# Prototype-enhanced prediction in graph neural networks for climate applications

N.Keshtmand

28.04.25

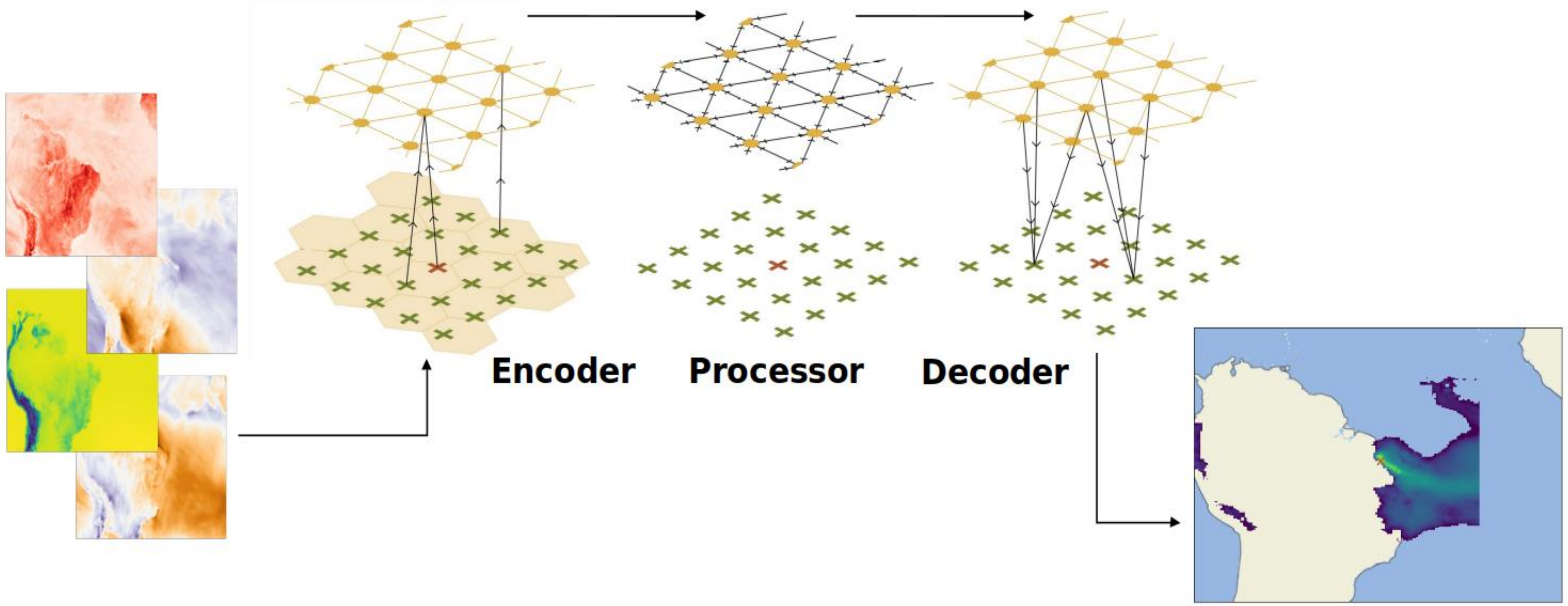
University of BRISTOL

# Motivation

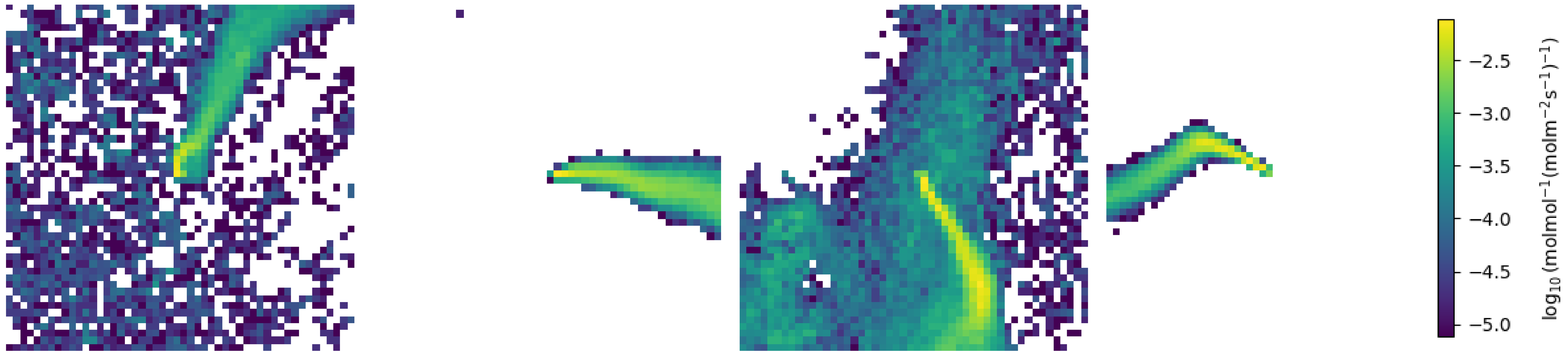
- Earth system modeling often relies on complex physics-based simulations which are computationally expensive.
- Machine learning (ML) models are increasingly being used to accelerate, or fully replace, these expensive simulations.
- Here, we introduce the concept of ‘prototypes’: an approximation of the emulator’s output provided as an input, serving as a prior  to help the emulator produce higher-quality predictions.

