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Blueprinting AI for Science at Exascale (BASE-II)

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Ai for Science
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Outline

1 Surrogate-modelling

2 Representation learning technique

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Emulating CO Line Radiative Transfer with Machine Learning

Shiqi Su, Frederik De Ceuster, Jaehoon Cha, Mark I Wilkinson, Jeyan Thiyagalingam, Jeremy Yates, Yi-Hang Zhu, Jan Bolte

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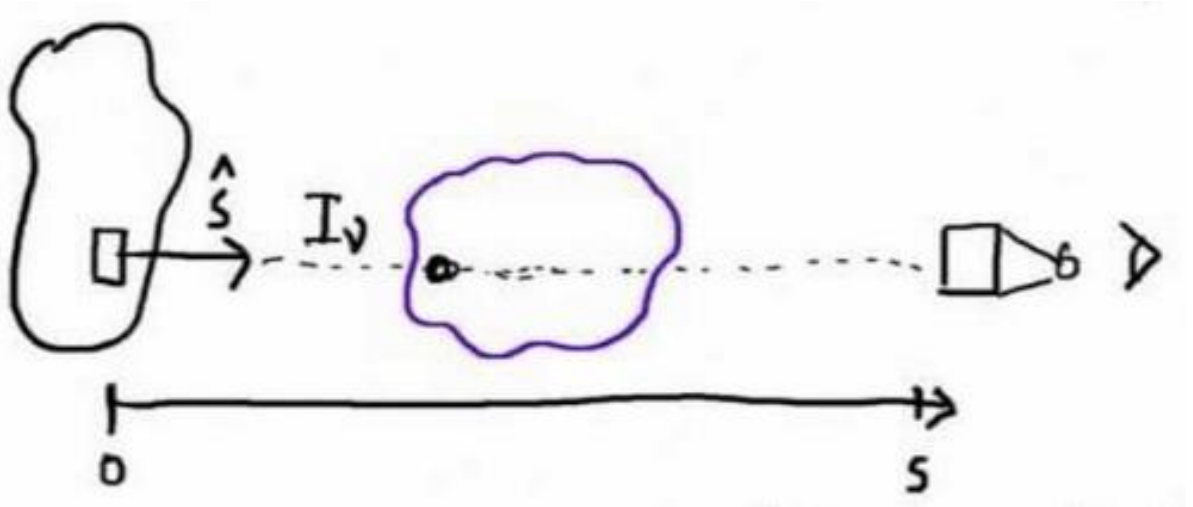
Emulating 3D Radiative Transfer Equation

- A linear partial integro-differential equation

$$\hat{n} \cdot \nabla I_\nu(\boldsymbol{x}, \hat{\boldsymbol{n}}) = \eta_\nu(\boldsymbol{x}) - \chi_\nu(\boldsymbol{x}) I_\nu(\boldsymbol{x}, \hat{\boldsymbol{n}}) + \oint d\Omega' \int_0^\infty \Phi_{\nu\nu'}(\boldsymbol{x}, \hat{\boldsymbol{n}}, \hat{\boldsymbol{n}}') I_\nu{}'(\boldsymbol{x}, \hat{\boldsymbol{n}}') d\nu'$$

- ❑ $\mathbf{x}$: spatial variable $(x, y, z) \in \mathbb{R}^3$
- ❑ $\hat{\boldsymbol{n}}$: direction of ray
- ❑ υ : frequency, $\frac{speed\ of\ wave}{wavelength} = \frac{c}{\lambda}$
- ❑ $I_\nu(x, \hat{n})$, radiative intensity
- ❑ $\eta_\nu(x)$, emission
- ❑ $\chi_\nu(x) I_\nu(\boldsymbol{x}, \hat{\boldsymbol{n}})$, absorption
- ❑ $\Phi(\cdot) I(\cdot)$, scattering



