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Effects of including the adjoint sea ice rheology on estimating Arctic ocean-sea ice state

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11 **Abstract.** The adjoint technique has been applied to the coupled ocean and sea ice models for sensitivity studies and
12 Arctic state estimation. However, the accuracy of the adjoint model is degraded by simplifications on the adjoint of
13 the sea ice model, especially adjoint sea ice rheology. As part of ongoing developments of coupled ocean and sea ice
14 estimation system, we incorporate and stabilize the adjoint of viscous-plastic sea ice dynamics (adjoint-VP) and
15 compare it with the adjoint of a free drift sea ice model (adjoint-FD) through assimilation experiments. Using the
16 adjoint-VP resulted in a further cost reduction of 7.9% in comparison to adjoint-FD with noticeable improvements in
17 ocean temperature over the open water and intermediate layers of the Arctic Ocean. Adjoint-VP more efficiently
18 adjusts uncertain parameters than adjoint-FD by involving different sea ice retreat processes. For instance, adjoint-
19 VP melts sea ice up to 1.0 m in the marginal seas from May to June through over-adjusting air temperature (>8 °C); adjoint-
20 VP reproduces the sea ice retreat with smaller adjustments on the atmospheric state within the prior uncertainty range.
21 The developments of the adjoint model here lay the foundation for further improving Arctic ocean and sea ice
22 estimation through comprehensively adjusting the initial conditions, atmosphere forcings, and model parameters.

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24



25 **1 Introduction**

26 The Arctic Ocean has experienced drastic changes and has been migrating to a new state over the past decades,
27 concerning the fast declining sea ice (Comiso et al., 2008; Kwok, 2018), increased inventory of freshwater in the
28 western Arctic (Proshutinsky et al., 2019), enhanced warm inflows from the Pacific Ocean (Woodgate et al., 2012)
29 and the Atlantic Ocean (Polyakov et al., 2017; Quadfasel et al., 1991), and increased ocean primary productivity
30 (AMAP, 2021). These changes amplify the local air and ocean temperature and potentially impact the climate and
31 weather of the Northern Hemisphere (Ma et al., 2022; Overland et al., 2021).

32 Over the recent years, progress has been made in satellite techniques (e.g., Kaleschke et al., 2001; Spreen et al.,
33 2008), in-situ observations (e.g., Toole et al., 2016; Morison et al., 2007; Polyakov et al., 2017; Proshutinsky et al.,
34 2009; Schauer et al., 2008), and coupled ocean and sea ice models. However, the lack of extensive Arctic observations,
35 especially direct observations of the state variables and fluxes through the water column, and deficiencies of the
36 coupled ocean and sea-ice model still obscure our understanding of the Arctic sea-ice changes and extremes. Accurate
37 predictions of sea ice is therefore also limited (e.g., Yang et al., 2020).

38 To fill the gaps, research groups have applied data assimilation techniques to ingest available observations into
39 coupled ocean and sea ice models, reconstructing spatio-temporal changes of the Arctic Ocean. The resulting
40 reanalyses are assumed to advance in fidelity since the development of models and data assimilation methods progress,
41 and observation numbers increase, providing invaluable information for understanding the Arctic changes and the
42 related ocean-atmosphere-ice heat and freshwater fluxes. Among the various data assimilation methods, an adjoint
43 method with a large assimilation window (years to decades) has been developed within the framework of Estimating
44 the Circulation and Climate of the Ocean (Heimbach et al., 2019; Stammer et al., 2002; Wunsch and Heimbach, 2007)
45 to create a dynamically consistent synthesis, permitting closed budget analysis (e.g., Buckley et al., 2014; Piecuch and
46 Ponte, 2012). Within the assimilation window, the adjoint method attempts to make the model simulation consistent
47 with available observations iteratively by correcting model uncertain inputs (control variables hereafter), including
48 initial conditions, atmospheric forcing, and model parameters to yield minimum misfits measured by an objective
49 function. An adjoint model (adjoint of the tangent linear approximation of the nonlinear model) is used as a spatio-
50 temporal interpolator to project the model-data misfits onto the gradient of a cost function with respect to the control
51 variables. Therefore, the accuracy of the adjoint model is crucial for the performance of the minimization and ultimately
52 the quality of the synthesis.

53 The adjoint method has been applied to the coupled ocean and sea ice system for adjoint sensitivities studies
54 (Heimbach et al., 2010; Kauker et al., 2009; Koldunov et al., 2013) and Arctic synthesis (Fenty and Heimbach, 2013;
55 Koldunov et al., 2017; Lyu et al., 2021b; Nguyen et al., 2021). However, due to the persistence of numerically
56 instability issues, the adjoint of sea ice dynamics is omitted (Forget et al., 2015; Nguyen et al., 2021; Fenty and
57 Heimbach, 2013; Mazloff et al., 2010) or simplified to a free-drift sea ice model (Koldunov et al., 2017; Lyu et al.,
58 2021a; Lyu et al., 2021b). Toyoda et al. (2019) described stabilizing the adjoint of full elastic–viscous–plastic sea-ice
59 dynamics and noted much weaker evolution of sensitivity to sea-ice velocity by $O(10^2)$ in the central Arctic Ocean
60 than the adjoint of free-drift sea ice dynamic. Therefore, using the adjoint of a free-drift sea ice dynamic may



61 overestimates the gradients of the cost function towards the sea-ice velocity and wind, which potentially impairs the
62 usefulness of the adjoint gradients and hinders the minimization of the model-data misfits.

63 In this study, we incorporate and stabilize the adjoint of a viscous-plastic sea ice dynamic (Hibler 1979; Zhang and
64 Hibler Iii, 1997), building on prior developments of the adjoint method in the Arctic Ocean (Fenty and Heimbach,
65 2013; Heimbach et al., 2010; Koldunov et al., 2017; Lyu et al., 2021b). Taking the unprecedented sea ice retreat
66 process in 2012 as an example, we evaluate the impacts of using the adjoint of full sea ice dynamics on estimating the
67 Arctic ocean and sea ice and sea-ice retreat processes.

68 The paper is organized as follows. In section 2, we introduce the model configurations and assimilation
69 experiments. We assess the assimilation results in section 3 regarding the residual errors. We examine adjustments of
70 the control variables in section 4 and compare sea ice retreat process from April 10, 2012 to September 20, 2012 in
71 section 5. Section 6 summarizes the results of this study.

72

73 **2 Model Configuration and Experiment Setups**

74 **2.1 The Coupled Ocean-Sea Ice Model and Assimilation System**

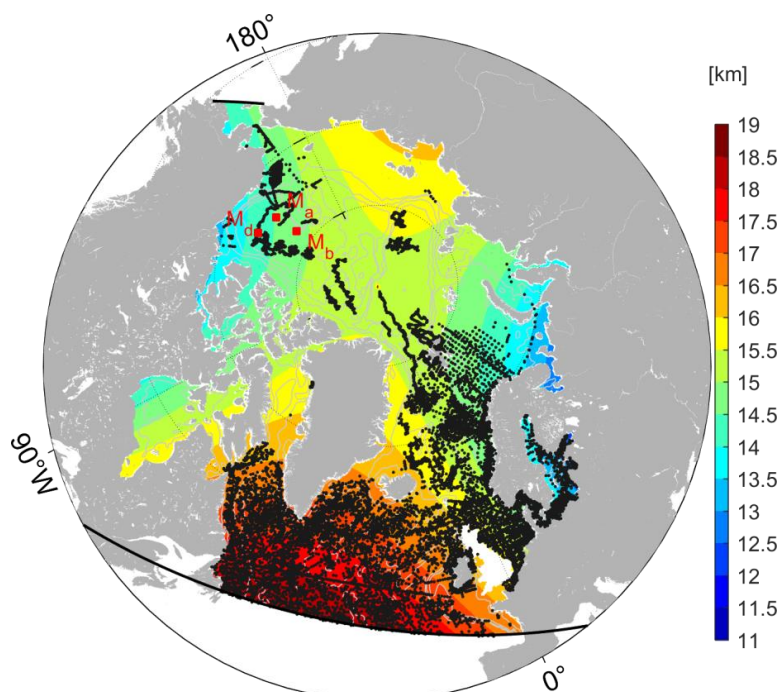
75 The data assimilation system is based on the adjoint method in the framework of ECCO, using the Massachusetts
76 Institute of Technology ocean general circulation model (MITgcm, Marshall et al., 1997) coupled with a zero-layer
77 dynamic-thermodynamic sea ice model of Hibler (1979). The sea ice dynamics are based on the viscous-plastic
78 rheology and are solved using a line successive over-relaxation algorithm (Zhang and Rothrock, 2000) and are
79 modified to facilitate the generation of adjoint model (Losch et al., 2010). The adjoint of the coupled ocean and sea
80 ice model is generated by the Transformation of Algorithms in FORTRAN (TAF, Giering and Kaminski, 1998).

