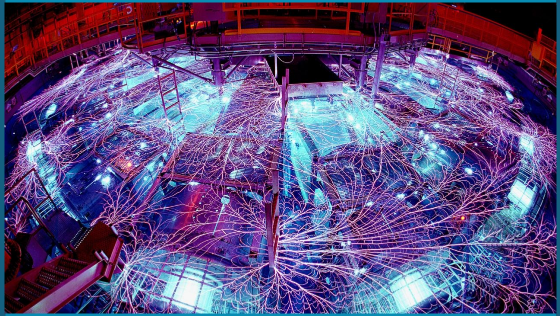
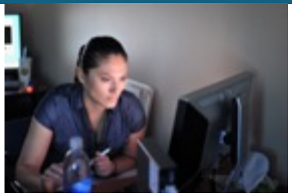
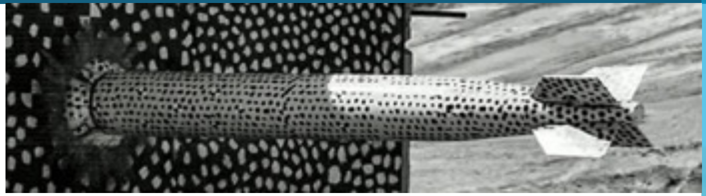
SAND2023-04286C

Developing a machine learning based spectral analysis tool to understand Argon gas puff implosion dynamics on Z







PRESENTED BY

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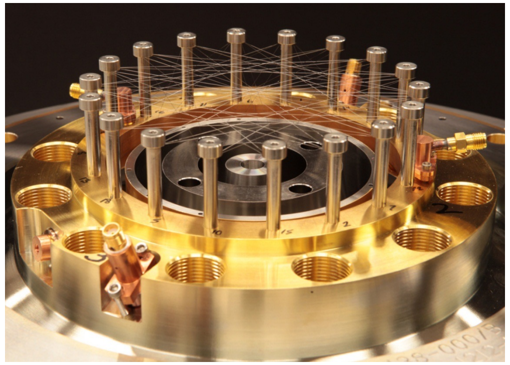
- Argon (Ar) gas puffs regularly produce > 350 kJ of x-rays at > 3 keV. Many outstanding questions regarding their fundamental physics can be answered through detailed spectral analyses.



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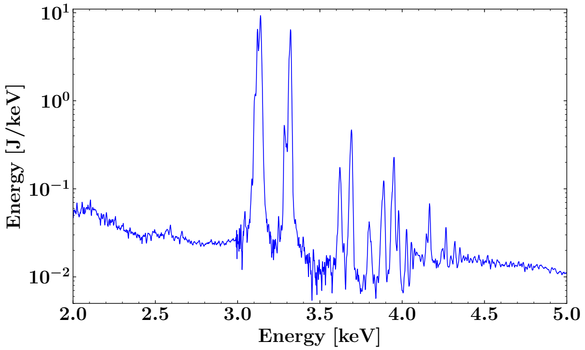
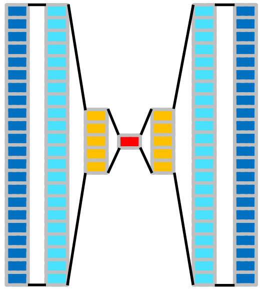


- We're in the process of developing an ML-based spectral model that outperforms traditional interpolation approaches in both accuracy and efficiency.

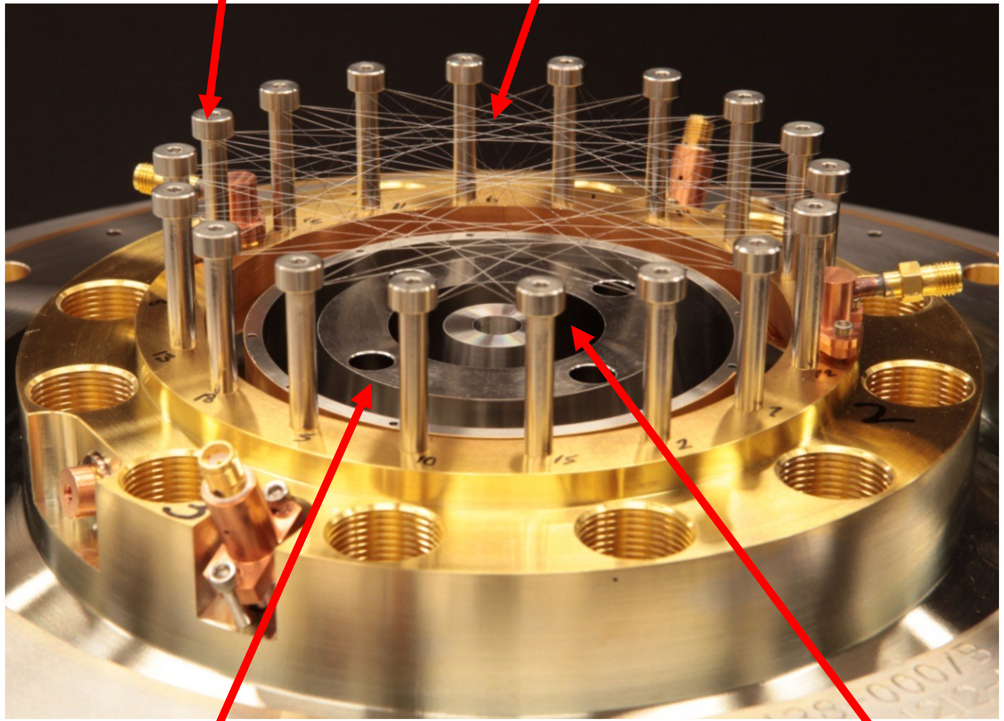


Coupling Bayesian statistics and ML models should allow us to develop a better understanding of Ar gas puffs.

The Ar gas puff on the Z-machine couples the accelerator current to the experimental gas.

Current return post

Wire mesh



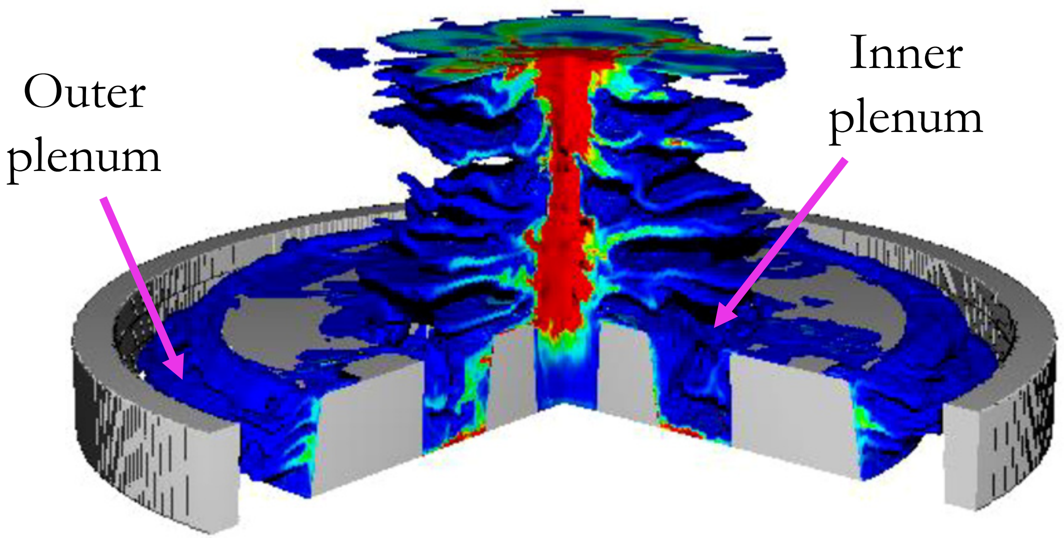
Harvey-Thompson et al. (2016), *Phys. Plasmas*

Outer gas nozzle plenum

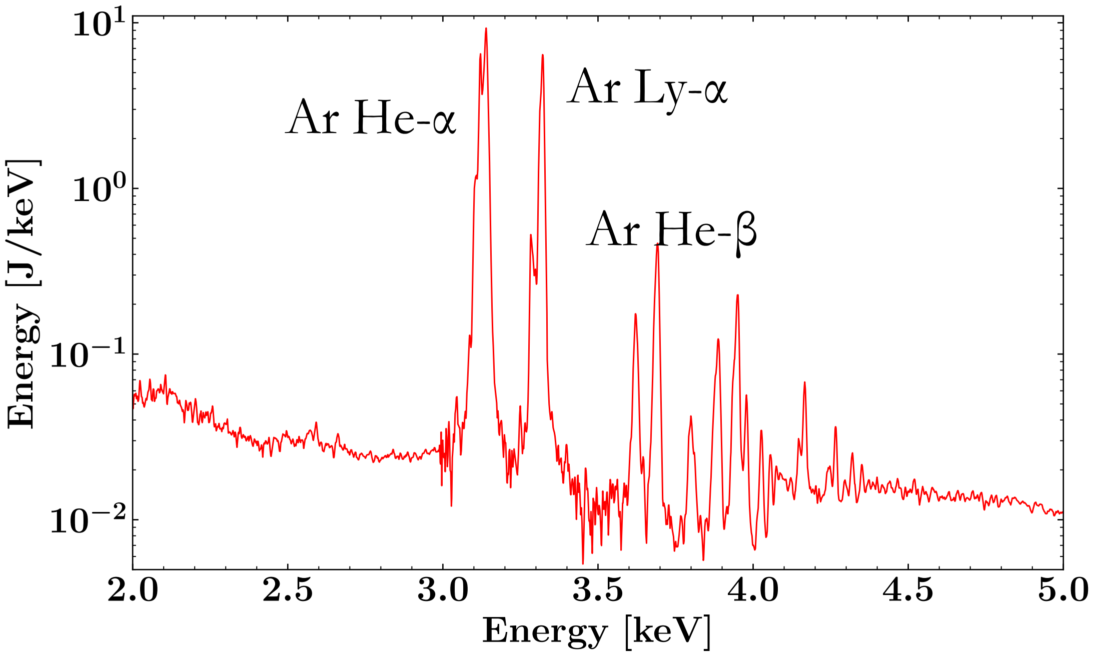
Inner gas nozzle plenum

- The Z-machine at Sandia National Laboratories supplies ~16 MA of current to the Ar gas puff platform.
- The outer gas shell conducts this current and begins to implode onto the inner shell.

