Potential methods for a machine learning based end-to-end digital twin of regional oceans, fisheries, and management

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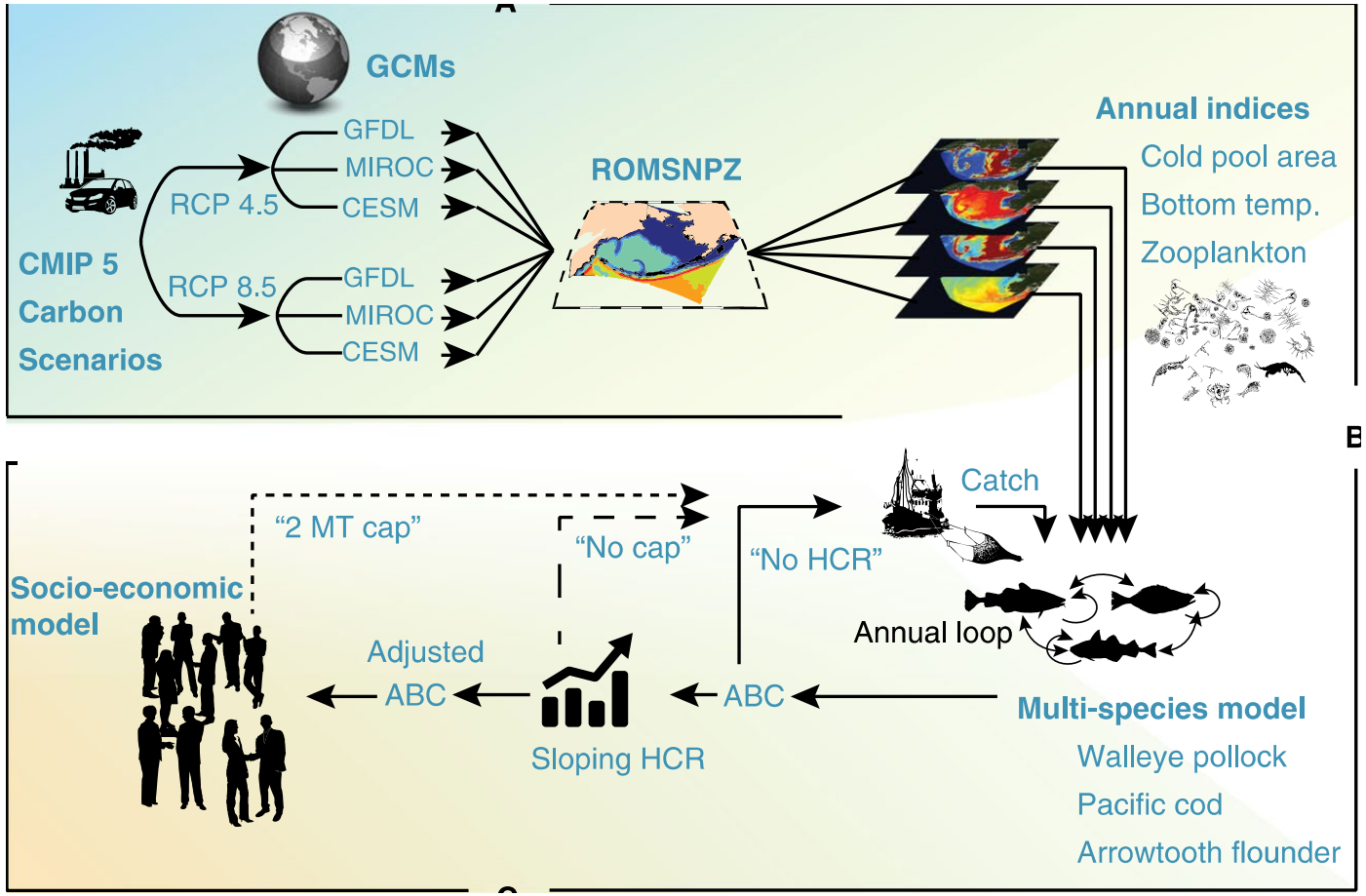
In collaboration with federal and non-federal colleagues:

Kirstin Holsman (AFSC), Wei Cheng (PMEL), Liz Drenkard (GFDL), many others!

Downscaled climate projections used in fisheries management strategy evaluation (figure from Alaska Climate Integrated Modeling program)

Ideally want really big ensembles for management applications

These can be very costly!



(Holsman et al 2020)

CEFI NEP10k Domain and Hindcast Configuration

Bathymetry (right, in meters): GEBCO 2020

Temporal Extent: 1993-2019 (27 years)

Atmospheric Forcing: ***JRA-55***

Tidal Forcing: TPXO

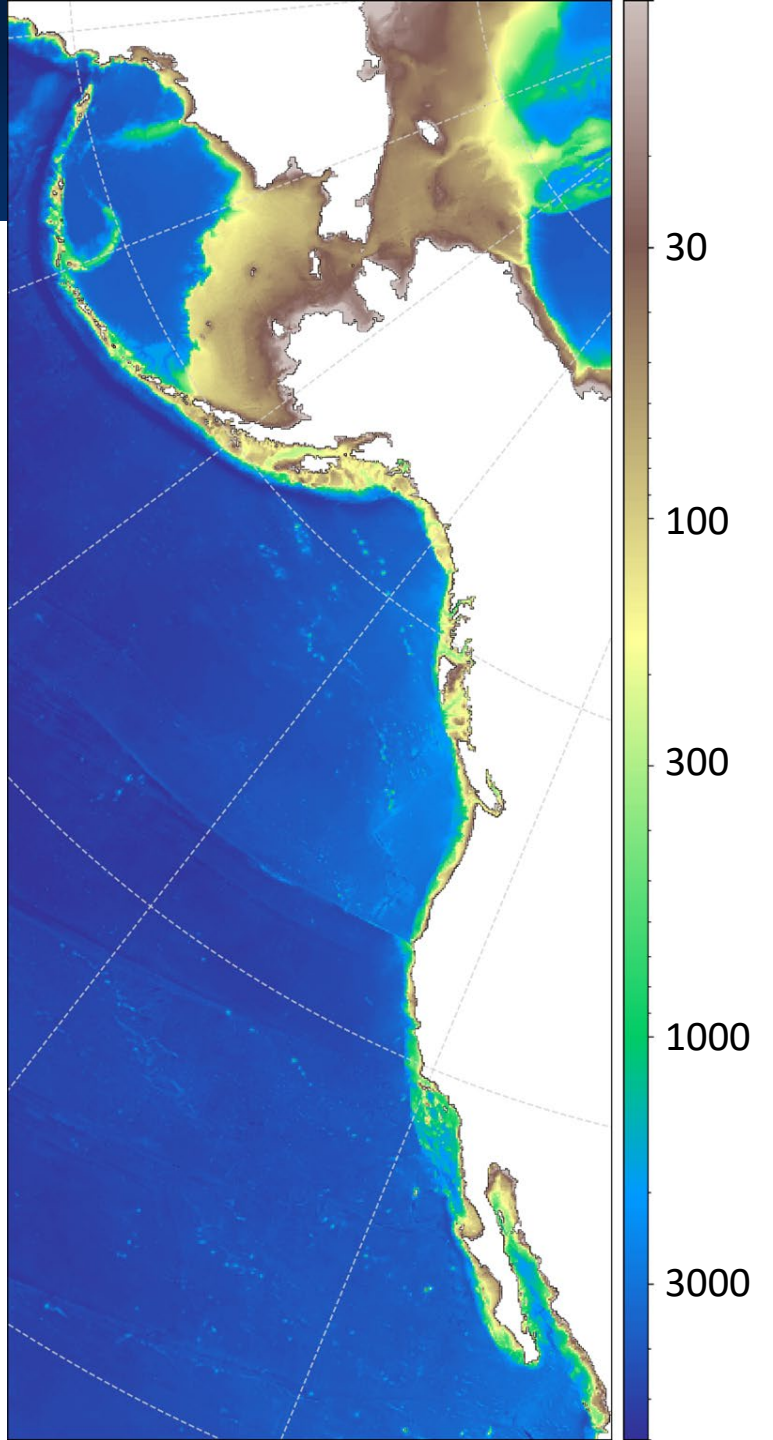
River Forcing

Freshwater: GloFAS, Beamer et al., (2016; GoA)

Initial and Boundary Conditions

Ocean Physics: GLORYS12

(modified slide from L. Drenkard)



Surrogate Modeling

- MOTIVATION: Regional models are computationally expensive!
- Output from a complex model can be used to train a ***surrogate*** which compactly approximates the behavior of the full system
- The use of a compact surrogate allows a broader range of model experiments, e.g.:
  - Broaden ensemble of predictions
  - Quantify sensitivities to forcing and parameters
- Here, we explore the use of ***Machine Learning*** to construct surrogates ("emulators") for regional NEP models
- Machine Learning can include EOF analysis (a form of "unsupervised learning"), Neural Networks, and Computer Vision approaches

EOFs have a long history of use to identify dominant geospatial patterns and their time variation

- Examples include:
  - ENSO
  - The Pacific Decadal Oscillation

- There are many others
  - Some (e.g. NPGO) are *not* the leading mode of variability!

