Virtual Spectroscopy and Surrogate Models at the European XFEL

Fady Bishara

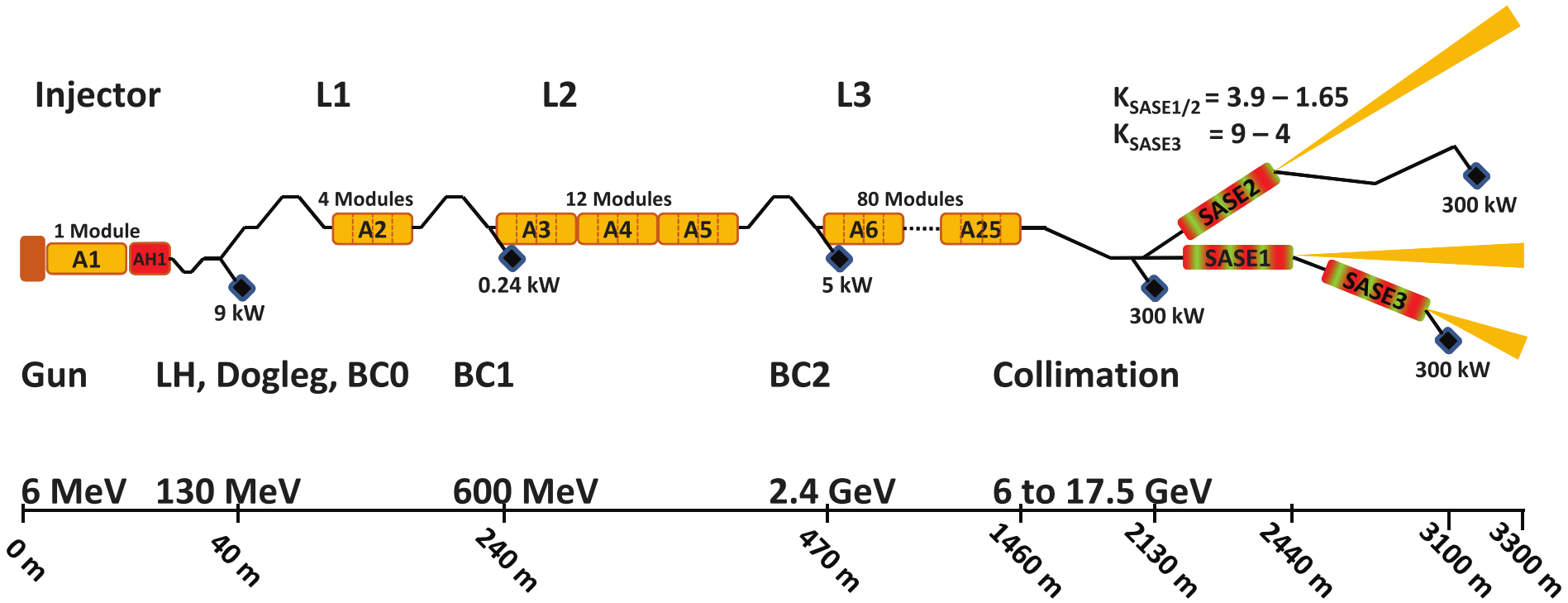
with: Danilo Enoque Ferreira de Lima + many others

Virtual Diagnostics Workshop

Frascati, 8 November 2024

European XFEL

EuXFEL: an amazing machine



[Modified figure, original from talk by W. Decking (DESY)]

EuXFEL: an amazing machine

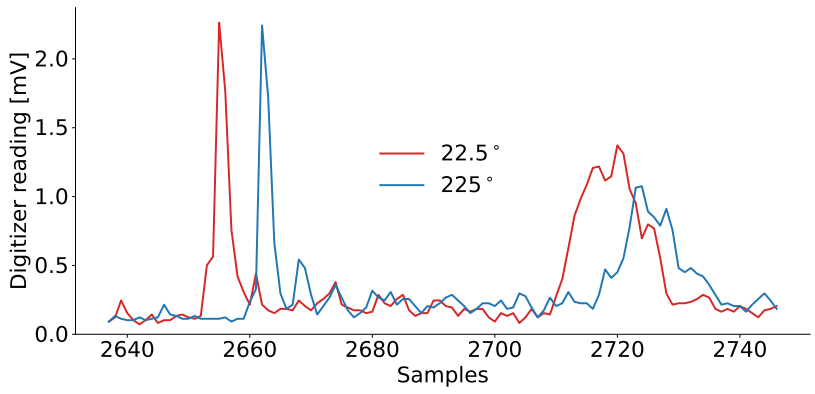
- Brilliant x-ray pulses for science
- Consistent spectral properties
- Extremely complicated system
- Massive amounts of **diagnostics** data
- Use this data to help operators and users
  - Virtual spectrometer: enhance physical diagnostics
  - Surrogate model: virtual diagnostics for users and machine operators

Virtual Spectrometer

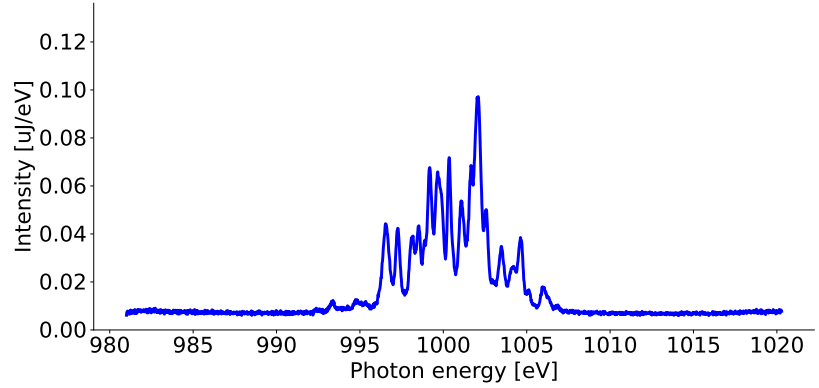
[Virtual Diagnostics]

Enhancing non-invasive X-ray diagnostics

Photo-Electron Spectrometer (PES)



Grating Spectrometer (GS)

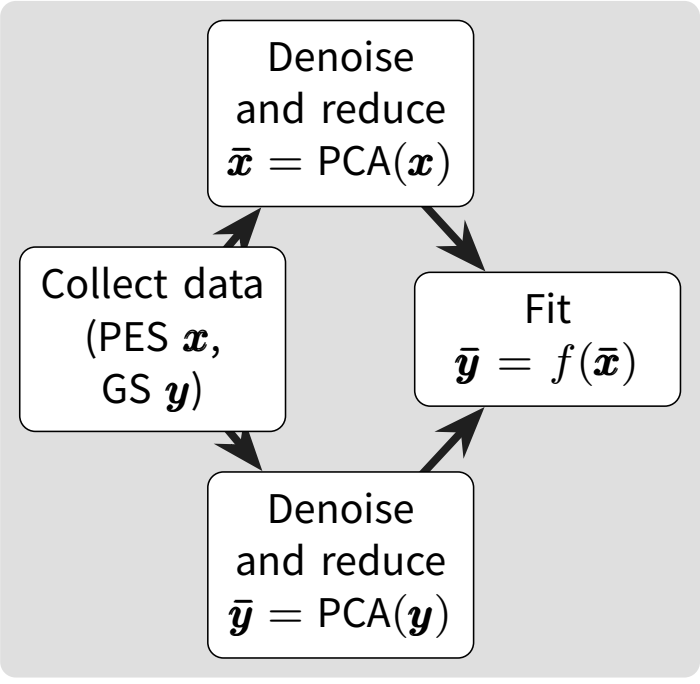


- ✔ Non-invasive
- ✔ Pulse-resolved
- 😐 Complex calibration
- 😐 Low resolution

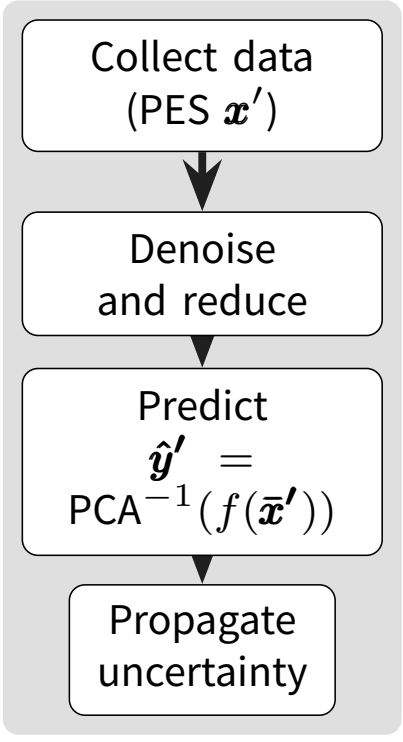
- 😐 Invasive
- 😐 Train-resolved
- ✔ Simple calibration
- ✔ High resolution