The resulting Ar gas implosion creates ~350 kJ of x-rays at > 3 keV.

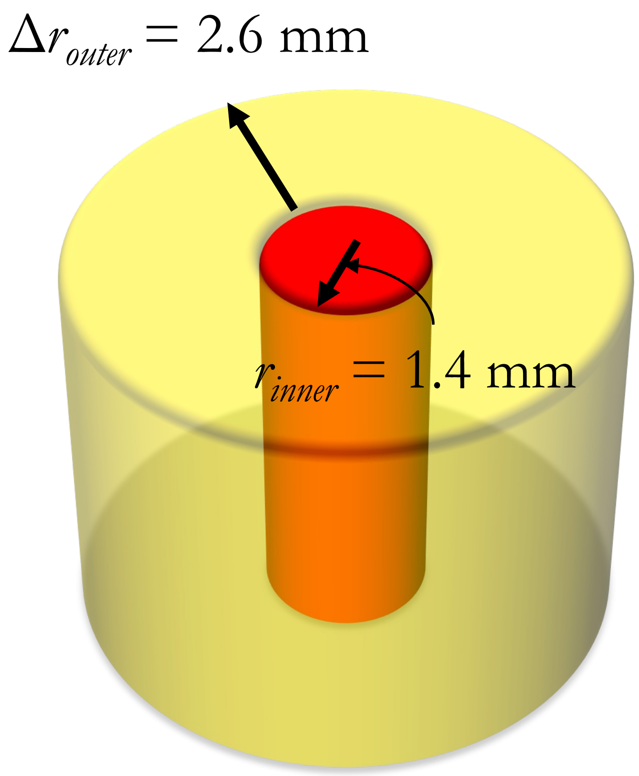


Harvey-Thompson et al. (2016), *Phys. Plasmas*



- The Z-machine at Sandia National Laboratories supplies 16 MA of current to the Ar gas puff platform.
- The outer gas shell conducts this current and begins to implode.
- Both gas shells implode on-axis simultaneously to create ~2 mm diameter, ~25 mm height pinch that reliably produces ~350 kJ of > 3 keV x-rays.

Ar gas puff spectra reveal significant gradients in the experimental spectra that may imply fundamental performance limits for this platform.

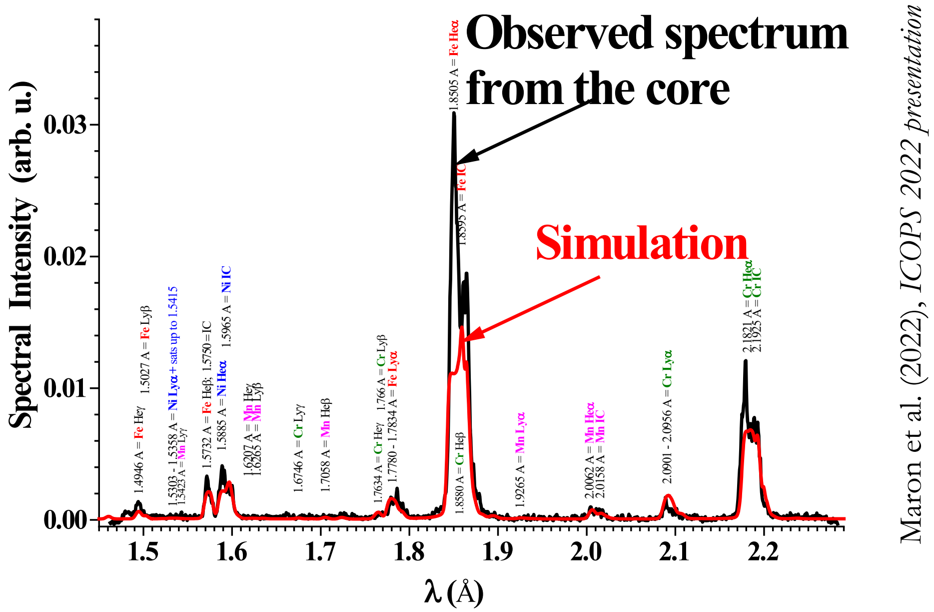


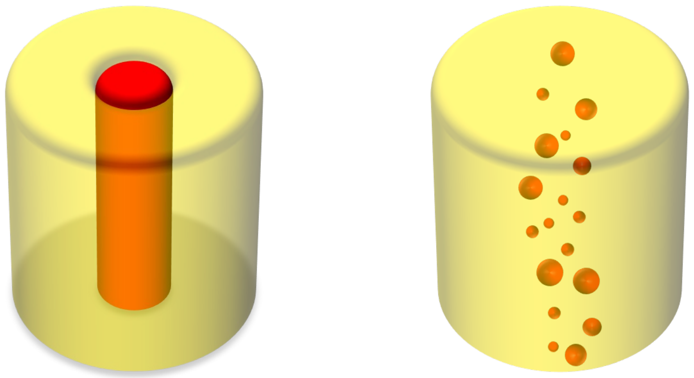
Layer	T_e [eV]	n_i [cm^{-3}]	Contained mass
Inner	2450	6.7×10^{19}	27%
Outer	110	2.5×10^{19}	73%

- Jones et al. (2015) used a 2-layer spectral model to study Ar gas puffs and found that inner layer radiates > 98% of K-shell yield, but only contains ~27% of mass.
- Other studies with similarly simple spectral assumptions have found the same limits.
- This knowledge could be crucial in designing future experiments and modeling this source at higher currents.

Jones et al. (2015), *Phys. Plasmas*

Spectra also imply that the annular plasma picture is inaccurate. A plasma with multiple mini-pinches matches the data better.





Annular plasma

Multiple mini-pinch plasma

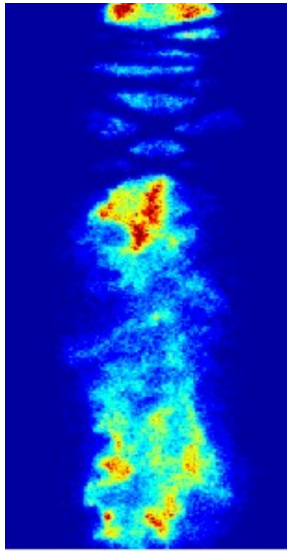
(not to scale)

- Maron et al. found that fitting spectra with the annular plasma assumption leads to significant opacity disagreements, especially for strong lines.
- Higher-fidelity spectral analyses that capture gradients can help solve several questions associated with the dynamics of imploding loads on Z.

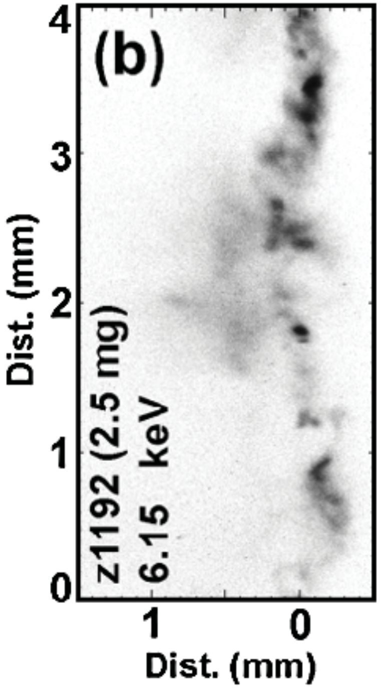
Many Z experiments are viewed as annular implosions. A Bayesian spectral analysis tool could help improve understanding of all these systems.

Platform	Elements needed
Gas puff	Ar, Kr
Wire arrays	Al, Ti, Fe, Cu
MagLIF	Fe, Co, Ni, Cu, Zn

Stagnation images

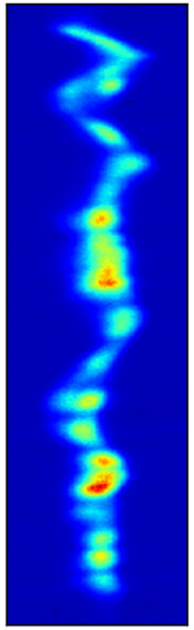


Ar gas puff



Sinars et al. (2008), *PRL*

Wire array



Knapp et al. (2022), *Phys. Plasmas*

MagLIF

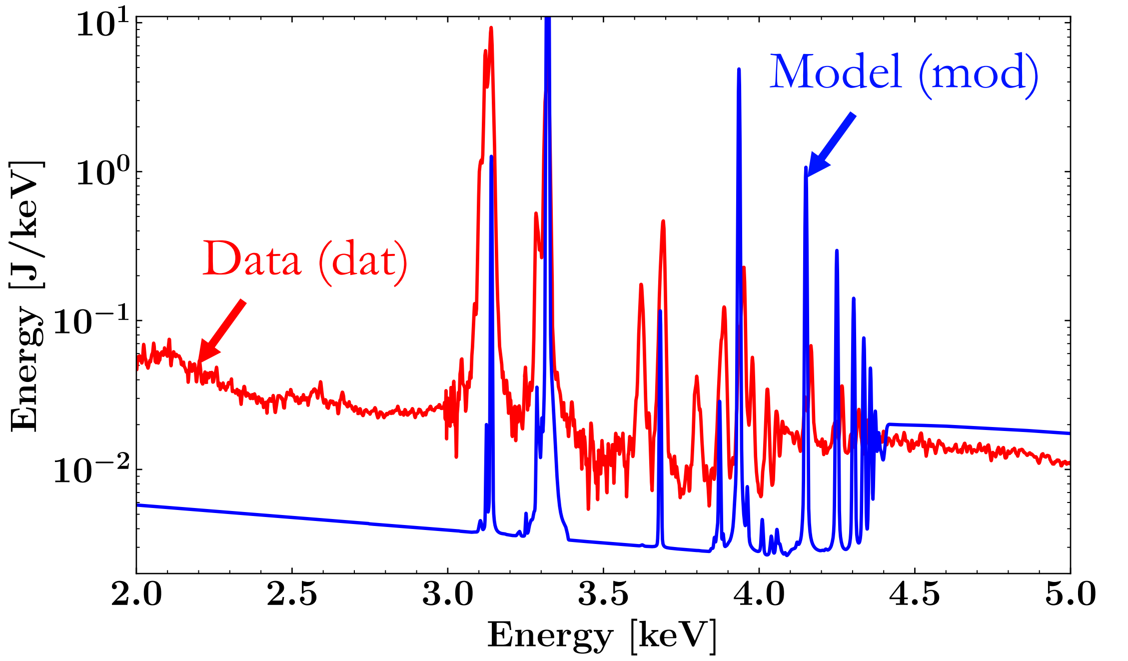
- The fundamental physics of the Z-machine force almost all experimental platforms to rely on the imploding plasma mechanism to produce their desired experimental outcomes.
- Imaging data captured for most Z experiments capture plasmas that have hot and cool regions.
- It is therefore important that we make our spectral model as general as possible so that it can be applied to a large number of Z experiments.

