# Cognitive Simulations and Virtual Diagnostics to Drive High Repetition Rate Laser Facilities

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Center for Extreme Data Management Analysis and Visualization

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# Ideas and Results are the Result of a Diverse Team

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- Ankita Shukla (ASU)
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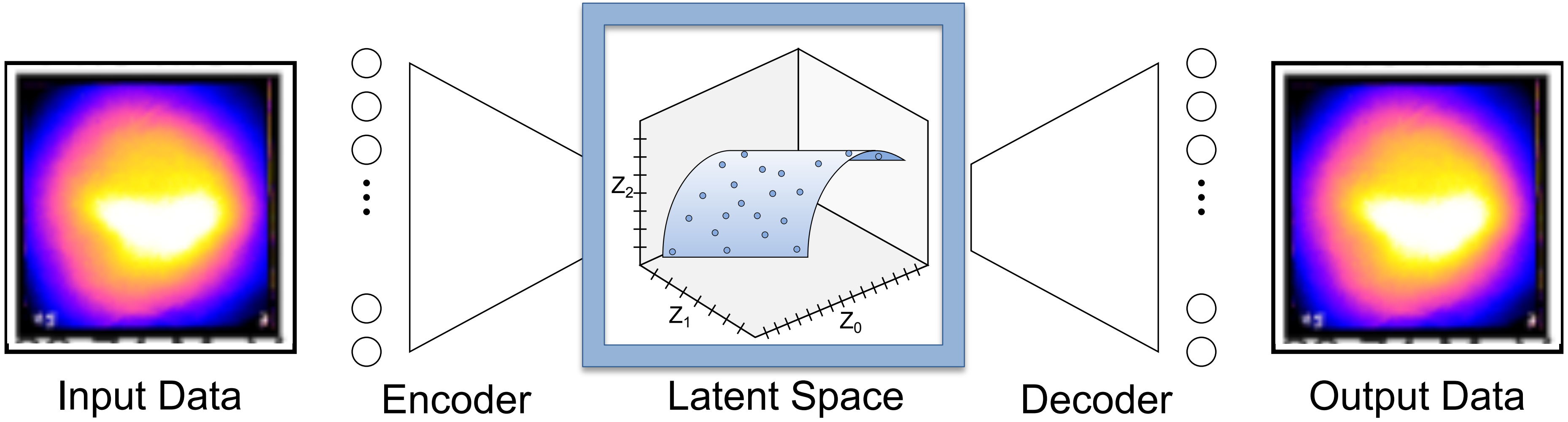
# Recent and Predicted Increases in Shot Rate Represent Significant Challenges and Opportunities and ML can Provide Solutions

- Upcoming high intensity short-pulse lasers will operate at >10Hz which represents a fundamental shift from toady's shot-per-hour approach
- **Opportunities:** Greatly increased data collection to drive down noise and explore larger parameter spaces
- **Challenges:** Traditional data processing and shot planning potentially wastes thousands of experiments
- Scientific Machine Learning has the potential to significantly improve the process
  - Multimodal data representation enable tight coupling of simulation ensembles and experiments
  - Robust sequential optimization techniques to create self-driving facilities

# Deep Learning Enables us to Jointly Encode Multi-Modal Data and Provides Generative Models to Decode Said Data Again

- Deep learning representations extract the fundamental degrees of freedom from complex data




$$Y \subset \mathbb{R}^n \xrightarrow[\text{Dimension reduction}]{n \gg m} Z \subset \mathbb{R}^m \xrightarrow[\text{Generative Model}]{} \bar{Y} \subset \mathbb{R}^n$$

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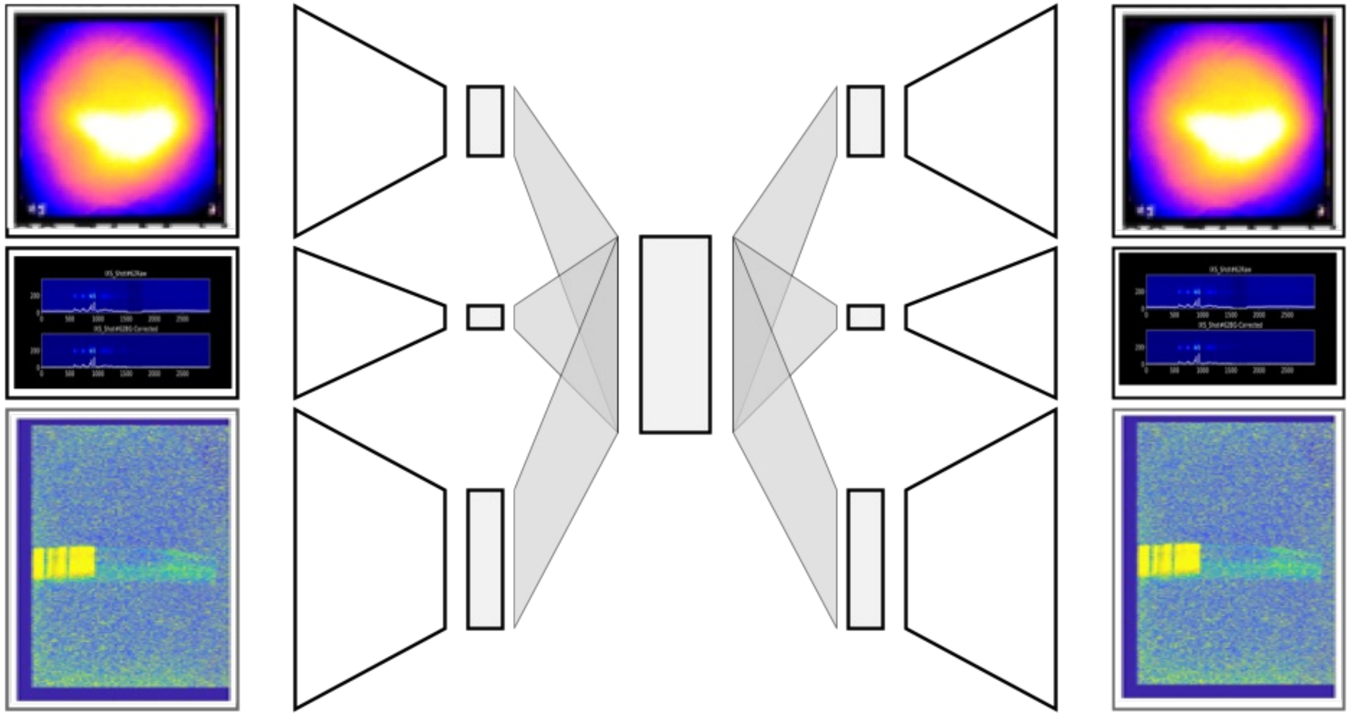
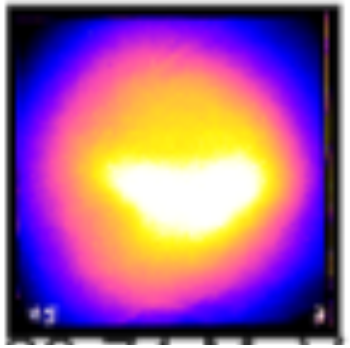


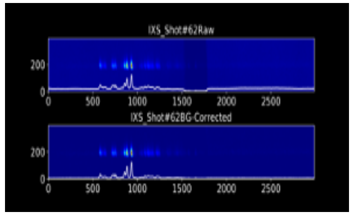
$$Y_0 \times Y_1 \times Y_2 \subset \mathbb{R}^n \qquad Z \subset \mathbb{R}^m \qquad \bar{Y}_1 \times \bar{Y}_2 \times \bar{Y}_3 \subset \mathbb{R}^n$$

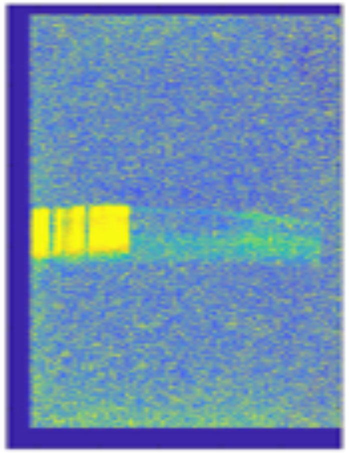
# Multi-Modal Data Representations Enable a New Class of Surrogate Models Capturing Much Richer Simulation Outputs

- Simulations enable us to predict outcomes for a variety of shot parameters

Shot Parameters







Internal state
Time series
Scalars
Diagnostics
…

$X \subset \mathbb{R}^p$

$Y_0 \times Y_1 \times Y_2 \subset \mathbb{R}^n$

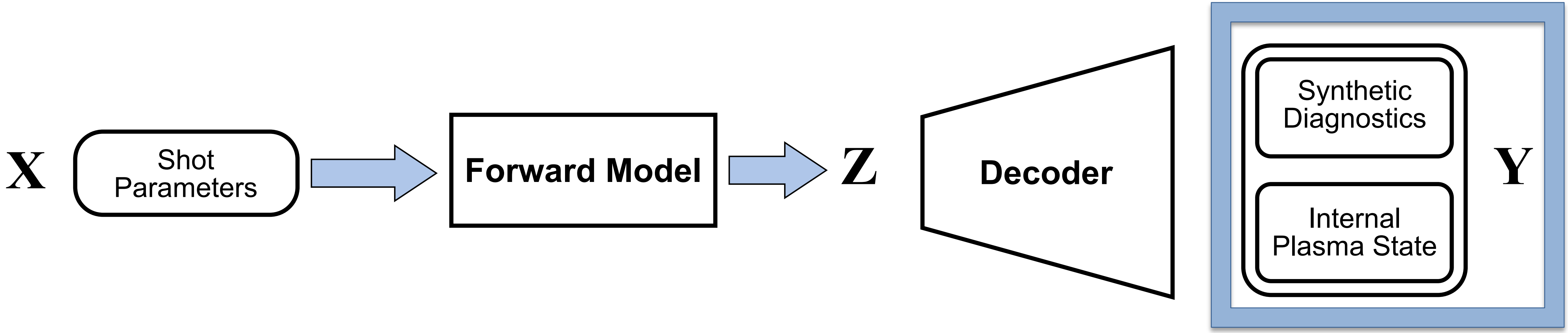
$G: Y_0 \times Y_1 \times Y_2 \rightarrow W \subset \mathbb{R}^q$

$F: X \rightarrow W$

$X \subset \mathbb{R}^p$ $\qquad$ $W \subset \mathbb{R}^q$

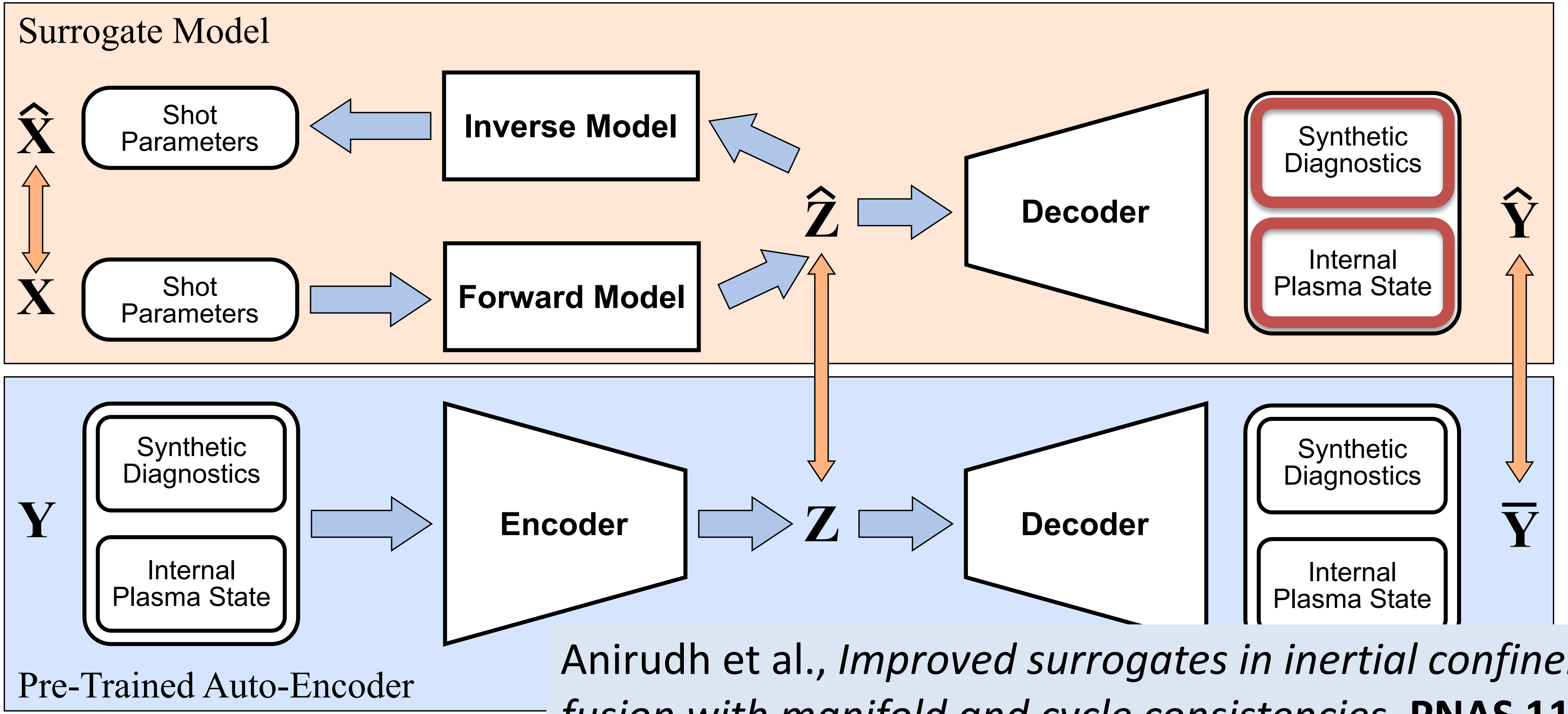
# Multi-Modal Data Representations Enable a New Class of Surrogate Models Capturing Much Richer Simulation Outputs

- Simulations enable us to predict outcomes for a variety of shot parameters
- Deep learning surrogates are not limited to figures of merit



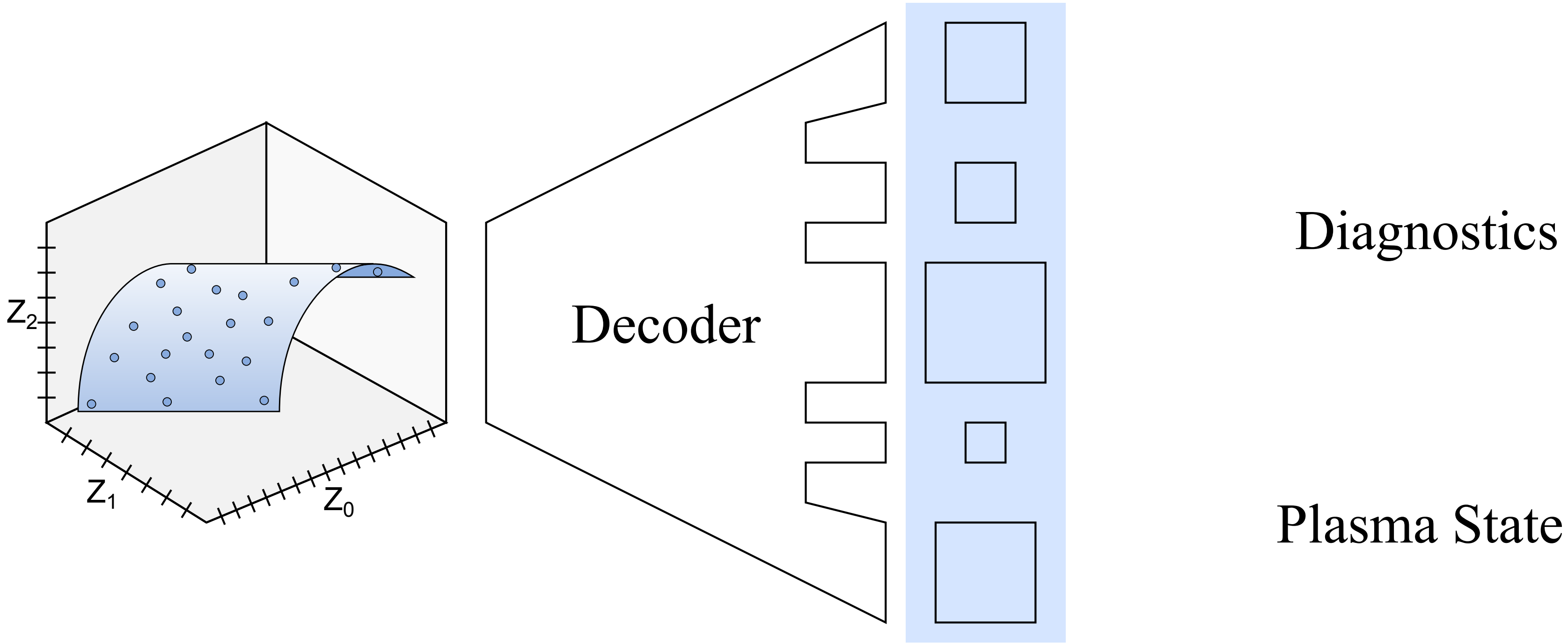

$$\boxed{Y \not\approx W}$$

# Coupling Forward and Inverse Models Provides a Self-Consistent Framework for Simulation Surrogates




Anirudh et al., *Improved surrogates in inertial confinement fusion with manifold and cycle consistencies*, **PNAS 117**

