

Emulating Greenland Ice Sheet Surface Melt Using Graph Transformer

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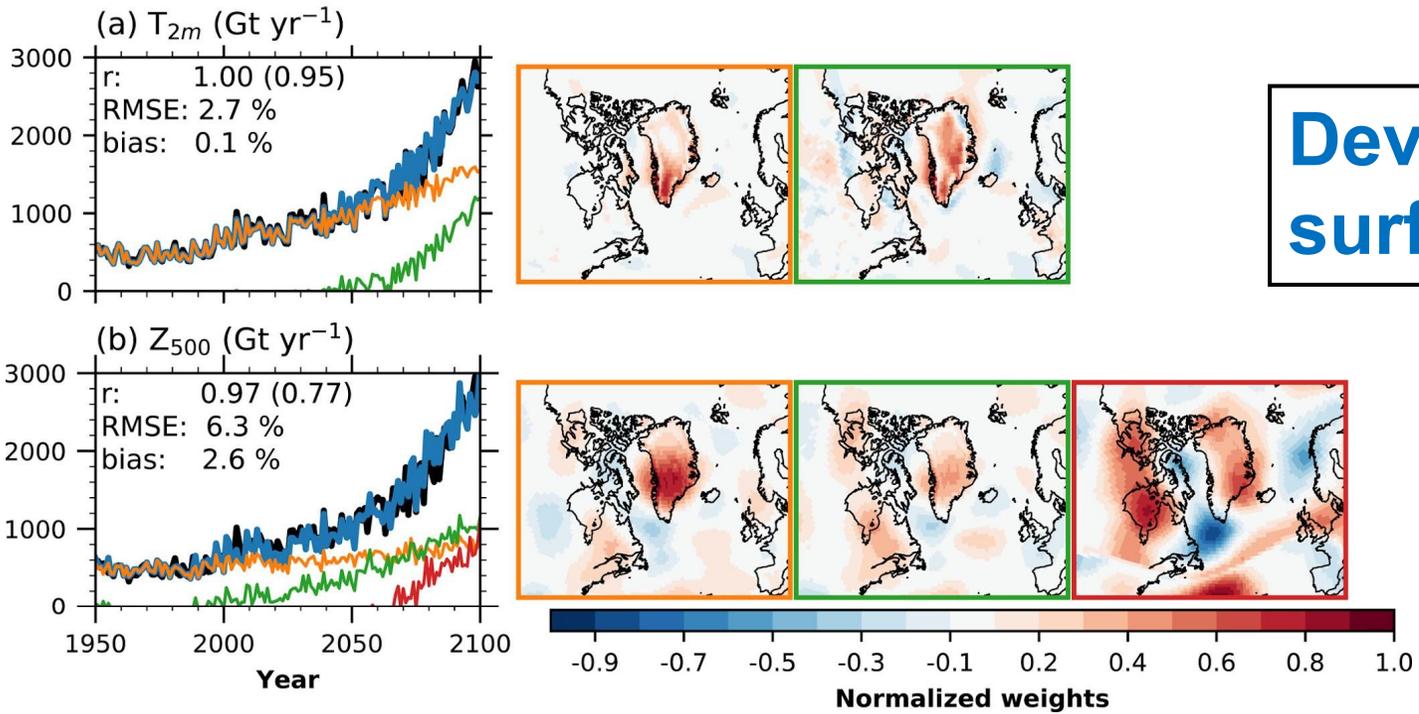
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LIWG meeting 2026
Feb

