Machine learning-based virtual diagnostic for longitudinal phase space prediction

C. Emma, A. Edelen, M. Alverson, G. White, A. Hanuka, M. J. Hogan, D. Storey, B. O'Shea, A. Scheinker, S. Gessner, A. Lutman, D. Bohler, L. Alsberg, V. Yakimenko

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U.S. DEPARTMENT OF ENERGY

Office of Science

FACET-II

Facility for Advanced Accelerator Experimental Tests

LCLS Linac Coherent Light Source

SLAC NATIONAL ACCELERATOR LABORATORY

Outline

1. ML-based virtual diagnostics - background and motivation

2. Virtual diagnostic examples:
    1. Previous studies at FACET and LCLS
    2. Single bunch simulations for FACET-II & proof-of-concept at LCLS
    3. Two-bunch simulations for FACET-II including TCAV effects

3. Optimization using LPS virtual diagnostics

4. Conclusions, challenges and next steps towards implementation

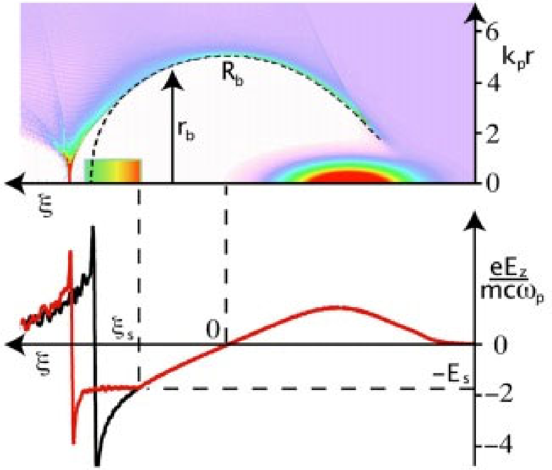
Longitudinal diagnostics for PWFAs/FELs

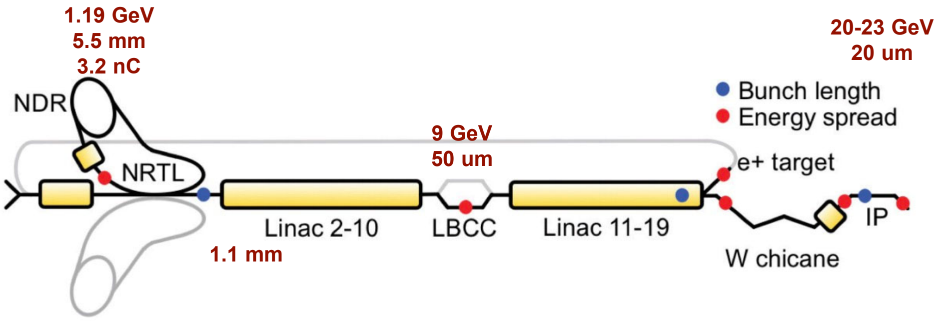
FACET (PWFA)

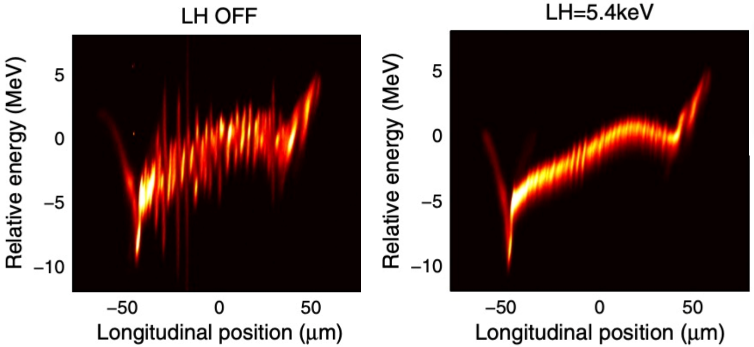
K. Bane SLAC PUB 3662 (1985)

Tzoufras et al., PRL **101,** 145002 (2008)

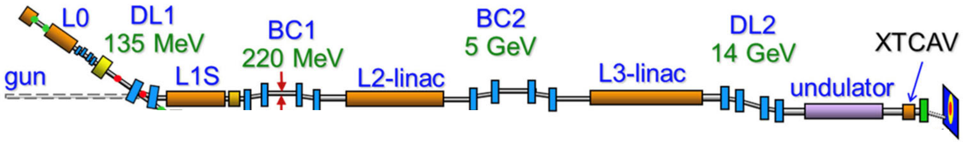
Ratner et al., PRSTAB **18,** 030704 (2015)







LCLS (FEL)



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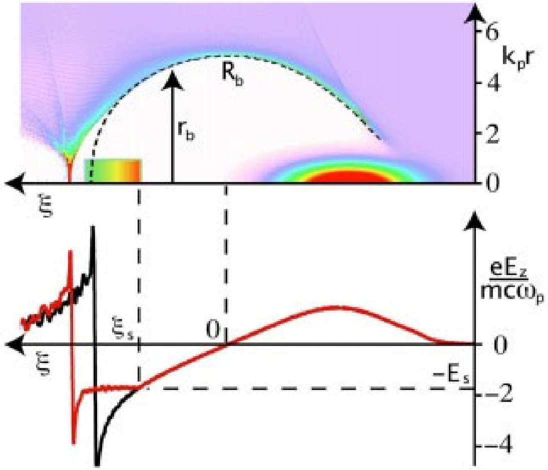

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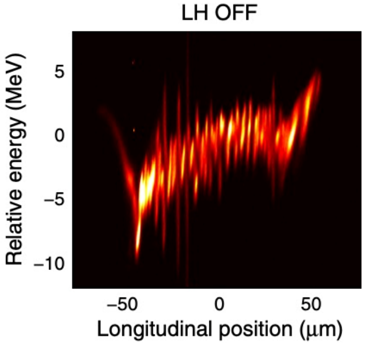
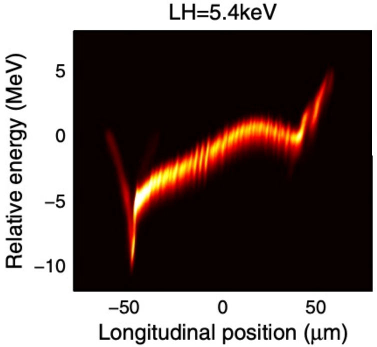




LCLS (FEL)

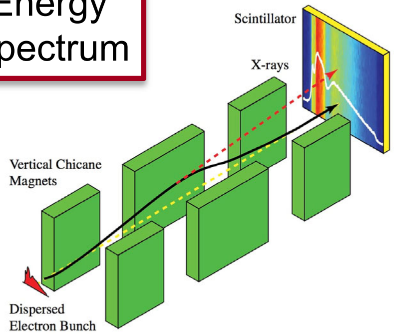
Quantities measured

$\Delta E/E \sim \%level$

$\sigma_z \sim 0.1 - 10\mu m$

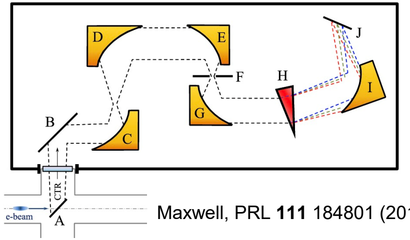
$\Delta z \sim 10 - 200\mu m$

Energy spectrum



Scheinker, Gessner, PRSTAB **18** 102801 (2015)

Bunch Profile

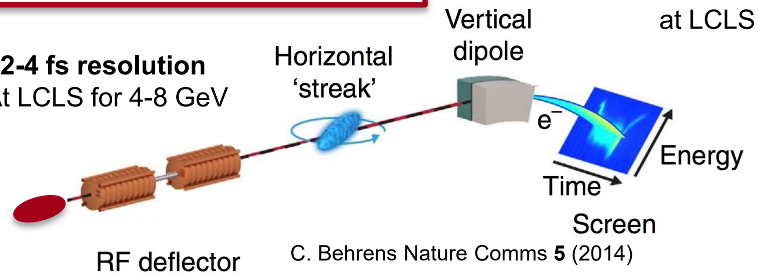


Maxwell, PRL **111** 184801 (2013)

~0.7 fs resolution at LCLS using OTR

Longitudinal Phase Space

~2-4 fs resolution At LCLS for 4-8 GeV



C. Behrens Nature Comms **5** (2014)

A. Edelen, J.P. Edelen, D. Erdstrom et al., Proc NAPAC 2016
A.L. Edelen et al IPAC 2018

Virtual diagnostics

Predict what the output of a diagnostic would look like when it is unavailable

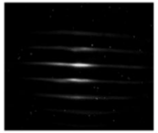
Fast physics-based simulation

ML model

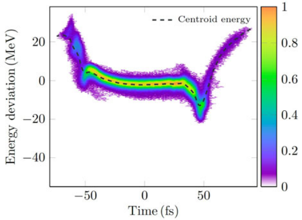
"Real-time" prediction of beam characteristics or explicit diagnostic output

Measured machine inputs (non-destructive)

Virtual diagnostic



$\epsilon_y, \langle y^2 \rangle, \langle yy' \rangle, \langle y'^2 \rangle$



Challenges with physics-based simulation approach:

Execution often still isn't so fast (sec-mins)

Can require HPC resources

Often takes much effort to replicate machine behavior!
(And even then, need to account for drifts)

Another approach:
Use a ML model

Once trained, neural networks can execute very quickly

Train on data from slow, high fidelity simulations
+
Train on measured data

A. Edelen, J.P. Edelen, D. Erdstrom et al., Proc NAPAC 2016
A.L. Edelen et al IPAC 2018

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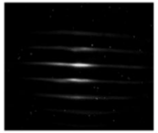

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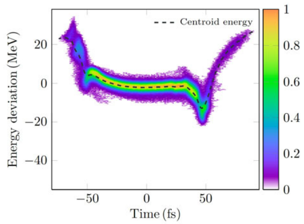

Challenges with p

Execution often

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fidelity simulations

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Joint benefits:

Additional information for user experiments

Additional signal to feedback on for LPS tuning

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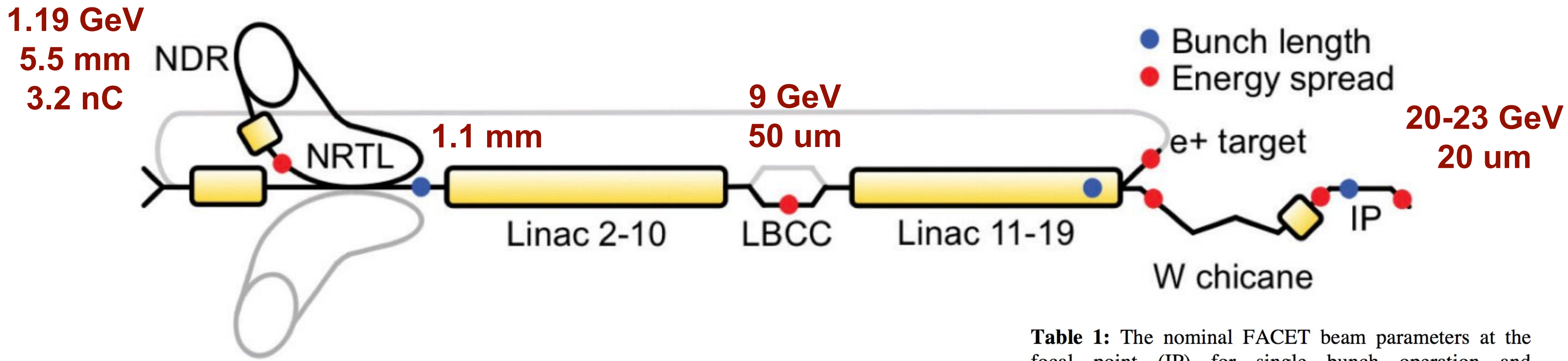
FACET schematic and parameters



- **Main goal:**
  demonstrate large energy gain for e-/e+ beams in single stage PWFA
- Beam generated by thermionic gun extracted from damping ring
- 2 km long accelerator with various systematic phase drifts, thermal drifts and time-varying uncertainties.
- Longitudinal diagnostics: TCAV, SYAG, EOS, DR bunch length monitors.
- **Challenge for diagnostics and control** - stabilize LPS and compression against drifts.

Table 1: The nominal FACET beam parameters at the focal point (IP) for single bunch operation and corresponding plasma parameters.

Parameter	Nominal Value
Energy	23GeV
Energy Spread (r.m.s.)	1.5%
Species	electrons or positrons
Charge per Bunch	3.2nC
Bunch Length	20μm
Transverse Size (x, y)	13μm, 5μm
Peak Current	20kAmps

E-beam profile prediction at FACET

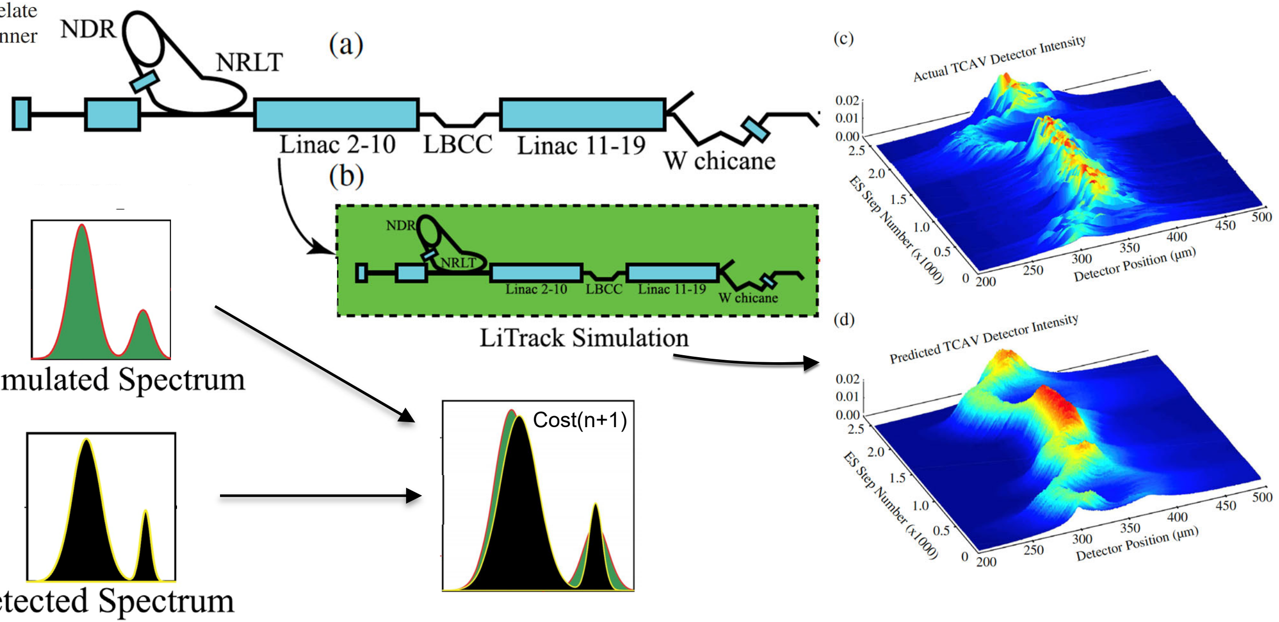
PHYSICAL REVIEW SPECIAL TOPICS—ACCELERATORS AND BEAMS **18,** 102801 (2015)

Adaptive method for electron bunch profile prediction

Alexander Scheinker[*]
Los Alamos National Laboratory, 1200 Trinity Drive, Los Alamos, New Mexico 87544, USA

Spencer Gessner[†]
SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California 94025, USA
(Received 16 June 2015; published 15 October 2015)

The measured energy spectrum is observed to correlate with the longitudinal bunch profile in a one-to-one manner



Guess machine parameters and simulate with LiTrack

Measure energy spectrum on SYAG

Compare LiTrack spectrum with SYAG

Adapt machine parameters to minimize difference

With "correct" machine parameters estimate longitudinal bunch profile based on LiTrack output LPS

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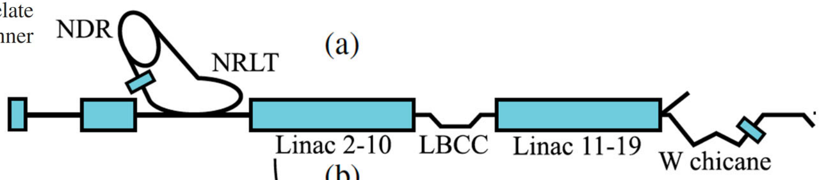
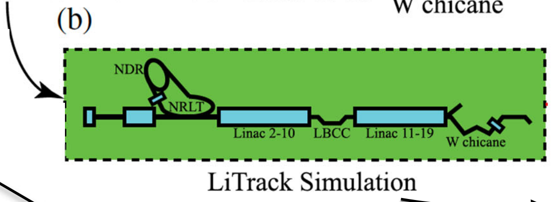
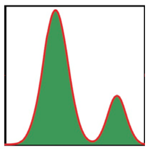
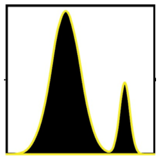