# Manifold Projections and Alignments Enable One to Integrate Experimental Data and Create Virtual Diagnostics



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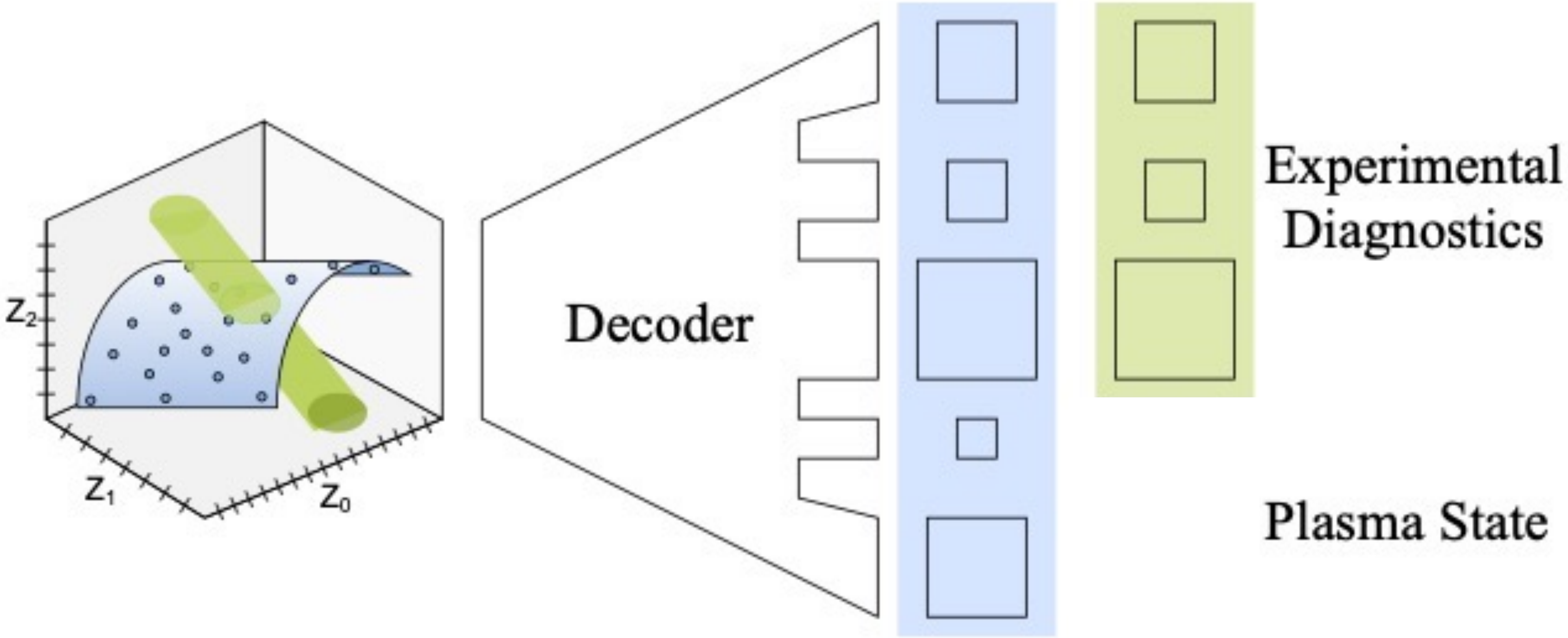

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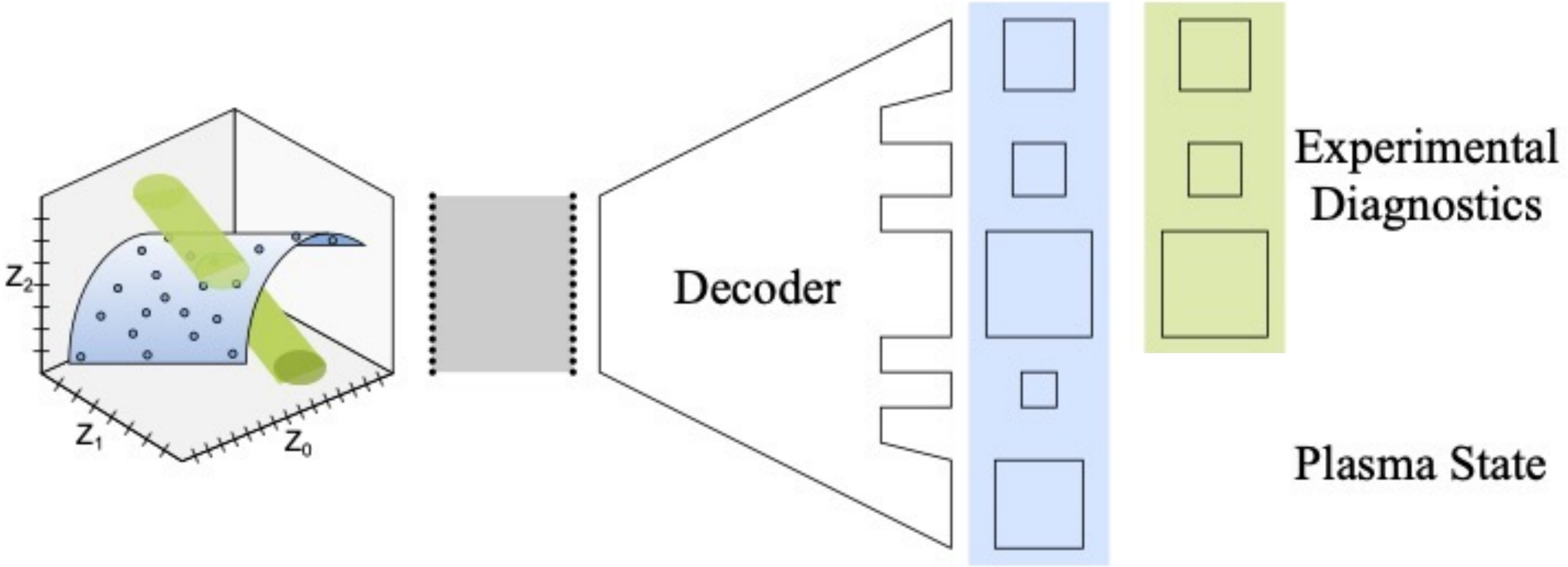
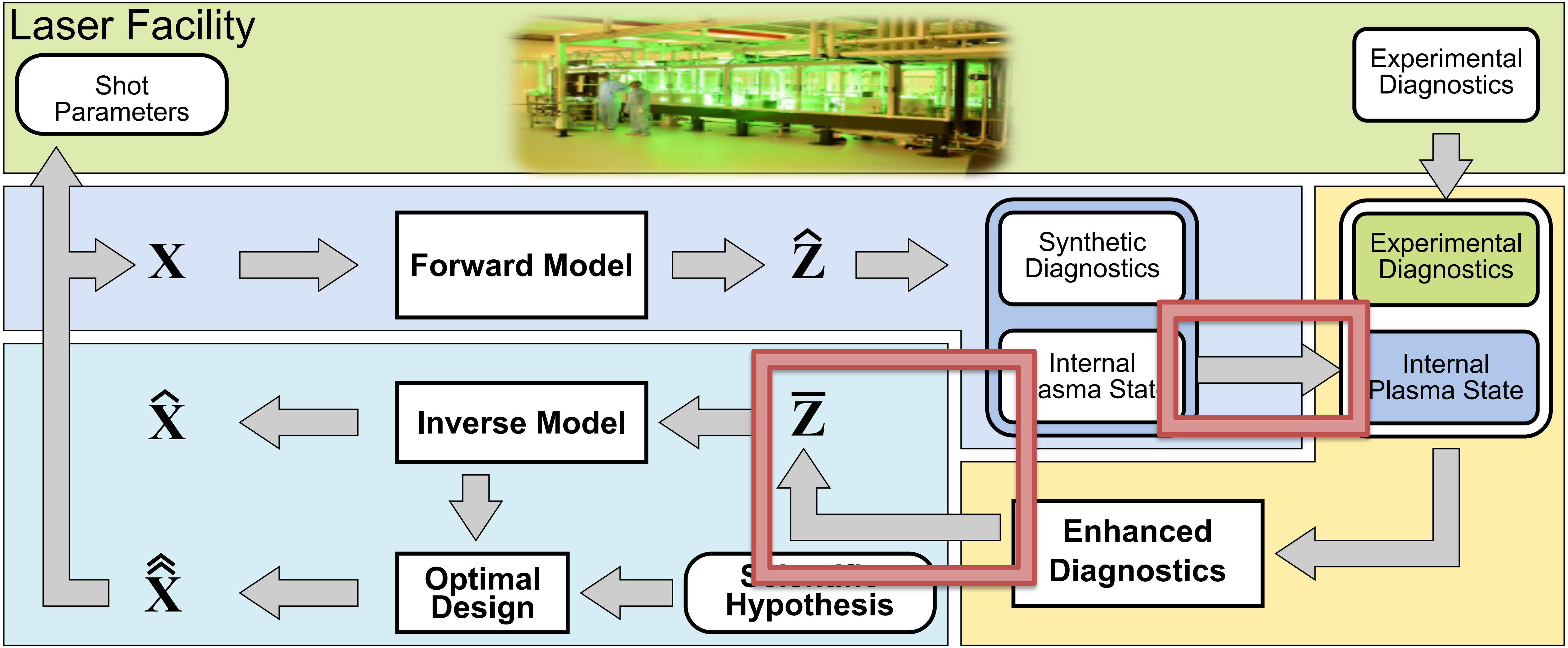


# Combining the Different Aspects Results in a Fully Automatic Loop to Drive High Repetition Laser Experiments



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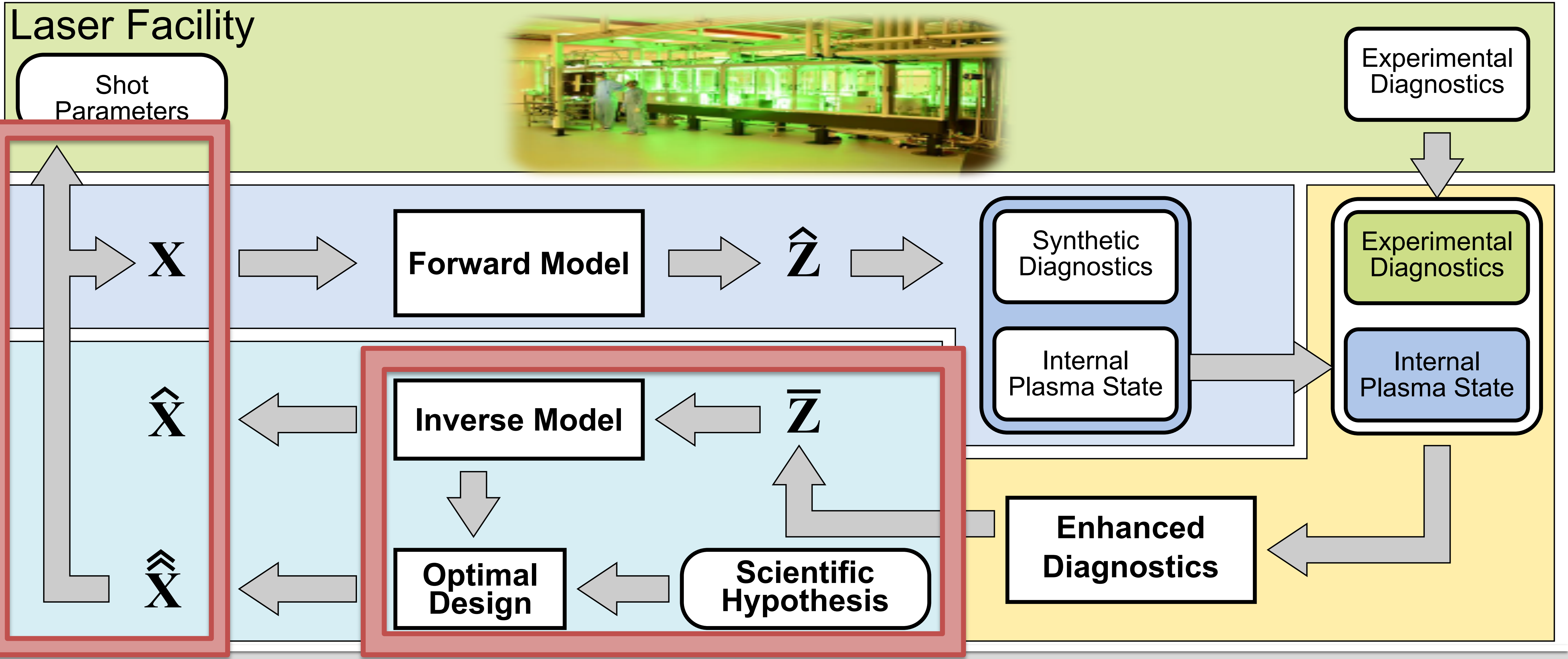

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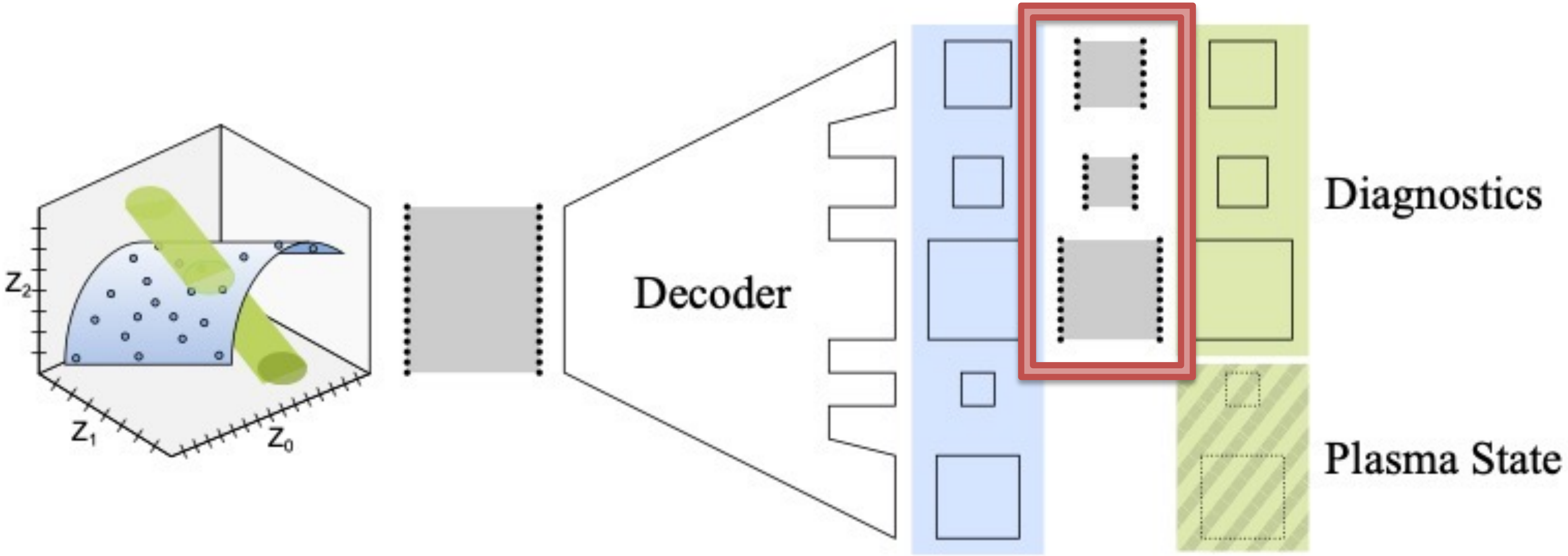
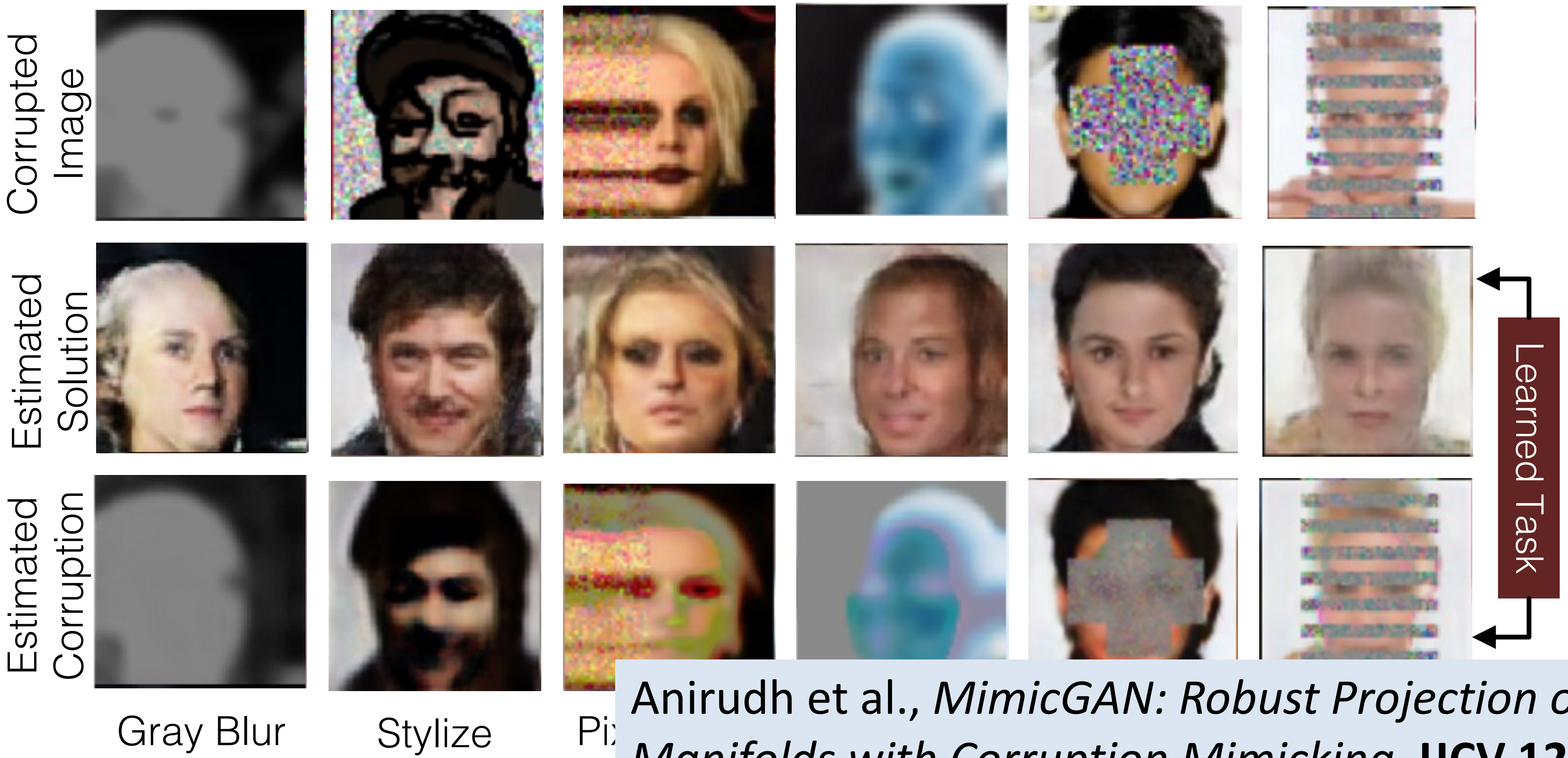


