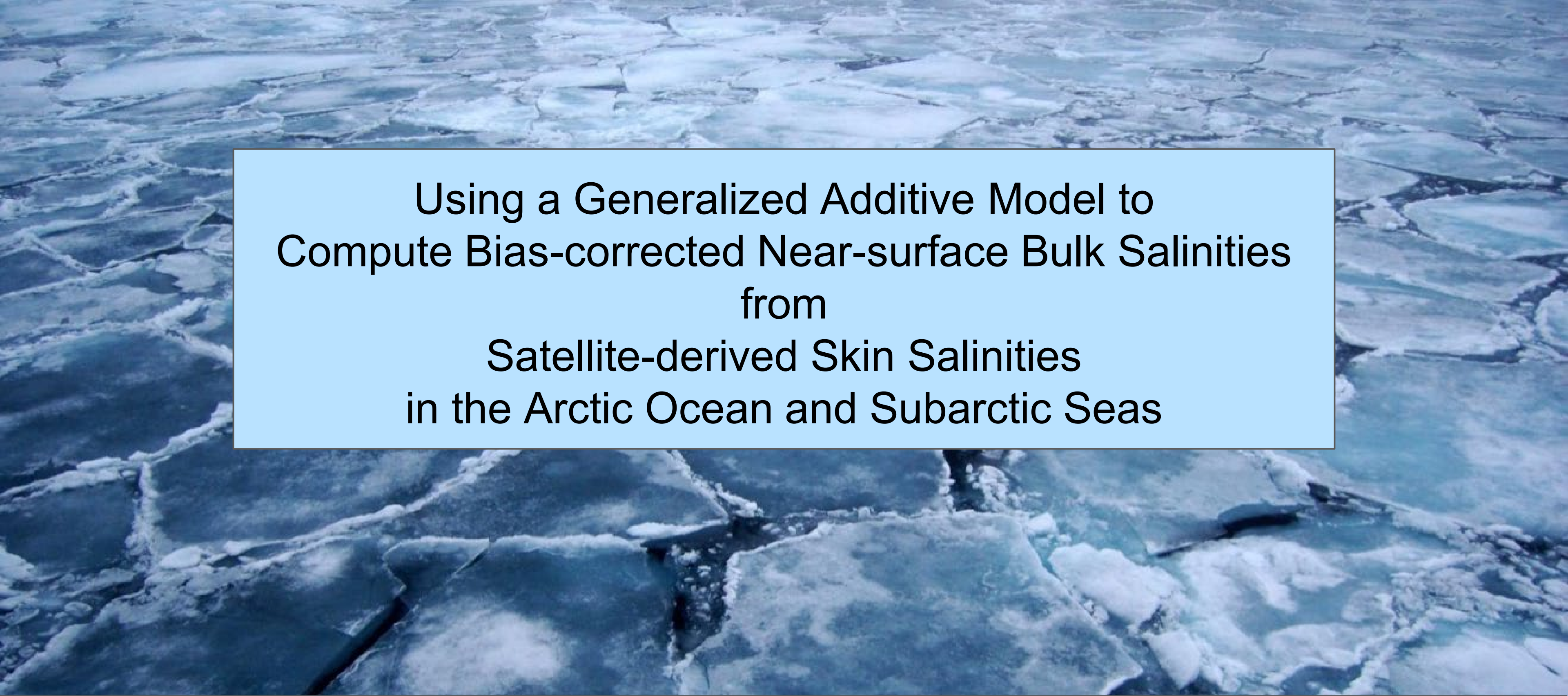

Using a Generalized Additive Model to Compute Bias-corrected Near-surface Bulk Salinities from Satellite-derived Skin Salinities in the Arctic Ocean and Subarctic Seas

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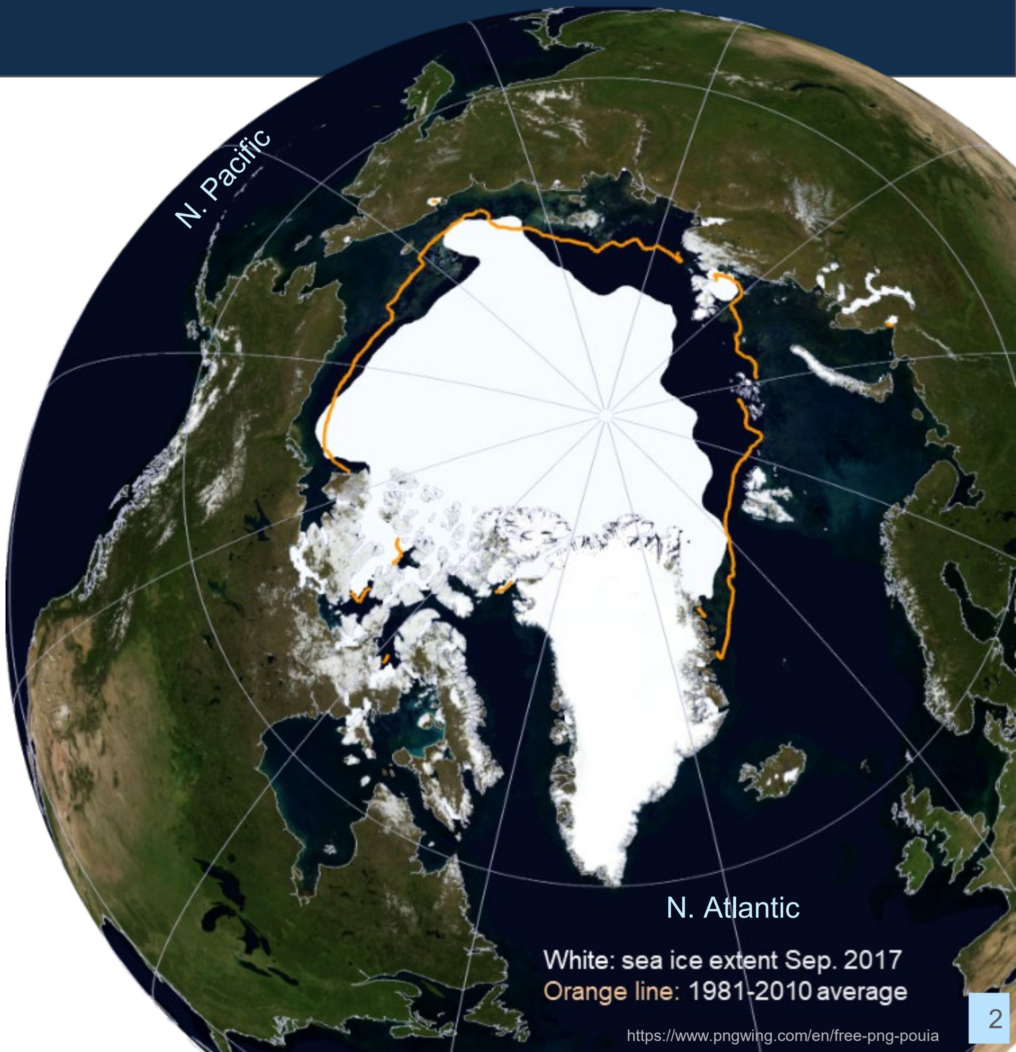
The Arctic Ocean