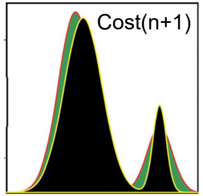


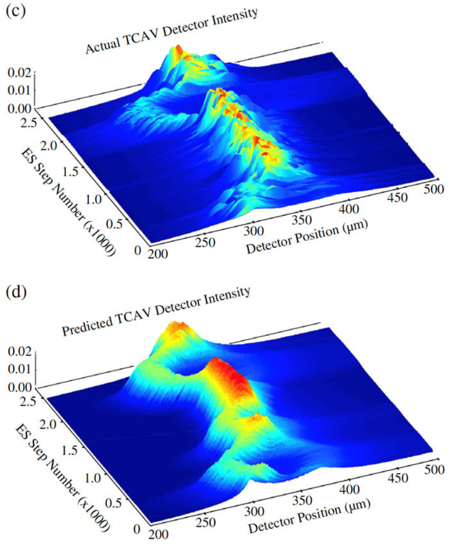


Simulated Spectrum



Detected Spectrum





Convergence Rate/Accuracy sensitive to initial parameter guess

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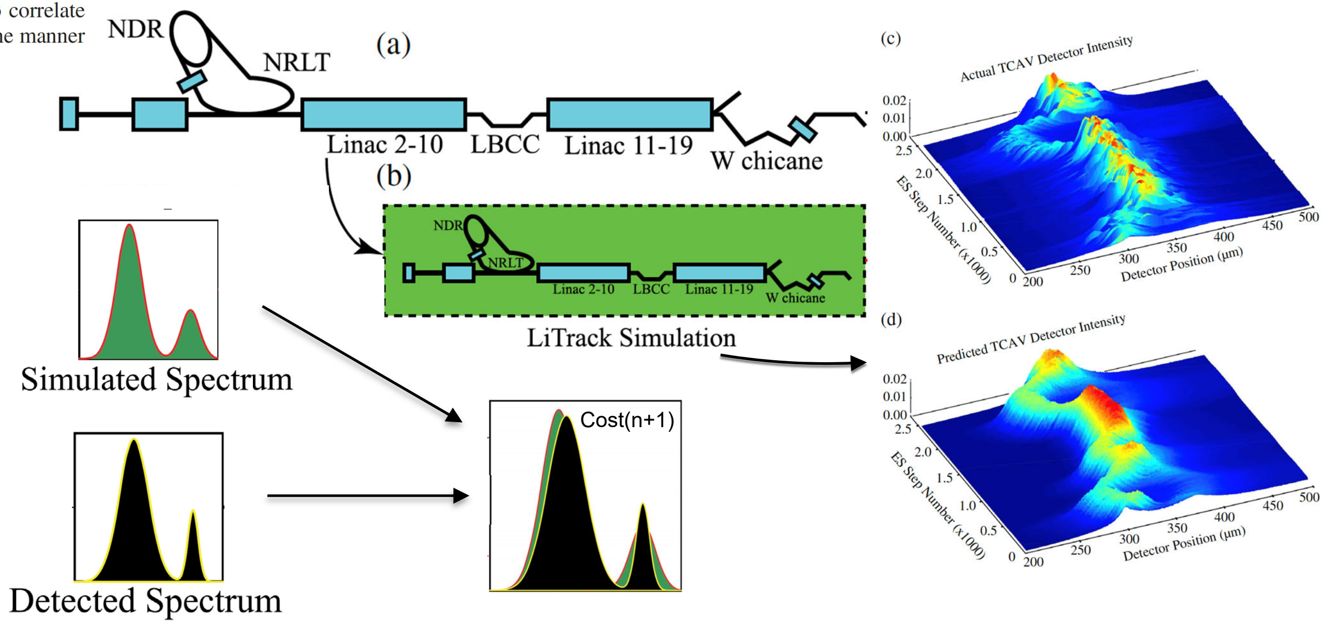
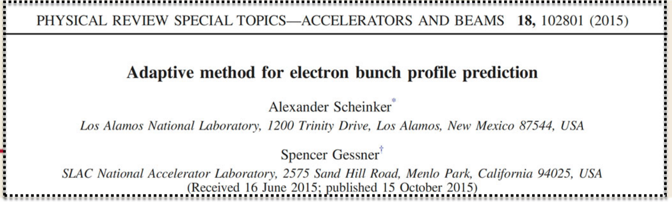


"Furthermore we hope to one day utilize LiTrackES as an actual feedback to the machine setpoints in order to tune desired e-beam properties"

E-beam profile prediction at FACET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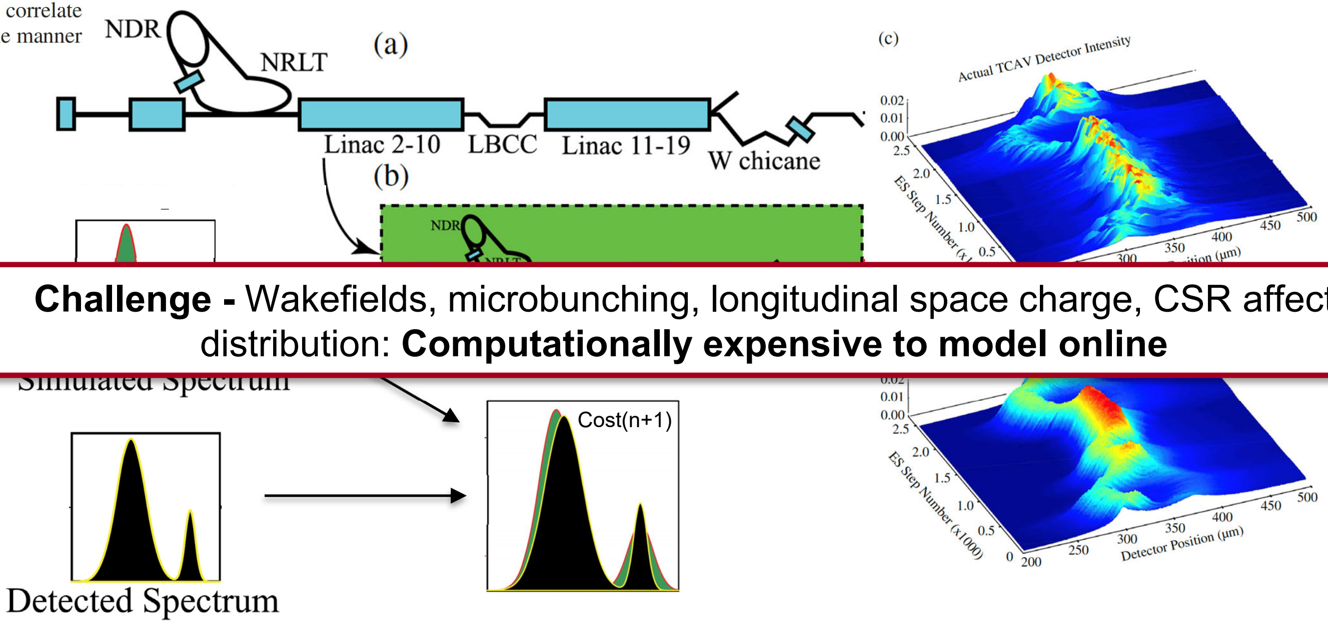


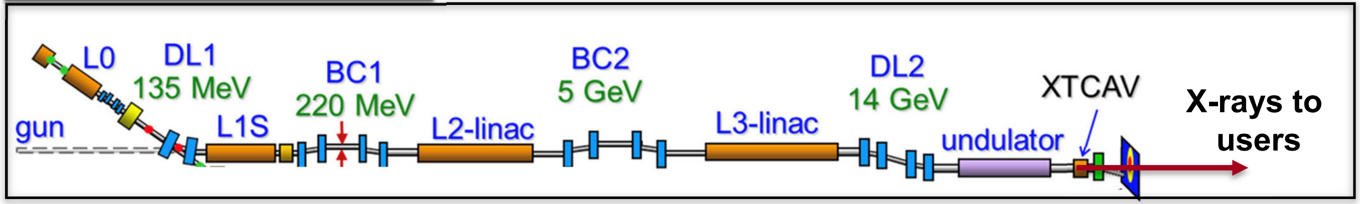
Challenge - Wakefields, microbunching, longitudinal space charge, CSR affect distribution: **Computationally expensive to model online**

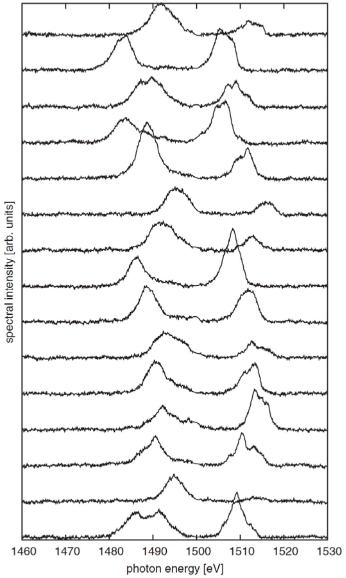
“Furthermore we hope to one day utilize LiTrackES as an actual feedback to the machine setpoints in order to tune desired e-beam properties”

ML-based prediction of X-ray properties at LCLS

- XFEL pulse properties intrinsically vary from shot to shot.
- Many experiments want full X-ray characterization shot to shot.