81 The pan-Arctic model covers the Arctic Ocean north of the Bering Strait and the Atlantic Ocean 44° N (Figure
82 1). In the horizontal, we use a curvilinear grid with a resolution of 12~15 km in the Arctic Ocean and ~18 km in the
83 north Atlantic Ocean. In the vertical, the system has 50 z-levels ranging from 10 m at the surface to 456 m in the deep
84 ocean. The open boundaries are provided by a 16 km Atlantic-Arctic Ocean simulation (Serra et al., 2010). At the
85 ocean surface, we use the atmosphere state from the National Centers for Environmental Prediction reanalysis 1
86 (NCEP-RA1, Kalnay et al., 1996) and bulk formulae to compute the momentum, heat, and freshwater fluxes. A virtual
87 salt flux parameterization simulates the dilution and salinification of rainfall, evaporation, and river runoff. The river
88 runoff is applied near the river mouth with seasonal-varying discharge (Fekete et al., 2002). Besides, the unresolved
89 vertical mixing is parameterized using the K-Profile scheme of Large et al. (1994). The bottom topography is derived
90 from ETOPO2 (Smith and Sandwell, 1997).

91 The adjoint method brings the model simulation close to available observations by iteratively adjusting control
92 variables to minimize a quadric target function J (cost function hereafter):

$$93 J(C_{ini}, C_{atm}(t)) = \sum_{t=1}^{T_1} [y(t) - E(t)x(t)]^T R^{-2} [y(t) - E(t)x(t)] + C_{ini}^T P^{-2} C_{ini} + \sum_{t=0}^{T_1} C_{atm}(t)^T Q_a^{-2} C_{atm}(t) \quad (1).$$

94



95 Figure 1. Model domain (enclosed by the black lines) and horizontal resolutions (shading). The black dots represent
 96 profile observations from EN4 datasets (Good et al., 2013), and the red rectangles show the three moorings from the
 97 Beaufort Gyre Exploration Project (BGEP).
 98
 99

100 With an assimilation window of one year (2012), the control variables consist of the initial condition (C_{ini}),
 101 including temperature, salinity, ice effective thickness, sea ice concentration, and daily atmosphere state on the model
 102 grid ($C_{atm}(t)$), which includes 10-m wind vectors, 2-m air temperature, 2-m specific humidity, precipitation,
 103 downwelling longwave, and net shortwave radiation. Overall, a total number of $\sim 2.7 \times 10^8$ variables are adjusted.

104 On the right hand of Equation (1), the first term measures the model-data misfits weighted by the inverse error
 105 covariance matrices (R^{-2}). The following section will introduce the available measurements and their uncertainties (R).
 106 $y(t)$ and $x(t)$ are observations and the model state at time t , respectively. $E(t)$ maps the model state $x(t)$ to the
 107 corresponding observations $y(t)$. The last two terms are background terms of the initial condition (C_{ini}) and the time-
 108 varying atmospheric forcing ($C_{atm}(t)$) weighted by their inverse error covariance matrices (P^{-2} and Q^{-2} , respectively),
 109 which penalize their adjustments and provide complete information on the controls. Following Lyu et al. (2021b),
 110 prior uncertainties of the time-varying atmosphere state (Q_a) depend on geographic locations. They are computed as
 111 the variance of the nonseasonal variability of the corresponding variables using the NCEP-RA1.

112 During the optimization process, the adjoint of the coupled ocean-ice model is used to compute the gradients of
 113 the cost function J to the control variables, and a quasi-Newton algorithm (Gilbert and Lemaréchal, 2006) is used to
 114 reduce the cost function J iteratively. The optimization process continues until the cost function cannot be further
 115 reduced.



116 2.2 Observations and Prior Uncertainties

117 Both satellite and in-situ measurements (Table 1) are used to constrain the model simulations. In addition, sea
 118 ice draft measurements by up-looking sonar from the Beaufort Gyre Exploration Project (see Figure 1 for the locations)
 119 are used to validate the assimilation results independently.

120 Prior uncertainties follow our previous Arctic-focused synthesis study (Lyu et al., 2021b). Uncertainties of
 121 temperature and salinity depend on the depth and are set to 0.6° C and 0.3 PSU at the surface and 0.02° C and 0.02
 122 PSU in the deep ocean; SIC uncertainties consist of representation errors (15% within 50 km from the coastlines and
 123 10% over the open water) and instrument errors. Because of higher errors in low SIC and lower errors over open water,
 124 we modify the representation uncertainties by multiplicative factors of 0.85, 1.20, 1.10, and 1.00 for the observed SIC
 125 ranges of 0.00, <15%, 15%–25%, and 0.25%, respectively.

126 SIT errors are provided by the datasets and interpolated to our model grid. SLA uncertainties are set to 3.0 cm.
 127 Sea ice drift uncertainties are dominated by representation errors and are set to 0.04 m/s. In addition, we reduce the
 128 weight of the temperature and salinity climatology (WOA18) cost component by a factor of 20 and 10 to avoid
 129 overfitting to the climatology.

130 **Table 1.** Assimilated measurements.

Date sets	Resolution	Source
sea level anomaly	7 km	Copernicus Marine Environment Monitoring Service, http://marine.copernicus.eu
Sea surface temperature	25km	Remote Sensing System, http://www.remss.com/measurements/sea-surface-temperature/
T&S profiles	–	Good et al. (2013), https://www.metoffice.gov.uk/hadobs/en4/
Sea ice concentration	25km	Kaleschke et al. (2001) and Spreen et al. (2008), SSMI(2011-2012), http://icdc.cen.uni-hamburg.de/1/daten/cryosphere.html
Sea ice thickness	25km	(Ricker et al., 2017), https://spaces.awi.de/pages/viewpage.action?pageId=291898639
Sea ice drift	62.5km	(Lavergne et al., 2019), https://osi-saf.eumetsat.int/products/osi-405-c
WOA18	1°	Zweng et al. (2018), https://www.nodc.noaa.gov/OC5/woa18/woa18data.html

131 2.3 Viscos-Plastic Sea Ice Dynamics and Its Adjoint

132 In the coupled ocean-sea ice model, the following equation governs ice motions:

$$133 \quad m \frac{d\vec{u}}{dt} = -mf\vec{k} \times \vec{u} + \tau_{air} + \tau_{ocn} - \nabla\phi(0) + \nabla \cdot \sigma \quad (2)$$

134 where m is ice mass and \vec{u} is ice motion vectors; τ_{air} and τ_{ocn} are the wind and ocean drags; $-\nabla\phi(0)$ is the tilt of
 135 the sea surface; and $\nabla \cdot \sigma$ is the divergence of the ice stress tensor σ_{ij} ($i=1,2$), representing the internal forces of sea
 136 ice.

137 In the viscous-plastic rheology of Hibler (1979), the stress tensor σ_{ij} is related to ice strain rate (ϵ_{ij}) and
 138 strength (P):

$$139 \quad \sigma_{ij} = 2\eta(\epsilon_{ij}, P)\epsilon_{ij} + [\zeta(\epsilon_{ij}, P) - \eta(\epsilon_{ij}, P)]\epsilon_{ij}\delta_{ij} - \frac{P}{2}\delta_{ij} \quad (3)$$

140 where δ_{ij} is the Kronecker delta ($\delta_{ij} = 1$ if $i=j$, otherwise 0). η and ζ are the bulk and shear viscosities, expressed
 141 as:



142
$$\zeta = \frac{P}{2\Delta_{reg}} \quad (4)$$

143
$$\eta = \frac{P}{2e^2\Delta_{reg}} \quad (5)$$

144 where

145
$$\Delta = [(\epsilon_{11}^2 + \epsilon_{22}^2)(1 + e^{-2}) + 2(1 - e^{-2})\epsilon_{11}\epsilon_{22} + 4e^{-2}\epsilon_{12}^2]^{\frac{1}{2}} \quad (6)$$

146 e is the ratio of normal stress to shear stress and is set to 2.0; $\Delta_{reg} = \max(\Delta, \Delta_{min})$ with Δ_{min} equals 1.0×10^{-10} . Sea

147 ice strain rate is computed as:

148
$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (7)$$

149 The ice strength P depends on sea ice effective thickness (H) and concentration (C):

150
$$P = P^*H \cdot \exp(-C^* \cdot (1 - C)) \quad (8)$$

151 P^* and C^* are the ice compressive strength constant and ice strength decay constant and are set to $2.75 \times 10^4 \text{ N m}^{-2}$

152 and -20.0.

153 The dependence of the internal force term ($\nabla \cdot \sigma$) on ice velocity is strongly nonlinear, leading to an unstable
154 adjoint of the coupled ocean-sea ice system. Therefore, previous studies (Koldunov et al., 2017; Lyu et al., 2021b)
155 used an adjoint of a free drift sea ice model (without adjoint of $\nabla \cdot \sigma$). Toyoda et al. (2019) pointed out that the full
156 adjoint of Equation (2) can be stabilized by eliminating the dependence of bulk and shear viscosities on strain rate
157 (ϵ_{ij}).