# Method

- We use the same Encoder-Processor-Decoder GNN architecture as Fillola et al. (2023)[1].
- Inputs include meteorology, topography as well as prototype (obtained using expert knowledge or a data-driven approach).
- We use footprints produced by NAME, the UK's Met Office LPDM for GOSAT measurements (Greenhouse gases Observing SATellite over Brazil for 2014-16.



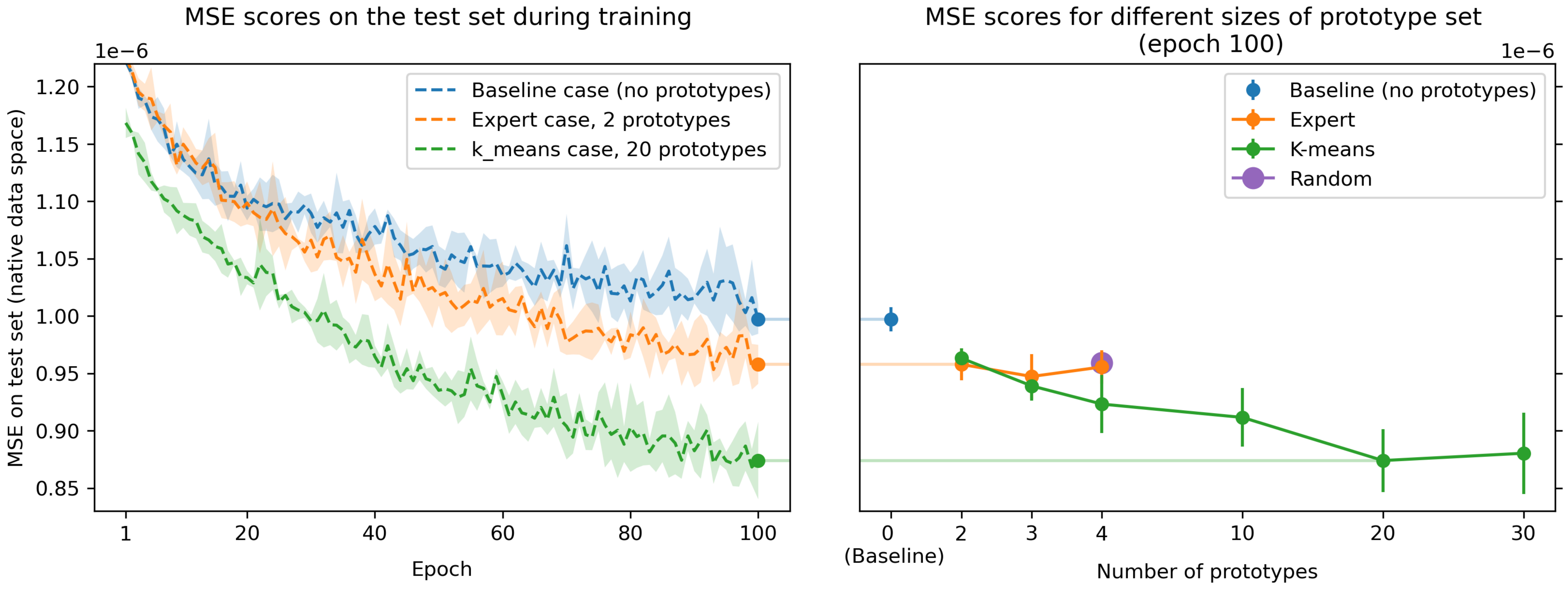

- Figure 1:GNN architecture used to predict footprints using meteorological inputs [1] based on graphcast [2].




- Figure 2: Example footprints used for prototypes.

# Results

- We compare the performance of a baseline model (0 prototypes [1], with our prototype approach for a range of n prototypes.
- We find that the data-driven approach, utilising prototypes selected with k-means, achieves better improvements on the baseline that the expert-driven method.



