Emulating Greenland Ice Sheet Surface Melt Using Graph Neural Network

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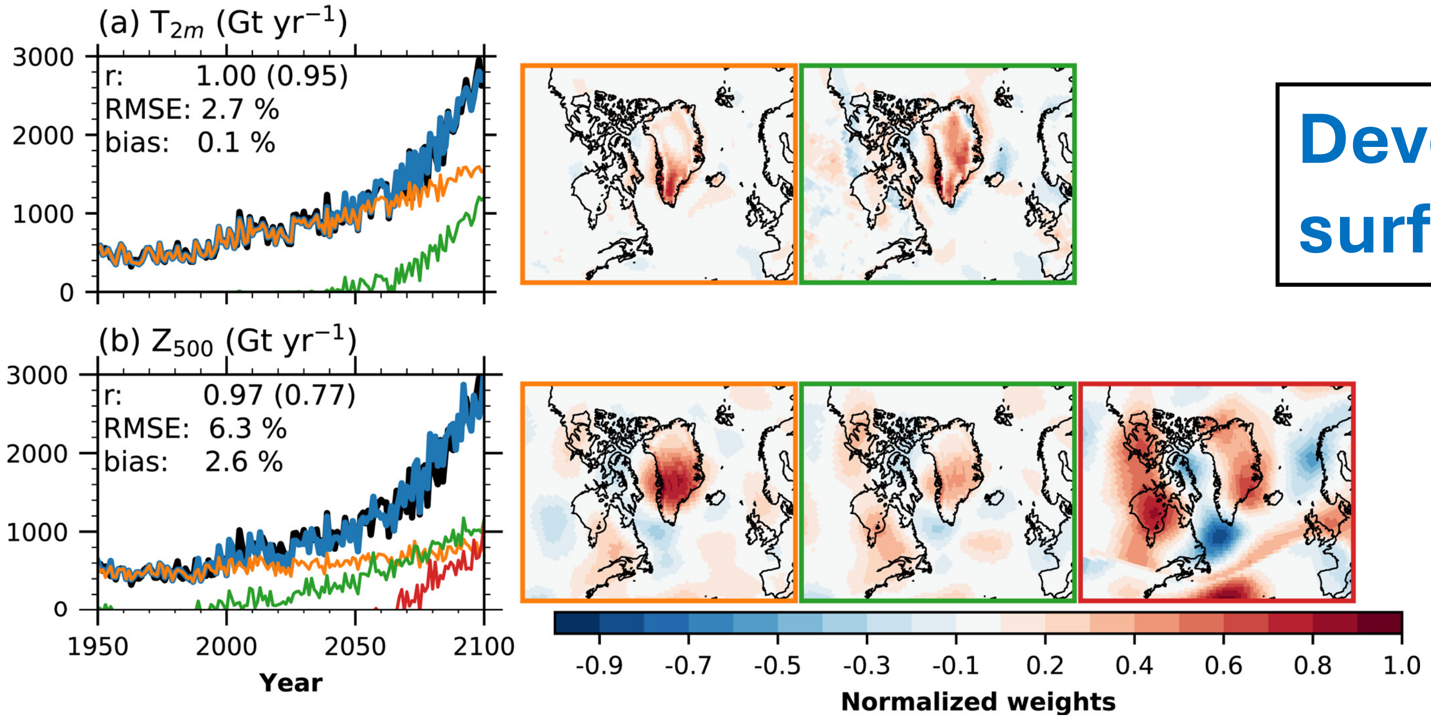
Motivation

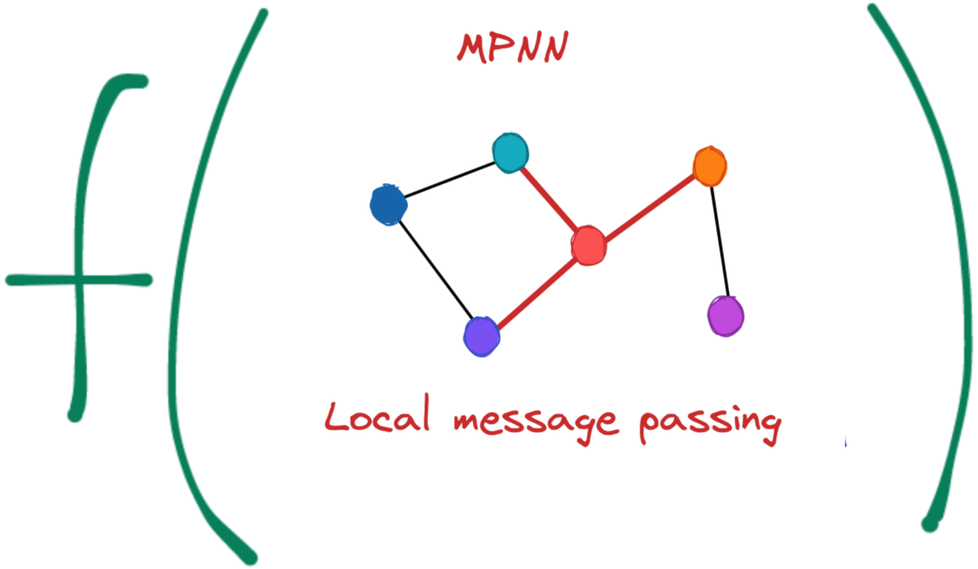
- Greenland Ice Sheet surface melt is driven by complex mechanisms involving both local and remote processes
- Most CMIP6 models lack realistic surface melt calculation over ice sheets