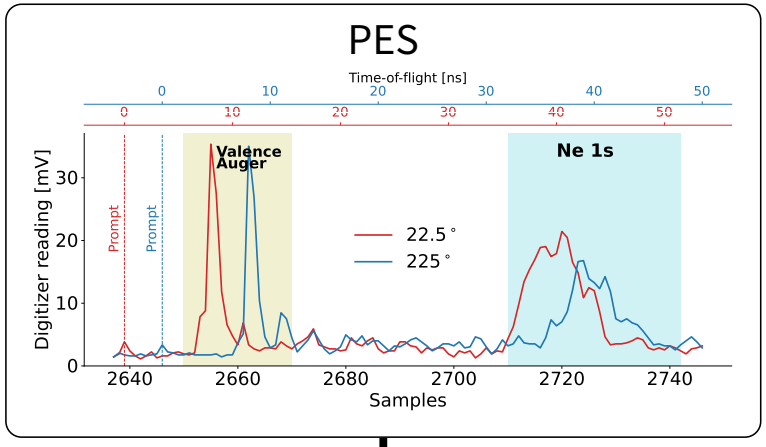
Enhancing non-invasive X-ray diagnostics: method

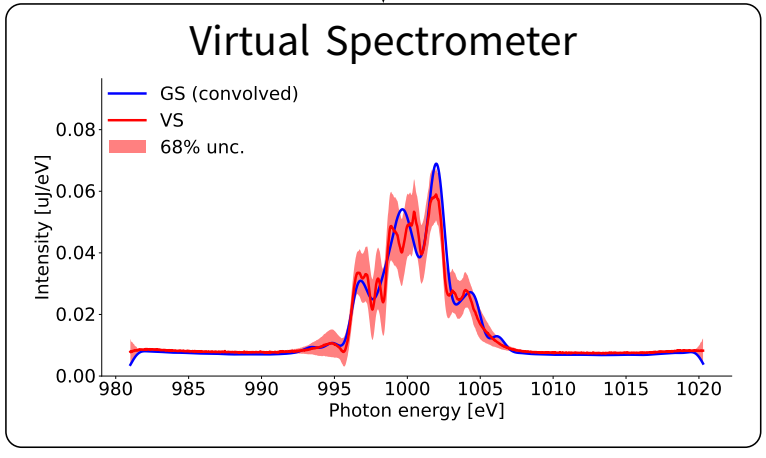
Training



Inference

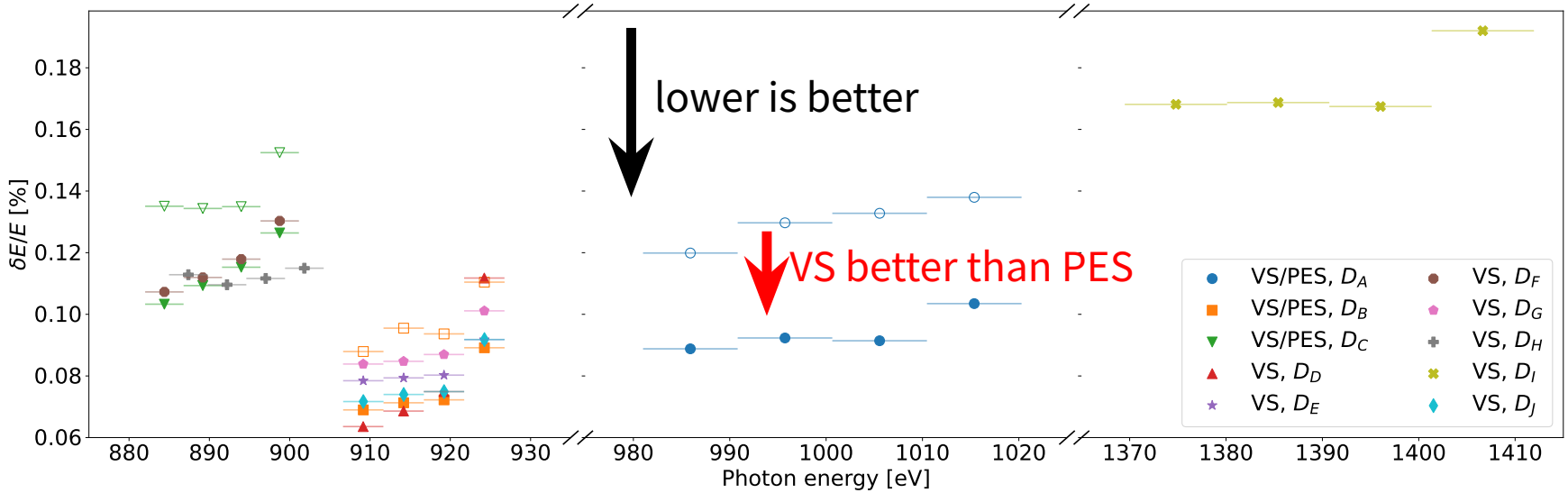






Virtual Spectrometer's resolution

- Systematic resolution studies under several conditions done
- Comparison with PES show better resolution
- Resolution calculated after training to inform scientists

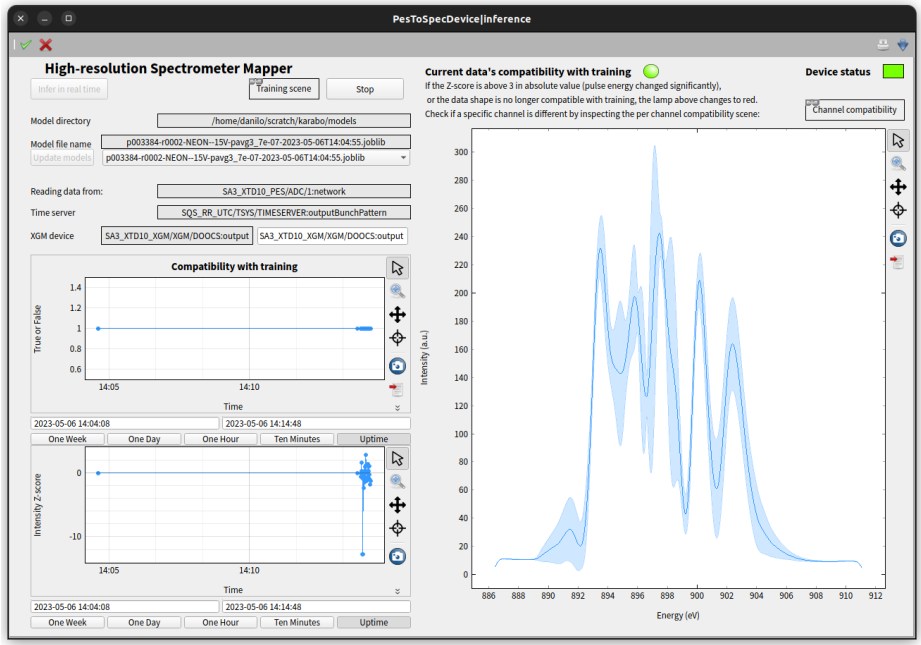


PES: open symbols; VS: full symbols.

[https://doi.org/10.21203/rs.3.rs-4610683/v1]

Deployment online and outlook

- Deployed w/ simple interface to retrieve data and integrate ML projects
- Combines advantages of low- and high-resolution devices:
  - ✔ Non-invasive
  - ✔ Pulse-resolved
  - ✔ Automated calibration
  - ✔ Improved resolution
- Design guidelines:
  - Embedded quality control
  - Resolution and uncertainty estimate
  - SASE principle guides denoising

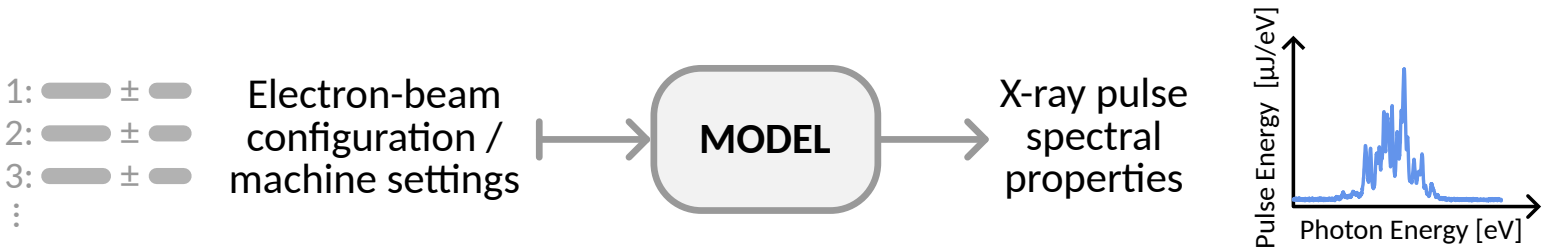


- Outlook:
  - Expand project for hard photons
  - Interpolate conditions to avoid pre-training stage

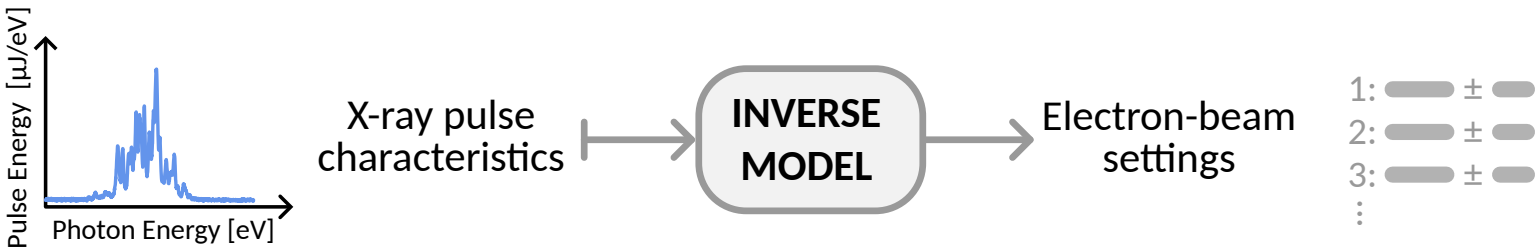
Beam Tuning

[Surrogate Model]

1 Give users valuable information about spectral properties non-invasively and at MHz rates while conducting experiments



② Give real-time guidance and feedback to assist operators to tune the machine to users' specification



Photon beam properties

- Central wavelength, bandwidth, Intensity, number of modes
- …

Table 3: Photon energy in keV as a function of magnetic gap and electron energy. Numbers in grey indicate gap settings that are unlikely to provide saturation.

