AI in Physics

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MEMORIAL
UNIVERSITY

THE NOBEL PRIZE IN PHYSICS 2024

Illustrations: Niklas Elmehed

John J. Hopfield   Geoffrey E. Hinton

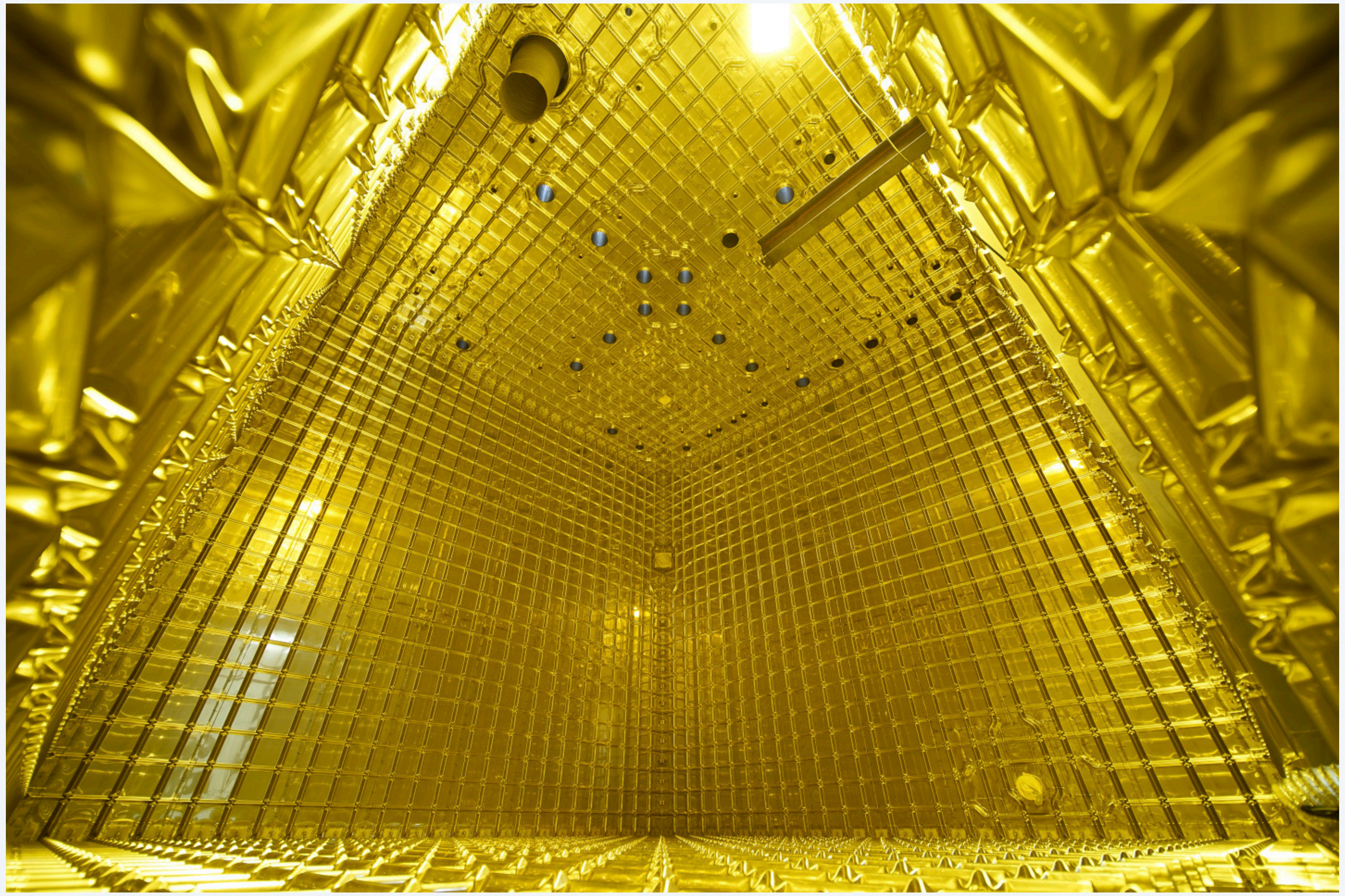
"for foundational discoveries and inventions
that enable machine learning
with artificial neural networks"

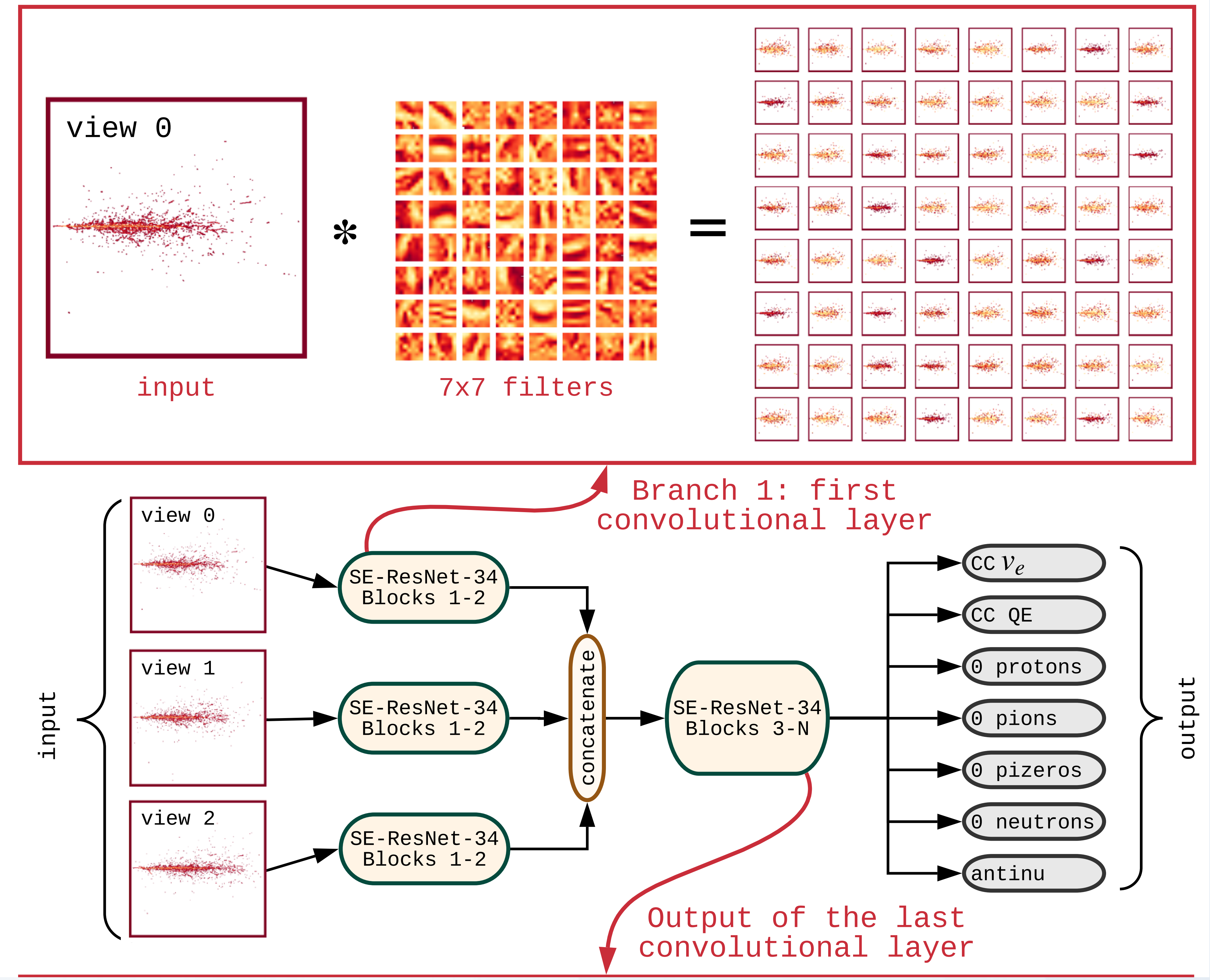
THE ROYAL SWEDISH ACADEMY OF SCIENCES

How is AI used in Physics?

Neutrinos

- What flavour of neutrino interaction has been observed?