Motivation

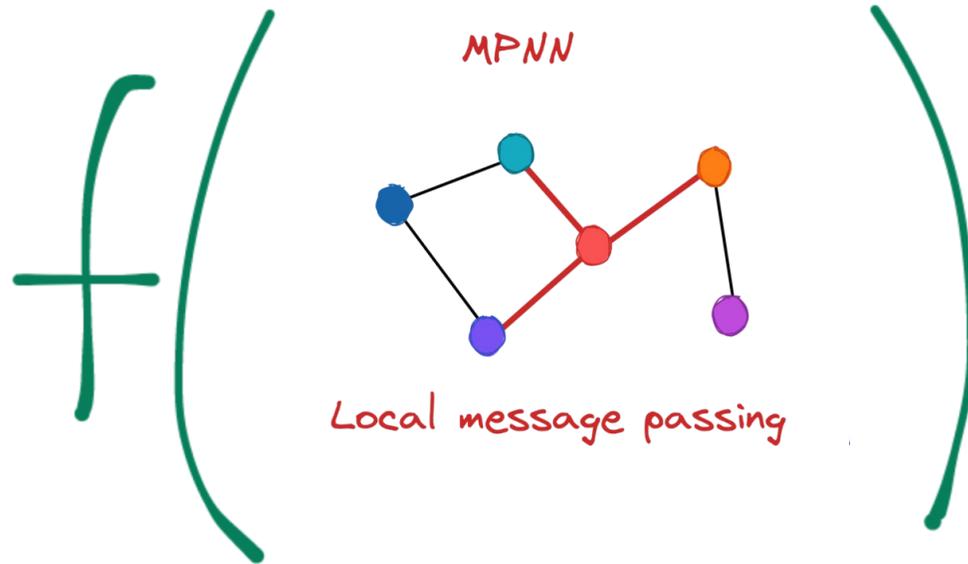
- Greenland Ice Sheet surface melt is driven by complex mechanisms involving both local and remote processes
- Simulating large ensembles of surface melt using climate models is computationally expensive and often impractical
- Most CMIP6 models lack realistic surface melt calculation over ice sheets



Develop an emulator for 2D surface melt fields

(Sellevoold et al., 2021)

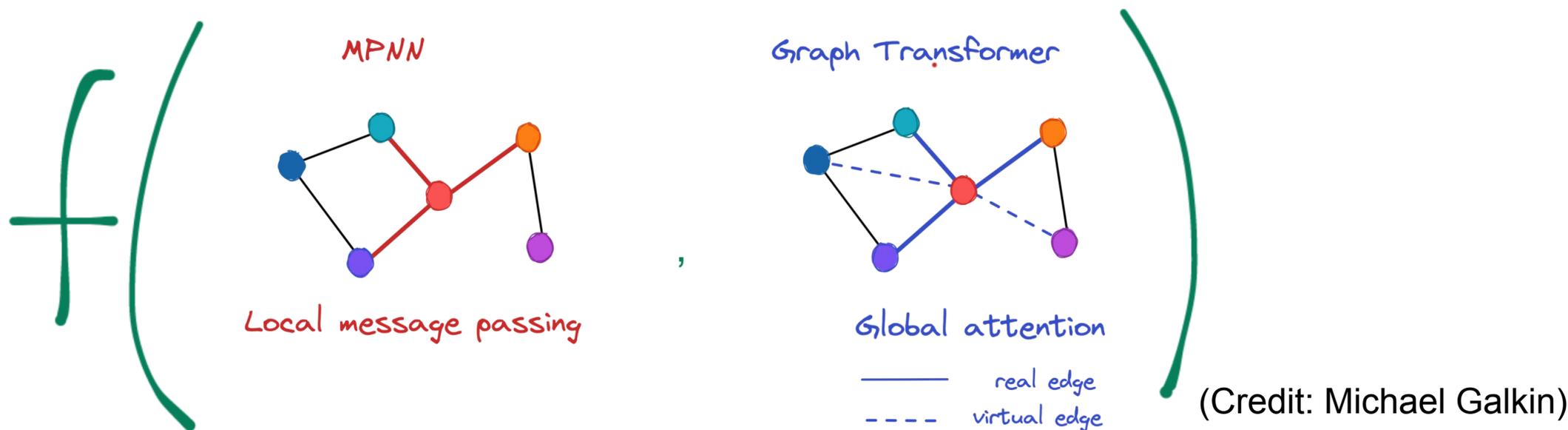
Method – Graph Neural Network (GNN)



(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



- 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

Training and Validation:

CESM2 large ensemble simulations (LENS2)

historical + SSP370 (1850-2014, 100 members)

first 90 members for training; last 10 members for validation

Testing:

CESM2 CMIP6 ensemble simulations

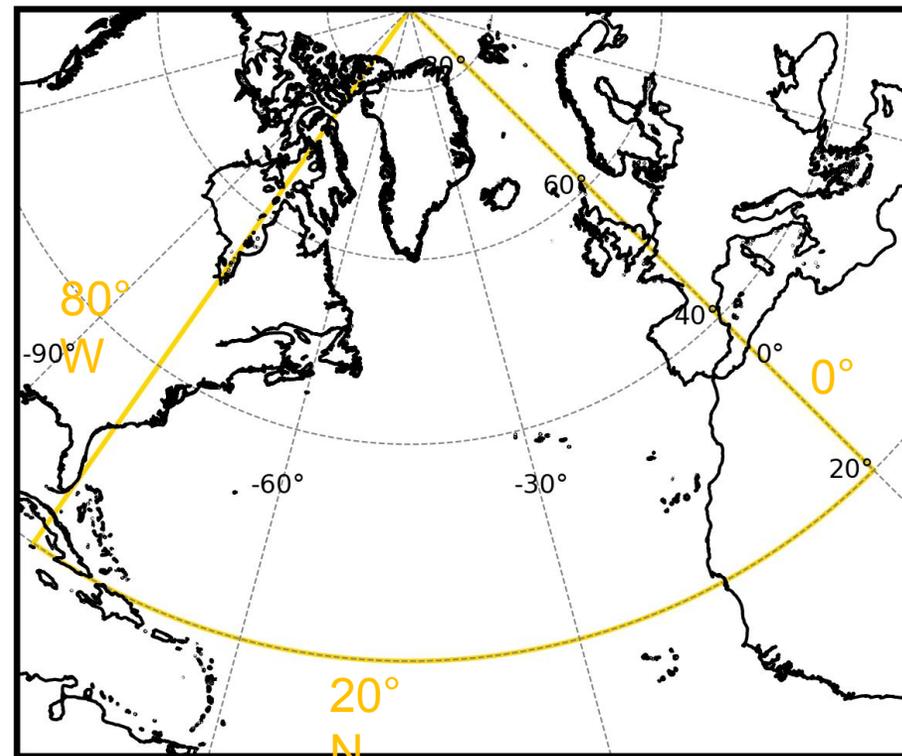
historical (11 members) + SSP1/2/3/5 (3 member each)

Input variables (JJA mean):

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

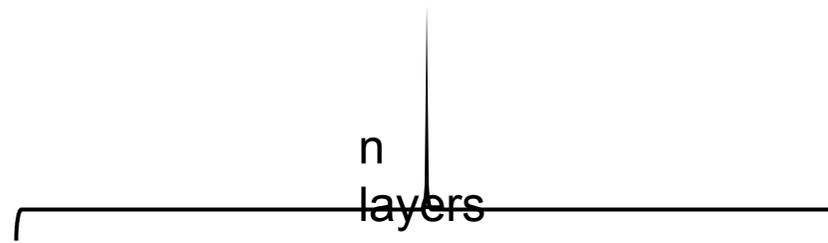
Output variable:

Annual surface melt



Region of
interest

Emulator structure



Input
variables

...

surface melt

lat/lon coordinates
as positional encoding

() ()

Loss function:

$$\mathcal{L} = \frac{1}{|\mathcal{M}|} \sum_{i \in \mathcal{M}} (w_i a_i) (\hat{y}_i - y_i)^2$$

