Opportunities for Edge Computing and ML across Science Domains

Ryan Coffee, Naoufal Layad, Jack Hirschman, Audrey Corbeil Therrien, Ryan Herbst, Jana Thayer
LCLS and the PULSE Institute, SLAC National Accelerator Laboratory

U.S. DEPARTMENT OF ENERGY Office of Science

SLAC NATIONAL ACCELERATOR LABORATORY

Abstract We present three current projects that span scientific domains yet share functional similarity for processing of sensor data: magnetic plasma confinement (DOE-FES), attoclock spectroscopy (DOE-BES), and Time-Tagged radiography (NIH). There is an opportunity for synergistic development of a streaming transformation pipeline from analog sensor signals into information dense representations.

Magnetic Confinement for Fusion Energy

Magnetic confinement for plasma fusion poses numerous challenges for real-time signal processing and control. So-called Edge Localized Modes (ELMs) can channel damaging energy bursts onto reactor walls. Low-latency machine learned control models could suppress or stabilize these self-destructive plasma oscillation modes. Such control requires real-time actionable diagnostic information regarding the spatially dependent state of the plasma.

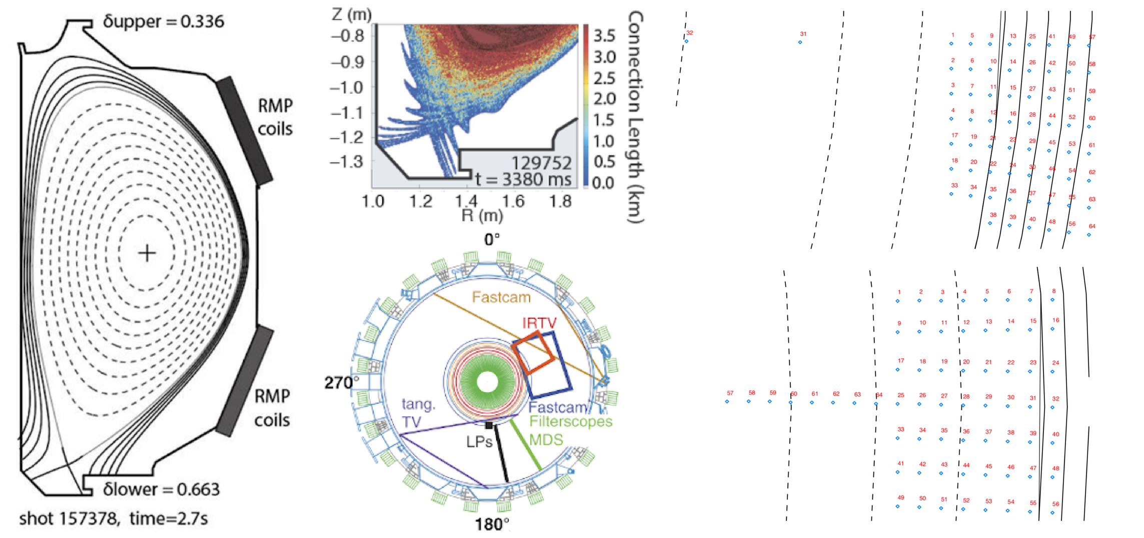

Figure 1. (left) Schematic of magnetic plasma confinement in a tokamak reactor as DIII-D shown here adapted from Refs. [1, 2]. (right) Example channel layouts for the Beam Emission Spectroscopy (BES) detector courtesy of Ref [3].

In Figure 2 we can see 3 individual points in the plasma using one of two types of diagnostic sensor, Beam Emission Spectroscopy (BES) and Electron Cyclotron Emission (ECE). We produce a rolling spectrogram of the signal (spectrum along vertical, time along horizontal) followed by a set of 2D convolution filters with logarithmic scaling to enhance mode visibility. Insets show similar frequency patterns across channels. Figure 3 (along poster bottom) shows that during a 2 second long shot, these shared patterns "breathe" during plasma evolution. The breathing represents the spatially correlated signals.