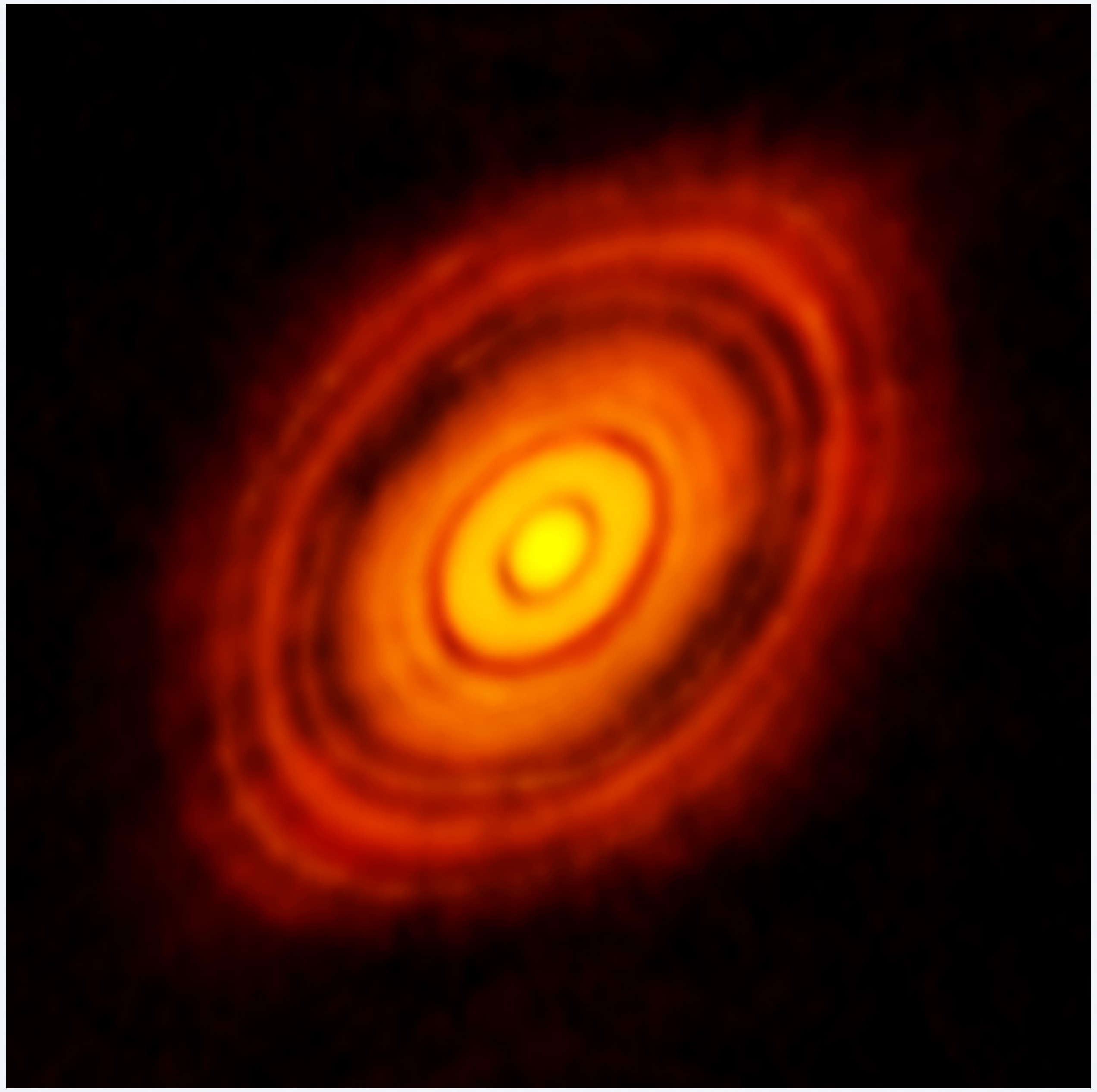


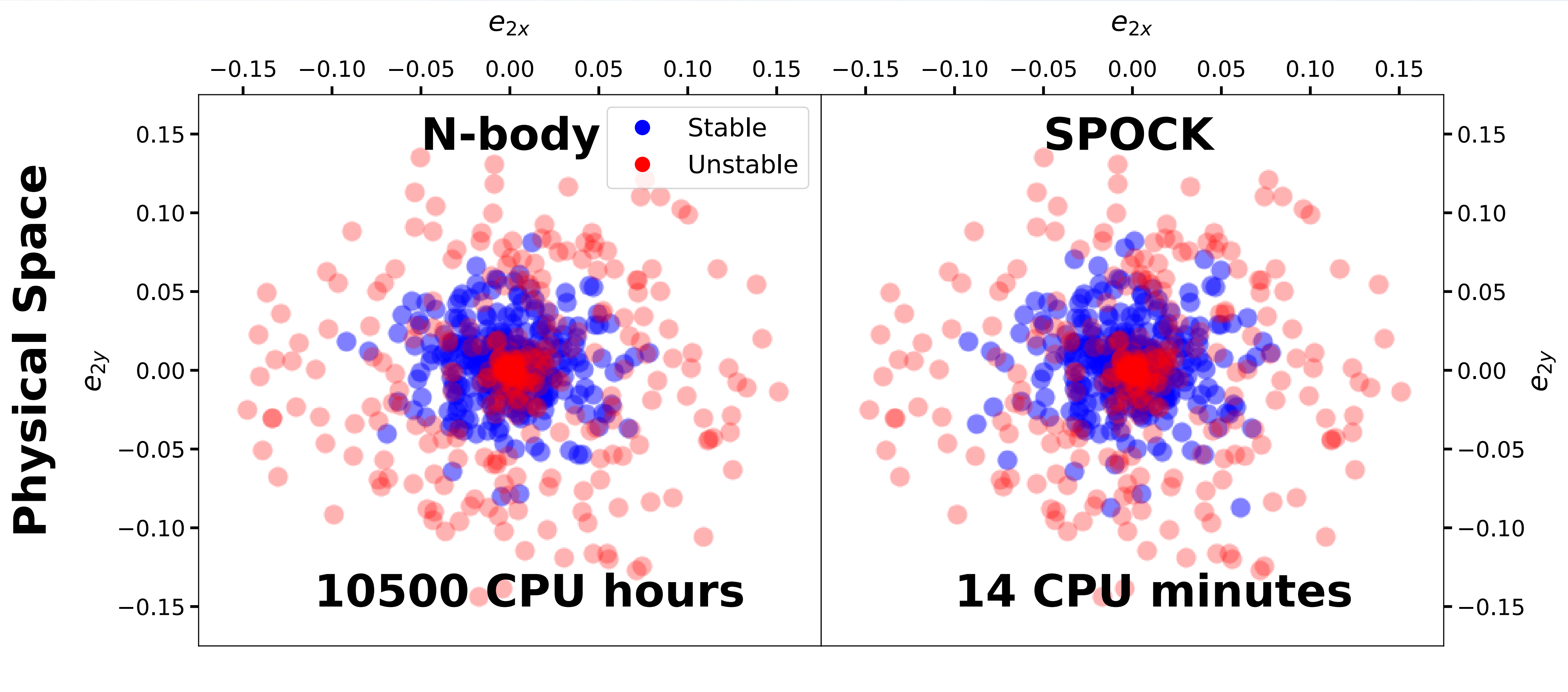


DUNE Collaboration *Phys. Rev. D* **102**, 092003 (2020) doi:10.1103/PhysRevD.102.092003

Exoplanets

- Which planetary system configurations are stable?