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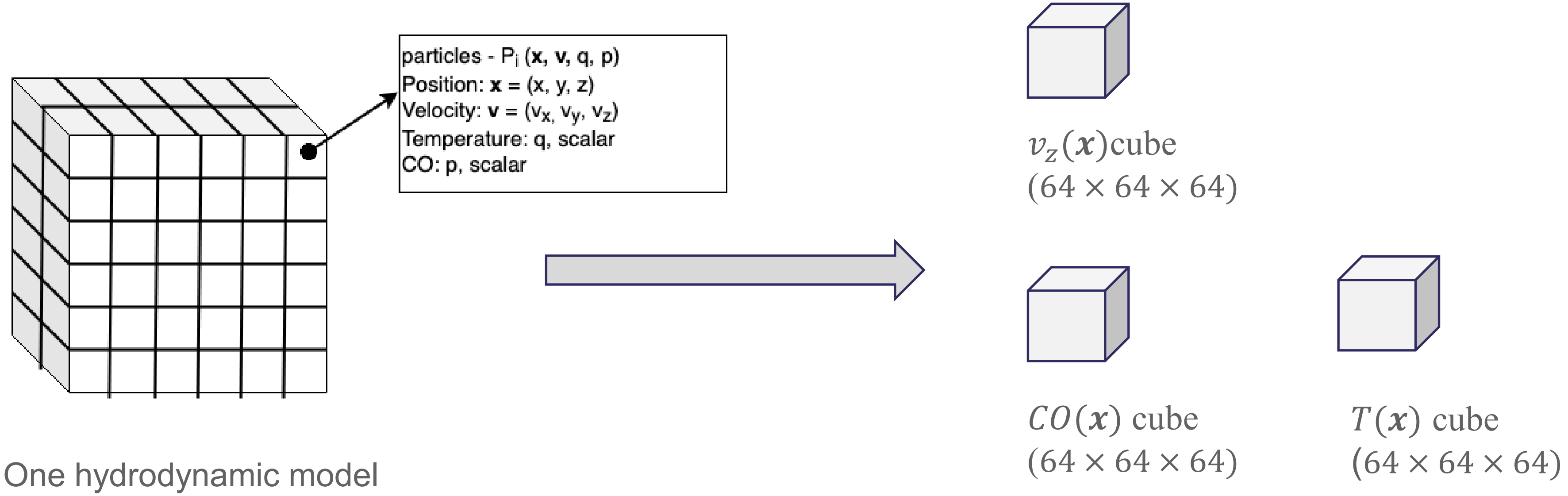
Surrogate Modelling

- The input is a hydrodynamic model, a mathematical framework describing the motion and behaviour of fluids, with a total size of around 7 TB.
- Under the assumption of local thermodynamic equilibrium (LTE), the spectral line model is fully determined by a few parameters.
- The model includes velocity along the z-axis, Carbon monoxide (CO) density, and temperature.



One hydrodynamic model

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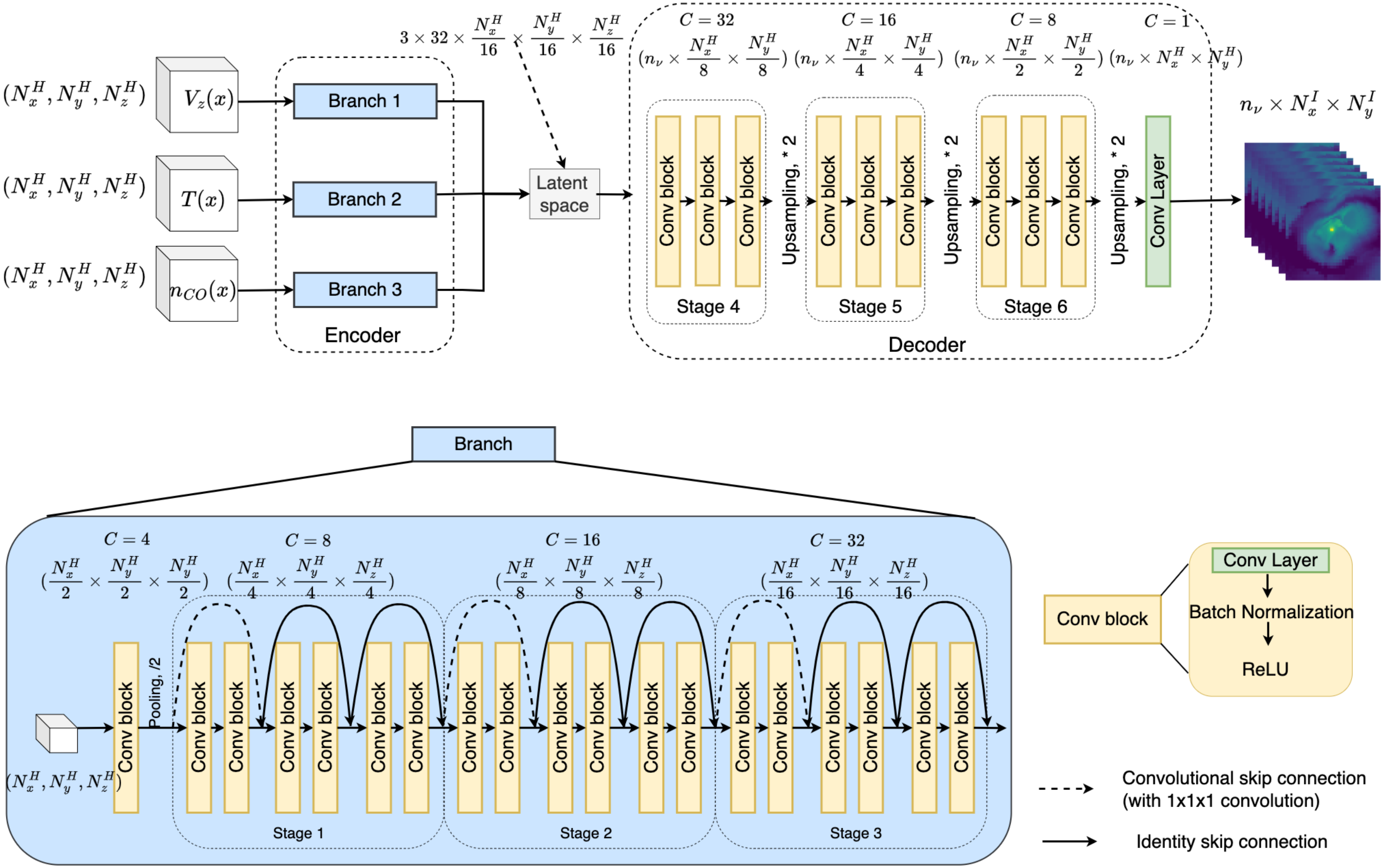
COEmuNet