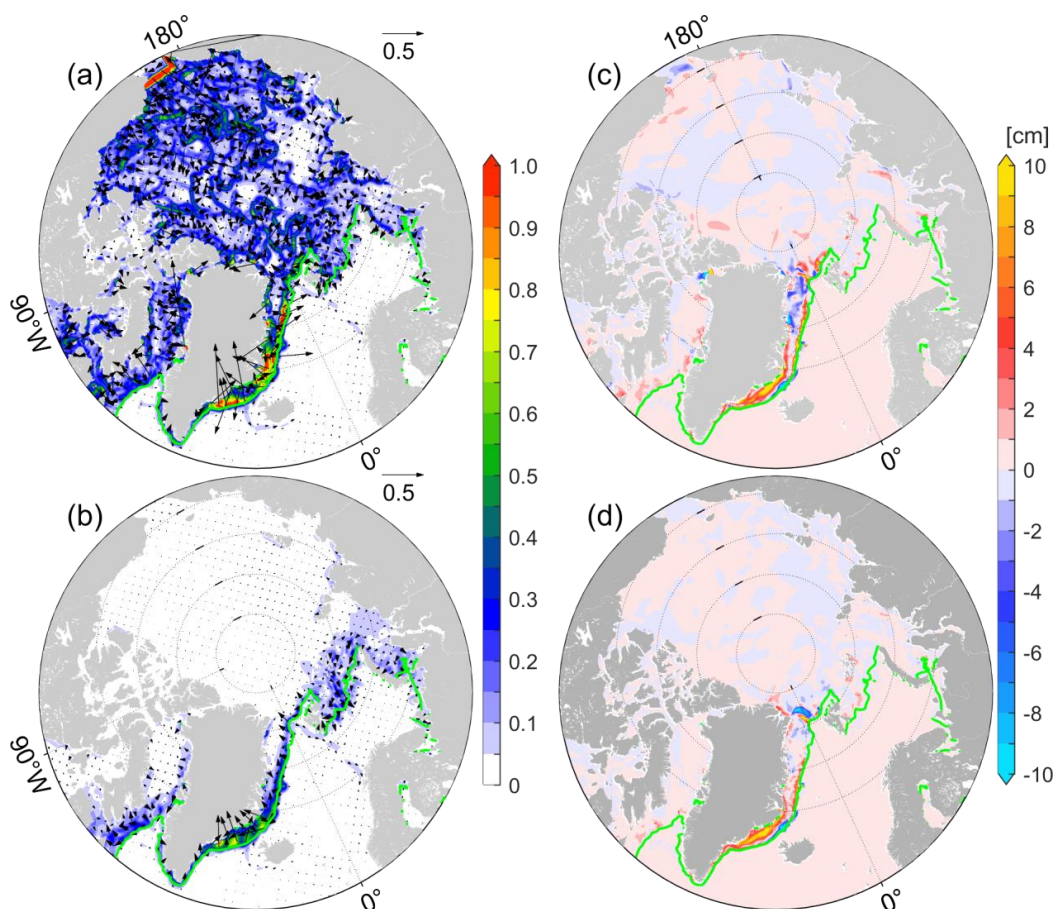
158 Following the study of Toyoda et al. (2019), we eliminate the dependence of bulk and shear viscosities on ϵ_{ij} in
159 the adjoint of Equation (2). Besides, we note that there are still strong sensitivities which hamper the convergence of
160 optimization. We set the adjoint sensitivities of ice velocity to zero if the local sensitivity is 50 times larger than the
161 global mean of their absolute values. The other modifications on the adjoint model are the same as in Lyu et al. (2021b).

162 Based on the adjoint of a free-drift sea ice model (adjoint-FD hereafter) and the viscous-plastic sea ice dynamics
163 (adjoint-VP hereafter), we compute over the period January 1 to 31 January 31, 2012 sensitivities of domain-integrated
164 sea ice volume with respect to the atmospheric forcings and the initial conditions. Similar to Toyoda et al. (2019),
165 adjoint-FD shows much stronger sensitivities to wind than adjoint-VP (Figure 2a, b) in the central Arctic Ocean. Along
166 the SIEs of the Atlantic sectors, adjoint-VP reveals that the towards-ice wind anomalies increase total sea ice (Figure
167 2b) since they prevent ice from drifting to the warm Atlantic water. However, adjoint-FD shows strong sensitivities
168 along the SIE of the Atlantic sectors, but both towards-ice and off-ice wind anomalies appear, potentially resulting in
169 ice convergence.

170 Furthermore, we add daily wind perturbations, computed by scaling the adjoint sensitivities (Figure 2a, b) that
171 the maximum perturbations are 1.0 m s^{-1} , to the 6-hourly wind from NCEP-RA1 and examine their impacts on sea ice
172 changes. As expected, sea ice effective thickness (Figure 2c, d) changes are mainly along the SIEs in the Atlantic
173 sectors, and wind perturbations from adjoint-FD lead to negative effective changes northeast of Greenland. In the
174 central Arctic Ocean with compact ice, the internal forces $\nabla \cdot \sigma$ contradicts the impacts of wind perturbations.
175 Therefore, despite the strong adjoint sensitivities to the wind in adjoint-FD, we note that the resulting wind



176 perturbations change effective thickness only slightly (Figure 2c), which is comparable to that in adjoint-VP (Figure
177 2d).



178
179 Figure 2. Sensitivities of total sea ice volume to wind vectors (in $0.1 \times \text{km}^3 (\text{m s}^{-1})^{-1}$, shadings for amplitudes) using the
180 adjoint of (a) a free-drift sea ice dynamic and (b) full viscous-plastic sea ice dynamics with modifications in section
181 2.3. Panels (c)-(d) are the mean effective thickness changes by perturbing the wind with the corresponding adjoint
182 sensitivities multiplied by a factor of 10^{-8} . The green lines are the SIE in January 2012.
183

184 Besides overestimating the sensitivities to wind, adjoint-FD may also degrade the usefulness of the adjoint
185 sensitivities in optimization. Therefore, we perform two assimilation experiments to comprehensively evaluate the
186 impacts of including the adjoint of sea ice rheology on ocean and sea ice estimation.

187 3 Model-Data Misfits Reductions and Residuals

188 3.1 Evaluation of the Optimization

189 In adjoint-FD and adjoint-VP, 13 and 32 iterations were performed before the cost function could not be further
190 reduced, resulting in an overall cost reduction of 32.3% and 40.2% (see Table 2 for details), respectively. Of the
191 individual cost constituents, satellite-observed SST and SIC contribute to $\sim 25.3\%$ and 39.7% of the total cost, which



192 are reduced significantly after optimization. The cost of temperature ($J_{profile_T}$) and salinity ($J_{profile_S}$) profiles are also
 193 considerably reduced, especially in the adjoint-VP experiment. The rest of the cost constituents are also brought down
 194 slightly. Overall, including the adjoint of sea ice rheology further reduces the total cost by 7.9% and individual cost
 195 constituents, especially J_{Sst} , $J_{profile_T}$ and $J_{profile_S}$. Based on iterations 0, 13 in adjoint-FD, and 32 in adjoint-VP of the
 196 optimization, we will focus on the sea ice state and ocean temperature to evaluate the impacts of using the adjoint of
 197 full sea ice dynamics.

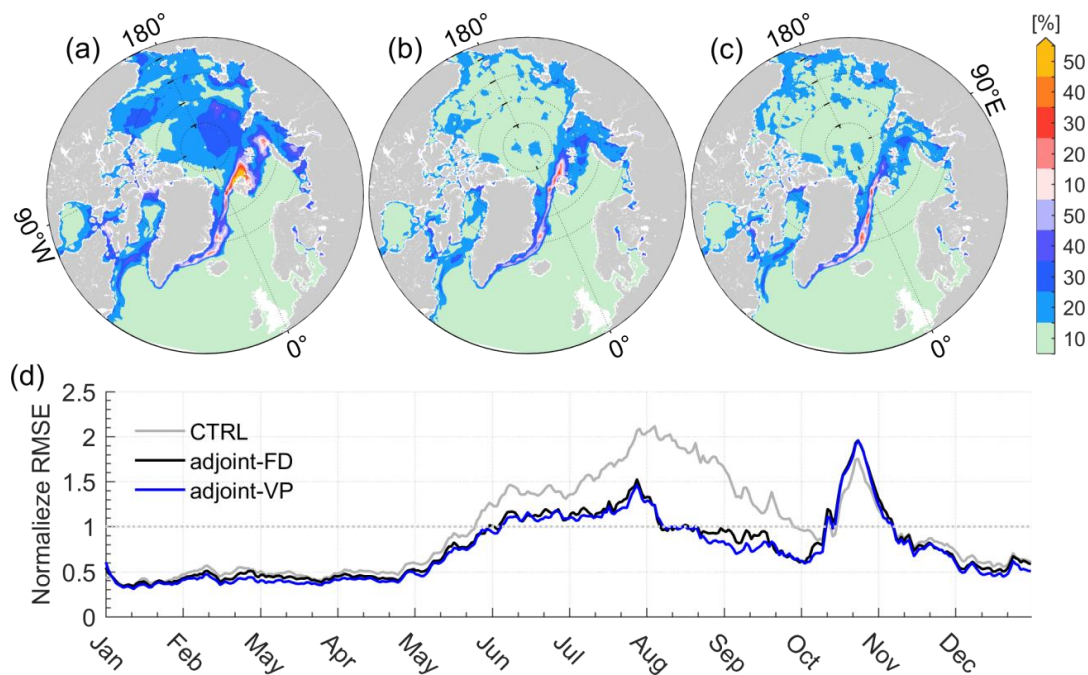
198 **Table 2.** Normalized costs and reductions in the two optimization runs.