Develop an emulator for 2D surface melt fields

(Sellevold et al., 2021)

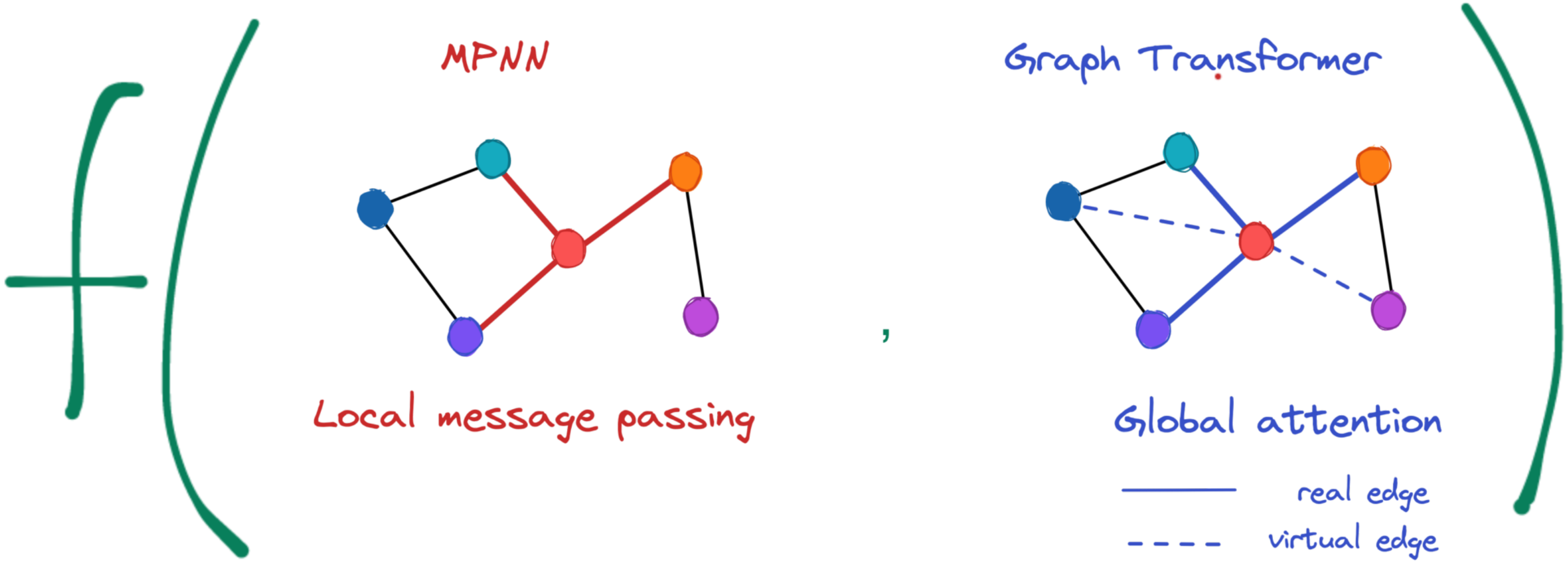
Method – Graph Neural Network (GNN)



(Credit: Michael Galkin)

- Unlike CNNs, GNNs can operate on unstructured grids
- Successfully applied in ML-based weather prediction models (e.g., GraphCast; Lam et al., 2023)

Method – Graph Transformer



(Credit: Michael Galkin)

- Combines local message passing and long-range impacts
- Integrates graph structure into the attention mechanism
- Applications include Artificial Intelligence Forecasting System (AIFS; Lang et al., 2024), molecular property prediction (e.g., GraphGPS; Rampášek et al., 2023)

Data

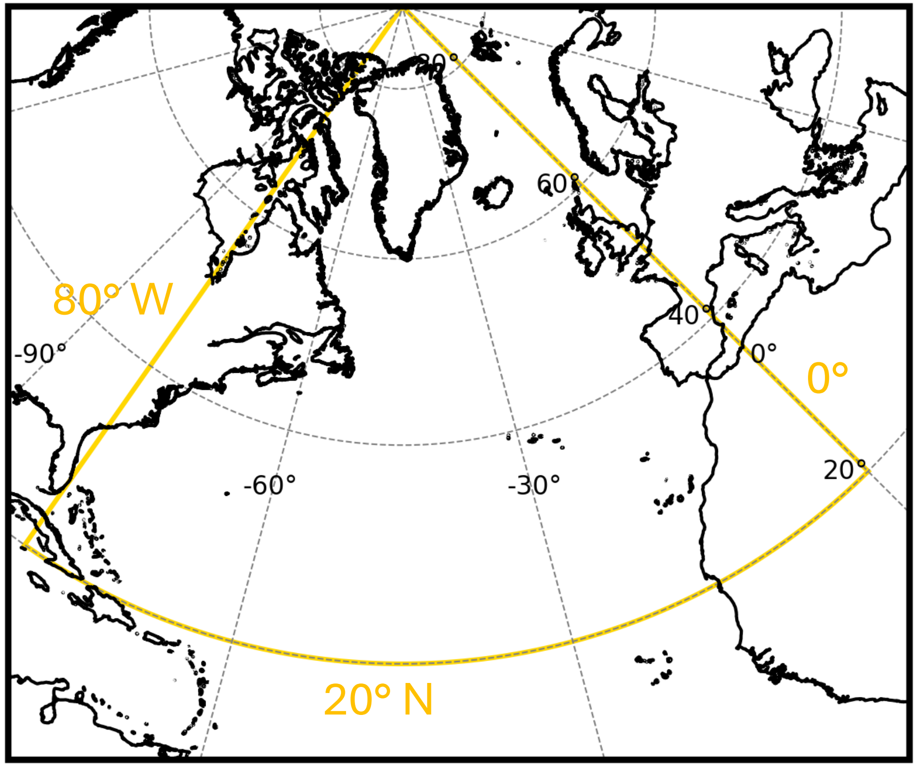
CESM2 CMIP6 historical simulations:

- First 10 members for training,
- The last member for evaluation (~11%)
- **Period:** 1850-2014

Input variables (JJA mean):

SW_{in}, LW_{in}, T_{2m}, Q_{2m}, U_{10}, PS, Z_{500}, SNOW, RAIN, LWP, IWV

Output variable: Annual surface melt



Region of interest

Emulator structure

n layers

Input variables

...

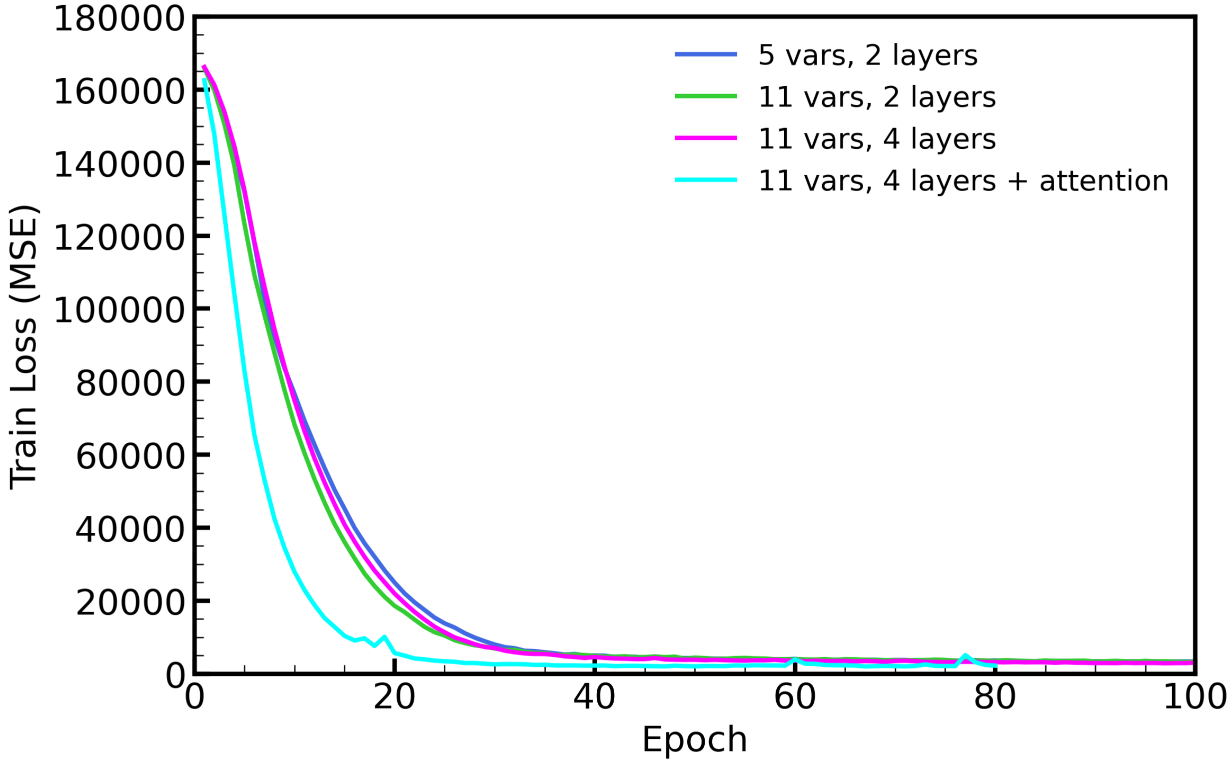
surface melt

lat/lon coordinates
as positional encoding

( ) ( )

Category	Setting / Value	Notes
Spatial Grid	75×65 grid	
Number of Layers	2 or 4 MPNN layers $\times$ 2-hop propagation	Effective 4-hop receptive field
Hidden Dimension	128	Hidden feature size
Optimizer	Adam	
Loss Function	Weighted Mean Squared Error (MSE) masked over the GrIS	Regression task
Neighborhood Size	4 nearest neighbors	Local graph structure

Training



Training speed:

- Without attention: 5-10 mins per epoch (Apple M1 Pro, 10-core CPU)
- With attention: ~30 mins per epoch (currently ran 80 epochs)
- Transferring to GPUs at TACC for acceleration