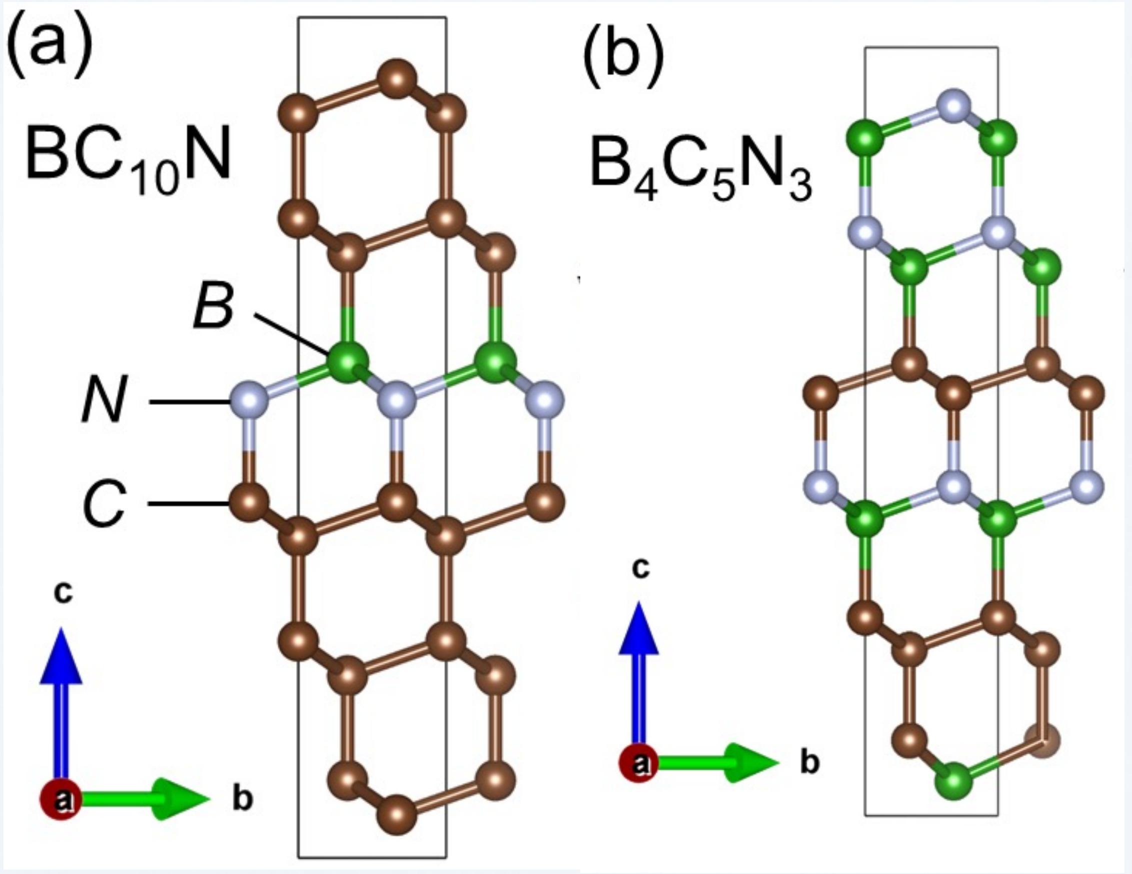


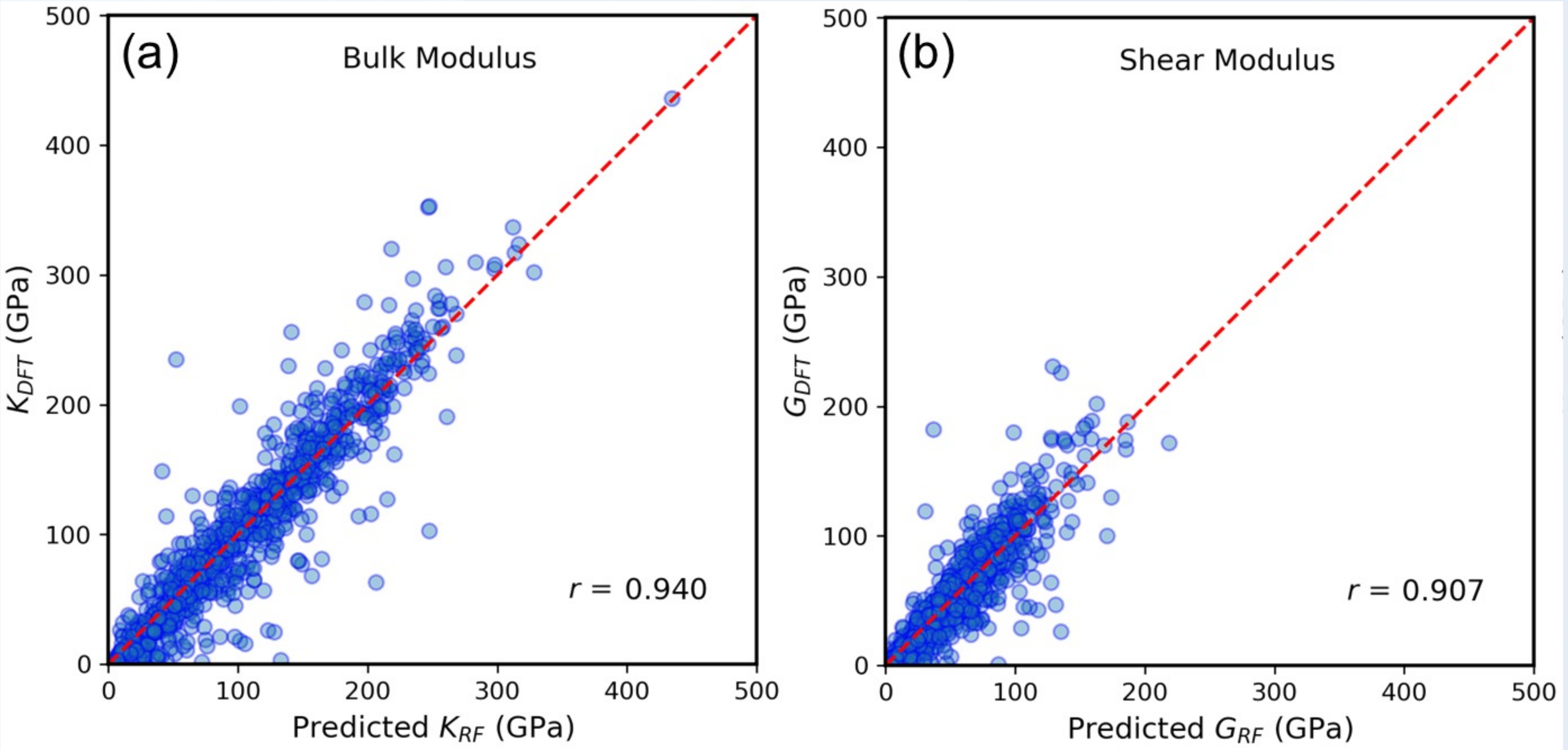


D Tamayo *et al.* *PNAS* **117** (31) 18194-18205 (2020) doi:10.1073/pnas.2001258117

Materials

- How hard are different crystalline structures?





W Chen *et al. npj Computational Methods* **7**:14 (2021) doi:10.1038/s41524-021-00585-7

Augmented Data Collection

- The **Large Hadron Collider** discards 99% of the data it collects.
- They use machine learning to help prioritize which events to store.

CMS Collaboration *Phys. Rep.* **115**, 678-772 (2025) doi:10.1016/j.physrep.2024.09.006

AI in Physics

Classification tasks

Regression tasks

Physics-Informed Neural Networks

- PINNs combine data-driven learning with physics-based constraints.
- The loss function is a combination of data loss and "physics" loss.

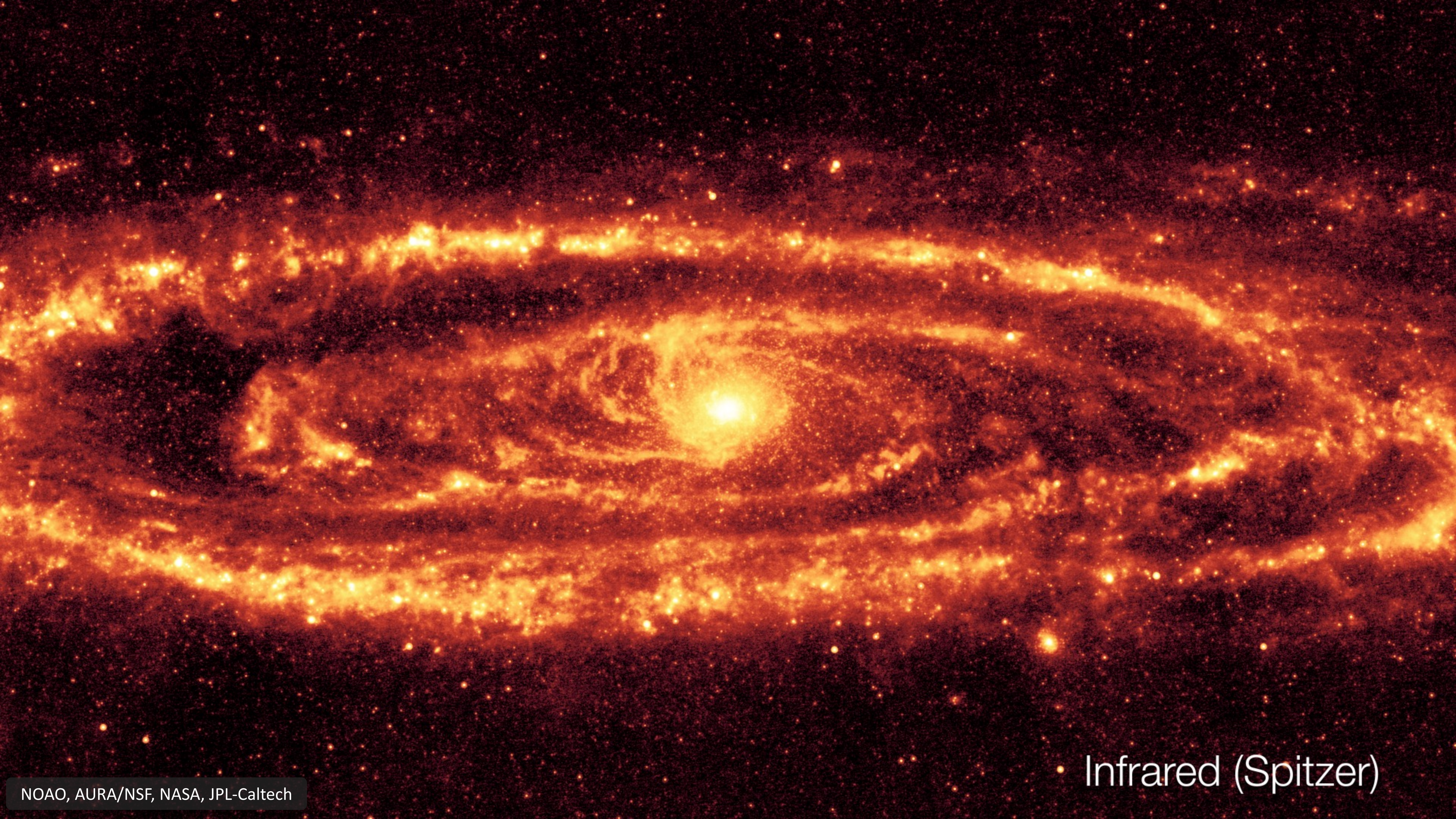
$$\mathcal{L} = \mathcal{L}_{\text{data}} + \lambda \mathcal{L}_{\text{physics}}$$

- The physics loss is the residuals from differential equations (difference between predicted and actual equation solution values).

- Curbs the problem of ML models predicting unphysical conditions (e.g., negative energy, faster than light speeds, etc.)