elevation
weight

Training

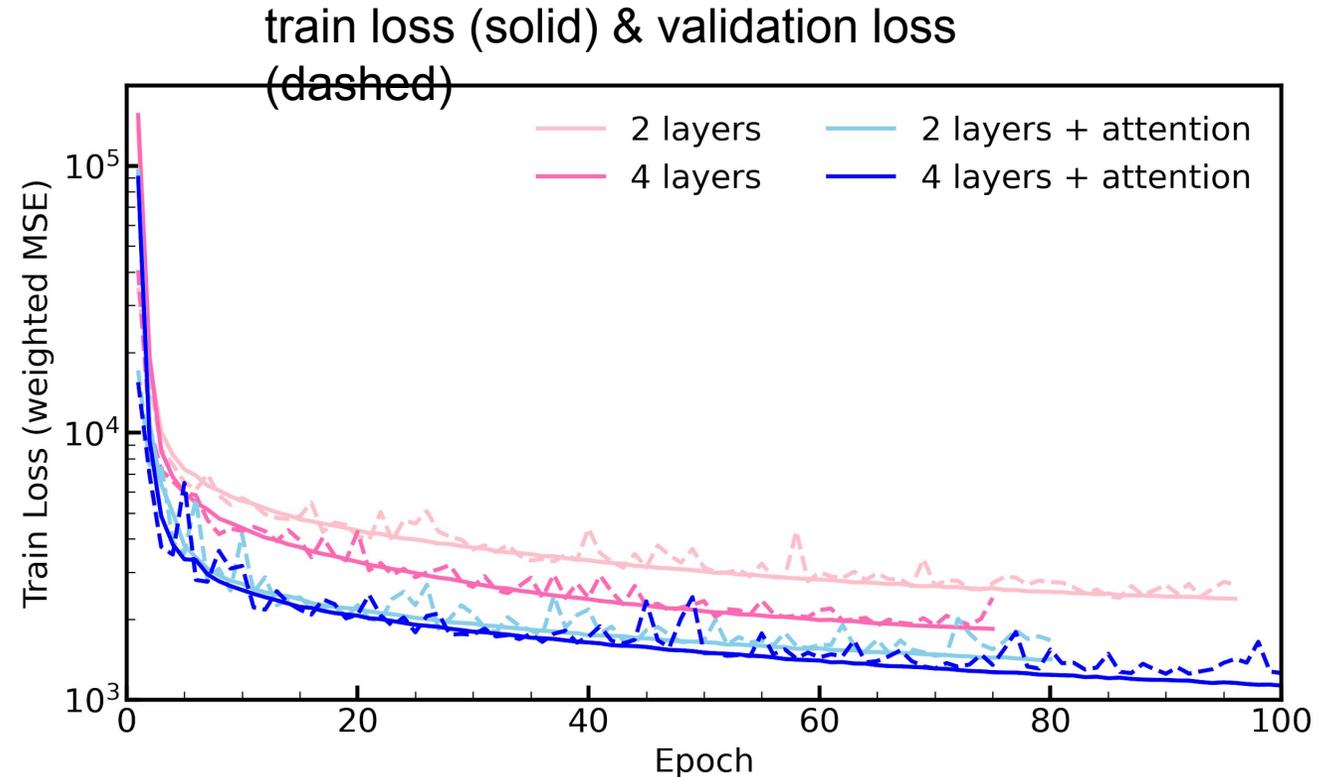
Training speed:

Apple M1 Pro, 10-core CPU

- Without attention: 5-10 mins per epoch
- With attention: ~30 mins per epoch

NVIDIA RTX A5000 GPU on TACC

- With attention: ~1 mins per epoch