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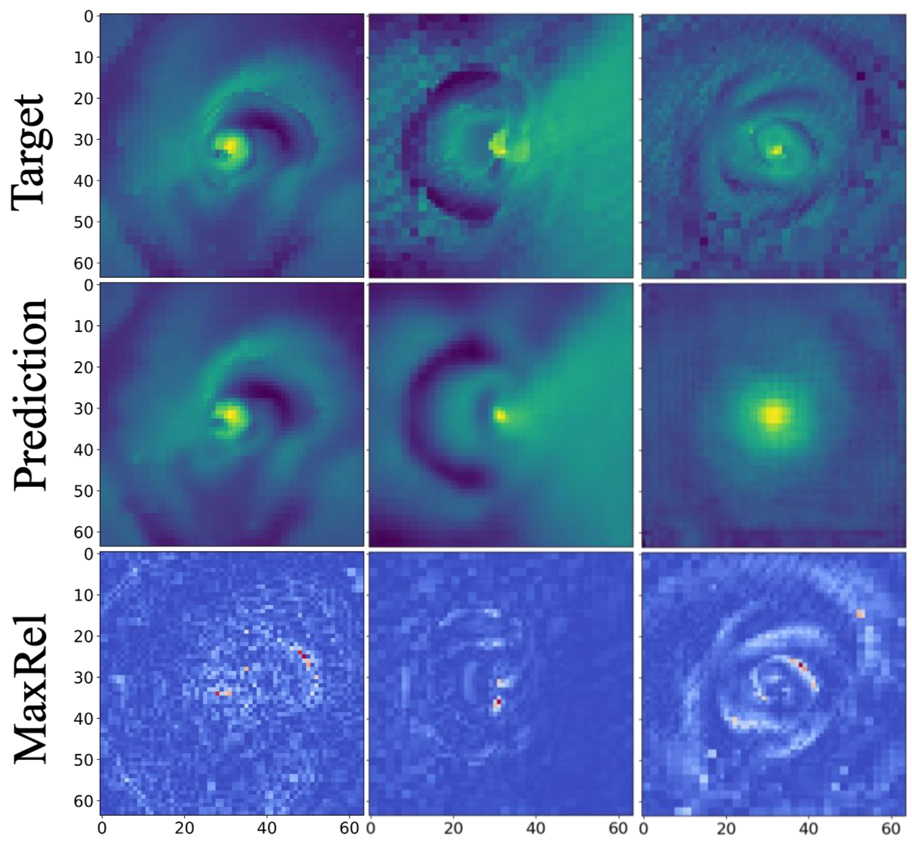
Results

- We trained the model to output the middle seven frequencies and randomly rotated the input 100 times.
- Total data size is about 7TB.
- The model contains 143,303,809 parameters, making a multi-GPU approach using data-distributed parallelism (DDP) necessary.
- We use four A100-40GB GPUs, and it takes one hour per epoch.