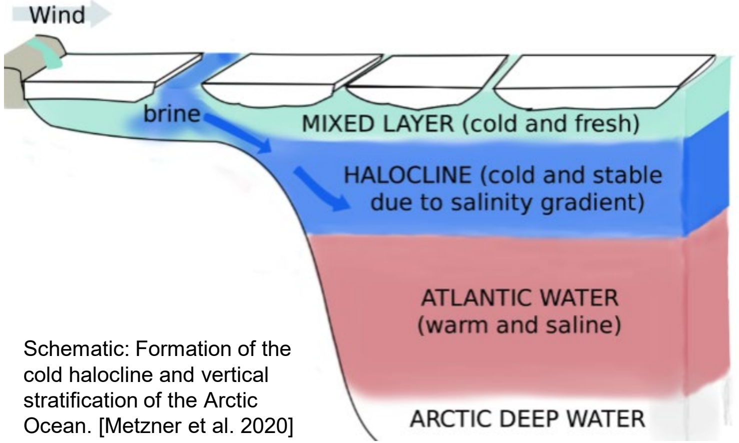
- Important seasonal and perennial global ice formation, with implications towards global climate
- Warming rate: ~3.8 times the global average
- Min sea ice extent shrinking: ~13% per decade (1979-present)
- Arctic summers forecasted to be “ice-free” as early as 2035
- Freshwater (low-salinity anomalies) exported to N. Atlantic impacts global-scale ocean circulation AMOC



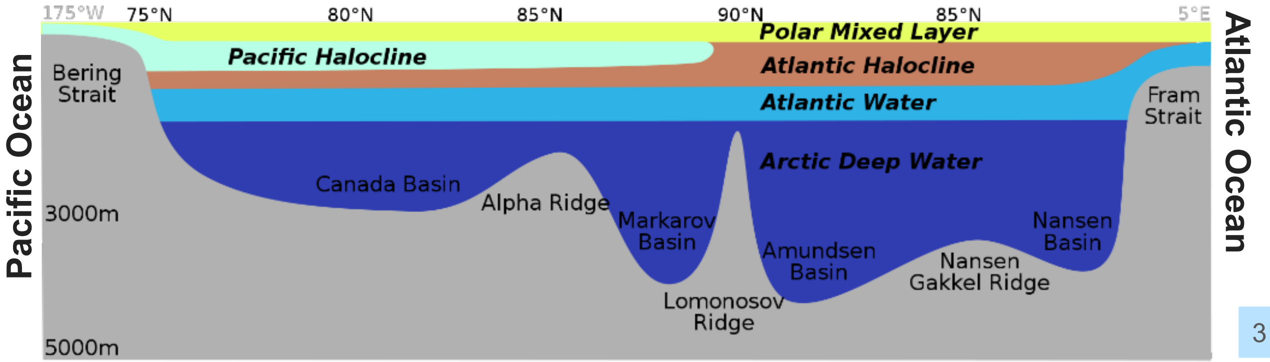
https://www.pngwing.com/en/free-png-pouia

Salinity in the Arctic Ocean

- **Salinity** governs the density structure of the quasi-isothermal Arctic Ocean
  - Influences ocean dynamics (e.g., circulation, vertical mixing), sea ice formation/melt, and ecosystem health
- Polar vertical stratification and overturning regulated by:
  - Saline water (Atlantic inflow, sea-ice growth)
  - Freshwater (river input, sea-ice melt)
- Accurate salinity measurements enable understanding climate-related changes and enhanced model representation/prediction of the Arctic's state and dynamics



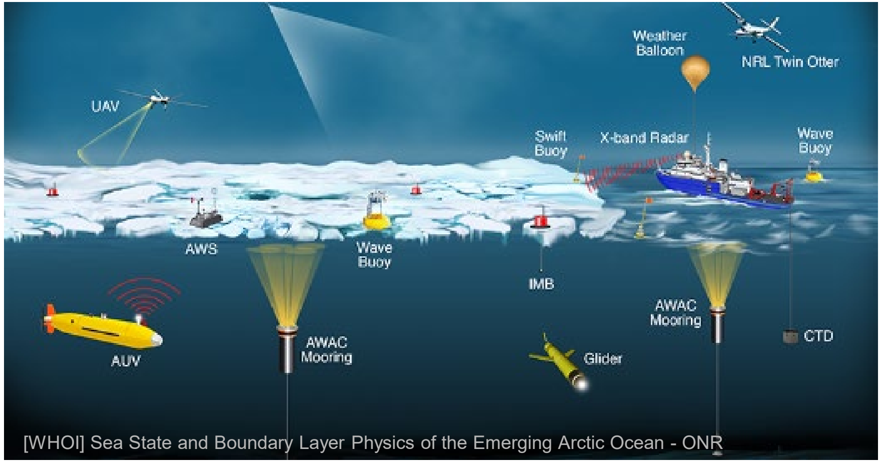
Schematic: Formation of the cold halocline and vertical stratification of the Arctic Ocean. [Metzner et al. 2020]



