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# The Arctic Subpolar gyre sTate Estimate (ASTE): Description and assessment of a data-constrained, dynamically consistent ocean-sea ice estimate for 2002–2017

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## Key Points:

- The 2002–2017 medium-resolution Arctic Subpolar gyre sTate Estimate (ASTE) is constrained to 10<sup>9</sup> satellite and in situ observations.
- Strict adherence to conservation laws ensures all sources/sinks can be accounted for, enabling application for meaningful budget analyses.
- ASTE captures the large-scale dynamics of the Arctic ocean-sea ice system including variability and trends in heat and freshwater storage.

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## Abstract

A description and assessment of the first release of the Arctic Subpolar gyre state Estimate (*ASTER1*), a medium-resolution data-constrained ocean-sea ice model-data synthesis spanning the period 2002–2017 is presented. The fit of the model to an extensive ( $O(10^9)$ ) set of satellite and in situ observations was achieved through adjoint-based non-linear least-squares optimization. The improvement of the solution compared to an unconstrained simulation is reflected in misfit reductions of 77% for Argo, 50% for satellite sea surface height, 58% for the Fram Strait mooring, 65% for Ice Tethered Profilers, and 83% for sea ice extent. Exact dynamical and kinematic consistency is a key advantage of *ASTER1*, distinguishing the state estimate from existing ocean reanalyses. Through strict adherence to conservation laws, all sources and sinks within *ASTER1* can be accounted for, permitting meaningful analysis of closed budgets, such as contributions of horizontal and vertical convergence to the tendencies of heat and salt. *ASTER1* thus serves as the biggest effort undertaken to date of producing a specialized Arctic ocean-ice estimate over the 21st century. Transports of volume, heat, and freshwater are consistent with published observation-based estimates across important Arctic Mediterranean gateways. Interannual variability and low frequency trends of freshwater and heat content are well represented in the Barents Sea, western Arctic halocline, and east subpolar North Atlantic. Systematic biases remain in *ASTER1*, including a warm bias in the Atlantic Water layer in the Arctic and deficient freshwater inputs from rivers and Greenland discharge.

## Plain Language Summary

A 2002–2017 ocean-sea ice product, *ASTER1*, is distributed for use in decadal climate studies in the northern high latitudes. The product is a model-data synthesis, merging approximately a billion satellite and in situ observations with a numerical model. The primary strength of *ASTER1* compared to most existing ocean reanalyses is that strict adherence to the equations describing the fluid flow and conservation laws is built into the product, thus making *ASTER1* free from artificial un-physical sources or sinks and associated “jumps” in the time-evolving state. Furthermore, the product is consistent with most available observations, both used in the synthesis and retained for independent verification. This indicates good large-scale representation of evolving sea-ice, ocean currents and water properties, including year-to-year variability and decadal trends in heat and freshwater storage in the Arctic and subpolar North Atlantic. Some systematic data-model differences remain in the product and highlight where extra data and/or model development will improve the next release. The product and underlying model configuration are freely available to the research community.

## 1 Introduction

The Arctic region has experienced large changes in recent decades. These include near-surface air temperature warming at twice the global rate (Richter-Menge & Jeffries, 2011), rapid decline in multi-year sea ice (Kwok & Cunningham, 2015), enhanced solar radiation absorption in the Western Arctic upper ocean (Timmermans et al., 2018), increased river and glacial discharge (Bamber et al., 2012, 2018; Proshutinsky et al., 2020), and increased influxes of freshwater from the Pacific (Woodgate, 2018) and heat from the Atlantic (Polyakov et al., 2011). Many of these changes have been suggested to trigger positive feedbacks. Enhanced shortwave absorption (Jackson et al., 2010; Perovich et al., 2011; Timmermans et al., 2018), enhanced air-ice-sea momentum transfer (Rainville & Woodgate, 2009; Martin et al., 2014), shoaling of the Atlantic Water layer (Polyakov et al., 2017, 2020), and enhanced heat flux through the Fram Strait (Q. Wang et al., 2020) have all been identified to both result from and further amplify sea-ice thinning.