Inference time (sec)	
Numerical solver	Surrogate model
2.67601	0.01181



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Discovering Interpretable Representations in Scientific Data

Jaehoon Cha, Jinhae Park, Samuel Pinilla, Kyle L Morris, Christopher S Allen, Mark I Wilkinson, Jeyan Thiyagalingam

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Why Learning Interpretable Representations Matters

Scientific data may look complex, but a few key factors often explain most of it.

- A 1D spectrum may have many wavelengths, but only a few peaks matter.
- A 2D image can be understood through shape, position, or orientation.

Interpretable representations help us

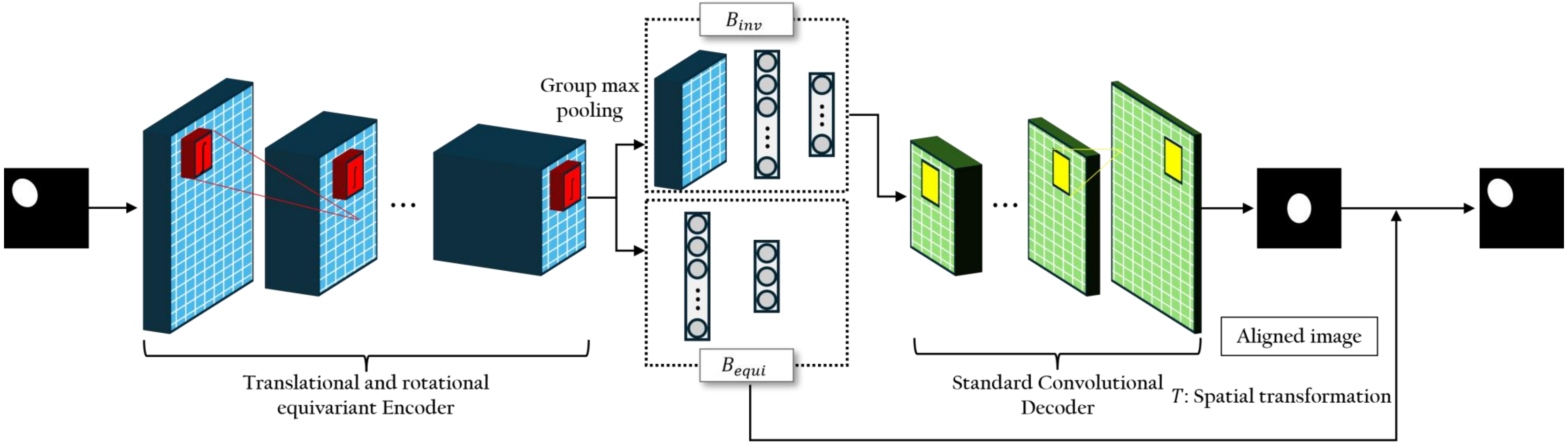
- Understand how our data varies.
- Cluster data in a meaningful way.
- Support discovery, and data collection.

Disentangled Representation

- A disentangled representation is a representation that separates the underlying factors of variation so each can be controlled independently.

Translational and rotational equivariant Encoder

- The encoder has stacks of rotated kernels to learn different orientations of objects.
- It enables learning both centroids and orientations of objects.
- However, this makes the encoder bigger.



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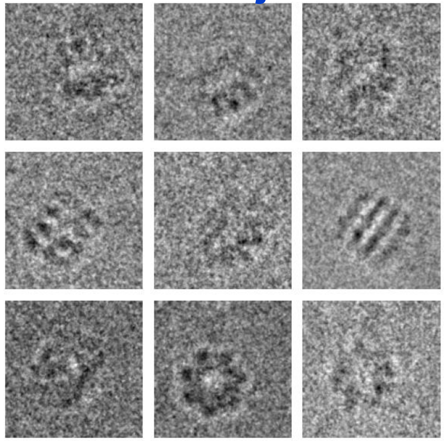
CryoEM single particle analysis