EOF analysis is based on *Singular Value Decomposition* of a matrix

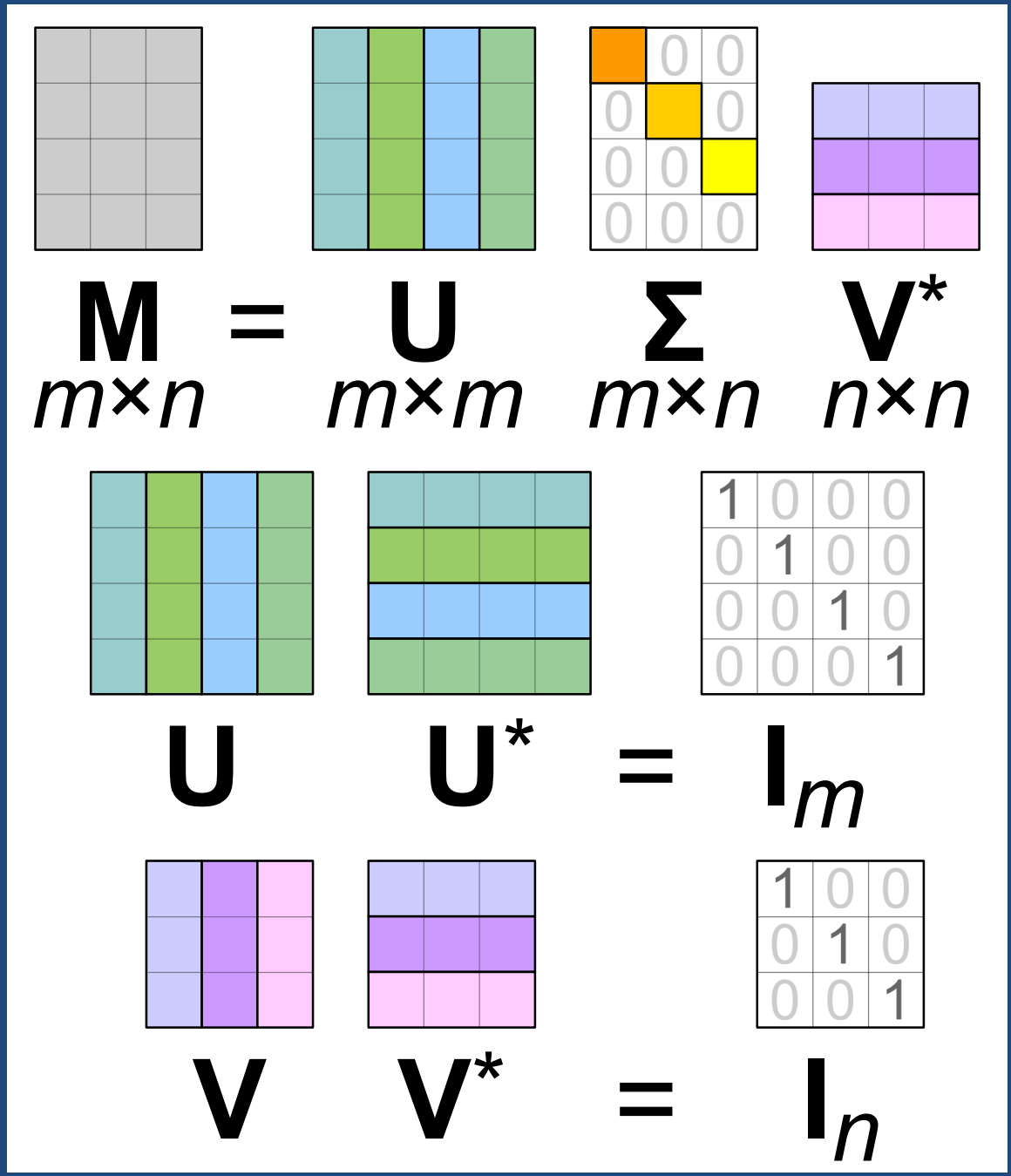
The two dimensions can really be anything:

space x time (univariate EOFs)

variable x time (Principal Components)

variable/space x time (multivariate EOFs)

FIGURE: By Cmglee - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=67853297



EOFs (PCA) can be used in hybrid dynamical-statistical downscaling for ensemble expansion