# MimicGAN is Able to Estimate a Wide Range of Corruptions and Correct the the Data Accordingly




Anirudh et al., *MimicGAN: Robust Projection onto Image Manifolds with Corruption Mimicking*, **IJCV 128**

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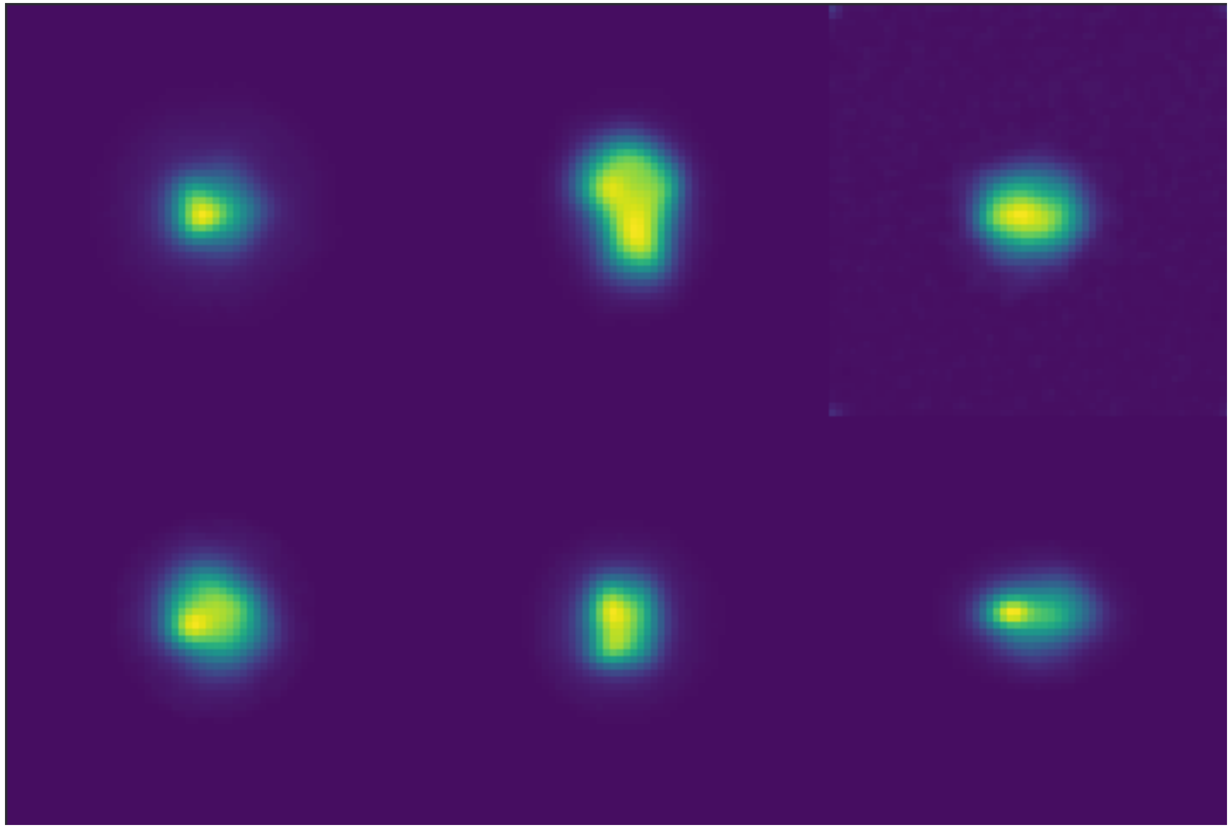
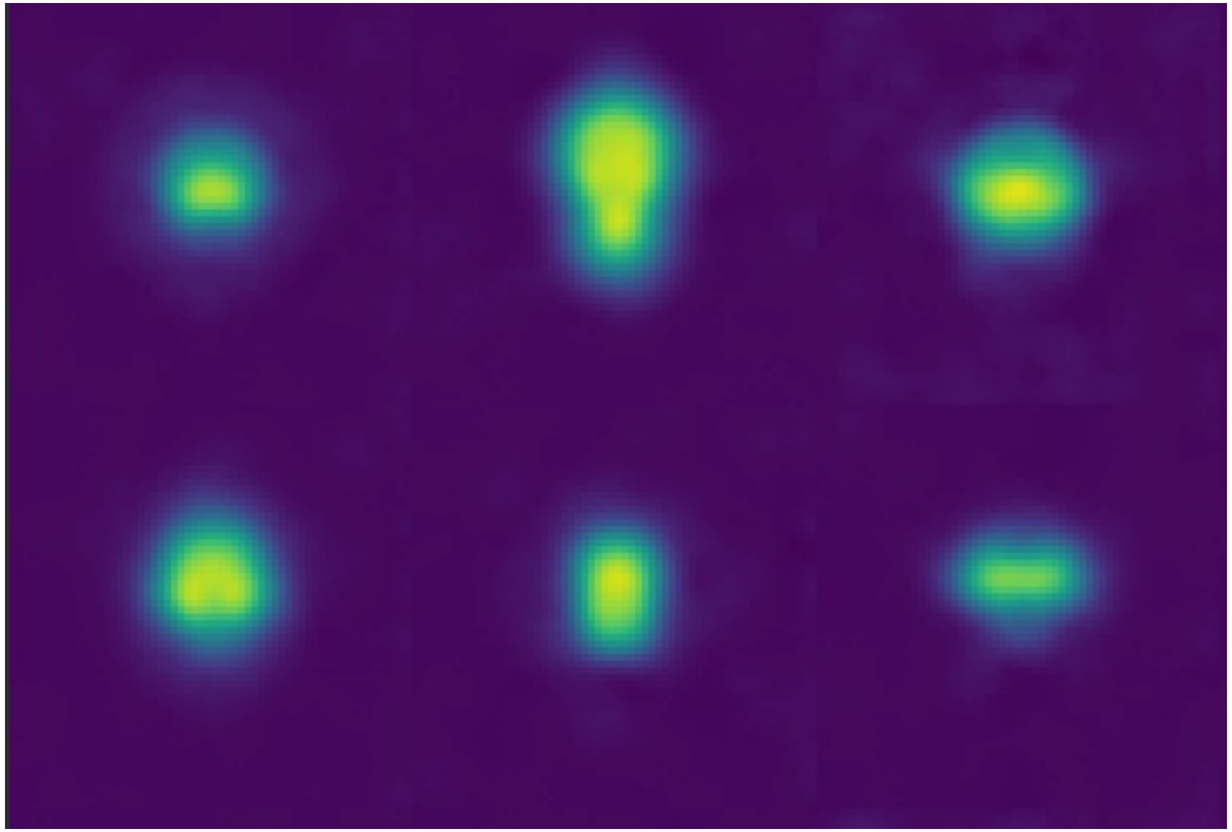


Experimental Xray Images



Equivalent 2D Hydra images

# Latent Spaces of Modern Generative Models can Express Out of Training and even Completely Out of Distribution Data

- Using large scale data modern generative models (e.g., StyleGAN) utilize powerful architectures to produce rich, yet very high-dimensional, latent spaces
  - These enable semantic interpretation and manipulation and enable transfer learning approaches
  - This leads to the idea of foundation models

**Picture:** *These people are not real – they were produced by our generator that allows control over different aspects of the image.*

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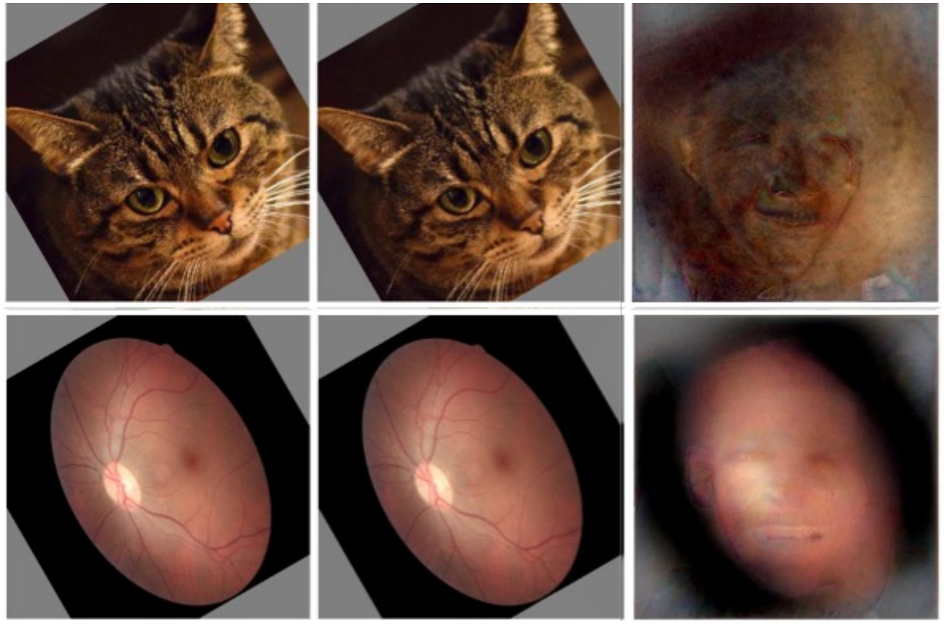
- Using large scale data modern generative models (e.g., StyleGAN) utilize powerful architectures to produce rich, yet very high-dimensional, latent spaces
  - These enable semantic interpretation and manipulation and enable transfer learning approaches
  - This leads to the idea of foundation models … except it is unclear where to get the data

True Proposed Baseline

**Might not need more data**

True Proposed Baseline



# Automatic Concept Discovery and Comparison Provides Intuitive Insights into the Fundamental Degrees of Variation Encoded in $Z$

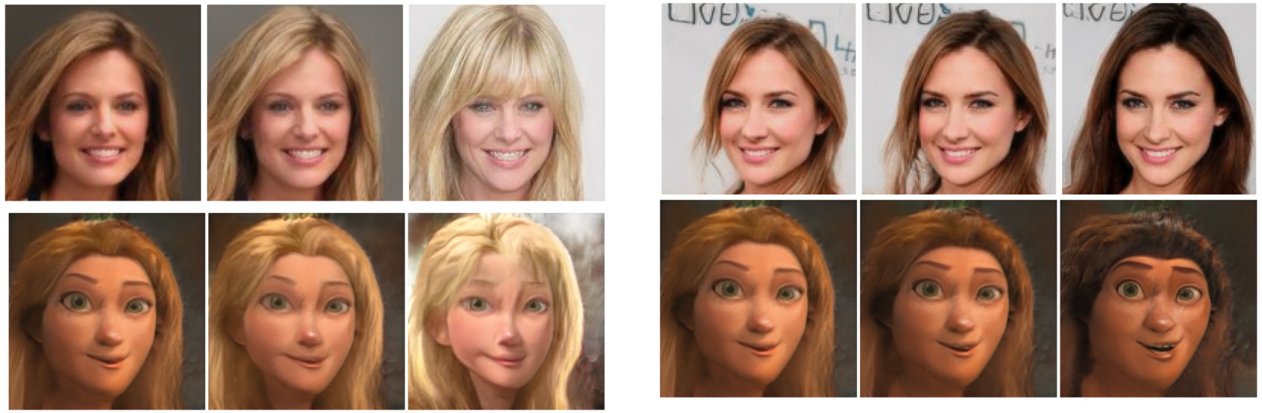
- Discovering and comparing concepts is how humans understand data and models
  - Essential for understanding many comparison tasks
  - Where does two surrogate models differ and in what way are they similar?
  - How and where does surrogate model differ from simulation
- Challenges
  - Often do not have one-on-one correspondence between dataset on sample level
  - There are a mixture of aligned and non-aligned factors
  - Need for a totally unsupervised solution
- Solution
  - Frame a joint concept discovery and concept alignment problem
  - Leverage a global latent representation to align shared and contrast unique concept (directions)

# Initial Results on Face Image Dataset: What are the Shared and Unique Factors between Real and Cartoon Images?

Face Photos

Cartoon Character Faces

Shared concepts



Concepts unique to cartoons

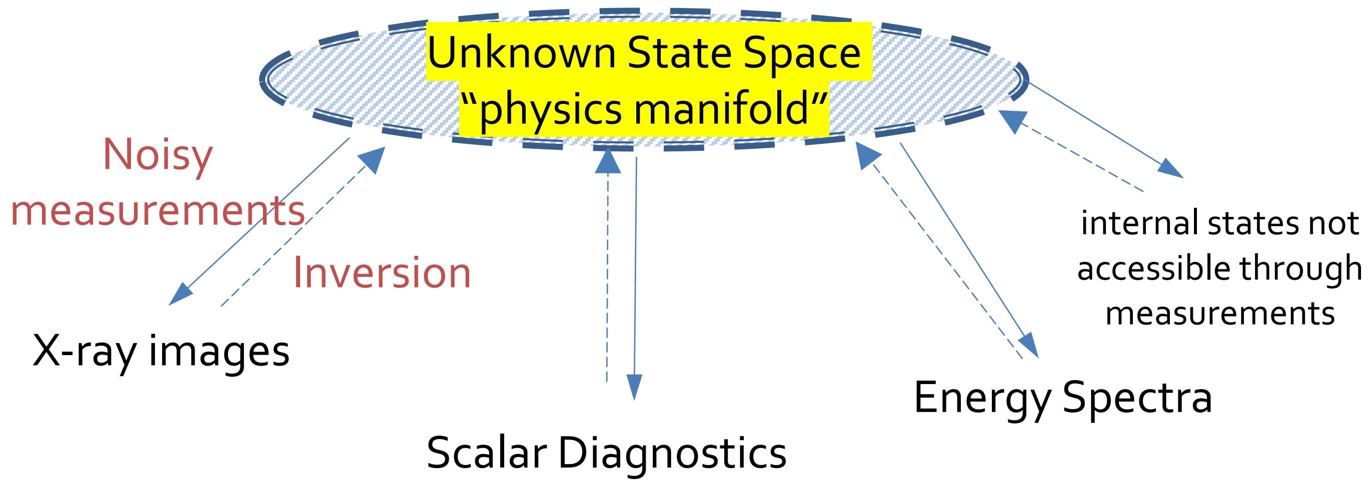
# The Next Steps for the Distribution Comparison/Alignment Research are Scientific Models and Ways to Improve Knowledge Transfer

- Physical applications
  - Evaluate on physical meaningful dataset with good ground truth
  - Expand to non-image or multi-modality dataset
  - Support users in understanding concepts

- Go beyond interpretation
  - Leverage the comparison insight to improve the existing models
  - A continuous mapping that account for distribution shift that facilitate better transfer learning