G Karniadakis *et al. Nat. Rev. Phys.* 3, 422-440 (2021) doi:10.1038/s42254-021-00314-5

Generative AI in Physics

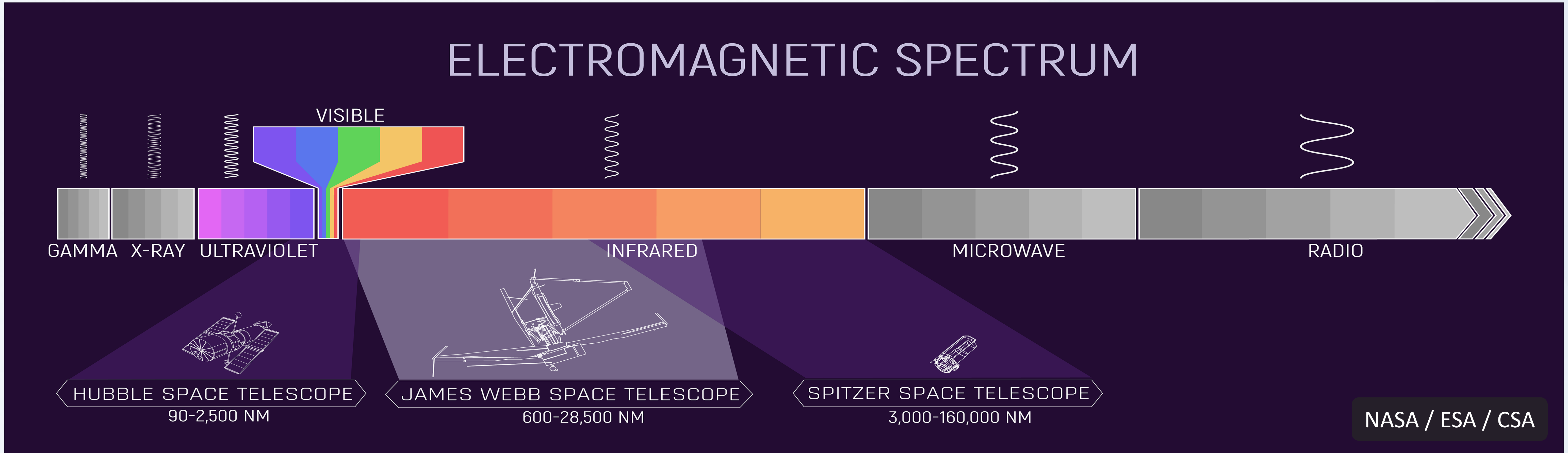

• Infrared (Spitzer)
NOAO, AURA/NSF, NASA, JPL-Caltech


Optical (NOAO)
NOAO, AURA/NSF, NASA, JPL-Caltech


Ultraviolet (SWIFT)
NASA / Swift

Galaxy Translation

- **Objective:** Translate galaxy images from one photometric band to another (e.g., infrared to ultraviolet).
  - **Band interpolation** – given two bands, find an intermediate band.
  - **Band extrapolation** – extend a sequence of bands.



Galaxy Translation

- **Architecture:** A ResNet-like supervised model consisting of residual blocks, up-sampling and down-sampling blocks.

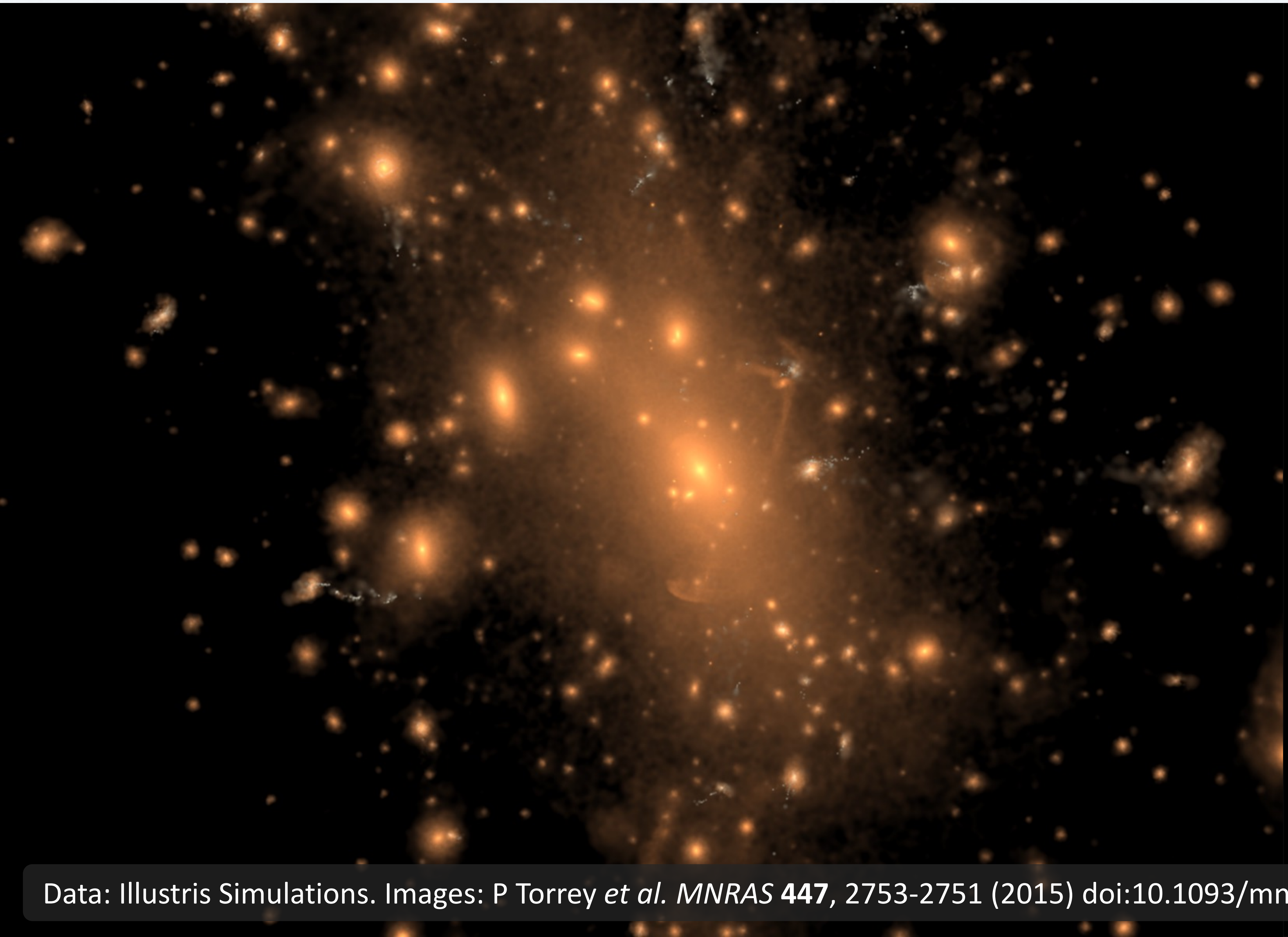
- **Loss function:** A combination of MAE and SSIM (structural similarity index).

$$\mathcal{L} = \mathcal{L}_1 + \lambda \mathcal{L}_{\text{SSIM}} \quad \text{where} \quad \mathcal{L}_{\text{SSIM}} = 1 - \text{SSIM}(Y, \hat{Y})$$

- Adding the SSIM Loss improved all generic and domain-specific metrics.