	Electron energy					
	SASE1 and SASE2 (λ_u=40 mm)			SASE3 (λ_u=68 mm)		
Magnetic gap	10.5 GeV	14 GeV	17.5 GeV	10.5 GeV	14 GeV	17.5 GeV
10 mm	2.3	4.1	6.4	0.26	0.47	0.73
12 mm	3.4	6.9	9.3	0.34	0.54	0.84
15 mm	5.5	9.8	15.3	0.45	0.80	1.25
20 mm	10.5	18.7	29.2	0.95	1.68	2.63
24 mm	14.9	26.5	41.4	1.5	2.6	4.1
28 mm	18.6	33.1	51.7	2.2		

[XFEL.EU TR-2011-001]

Electron beam parameters

- Phase space
- Undulator parameters

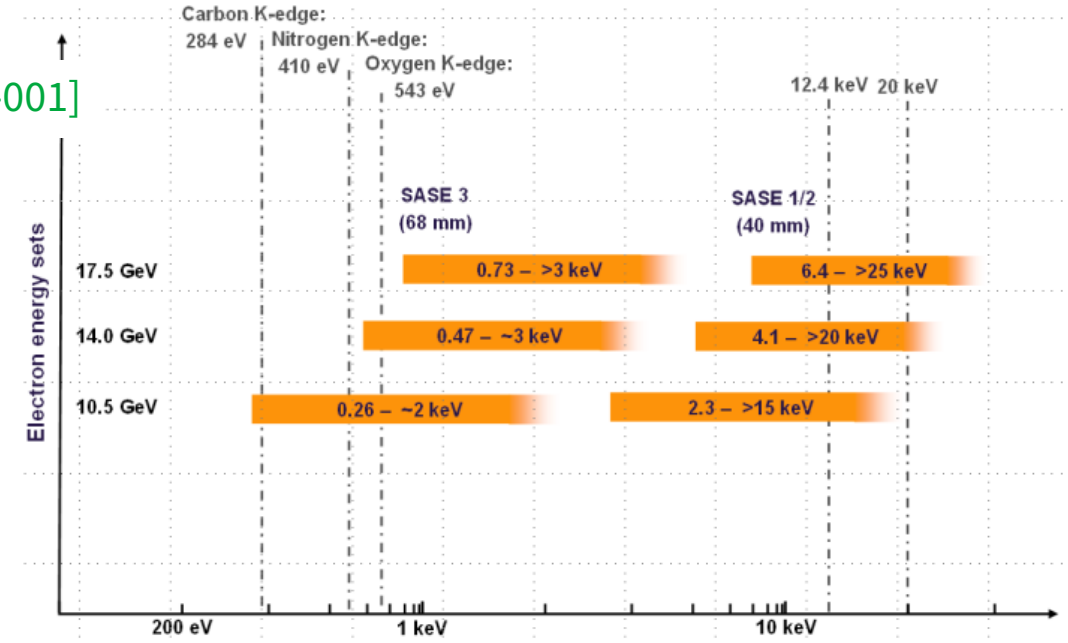
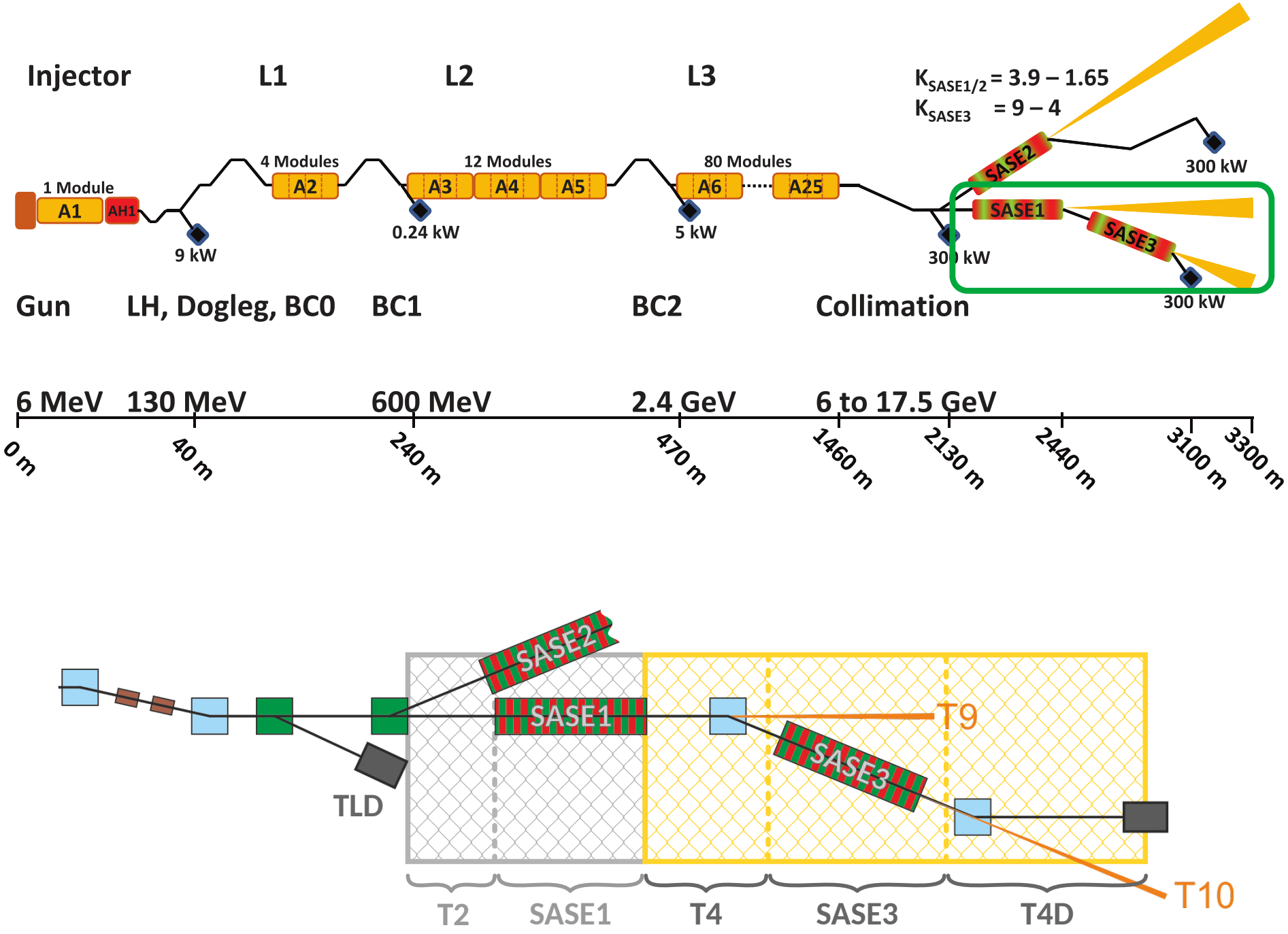


Figure 1: Photon energy ranges of SASE1, SASE2, and SASE3 undulators for the electron energies 10.5, 14, and 17.5 GeV. While the low energy cut-offs are fixed (compare with Table 3), the highest accessible energies are determined by the electron beam parameters and the magnetic length of the undulators.