Bayesian inversion is a powerful tool, but requires an efficient spectral calculation model.

Bayes' Theorem:

$$P(\text{mod}|\text{dat},\text{bac}) = \frac{P(\text{dat}|\text{mod},\text{bac})P(\text{mod},\text{bac})}{P(\text{dat},\text{bac})}$$

bac: background knowledge



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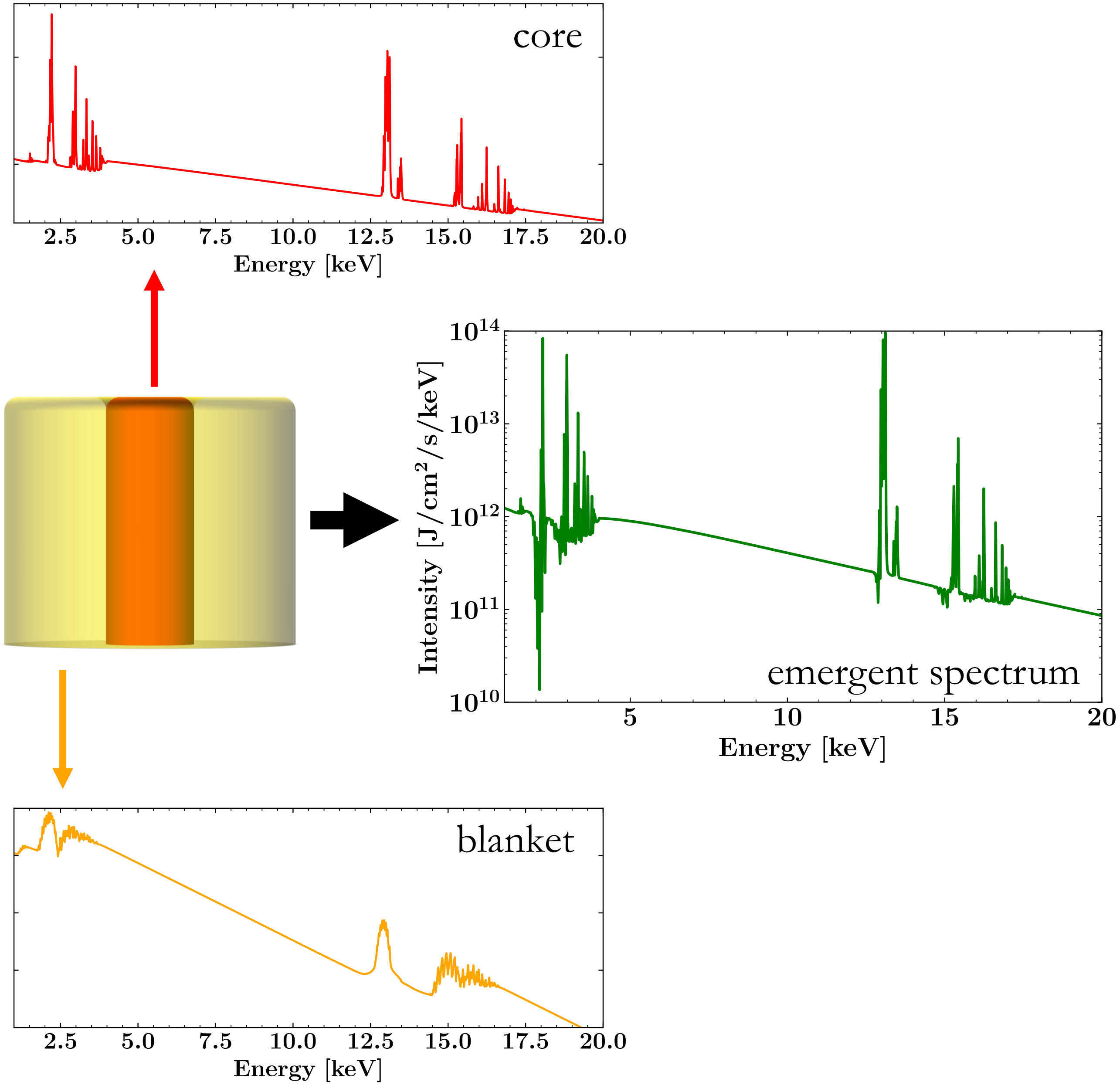
- Imaging data captured for most Z experiments capture plasmas that have hot and cool regions.
- It is therefore important that we make our spectral model as general as possible so that it can be applied to a large number of Z experiments.
- Bayesian inversion is a powerful framework to derive plasma gradients and distinguish between different plasma structure assumptions.
- A computationally efficient spectral model is needed for Bayesian inversion.

The SCRAM* atomic modeling code can calculate the data needed for Bayesian inversion. Unfortunately, SCRAM is computationally inefficient.



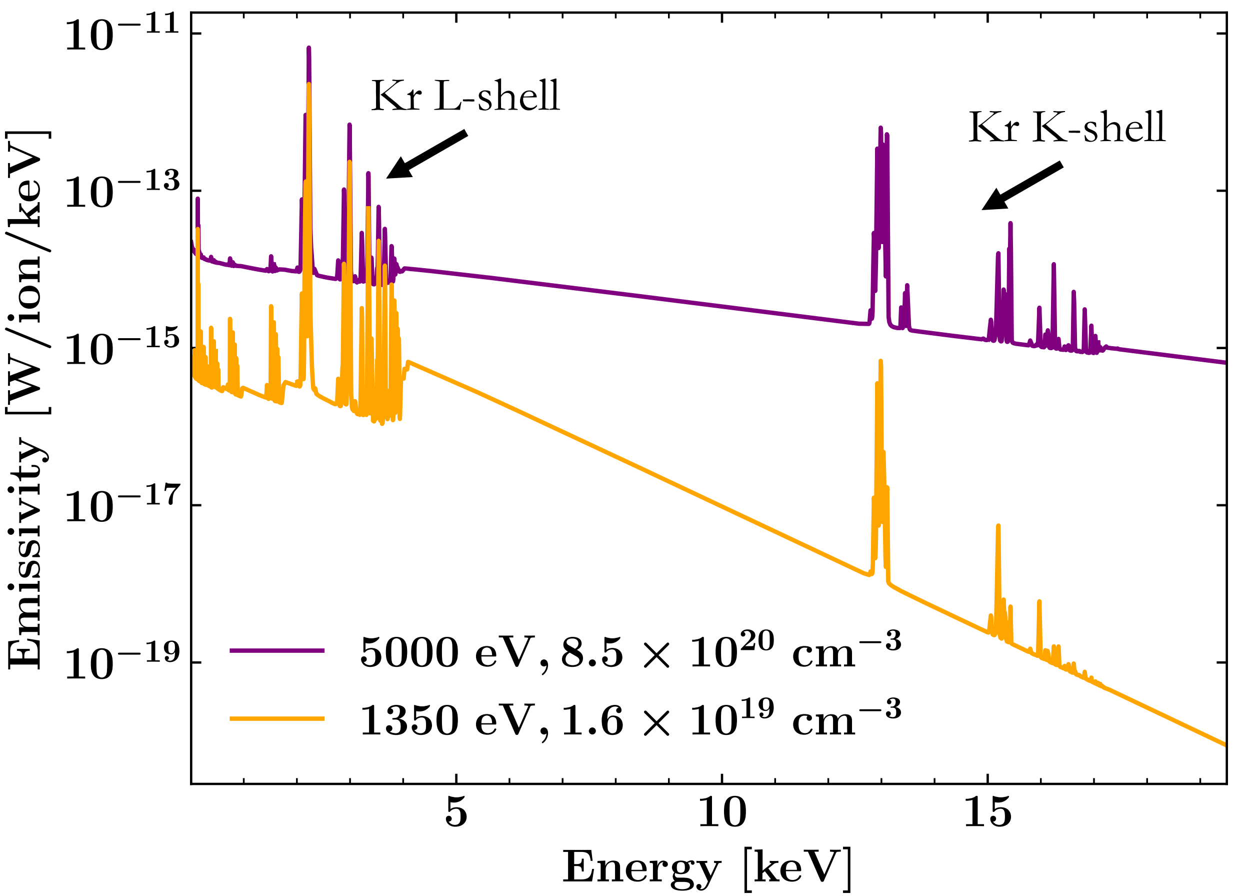
- The equation of radiative transfer can be written as follows:

$$I_\nu = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau'_\nu} e^{-\tau'_\nu} \frac{j_\nu}{\kappa_\nu} d\tau'_\nu$$

- As the ray traverses each plasma region, its intensity (I_ν) can get altered by opacity and emissivity.
- The opacity and emissivity are dependent on the plasma conditions in each region.
- The more plasma layers we include in our model, the more complicated/expensive these calculations become.
- SCRAM* is a detailed atomic physics code that can provide the needed input data.
- SCRAM is too slow for Bayesian inversion.