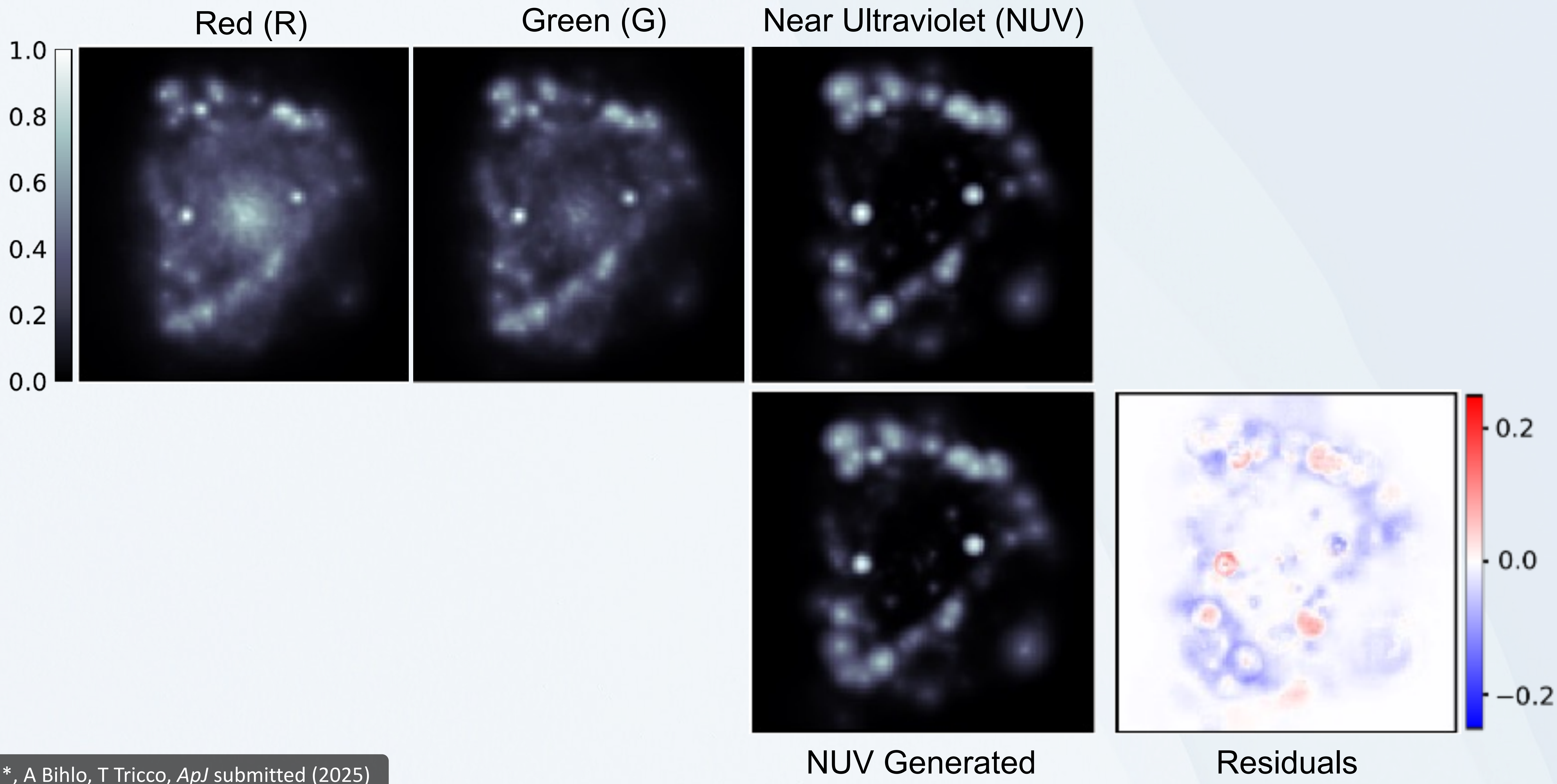
Training Data – Simulated

- Simulated galaxy images from the Illustris simulations.
- Includes 36 bands from 151 nm (ultraviolet) to 7090 nm (mid-Infrared).



Data: Illustris Simulations. Images: P Torrey *et al.* *MNRAS* **447**, 2753-2751 (2015) doi:10.1093/mnras/stu2592

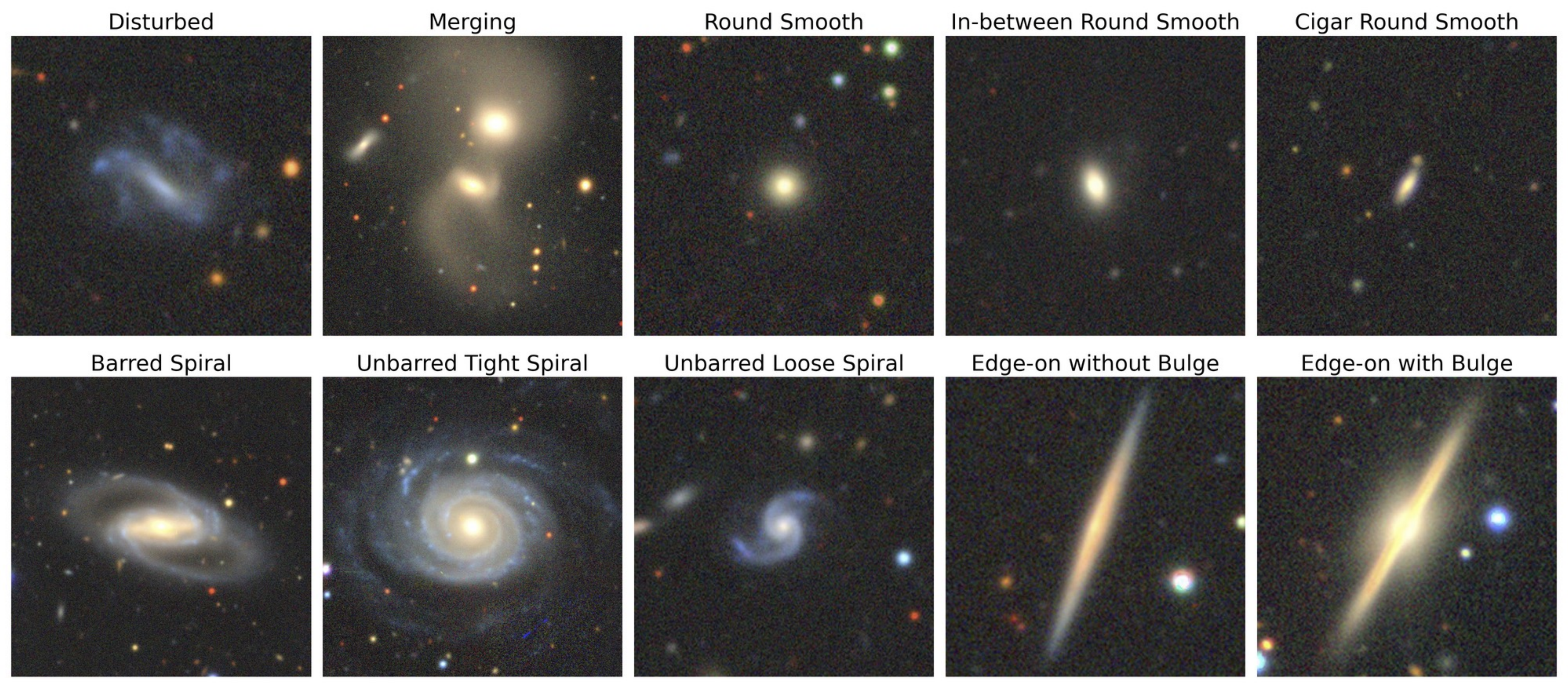
Extrapolation on Simulated Data (Illustris)



Y Zaazou*, A Bihlo, T Tricco, *ApJ* submitted (2025)

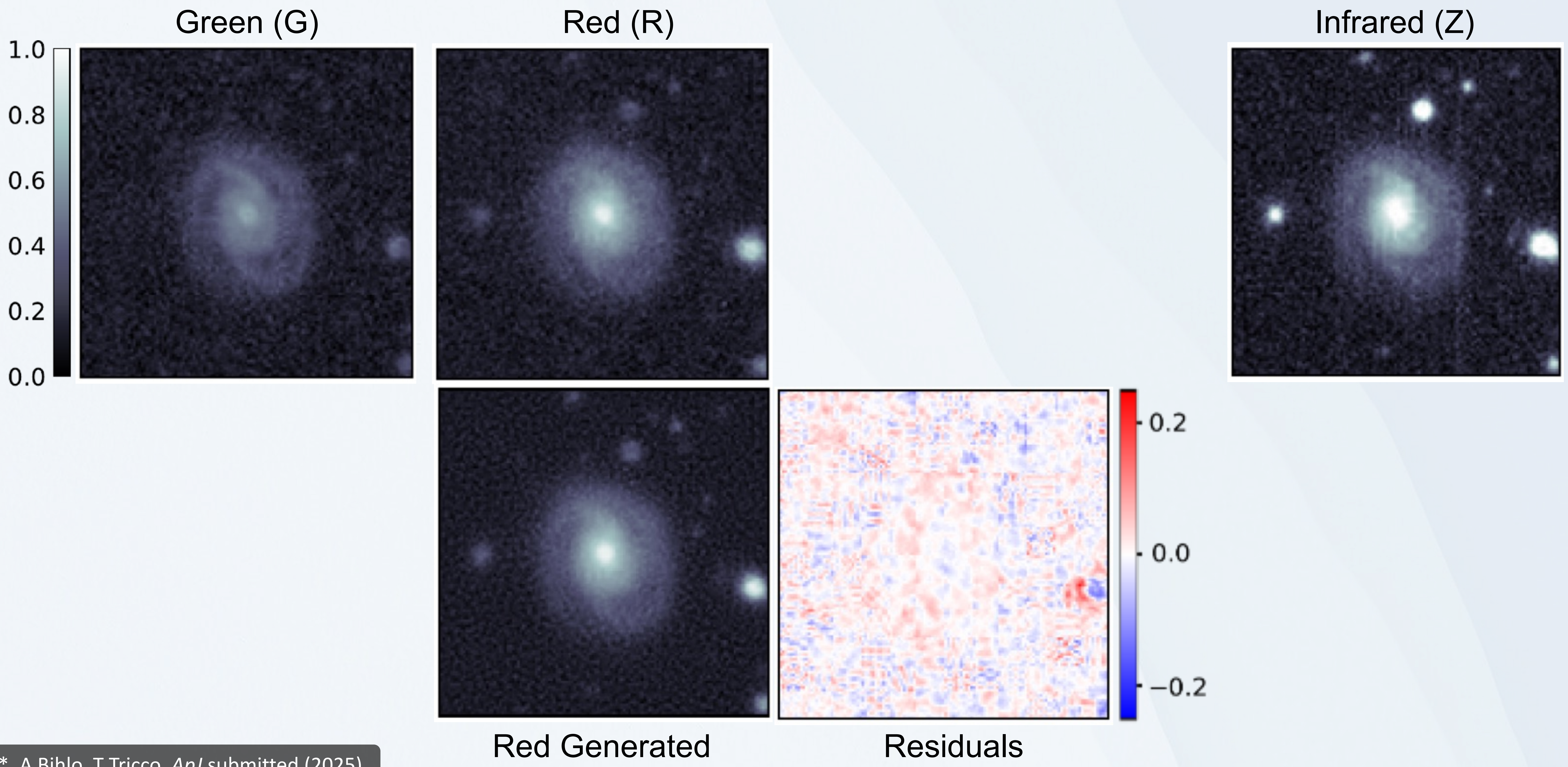
Training Data – Real

- Galaxy images from DECaLS – Dark Energy Camera Legacy Survey.
- Includes 450 nm to 900 nm (green, red, near-infrared).