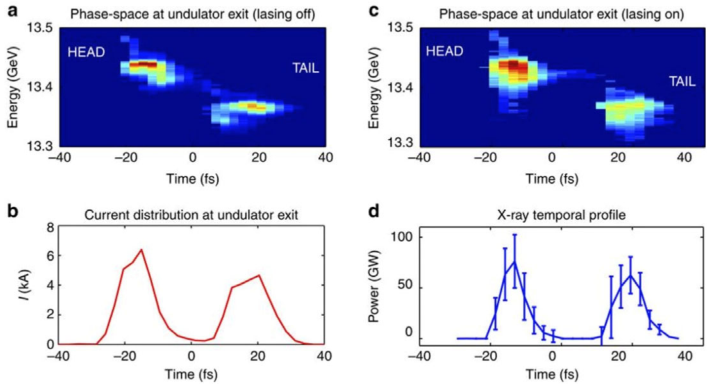
LCLS accelerator schematic





Two color single-bunch and two-bunch examples

Lutman et. al., PRL **110**, 134801 (2018), Marinelli et. Al., Nat. Comms, **6** 6369, (2015)



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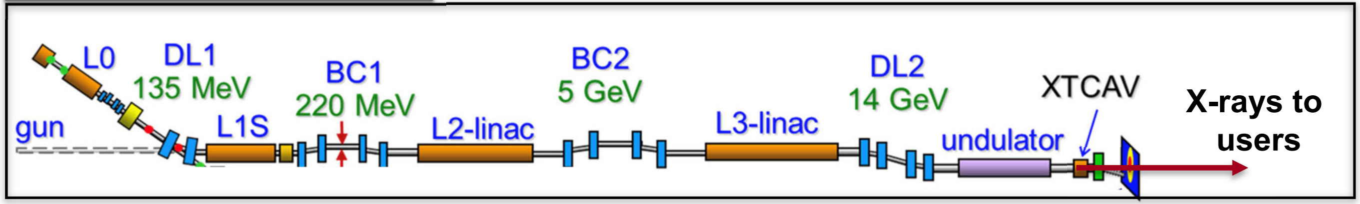
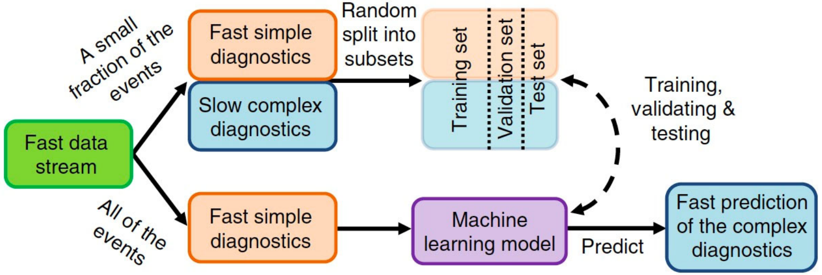
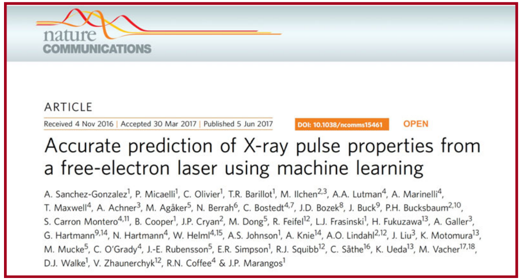
- Many experiments want full X-ray characterization shot to shot.
- Use fast diagnostics and ML model to predict output of slow diagnostics.
- Promising result for high rep-rate FEL facilities.

LCLS accelerator schematic



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ARTICLE

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Accurate prediction of X-ray pulse properties from a free-electron laser using machine learning

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.D. Bozek[8], J. Buck[9], P.H. Bucksbaum[2,10], S. Carron Montero[4,11], B. Cooper[1], J.P. Cryan[2], M. Dong[5], R. Feifel[12], L.J. Frasinski[1], H. Fukuzawa[13], A. Galler[3], G. Hartmann[9,14], N. Hartmann[4], W. Helml[4,15], A.S. Johnson[1], A. Knie[14], A.O. Lindahl[2,12], J. Liu[3], K. Motomura[13], M. Mucke[5], C. O'Grady[4], J.-E. Rubensson[5], E.R. Simpson[1], R.J. Squibb[12], C. Såthe[16], K. Ueda[13], M. Vacher[17,18], D.J. Walke[1], V. Zhaunerchyk[12], R.N. Coffee[4] & J.P. Marangos[1]

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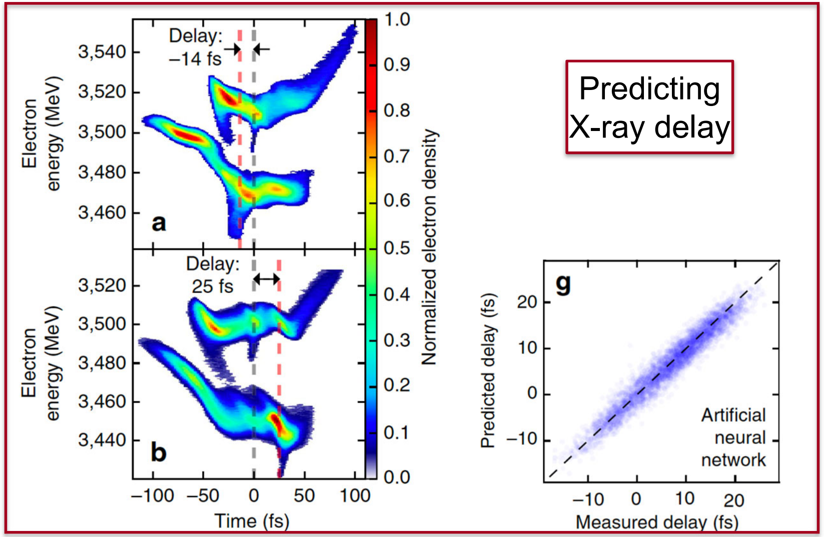

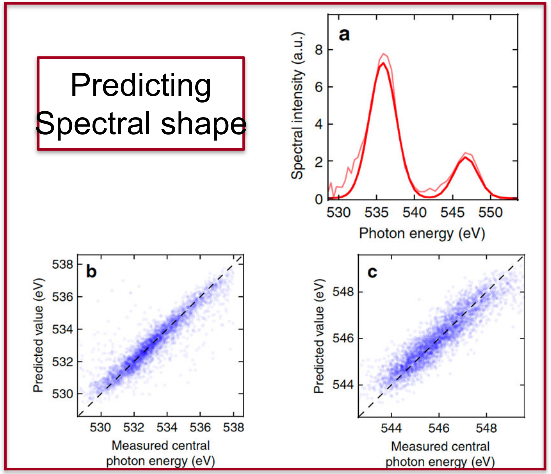

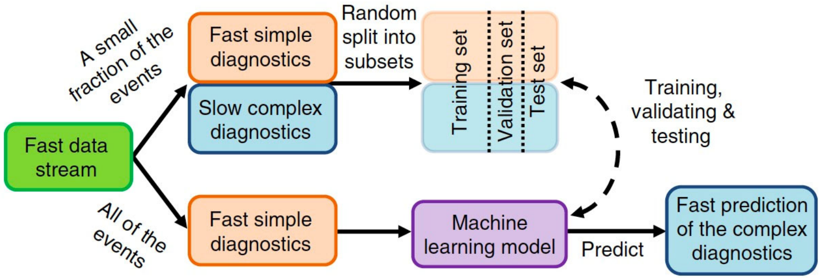

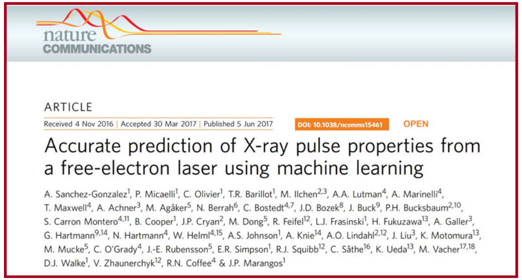
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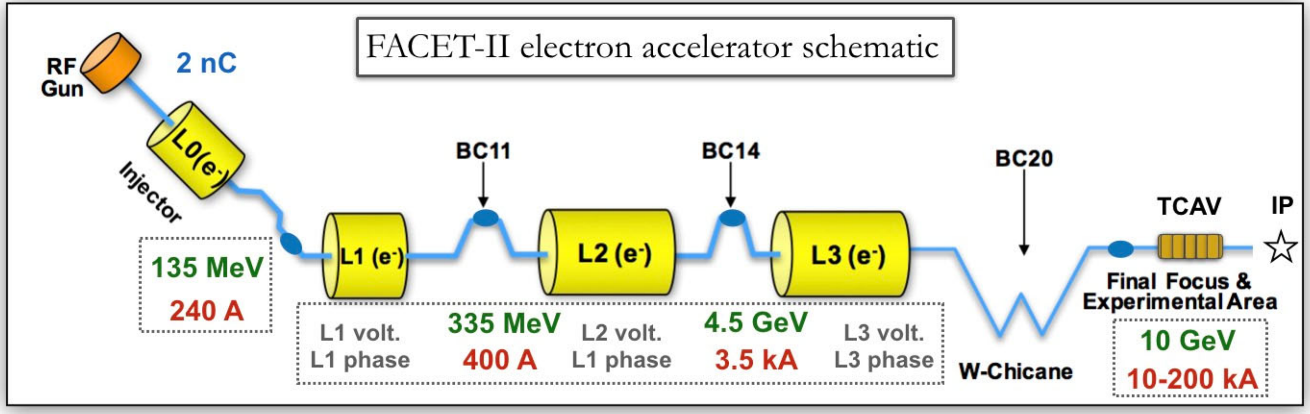
FACET-II schematic and parameters