*Hansen, (2011), *Can. J. Phys.*

Logarithmic interpolation has traditionally been used to efficiently derive the plasma opacities and emissivities.

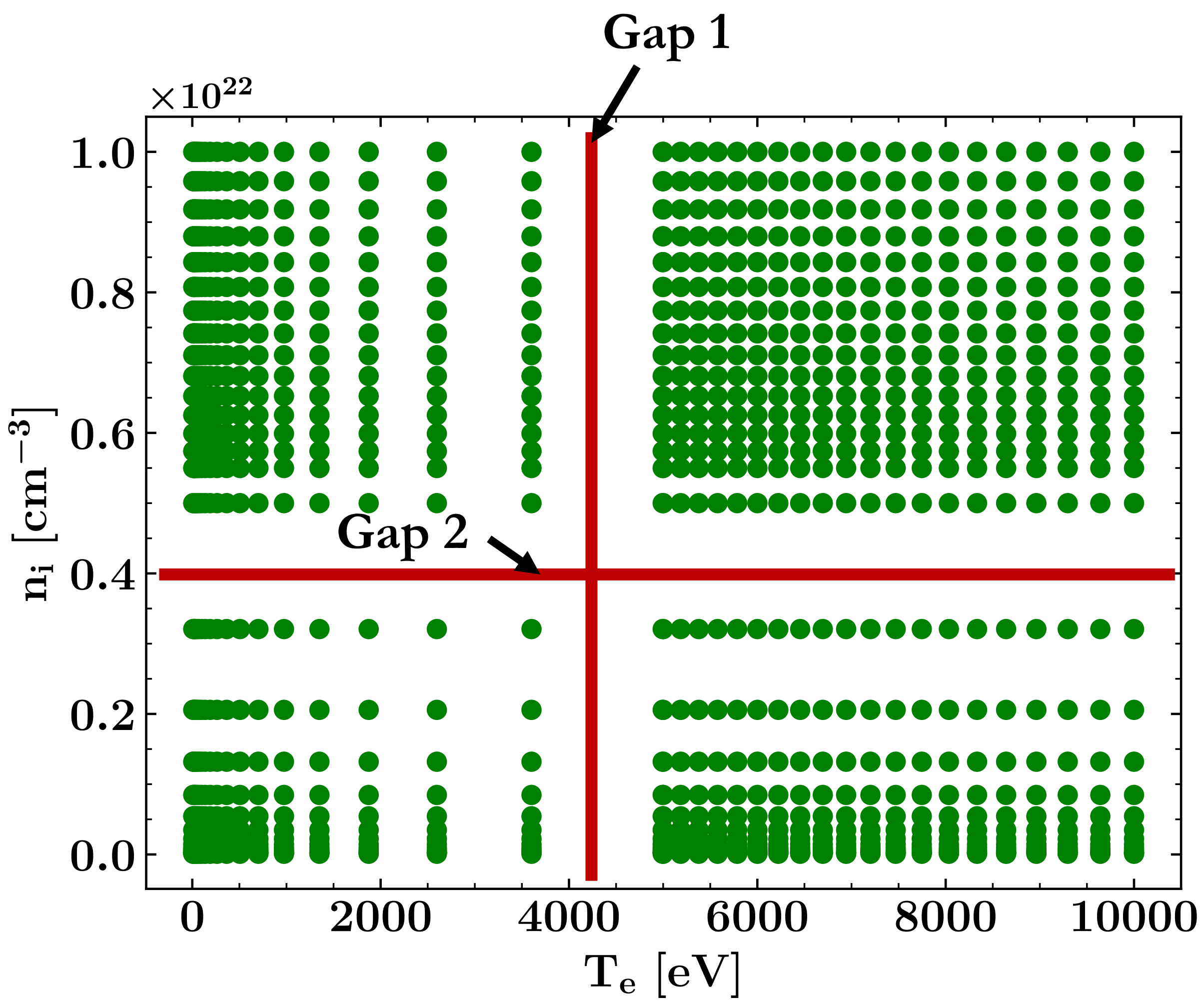


- Historically, logarithmic interpolation has been the preferred tool for spectral interpolation.
- For experimental parameters found at Z, the following table would be adopted for logarithmic interpolation:

Parameter	Range	Steps
T_e	10 – 10,000 eV	40
N_i	10^{19} – 10^{22}	30
$h\nu$	1 – 20,000 eV	20,000

- We calculate these 1200 spectra for krypton using SCRAM.
- Kr spectra are more complex than Ar spectra and allow us to test limits of logarithmic interpolation.

Logarithmic interpolation has traditionally been used to efficiently derive the plasma opacities and emissivities.

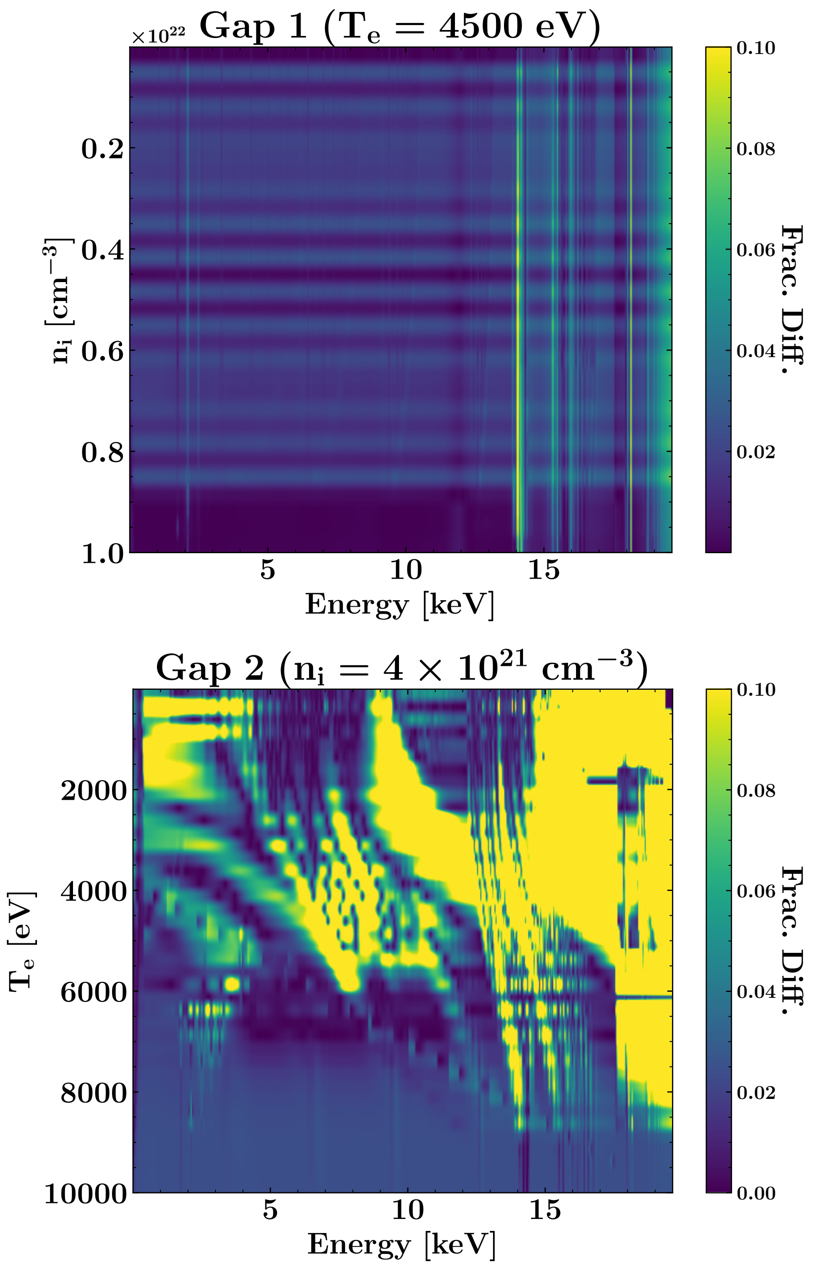


- We use a data distribution that leaves deliberate gaps:

Gap	N_i range	T_e range	Steps
1	$10^{19} - 10^{22}$	4500 eV	30
2	4×10^{21}	10 – 10,000 eV	40

- These gaps are designed to provide a basis of comparison between logarithmic interpolation and machine learning accuracy.

Logarithmic interpolation performance is uneven across the two gaps and any attempt to improve performance will result in higher computational costs.