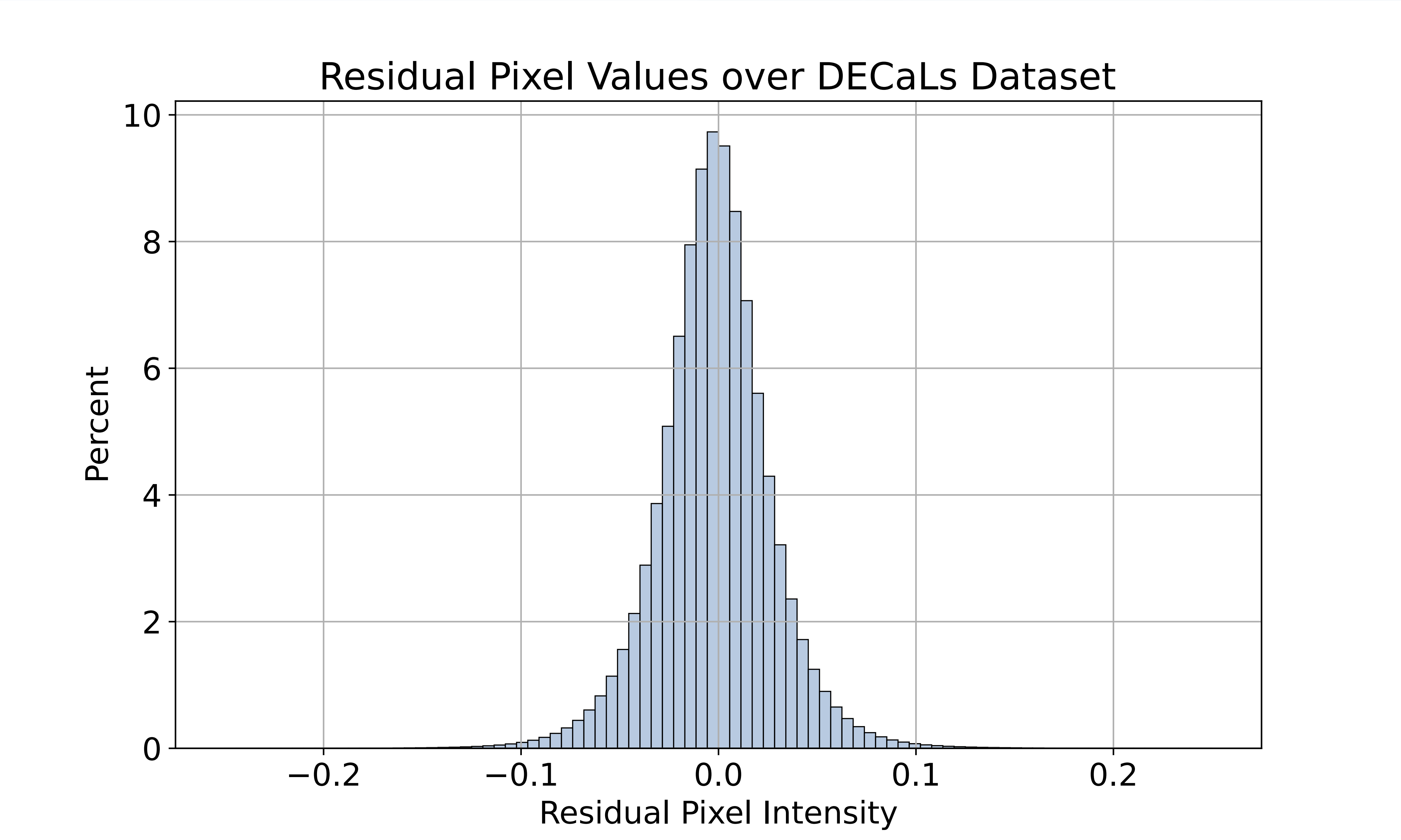
Data: DECaLS/Galaxy Zoo. Images: H Leung, J Bovy *MNRAS* **483,** 3255-3277 (2019) doi:10.1093/mnras/sty3217

Interpolation with Real Data (DECaLS)



Y Zaazou*, A Bihlo, T Tricco, *ApJ* submitted (2025)

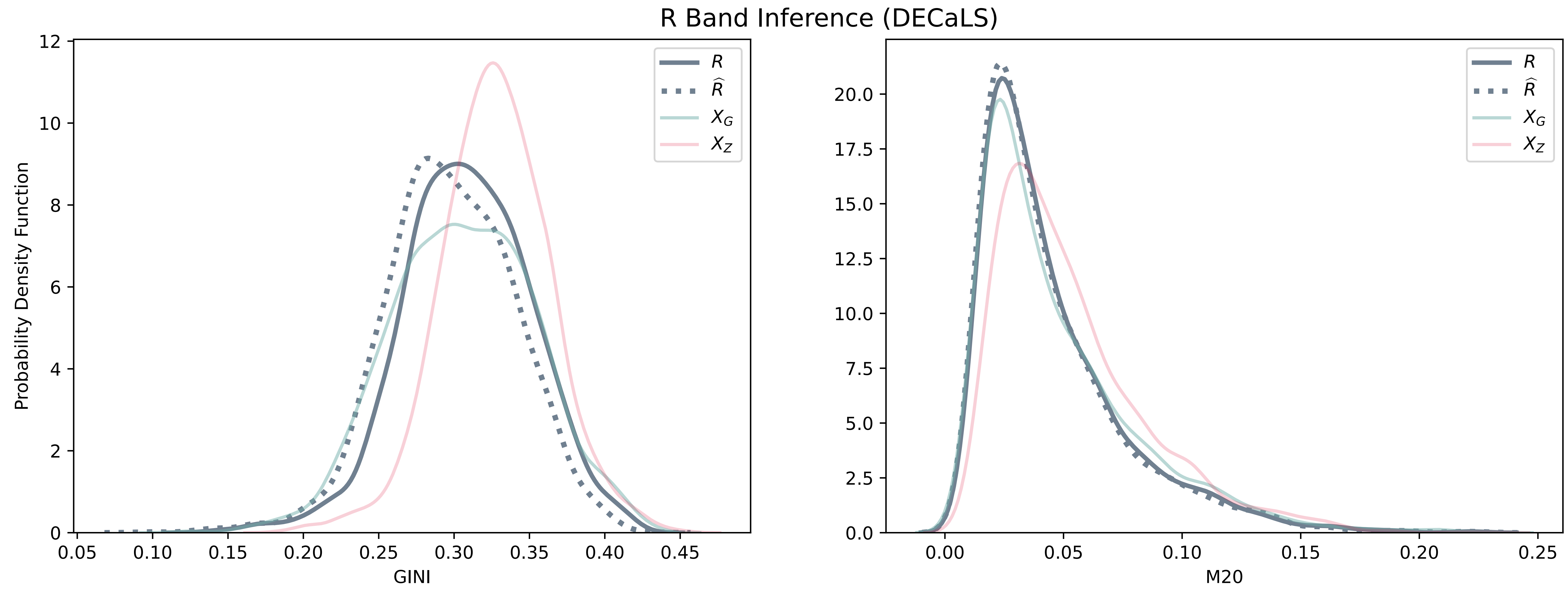
Residual Distributions



- Distribution of per-pixel residuals across the DECaLS testing dataset.
- Normally distributed (no skew). 99% of residuals are less than 0.09.

Y Zaazou*, A Bihlo, T Tricco, *ApJ* submitted (2025)

Domain-Specific Metrics

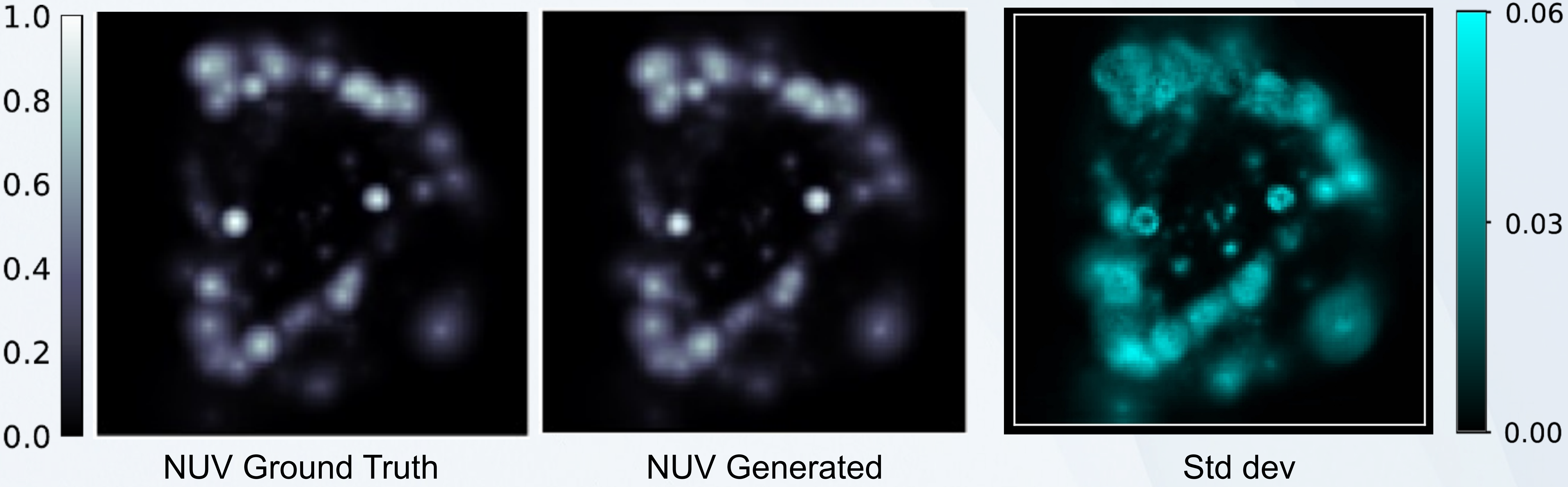


- Gini coefficients quantify the per-pixel distribution of light in a galaxy.
- M20 relates the brightest 20% to the overall galaxy’s light distribution.