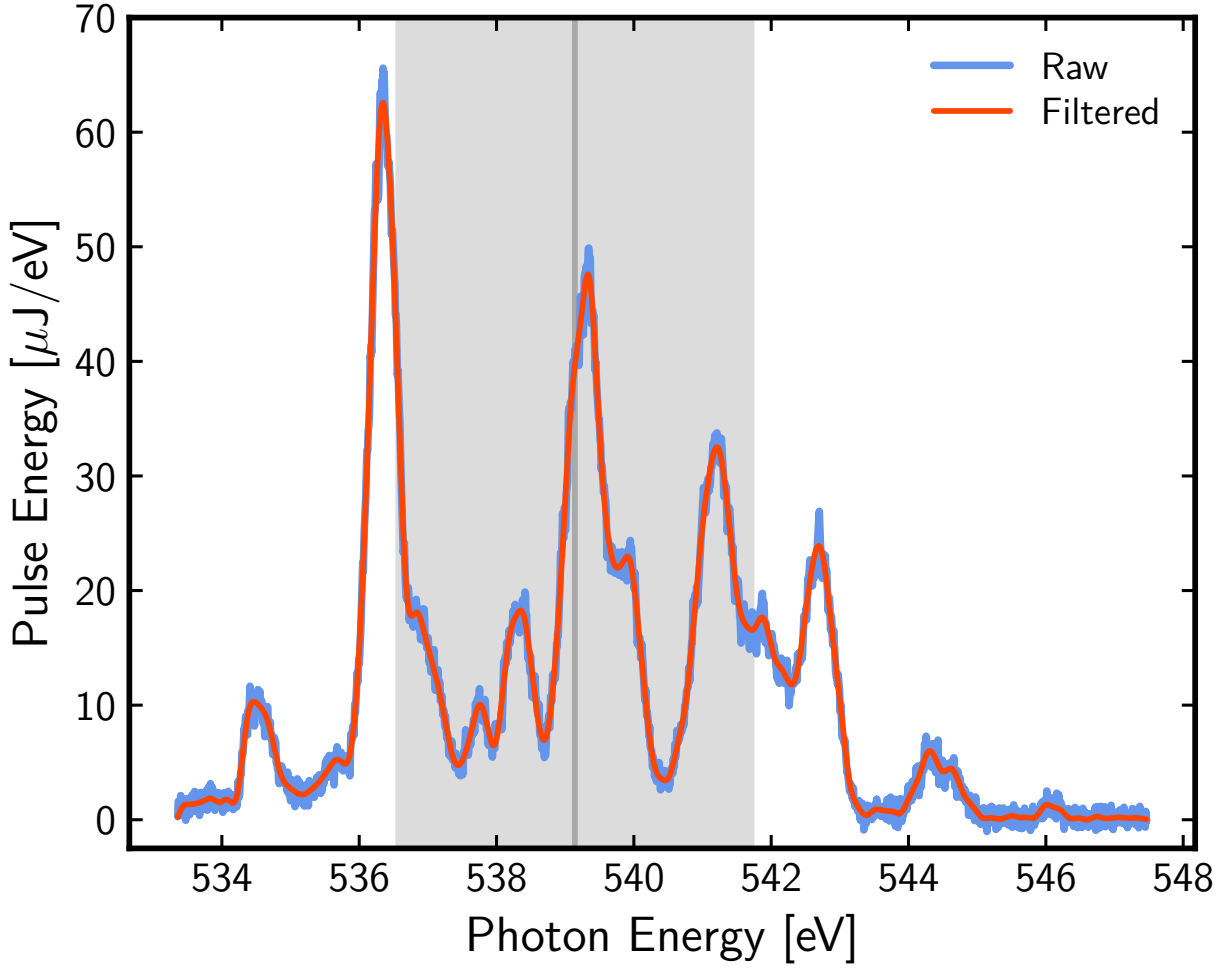
Roadmap

- Identify relevant parameters / collect data
- *Clean* the data (de-noising, feature engineering)
- Statistical analysis
- Model building
- **Interpretability** and uncertainty quantification

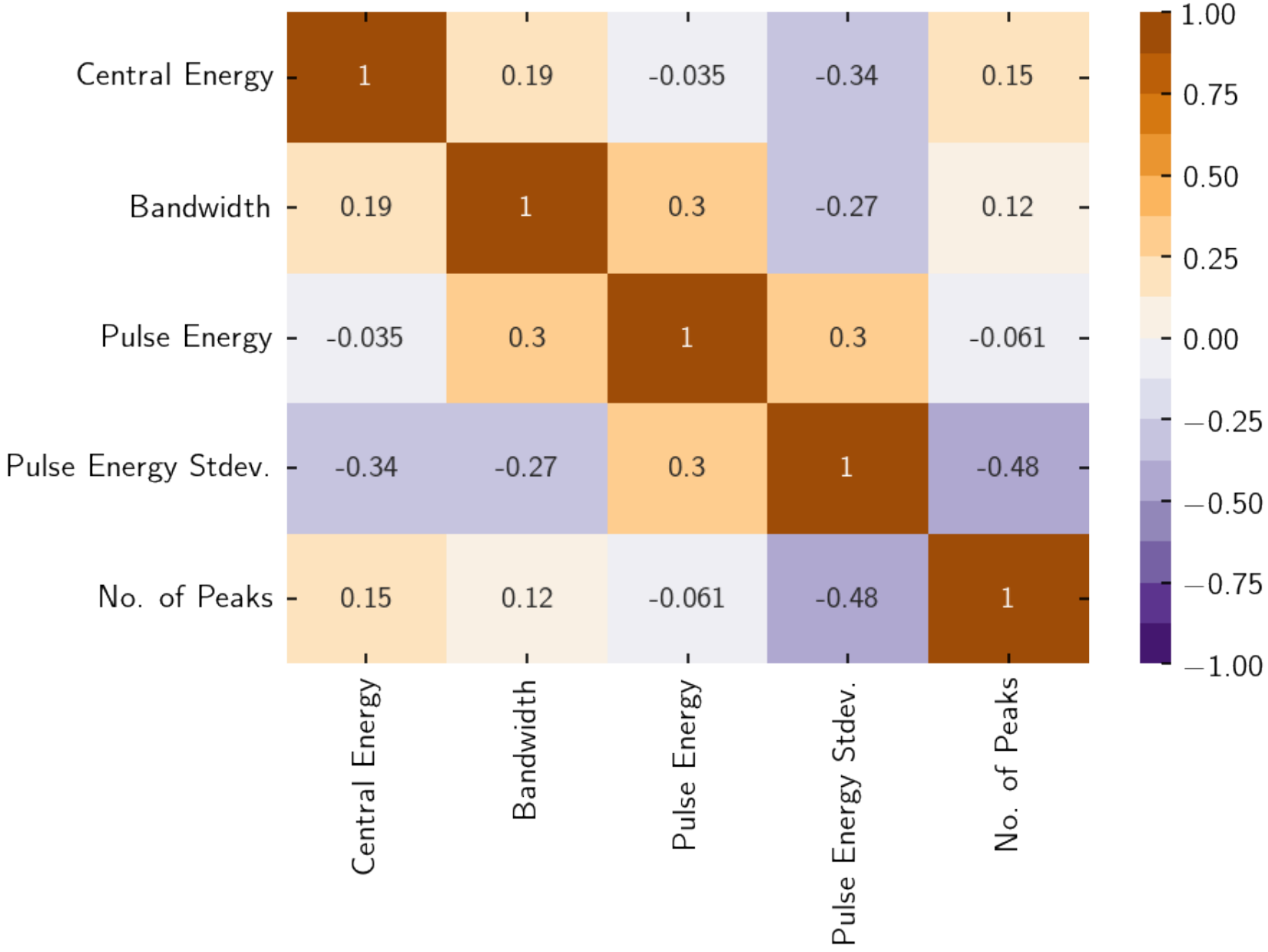

Injector
L1
L2
L3
$K_{SASE1/2}$ = 3.9 – 1.65
K_{SASE3} = 9 – 4
1 Module
A1
AH1
4 Modules
A2
12 Modules
A3
A4
A5
80 Modules
A6
A25
9 kW
0.24 kW
5 kW
300 kW
SASE2
SASE1
SASE3
300 kW
300 kW
Gun
LH, Dogleg, BC0
BC1
BC2
Collimation
6 MeV
130 MeV
600 MeV
2.4 GeV
6 to 17.5 GeV
0 m
40 m
240 m
470 m
1460 m
2130 m
2440 m
3100 m
3300 m
SASE2
SASE1
T9
SASE3
TLD
T10
T2
SASE1
T4
SASE3
T4D

