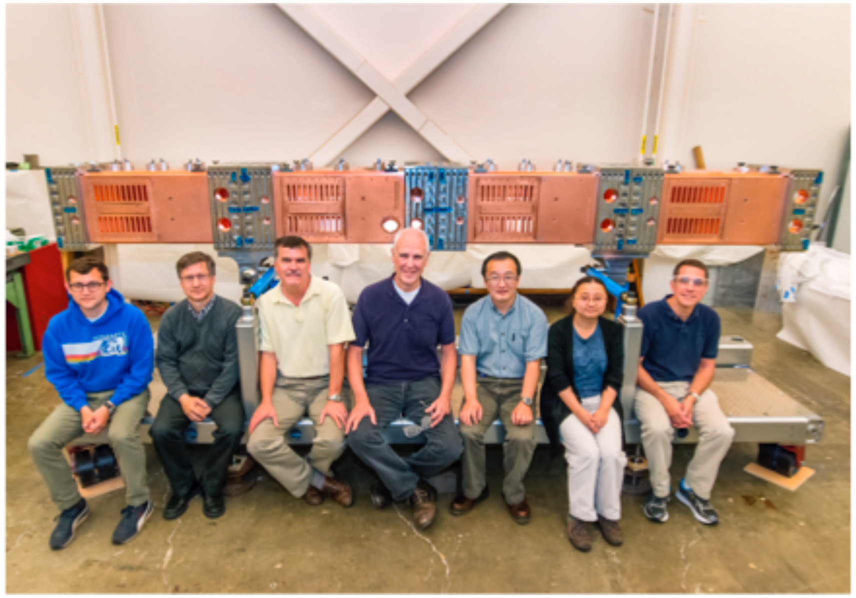


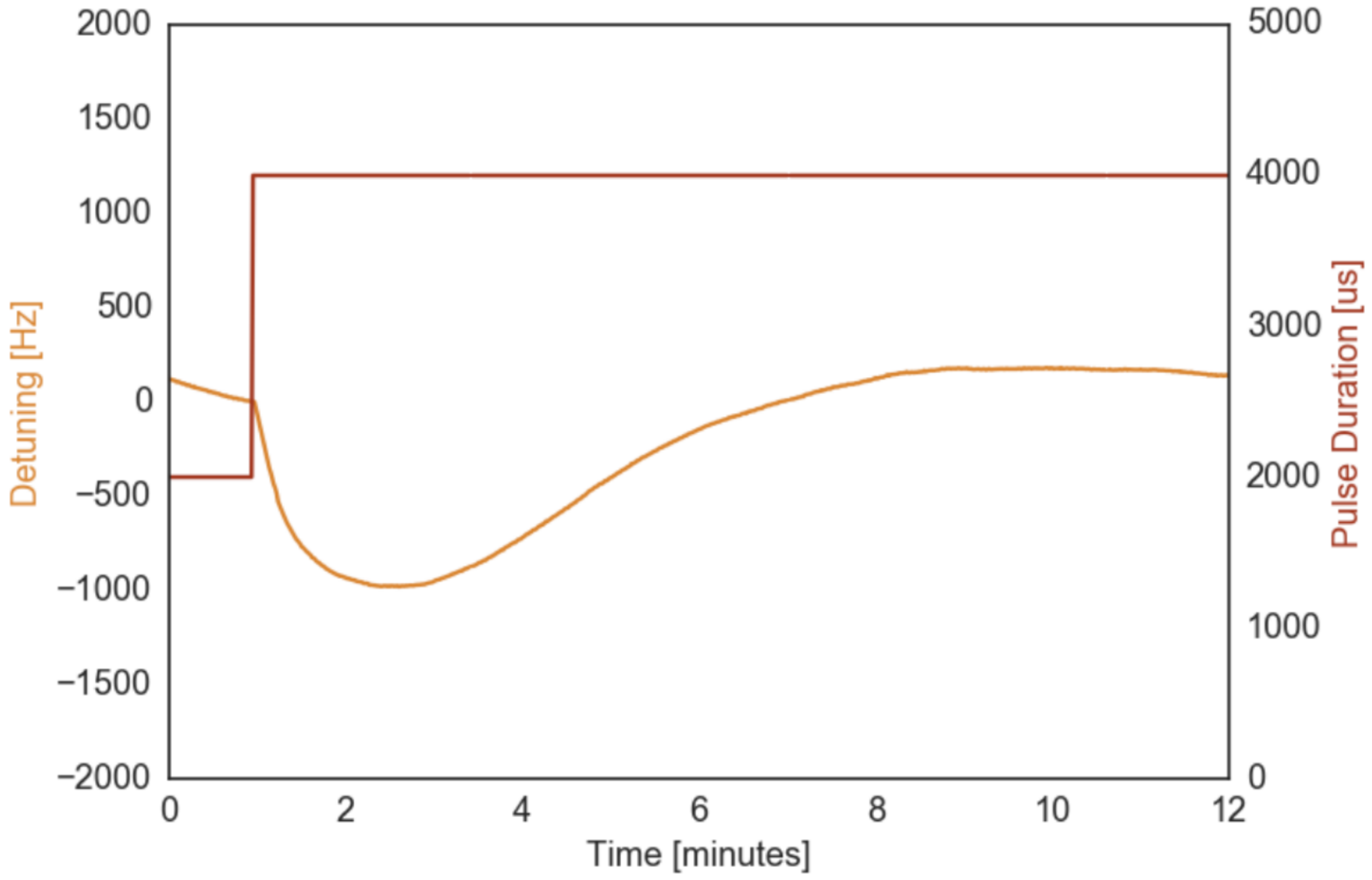
Photo: J. Steimel

Constructed by LBNL



High-intensity RFQ for the PIP-II Injector Experiment (PXIE)

— Time delays
— Large, dynamic frequency response
— Tight tolerances
— Coupling
— Recursive behavior
— Three controllable parameters



PI frequency control during pulsed RF operation for a 2-ms increase in pulse duration and a cavity field of 65 kV