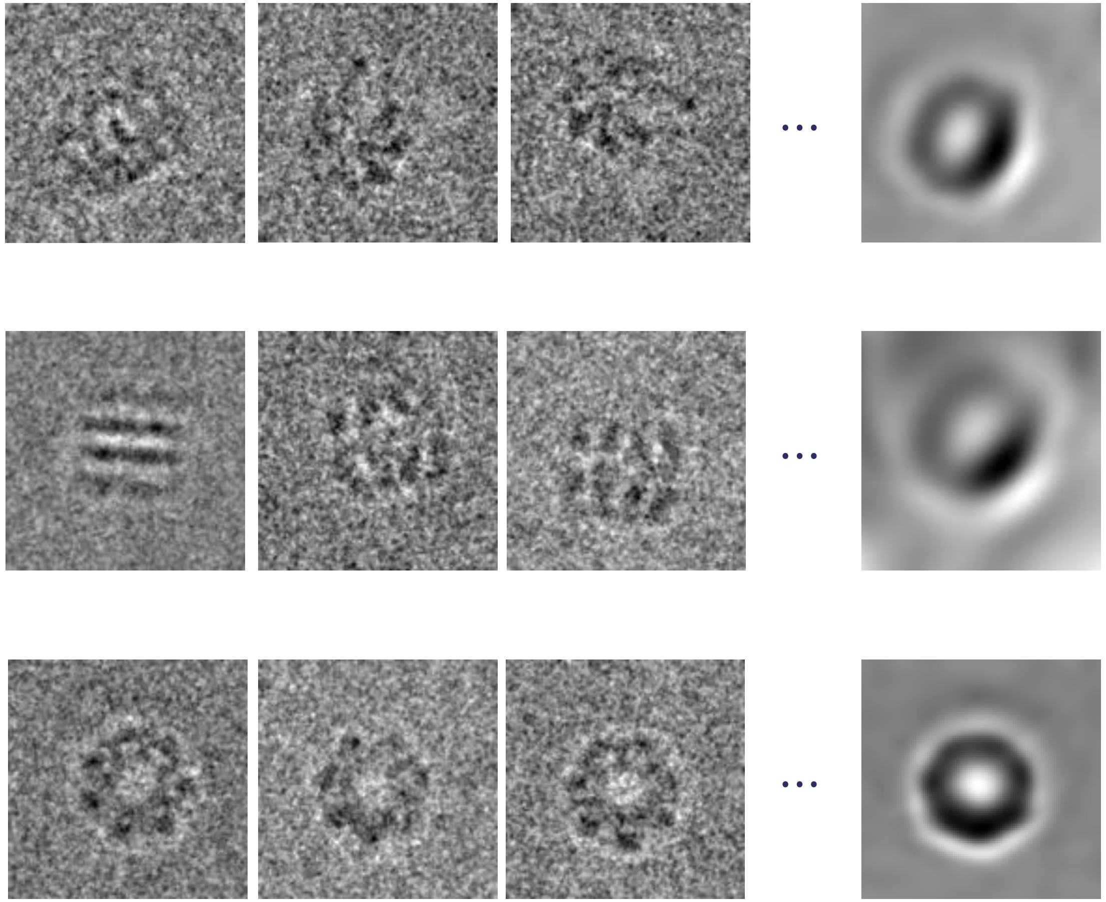
- The cryoEM single particle analysis method generates 2D projection images with low signal-to-noise ratios.
- Grouping 2D projections of the molecule captured from similar viewing angles (or object poses) and aligning them using in-plane rotations and translations improves the signal-to-noise ratio, enabling more effective 2D image analysis.