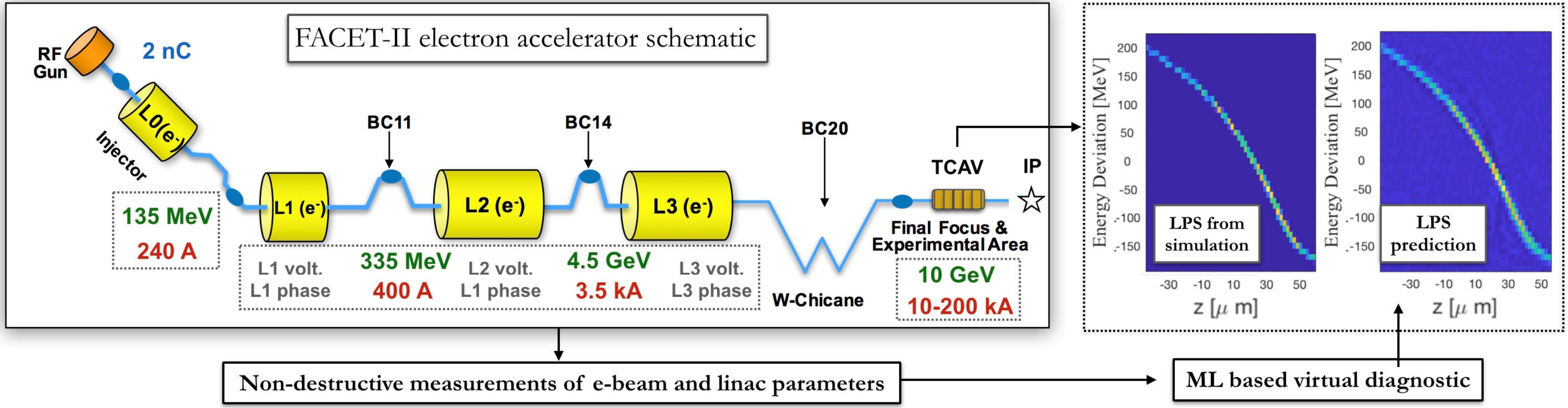


- **Main goal:** demonstrate energy depletion of drive bunch and preservation of emittance.
- RF photo injector replaced thermionic gun + damping rings
- **Challenges for diagnostics and control** -
  - measure LPS and stabilize compression w.r.t. shot-to-shot jitter of linac parameters.

Table 1. Comparison of bunch parameters for the two input bunches (drive and trailing) and the output bunch (accelerated trailing bunch) at the interaction point and exit of the plasma, respectively, for the earlier FACET I facility and for the expected (nominally) FACET II operation.

	Facet I (delivered) [27]	FACET II (expected/simulated)
Drive bunch		
Drive and trailing energy	21 GeV	10 GeV
Charge/σ_z/I_{peak}/σ_r	600 pC/30 μm/ 6 kA/30 μm	1.6 nC/13 μm/ 15 kA/4 μm
$\delta E/E$	0.8% r.m.s	0.15% rms
Normalized emittance	200 $\times$ 50 μm (with Be foil)	<7 $\times$ 3 μm (without Be foil)
Trailing bunch		
Trailing Energy	21 GeV	10 GeV
Charge/σ_z/I_{peak}/σ_r	350 pC/50 μm/ 2.1 kA/30 μm	0.5 nC/6.4 μm/ 7.5 kA/4 μm,
$\delta E/E$	1.5% rms	<1% rms
Accelerated bunch		
Final energy spread	<5%	1%
Energy gain	9 GeV (max)	>10 GeV
Efficiency	30% (max)	50%
Emittance preservation	No	Yes

LPS virtual diagnostic for FACET-II

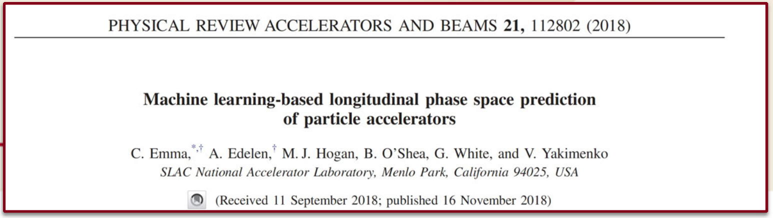


- Virtual diagnostic is trained with 5^5 simulations scanning linac/beam parameters within expected jitter ranges

- Inputs fed to ML model include random error to simulate measurement accuracy.

Simulation parameter scanned	Range
L1 & L2 phase [deg]	± 0.25
L1 & L2 voltage [%]	± 0.1
Bunch charge [%]	± 1
Input to ML model	Accuracy
L1 & L2 phase [deg]	± 0.1
L1 & L2 voltage [%]	± 0.05
I_{pk} at BC (11,14,20) [kA]	$\pm(0.25, 1, 5)$
ϵ_n at BC (11,14) [μm]	± 1
Beam centroid BC (11,14) [m]	

FACET-II Single bunch simulations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Machine learning-based longitudinal phase space prediction of particle accelerators

C. Emma,[*,†] A. Edelen,[†] M. J. Hogan, B. O'Shea, G. White, and V. Yakimenko
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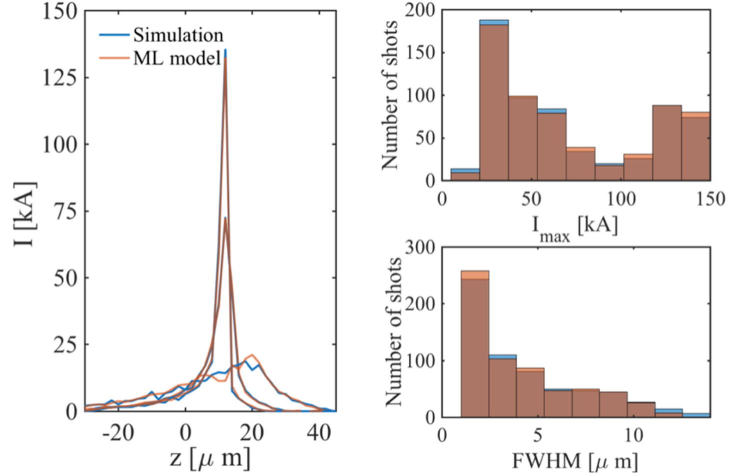

Simulation parameter scanned	Range
L1 & L2 phase [deg]	± 0.25
L1 & L2 voltage [%]	± 0.1
Bunch charge [%]	± 1
Input to ML model	Accuracy
L1 & L2 phase [deg]	± 0.1
L1 & L2 voltage [%]	± 0.05
I_{pk} at BC (11,14,20) [kA]	$\pm(0.25, 1, 5)$
ϵ_n at BC (11,14) [μm]	± 1
Beam centroid BC (11,14) [m]	

- ML predictions *given 10 scalar diagnostic readings as inputs* show good agreement with the current profile output at the IP.

FACET-II Single bunch simulations

PHYSICAL REVIEW ACCELERATORS AND BEAMS **21**, 112802 (2018)

Machine learning-based longitudinal phase space prediction of particle accelerators

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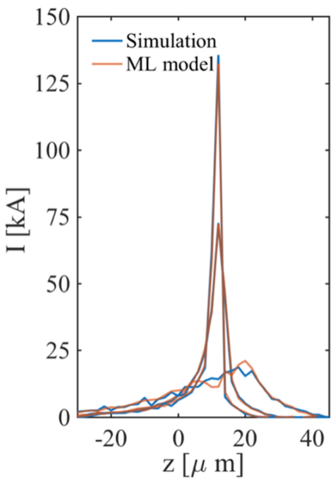

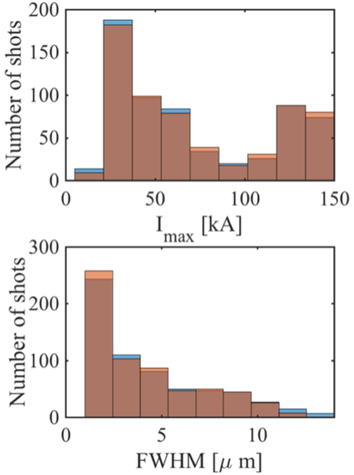

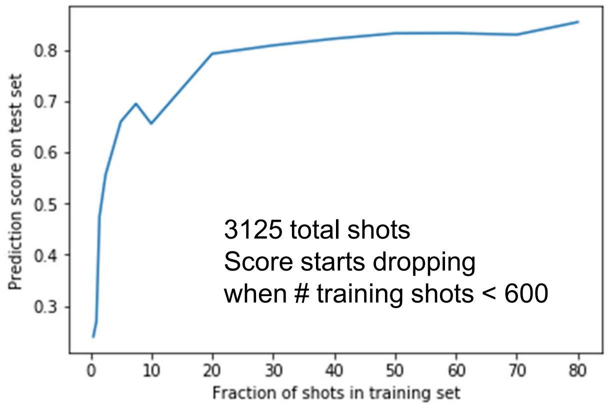

Simulation parameter scanned	Range
L1 & L2 phase [deg]	±0.25
L1 & L2 voltage [%]	±0.1
Bunch charge [%]	±1
Input to ML model	Accuracy
L1 & L2 phase [deg]	±0.1
L1 & L2 voltage [%]	±0.05
I_{pk} at BC (11,14,20) [kA]	$\pm(0.25, 1, 5)$
ϵ_n at BC (11,14) [μm]	±1
Beam centroid BC (11,14) [m]	

- ML predictions *given 10 scalar diagnostic readings as inputs* show good agreement with the current profile output at the IP.
- At least ~ 600 shots necessary to achieve good accuracy for these jitter ranges.
- Some shots (I_{max} > 60 kA) are beyond the resolution of the TCAV. A robust way of tagging these shots is important for us to trust the output of the virtual diagnostic.