Spectral properties

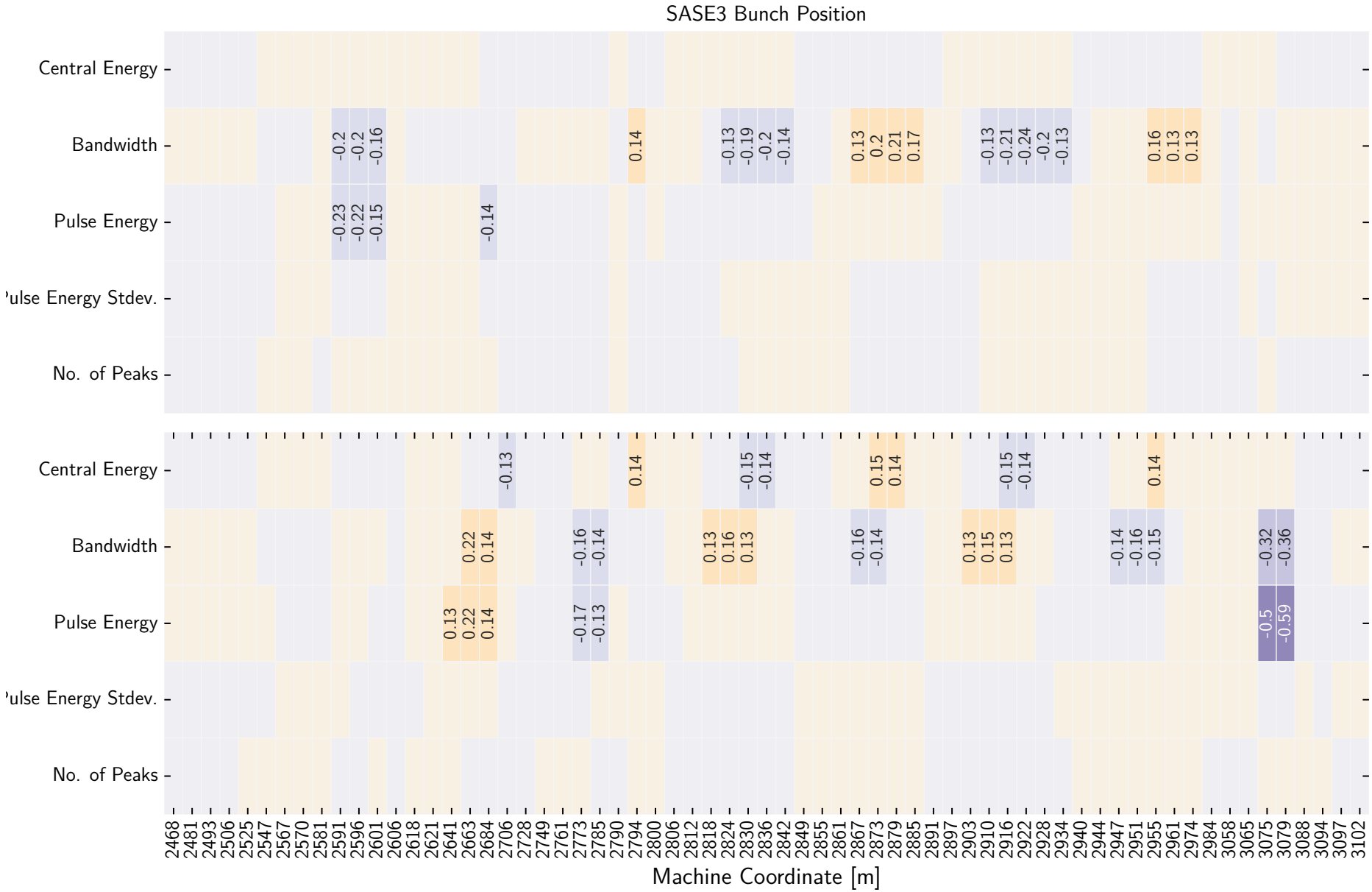
- Central energy
- Bandwidth
- Pulse energy
- Pulse energy var.
- Number of peaks



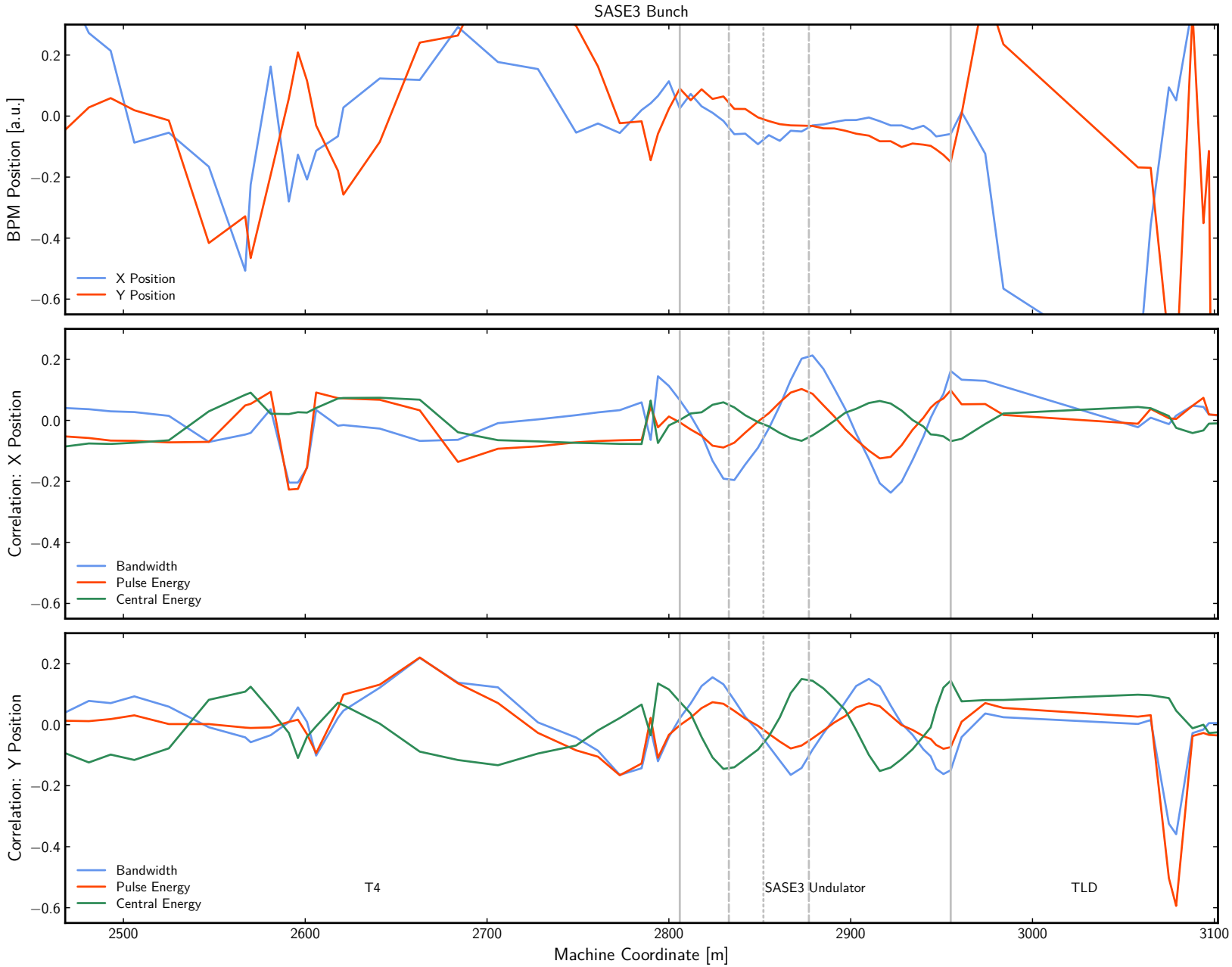
Correlations



Correlations



Correlations



Summary and Outlook

Virtual spectrometer: deployed @ MHz repetition rate $\rightarrow$ enhances photo-electron spectrometer

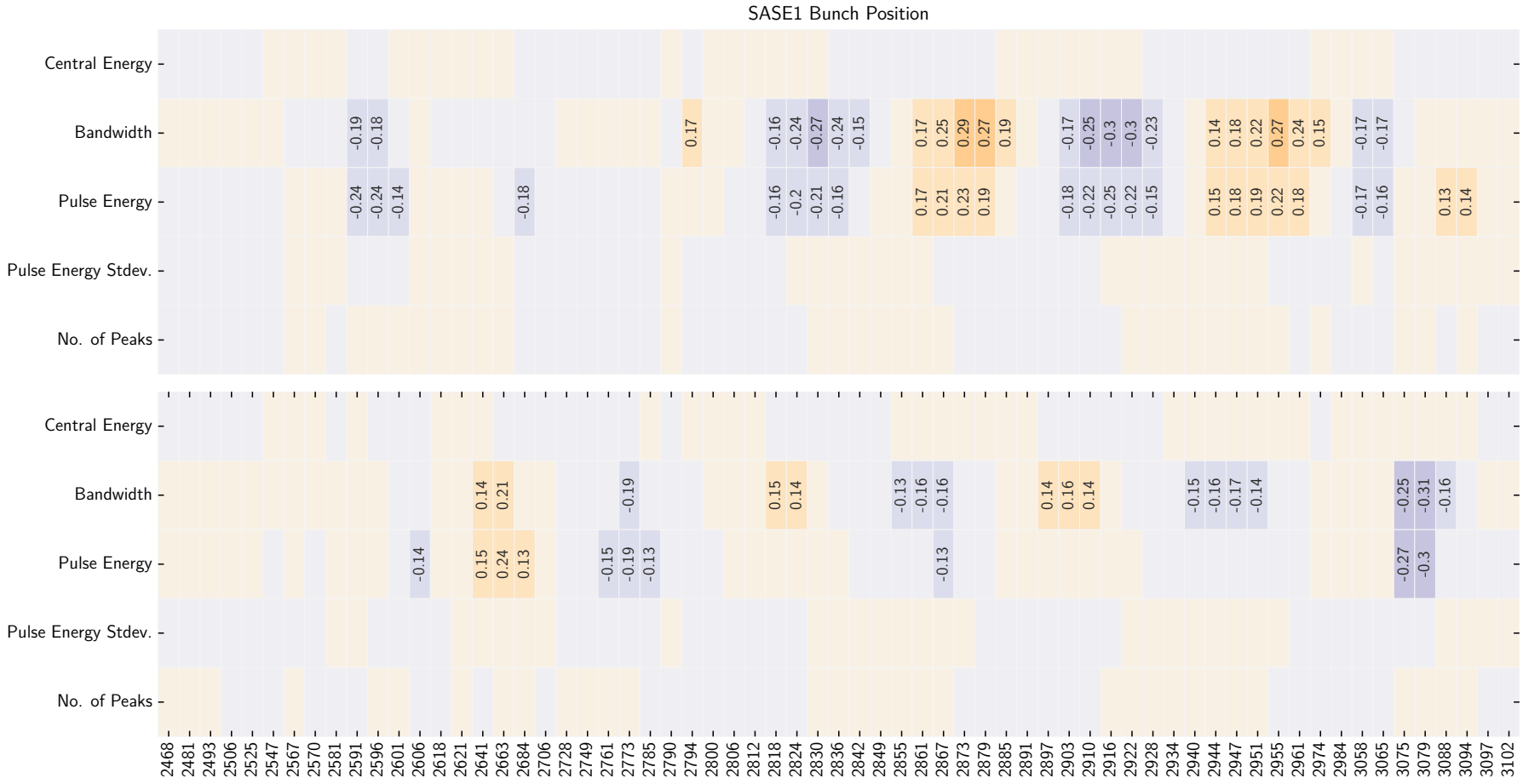
- Expand project for hard photons
- Interpolate conditions to avoid pre-training stage