Evaluation

Emulate JJA melt

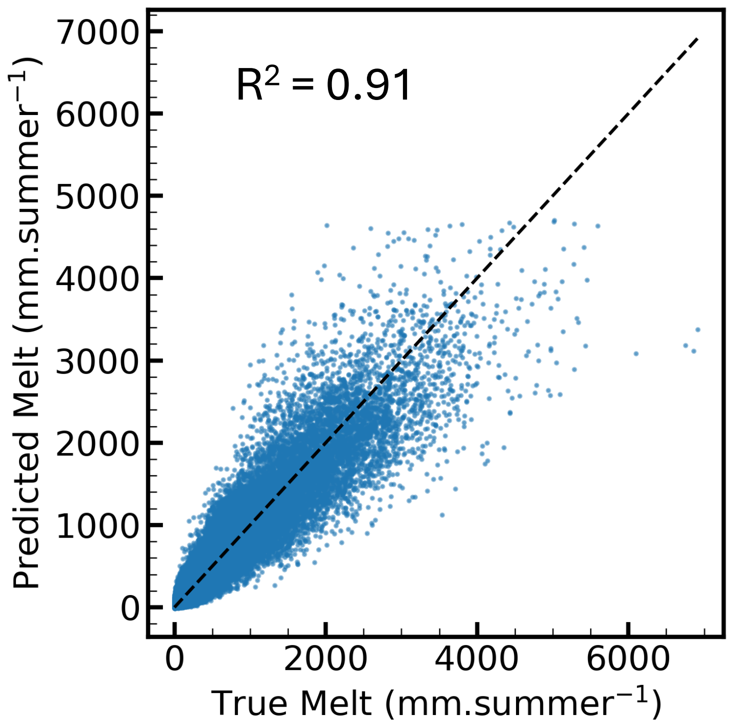
	RMSE (mm)	Bias (mm)	R^2 score
5 vars, 2 layers	117.29	-12.19	0.91
11 vars, 2 layers	117.95	0.88	0.91
11 vars, 4 layers	118.85	-1.3	0.91
11 vars, 4 layers, + attention	111.72	3.21	0.92

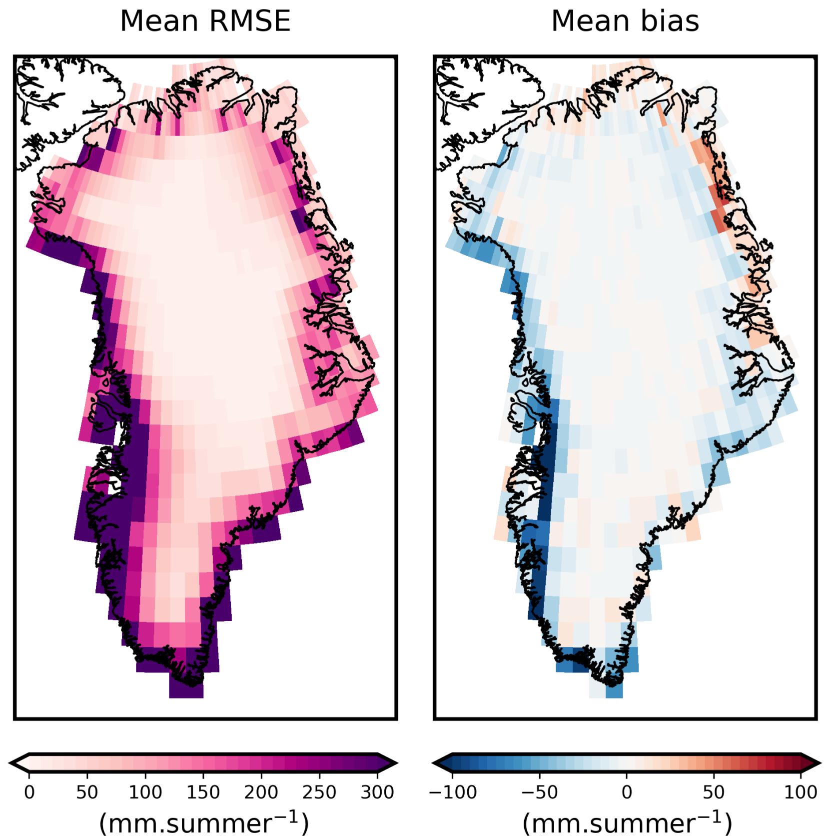
Emulate annual melt

	RMSE (mm)	Bias (mm)	R^2 score
5 vars, 2 layers	130.73	-5.72	0.91
11 vars, 2 layers	135.62	-22.74	0.91
11 vars, 4 layers	130.37	-14.57	0.91
11 vars, 4 layers, + attention	127.60	13.86	0.92

- Emulating annual melt is more challenging
- Some input variables may be redundant
- Adding attention slightly decrease RMSE and increase R^2