FACET-II Single bunch simulations

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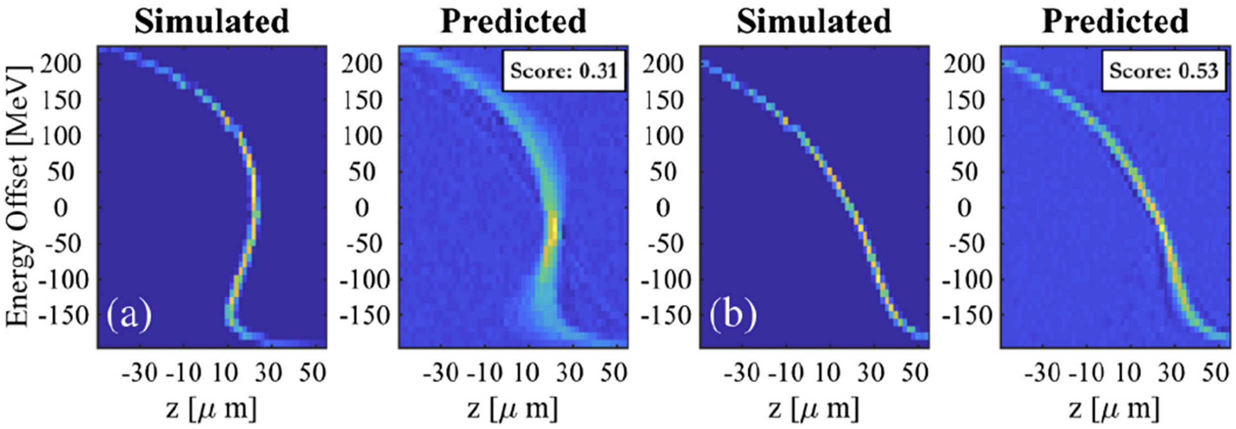

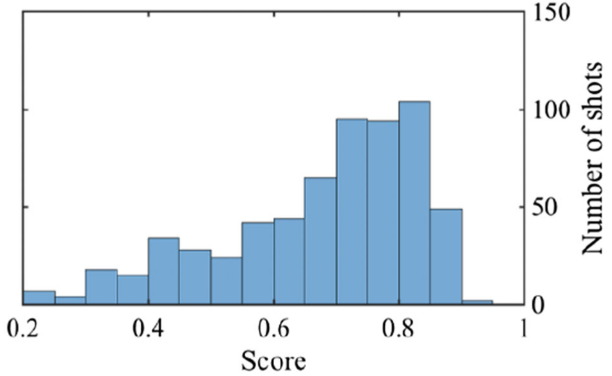

- Results for the LPS prediction show similar agreement between NN and simulation.

$$\text{score} \equiv R^2 = 1 - \frac{\Sigma_{i,j}(x_{ij}^{\text{true}} - x_{ij}^{\text{predicted}})^2}{\Sigma_{i,j}(x_{ij}^{\text{true}} - \bar{x}^{\text{true}})^2}$$

FACET-II Single bunch simulations

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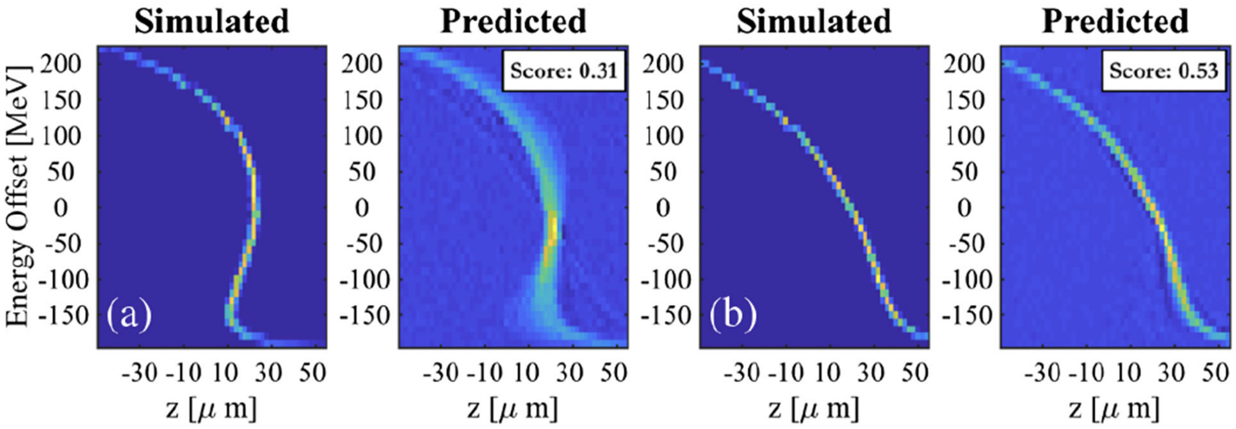
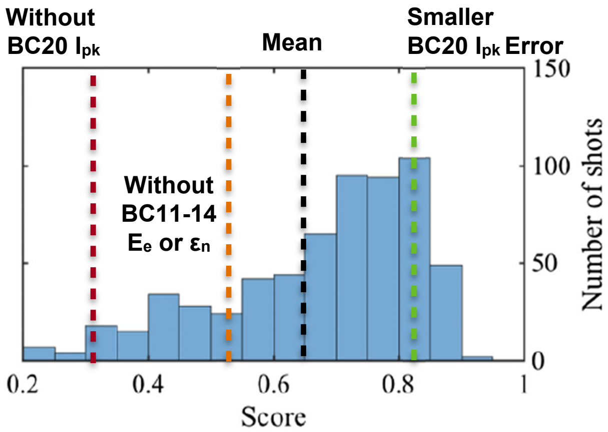
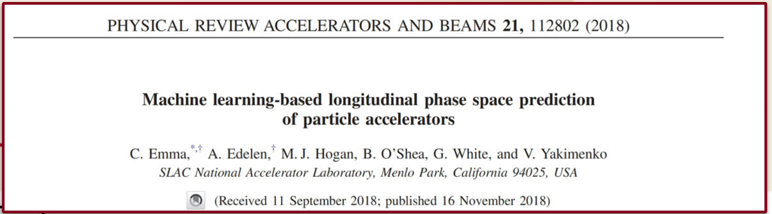




- Results for the LPS prediction show similar agreement between NN and simulation.
- Sensitivity study (removing diagnostics from ML input) shows that the most critical diagnostic is the peak current measurement after BC20.

$$\text{score} \equiv R^2 = 1 - \frac{\Sigma_{i,j}(x_{ij}^{\text{true}} - x_{ij}^{\text{predicted}})^2}{\Sigma_{i,j}(x_{ij}^{\text{true}} - \bar{x}^{\text{true}})^2}$$

LCLS experimental proof of concept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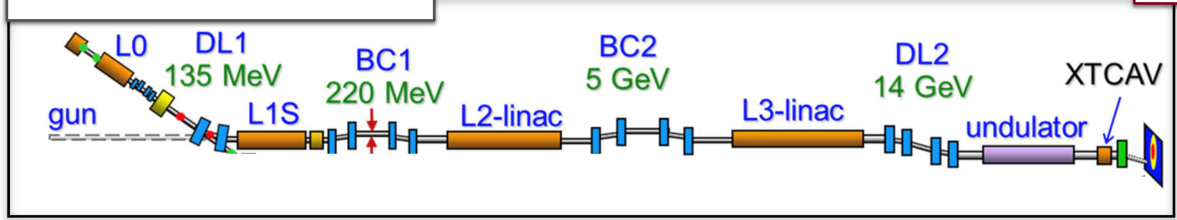
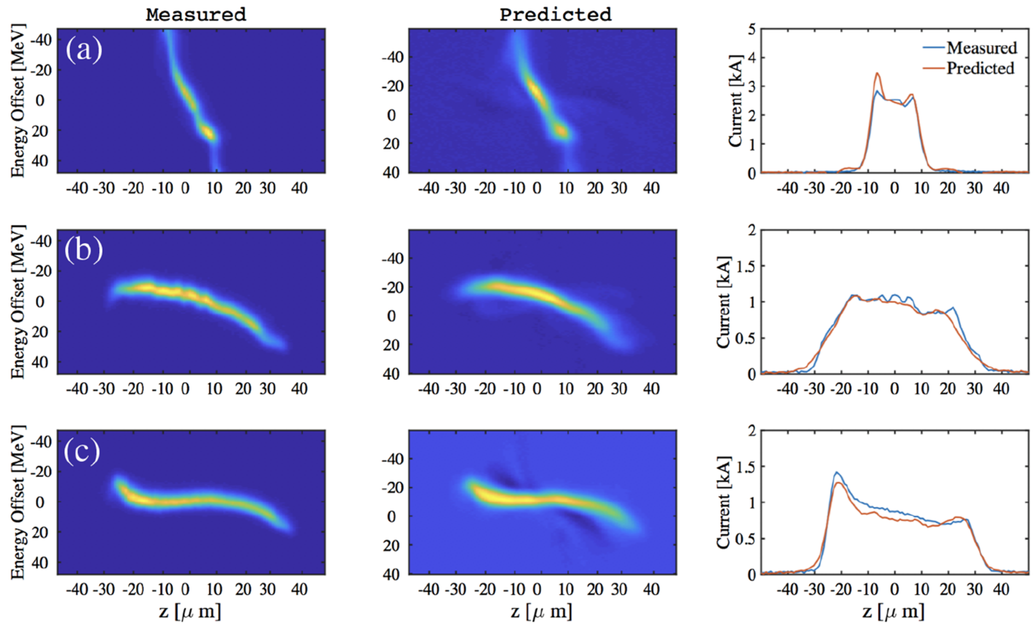
LCLS accelerator schematic





LCLS Experiment:

Machine parameters scanned:
L1s phase from -21 to -27.8 deg

BC2 peak current from 1 to 7 kA

Inputs to ML model:
L1s voltage & phase readbacks,
L1x voltage, BC1 and BC2 current

- ML prediction of LPS/current profile from **five** scalar inputs agrees well with measurements.