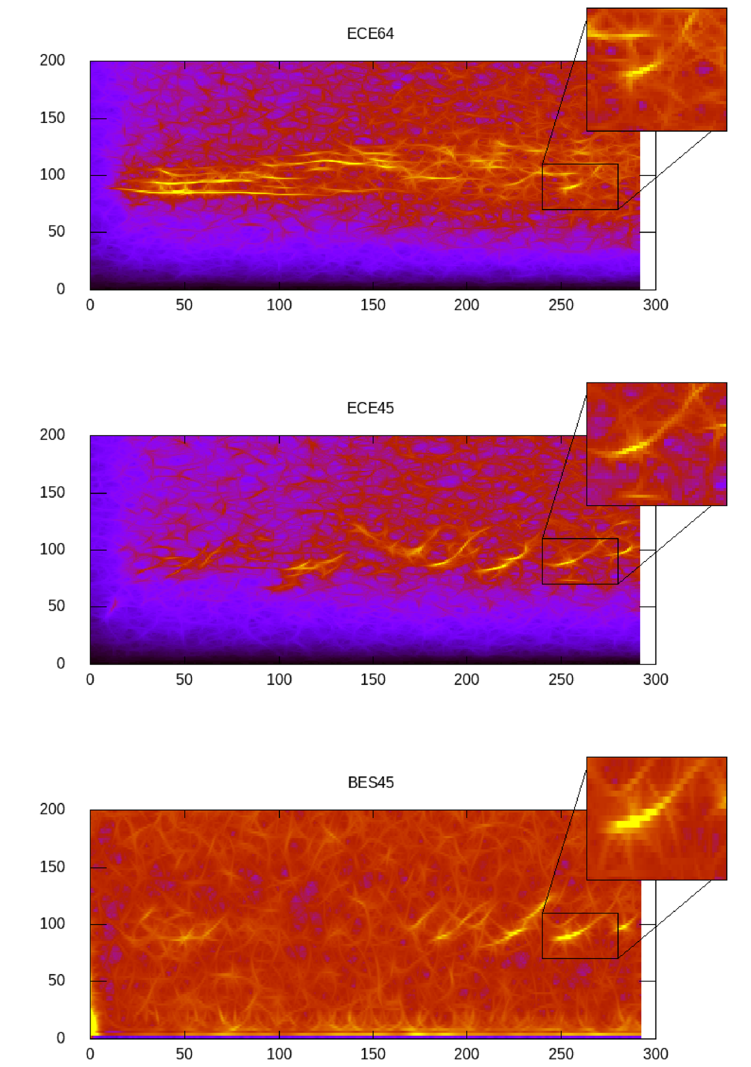

Figure 2. The top 2 panels show two of the 40 ECE channels. The bottom panel shows one of the 64 total BES channels. Each panel shows the 2D Fourier power spectrogram (frequency along vertical, time within shot along the horizontal). Insets show that cross-channel, even cross-diagnostic, matched patterns motivate deeper layers that collate upstream single channel layer outputs.

Dynamic Configurations

- The BES and ECE channel layouts do not resemble conventional imaging sensors where deep neural networks have enjoyed wide application,
- BES layouts are re-configured for each experimental campaign,
- Irregular physical layouts are ill formed for conventional convolutions,
- Spatial dependence of channel correlations are key to locating edge instabilities, e.g. Edge Localized Modes (ELMs),
- The lab-frame to plasma-frame correspondence varies with the state of the plasma which we are trying to predict.

Simulation Challenge

- Highly non-linear system that incurs some of the highest computational costs for simulations, e.g. challenging for Summit@ORNL,
- Accelerating simulations with less costly surrogate models is an active research effort.

Data starved

- Scientific papers can be based on only one shot of 2 second duration,
- Rare modes show less than 100 examples,
- Conventional "augmentation" methods of rotation and translation are inappropriate (until surrogate models can be trained),
- ML-based classification efforts rely heavily on a "golden standard" of just over 1000 shots, each with only a few labeled ROIs. [4]