Cost constituent	Control run	Adjoint-FD		Adjoint_VP	
	Normalized cost (%)	Normalized cost (%)	Percentage reduction (%)	Normalized cost (%)	Percentage reduction (%)
J_{Total}	100	67.7	32.3	59.8	40.2
J_{SLA}	2.2	2.1	4.6	2.1	4.6
J_{SST}	25.3	15.4	39.1	12.9	49.0
$J_{profile_T}$	6.9	6.5	5.8	4.3	37.7
$J_{profile_S}$	5.8	5.9	-1.7	4.5	22.4
J_{SIC}	39.7	18.4	53.7	18.1	54.4
J_{SIT}	3.6	3.1	13.9	2.7	25.0
J_{SID}	4.5	4.4	2.2	4.3	4.4
J_{WOA_T}	6.6	6.6	0.0	6.2	6.1
J_{WOA_S}	5.4	5.3	1.9	4.7	13.0

199

200 **3.2 Sea Ice State**

201 **3.2.1 Residual Errors of SIC and SIT**



202



203 Figure 3. Root mean square errors (RMSEs) of SIC between the satellite measurements and (a) the control run, (b)
204 adjoint-FD, and (c) adjoint-VP, respectively. Panel (d) shows the temporal variations of RMSEs in the three
205 simulations.

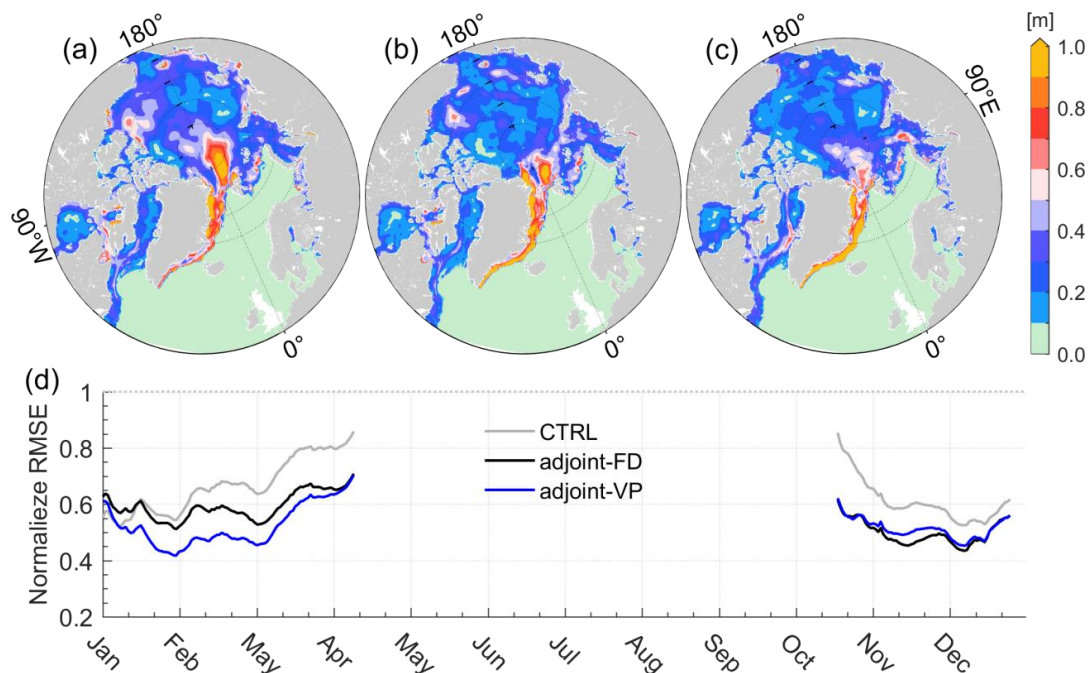
206
207 Satellite visual, infrared, and microwave technologies have been applied to monitor SIC with high frequencies
208 and quality, which is of high priority in the global and Arctic-focused synthesis (Chevallier et al., 2017; Uotila et al.,
209 2019). Previous studies (Fenty and Heimbach, 2013; Lyu et al., 2021a; Lyu et al., 2021b) indicated that SIC could be
210 improved significantly by adjusting the atmospheric forcings slightly. Here, we explore the residual errors in the
211 optimization runs.

212 The root mean square errors (RMSEs) of SIC averaged over 2012 (Figure 3a-c) and normalized by the prior
213 errors and averaged over the model domain (Figure 3d) show the geographical distribution and temporal evolution of
214 SIC errors, respectively. The normalized RMSEs should be close to 1.0 if the optimization found a model simulation
215 consistent with the observations and the prior uncertainties.

216 The control run (Figure 3a) shows pronounced RMSEs in the Beaufort Gyre (~15%), the central Eurasian Basin
217 (15%~20%), the marginal seas (15%~20%), and sea ice extent regions of the Atlantic sector (30%-50%). The
218 normalized RMSEs reveal that SIC errors remain small (~0.5) and grow quickly from May-September when the sea
219 ice melts (Figure 3d). Normalized RMSEs up to 1.5 are observed in October, but quickly drop in November (Figure
220 3d).

221 Both assimilation experiments reduce the SIC errors to less than 5% in the central Arctic Ocean and 10% in the
222 marginal seas. SIC errors up to 20% exist in the Atlantic sector, where sea-ice shows strong nonlinearity and the
223 tangent linear model could only capture part of the sea-ice changes (Appendix B in Lyu et al., 2021a). Normalized
224 SIC errors from May to September have also been reduced close to 1.0 by assimilation of the daily SIC observations
225 (Figure 3d). However, SIC errors in October remain significant (Figure 3d) since the observed sea ice recovered much
226 faster than in the three simulations (not shown here). This delayed sea ice recovery in the model may related to model
227 uncertain parameters, such as demarcation thickness between thin and
228 thick ice which decides the initial sea ice thickness formed in open water.

229 The control run shows sea ice thickness errors up to 1.0 m in regions north and south of the Fram Strait and
230 around 0.4~0.7 m in the Beaufort Gyre. In the Beaufort Gyre, the SIT errors are reduced to less than 0.3 m in adjoint-
231 VP (Figure 4c) and around 0.3-0.5 m in adjoint-FD (Figure 4b). Similar to SIC errors, SIT errors up to 1.0 m remain
232 along the East Greenland Current, which seems to increase in the two assimilation experiments. The temporal
233 evolutions of normalized RMSEs show that SIT errors grow quickly from February to April (Figure 4d). Both
234 assimilation experiments bring down the SIT errors, especially in adjoint-VP from January to April (Figure 4d).
235 However, the normalized RMSEs of SIT averaged over the model domain remain smaller than 1.0 and seem to grow
236 larger during the melting season, indicating that the prescribed constant error is not entirely appropriate. More accurate
237 SIT observations (e.g., halve the uncertainties) and SIT observations during the melting season are required to facilitate
238 a significant impact on the solution.