Early stopping criterion: if validation loss did not improve for 10 consecutive epochs, save the model parameters corresponding to the minimum loss

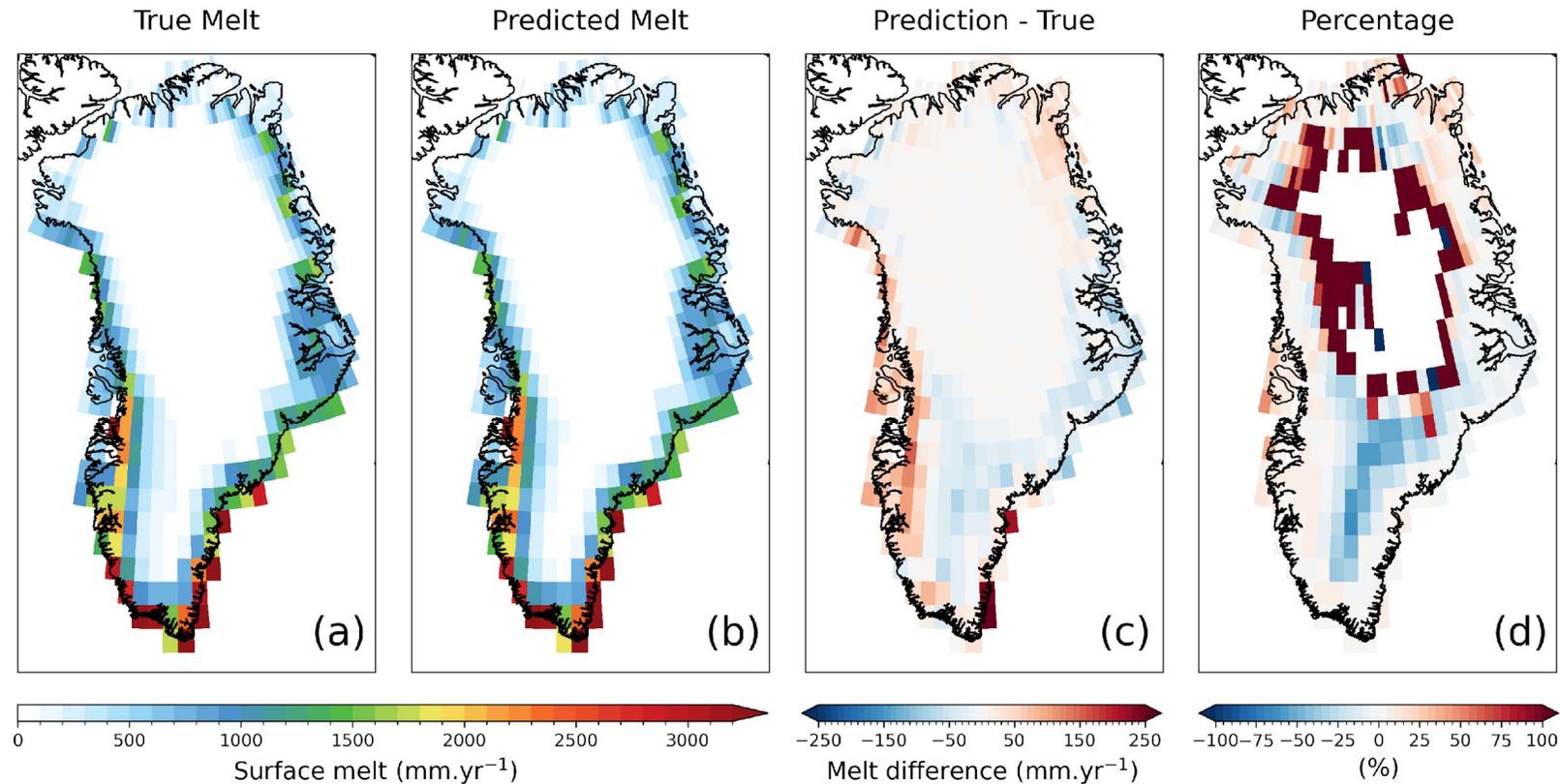
Evaluation – For all ice sheet grid cells