Y Zaazou*, A Bihlo, T Tricco, *ApJ* submitted (2025)

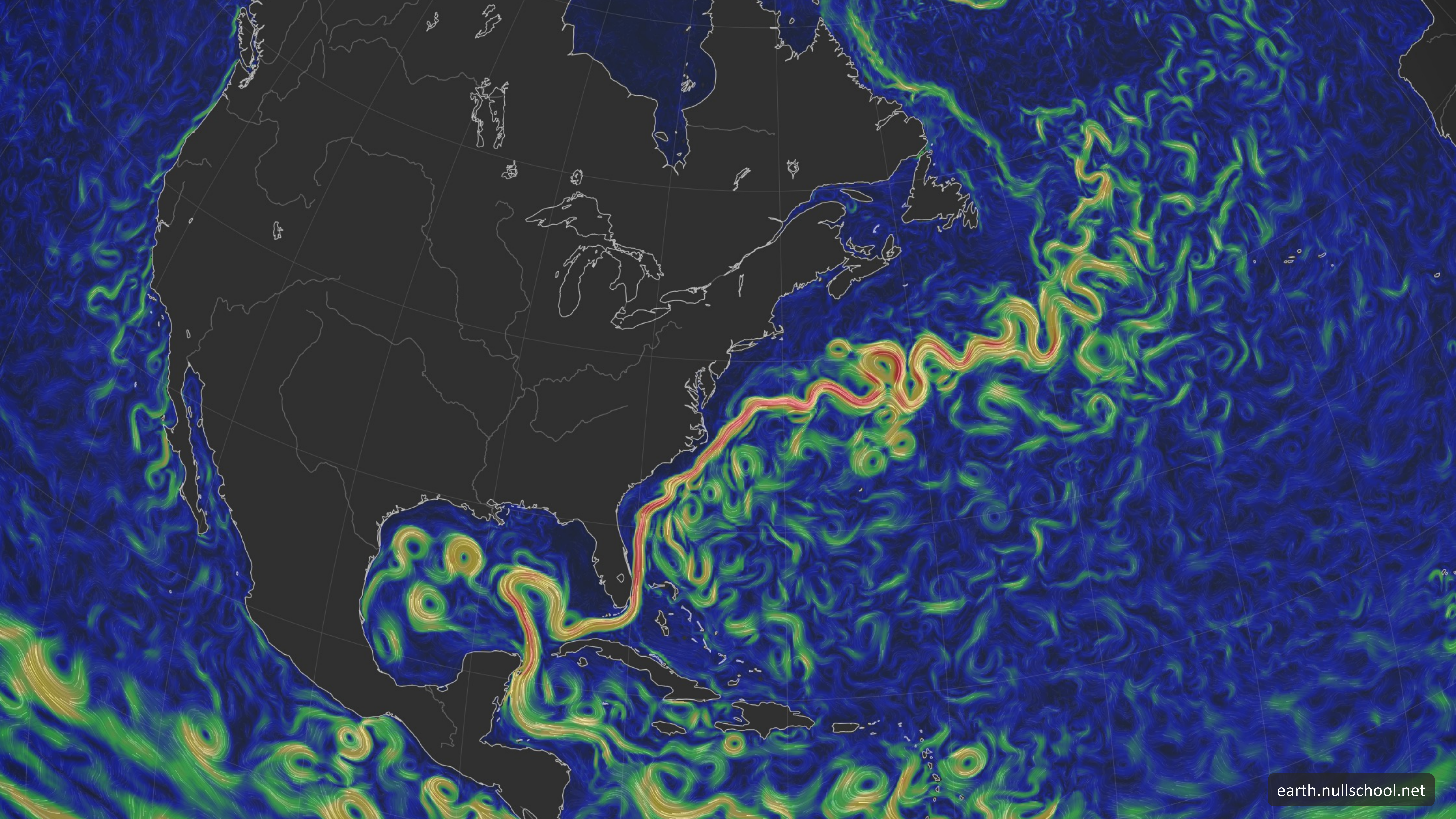
Uncertainty Estimation

- Re-trained extrapolation model (R, G to NUV) multiple times with different random seeds.
- “donut-like” uncertainties – location is accurate, with the most dominant uncertainty on the size and intensity.

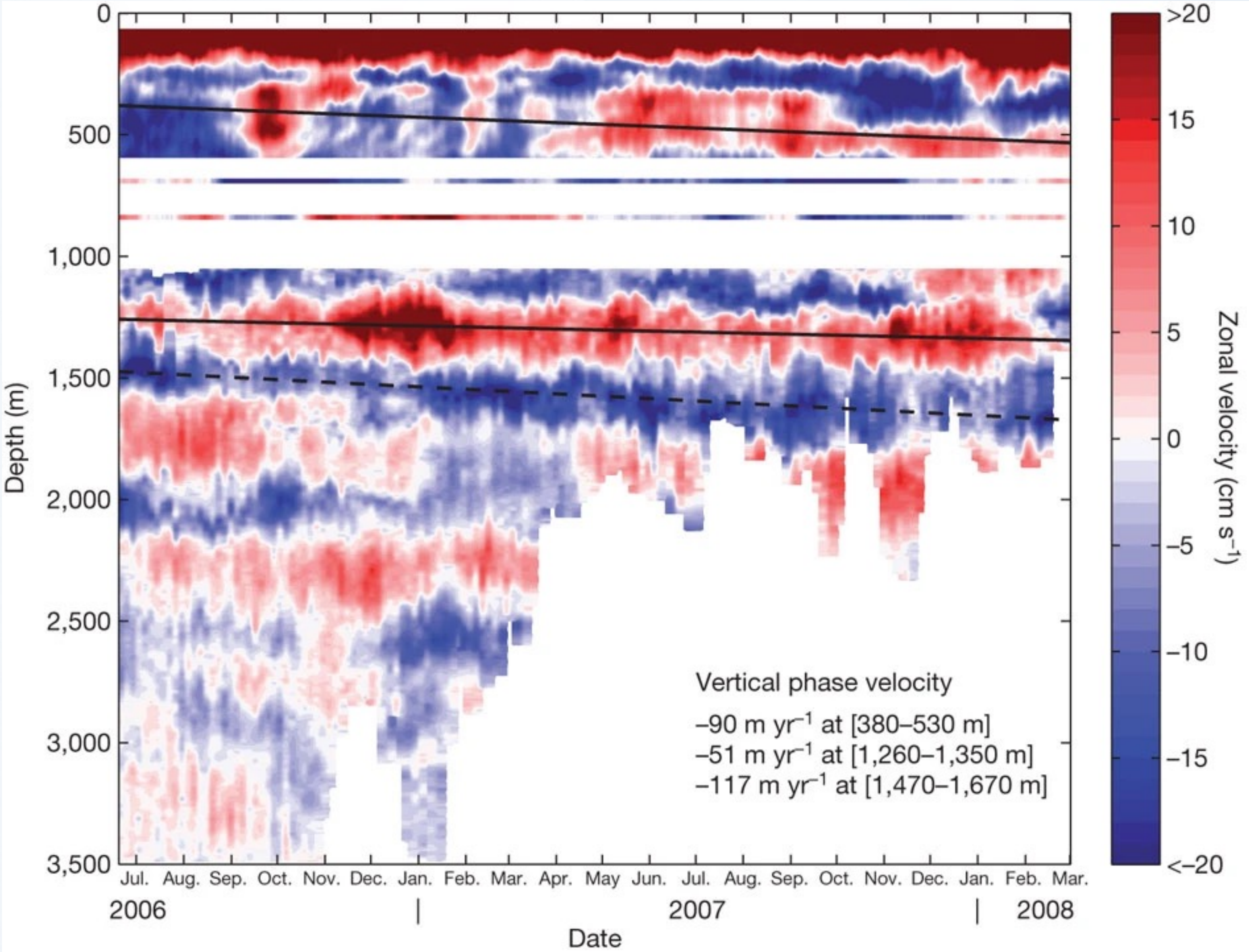


Y Zaazou*, A Bihlo, T Tricco, *ApJ* submitted (2025)

AI as an Interpretability Tool


earth.nullschool.net

Equatorial Deep Jets



P Brandt *et al. Nature* **000**, 1-3 (2011) doi:10.1038/nature10013

AI as a Pathfinder

- We want to understand the conditions under which **coherent jets abruptly reverse direction.**