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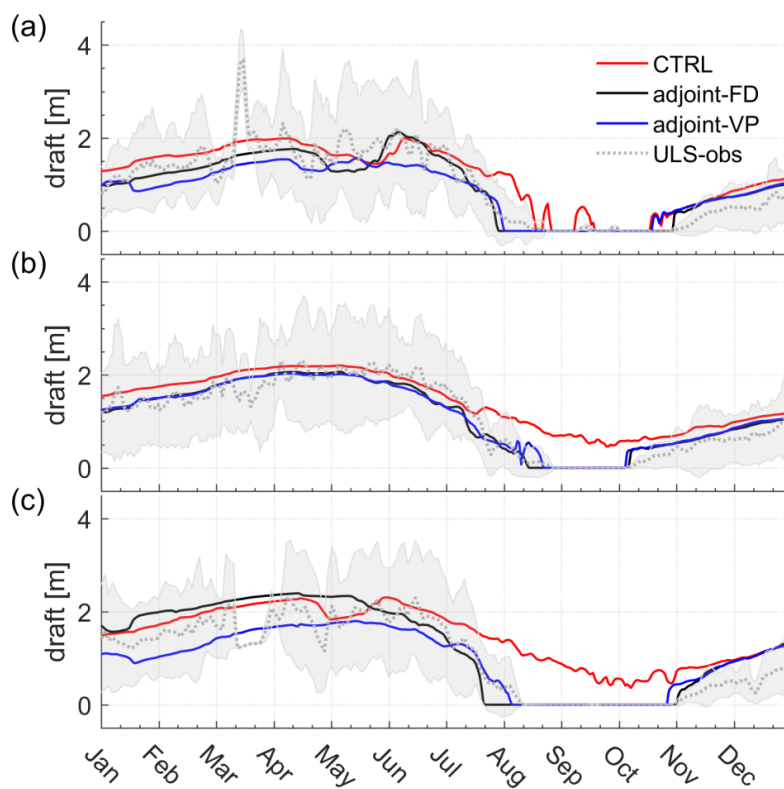
240 Figure 4. Root mean square errors (RMSEs) of SIT between the satellite measurements and (a) the control run, (b)
 241 adjoint-FD, and (c) adjoint-VP. Panel (d) shows the temporal variations of RMSEs in the three simulations.
 242

243 3.2.2 The BGEP Mooring Measurements

244 Independent sea ice draft measured by up-looking-sonar (ULS) from BGEP moorings (M_a , M_b , and M_d in
 245 Figure 1) is used to validate the simulated sea-ice draft. The simulated snow depth (d_{snow}) and SIT (d_{SIT}) are used to
 246 compute the sea ice draft following Tilling et al. (2018):

$$247 \text{draft} = \frac{\rho_i \times d_{SIT} + \rho_s \times d_{snow}}{\rho_w} \quad (9)$$

248 where ρ_i , ρ_s , ρ_w are the density of sea-ice, snow, and water and are set to 910.0, 330.0, and 1027.5 kg m⁻³ as in our
 249 model.



250

251 Figure 5. Daily time series of sea ice draft (grey lines) and the daily standard deviation (shadings) at the mooring
 252 locations (a) M_a , (b) M_b , and (c) M_d compared with the three model runs (see the legends). ULS-observed sea ice
 253 draft is smoothed with 5-days running average.

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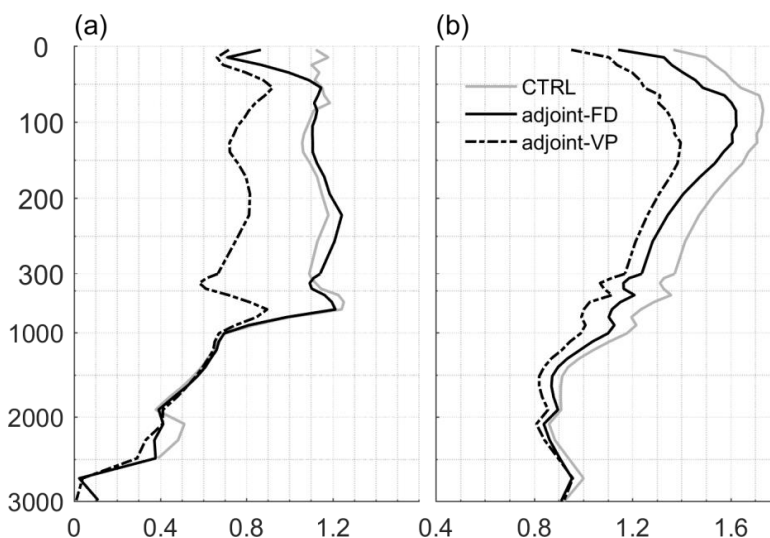
255 3.3 Ocean Temperature

256 Ocean temperature changes are closely related to sea ice changes. Adjoint-VP introduces more pronounced ocean
 257 temperature changes than adjoint-FD. Here, we explore ocean temperature changes after assimilation.

258 Temperature profiles in the Arctic Ocean are much less than in the North Atlantic Ocean (black dots in Figure
 259 1). In the Arctic Ocean, adjoint-FD only reduces temperature errors over the top 20 m, while adjoint-VP reduces
 260 temperature errors up to 0.4°C over the top 1000 m (Figure 6a). In the North Atlantic Ocean, adjoint-VP results in
 261 more pronounced RMSEs reduction up to 0.3°C than adjoint-FD (Figure 6b).

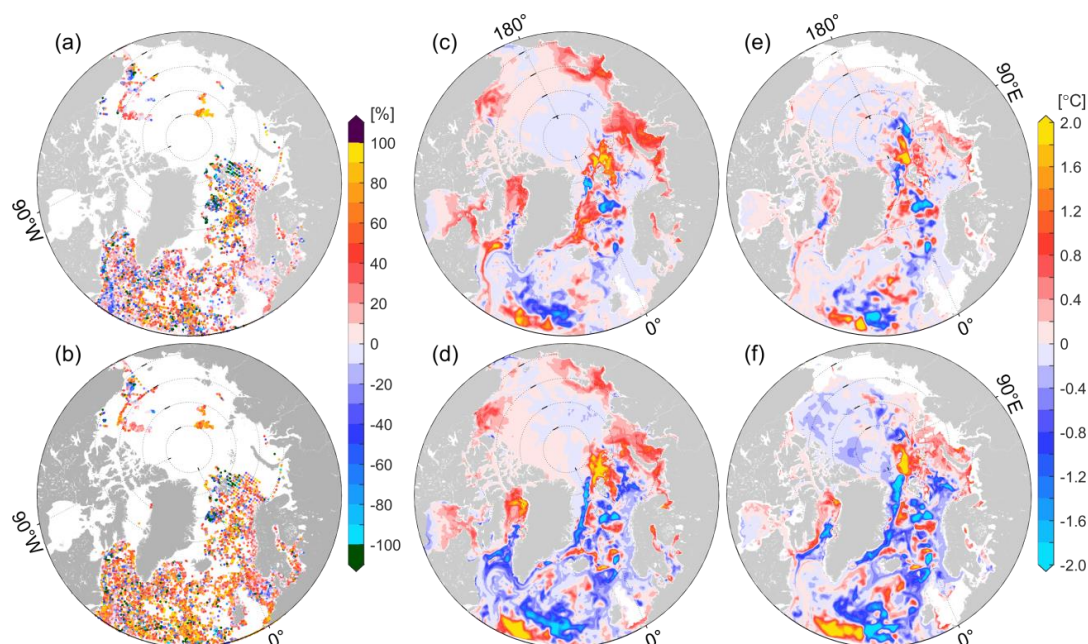
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263



264 Figure 6. Root mean squares errors of potential temperature (a) in the Arctic Ocean and (b) the North Atlantic Ocean
265 in the three runs.
266
267

268 Relative temperature error reductions over the top 50 m reveal an overall improvement of temperature with
269 occasional degradations (Figure 7a, b). Adjoint-VP results in a more significant error reduction than adjoint-FD in the
270 North Atlantic Ocean (Figure 7a, b). In the southern Beaufort Gyre, the Laptev and Kara seas, and north of Svalbard,
271 both adjoint-VP and adjoint-FD increase the ocean temperature (over 50 m) since the two optimization runs reproduce
272 the early retreat of sea ice well, allowing more solar heating of the open water. In the North Atlantic Ocean, adjoint-
273 VP achieves more considerable temperature changes than adjoint-FD both over the top 50m (Figure 7c, d) and from
274 50m-700m (Figure 7e, f). In the Arctic Ocean, In the layer of 50-700 m, adjoint-VP further introduced negative
275 temperature corrections between 50-700 m (Figure 7f), especially near the profiles locations (see dots in Figure 7b),
276 resulting from more iterations performed.