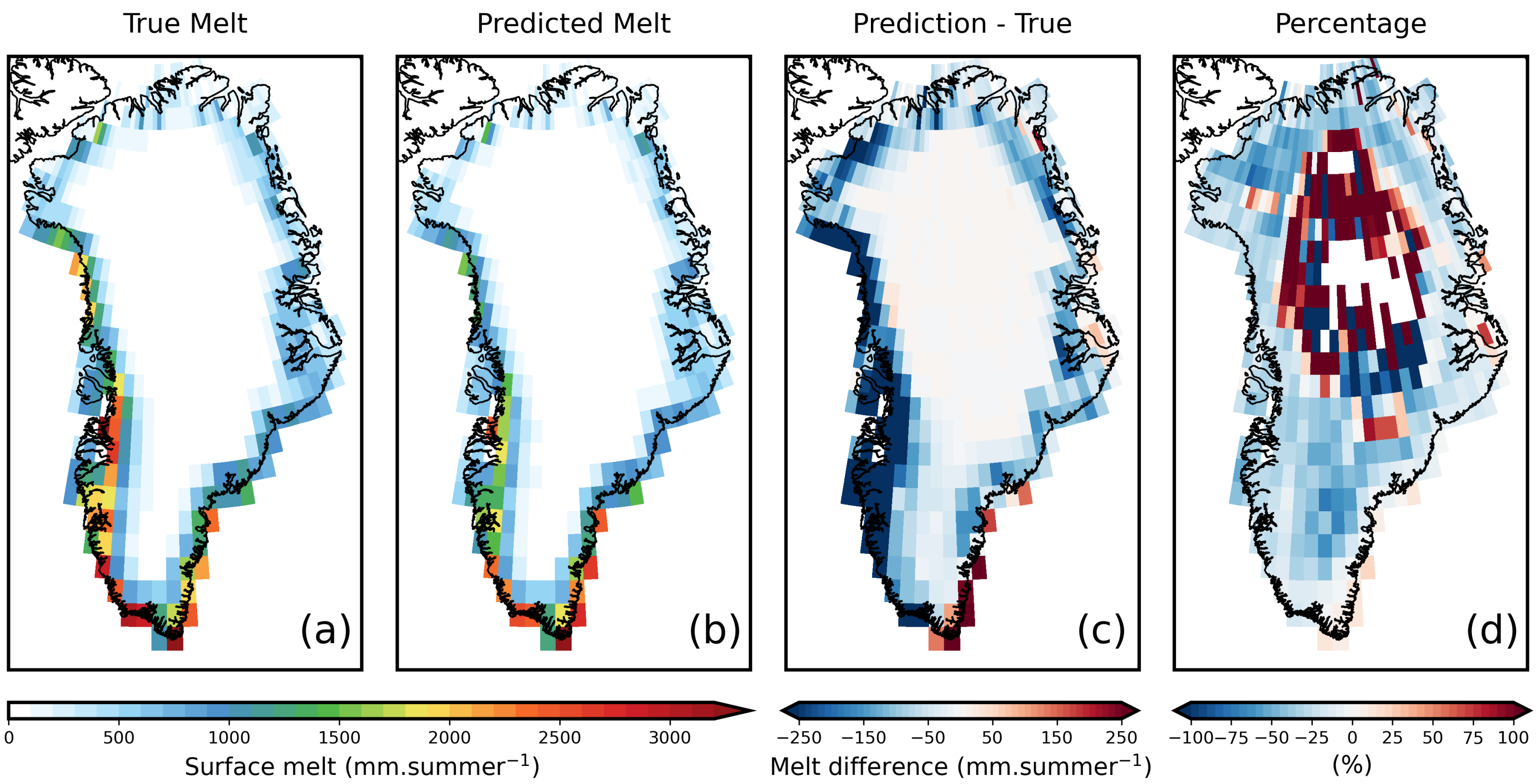
Evaluation – Averaged over 1850-2014





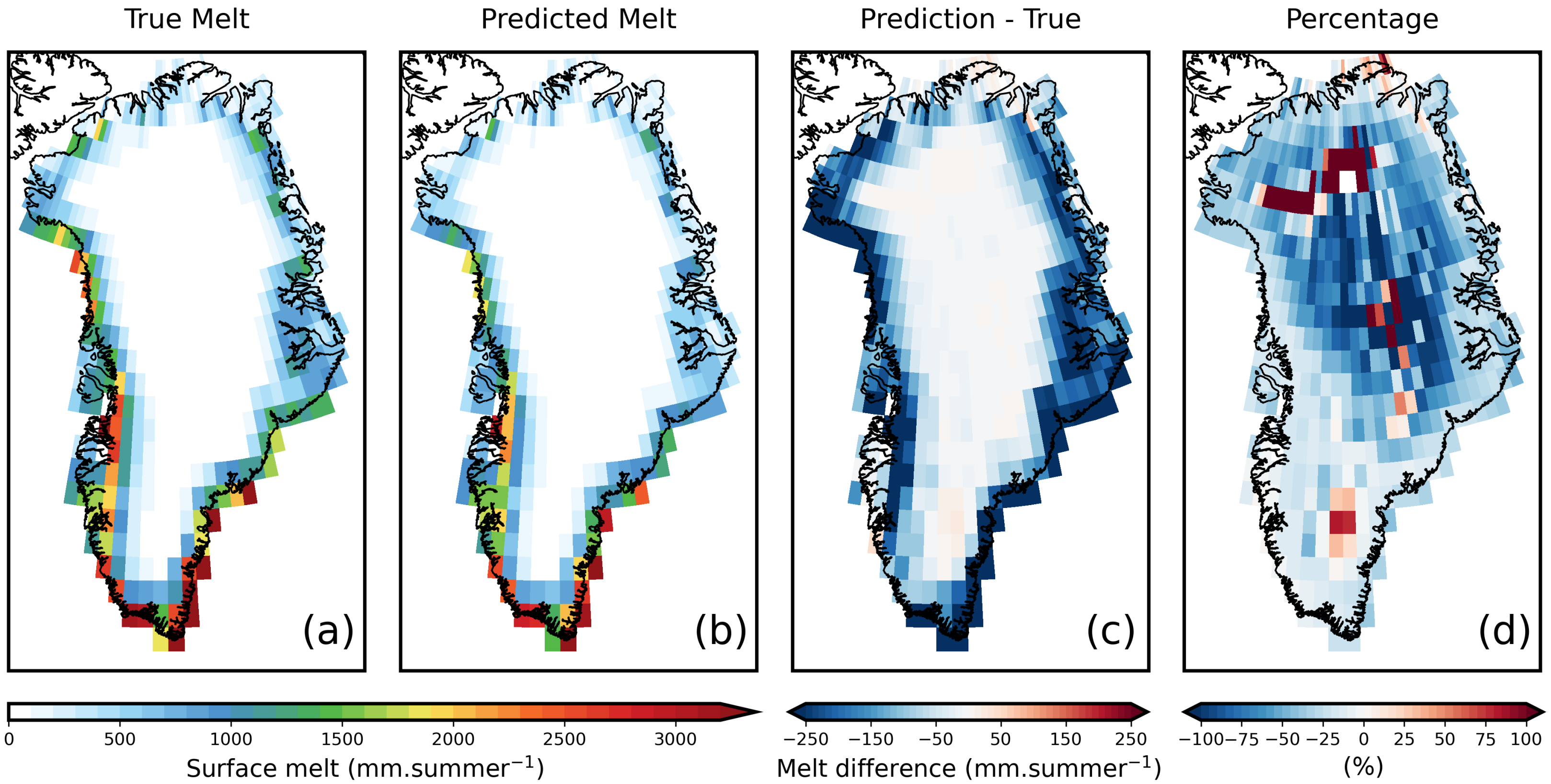
- Larger RMSE and bias over marginal regions

Evaluation – Example of one single year (1990)