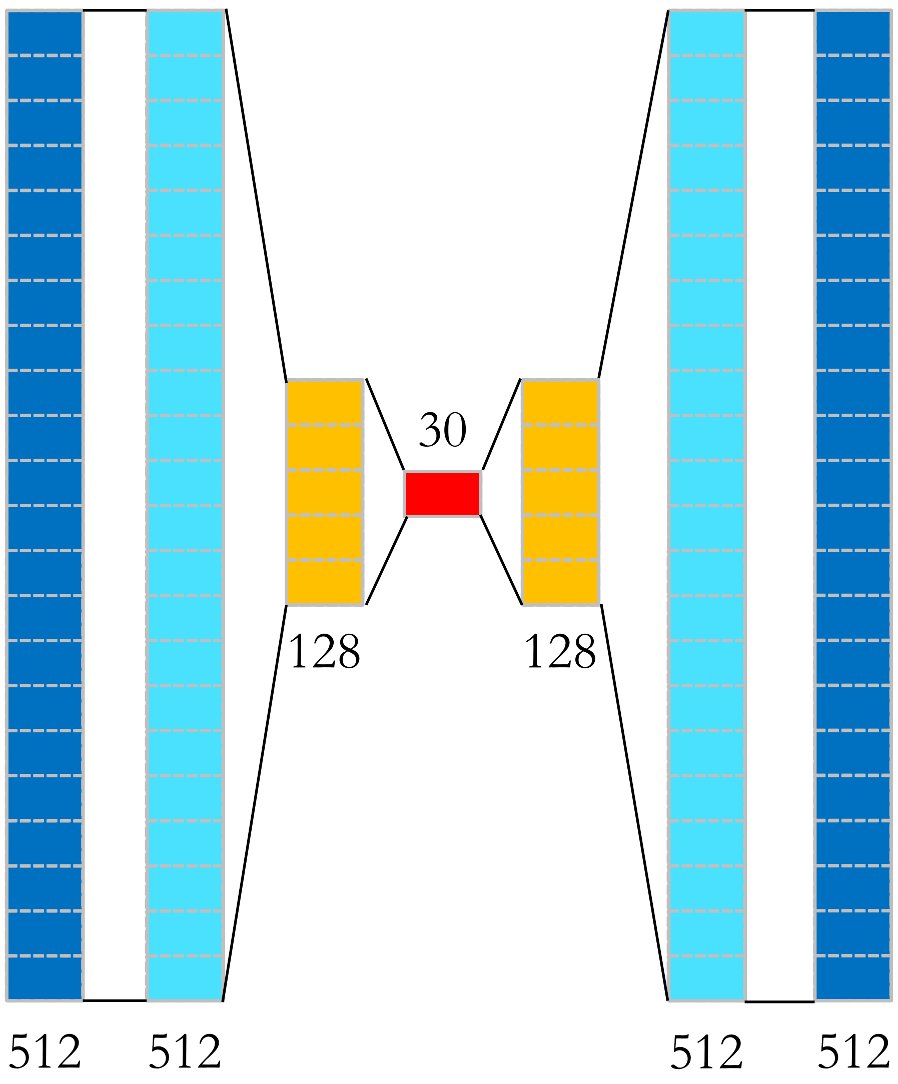


- We calculate the fractional difference between interpolation and truth as:

$$\text{Frac. Diff.} = \frac{|\text{truth} - \text{interpolation}|}{|\text{interpolation}|}$$

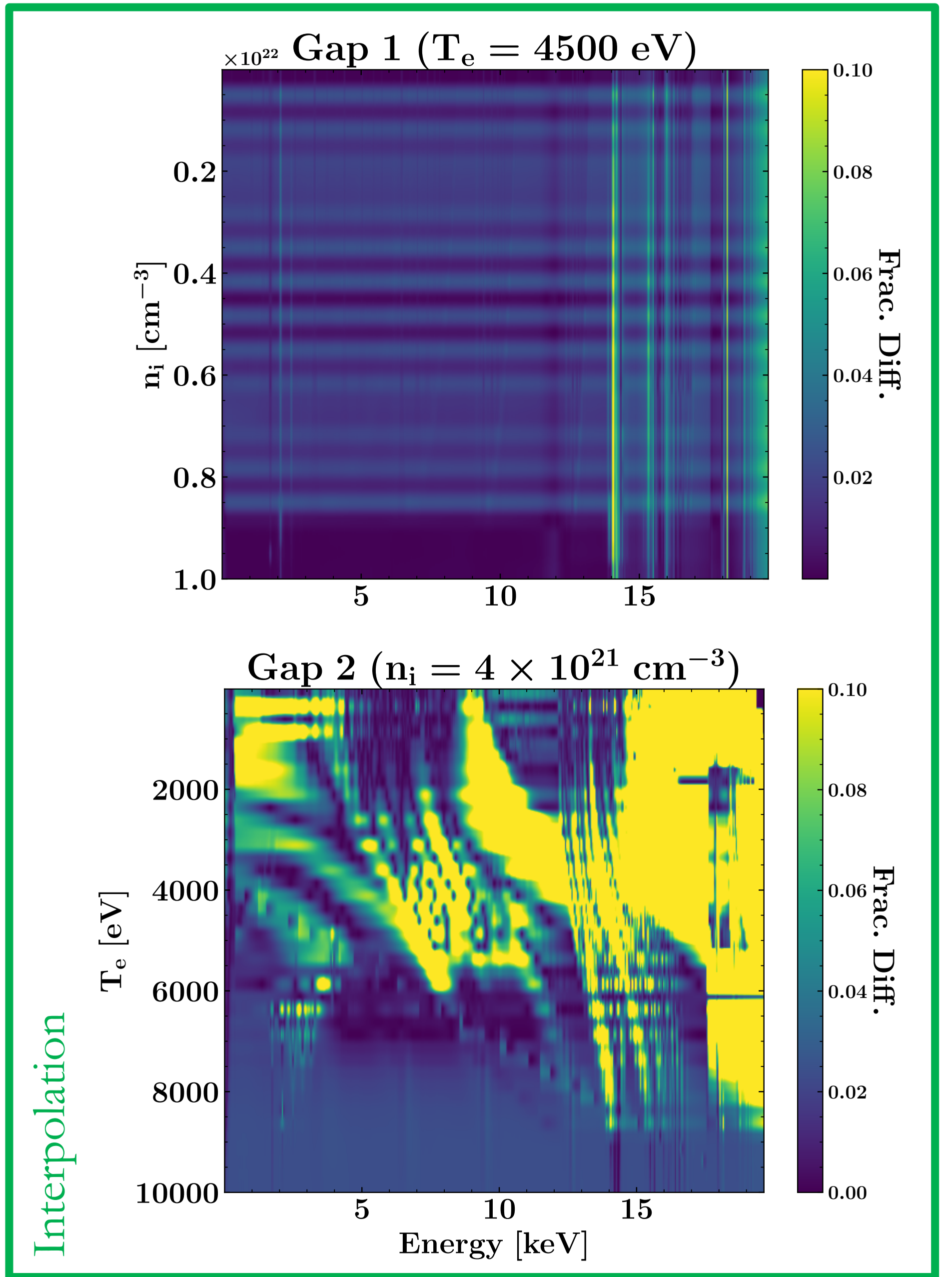
- Interpolation struggles to capture lower temperatures correctly, but gets the $T_e = 4500$ eV spectra correct across all densities.
- Improving the accuracy of the interpolation would require a larger input data files, which would make the interpolating more unwieldy and slower.

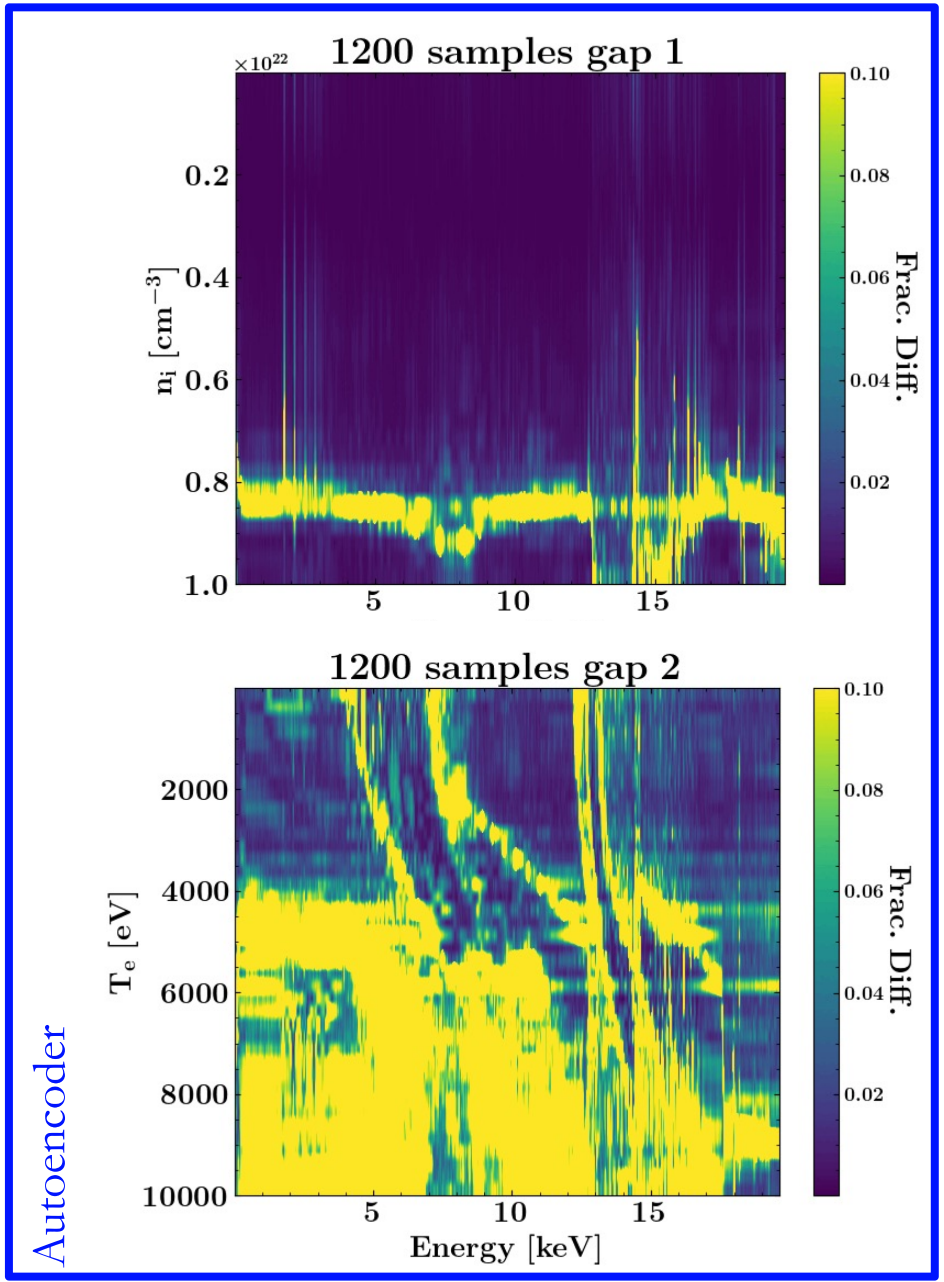
Machine learning models provide an attractive alternative to logarithmic interpolation since they can potentially predict spectra with higher accuracy.