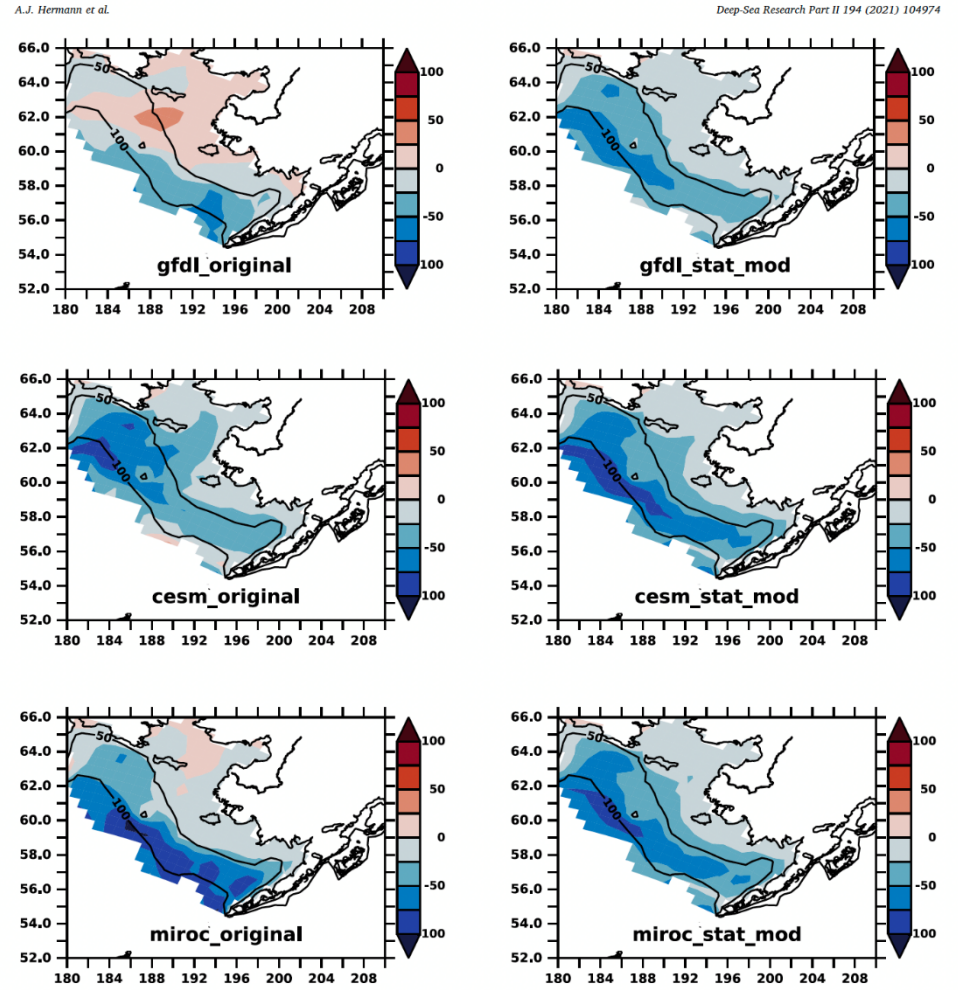
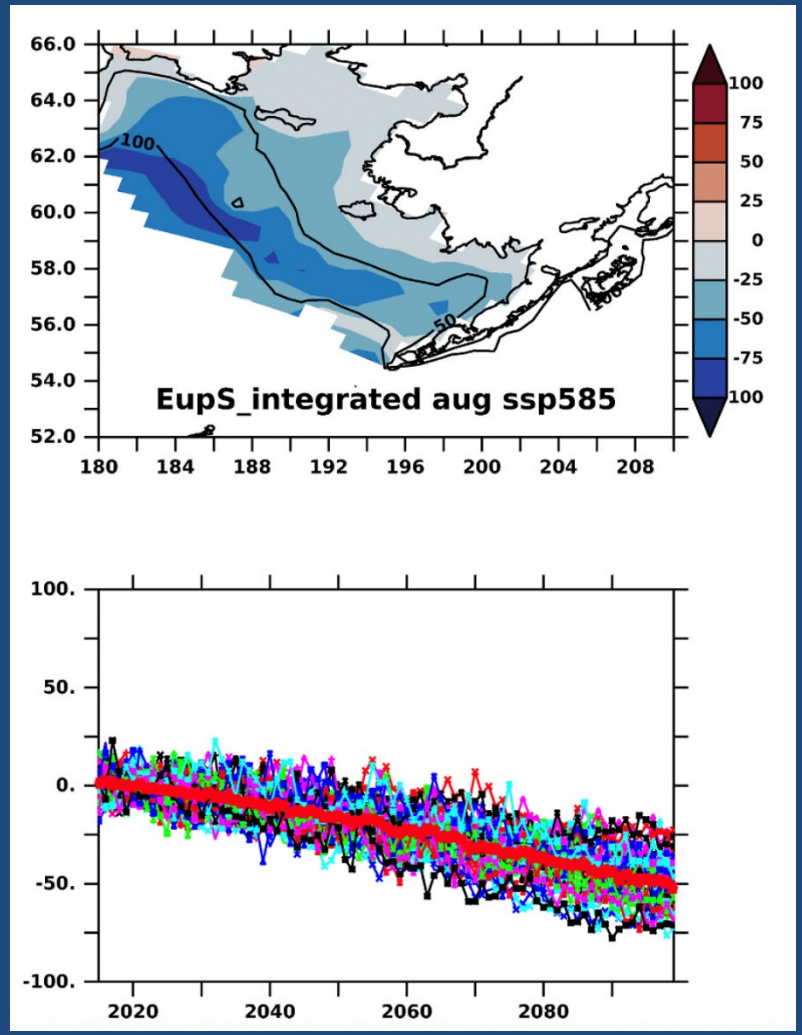
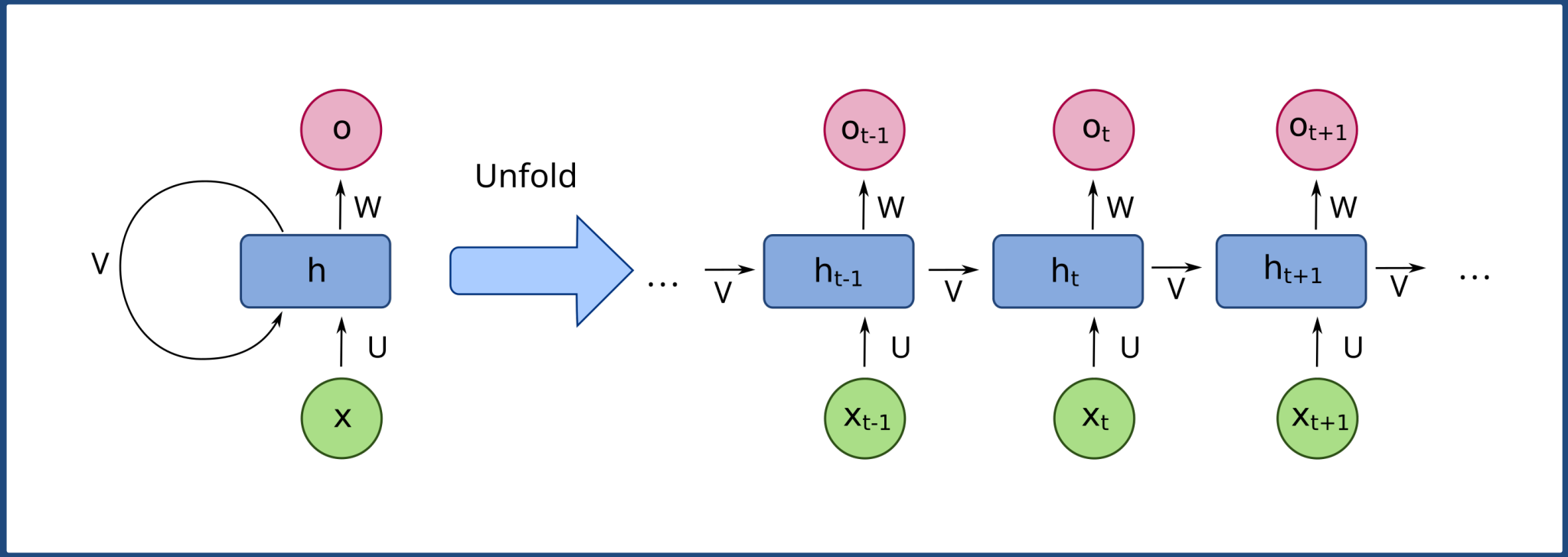


Fig. 21. As in Fig. 19, for July depth-integrated shelf Euphausiids (EupS, mg C m^{-2}).



Hermann et al. 2021, Deep-Sea Res II

EOFs have associated time series. Recurrent Neural Networks (RNNs) can be used to relate sets of time series. Long Short-Term Memory (LSTM) is a type of RNN



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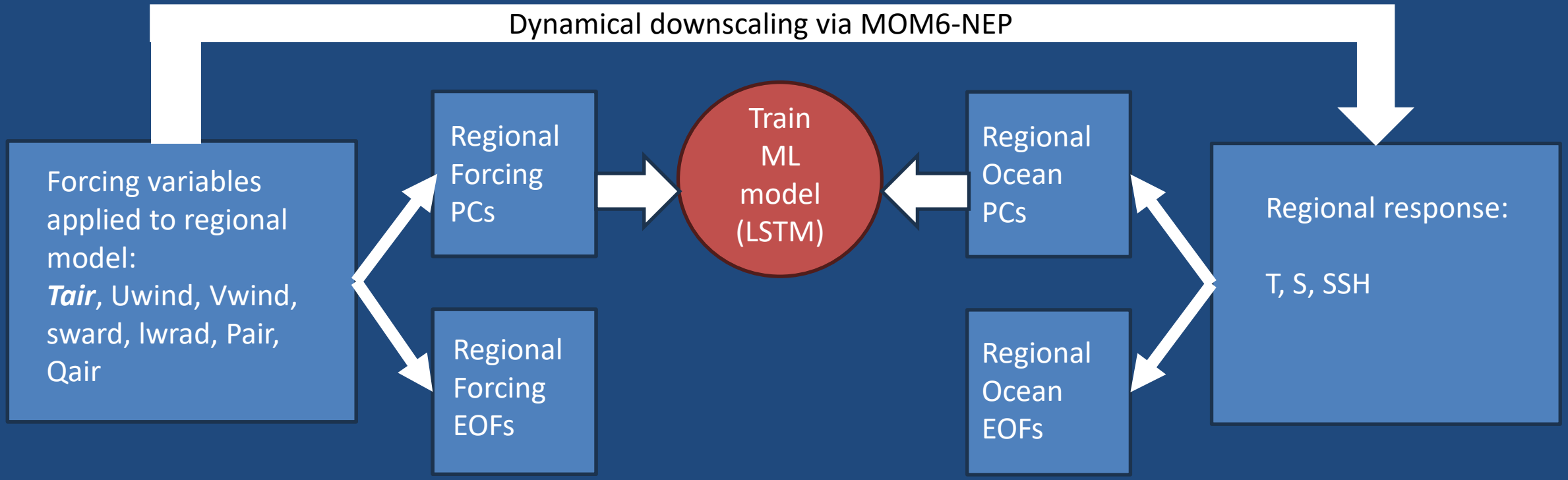
ML method #1: EOFs and Long Short-Term Memory

dynamically downscale, calculate forcing and response EOFs of monthly anomalies, then train the ML model to relate the PCs