- Emulator captures the general spatial pattern but underestimates high melt values

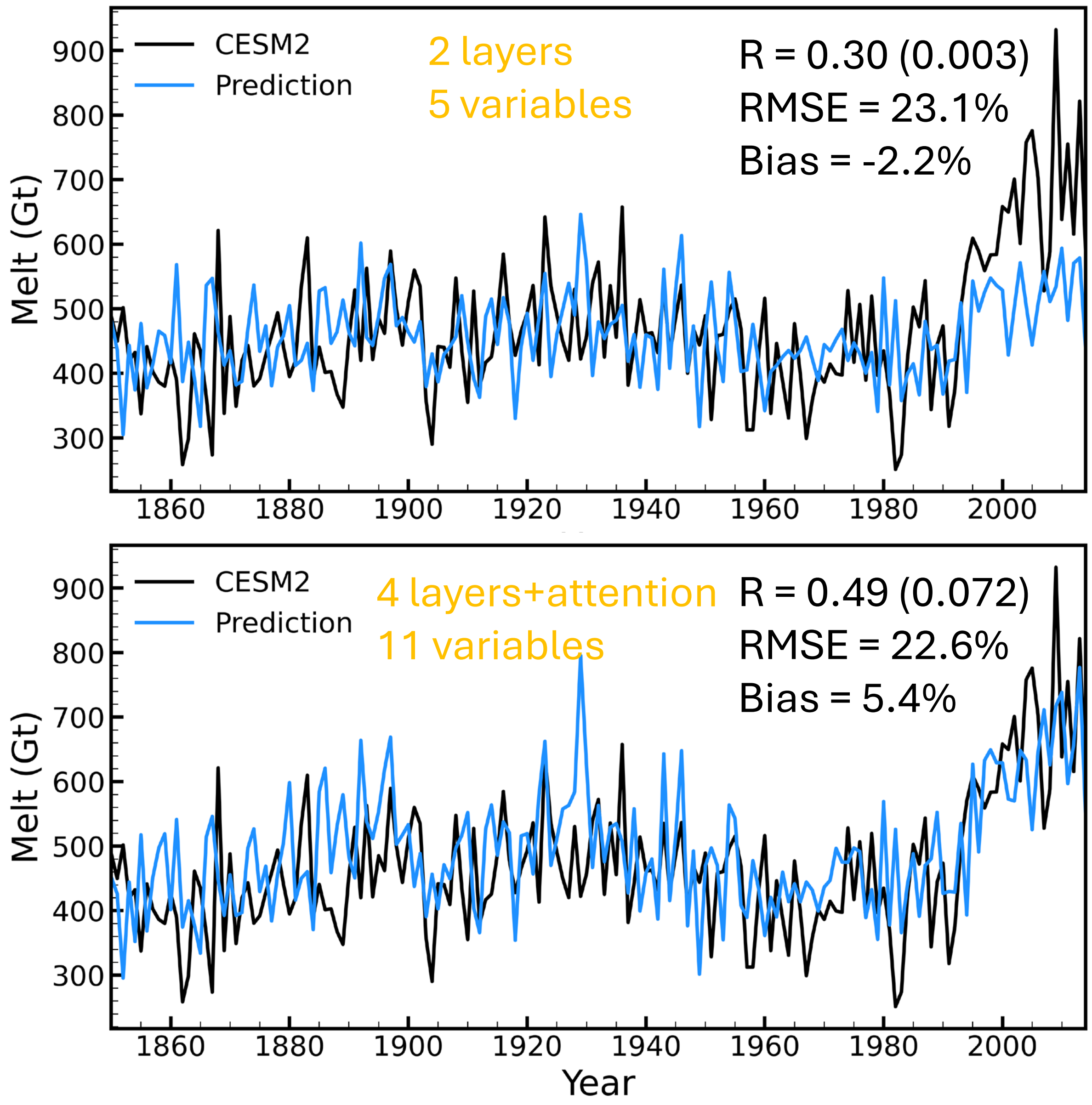
Evaluation – Example of one single year (2014)