277

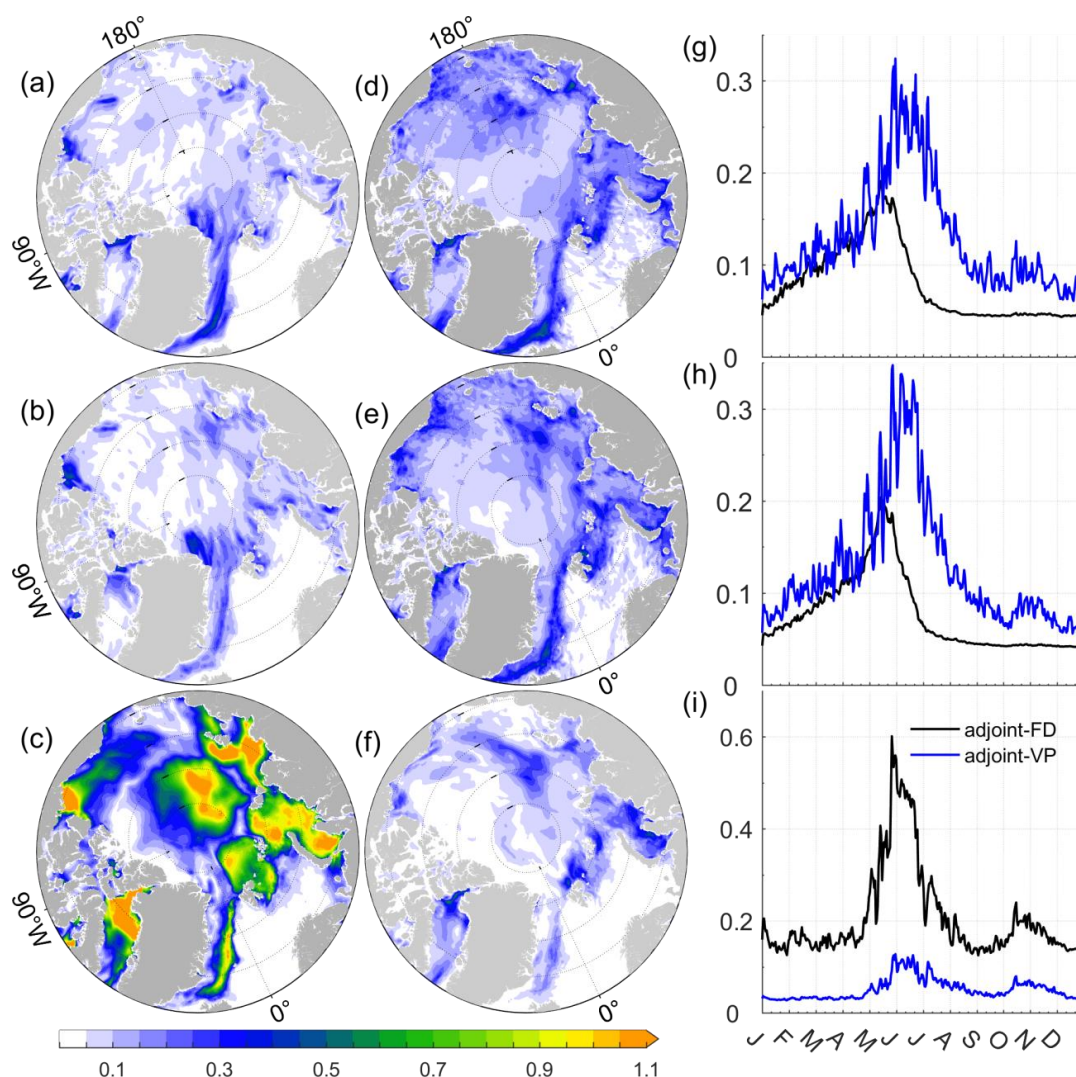
278 Figure 7. Relative temperature error reduction ($-\frac{|T_{opti}-T_{obs}|-|T_{ctrl}-T_{obs}|}{|T_{ctrl}-T_{obs}|} \times 100\%$) over the top 50 m at the profile
 279 locations in (a) adjoint-FD and (b) adjoint-VP. Values >100% means over-adjustment. Panels (c) and (d) are
 280 temperature differences of adjoint-FD and adjoint-VP to the control run averaged over the top 50m, respectively.
 281 Panels (e) and (f) are the same as Panels (c) and (d), but for layers 50-700m.
 282

283 In summary, adjoint-FD and adjoint-VP reproduce the SIC variations well in the Arctic Ocean, which further
 284 reduces ocean temperature errors over the top layer by improving atmosphere-ocean heat flux. adjoint-VP achieves
 285 more significant corrections to the ocean temperature over the open water and in the intermediate layer of the Arctic
 286 Ocean than adjoint-FD.

287 4 Adjustments of the Control Variables

288 The adjoint models project the model-data misfits onto the gradient of the objective function with respect to all
 289 control variables simultaneously, which is used by the optimization algorithm to adjust the control variables. In this
 290 section, we compare adjustments of the control variables in the adjoint-FD and adjoint-VP, and evaluate contributions
 291 of individual adjustments of the control variables on the cost function reduction.

292 Among all the control variables, wind vectors and 2-m air temperature are adjusted considerably in adjoint-FD
 293 and adjoint-VP, which also show significant differences. Besides, adjoint-VP induce more pronounced adjustments of
 294 initial temperature and salinity than adjoint-FD (not shown here).
 295



296

297 Figure 8. Adjustments of (a) wind u -component, (b) wind v -component, and (c) 2 meter air temperature normalized
 298 by their prior uncertainties in adjoint-FD and averaged over 2012. Panels (d)-(f) are similar to (a)-(c) but for adjoint-
 299 VP. Panels (g)-(i) are area average of the adjustments of the wind u -component, wind v -component, and 2-m air
 300 temperature normalized by their prior uncertainties in adjoint-FD and adjoint-VP.

301 Moderate wind vector adjustments (with normalized adjustments of 0.2~0.3) occur over the seasonal ice-covered
 302 regions (Figure 8a, b, d, and e) with more pronounced adjustments in adjoint-VP (Figure 8d, e) than adjoint-FD (Figure
 303 8a, b). Besides, maximum adjustments of wind vectors appear in June in adjoint-VP but in May in adjoint-FD (Figure
 304 8g). adjoint-FD adjusts 2-m air temperature more significantly than adjoint-VP in the Arctic Ocean (Figure 8c, f)
 305 and throughout 2012 (Figure 8i).

306 In adjoint-FD, the 2-m air temperature adjustments normalized by their prior uncertainties exceed 1.0 over the
 307 seasonal sea ice-covered regions and the central Arctic Ocean (Figure 8c). While adjoint-VP adjust 2-m air



308 temperature moderately with normalized adjustments of ~0.2-0.3 over the seasonal sea ice-covered regions. The
 309 maximum adjustments occur in June in the two optimization runs (Figure 8i).

310 **Table 3.** Contributions of adjustments of 2-m air temperature, wind vectors, initial temperature and salinity (Initial T
 311 &S), and the remaining control variables (including initial sea ice effective thickness and concentration, 2-m specific
 312 humanity, precipitation, downwelling longwave, and net shortwave radiation) on the total cost reduction, SIC, SST,
 313 and temperature profiles in the two optimization runs.

	Adjoint-FD (%)				Adjoint-VP (%)			
	2-m air temperature	Wind vectors	Initial T & S	The rest	2-m air temperature	wind	Initial T & S	The rest
J_{total}	29.0	17.5	6.0	3.0	5.3	52.6	25.1	5.0
J_{SIC}	25.5	19.8	2.4	1.2	4.5	64.9	10.1	2.4
J_{SST}	41.0	8.6	10.1	5.5	8.4	47.4	29.6	6.4
$J_{prof,T}$	3.9	4.9	4.3	4.3	4.4	40.9	182.0	7.9

314 By replacing the adjusted initial temperature and salinity, wind vectors, 2-m air temperature, and the remaining
 315 control variables (including initial sea ice effective thickness and concentration, 2-m specific humanity, precipitation,
 316 downwelling longwave, and net shortwave radiation) with their original values and estimate their contributions to the
 317 total cost reductions and individual components, including SIC, SST, and temperature profiles (see Table 3).
 318

319 The small contributions of adjustments of the remaining control variables (“The rest” in Table 3) variables to the
 320 cost function reductions in adjoint-FD and adjoint-VP highlight the importance of adjustments on the initial
 321 temperature and salinity, wind vectors and 2-m air temperature simultaneously. In adjoint-FD, adjustments of 2-m air
 322 temperature and wind vectors dominate the cost function reduction, especially SIC components. In contrast, adjoint-
 323 VP rely more on adjustments of wind vectors and initial temperature and salinity. Besides, the more pronounced water
 324 temperature improvements (see Figure 7) in adjoint-VP are mostly attributed to adjustments of initial temperature and
 325 salinity (Table 3).

326 Overall, adjoint-FD improves the model simulation through adjusting 2-m air temperature strongly and wind
 327 vectors moderately. Adjoint-VP adjusts initial conditions, 2-m air temperature, and wind vectors moderately while
 328 achieving a much larger reduction of the model-data misfits. This leads to the conclusion that the large 2-m air
 329 temperature adjustments in adjoint-FD are likely an overcompensation for wind errors that could not be corrected
 330 appropriately because of large errors in the respective cost function gradients.