Number in parentheses represents evaluation based on all but SSP5 data.

Model	RMSE (mm)	Bias (mm)	R² score
Linear regression	154.99 (121.49)	6.44 (18.80)	0.93 (0.95)
Random Forest	139.91 (110.99)	3.80 (14.78)	0.94 (0.96)
GNN (2 layers)	80.64 (67.89)	6.62 (10.91)	0.98 (0.98)
GNN (4 layers)	70.30 (57.41)	-11.45 (-6.91)	0.99 (0.99)
GT (2 layers)	65.99 (53.43)	-9.93 (-6.01)	0.99 (0.99)
GT (4 layers)	65.33 (54.68)	6.53 (9.96)	0.99 (0.99)

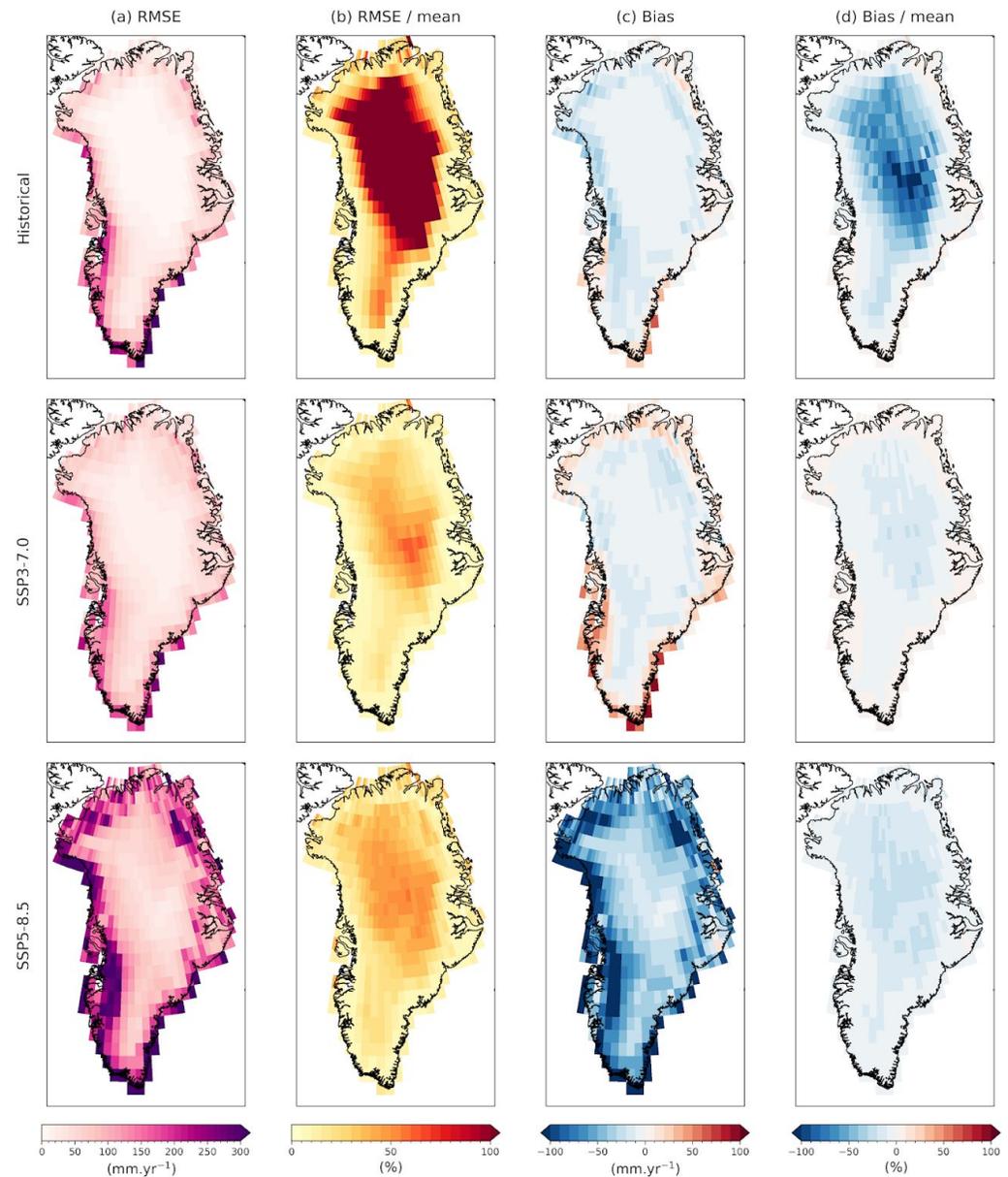
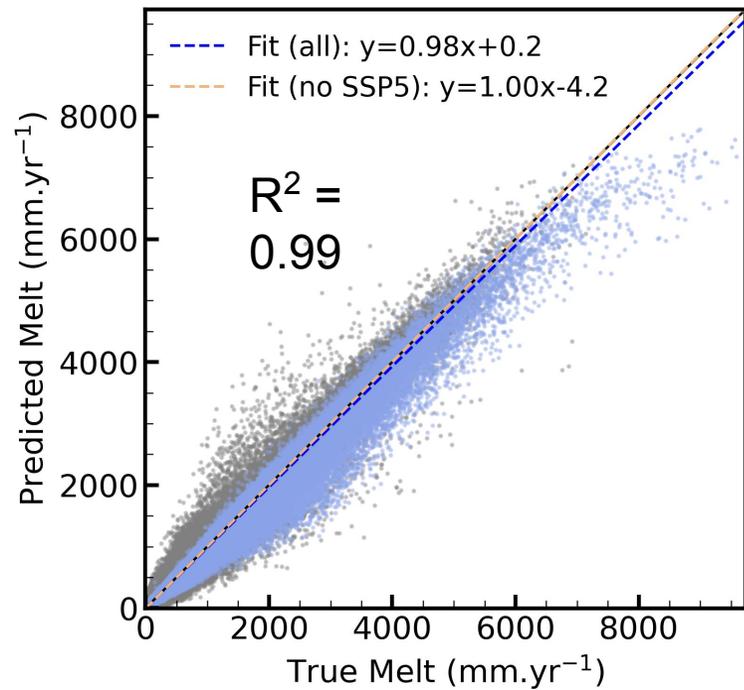
- The Graph neural network (GNN) models outperforms the per-grid-cell baseline methods
- The Graph Transformer (GT) models outperforms pure GNN models

Evaluation – Example of one single year (2014)