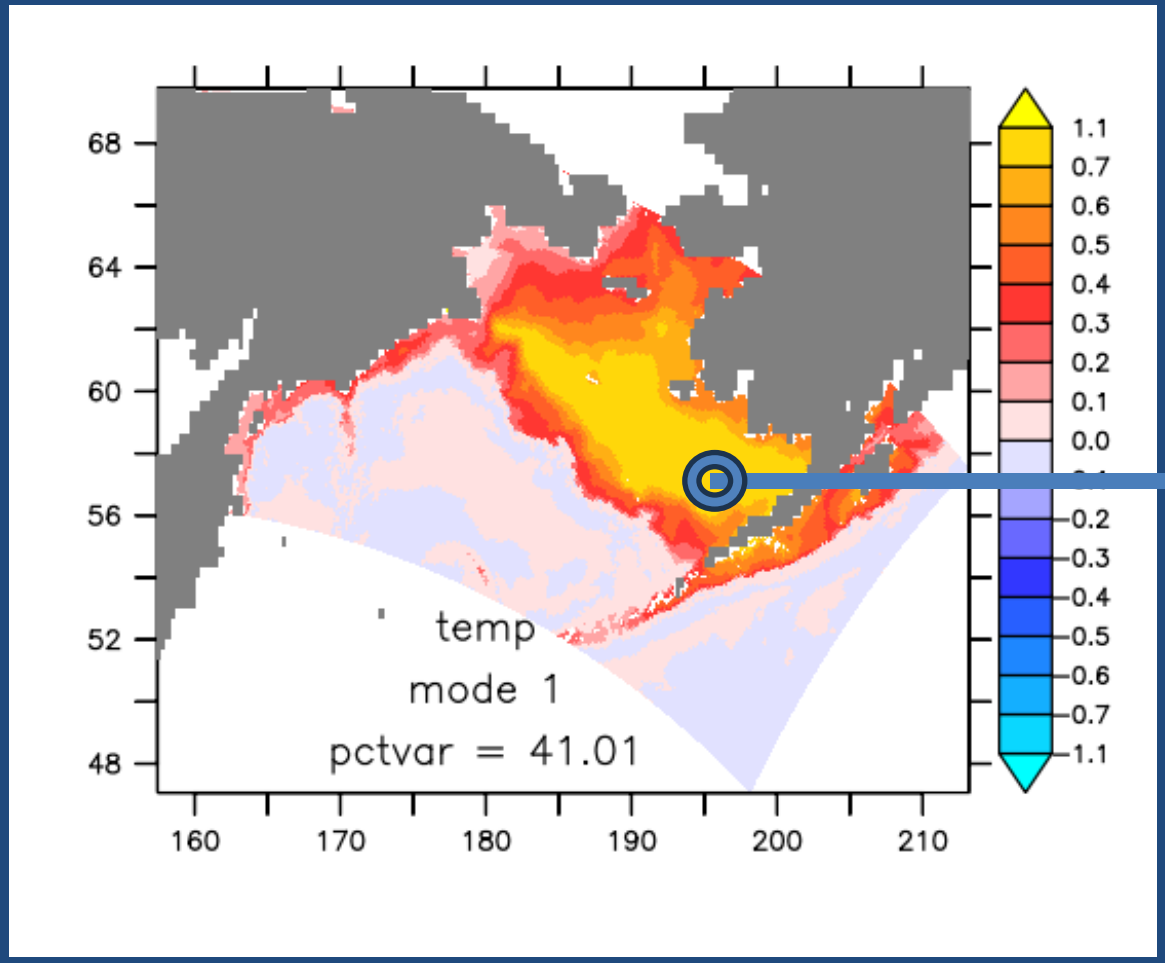
- Include the past 12 months of forcing for training and emulation
- Include top 20 PCs of each forcing (2D) and top 20 PCs of each response variable (3D)
- Use 400 LSTM "neurons" in the LSTM
- Optimization target for each "training session" can be a single PC of a single regional response variable or ***can train all variables/modes simultaneously***

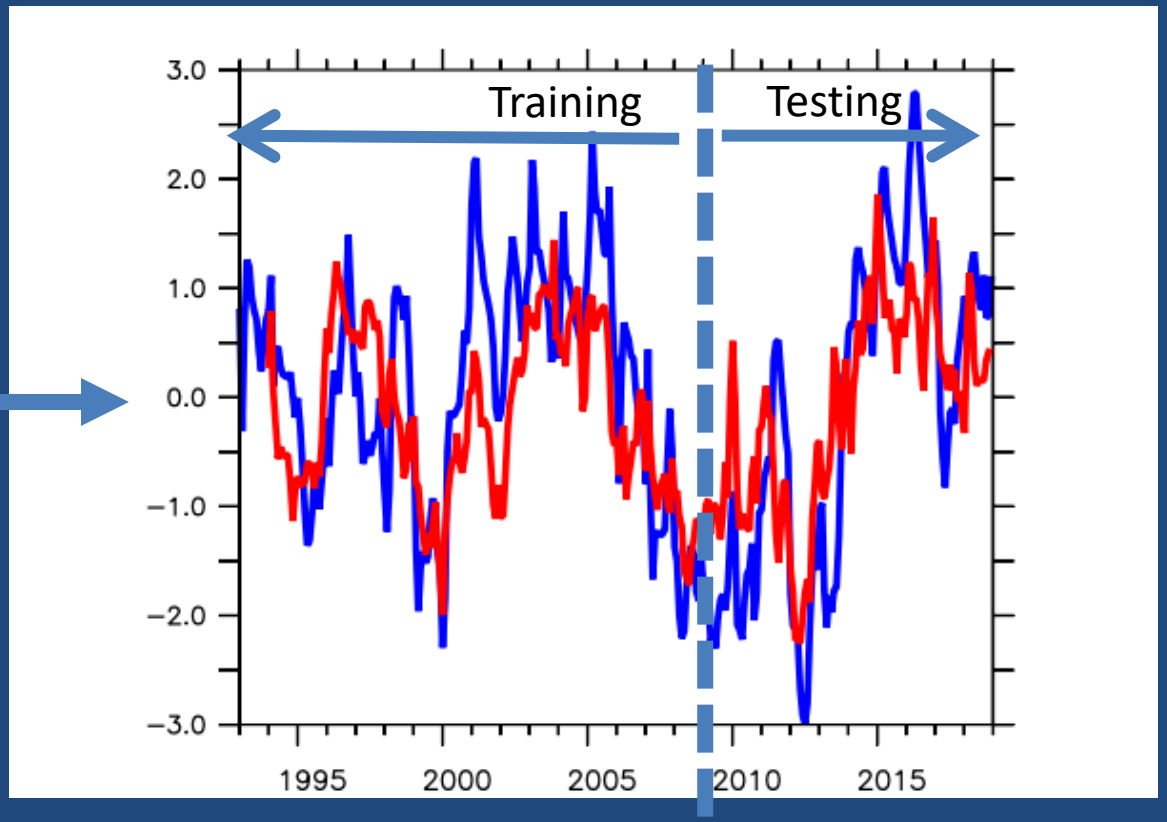
Temperature (deg C) results for the BERING SEA SHELF

Left panel: leading mode ***3D*** EOF of bottom temperatures

Right panel: monthly anomalies of bottom temperature at mid-shelf mooring "M2"

(Blue = MOM6-NEP; Red = Emulator, ***summed over all EOF modes***)

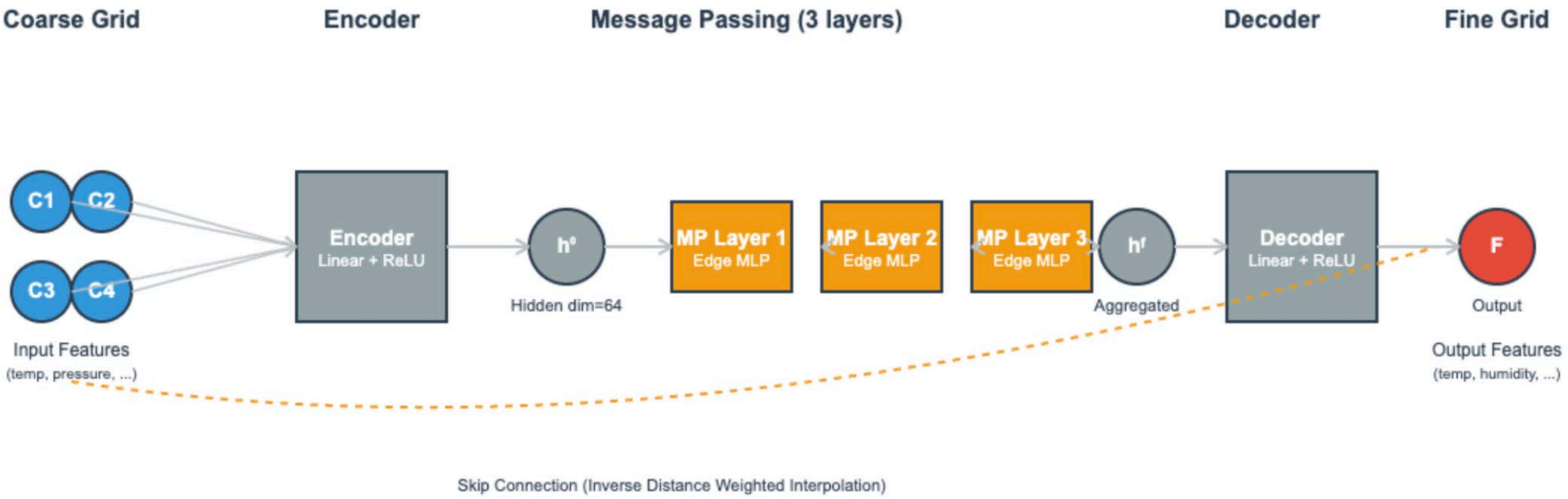




ML method #2: Graph Neural Network (GNN)