Examples of 2D Protein Projections



2D projections

Average of projections



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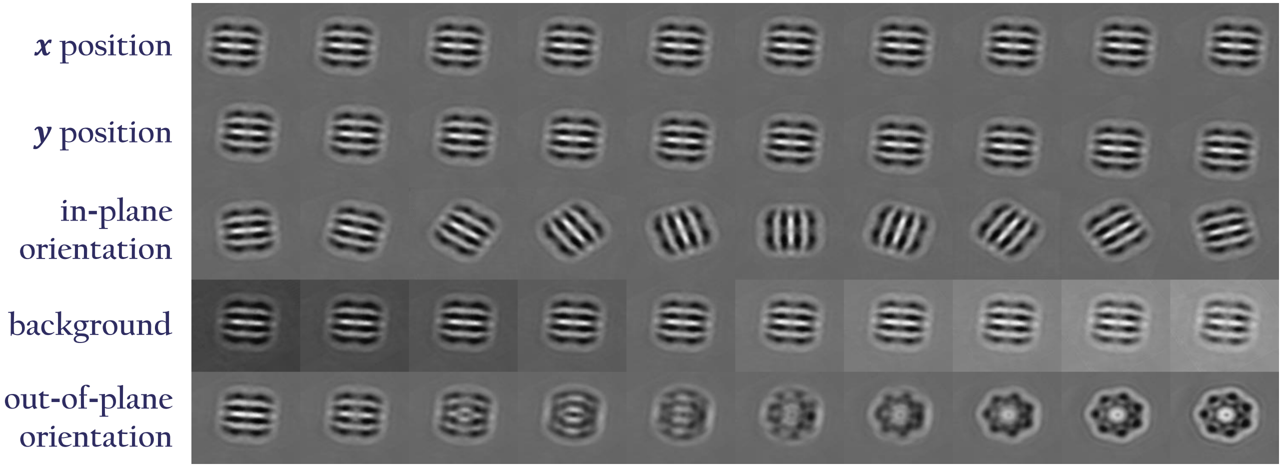
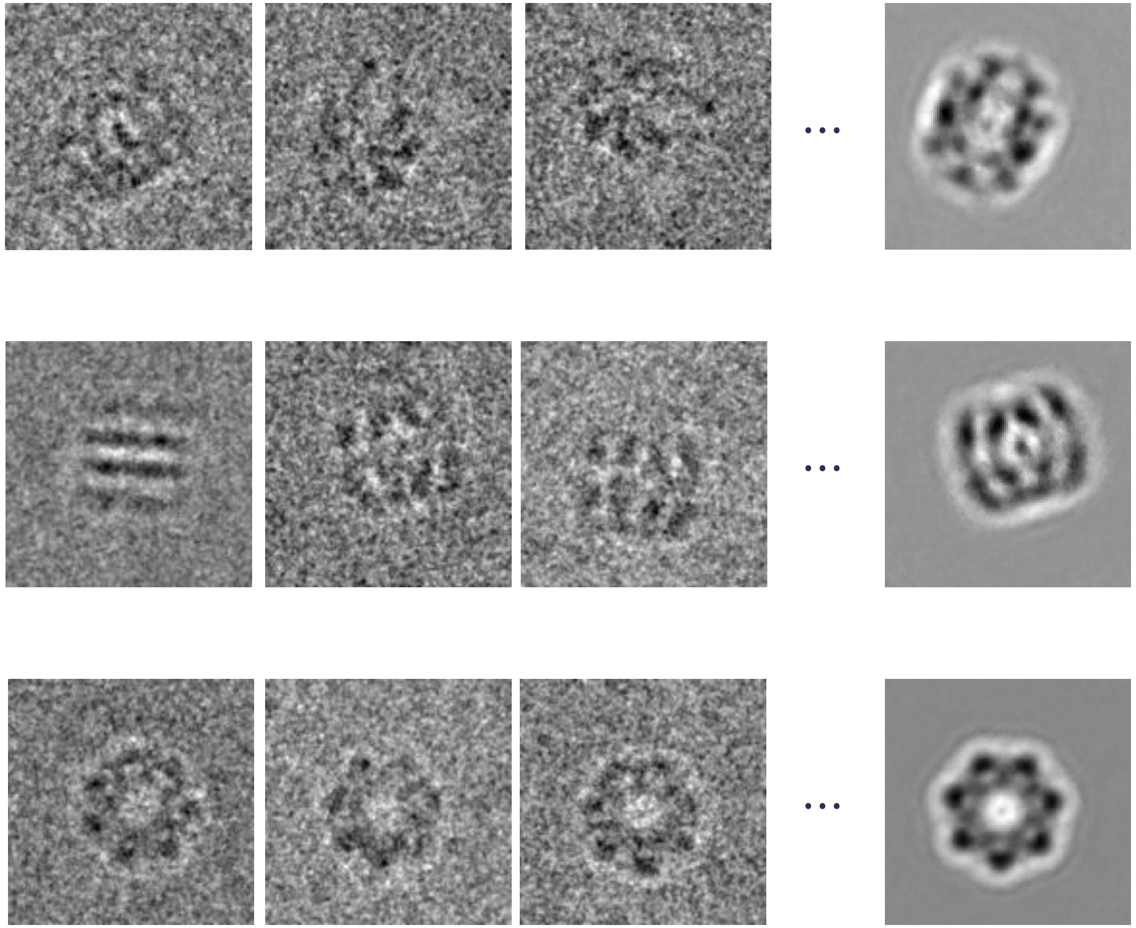
Extracting 2D particles from Cryo-EM