Distribution of the major water mass in the Arctic Ocean along a vertical section from Bering Strait over the geographic North Pole to Fram Strait. As the stratification is stable, deeper water masses are denser than the layers above. [Gonçalves-Araujo, Rafael (2016)]

Arctic Observations

In situ Measurements



[WHOI] Sea State and Boundary Layer Physics of the Emerging Arctic Ocean - ONR

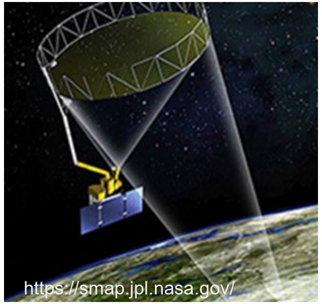
Pros:

- Direct measurement
- Subsurface ocean

Cons:

- Non-uniform spatial and temporal distribution
- Constrained by environmental conditions and remote locations

Satellite Missions


https://smap.jpl.nasa.gov/

Soil Moisture Active Passive (SMAP)


http://www.esa.int/SPECIALS/smos/

Soil Moisture and Ocean Salinity (SMOS)

Also: Aquarius (ended 2015) and CIMR (future mission)

Pros:

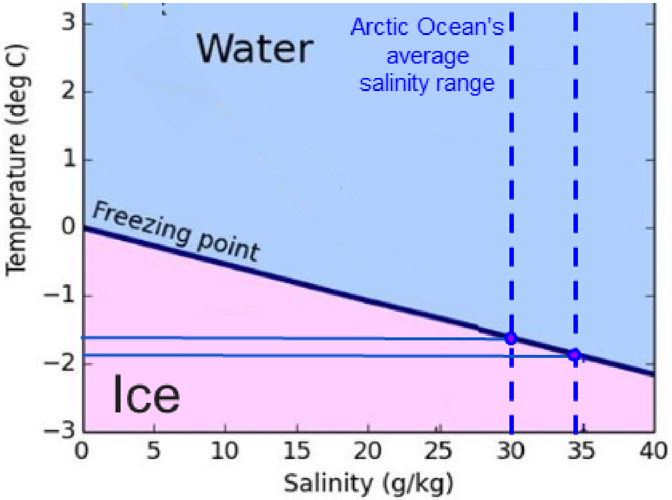
- Global coverage
- Uniform temporal coverage

Cons:

- Indirect measurements
- Restricted to sea surface (skin) in open water
- Diverse sources of errors:
  - Radiometer
  - Antenna
  - System pointing
  - Solar & Galactic noise
  - Ionosphere
  - Atmosphere
  - Rain (total liquid water)
  - Sea Surface Roughness
  - Sea surface temperature
  - Land/Ice contamination

Satellite Salinity Retrievals

- The relationship between conductivity and salinity allows for the remote sensing of salinity
- SMOS/SMAP at a frequency band 1.4 Ghz ("L-band")
- Brightness temperature (T_B) can be related to the surface seawater's temperature and dielectric coefficient.



Brightness Temperature: T_B

$$T_B = e\,T$$

e = Emissivity

T = Physical Temperature

$$e = 1 - R^2$$

$$= 1 - \left|\frac{1-\sqrt{\varepsilon}}{1+\sqrt{\varepsilon}}\right|^2 \quad \text{(normal incidence)}$$

Relative Dielectric Constant: ε(f,S,T)

$$\varepsilon = \varepsilon_\infty + \underbrace{\frac{\varepsilon_s - \varepsilon_1}{1 + j\omega\tau_1} + \frac{\varepsilon_1 - \varepsilon_\infty}{1 + j\omega\tau_2}}_{\text{Response of molecular dipole; One term at low frequency with additional terms at higher frequency}} - j\frac{\sigma}{\omega\varepsilon_o}$$

Response of molecular dipole; One term at low frequency with additional terms at higher frequency

Effect of current (moving ions)

ε(f,S,T)

S - Salinity

T - Temperature

f - electromagnetic frequency

Research Outlook

Research Goal

Develop a robust methodology for a bias-corrected, satellite-derived near-surface ("bulk") salinity product in the Arctic region to enable exploiting satellite measurements at high-latitudes for numerical modeling

Objectives

1. Improve the accuracy of bulk salinity predictions by leveraging in situ data and a machine-learning-based approach (Generalized Additive Model; GAM)

2. Develop a comprehensive GAM calibration process, addressing biases and ensuring robust generalization to diverse marine conditions