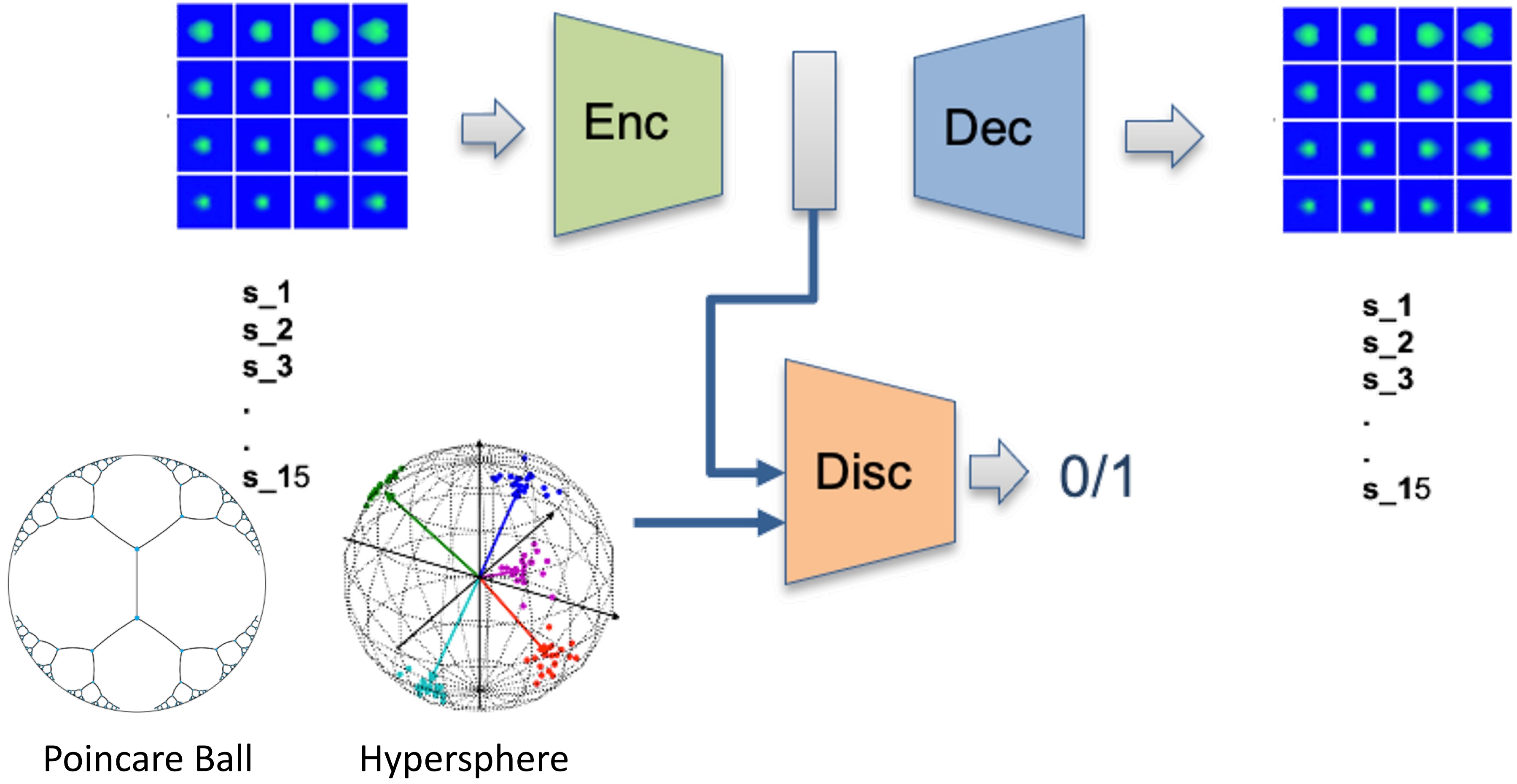
# Different Geometric and Structural Priors Lead to Latent Spaces Producing More Diverse Sampling and Better Optimization

- Existing data-driven feature learning solutions assume that latent spaces are Euclidean.
- In many problems, the physics manifold might correspond to a curved manifold creating a potential mismatch
- Better "geometric priors" in the latent space can help improve the quality of latent spaces → better predictive modeling.



# We Enforce Soft Geometric Constraints by Exploiting the Discriminator Network in the Wasserstein Autoencoder

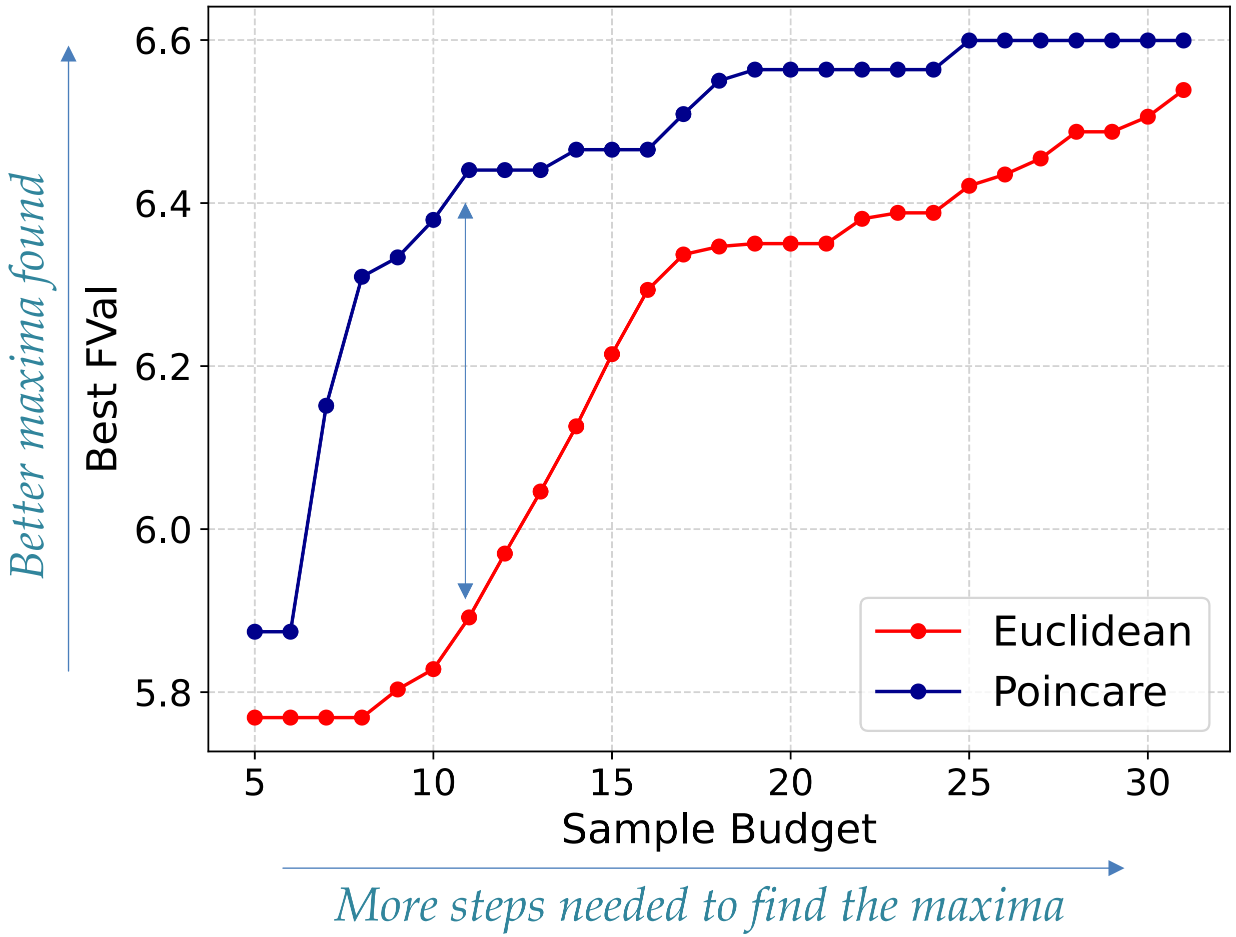
- Easier to enforce
- More flexible
- Enables mixed/ hierarchical spaces



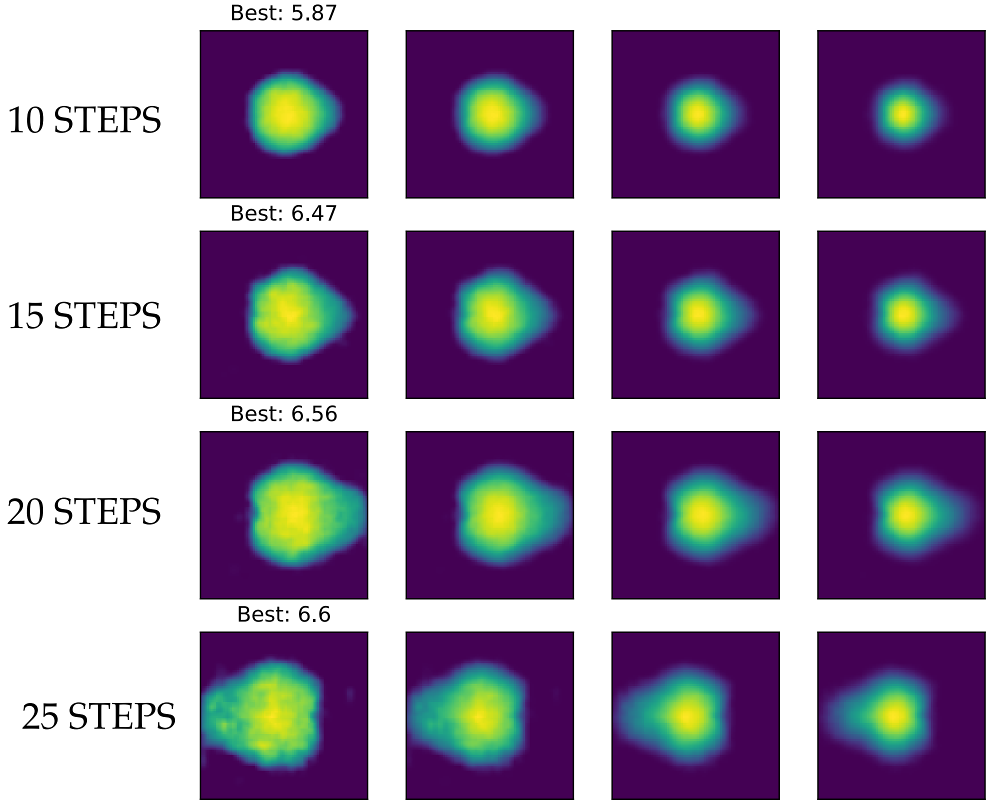
# Initial Results Suggest Hierarchical Latent Spaces Improve Sequential Optimization Likely due to Better Sampling

Optimizing for total Image brightness

*Significantly faster, and better maxima with Poincare models*

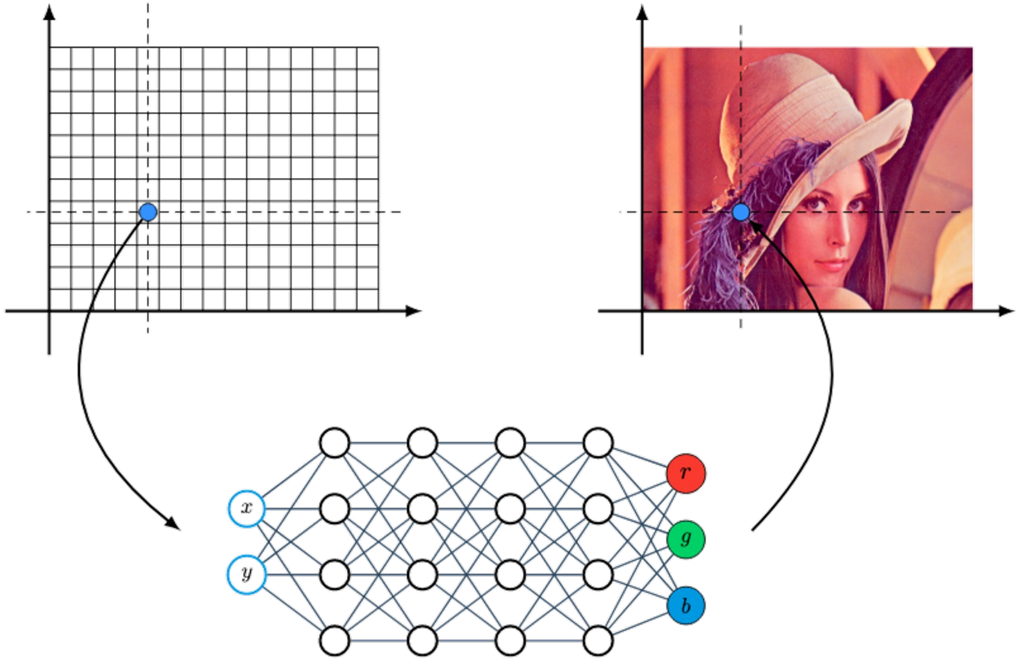


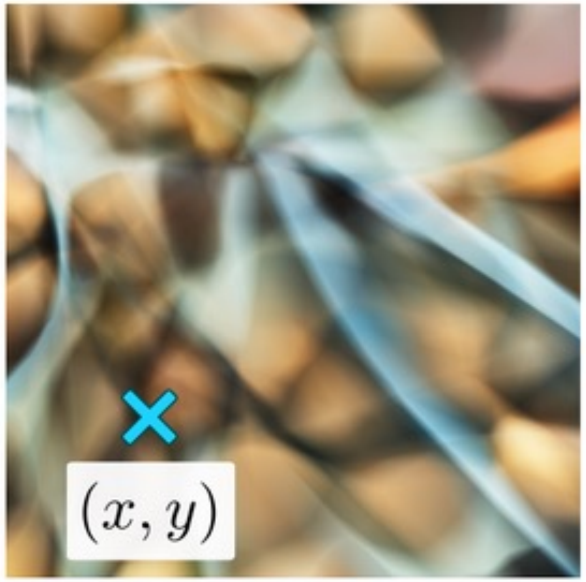

Best solution discovered so far



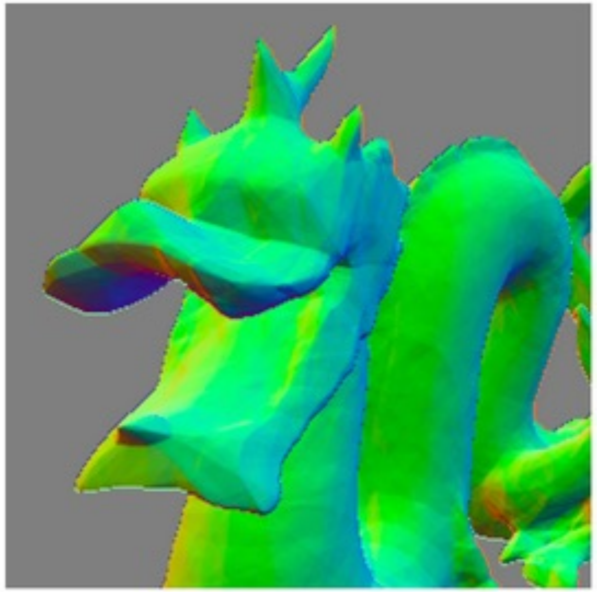
# Conventional DNN Surrogates Cannot Recover Higher Frequency Content Even in Very Low Dimensions

- An image can be viewed as a function defined in a continuous 2D (or 3D) domain with lots of data but high frequencies.
- Representing images using standard MLPs usually fails because we cannot recover even moderate frequencies reliably



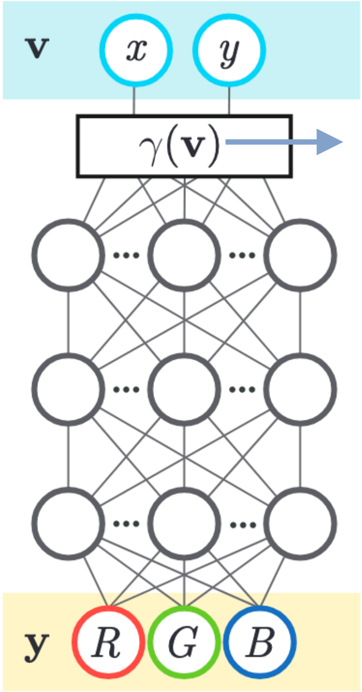

2D image



3D shape

# Fourier Feature Networks – A new family of neural network surrogates

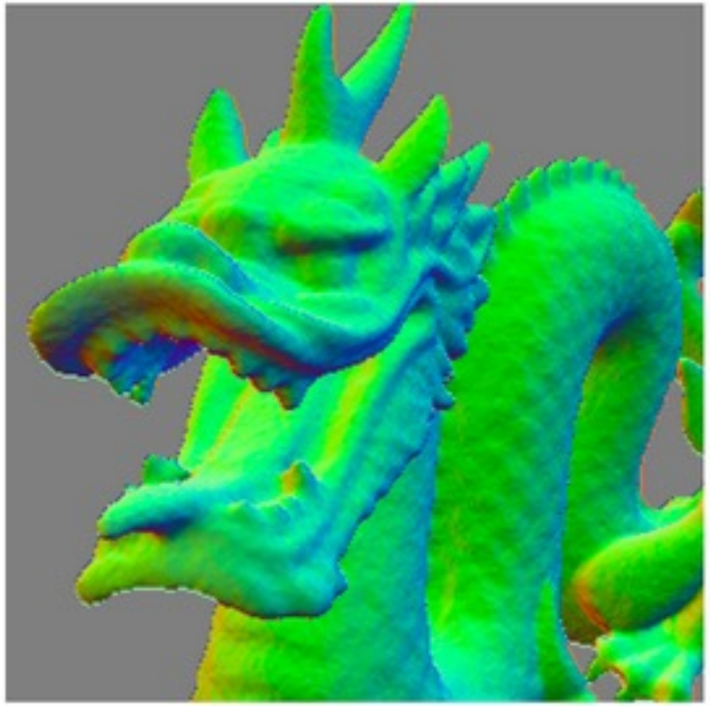
- Bochner's theorem allows the use of random Fourier features to approximate any arbitrary stationary (shift-invariant) kernel