Latent traversals



2D projections

Average of projections after alignment



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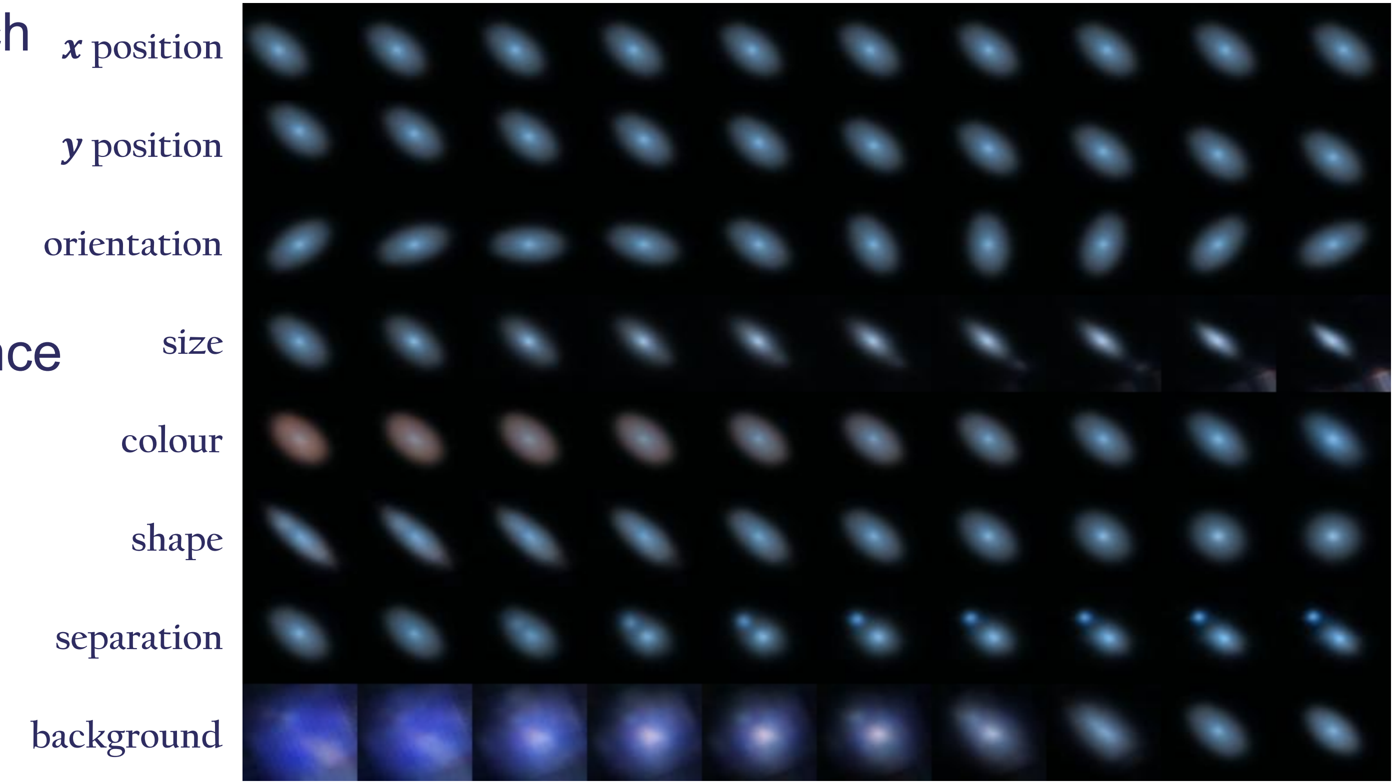
Galaxy Images

- The pose of galaxy images does not affect their intrinsic properties, highlighting the importance of an unsupervised approach to learn semantic representations of galaxies while capturing their pose information.

- In this study, we evaluate the performance of a disentanglement model using the Galaxy-Zoo dataset.

- The results demonstrate that the model effectively identifies key features of the dataset, including pose, size, colours, shape, separation, and background.

Galaxy-Zoo from astronomy with DiRAC (Mark Wilkinson)



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