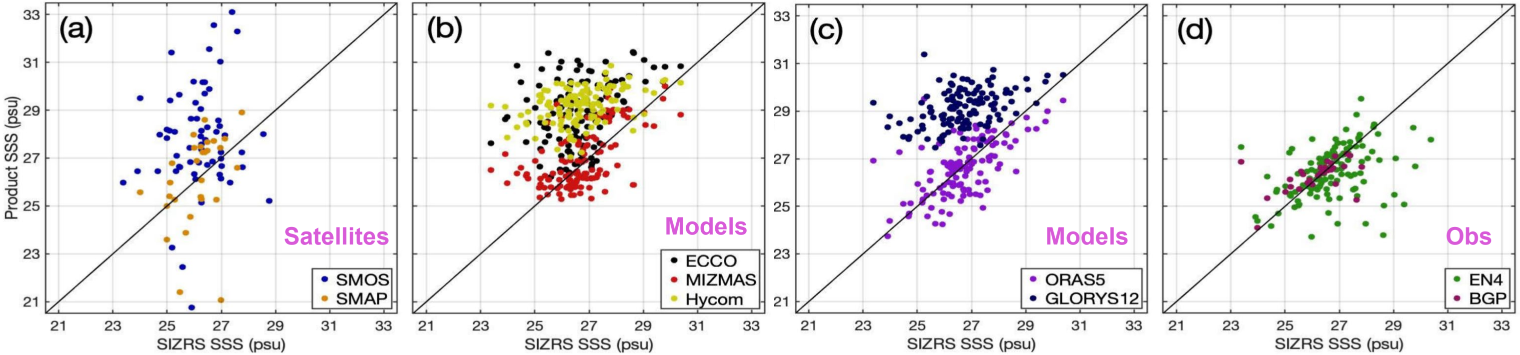
3. Enhance the methodology for bias-corrected bulk salinity, contributing to more reliable and precise predictions

4. Generate a gridded bulk salinity product for integration into ocean models, facilitating data assimilation and operational applications

Research Outlook

Scientific Impact

- Advance understanding of the intricate relationships between SSS, ocean state & dynamics, biogeochemical factors, and climate trends in the Arctic
- Provide a methodology to improve the representativeness and bias-corrections of satellite salinity measurements at high-latitudes
- Increase the usability of satellite SSS data, improving temporal and spatial coverage while enhancing data assimilation in ocean models.
- Facilitate more accurate forecasting of SSS, aiding in climate research and contributing to informed decision-making in the face of ongoing Arctic environmental changes.

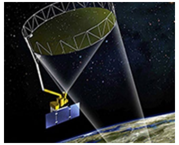


Scatter diagrams of Arctic Ocean (Beaufort Sea) sea surface salinity (SSS) of Seasonal Ice Zone Reconnaissance Surveys (SIZRS; 2 m) to (**a**) satellite missions, and of SIZRS (5 m) to (**b**,**c**) ocean model simulations, and (**d**) in–situ observations during SIZRS AXCTD drops. Black line signifies equivalent salinity values (psu). [Hall et al., 2022]

Data

Satellite Sea Surface Salinity

ESA's SMOS L2	06/2010 - 12/2022
JPL's SMAP L2	04/2015 - 12/2022


SMAP: https://smap.jpl.nasa.gov/


SMOS; http://www.esa.int/

In Situ Measurements

SUMD	Surface Underway Marine Database (NOAA/NCEI)	06/01/2010 - 12/31/2022
WOD	World Ocean Database (NOAA/NCEI)	06/01/2010 - 09/15/2022
MEOP	Marine Mammals Exploring the Oceans Pole to Pole	06/01/2010 - 05/09/2018
OMG	Oceans Melting Greenland (NASA)	07/07/2016 - 09/16/2021
MOSAiC	Multidisciplinary drifting Observatory for the Study of Arctic Climate (NOAA/PSL)	07/01/2020 - 07/28/2020
SD	Saildrone - Arctic 2019 Expedition (NOAA, NASA)	05/18/2019 - 10/08/2019
SASSIE	Salinity and Stratification at the Sea Ice Edge (NASA)	08/11/2022 - 10/05/2022

OAFlux Parameters

WHOI OAFlux Project: Objectively Analyzed air-sea Fluxes (OAFlux) for the Global Oceans

https://oaflux.whoi.edu/data-access/

Latent Heat Flux (Q_{LH}); Sensible Heat Flux (Q_{SH}); Wind speed at 10m (U); Specific air humidity at 2m (q_a); Air Temperature at 2m (T_a); Sea Surface Temperature (T_s); Moisture flux/ocean evaporation (Evp)

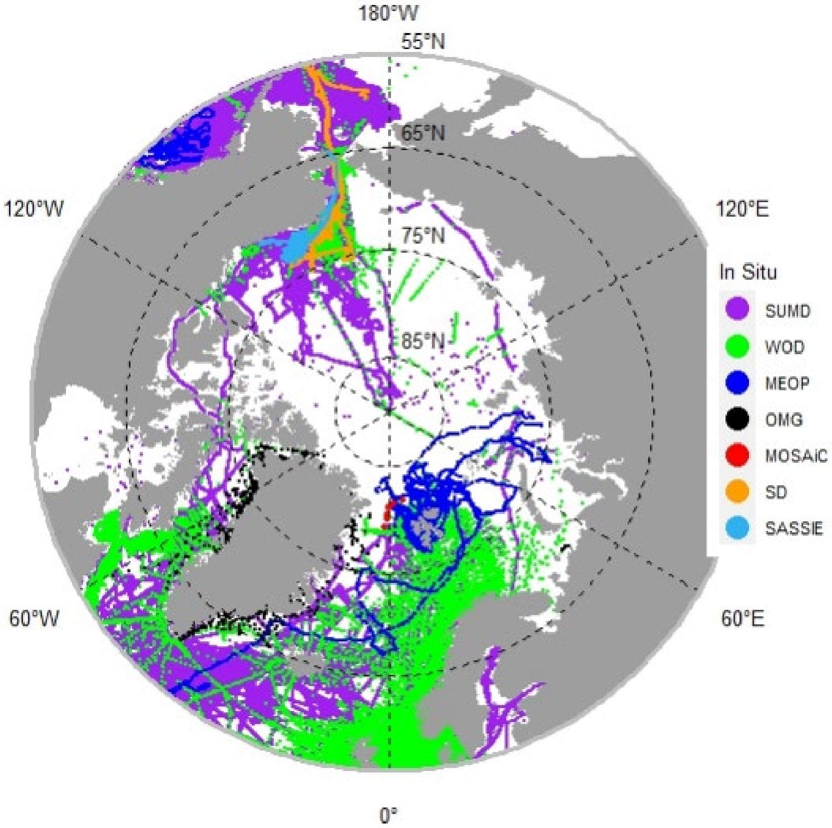


Figure. Arctic Ocean with in situ measurement locations between 0-5 m and June 2010 - Dec. 2022.