Gaussian Fourier basis

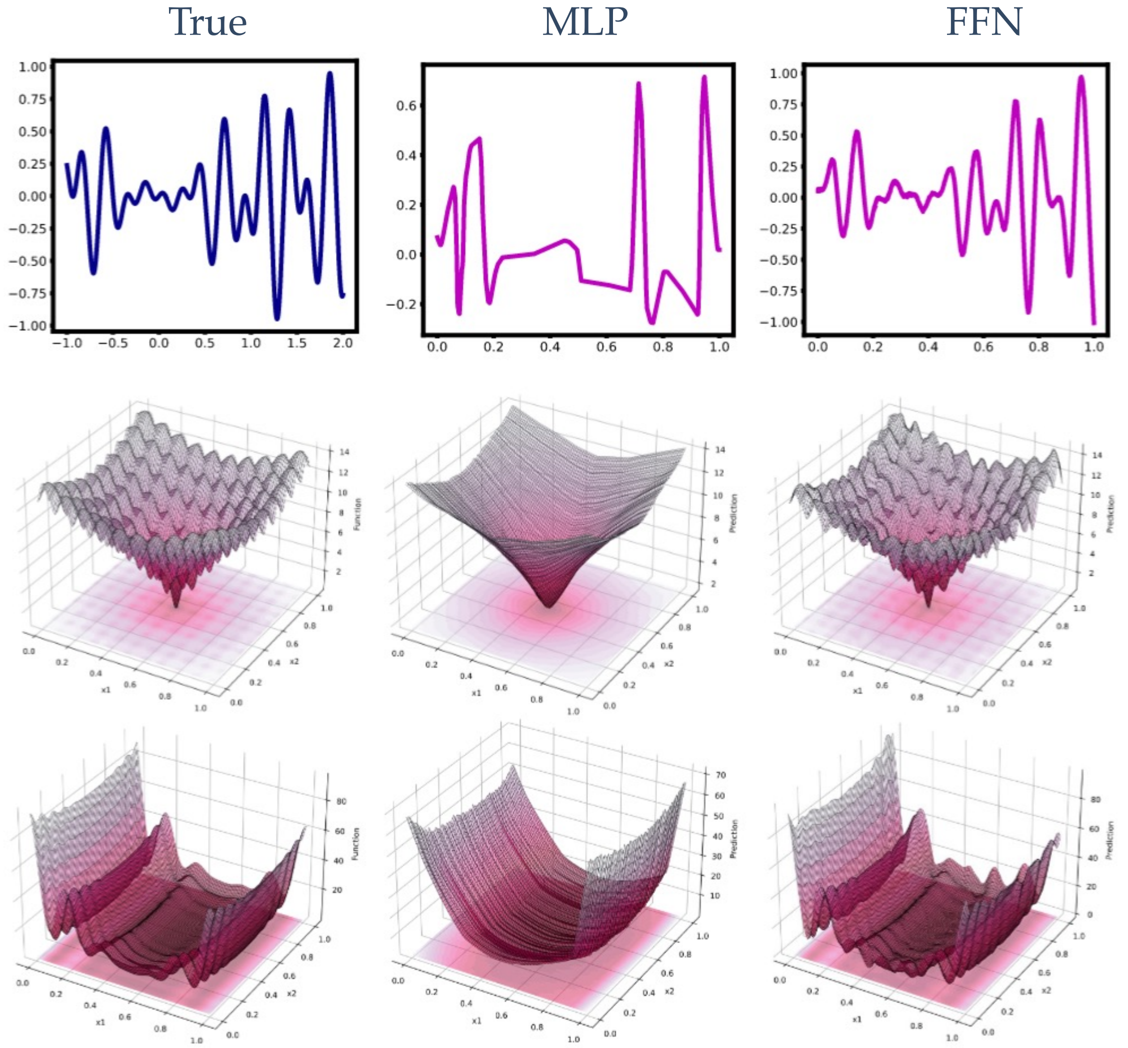
1. what frequencies?
2. how many components?

2D image



3D shape

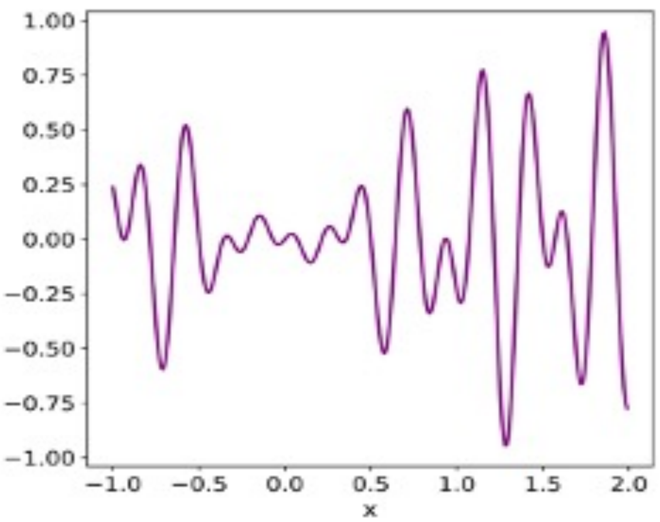
# Fourier Feature Networks produce significantly higher quality regression functions than MLPs of the same complexity



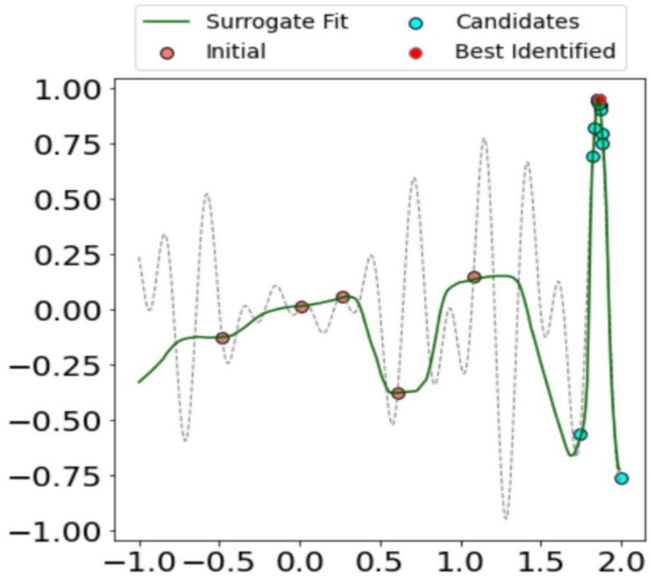

| Dataset | MLP | | | FF | | |
|---|---|---|---|---|---|---|
| | RMSE | RSE | SMAPE | RMSE | RSE | SMAPE |
| Multi Optima | 0.21 | 0.61 | 99.2 | **0.02** | **0.05** | **17.1** |
| Ackley | 0.59 | 0.23 | 5.4 | **0.45** | **0.18** | **3.4** |
| Levy | 9.04 | 0.53 | 40.7 | **1.49** | **0.08** | **8.1** |
| Griewank | 0.18 | 0.33 | 20.1 | **0.05** | **0.09** | **5.9** |
| Holder | 2.11 | 0.67 | 69.4 | **1.05** | **0.33** | **40.8** |

$$\mathrm{RSE} = \frac{\sqrt{\sum (y-\hat{y})^2}}{\sqrt{\sum (y-\mu_y)^2}} \qquad \mathrm{SMAPE} = \frac{100}{n} \frac{|y-\hat{y}|}{0.5(|y|+|\hat{y}|)}$$

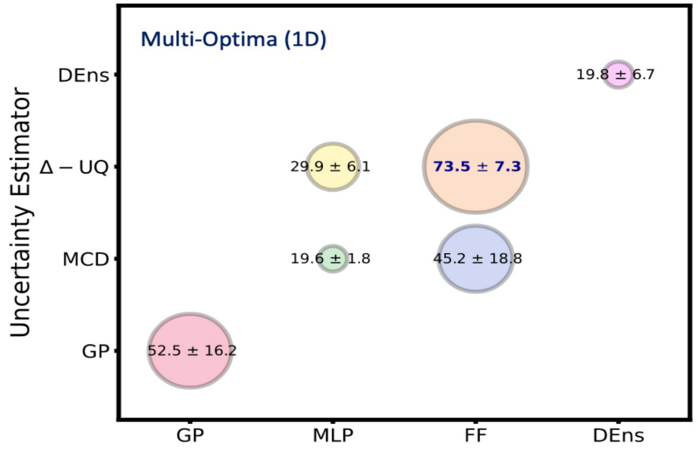
# Together With Δ-UQ New Deep UQ Approach FFNs Consistently Outperform Baselines in Sequential Optimization

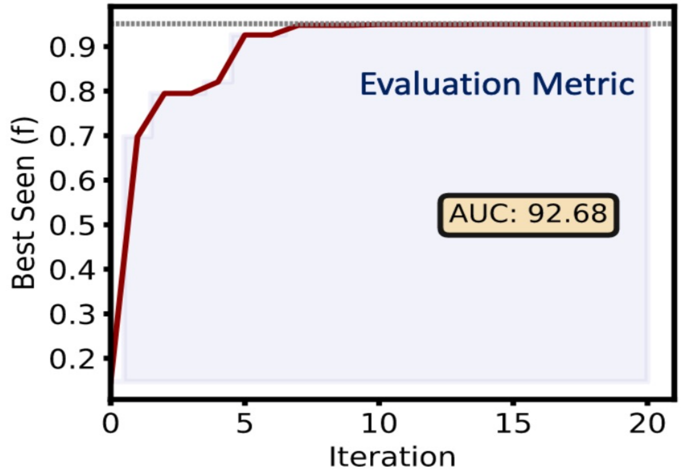



1D Multi optima




FFN + Delta-UQ




MCD: Monte-Carlo Dropout

DEns: Deep Ensembles

GP: Gaussian Processes

FF: Fourier Feature Networks

MLP: Multilayer Perceptron (ReLU)

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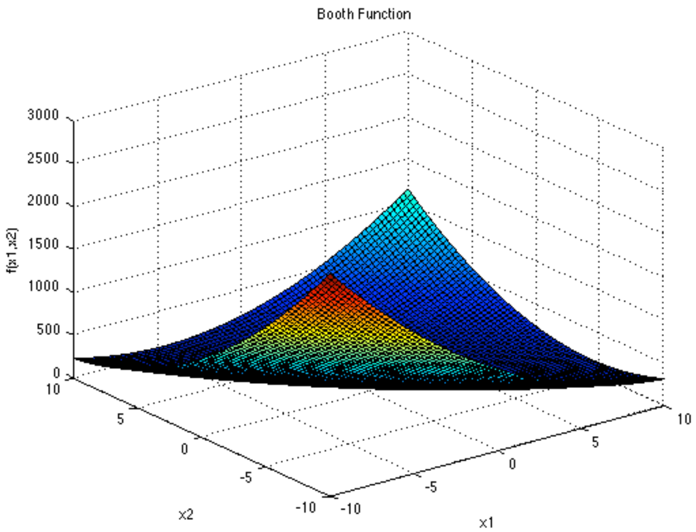