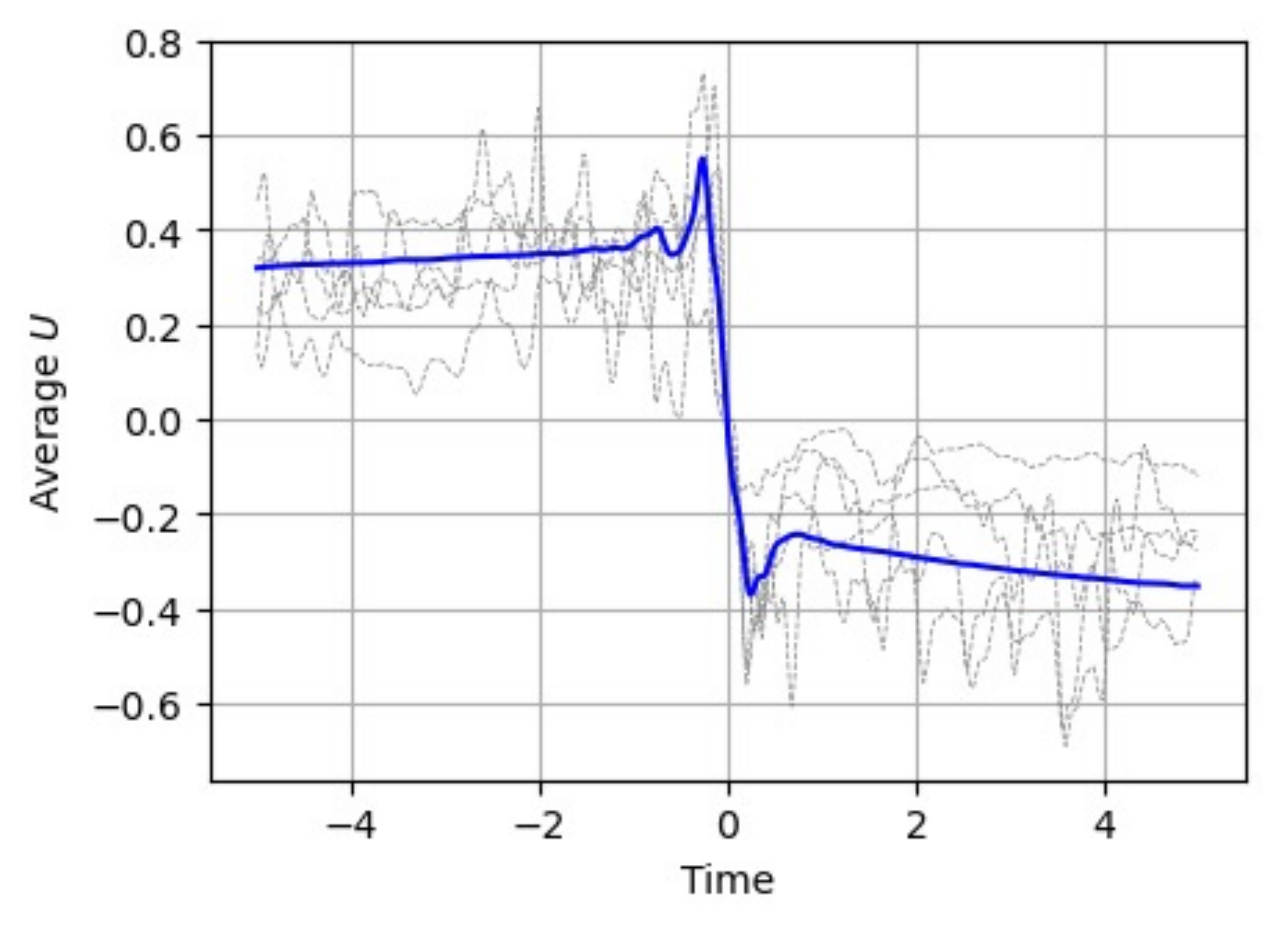
- Our data is generated by a simplified statistical model of stratified, two-dimensional turbulence.
  - Describes the flow in terms of stream functions (excited & sheared).
  - Includes stochastic energy injection to drive turbulence.

- Ensemble average our data over 10,000 realizations.

The Reversal Phenomenon

Coherent mean positive flow abruptly transitions to coherent mean negative flow.

Jet Velocity



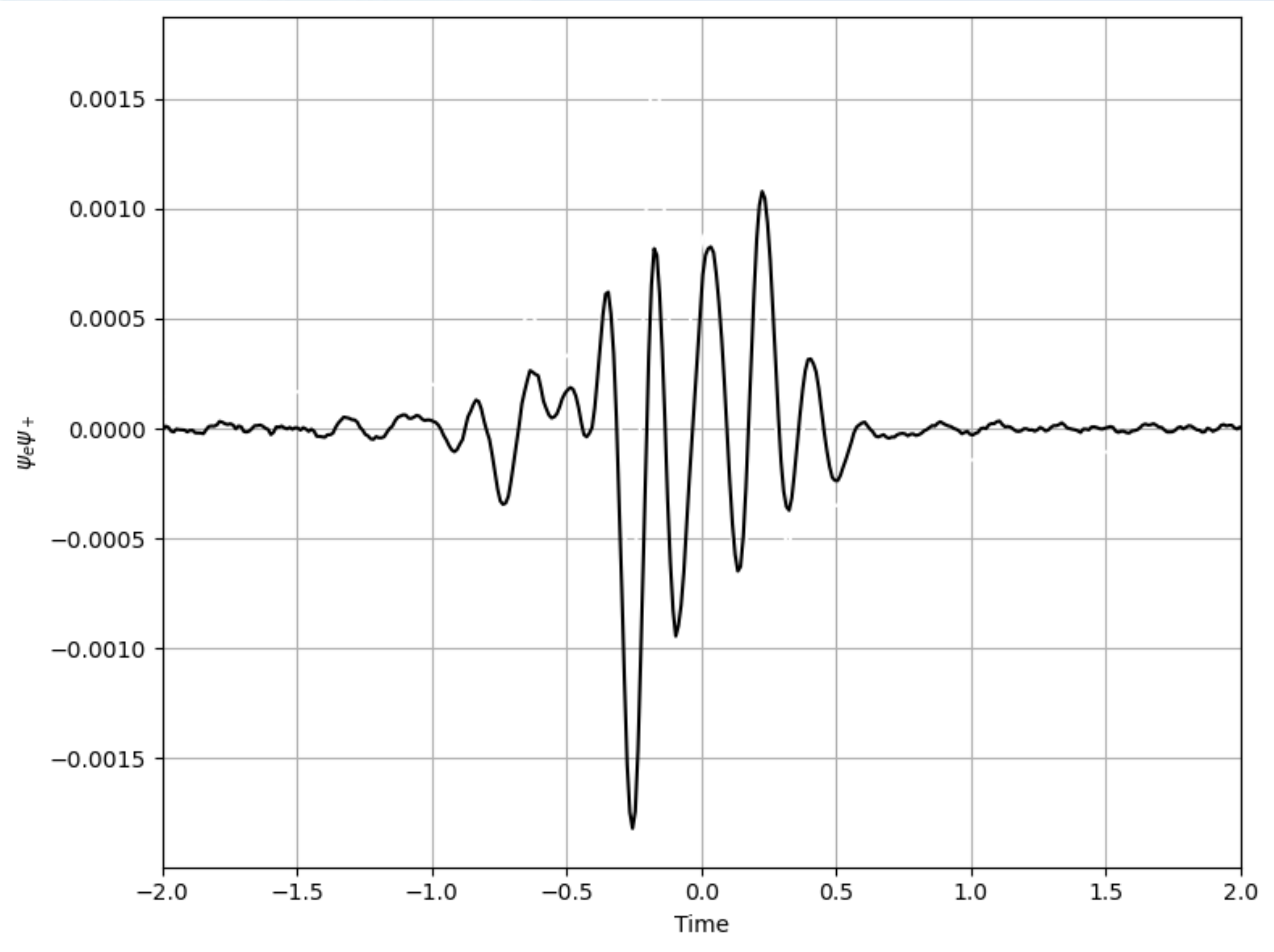
B Sanu*, J Fitzgerald, T Tricco, *in prep* (2025)

A Complicated Process

- This is a complicated process.

- Not so abrupt!
- There is a lead time before the velocity abruptly reverses.

Covariance of Excited and Sheared Stream Functions



B Sanu*, J Fitzgerald, T Tricco, *in prep* (2025)

Questions

- How early does a jet reversal start?
- What are the key moments that trigger a jet reversal?
- At what point is a jet reversal “locked in” (unavoidable)?

B Sanu*, J Fitzgerald, T Tricco, *in prep* (2025)

AI as an Explainability Tool

- We think we can use AI to answer these questions:
  - AI explainability tools (e.g., Shap, Accumulated Local Effects, etc),
  - Transformer models with the attention mechanism.
- Given a sequence of turbulent states, how far in advance can the model predict a jet reversal event?
- What are the key states or points in time that predict a reversal?

B Sanu*, J Fitzgerald, T Tricco, *in prep* (2025)

Parting Thoughts

AI in Physics Parting Thoughts

- Physics helped create AI. But how can physics now benefit from AI?

- AI Advantages:
  - Speed of results (once training has been done!).
  - Data quantity is increasing – AI performs better with more data.

- AI Challenges:
  - Black box nature of AI. Physicists need explainability.
  - Lack of scientific robustness and reliability of models.