Salinity Observations

Satellites

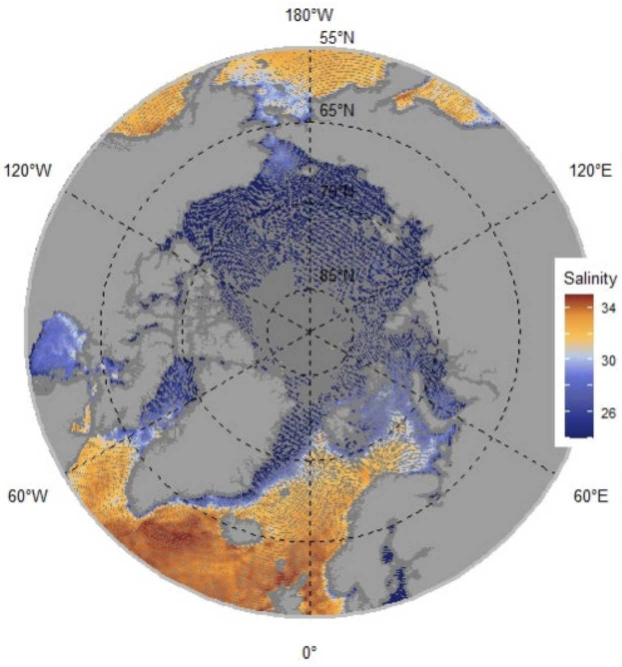


Figure. ESA SMOS salinity [psu] average during June 2010 - Dec. 2022.

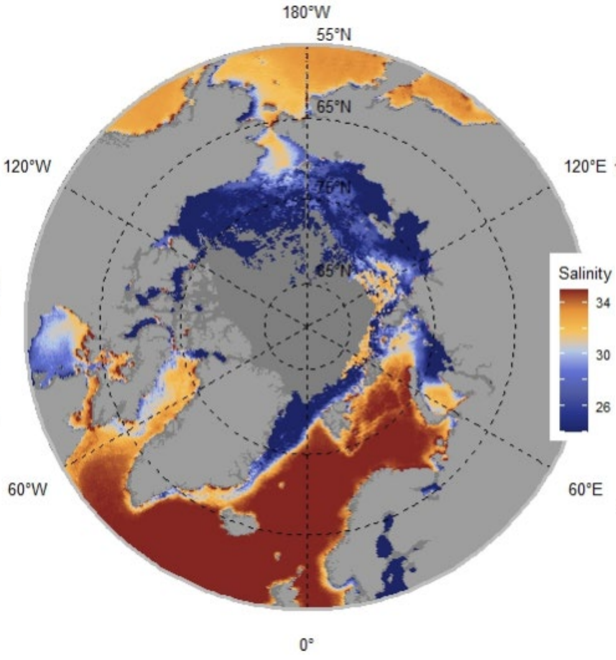


Figure. NASA's SMAP salinity [psu] average during April 2015 - Dec. 2022.

In situ

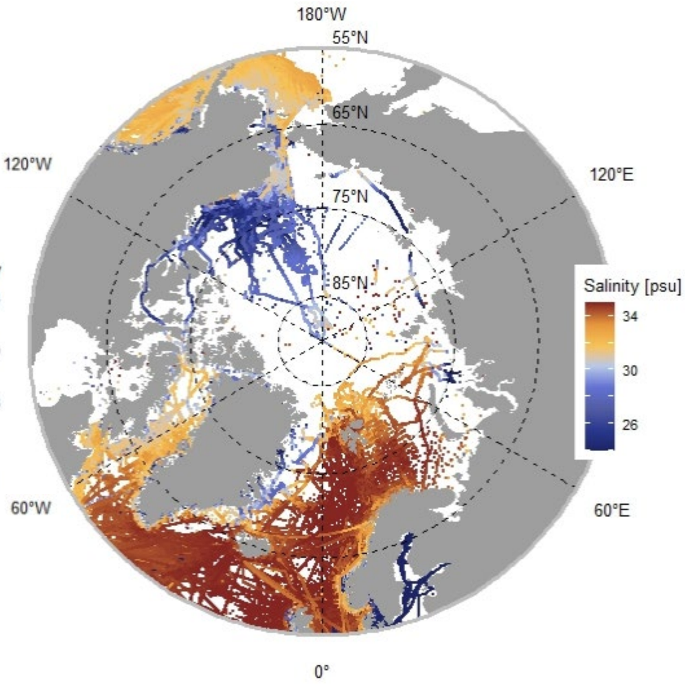
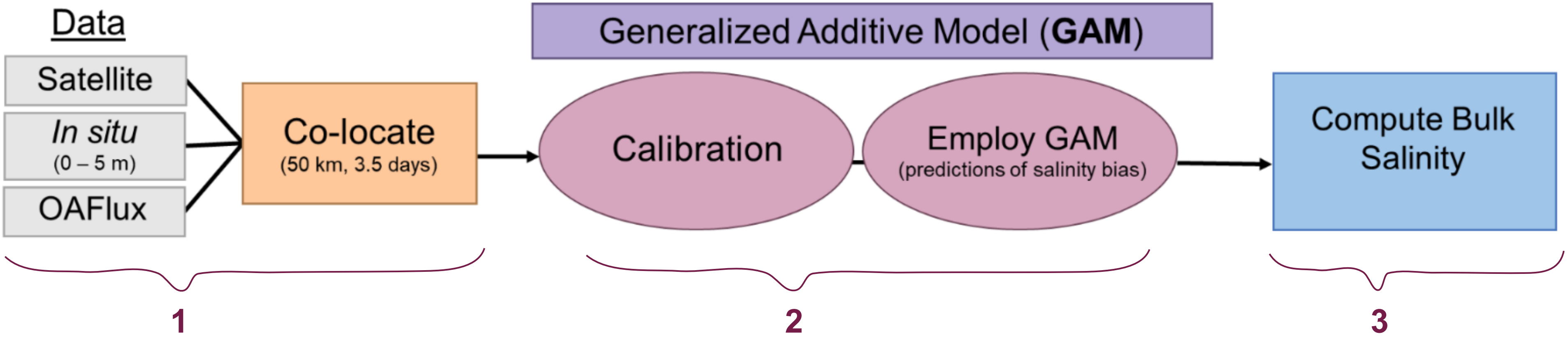


Figure. In situ (0-5m) salinity [psu] average during June 2010 - Dec. 2022.