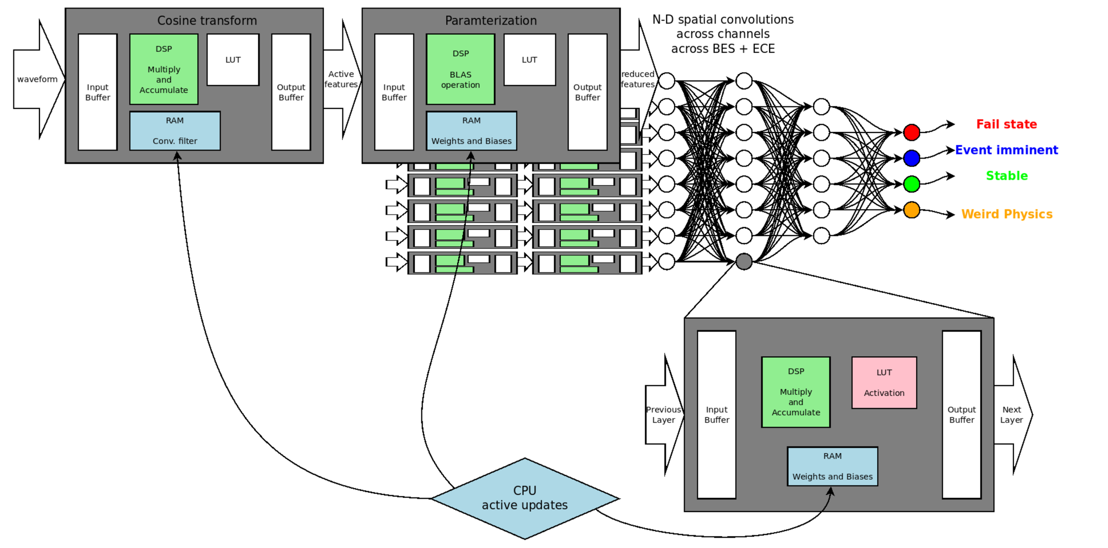

Figure 4. Proposed FPGA-based data flow for pre-analysis "featurization" and plasma state inference.

Pre-processing

- A "patch" of rolling spectrogram image, windowed power spectrum along vertical columns in time-steps along the horizontal dimension.
- Computational efficiency of discreet cosine transform (DCT) to optimally increase information density,
- Pattern of behaviors for hot features across channels in deeper collating layers.

Attoclock Spectroscopy for LCLS-II

Attoclock spectroscopy aims to resolve attosecond scale molecular electronic re-configurations by using soft x-ray resonant absorption and photo-emission signals. Relevant methods [5, 6] rely on reconstruction of each x-ray shot. The LCLS has therefore recently designed an angular array of electron time-of-flight (ToF) spectrometers colloquially known as the "CookieBox" (Fig. 5). The drift time of emitted electrons is mapped to emission energy by accounting for electrostatic control fields in each ToF, a $\log(t) \mapsto \log(E)$ mapping. One dresses the gas-phase molecule in a circularly polarized optical field such that the electron emission experiences a time-angle dependent energy shift. [7–9], producing a so-called sinogram as shown in Fig. 6.