Beam tuning: surrogate model to gives users real-time virtual diagnostics @ MHz repetition rates *and* guide operators in tuning and control

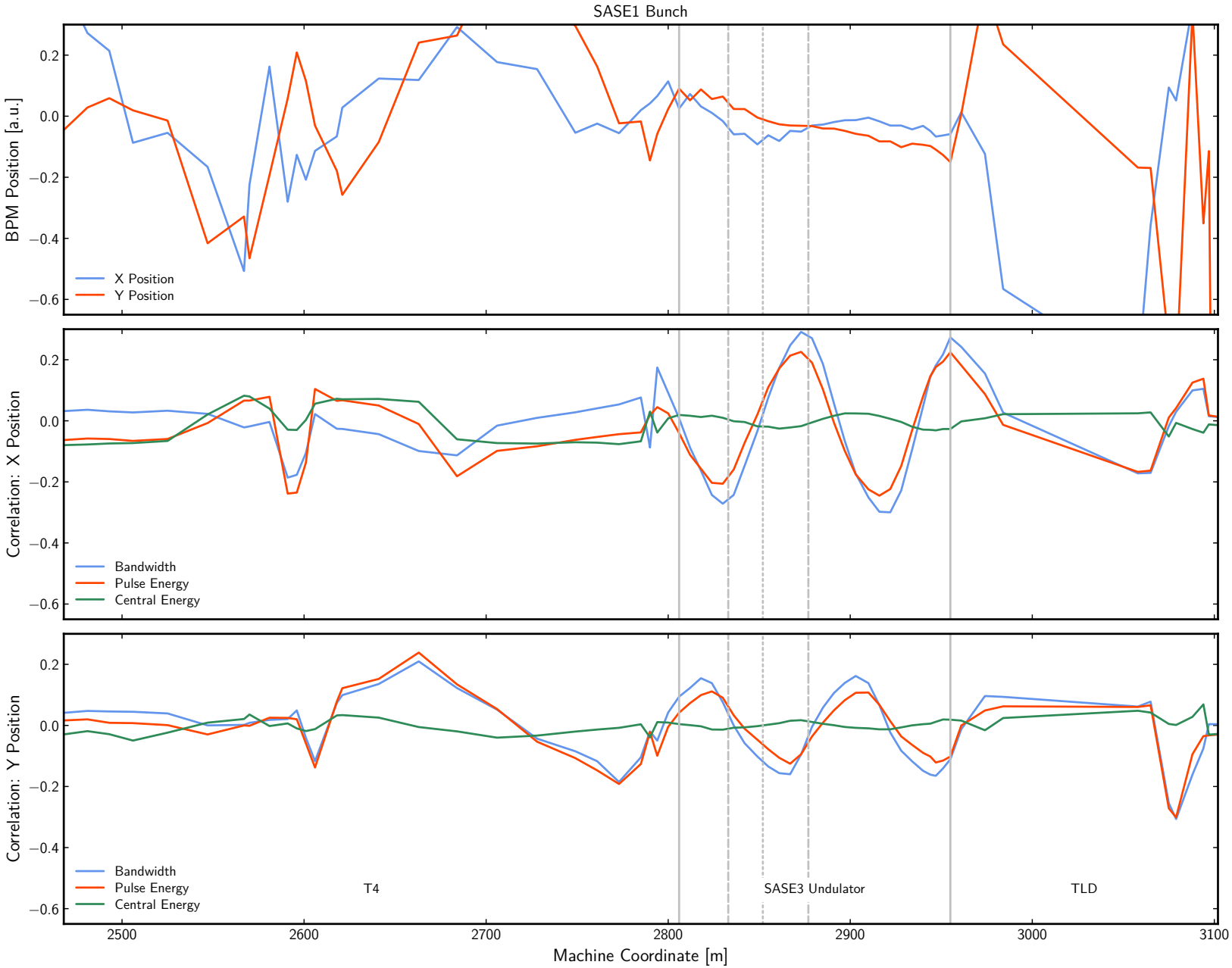
- Much more data to analyze
- Build a model to predict spectral properties