Methodology



1. Initial data (satellite, in situ, and OAFlux parameters) are co-located within 50 km and 3.5 days
    > In situ data: ~80% train the GAM, ~20% cross-validate output

1. Machine-learning-based approach, GAM, predicts salinity bias to original satellite observations

2. Output: bias-corrected near-surface bulk salinity product

GAM: Generalized Additive Model

Why GAM?

- Offers a flexible and interpretable framework that accommodates the complex and non-linear relationships inherent in the dynamic marine environment
- Has a history rooted in statistical regression techniques: similar to a linear regression model, but allows for the non-linear combination of variables to estimate our target variable (salinity bias)
- Predictions are made by using predictors as inputs. Aims to balance salinity bias and variance of its predictions through a regularization term. This regularization term prevents the machine-learning method from over-fitting to a particular training dataset
- Cross-validation is done to guarantee that the GAM does not overfit to the training data and to verify the predictions are accurate

Using the GAM

- Machine-learning algorithm to predict salinity bias between in situ and satellite data between 0 - 5 meters
- Incorporates smooth functions and linear components: captures nuanced spatiotemporal patterns associated with SSS, considering factors such as OAFluxes, systematic satellite errors, and geographical coordinates

GAM: Calibration Process

<u>At each location and time:</u>

A) Calculate thermodynamic properties and empirical coefficient ("λ"):

$$\lambda = \left\{1 + \left[\frac{16 \times (Q_{sens} + Q_{lat} + (0.99 \times 5.67e^{-8} \times (\mathrm{SST}+273.16)^4) + \frac{s\beta c_p Q_{lat}}{\alpha L_e}}{\left(\frac{\tau}{\rho}\right)^2 \times k^2}\right]\right\}$$

[from: Yu (2010)]

B) Calculate salinity bias (used as the response in GAM formula)

$$\mathrm{Sbias} = \mathrm{SSS}_{insitu} - SSS_{skin}$$

C) Use GAM to predict bulk-salinity bias in satellite-derived SSS data

$$\Delta SSS_{bulk}(x,y,t) = f_0 + f_1(t) + f_2(\Delta SSS) + f_3(SSS_{skin}) + h(SSS_{skin}, SST, \lambda, w_{inv}, Q_{sens}, Q_{lat}, E, q_{hum}, \Delta SSS)$$

D) Average salinity biases over satellite data period

$$\Delta SSS_{bulk}(x,y) = \overline{\Delta SSS_{bulk}(x,y,t)}$$

E) Add temporally-averaged bias correction term to satellite-derived SSS

$$SSS_{bulk}(x,y,t) = SSS_{skin}(x,y,t) + \Delta SSS_{bulk}(x,y)$$

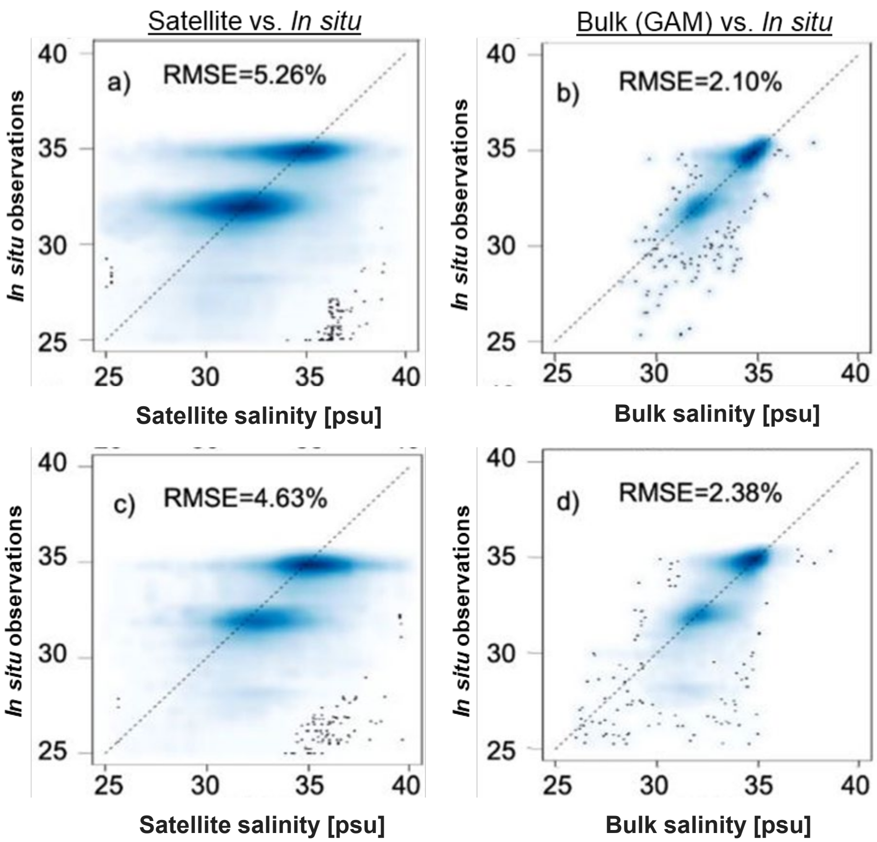
Term	Description
$f_i(\cdot)$	Smoother functions for i = 0…3
$h(\cdot)$	Tensor product of pairwise variables
SSS_{skin}	Satellite-derived SSS from SMAP
x , y	Longitude, Latitude
t	Julian day relative to January 1 of 1970
z	Depth of the *in situ* observations [m]
λ	Empirical coefficient
Q_{sens}	Sensible heat flux (OAFlux)
Q_{lat}	Latent heat flux (OAFlux)
SST_{bulk}	Sea-surface temperature [°C] (OAFlux)
E	Evaporation (OAFlux)
q_{hum}	Near-surface humidity (OAFlux)
τ	Wind stress (OAFlux)
ρ	*In situ* density *
L_e	Latent heat of evaporation *
α	Thermal expansion coefficient *
β	Haline contraction coefficient *
c_p	Specific heat of seawater *
w_{inv}	= $(\tau/\rho)^{-1/2}$, function of the inverse wind stress
p	Pressure
k	Thermal conductivity of seawater [W m^{-1} K^{-1}]
v	= 1.4 x 10^{-6} , kinematic viscosity of seawater
g	= 9.806 m^2 s^{-1} , acceleration due to gravity
ΔSSS	= $f_c \, \mathrm{SSS}_{skin} \lambda E w_{inv}$, **bias correction**, f_c is determined with the GAM