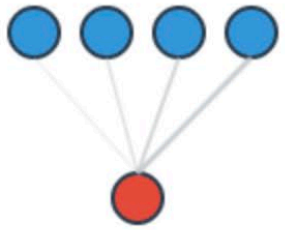
- EOFs focus on broad-scale patterns; GNN is more “local”: each fine node of the ocean model pays the most attention to *nearby* forcing
- Hidden layers focus on relating a set of input features (e.g. air T, winds) to a set of output features (e.g. T, S at various depths)
- Each fine node is treated as a separate “sample” in training
- Can train with ocean values or ocean *tendencies,* which is more analogous to the original dynamical model

GNN Architecture for Spatial Downscaling



Bipartite Graph:

Each fine node connects to
k=4 nearest coarse neighbors



Edge weights: 1/distance

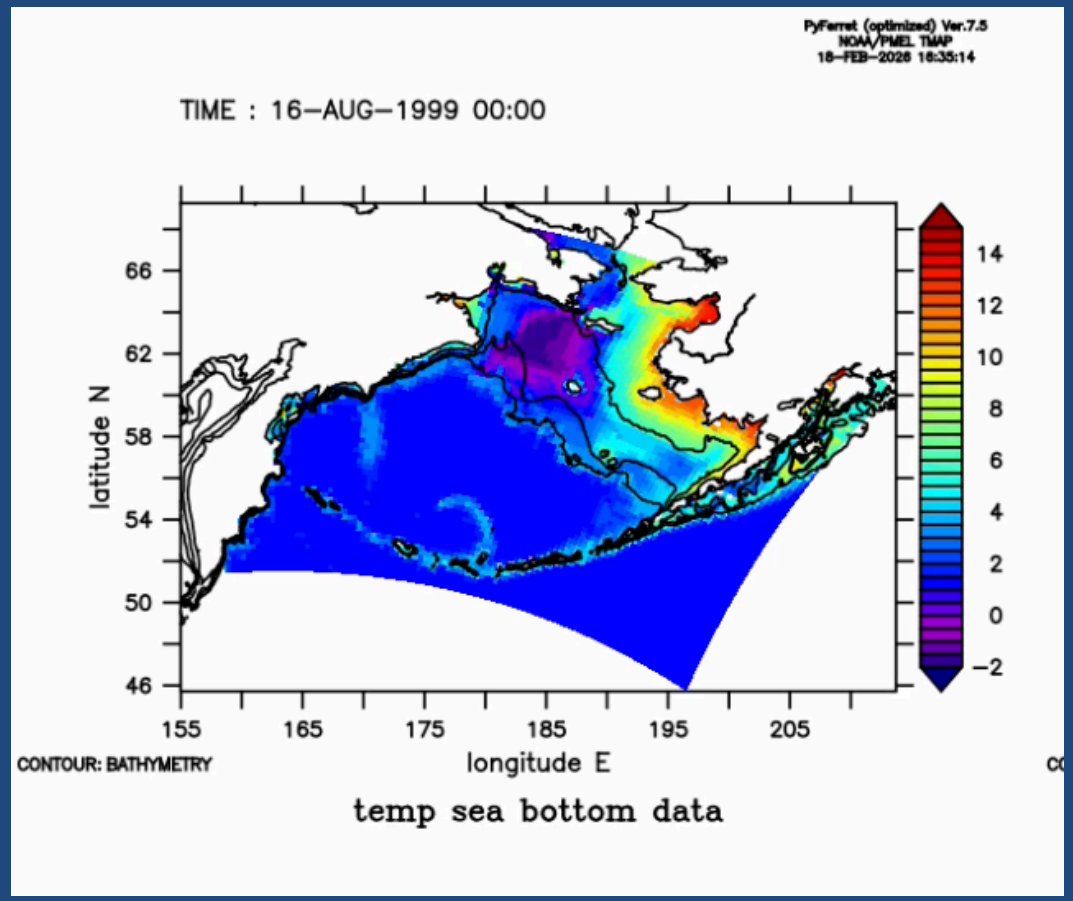
Legend:

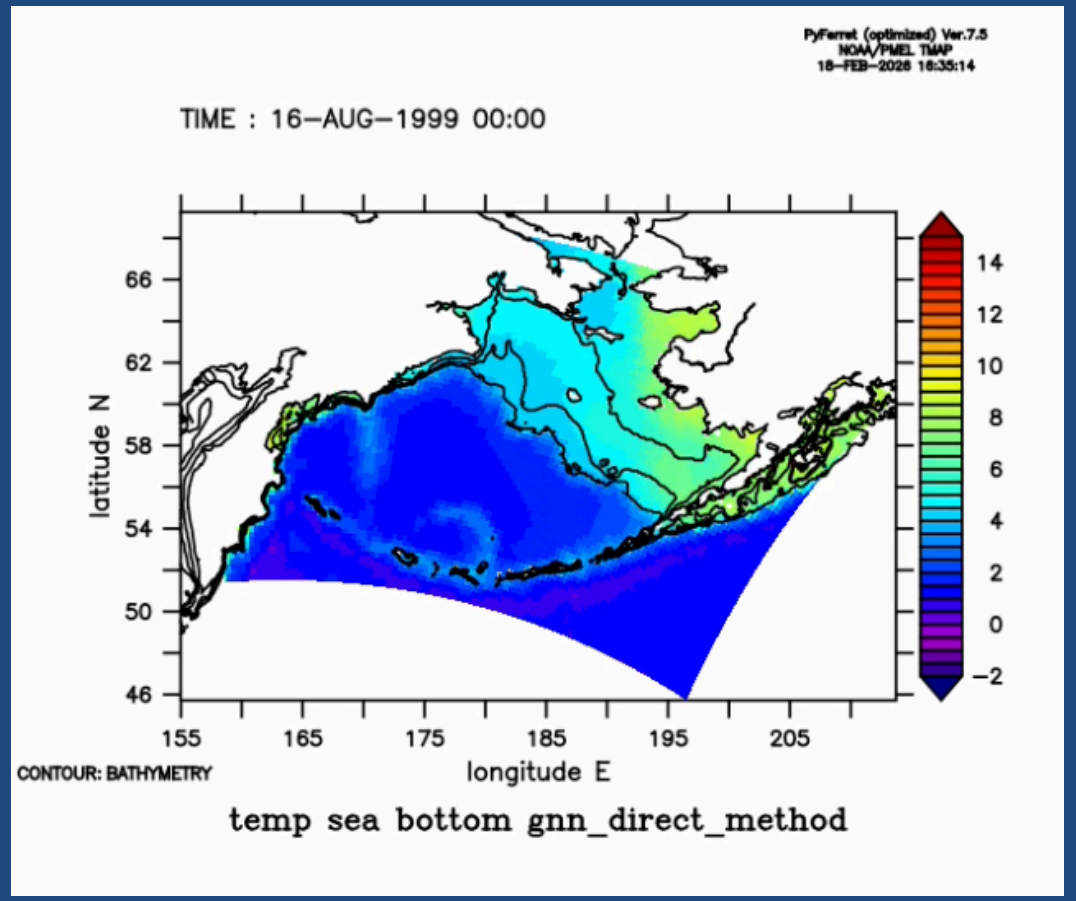
- Coarse node
- Fine node
- Hidden state

Key Features:

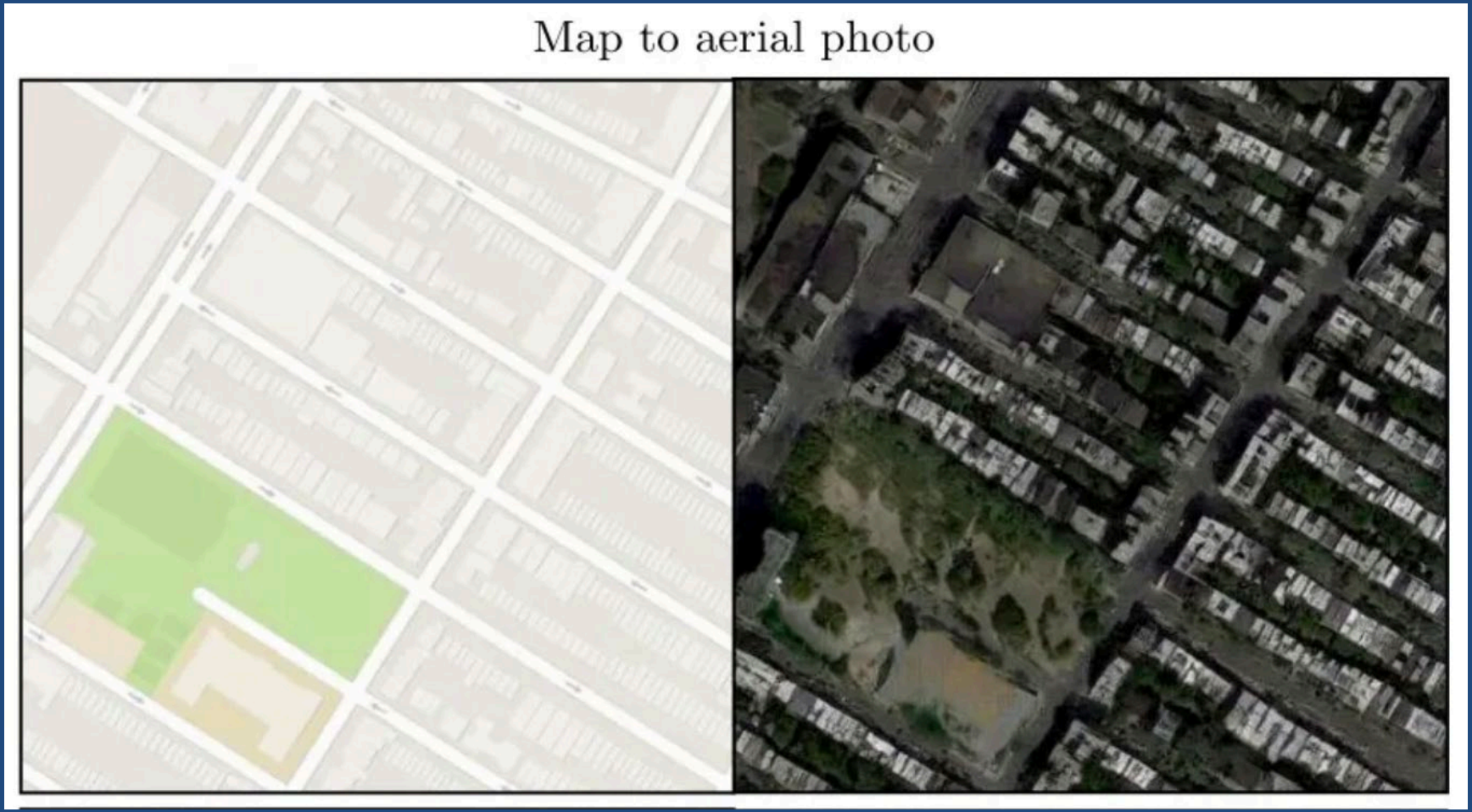
- k=4 nearest neighbors for each fine point
- 3 message passing layers
- Skip connection for residual learning

GNN method reproduced some broad spatial patterns but still failed on the details





ML method #3 (computer vision): Pix2Pix used for ***super resolution*** (image sharpening)



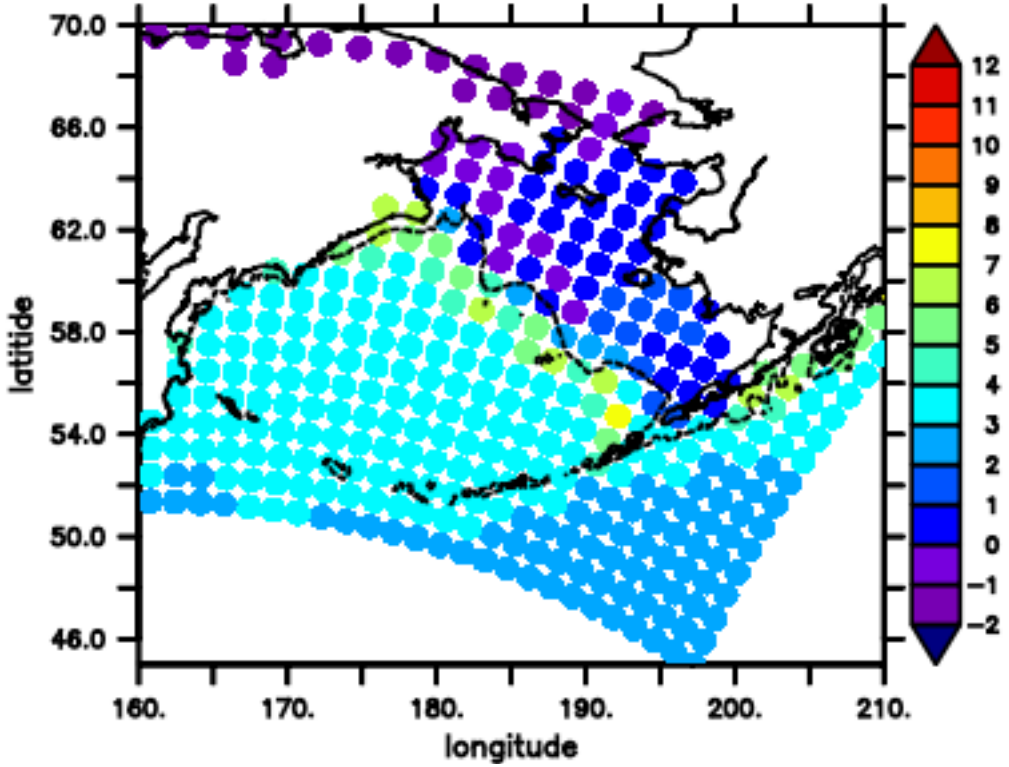
Pix2Pix uses a CNN-based U-Net architecture to generate a fine-scale image from coarse-scale image(s). A PatchGAN discriminator ultimately forces the weights to reproduce both coarse and fine scale patterns



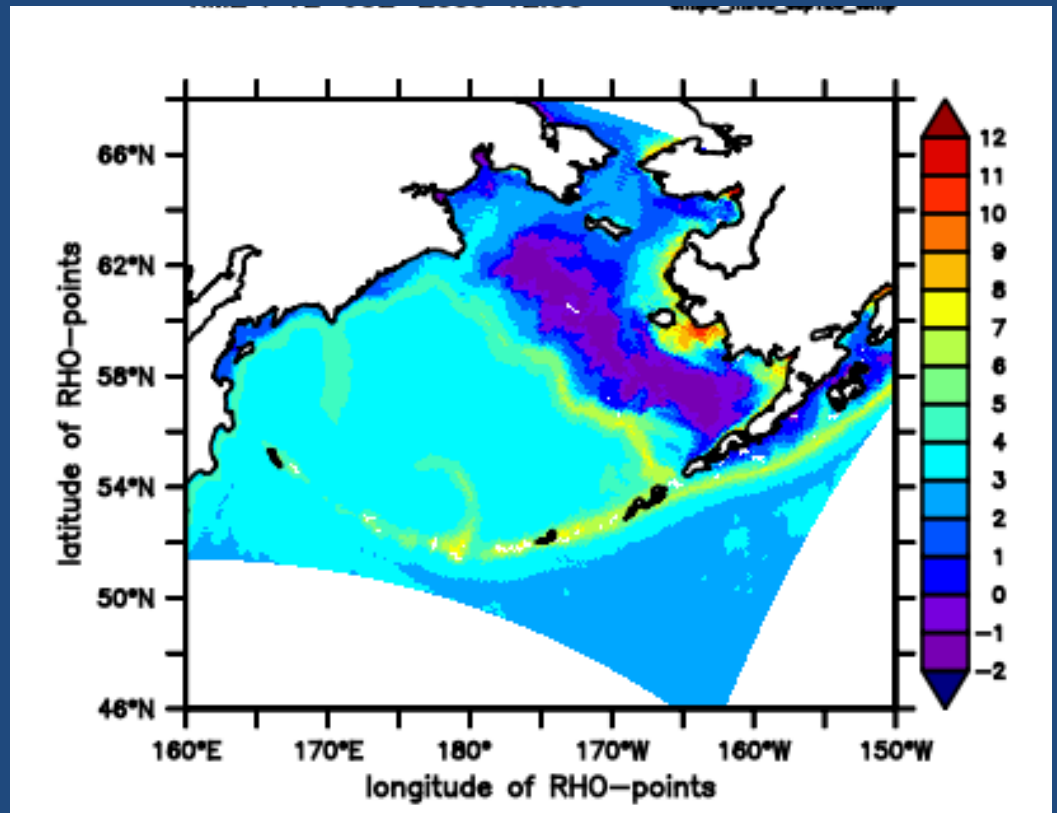
- A succession of levels translate the image(s) into a latent space with reduced spatial dimensions but enhanced number of features, then expands back up to the desired final resolution
- “Skip connections” allow interpolation of the coarse image to the fine image as a starting point for the optimization