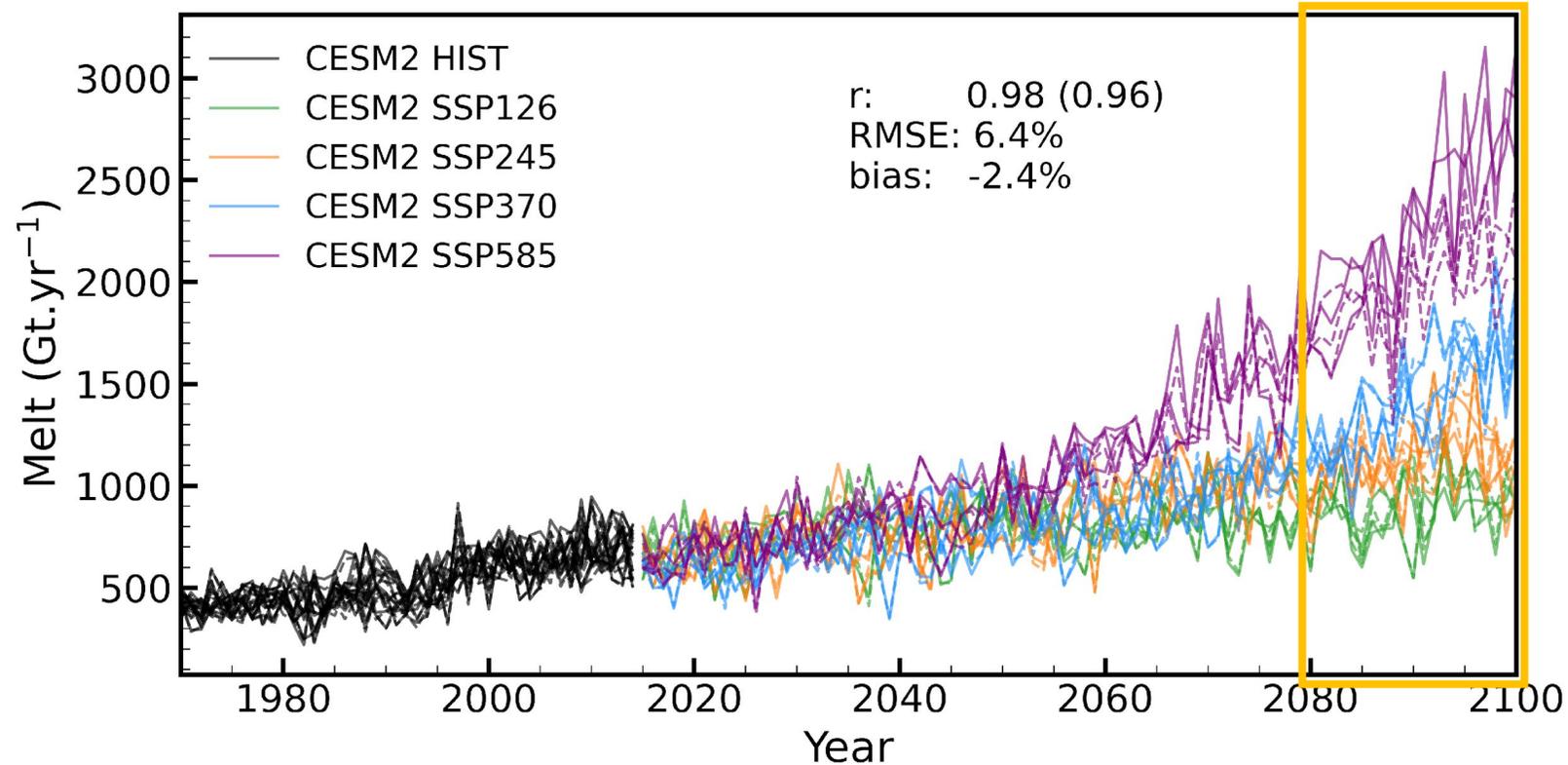


- Emulator captures the general spatial pattern but overestimates (e.g., CW, SW, NE basins) or underestimates high melt values (in other basins)

Evaluation – Averaged over 1850-2014 or 2015-2100



Evaluation – Integrated surface melt



- The emulator underestimates integrated surface melt when conditions are out of the training sample distribution

Take-aways

- The Graph Transformer emulator produces reasonable CESM2 annual surface melt fields and captures interannual variability well
- Relatively large bias exists over the ice sheet margins
- The emulator shows some but limited generative ability for out-of-sample prediction

Next steps

- Optimize the emulator
- Conduct feature attribution analyses to identify key atmospheric variables and regions controlling surface melt
- Apply the trained emulator across all CMIP6 models to generate an ensemble estimate of GrIS surface melt

Reference

Sellevoold, 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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This work is funded by the National Science Foundation HDR iHARP institute (Grant OAC,2118285)