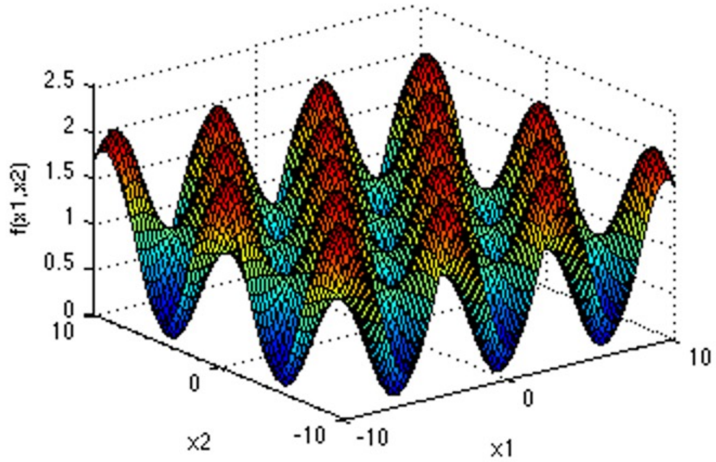


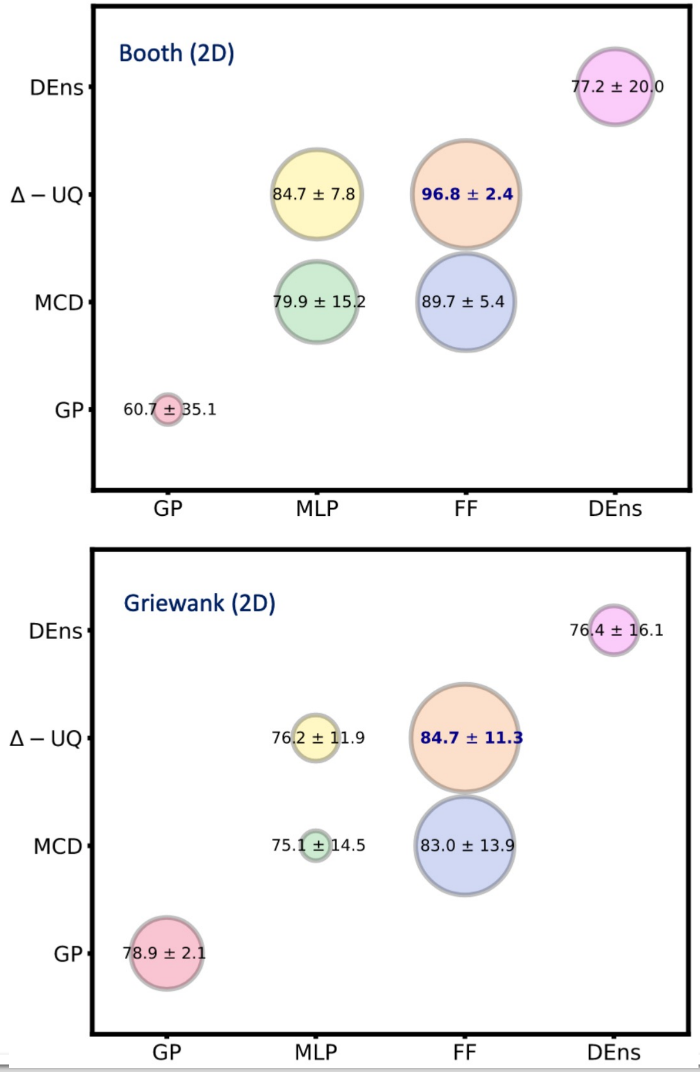


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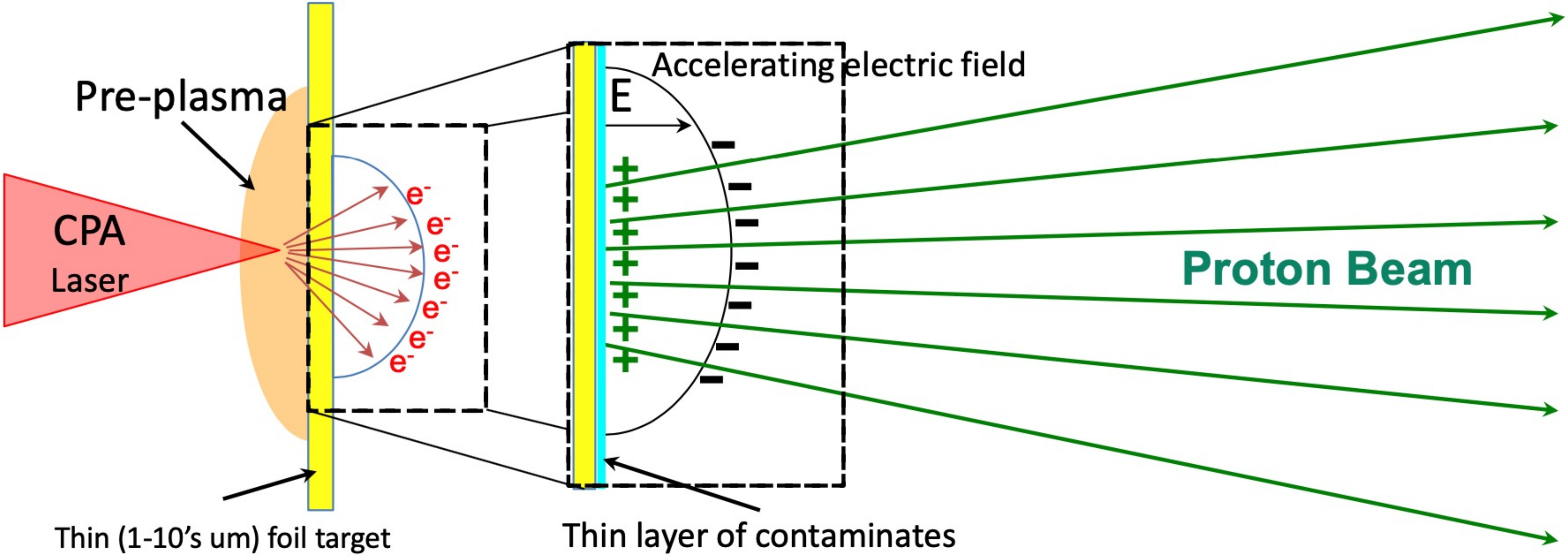
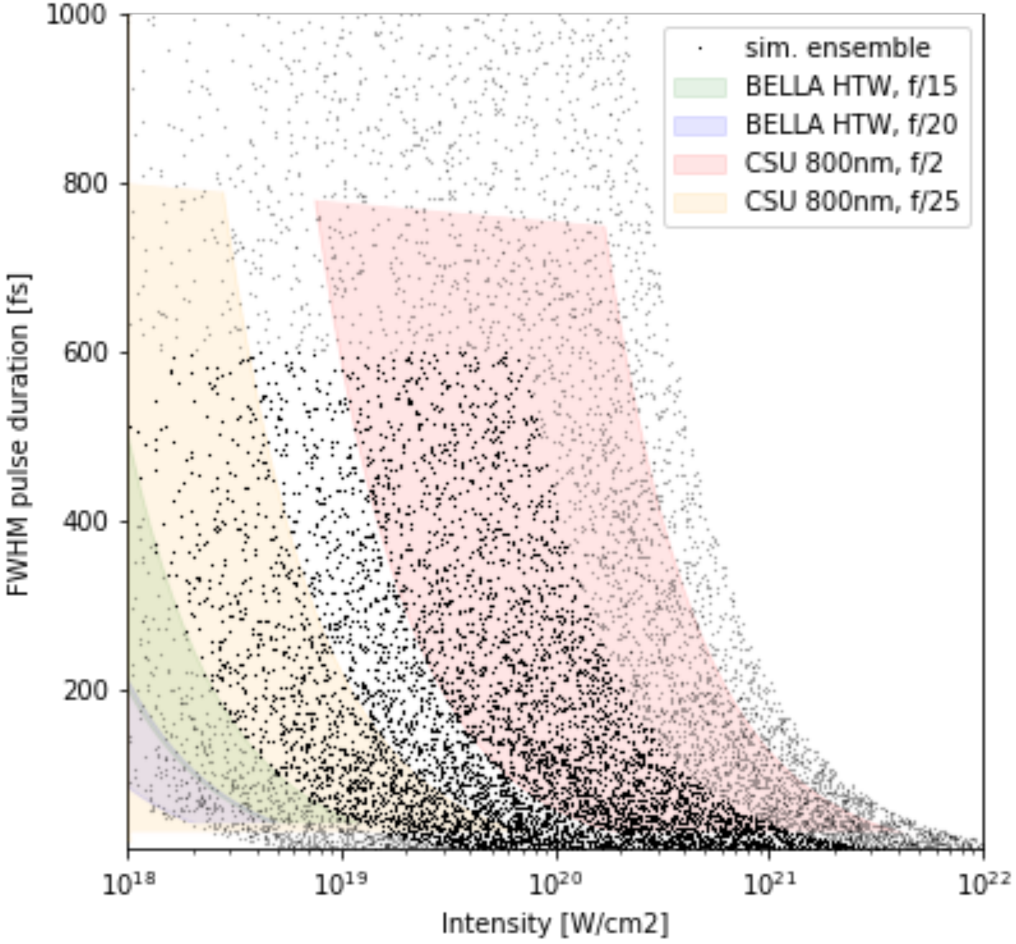
# We are Interested in Short-Pulse Lasers Able to Create MeV Energy Proton Beams for Future Diagnostics

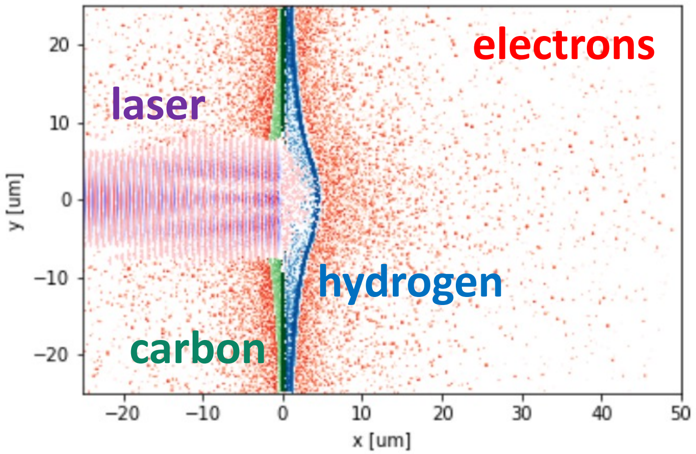


# Working with 10k+ Simulations Targeted to Match ALEPH (CSU) Experiments Including Spectral Pulse Shaping

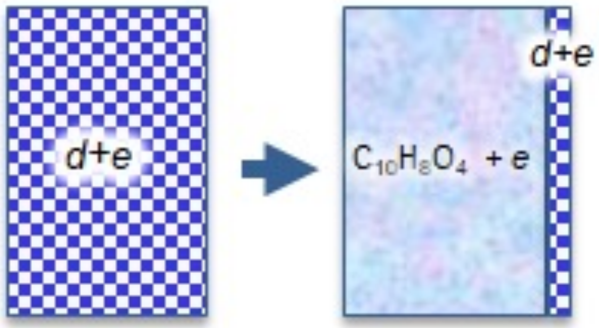
C + H target tailored to experiment



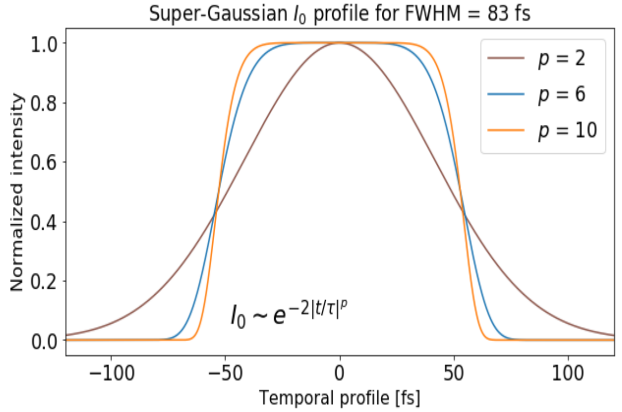

Multi-dimensional modeling

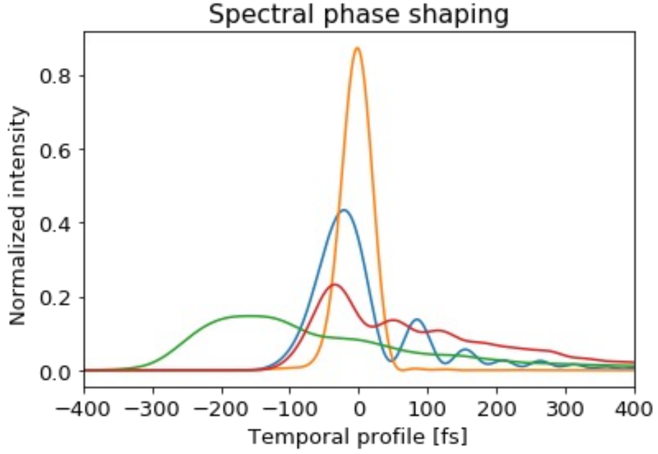



Material properties

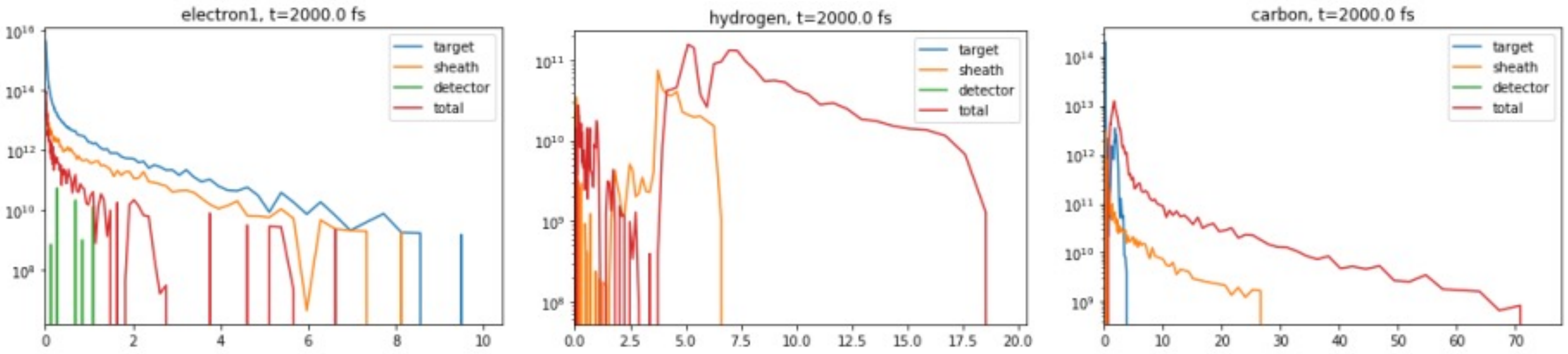



Shaped laser pulses



# Simulation Outputs are Spectra of Various Species at Different Locations as well as Simulated Diagnostics such as PROBIES



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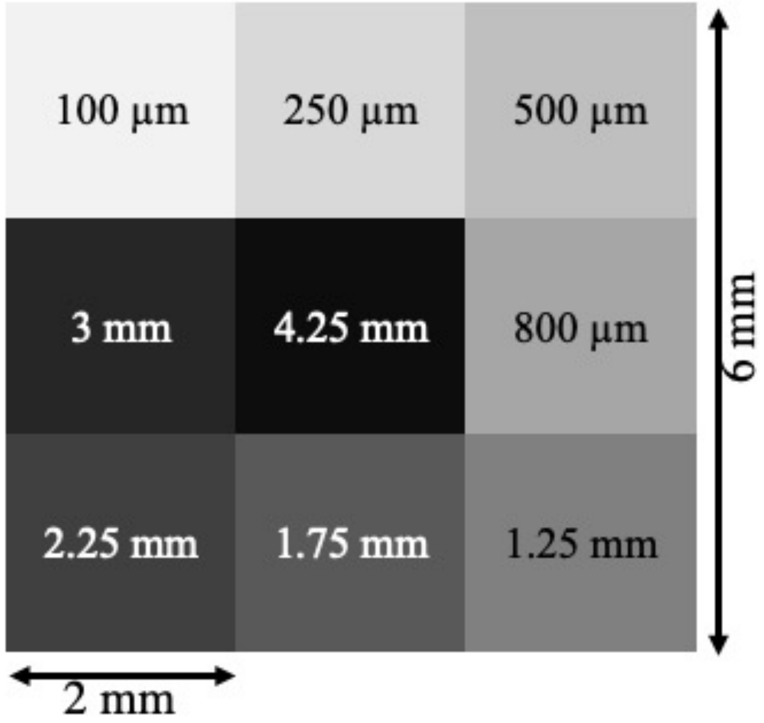
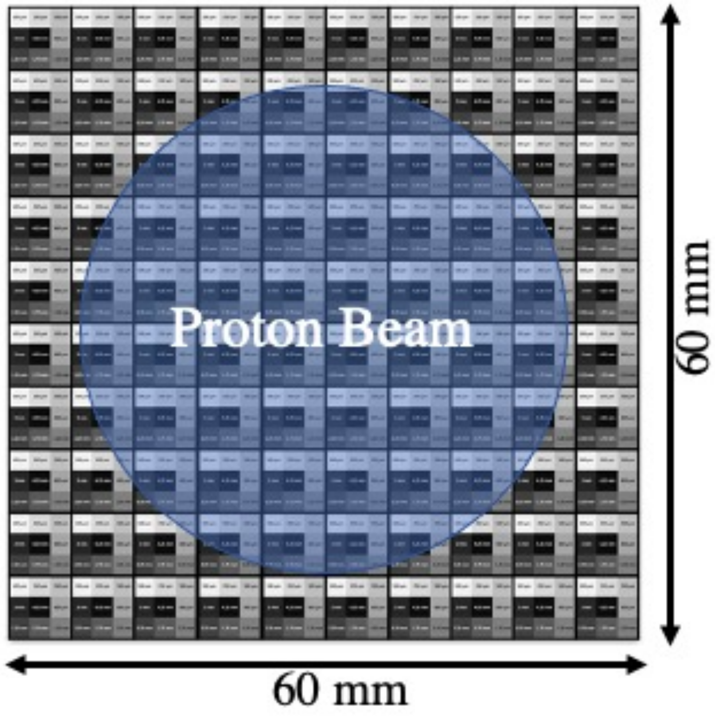
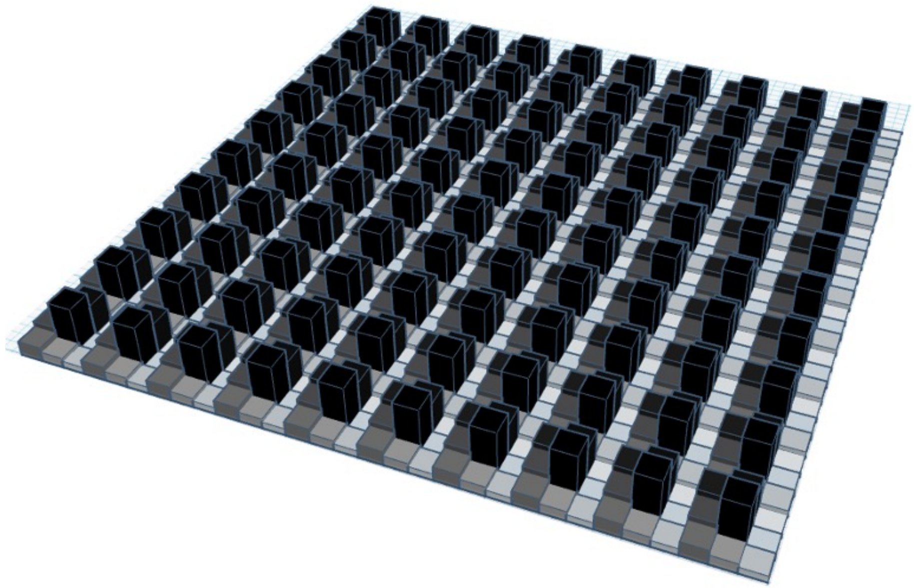
Local Mask of Thicknesses