331 5 The Impacts On Sea Ice Retreat Processes

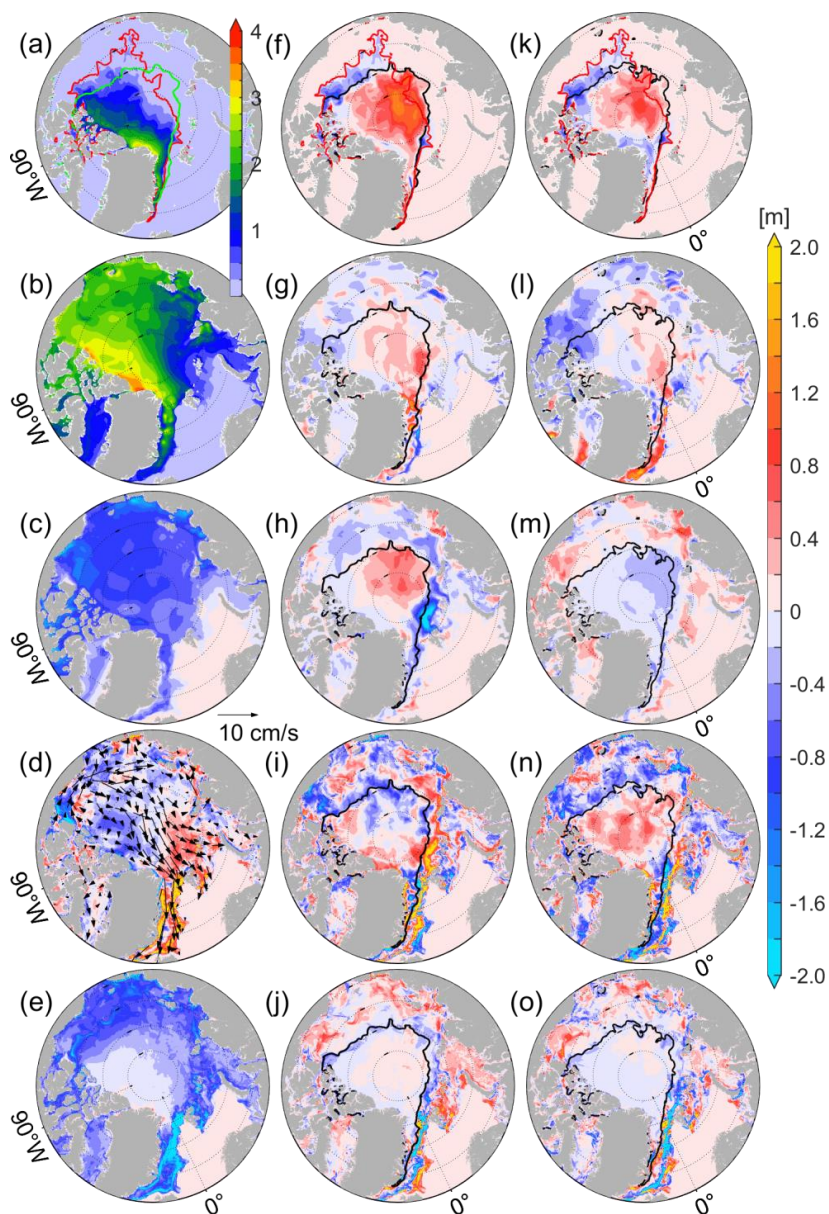
332 A unique characteristic of the adjoint-based synthesis is that its physical processes are described by the governing
 333 equations of the model, allowing us to quantify the sea ice loss and the contributions of ice dynamics and sea ice-
 334 ocean-atmosphere fluxes through a closed budget analysis. Since the two optimization runs reproduce the retreat of
 335 sea ice cover well, we further explore sea-ice effective thickness changes based on the model governing equations:

$$336 \quad H_{Sep} = H_{Apr} + \int (-\nabla \cdot (\bar{u}h) + F_{oi} + F_{ai} + F_{res}) dt \quad (10).$$

337 Ice effective thickness on September 20 (H_{Sep}) depends on effective thickness on April 10 (H_{Apr}), ice advective
 338 flux ($-\nabla \cdot (\bar{u}h)$), ocean-sea ice heat flux (F_{oi}) depending on ocean temperature difference to freezing temperature
 339 (Maykut and Mcphee, 1995), atmosphere-sea ice flux (F_{ai}) consisting of radiation and turbulence fluxes, and a residual



340 term (F_{res}) including a snow flooding effect and a source term to correct negative effective thickness to zero. Since
 341 contributions of the residual terms are small, we will not show them in the analysis below.



342
 343
 344 Figure 9. Sea ice effective thickness on (a) September 20 and (b) April 10, and ice changes due to (c) F_{ais} , (d) F_{adv} ,
 345 and (e) F_{oi} . Panels (f)-(j) and (k)-(o) are differences in the corresponding terms to the control run for (f-j) adjoint-FD
 346 and (k)-(o) adjoint-VP, respectively. The green and red lines are the September SIEs from satellite measurement and
 347 the three runs, respectively.
 348



349 In the control run, the September sea ice covers more area than satellite observations in the Pacific sectors and
350 less area in the eastern Eurasian Basin (red and green lines in Figure 9a). On April 10, effective thickness is up to 1.5
351 m in the Eurasian Basin and ~2.0-2.5m in the Pacific sectors (Figure 9b). From April 10 to September 20, atmosphere-
352 sea ice heat flux melts the ice from the top, which is more pronounced in the Pacific sectors (-1.0~-2.0 m) than in the
353 Eurasian Basin and the central Arctic Ocean (-0.6 m, Figure 9c). F_{adv} moves ice from the central Arctic Ocean to the
354 western Eurasian Basin and out through the Fram Strait (Figure 9d), which is then melted by the warm Atlantic water
355 (Figure 9e). Besides, ocean-sea ice heat flux melts sea ice up to -1.2 m over the seasonal sea ice-covered areas (Figure
356 9e).

357 Adjoint-FD and adjoint-VP reproduce the observed September SIE very well (black lines in Figure 9f, k). The
358 two optimization runs remove the extra sea ice the Pacific sectors of the control run in comparison to the satellite
359 observations (areas enclosed by the red and black lines in Figure 9f, k) through F_{adv} (Figure 9i, n). At the same time,
360 in the central Arctic Ocean, adjoint-FD and adjoint-VP thicken the sea ice up to 1.2 and 0.8 m (Figure 9f, k),
361 respectively.

362 On April 10, adjoint-FD/adjoint-VP show thinner sea ice by -0.2/-0.6 m in the southern Beaufort Gyre and the
363 marginal seas (Figure 9g, l) and thicker sea ice in the Eurasian Basin and the central Arctic Ocean by 0.4 m. During
364 the melting season, adjoint-FD and adjoint-VP show differences mainly in F_{ai} (Figure 9h, m) and F_{adv} (Figure 9i, n).
365 In adjoint-FD, F_{ai} melts more ice in the seasonal sea ice-covered regions (-0.4~-2.0 m) and less ice in the central Arctic
366 Ocean up to 0.6 m (Figure 9h), contributing to the increased effective thickness in September in the central Arctic
367 Ocean. In adjoint-VP, the thickened September ice thickness in the central Arctic Ocean is mainly induced by F_{adv}
368 through ice convergence (Figure 9n). Both adjoint-FD and adjoint-VP enhance ice loss in the marginal seas and the
369 southern Beaufort Gyre (Figure 9j, o) with similar patterns and amplitudes, reflecting that basal melting is mainly
370 related to the SIC changes through ice-albedo feedbacks.

371 We note that a much stronger sea ice loss process occurs from May 10 to June 10 in adjoint-FD than in adjoint-
372 VP, mainly related to surface melting anomalies. During this period, the Arctic Ocean observations rely most on SIC
373 measurements. Both the two optimization run reproduce the observed SIEs well (green and red lines in Figure 10a, d,
374 and b, e), with adjoint-VP (Figure 10b) slightly better than adjoint-FD in the Barent and Kara Seas on June 10 (Figure
375 10e).