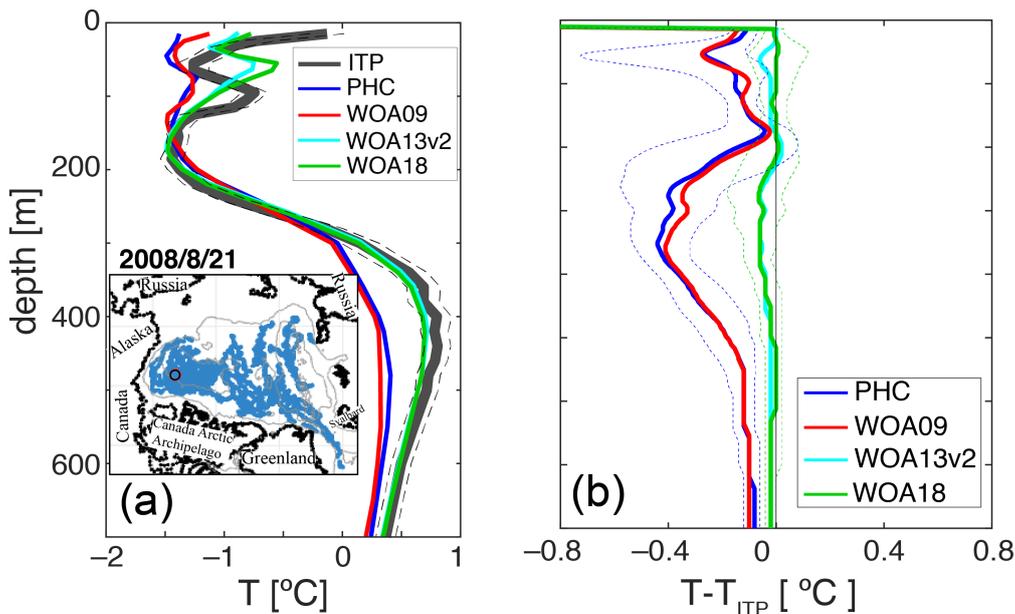
66 Some of the recent changes in the observed Arctic Ocean heat content have been  
67 traced back upstream into the North Atlantic (e.g., Årthun & Eldevik, 2016), and linked  
68 to pulsed warming of the Atlantic Water (AW) inflow (Mulwijk et al., 2018). Tracking  
69 these pulses provides a useful estimate of characteristic circulation and residence timescales  
70 within Arctic Ocean’s boundary currents. For example, it is estimated to take  $O(1-3 \text{ yr})$   
71 for these heat pulses to be carried by the Norwegian Atlantic Current from the Green-  
72 land Scotland Ridge (GSR) to the Fram Strait (Årthun & Eldevik, 2016). After pass-  
73 ing through the Fram Strait, it is estimated that these pulses remain in the Arctic for  
74  $O(15-25\text{yr})$  exiting via the Fram Strait after following either a complete circumpolar path-  
75 way or a shorter circumnavigation of the Eurasian Basin (Karcher et al., 2011; Polyakov  
76 et al., 2011; Timmermans & Marshall, 2020).

77 Similar characteristic timescales emerge from considering the large-scale redistribu-  
78 tion of freshwater in the Arctic. For example, theoretical arguments suggest multi-  
79 decadal timescales for eddy-driven equilibration between the Beaufort Gyre’s circulation  
80 and freshwater content (Manucharyan et al., 2016). Similar timescales also emerge from  
81 considering geometrical constraints on the dynamics of inter-basin exchange to infer resi-  
82 dence times within the Arctic (Haine et al., 2015).

83 It is clear that investigations of mechanisms setting the time-mean and evolving  
84 state of the Arctic and exchanges with surrounding oceans must be supported by basin-  
85 scale estimates of the ocean-sea ice state. Historically, these observations have been ex-  
86 tremely sparse, and in the absence of observational constraints, realistic simulation of  
87 the Arctic and sub-Arctic ocean-sea ice state has remained challenging. There has been  
88 a notable increase, however, in observational coverage since the 2000s. Increasing avail-  
89 ability of *in situ* observations of sub-surface ocean hydrography and oceanic transports  
90 across Arctic gateways continues to improve our understanding of key processes, includ-  
91 ing interior eddy activity and mixing (Timmermans et al., 2012; Cole et al., 2014; Zhao  
92 et al., 2016; Bebieva & Timmermans, 2016), and the transformation and redistribution  
93 of watermasses (Proshutinsky et al., 2009; Rabe et al., 2014; Pnyushkov et al., 2015; Tim-  
94 mermans & Jayne, 2016; von Appen, Schauer, Hattermann, & Beszczynska-Möller, 2015;  
95 Polyakov et al., 2017; Timmermans et al., 2018). In the upper ocean, satellite altime-  
96 try (Kwok & Morison, 2016), gravimetry (Peralta-Ferriz et al., 2014), and sea ice obser-  
97 vations have allowed a more accurate estimate of Ekman transport (Meneghello et al.,  
98 2018) and inventory of freshwater in the Western Arctic (Proshutinsky et al., 2019, 2020).