Spatial Arrangement




Manufactured Filter



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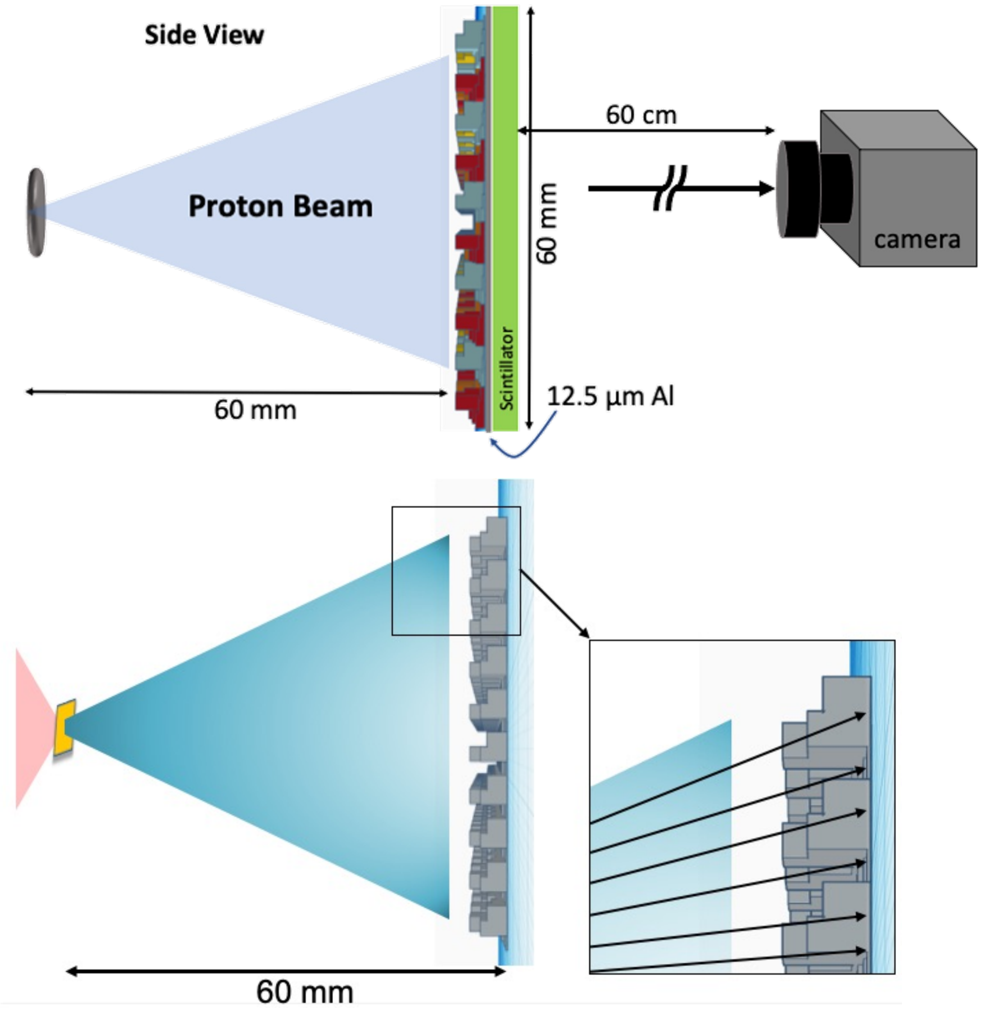
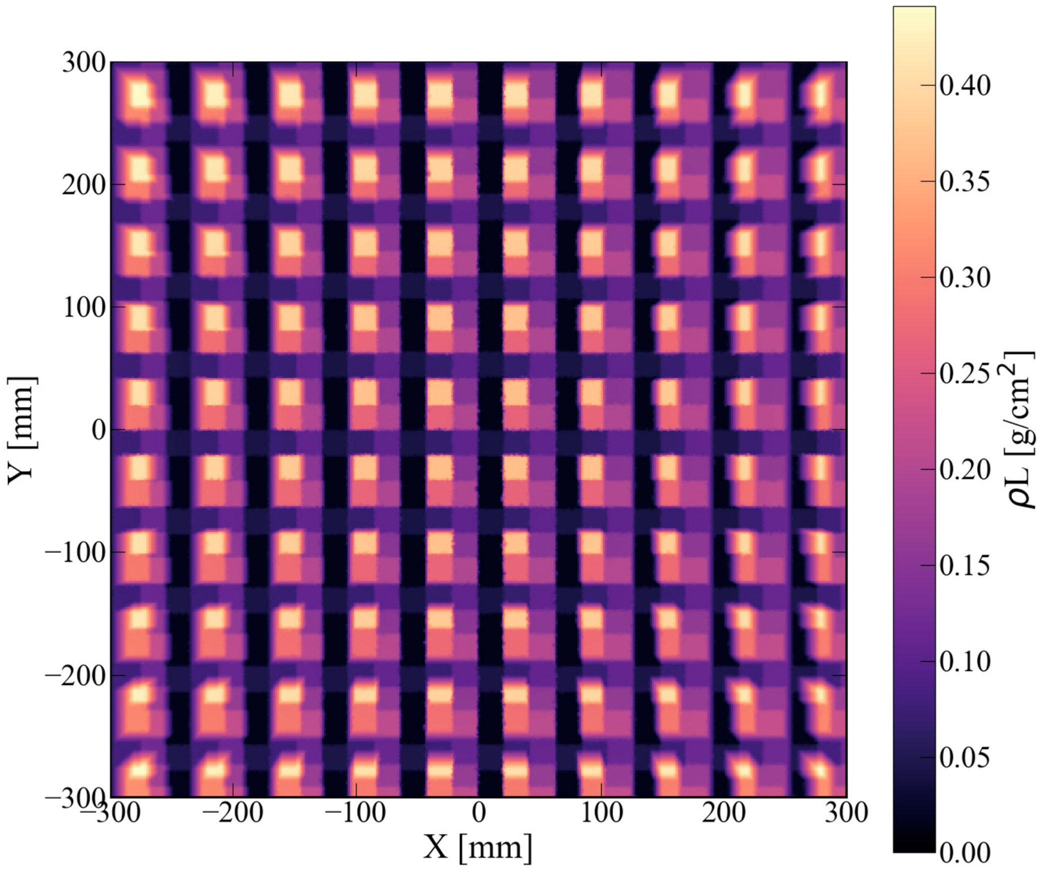
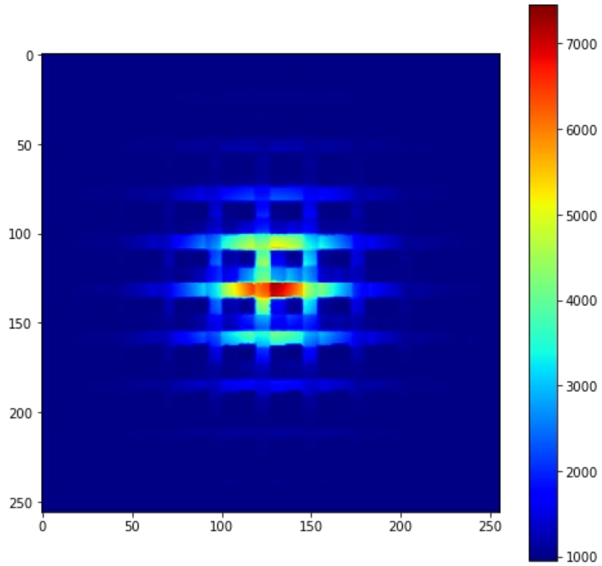


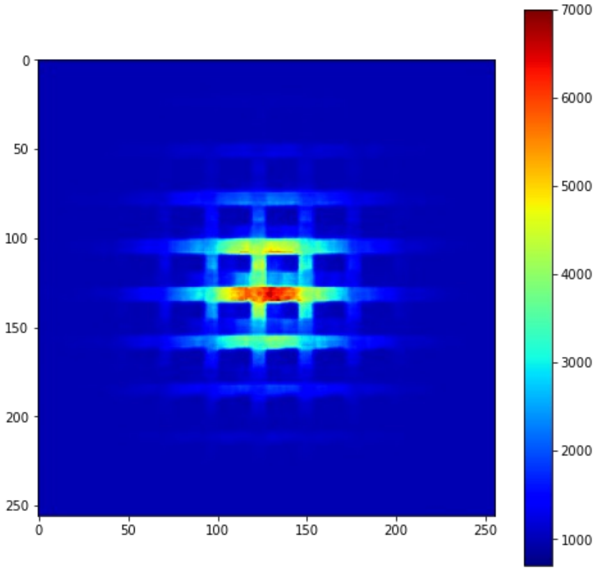



# We can Build Multimodal Forward Models that Jointly Predict PROBIES Images and Spectra

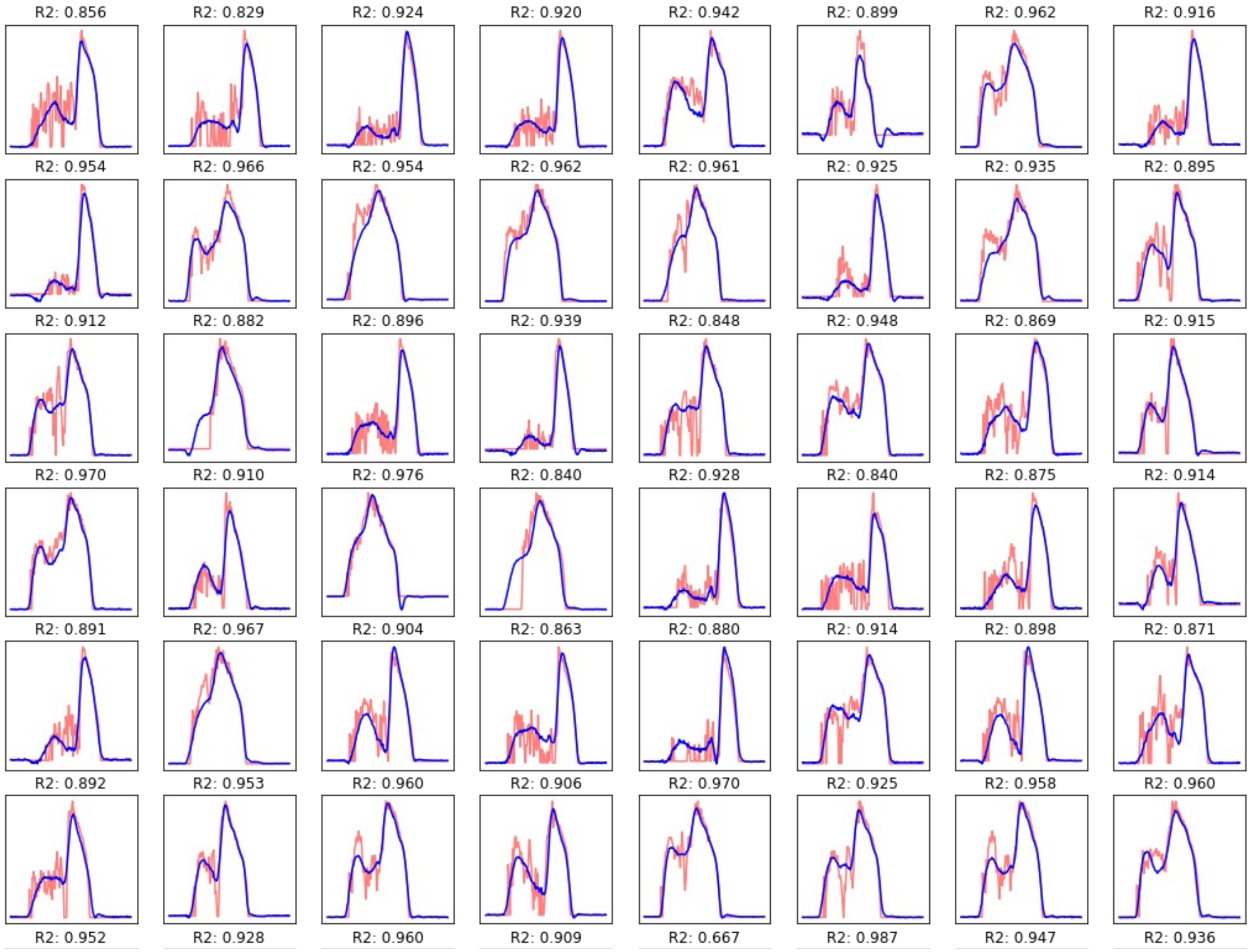
- **Inputs**: Epmax, Etot, alpha, log(I), preplasma_scale_length, pulse_length, target_density, target_thickness