LCLS experimental proof of concept

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Machine learning-based longitudinal phase space prediction of particle accelerators

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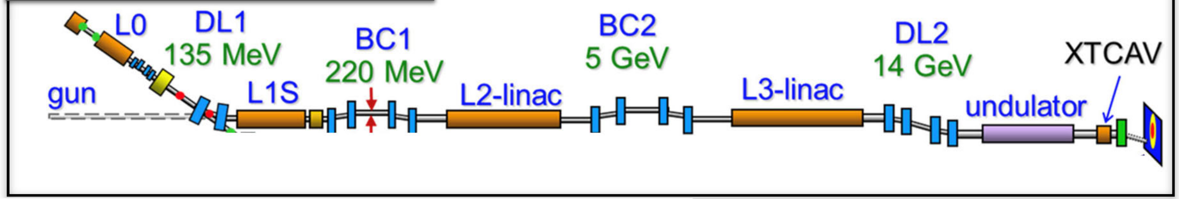

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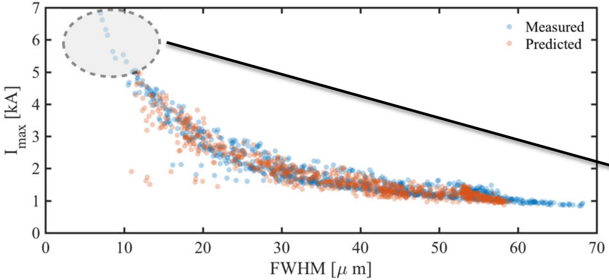
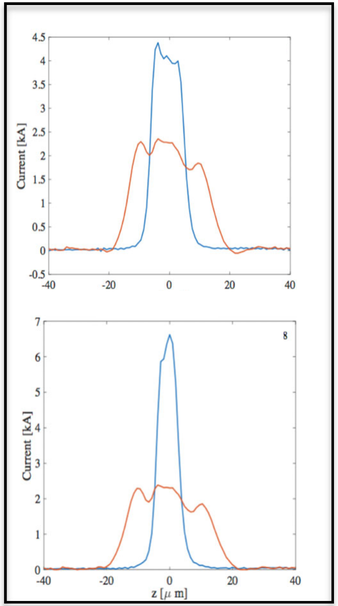
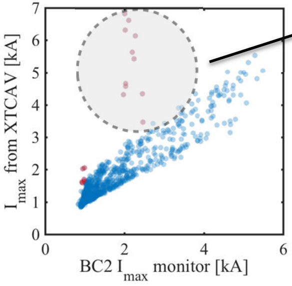




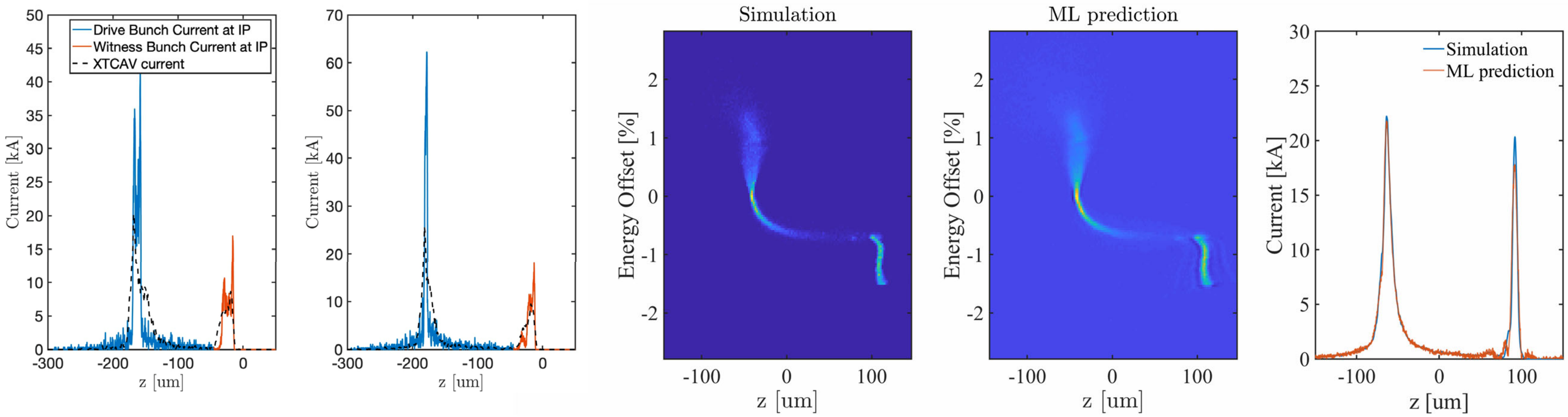
Shots with 'bad' prediction circled



- ML prediction of LPS/current profile from **five** scalar inputs agrees well with measurements.
- Bad predictions can result from large discrepancy between diagnostic input (e.g. BC2 current) and XTCAV current (see bad shots).
- Flagging bad shots (e.g. with redundant diagnostic) is important for trusting virtual diagnostic prediction.

FACET-II Two-bunch simulations with TCAV

Single shots

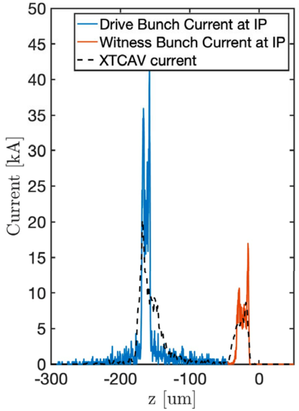


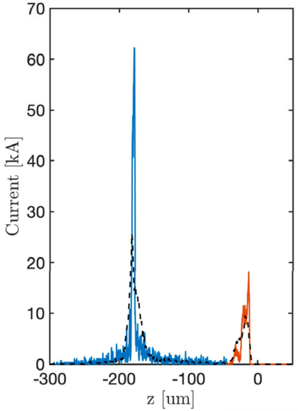
Good agreement in between ML prediction and simulated TCAV measurement

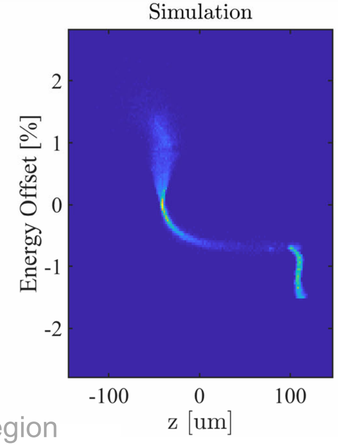
Parameter	*L1 & L2 phase*	*L1 & L2 volt*	*Bunch Charge*
Scan Range	*± 0.25 deg*	*± 0.25 %*	*± 1 %*
F2 Baseline	*± 0.1, 0.2 deg*	*± 0.1,0.25 %*	*± 1 %*

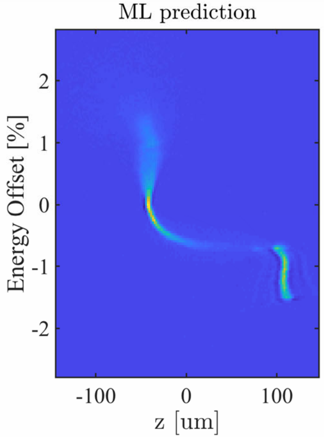
FACET-II Two-bunch simulations with TCAV