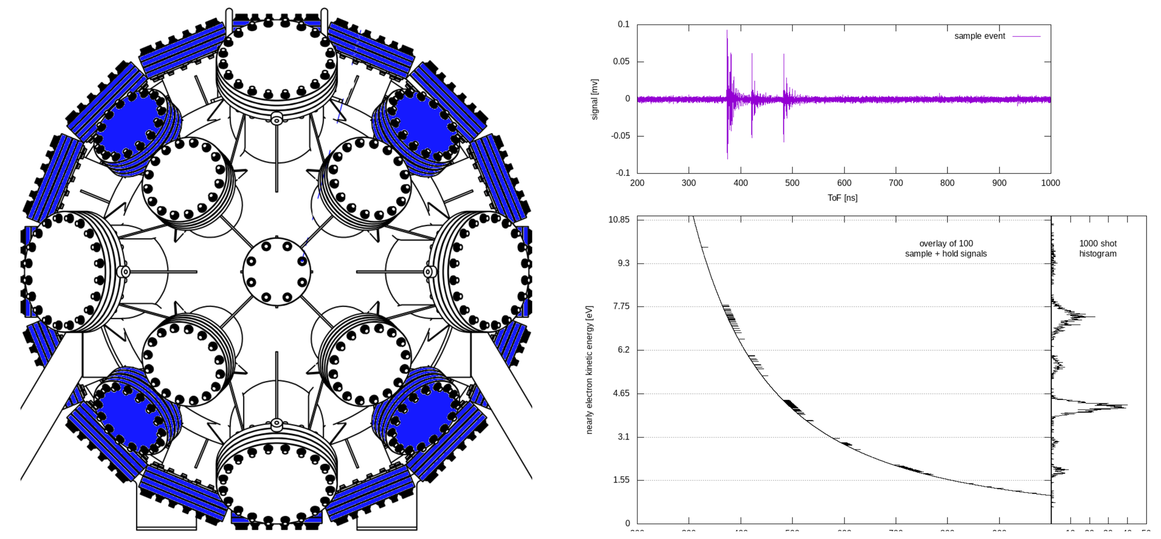

Figure 5. (left) The CookieBox detector array, blue indicates the 20 ToF spectrometer angles, the x-ray beam is directed central and coming out of the page. (right) Fitted logarithmic mapping from time-of-flight to energy optimizes resolution distribution.

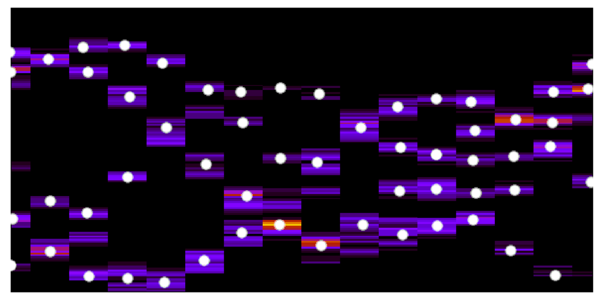

Figure 6. Example angular emission for the attoclock spectroscopy case for a few spike spike shot. Note that sinogram reconstruction algorithms are commonplace in the radiography community.

Dynamic configuration

- Any or all 20 angles (blue in Fig. 5) can be populated with ToFs, each with potentially different (and drifting) retardation, e.g. energy windows
- Cross-channel correlations represent the relevant sinograms of Fig.6 and would be collated similarly as in FES case.
- FPGA implemented networks for initial phase achieve desirably low few μ-second scale latency [10].

Data and Simulation rich

- Parasitic operation as on-line FEL diagnostic with feedback to accelerator control system,
- Currently building Edge@LCLS$\Longleftrightarrow$ALCF@Argonne data$\Longleftrightarrow$model exchange.

Time-Tagged Radiography for ToF-PET

Transferring the x-ray timing methods from the LCLS to time-of-flight Positron Emission Tomography (ToF-PET) could deliver a 100-fold improvement in imaging resolution and allow direct image reconstruction. [11] We are therefore pursuing a joint project with Stanford Radiology to significantly improve the coincidence time resolution based on the 2D-spectrogram timing method.

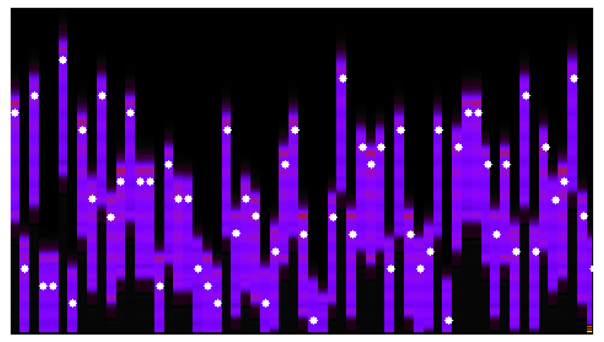

Figure 7. Two-dimensional spectrogram encoding [12, 13] of femtosecond time-resolved x-ray material interaction. Each column of the image represents the spectral encoded arrival time of a photon for a particular spatial location.

Static configuration

- Spectrum $\mapsto$ time mapping along each column varies with temperature and drive-laser intensity,
- Inter-column correlations encode the spatial mode of the x-ray pulse,
- The space $\mapsto$ column mapping is fixed but pathological and so must be collated in deeper layers as in the Fusion and Attoclock examples,

Open Data/Model Marketplace for All

The common theme across all three use cases of Edge Computing and ML is that they will all similarly and actively transform the raw signals into actionable information. Adoption of an open data and model marketplace would encourage sharing of validated methods over "hand rolled" fragile methods, ensure data integrity, and enable forensic provenance reconstruction.

- Searchable such that data and models where use cases have high degrees of functional overlap,
- Encode the data transformation chain in a record that identifies active models,
- Model versions would include identifiers to the training and validation sets.