- Emulator captures the general spatial pattern but underestimates high melt values

Evaluation – Integrated surface melt

- Emulator does not capture interannual variability well
- Adding global attention helps capture the increase in melt due to warming



Take-aways

- The GNN-based emulator produces reasonable JJA surface melt fields, but improvements are needed, especially over lower-elevation regions

Next steps

- Incorporate SSP simulations into training
- Perform sensitivity experiments to assess the impact of input variables and modeling choices (e.g., gradient loss)
- Conduct feature attribution analyses (e.g., GraphSHAP) to identify key variables and regions controlling surface melt
- Apply the trained emulator across all CMIP6 models to generate an ensemble estimate of GrIS surface melt
- (Probabilistic prediction)

Reference

Sellevold, R., & Vizcaino, M. (2021). First application of artificial neural networks to estimate 21st century Greenland ice sheet surface melt. Geophysical Research Letters

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Lang, Simon, Mihai Alexe, Matthew Chantry, Jesper Dramsch, Florian Pinault, Baudouin Raoult, Mariana CA Clare et al. "AIFS--ECMWF's data-driven forecasting system." arXiv preprint arXiv:2406.01465 (2024).

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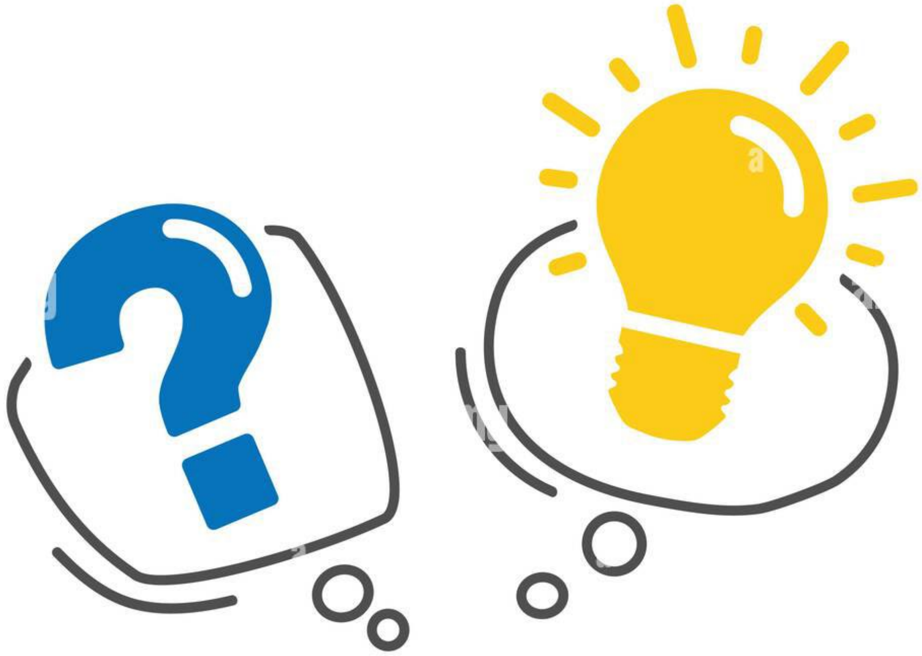
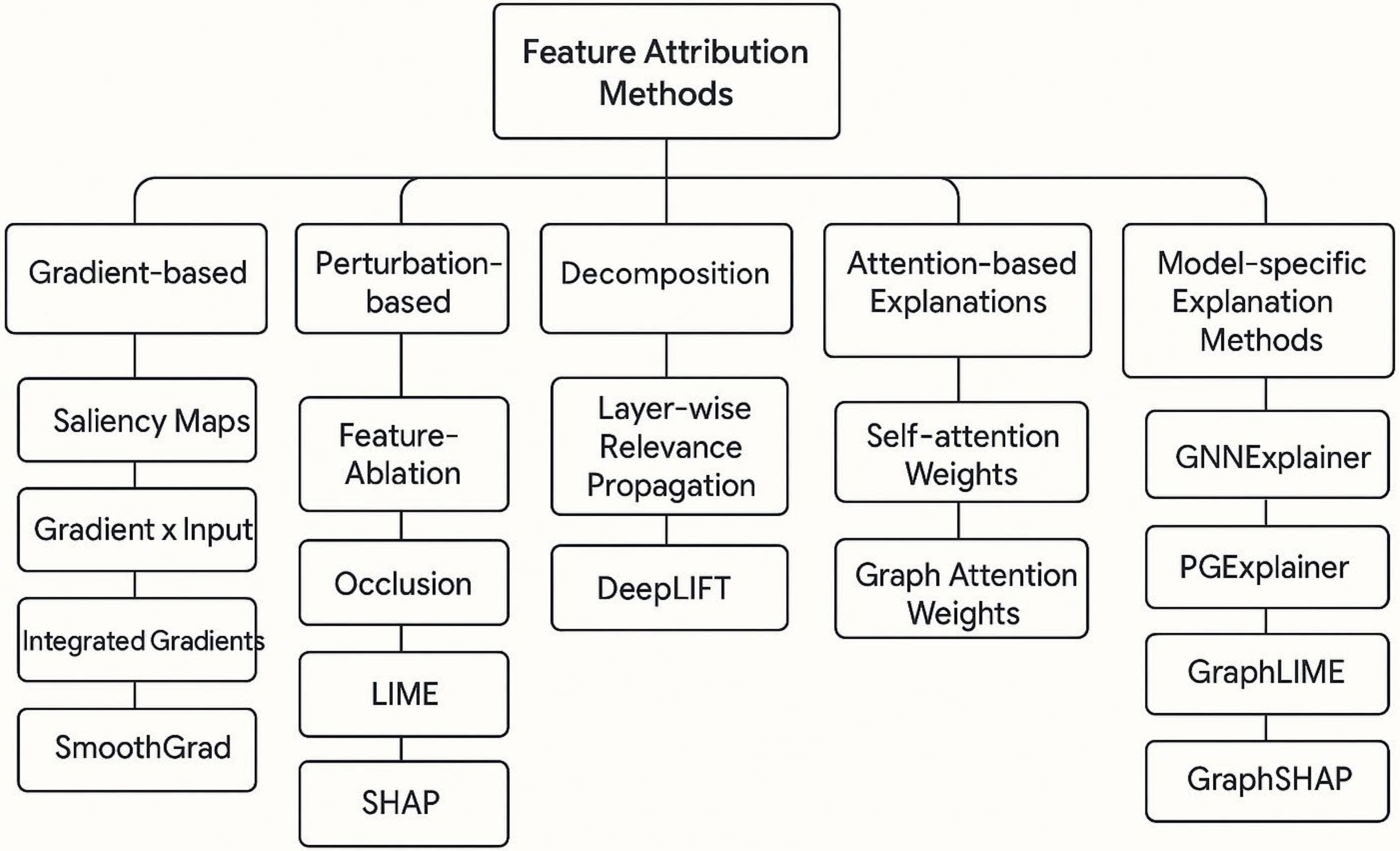
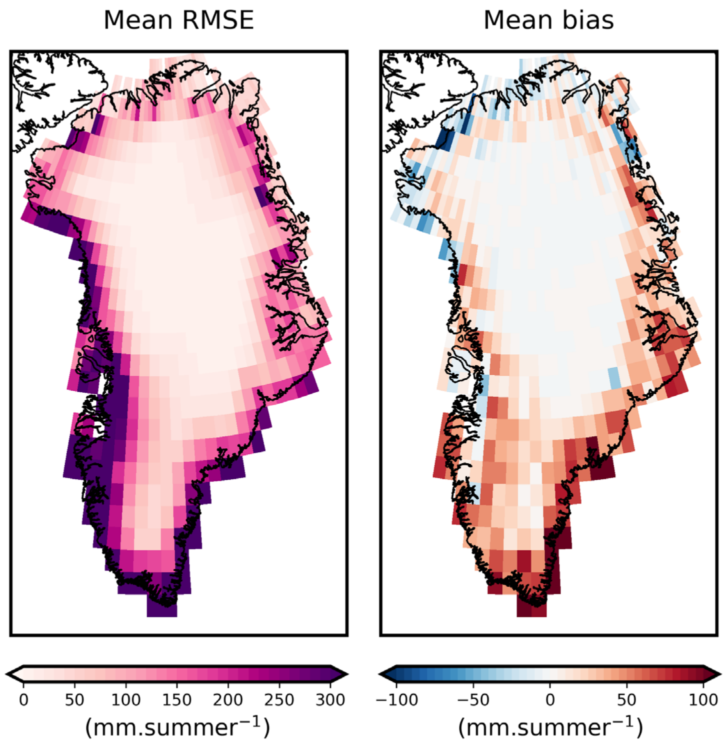



Feature Attribution Methods
Gradient-based
Perturbation-based
Decomposition
Attention-based Explanations
Model-specific Explanation Methods
Saliency Maps
Gradient x Input
Integrated Gradients
SmoothGrad
Feature-Ablation
Occlusion
LIME
SHAP
Layer-wise Relevance Propagation
DeepLIFT
Self-attention Weights
Graph Attention Weights
GNNExplainer
PGExplainer
GraphLIME
GraphSHAP

1850-2014 mean



2014