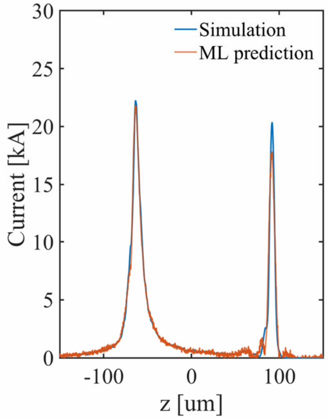
Single shots





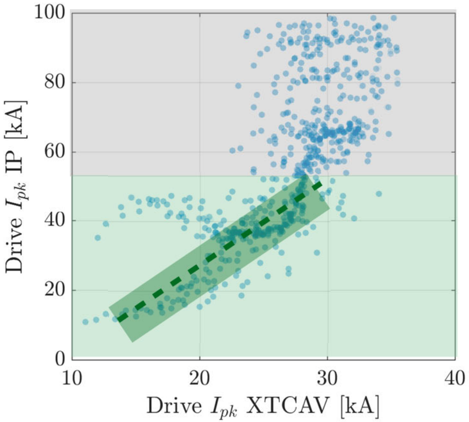




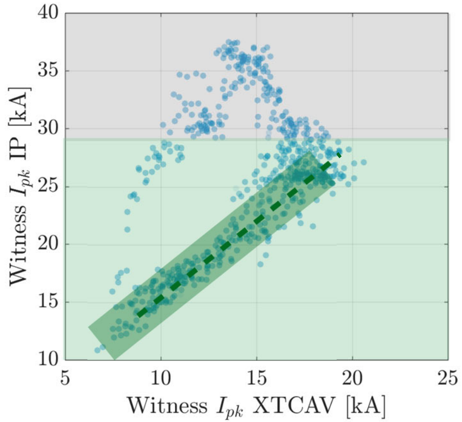


All shots

Good measurement region



Bad measurement region



Good agreement in between ML prediction and simulated TCAV measurement

Using the ML prediction with additional input (e.g. correlations with other diagnostics) will add confidence in agreement between measured LPS and LPS at the IP

Outline

1. ML-based virtual diagnostics - background and motivation

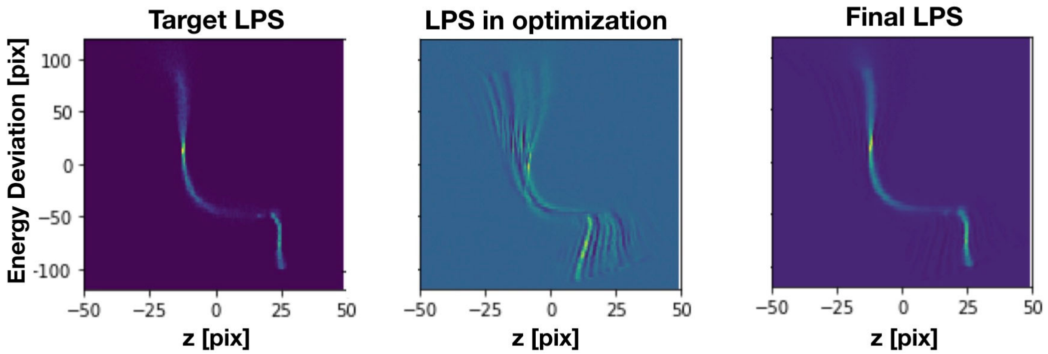
2. Virtual diagnostic examples:
    1. Previous studies at FACET and LCLS
    2. Single bunch simulations for FACET-II & proof-of-concept at LCLS
    3. Two-bunch simulations for FACET-II including TCAV

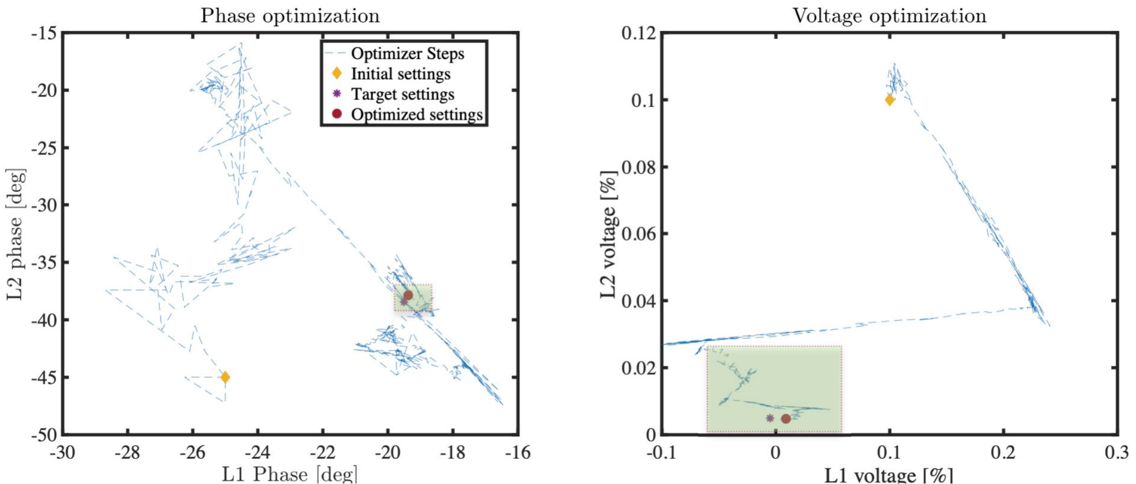
3. Optimization using LPS virtual diagnostics

4. Conclusions, challenges and next steps towards implementation

Optimization for two-bunch at FACET-II

- ML prediction of LPS used with conventional optimizer to tune L1-2 phases/voltages for desired LPS.
- Initial settings outside training set of ML model.
- Model shows ability to interpolate within training data.



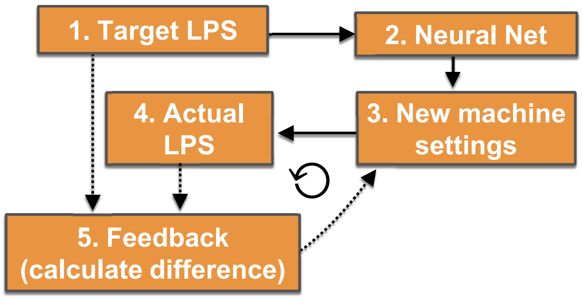


Optimization using ML *inverse model*

NN provides "smart" initial guess for optimizer - avoids getting stuck in local minima to converge to correct solution

- Goal is decrease tuning time and improve beam quality for target beam parameters

Flow diagram for the NN + feedback

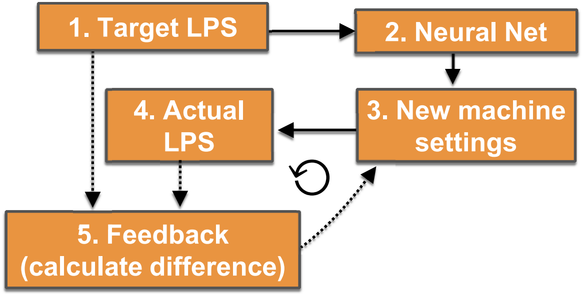


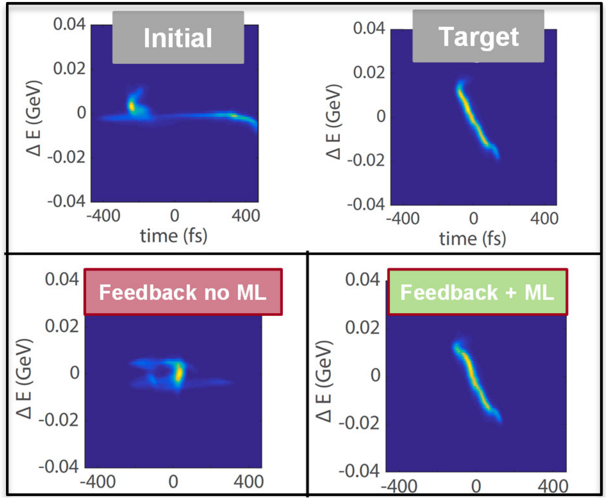
Optimization using ML *inverse model*

NN provides "smart" initial guess for optimizer - avoids getting stuck in local minima to converge to correct solution

- Goal is decrease tuning time and improve beam quality for target beam parameters
- NN and an optimizer used to automatically change machine parameters to obtain a desired LPS
- By making an initial guess using the NN, the optimizer feedback is able to achieve the desired LPS

Flow diagram for the NN + feedback





PHYSICAL REVIEW LETTERS **121,** 044801 (2018)

Demonstration of Model-Independent Control of the Longitudinal Phase Space of Electron Beams in the Linac-Coherent Light Source with Femtosecond Resolution

Alexander Scheinker,[1,*] Auralee Edelen,[2] Dorian Bohler,[2] Claudio Emma,[2] and Alberto Lutman[2]
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[2]*SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, California 94025, USA*

Conclusion and future work

- We are developing an ML-based virtual diagnostic for single shot prediction of the 2D LPS of e-beam linacs.
- Our work shows the feasibility of the virtual diagnostic for predicting the LPS given few non-destructive diagnostic inputs and LPS in simulation (FACET-II) and experiment (LCLS).
- Successful implementation + integration with non-ML diagnostics will provide additional information for users and a signal for LPS feedback, tuning and control.
- Resolution limits of TCAV at FACET-II result in discrepancies between predicted current profiles and actual current at IP. Tagging high vs low current shots important for trusting prediction.
- **Challenges to address:** Accurate quantification of robustness/model uncertainty, retraining strategies, how best to combine machine + simulation data, scale to complex operation modes.

Thank you!

Many thanks to the following colleagues who contributed to this work:
A. Edelen, G. White, A. Scheinker, B. O'Shea, A. Hanuka, D. Storey, M.J. Hogan, V. Yakimenko, S. Gessner, A. Lutman, D. Bohler, L. Alsberg, M. Alverson, LCLS Operations Group