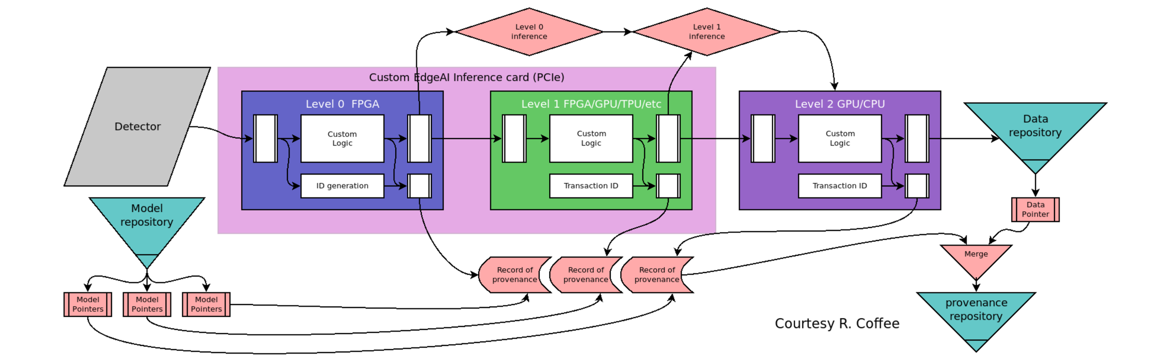

Figure 8. Proposed development of an integrated dataflow transformation with integrated provenance tracking.

Acknowledgements

The work represented here spans multiple projects supported by multiple agencies as follow: DOE-FES FWP 100636 "Machine Learning for Real-time Fusion Plasma Behavior Prediction and Manipulation", DOE-BES FWP 100498 "Enabling Long Wavelength Streaking for Attosecond X-ray Science", SLAC-LDRD "Machine Learning for Data Reduction at LCLS-II: A Path Toward 1 MHz Detection", DOE-BES FWP 100643 "Actionable Information from Sensor to Data Center", NIH PN 5R01EB023903-04 "A new direction to achieve ultra-fast timing for positron emission tomography".

References

[1] L. Cui *et al.*,. The energy confinement response of DIII-d plasmas to resonant magnetic perturbations. *Nuclear Fusion*, 57(11):116030, aug 2017.
[2] R. A. Moyer *et al.*,. Imaging divertor strike point splitting in rmp elm suppression experiments in the diii-d tokamak. *Review of Scientific Instruments*, 89(10):10E106, 2018.
[3] David R. Smith. private communication.
[4] William Heidbrink. The labeled dataset is the result of a single expert hand identifying likely regions of particular types of fluctuating modes.
[5] Wolfram *et al.*,. Helml. Ultrashort free-electron laser x-ray pulses. *Applied Sciences*, 7(9):915, 2017.
[6] Taran *et al.*,. Driver. Attosecond transient absorption spooktroscopy: a ghost imaging approach to ultrafast absorption spectroscopy. *Phys. Chem. Chem. Phys.*, 22:2704–2712, 2020.
[7] N. Hartmann *et al.*,. Attosecond time–energy structure of x-ray free-electron laser pulses. *Nat. Photon.*, 12:215, 2018.
[8] Siqi Li *et al.*,. Characterizing isolated attosecond pulses with angular streaking. *Opt. Express*, 26(4):4531–4547, Feb 2018.
[9] R. *et al.*,. Heider. Megahertz-compatible angular streaking with few-femtosecond resolution at x-ray free-electron lasers. *Phys. Rev. A*, 100:053420, Nov 2019.
[10] *et al.*,. Corbeil Therrien. Machine learning at the edge for ultra high rate detectors. pages 1–4, 10 2019.
[11] Li Tao *et al.*,. Ionizing photon interactions modulate the optical properties of crystals with femtosecond scale temporal resolution. *Physics in Medicine Biology*, 2021.
[12] Hartmann N. *et al.*,. Sub-femtosecond precision measurement of relative x-ray arrival time for free-electron lasers. *Nat. Photon.*, 8:706, 7 2014.
[13] Ryan N. *et al.*,. Coffee. Development of ultrafast capabilities for x-ray free-electron lasers at the linac coherent light source. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 377(2145):20180386, 2019.

Figure 3. Sample of Beam Emission Spectroscopy measurements sampling the inter-channel covariance versus time during the shot.