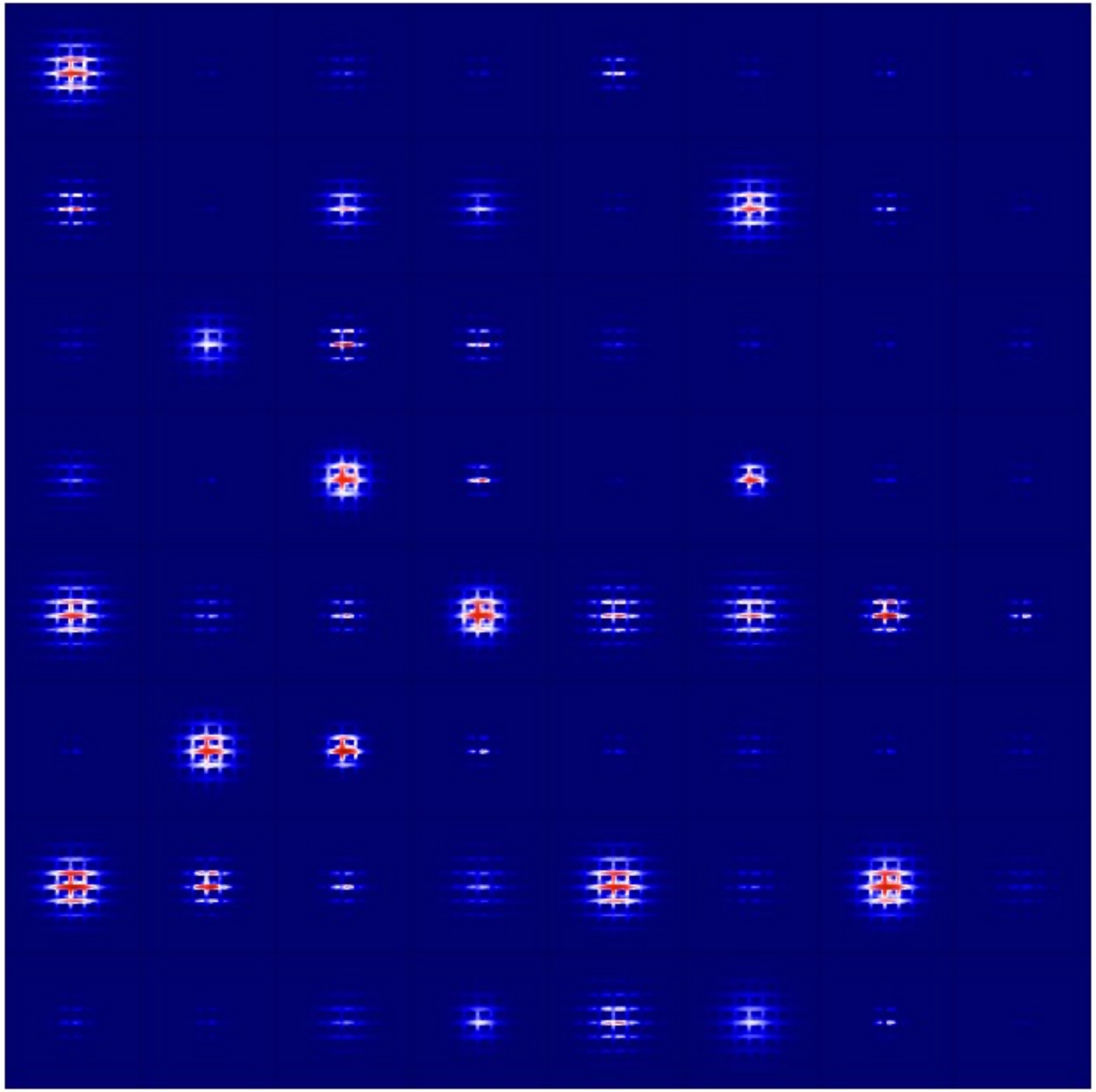



Ground truth

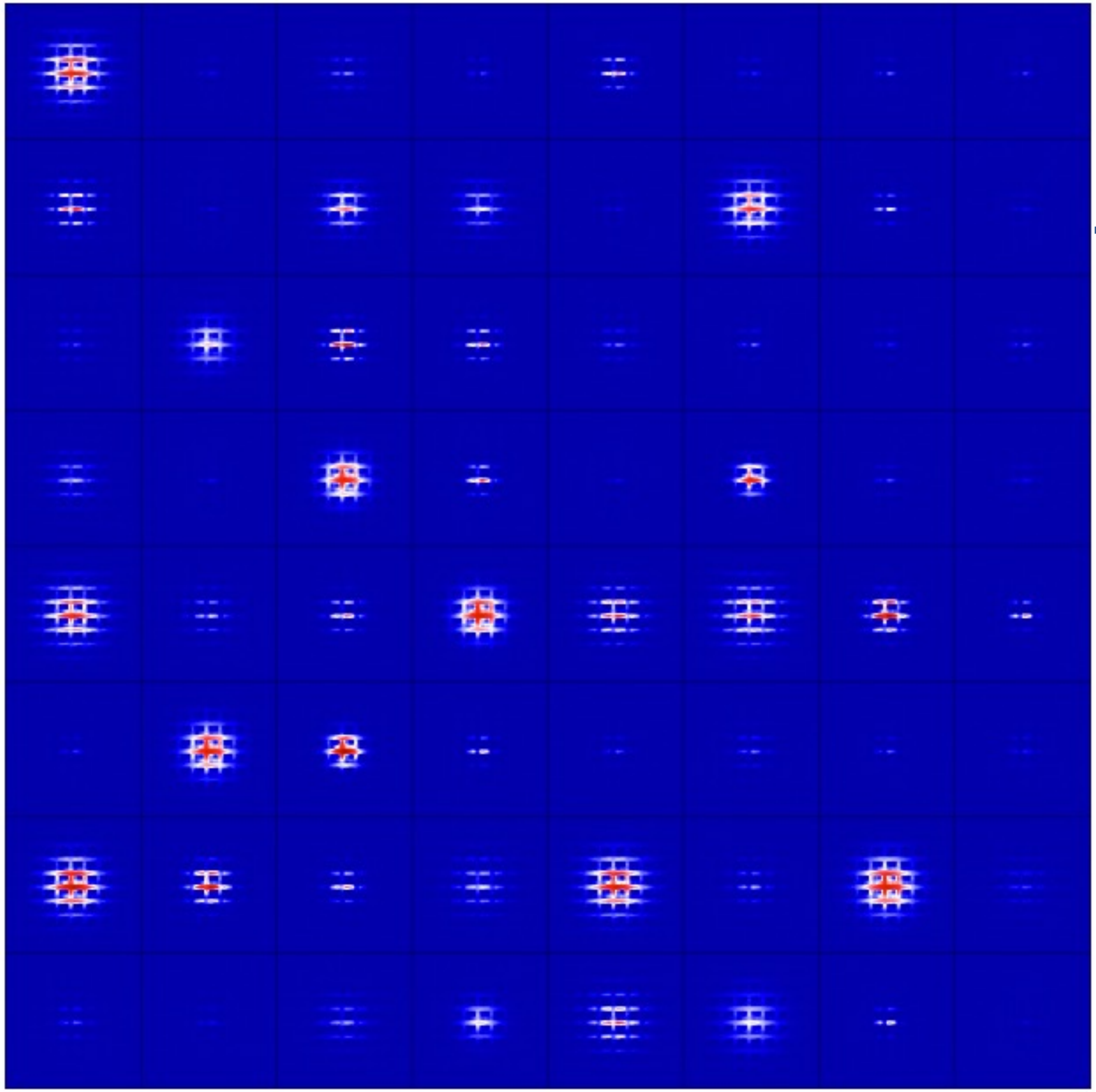



Predicted





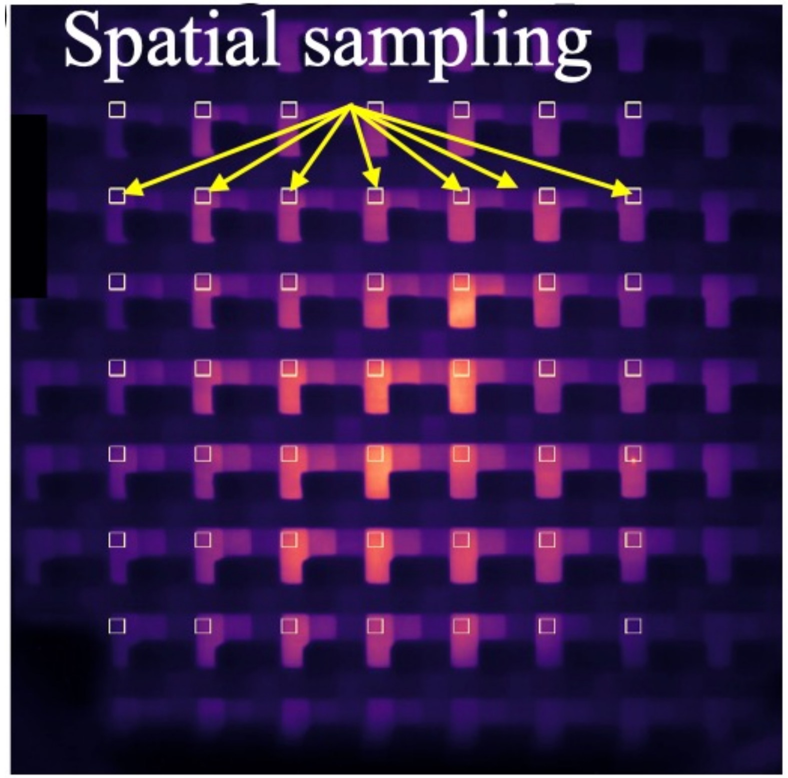
Ground truth

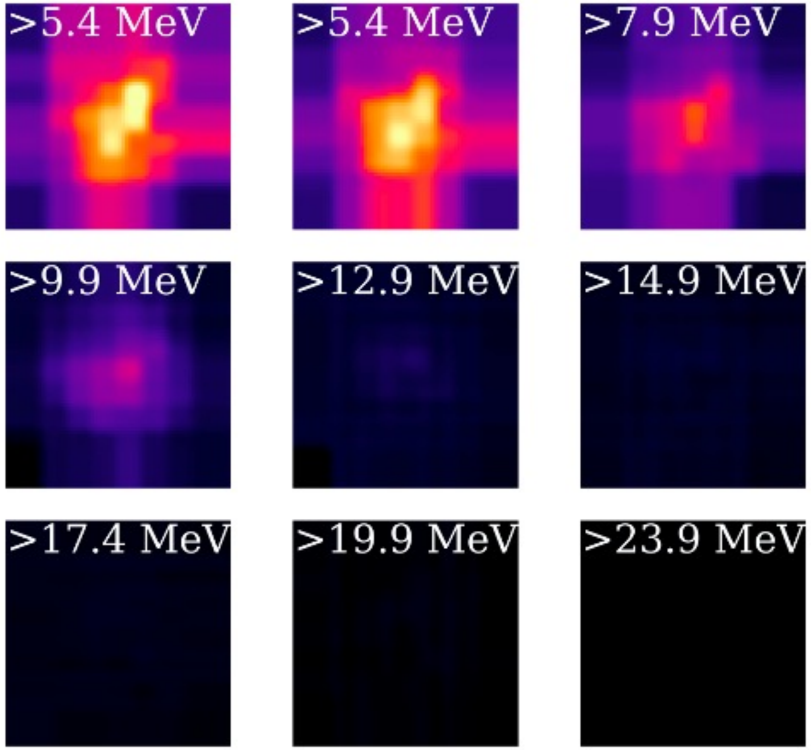


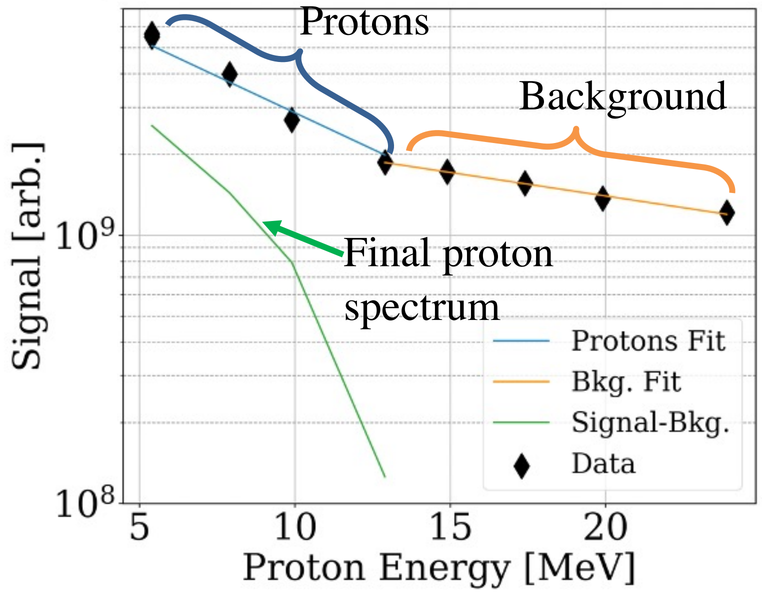
Predicted

# Similar Models Also Enable Fast Diagnostics Necessary for Real-Time Analysis and Experimental Steering

| 1) Sample the data | 2) Interpolate new images | 3) Reconstruct proton spectrum |
|---|---|---|

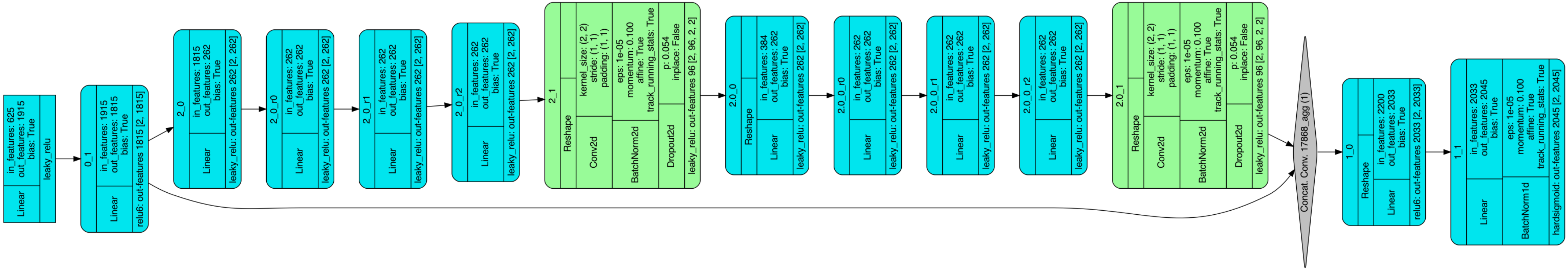


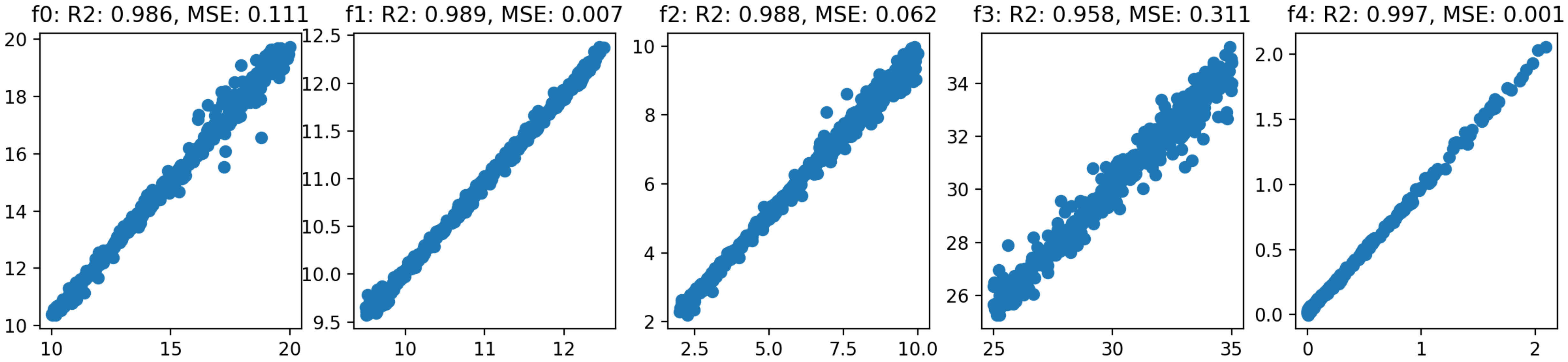
# Similar Models Also Enable Fast Diagnostics Necessary for Real-Time Analysis and Experimental Steering

- Neuroevolution, a genetic algorithm-based neural architecture search, provides flexible and unbiased approach to create optimal architectures
- PROBIESNet-Zero: High performing architecture for PROBIES evolved from ”scratch” to derive five scalar diagnostics from 300x300 PROBIES images



# Similar Models Also Enable Fast Diagnostics Necessary for Real-Time Analysis and Experimental Steering

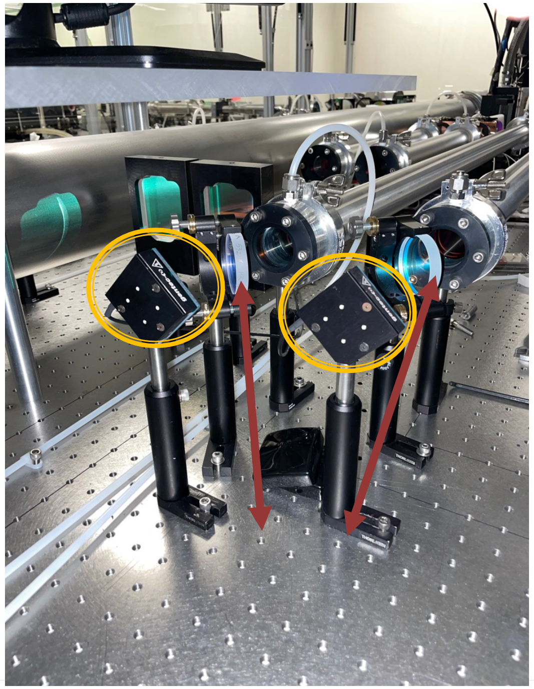
- PROBIESNet-Zero reached average R2 of 0.98 compared to 0.91 of previous human developed architectures in predicting *amplitude, ion temperature, maximum proton energy, divergence beam angle,* and *total energy*

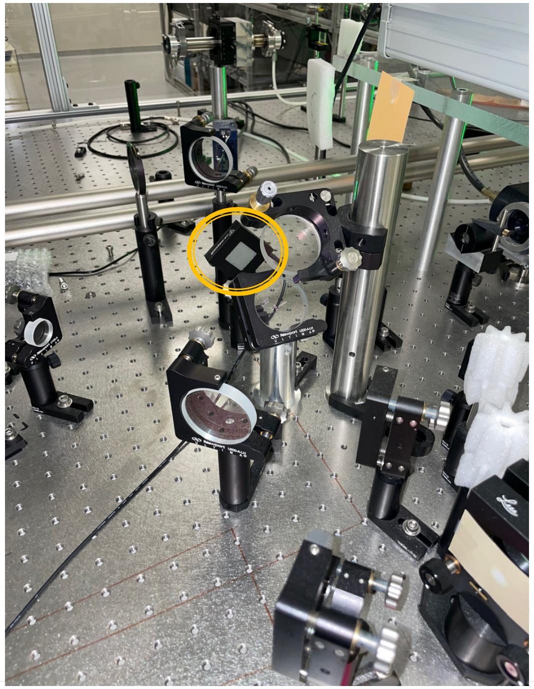
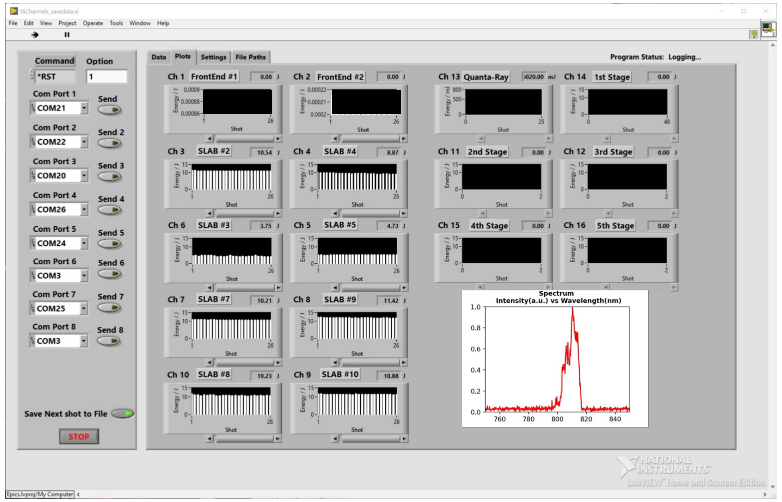


# Integrating Both Control Inputs, Beam Characterization, Diagnostic Outputs, and Sequential Optimization Through EPICS

- EPICS provides a common control system
  - Mature technology
  - Distributed processing is scalable and avoid common bottlenecks
- Demonstrated "first light" at ALEPH

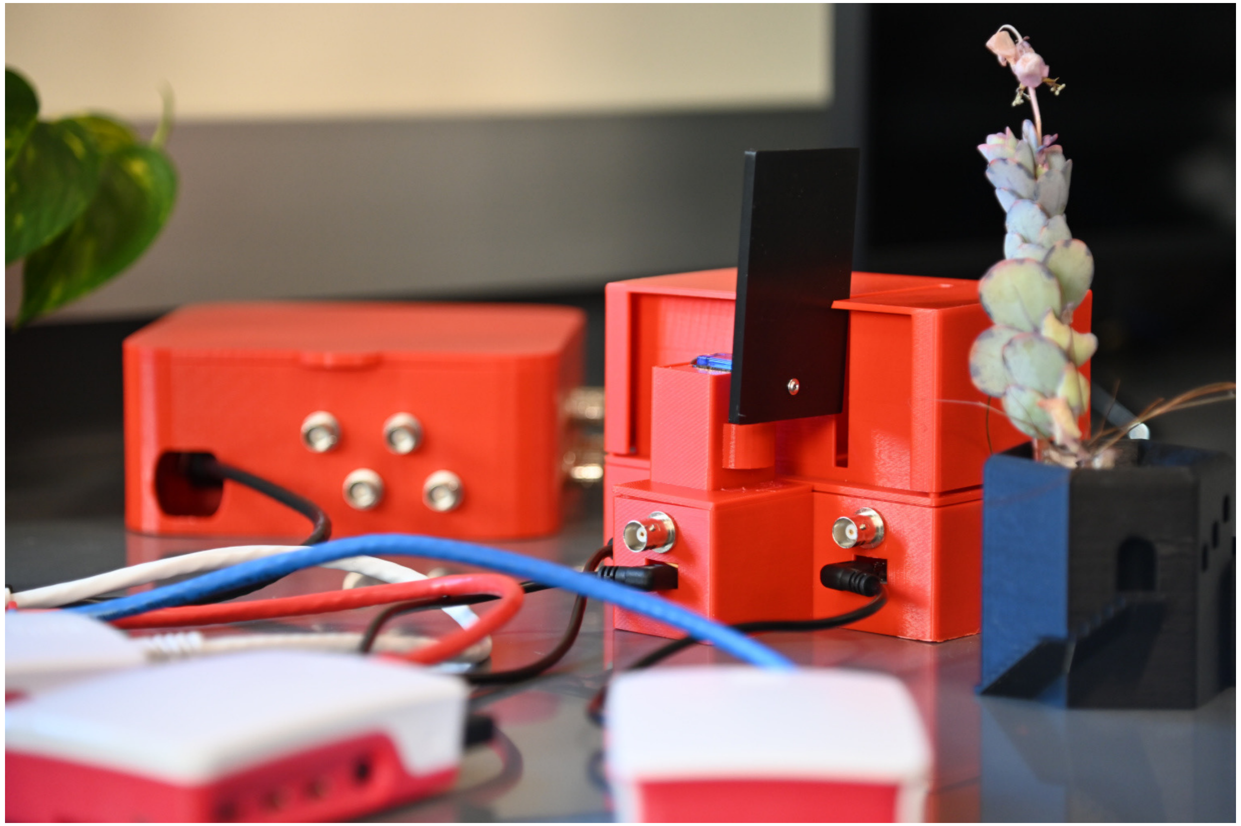
EPICS



# We are Facilitating EPICS Integration by Building and (Soon) Shipping Simple Sidekick Systems Developed at CSUCI

- Models a full control system coupling
  - Light sources (6 LEDs)
  - Detectors (a phototransistor)
  - Shutter (swings an object to block light)
  - Raspberry PIs or similar computers
  - Wired local area network
  - Full EPICS installation
- Enables CS/ML researchers to develop and debug portable control loops
- Provide all partners common test systems
  - LLNL
  - NVIDIA
  - CSU
  - Kansas City NSC



http://scottfeister.com/sidekick

# Many Challenges Remain at All Fronts but the Integration of Experiments, Simulations, and ML Promises Great Opportunities

- Integrating additional diagnostics and multiple spectra into the modeling
- Develop UQ driven sequential optimization loop
- Harmonize pulse shape control between simulations and experiments (SLAC)
- Integrate automatic control at CSU including guaranteeing laser safety
- Preparing for first demonstration at the end of May

CASC

Center for Applied Scientific Computing

Lawrence Livermore National Laboratory