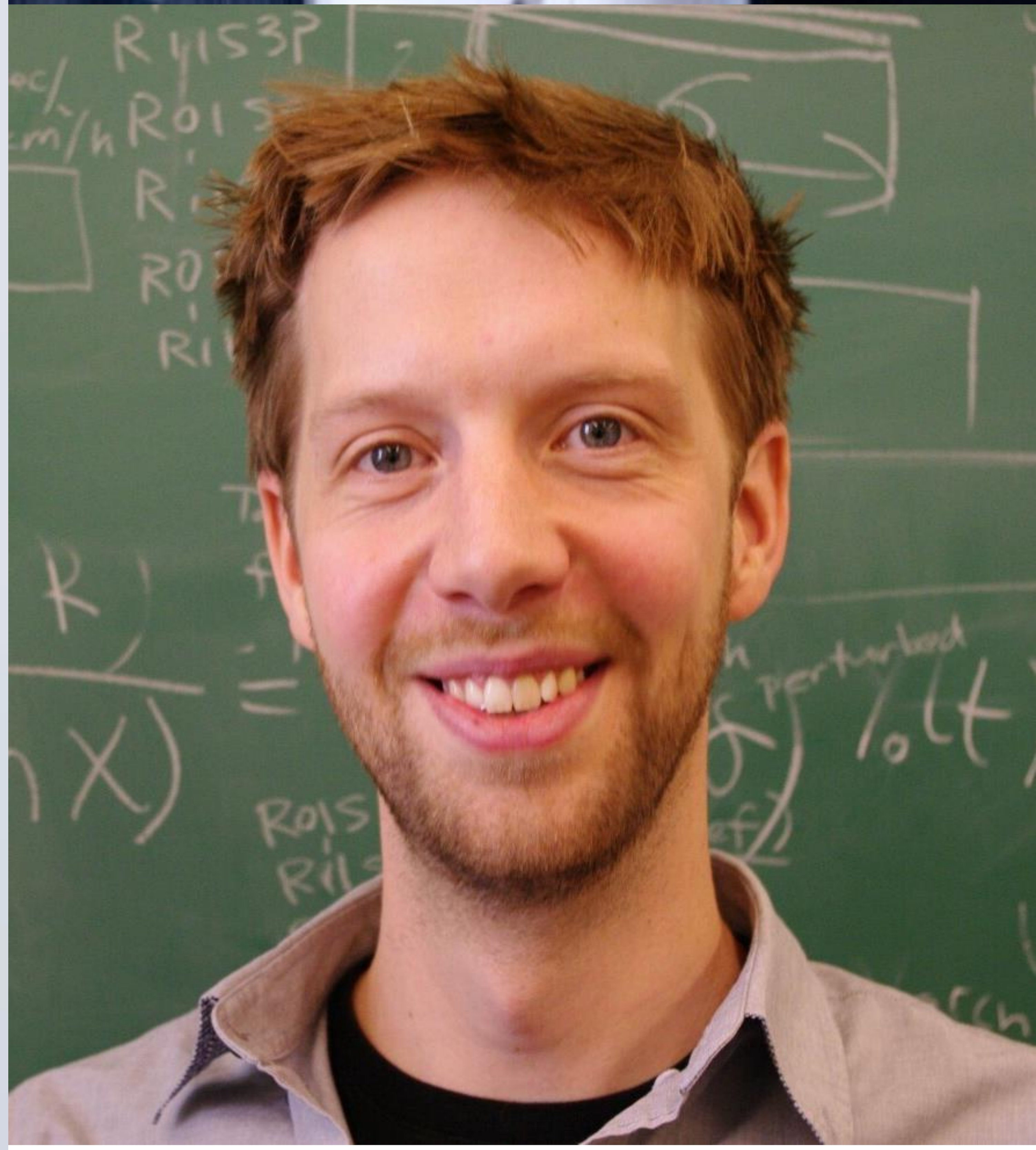

- Figure 3: Comparison of different models. The left panels show training curves for three selected models averaged over three seeds (shaded area shows standard distribution). The right panels show the mean score at epoch 100 for different prototype sets and sizes. Error bars show standard deviation across three seeds.

# Conclusion and future work

- We demonstrate a structured, easy-to-implement approach to improve GNN-based footprint predictions where footprints predicted using prototypes achieve better MSE scores.
- Future work will focus on explore other applications of prototypes, collaborating with domain experts and those developing emulators, since it is likely that other physical emulators could benefit from incorporating prototypes into their emulation pipeline.

# Acknowledgements


- Coauthors: Elena Fillola, Jeffrey Nicholas Clark, Raul Santos-Rodriguez and Matthew Rigby.
- NK, JNC and MR are funded by the Self-Learning Digital Twins for Sustainable Land Management grant [grant number EP/Y00597X/1]. EFM is funded by a Google PhD Fellowship. RSR is funded by the UKRI Turing AI Fellowship [grant number EP/V024817/1].

# References


- [1] E. Fillola, R. Santos-Rodriguez, and M. Rigby, "A graph neural network emulator for greenhouse gas emissions inference," Copernicus Meetings, Tech. Rep., 2024.
- [2] R. Lam, A. Sanchez-Gonzalez, M. Willson, P. Wirnsberger, M. Fortunato, F. Alet, S. Ravuri, T. Ewalds, Z. Eaton-Rosen, W. Hu et al., "Graphcast: Learning skillful medium-range global weather forecasting," arXiv preprint arXiv:2212.12794, 2022