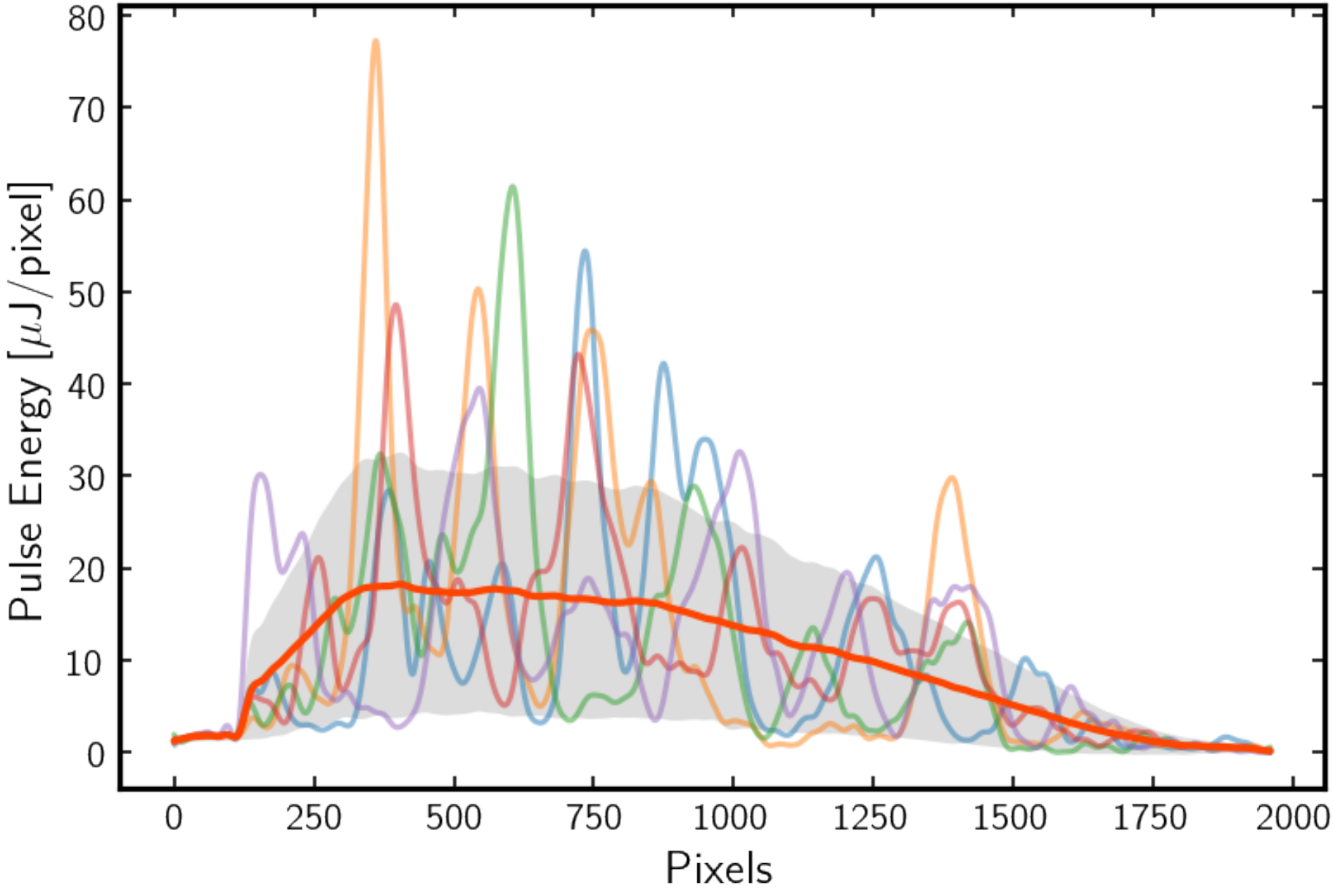
Additional Material

Correlations

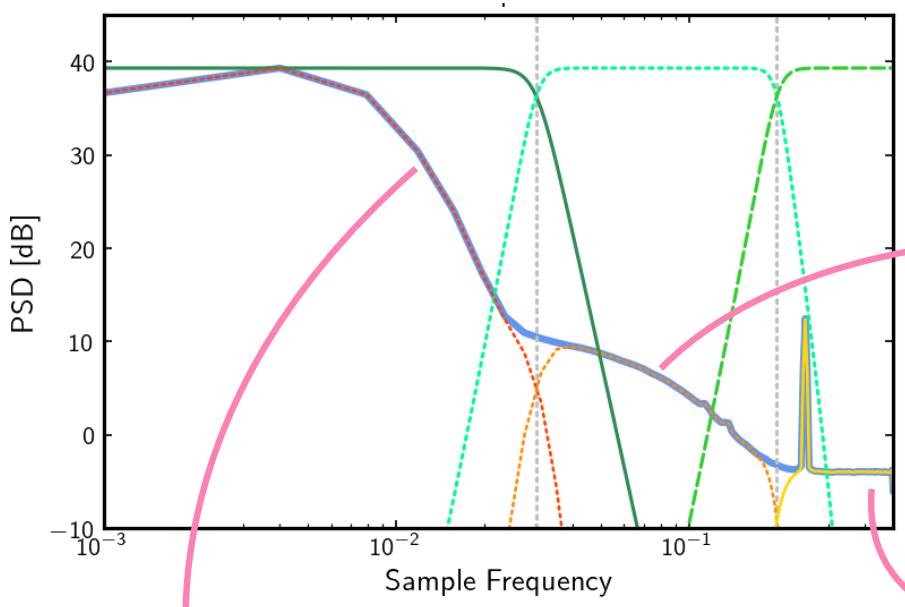


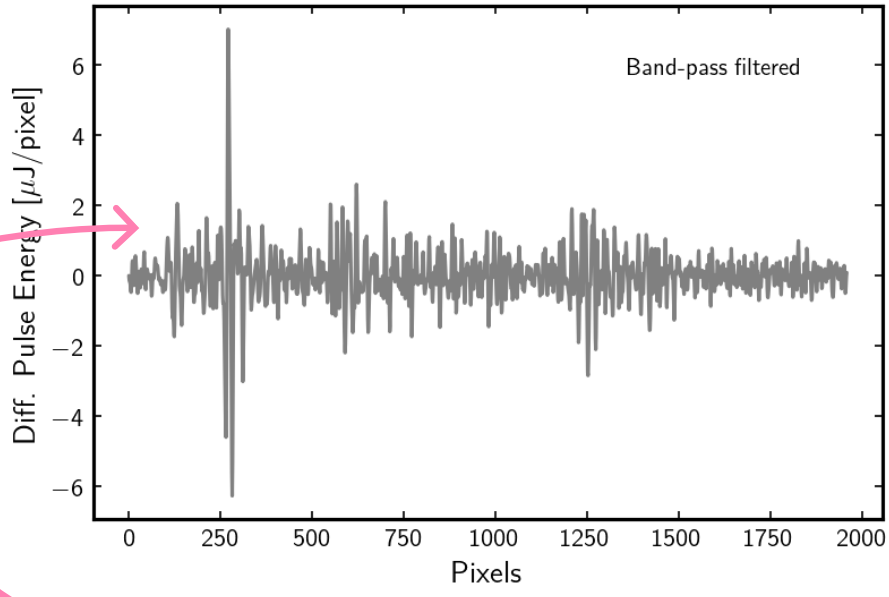
Correlations

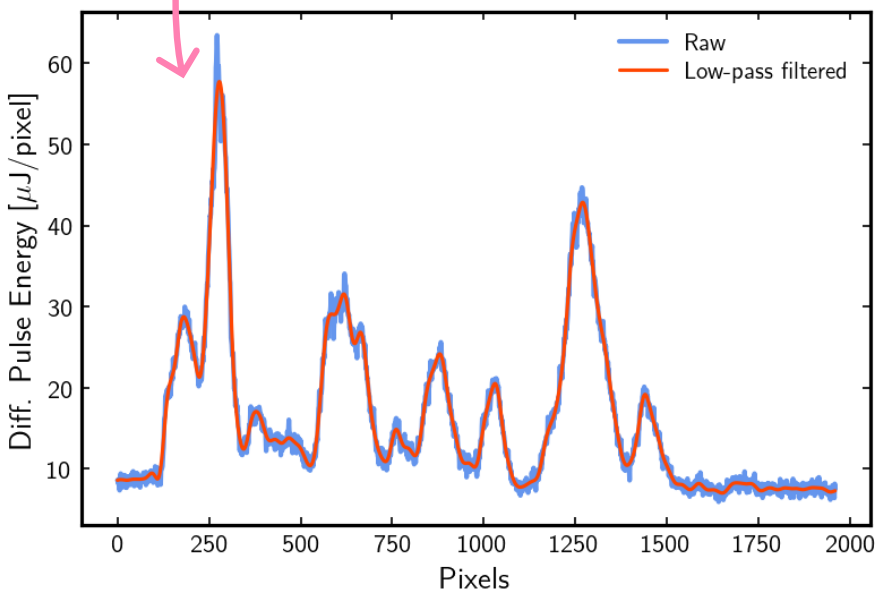


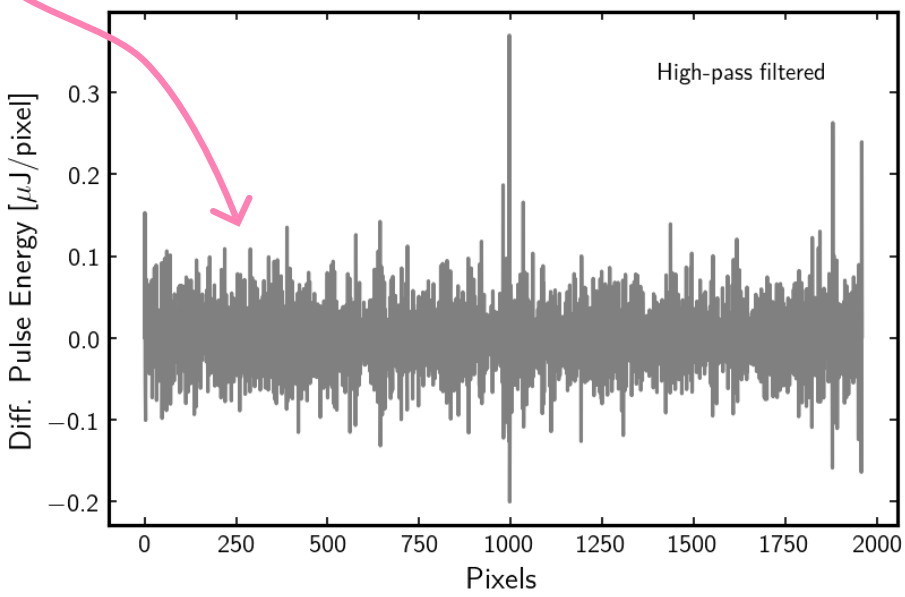

Pulse Energy [μJ/pixel]
0
10
20
30
40
50
60
70
80
0
250
500
750
1000
1250
1500
1750
2000
Pixels