- Machine learning models can be trained off-line, making them potentially superior of interpolation.
- We developed an autoencoder that compresses the 20,000 photon energy points down to 30 points.
- The latent dimension is constrained by the fact that we have to relate T_e and n_i to the latent spectra.
- We train this network using 1200, 5000, 10000, 15000, and 30000 samples, comparing performance to the interpolator at each step.

The autoencoder exceeds interpolator performance with > 10,000 training sets. This highlights a potential path forward.





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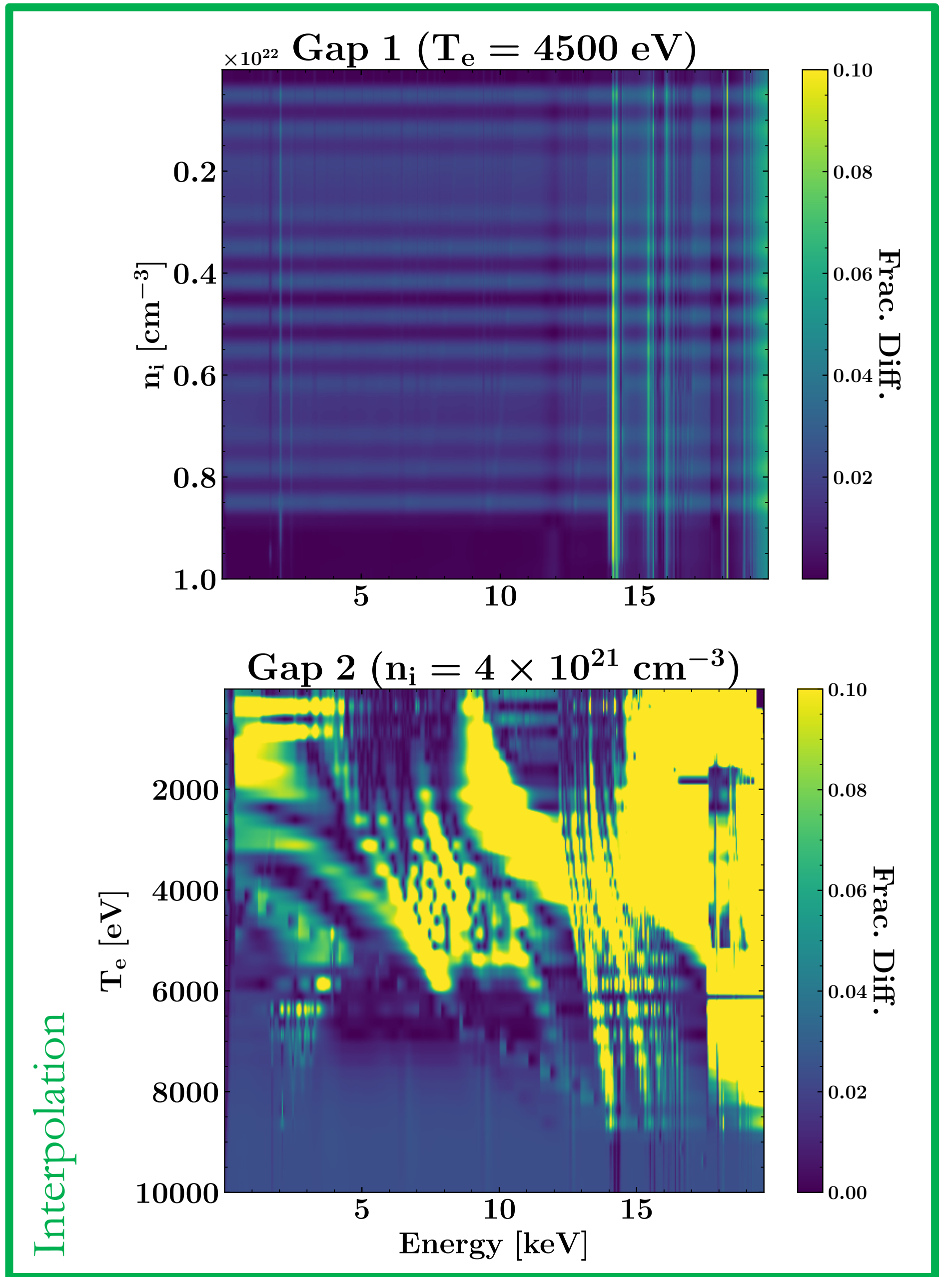