* calculated using TEOS-10

Context

BEC's SMOS

NASA's SMAP

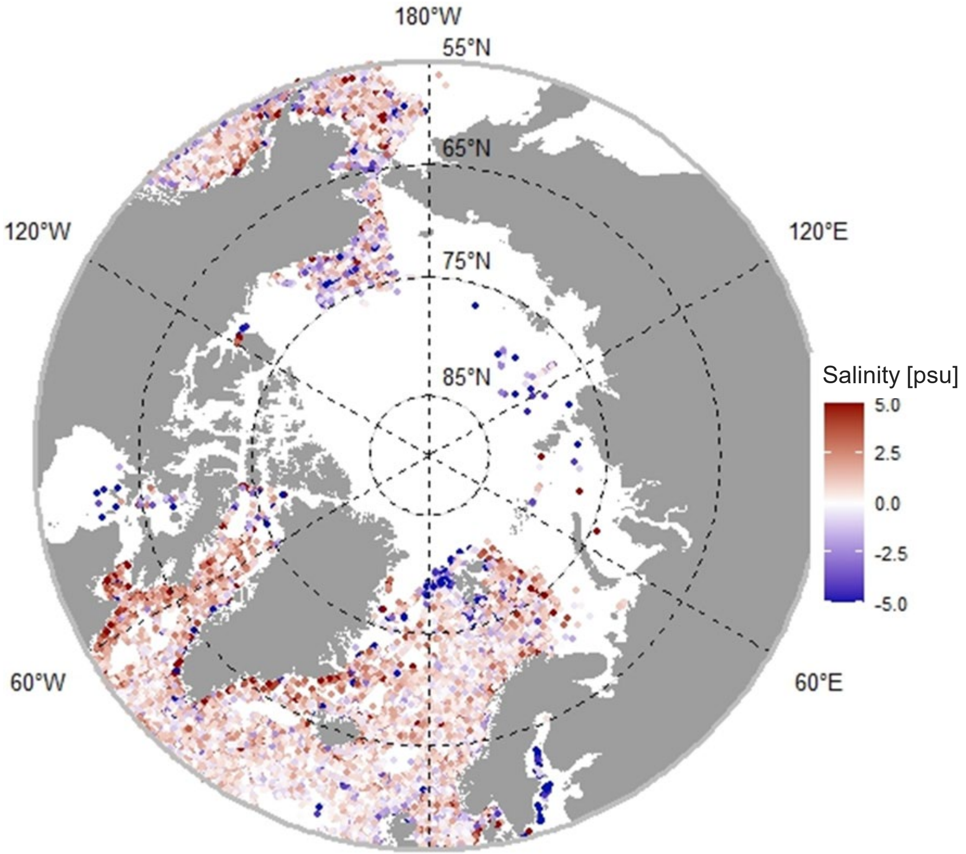


> Bias-correction algorithm (GAM) reduced the root-mean-square error when comparing in situ salinity with skin (satellite) salinity versus when comparing in situ salinity with the computed bulk salinity

Comparison between in situ salinity and (a,c) satellite-derived salinity and (b,d) GAM-produced bulk salinity. The top row uses BEC's SMOS salinity while the bottom row utilizes NASA's SMAP salinity. Deeper blue regions correlate to denser points and individual dots represent outliers. The dashed line indicates salinity of equal psu. The root-mean-squared error (RMSE) are shown for each comparison. [Adapted from Trossman & Bayler, 2022]

Current Efforts

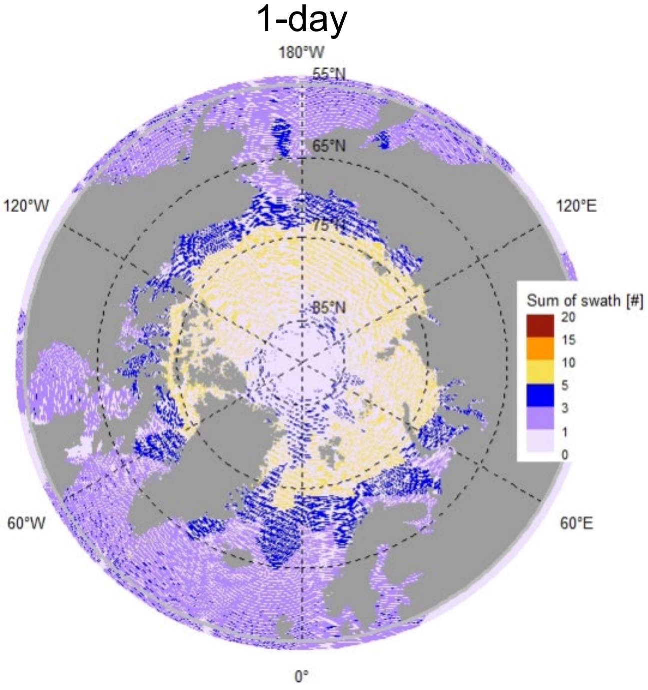
- Mitigating large satellite salinity values due to land/ice contamination, particularly at the sea-ice edge and the edge of Greenland
- Evaluating different parameterizations in the GAM, aiming to explain a higher percentage of deviance (best: ~77.8%)
- Refining methodologies by comparing different spatiotemporal thresholds during the co-location and cross-validation processes