From: Rampal N, Hobeichi S, Gibson PB, et al. Enhancing Regional Climate Downscaling through Advances in Machine Learning. *Artif. Intell. Earth Syst.. 2024;3(2): e 230066. doi:10.1175/AIES-D-23-0066.1*

Train the network to translate coarsely resolved bottom temperatures (from CMIP6) into finely resolved bottom temperatures (from ACLIM ROMS dynamical downscaling). Train with GFDL and MIROC ssp585 results; Validate using ssp126 results



CMIP6 MIROC (100 km spacing)

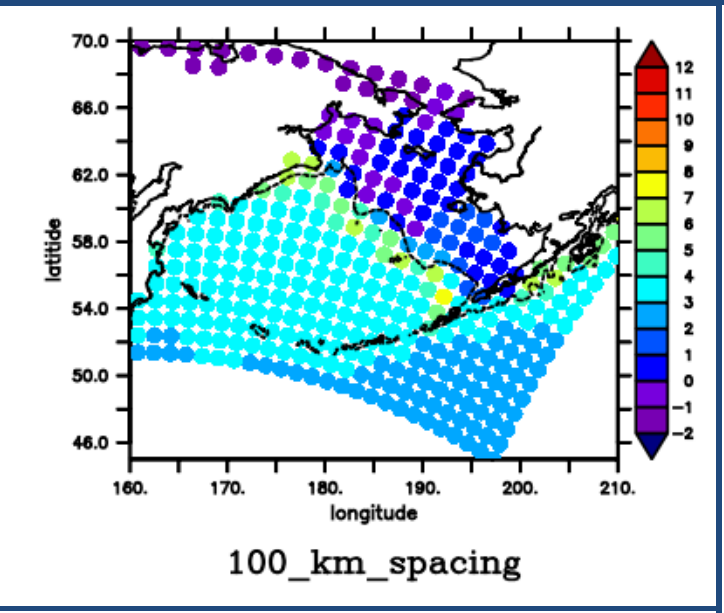


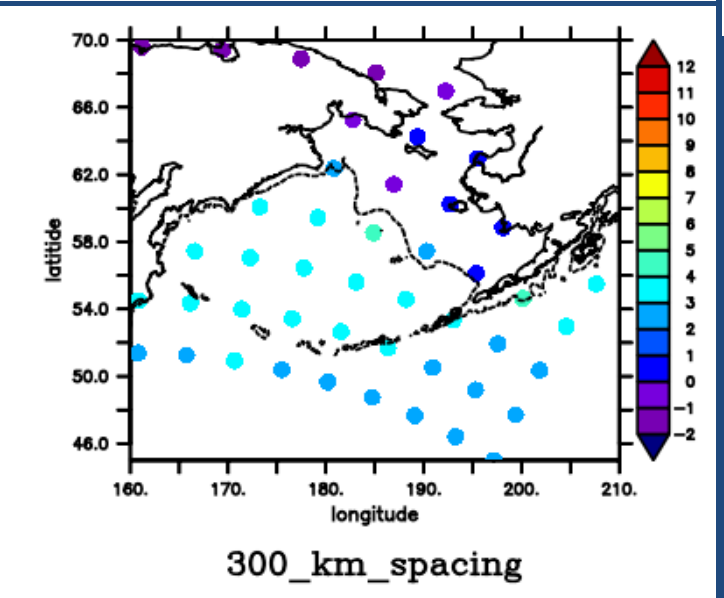
ROMS (10 km spacing)

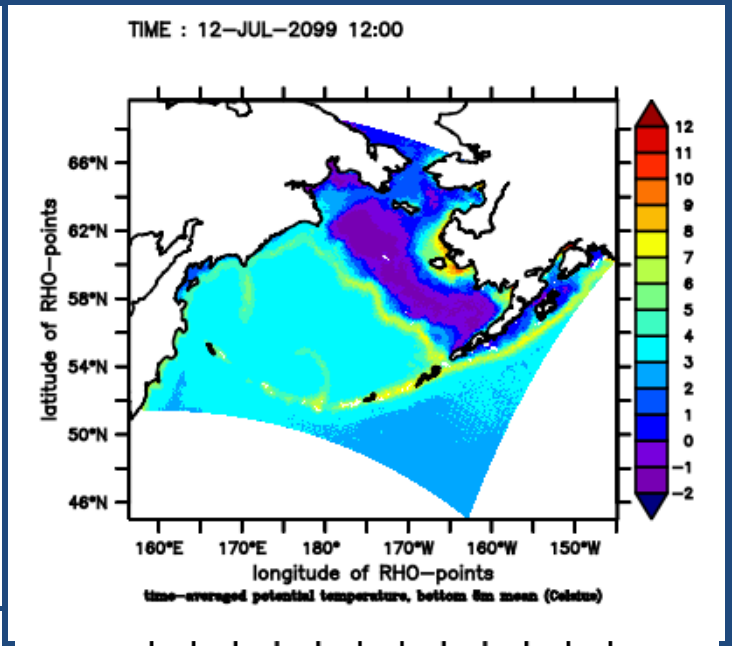
Pix2Pix emulator captures most spatial details…

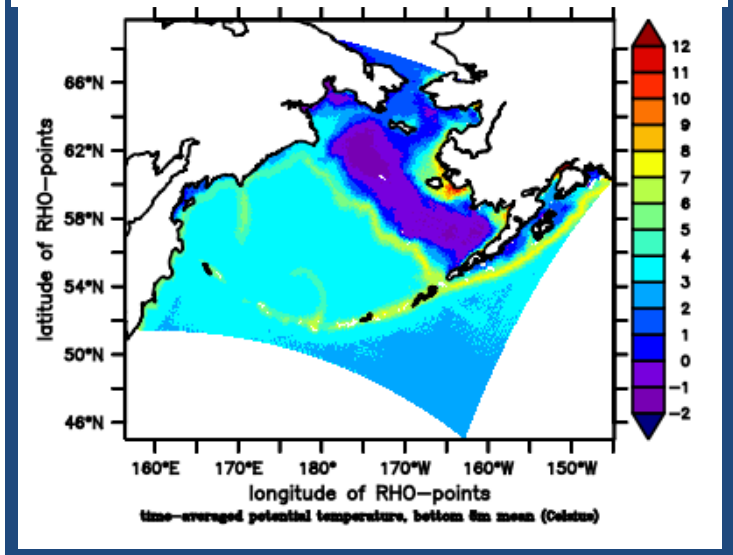


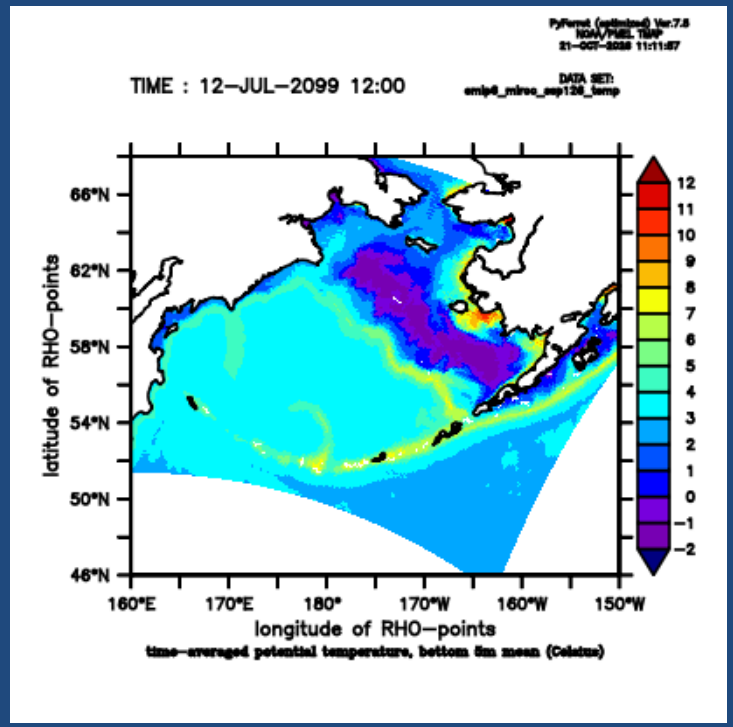
and works well even with lower resolution input!