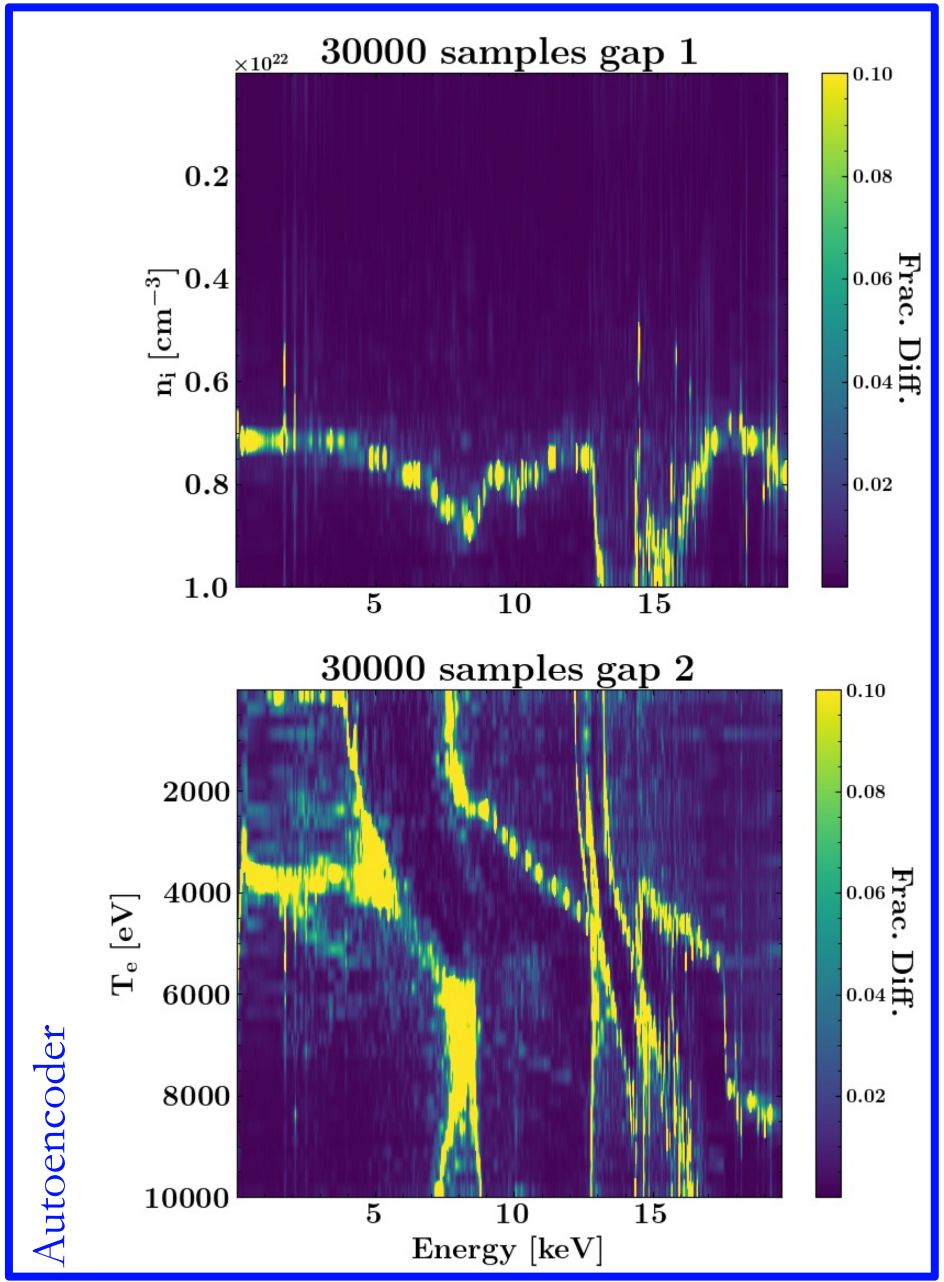

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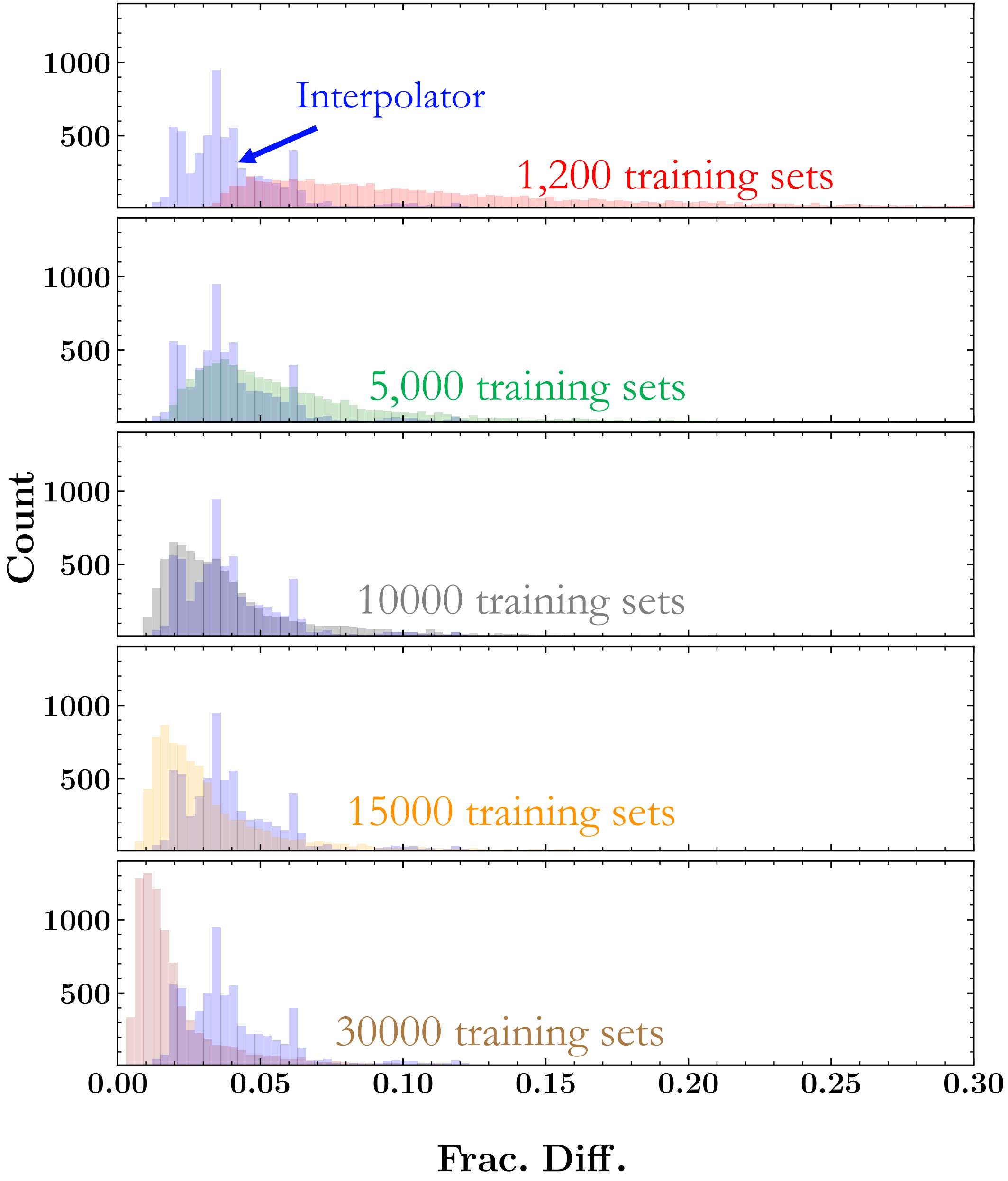
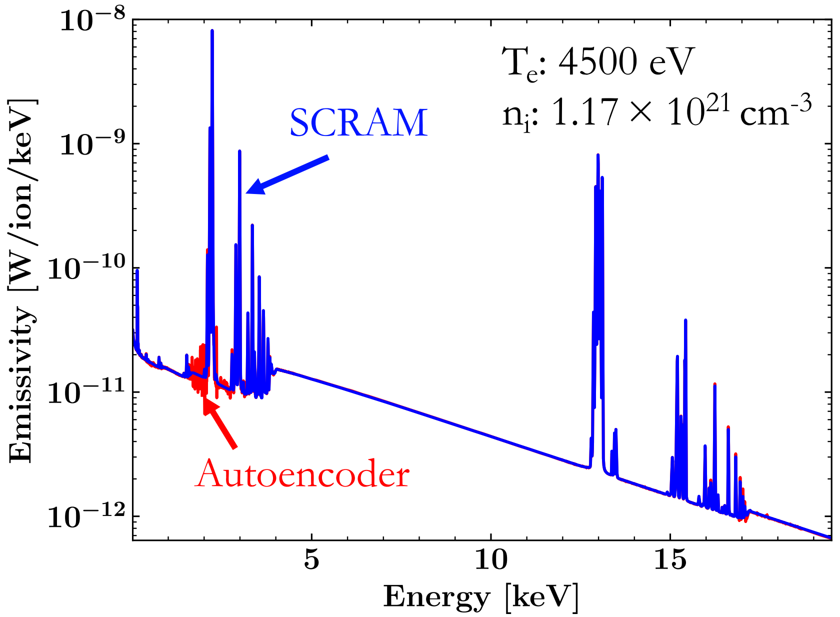


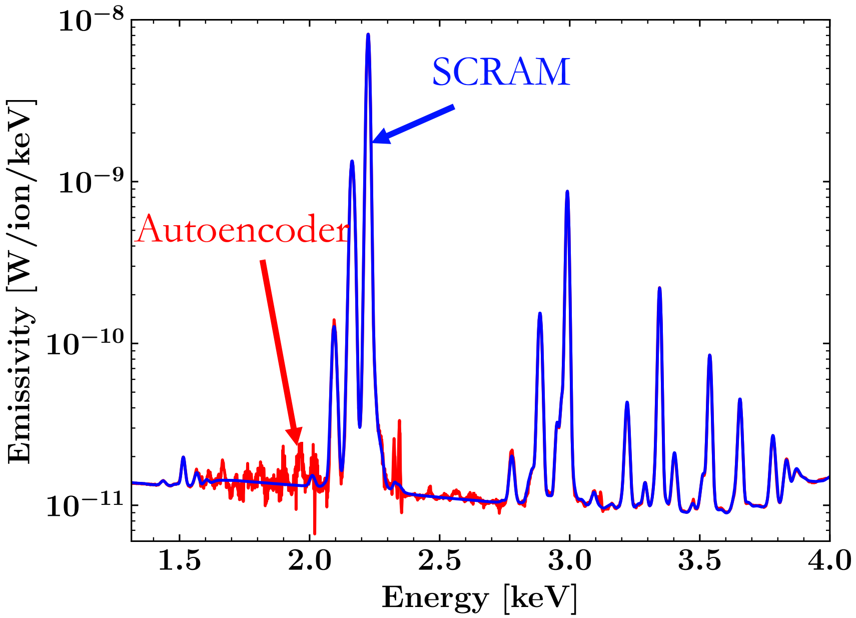
- To quantitatively estimate performance differences between interpolator and autoencoder, we compare histograms of fractional differences at each photon energy averaged over the two test datasets.

- We find that interpolator and autoencoder performance roughly match at ~10,000 training sets.

- With 30,000 training sets, the autoencoder performance far exceeds the interpolator.

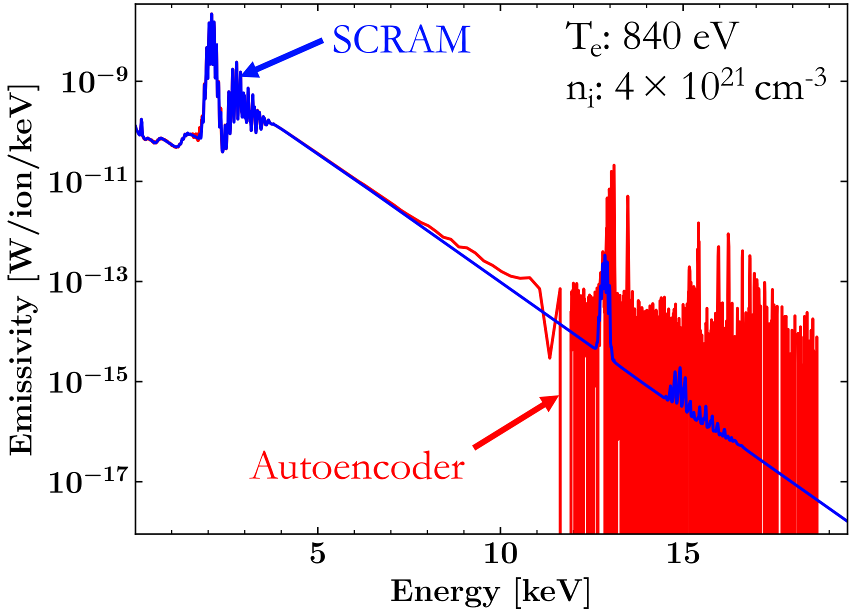
The autoencoder struggles with reproducing lower energy spectral regions around Kr L-shell lines.

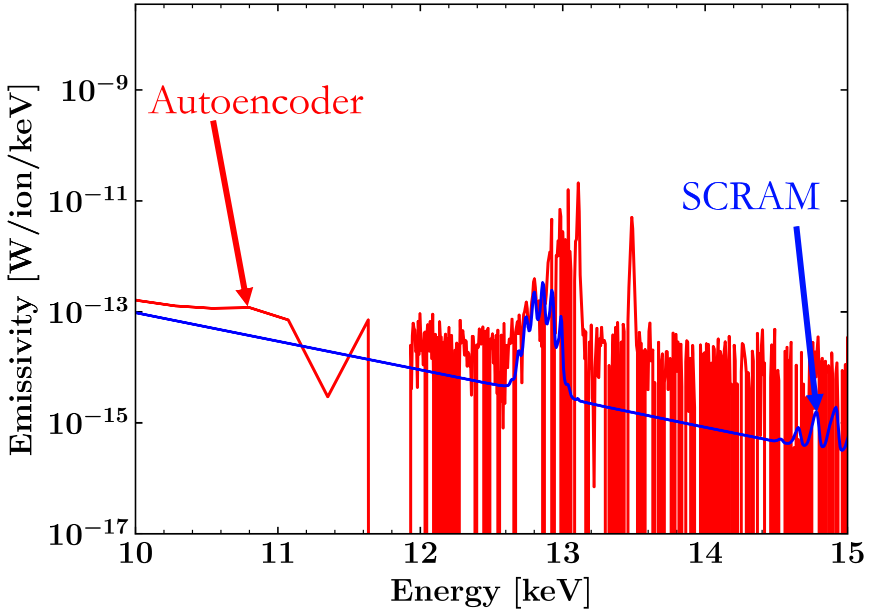




- Our autoencoder model predicts most spectral regions very accurately, but struggles around the strongest Kr L-shell lines in high-temperature regions.