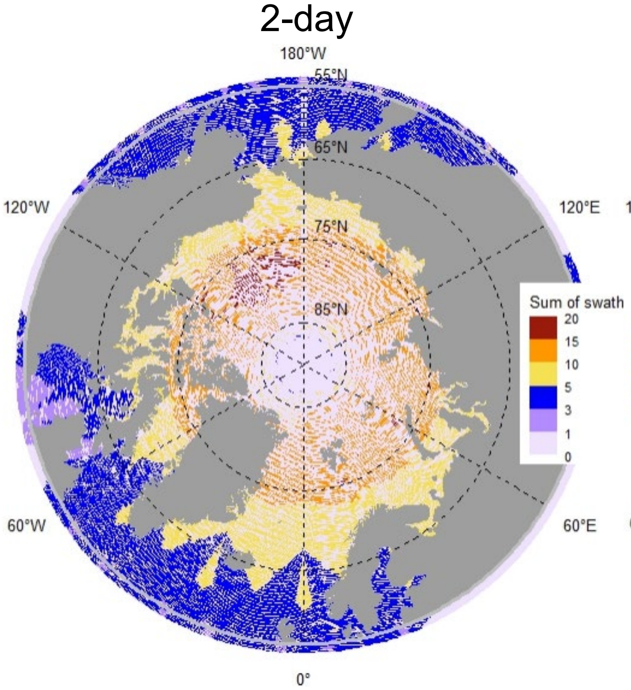


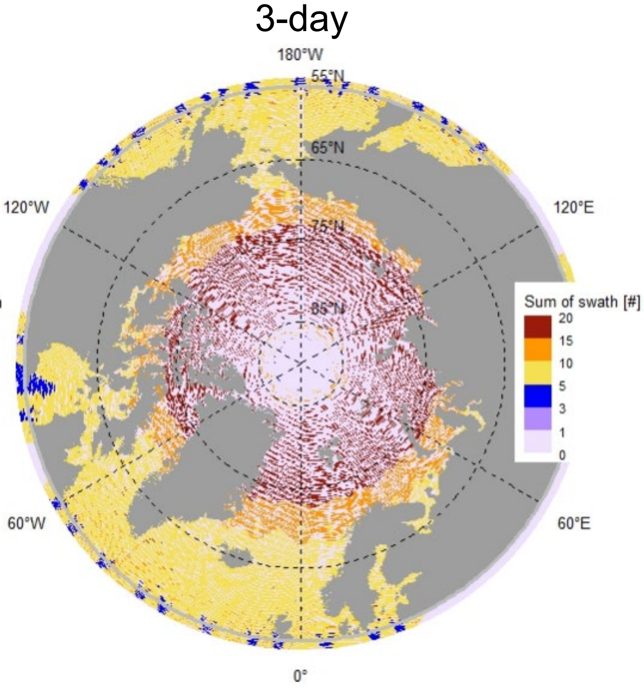
Salinity biases [psu] between the GAM-produced bulk salinity minus untrained in situ observations (0–5 m) between June 2015 – Dec. 2022 in the northern high-latitudes (55 – 90°N).

Spatial & Temporal Thresholds

Satellite [SMOS] swath revisits







Thresholds used: 3.5 days & 50 km

Expanding thresholds to: 1, 2, 3 days @ 50 km, 37.5 km, 25 km, & 12.5 km (12 total combinations)

Broader Impacts

Extended Applications

- Our algorithm is extensible to different depth ranges, providing adaptability of the bias-corrected bulk salinity to model top-layer thickness
- This methodology, applicable to both the Arctic and Antarctic regions, has uncertainties subject to the temporal-spatial resolution of the training data

Blue Economy

- Prediction of sea-ice growth/melt, enabled by integrated salinity impacts, will inform on Arctic accessibility in the near future
- Large economic opportunities and risks: shipping, fisheries, oil/gas mining, deep-water resource extraction, and tourism

Connections to other projects

- CEFI - Climate-Ecosystems-Fisheries Initiative
- ESA's Copernicus Imaging Microwave Radiometer (CIMR) mission (launch expected 2029)
- UN Ocean Decades

Conclusions

- Salinity is vital for understanding Arctic Ocean dynamics, with further effects on the global thermohaline circulation and climate
- GAM reduces the root-mean-square error (RMSE) between satellite SSS and in situ salinity (0–5 m) in the Arctic Ocean and subarctic seas; further refinements should focus on regional characteristics and methodologies
- Enhancing the GAM through refining input data quality, adjusting interaction terms, applying different spatiotemporal thresholds, and evaluating residuals for patterns or systematic errors may help reduce the RMSE further
- Increasing the usability of satellite SSS data improves temporal and spatial coverage while enhancing data assimilation in ocean models

Reference:

Trossman, D., and E. Bayler (2022), An Algorithm to Bias-Correct and Transform Arctic SMAP-Derived Skin Salinities into Bulk Surface Salinities. *Remote Sens., 14*, 1418. https://doi.org/10.3390/rs14061418

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