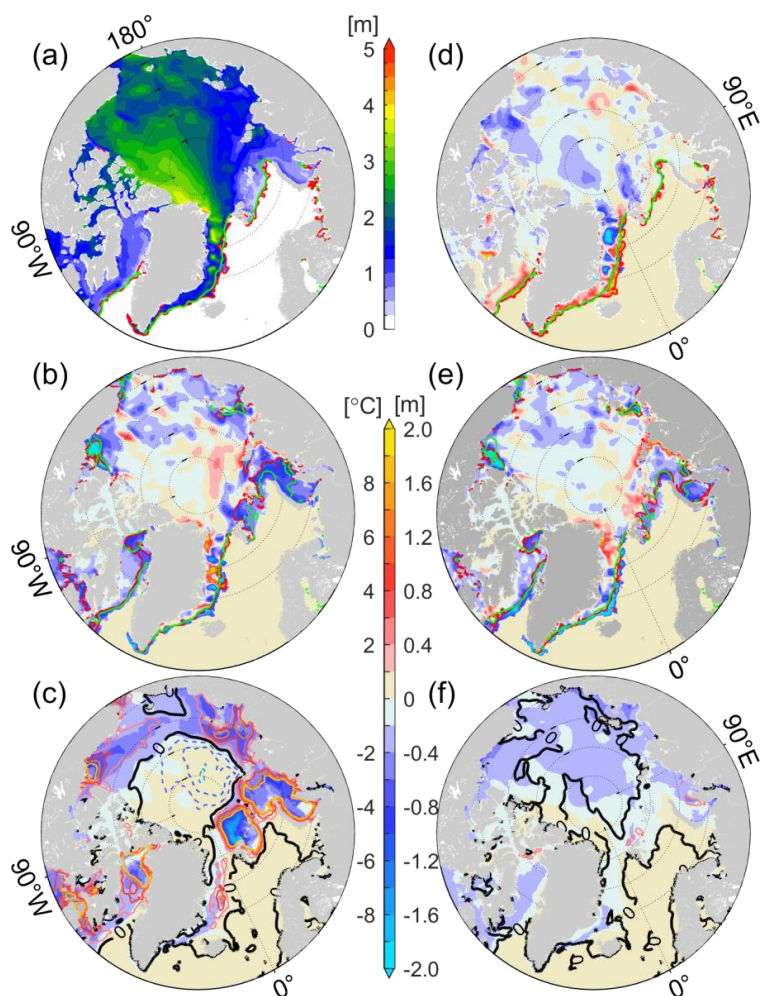
376 On May 10, sea ice has been thinned to ~1.0 m between the central Arctic Ocean and the Chukchi Sea (Figure
377 10a). adjoint-VP shows thinner ice up to -0.6 m than adjoint-FD in the southern Beaufort Gyre, north of Svalbard and
378 Franz-Josef-Land (Figure 10d).

379 From May 10 to June 10, sea ice is melted in the southeastern Beaufort Gyre, the Laptev Sea, the Kara Sea, and
380 north of Svalbard and Franz-Josef-Land, creating open water and polynya (Figure 10b, e), with adjoint-FD (Figure
381 10b) shows much stronger melting than adjoint-VP (Figure 10e). In the Kara and Barents Seas, the intense ice melt in
382 adjoint-FD leads to a further retreat of SIEs (red line in Figure 10b) compared with observations and adjoint-VP (red
383 line in Figure 10e) by June 10.

384 In adjoint-FD, surface melting contributes to strong sea ice thinning up to 0.8-2.0 m (shading in Figure 10c),
385 mainly caused by 2-m air temperature adjustments (contours in Figure 10c). As shown, 2-m air temperature is



386 increased by more than 8°C in the marginal seas (prior air temperature uncertainties are $\sim 2\text{--}5^{\circ}\text{C}$) to facilitate the
 387 intense surface melting. In the central Arctic Ocean, negative 2-m air temperature adjustments up to -6°C result in
 388 little ice melt. In contrast, adjoint-VP shows surface melting of -0.4 m with reasonable air temperature adjustments
 389 ($< 2^{\circ}\text{C}$, Figure 10f).



390

391 Figure 10. (a) Sea ice effective thickness on May 10 in adjoint-FD. Panels (b) and (c) are the sea ice effective thickness
 392 changes and contributions from atmosphere-sea ice heat flux $\int F_{ai}$ from May 10 to June 10. Panel (d) is sea ice
 393 effective thickness differences between adjoint-VP and adjoint-FD (adjoint-VP minus adjoint-FD) on May 10. Panels
 394 (e)-(f) are similar to Panels (b)-(c) but for adjoint-VP. The red and green lines indicate the model-simulated (a-b for
 395 adjoint-FD; d-e for adjoint-VP) and satellite-observed sea ice extent on (a, d) May 10 and (b, e) June 10. The contours
 396 in panels (c) and (f) show the adjustments of 2-m air temperature (see the legend for the amplitude).
 397

398 Overall, the two optimization runs successfully reproduce the sea ice retreat process in 2012 by assimilating
 399 satellite and in-situ measurements. However, the sea ice retreat processes differ in the two optimized solutions,
 especially from May to June, when Arctic Ocean observations rely mostly on satellite-measured SIC. Considering the



400 amplitude of air temperature adjustments, the adjustments of the control variables in adjoint-VP are more reasonable
401 than adjoint-FD, and adjoint-VP seems to project model-data misfits to the control variables more reasonably than
402 adjoint-FD.

403 **6 Conclusions**

404 The adjoint model is a powerful way to calculate sensitivities of a target function to model variables and has been
405 applied to the coupled Arctic ocean and sea ice models for sensitivity studies (Heimbach et al., 2010; Kauker et al.,
406 2009; Koldunov et al., 2013) and state estimate (Fenty and Heimbach, 2013; Koldunov et al., 2017; Lyu et al., 2021b;
407 Nguyen et al., 2021). However, due to the persistent instability issues, traditionally the adjoint of sea ice dynamics
408 was excluded or simplified to the adjoint of a free-drift sea ice model, which potentially hampers the accuracy of the
409 coupled ocean and sea ice estimation.

410 Based on the study of Toyoda et al. (2019) and the coupled ocean-sea ice modeling and adjoint assimilation
411 system (Lyu et al., 2021a), we stabilize the adjoint of a viscous-plastic sea ice dynamic model and test the impacts of
412 including the rheology on estimating the spatio-temporal variations of Arctic ocean and sea ice state.

413 Two optimizations with included and excluded rheology were performed and both show reduced SIC and SIT
414 errors and both reproduce the sea ice retreat well. With the improved SIC retreat processes, adjoint-FD and adjoint-
415 VP also show similar ocean temperature changes in the marginal seas and the southern Beaufort Gyre since solar
416 radiation heats the open water quickly as the sea ice retreats. With the improved adjoint of sea ice dynamics, adjoint-
417 VP allows much stronger adjustments of the initial temperature, resulting in a much more significant improvement in
418 the temperature in the North Atlantic Ocean and the intermediate layer (50-700 m) of the Arctic Ocean.

419 Despite that adjoint-FD compute much stronger sensitivities of the cost function to the wind vectors than adjoint-
420 VP, we note that adjoint-FD adjusts more (less) on 2-m air temperature (wind vectors) than adjoint-VP. It seems that
421 adjoint sensitivities of wind vectors in adjoint-FD is less efficient to reduce the cost function than adjoint-VP during
422 the optimization. And adjoint-FD adjusts 2-m air temperature strongly to reduce the model-data misfits while adjoint-
423 VP adjusts all the control variables considerably to improve the model simulation.

424 Using a sea ice budget analysis, we further examine the sea ice retreat processes in adjoint-FD and adjoint-VP.
425 The control run simulates extra ice in the Pacific sector on 20. September, which is removed through ice advective
426 flux in the optimization runs. At the same time, sea ice in the central Arctic Ocean is thickened compared with the
427 control run caused by reduced surface melting in adjoint-FD and ice convergence in adjoint-VP. We note that adjoint-
428 FD and adjoint-VP show different ice thinning processes from May 10 to June 10 and in the marginal seas. Adjoint-
429 FD showed thicker ice in the marginal seas than adjoint-VP, which is melted by increasing the air temperature
430 enormously (up to 8° C). In adjoint-VP, sea ice thinning is moderate with more reasonable adjustments of air
431 temperature. Therefore, the improvement of the adjoint model in adjoint-VP maps the model-data misfits better to the
432 control variables than adjoint-FD.



433 Parameter uncertainties significantly impact ocean and sea ice simulations (Lu et al., 2021; Massonnet et al.,
434 2014; Sumata et al., 2019), and a lack of direct observations of key parameters potentially result in biases in the model
435 simulation and predictions. The development of the adjoint of the viscous-plastic sea ice dynamics further introduces
436 three parameters, including ice compressive strength constant (P^*), ice strength decay constant (C^*), and ration of
437 normal stress to shear stress (e), into the adjoint model. Sensitivities of the model uncertain parameters could be
438 calculated with the adjoint of the coupled ocean-sea ice model, providing chances to further improve ocean-sea ice
439 estimates through jointly estimating state and parameters.

440 **7 Data availability**

441 The data used to create the plots in the paper are available at Pangaea (<https://issues.pangaea.de/browse/PDI-33039>).
442 Assimilated observations are listed in Table 1; and the up-looking sonar observed sea ice draft are from the Beaufort
443 Gyre Exploration Project (BGEP, <https://www2.who.edu/site/beaufortgyre/>).

444

445 *Author contribution.* G. Lyu designed the experiments, conducted the experiments and analysis. A. Koehl contributed
446 to the experiment design and interpretations. G. Lyu wrote the first draft. A. Koehl, D. Stammer, X. Wu, and M. Zhou
447 contributed to reviewing and editing the manuscript.

448

449 *Competing interests.* The authors declare that they have no conflict of interest.

450

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457 and the Beaufort Gyre Exploration Project for archiving and sharing the EN4, the along-track SLA, and sea ice draft
458 datasets used in assimilation and independent validation.

459

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