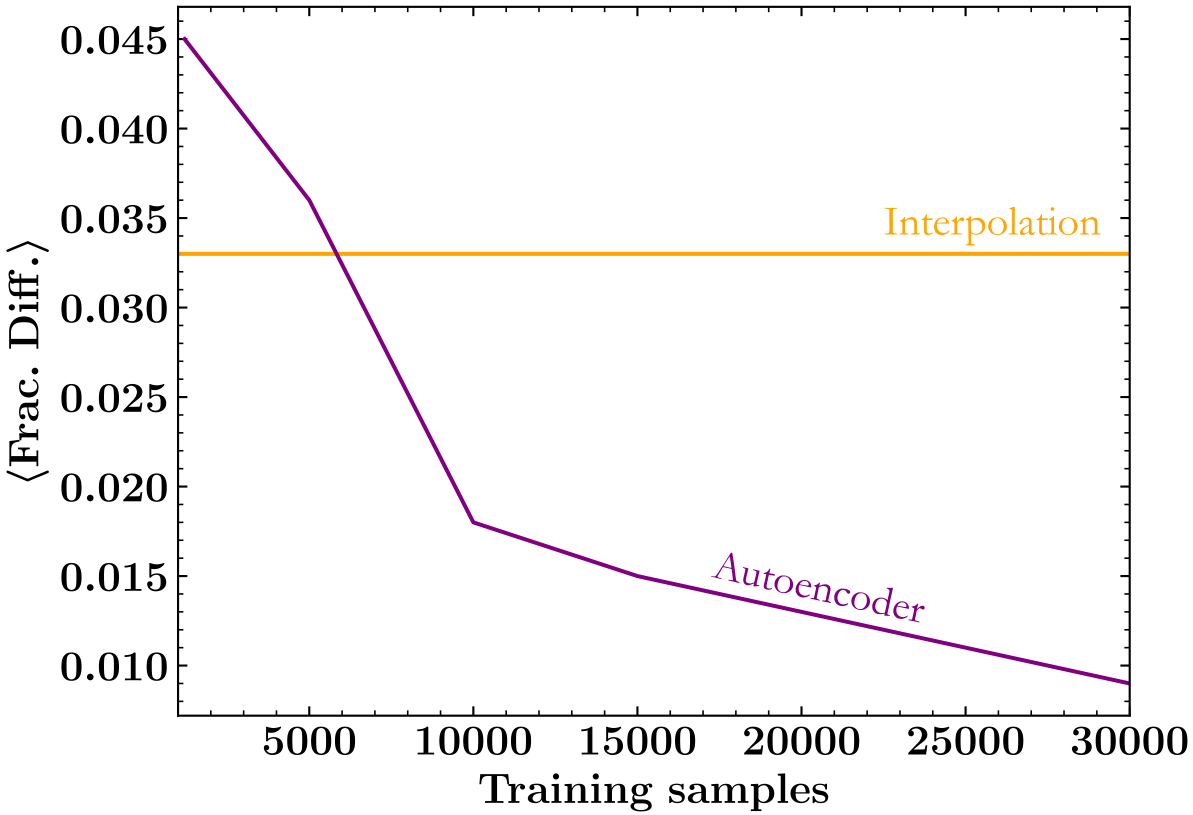
The autoencoder also struggles with reproducing Kr K-shell lines at low temperatures and high densities.





- Our autoencoder model predicts most spectral regions very accurately, but struggles around the strongest Kr L-shell lines in high-temperature regions.
- In cooler regions, the autoencoder struggles to properly capture the the K-shell lines, as well as the continuum.
- Some of these oscillations can be traced back to the scaling methodology used during the data preparation process.

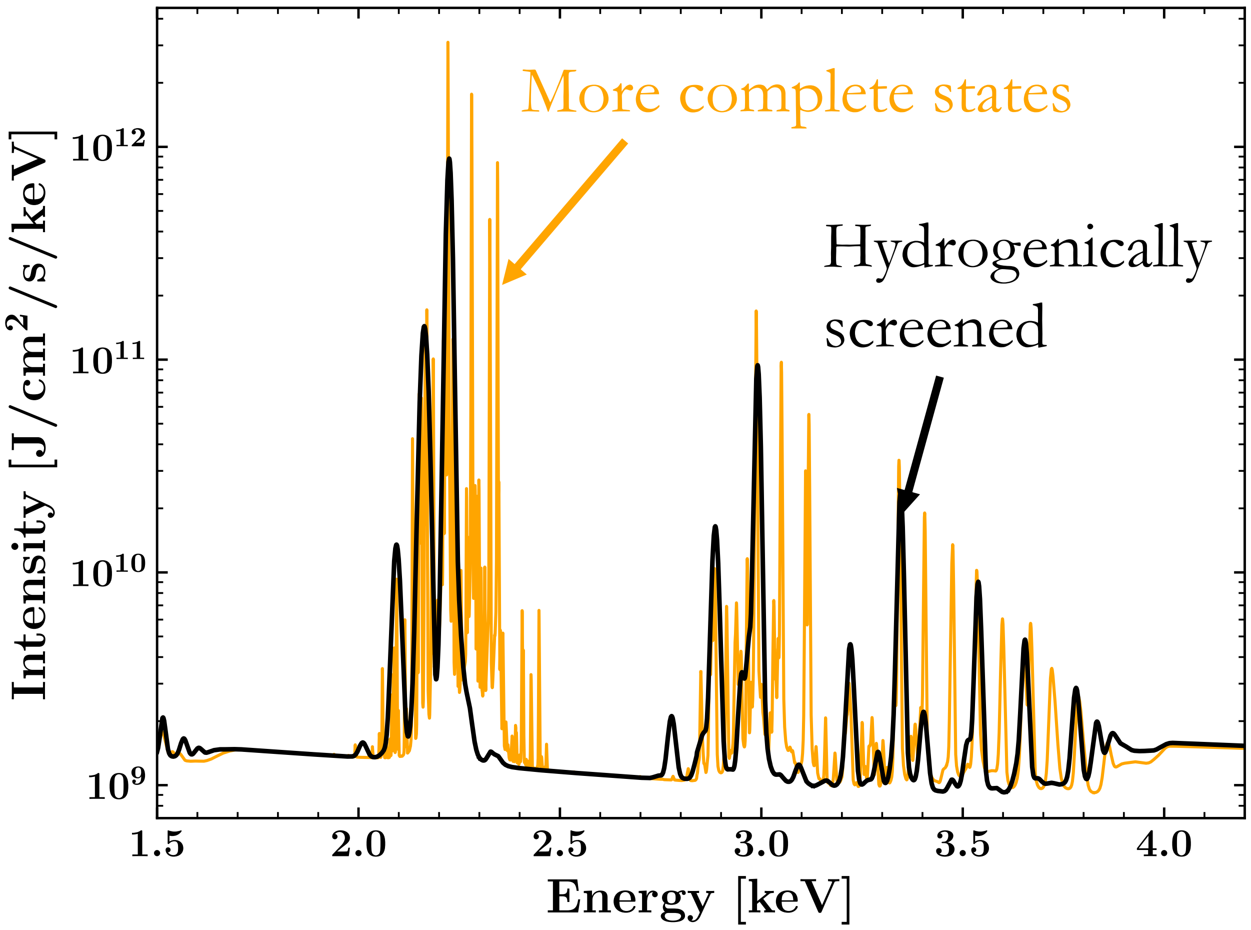
Despite the work left to be done on our spectral ML model, we are already outperforming interpolation and can improve ML model performance.



Case	Time per prediction [ms]
interpolation	2.99 ± 0.14
autoencoder	2.03 ± 0.09
SCRAM	$3 \times 10^5 – 2 \times 10^6$

- A relatively simple autoencoder structure with a modest amount of training data has enabled us predict spectra more accurately than a log-interpolation approach.
- We only attempted to roughly optimize the autoencoder, so more performance gains could be achieved.
- The autoencoder can also predict spectra more quickly compared to the log interpolator.
- The fractional difference maps shown earlier can also guide us which plasma parameter regions may require more training data.
- Adding ‘training data’ to the interpolator is much more difficult.

Future work includes exploring convolutional networks, transfer learning, and including radiation fields in our training data.



- Using convolutional networks may increase computational performance and mitigate oscillations.
- All models in this presentation were trained on hydrogenically screened data, but SCRAM also produces more realistic spectra. Transfer learning may be useful here.
- Radiation fields also have not been included in the training data.
- We would also like to expand to other elements.
- Gluth et al. (2020), Vander Wal et al. (2021) have tackled similar problems with success.
- We're very interested in opening collaborations on these issues and look forward to further suggestions from the audience.

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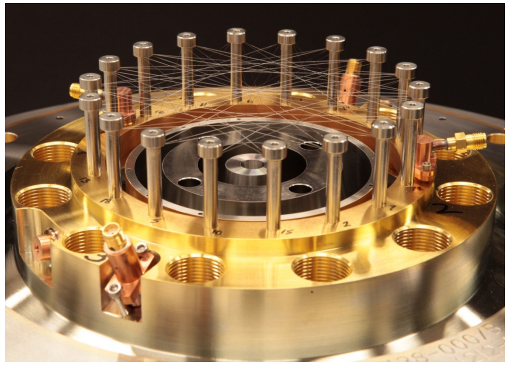

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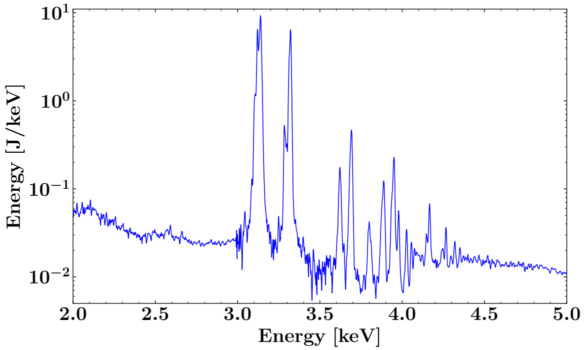

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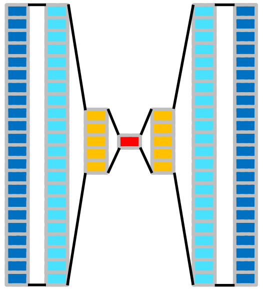

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