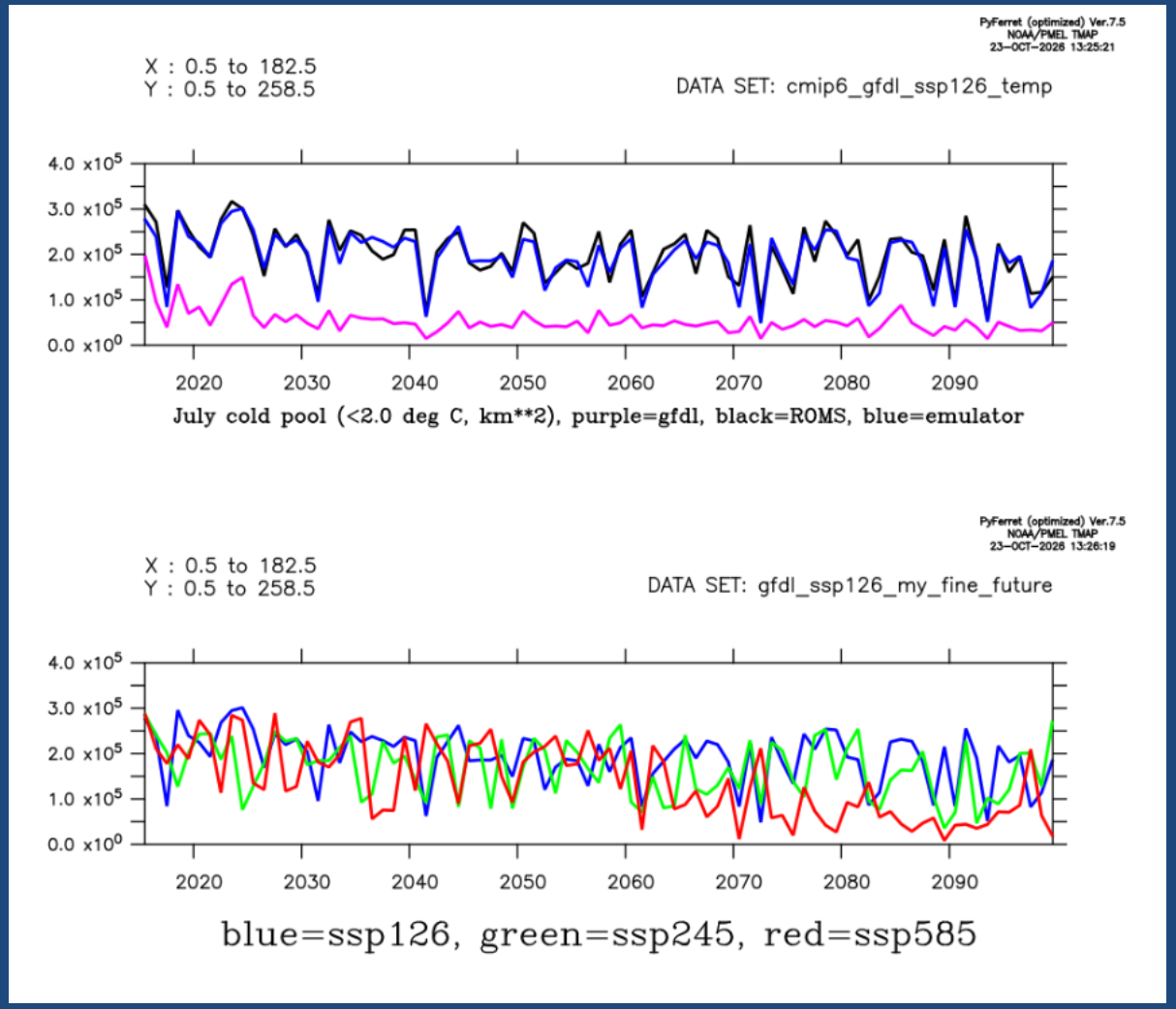


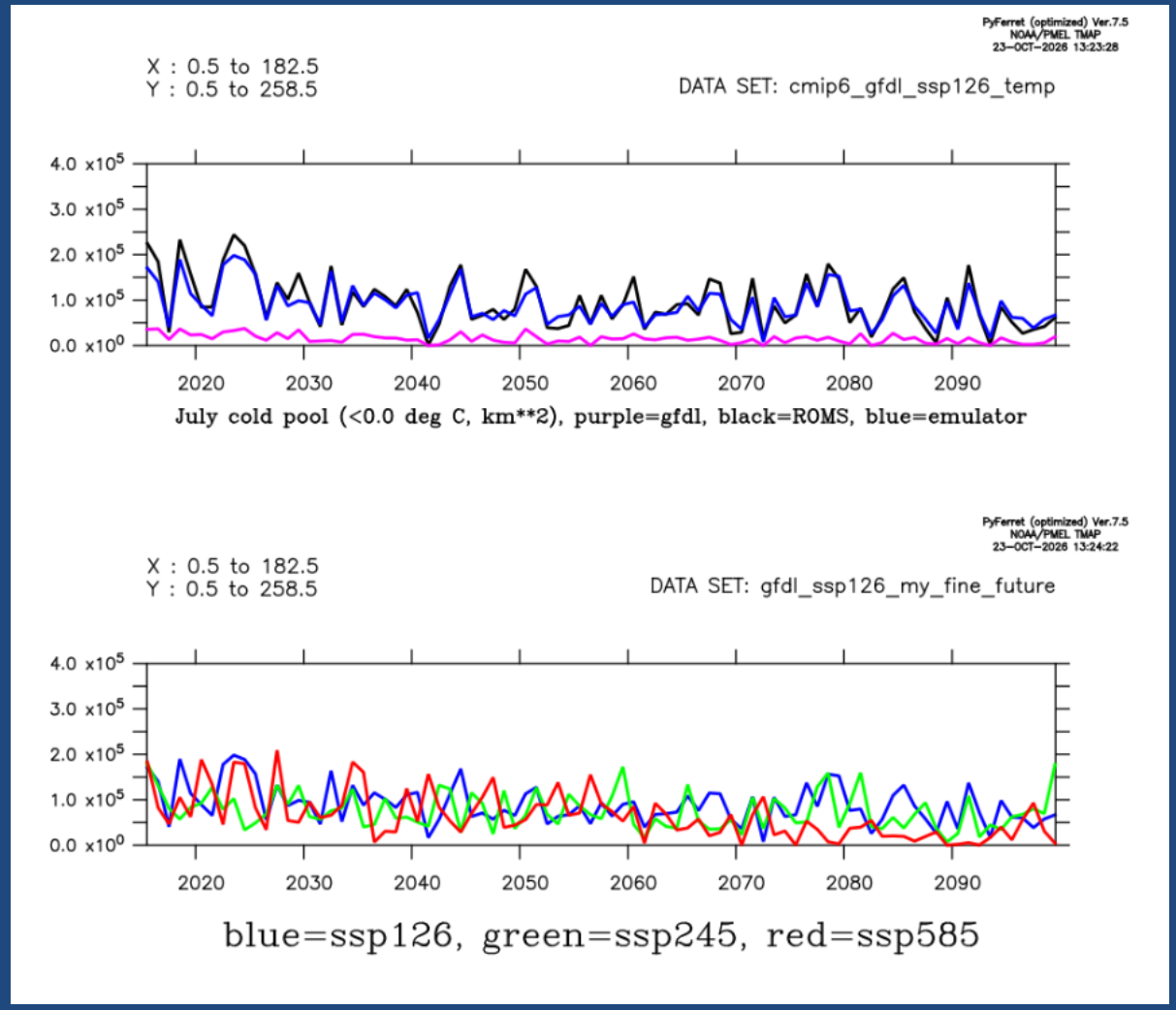






This emulator allows us to rapidly expand our ssp126, ssp585 ensemble. Here we have added ssp245 to July projections of the Bering Sea cold pool





Conclusions and next steps

- Machine Learning methods show increasing promise as ***fast*** (~10^6 x faster) downscaling model emulators which capture spatial detail
- EOF/LSTM/GNN methods each captured some broad-scale patterns but all struggled with capturing details
- A CNN-based image sharpening method (U-Net CGAN; Pix2Pix) did well at both broad-scale patterns and details
- Atmospheric science community is now using CNN for downscaling
- Next steps:
  - *Experiment with multivariate input (e.g. winds, SST)*
  - *Experiment with multivariate output (e.g. zooplankton)*

How this is relevant to full “digital twins”

- It is difficult to meld multiple complex fish management, biogeochemical and food web models together with mutual feedbacks (e.g. top-down and bottom-up effects)
- If we can develop simple and robust *emulators* of each of those complex models, we could *couple the emulators* to achieve a holistic digital twin
- Robust coupled emulators would allow rapid exploration of management strategies in the virtual world, and rapid assessment of optimal sampling strategies.