Filtering

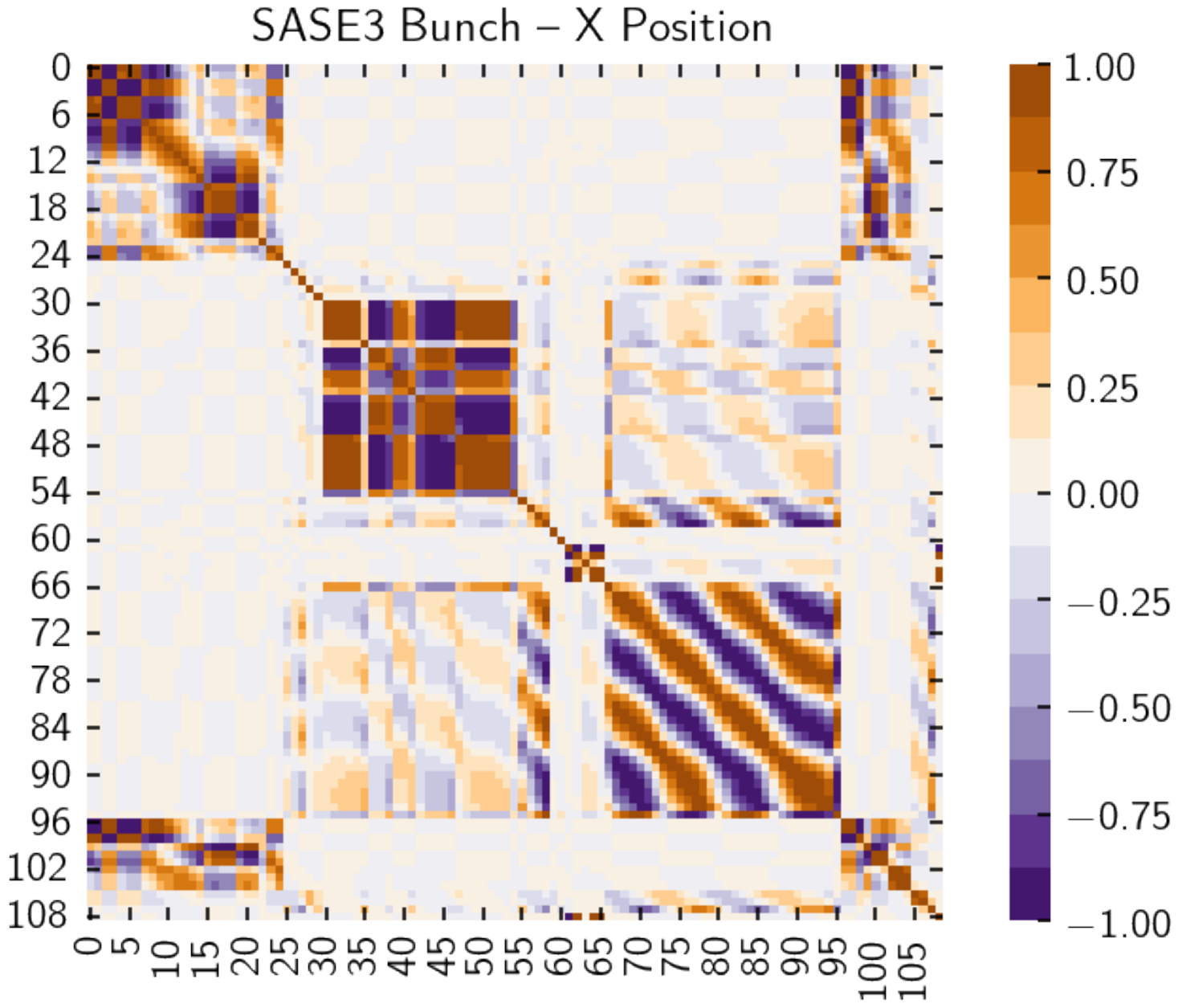

PSD [dB]
Sample Frequency


Band-pass filtered
Diff. Pulse Energy [μJ/pixel]
Pixels

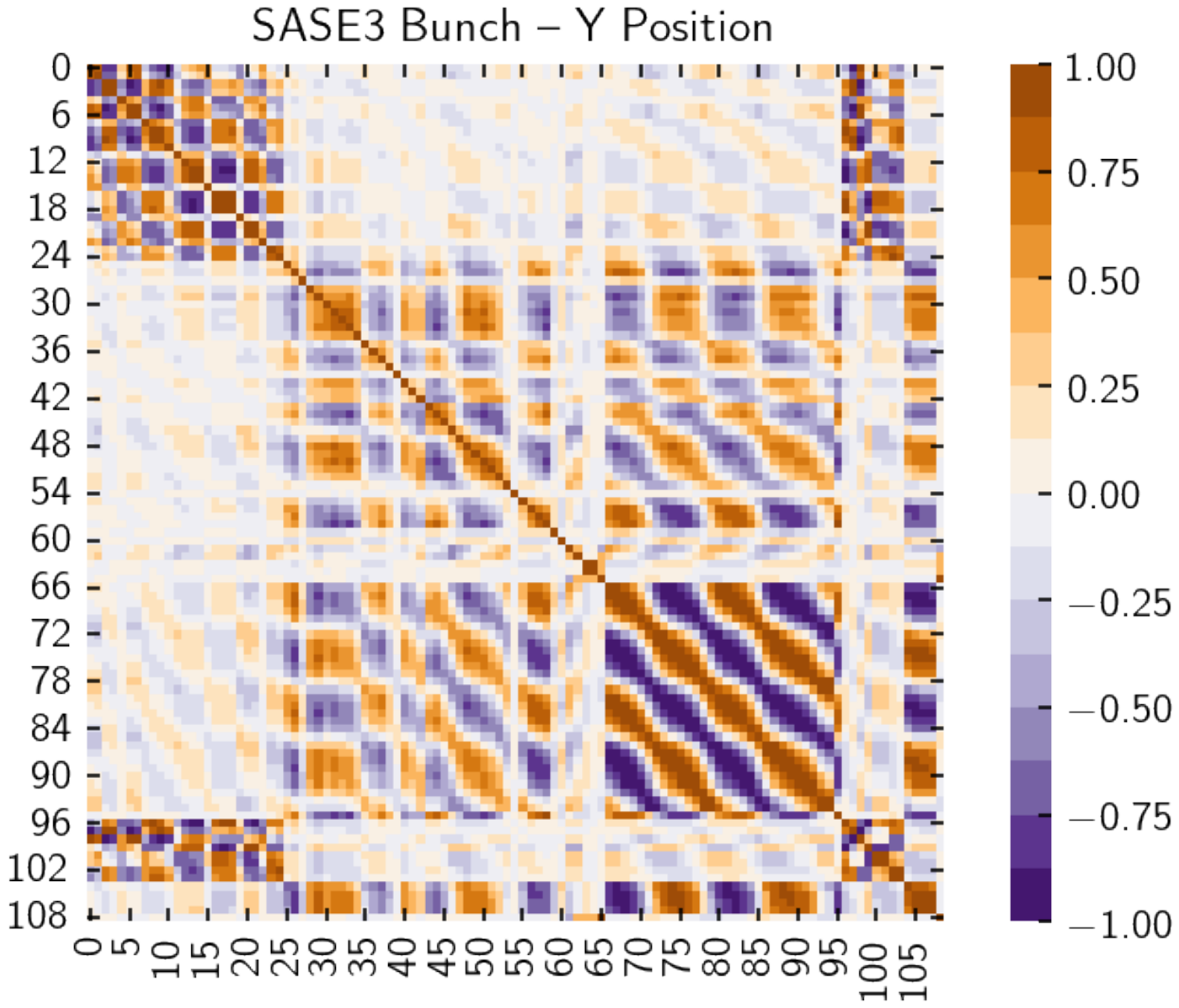

Raw
Low-pass filtered
Diff. Pulse Energy [μJ/pixel]
Pixels


High-pass filtered
Diff. Pulse Energy [μJ/pixel]
Pixels

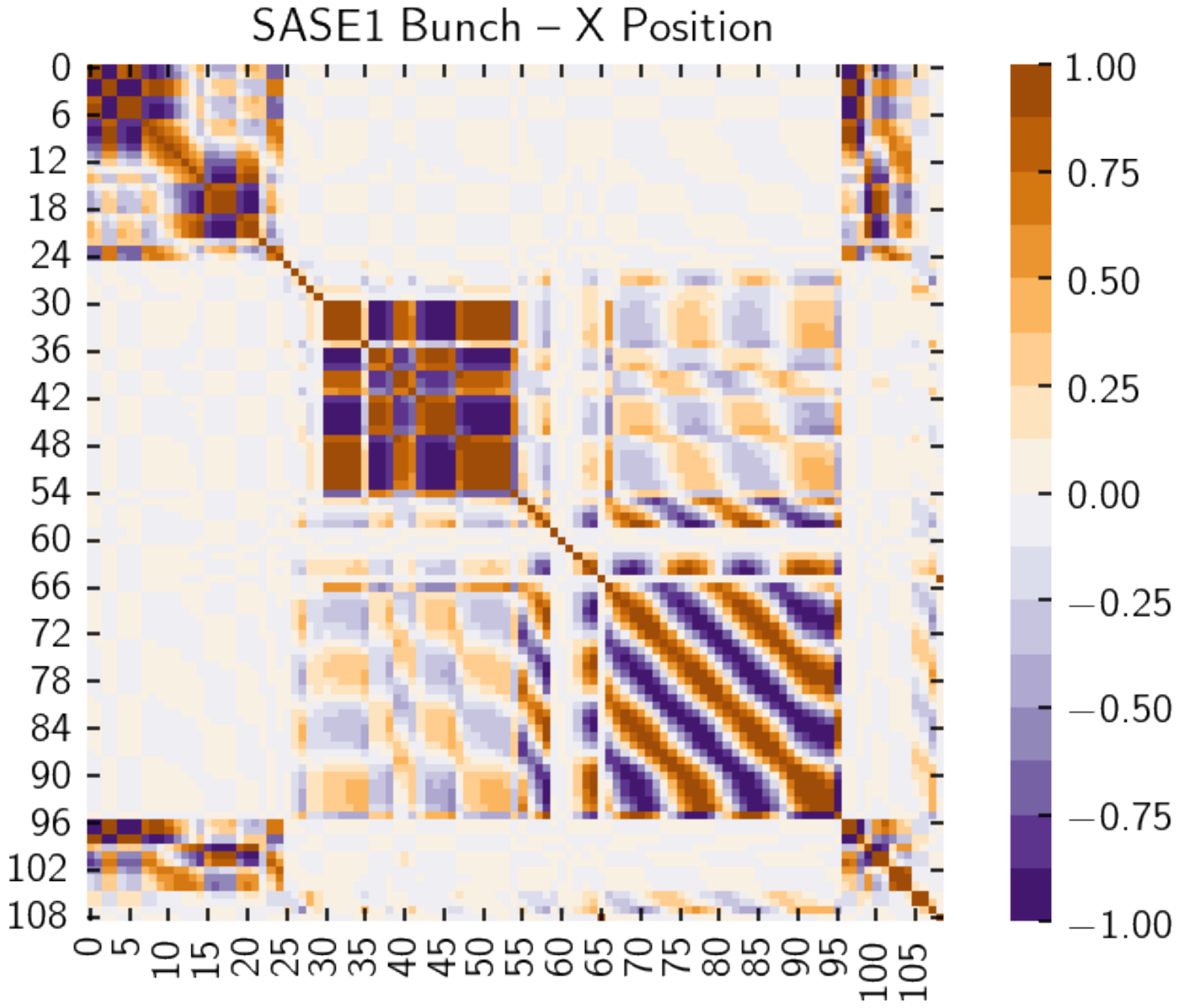
Bunch position monitors: T4, SASE3, TLD



Bunch position monitors: T4, SASE3, TLD



Bunch position monitors: T4, SASE3, TLD



Bunch position monitors: T4, SASE3, TLD