99 In parallel with increased observational coverage, great progress has also been made  
100 using theoretical and modeling frameworks to advance our understanding of Arctic Ocean  
101 dynamics, for example, elucidating the importance of eddies in gyre equilibration (as noted  
102 above, Manucharyan & Isachsen, 2019; Meneghello et al., 2017) and vertical heat redistri-  
103 bution (Polyakov et al., 2017). Despite this progress, confident assessment of the lo-  
104 cal time-mean state, interannual variability and identification of robust decadal trends  
105 remains a great challenge (Timmermans & Marshall, 2020) due to multiple factors (Holloway  
106 et al., 2007; Q. Wang et al., 2016b, 2016a; Ilicak et al., 2016; Docquier et al., 2019). The  
107 most important amongst these factors is the lack of direct observations throughout the  
108 full water column, including at the air-ice-ocean interface, in and just below the mixed  
109 layer, along the Atlantic Water (AW) boundary current pathway, and at the shelf-basin  
110 regions that connect the dynamics of this energetic current and the relatively quiescent  
111 Arctic Ocean interior (Timmermans & Marshall, 2020).

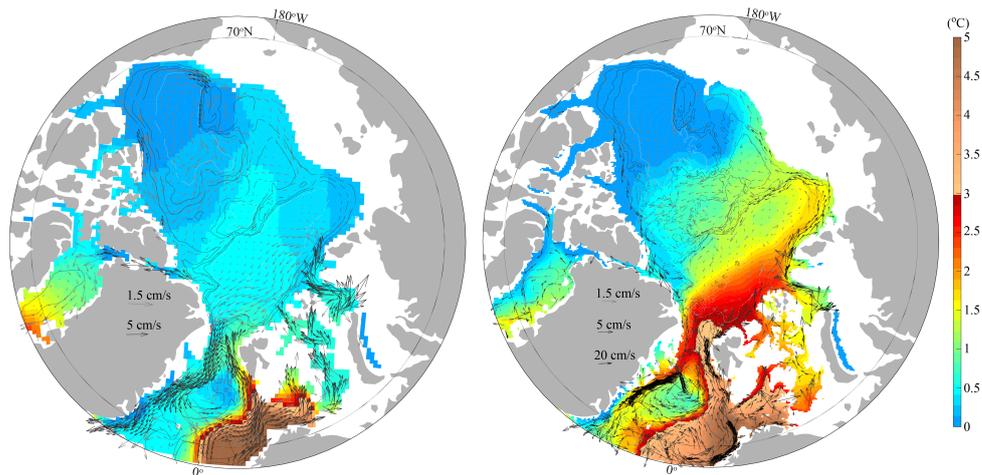
112 To fill in these gaps, the community has constructed climatologies (e.g., WOA13  
113 version 2 and WOA18, Locarnini et al., 2018; Zweng et al., 2018) and data-model syn-  
114 theses (Stammer et al., 2016; Uotila et al., 2019; Carton et al., 2019) which are assumed  
115 to have higher fidelity as the repository of incorporated data grows. The improved fit  
116 between the latest climatology and existing observations is far superior to that seen in  
117 older climatologies. For example, in the Western Arctic interior, Ice Tethered Profilers  
118 (ITP) consistently report warmer temperatures (Fig. 1) than provided by both the Po-



**Figure 1.** Comparison between ITP-derived temperature and the climatologies from the Polar Hydrography Center (PHC, blue), World Ocean Atlas 2009 (WOA09, red), 2013 version 2 (WOA13v2, cyan), and 2018 (WOA18, green). Panel (a) shows this comparison for a single ITP profile on August 21, 2008 (thick dark gray, with the observational uncertainty shown by the thin dashed black lines). The location of the profile is shown in the inset. Panel (b) shows the 50th percentile difference between all ITP temperature profiles in the Canada Basin and the four climatologies. The dotted lines show the 30th and 70th percentile differences.

119 lar Hydrographic Climatology (PHC, Steele et al., 2001) and the World Ocean Atlas 2009  
 120 (WOA09, Locarnini et al., 2010; Antonov et al., 2010), but are in close agreement with  
 121 WOA18. Here it is important to note that this close agreement at the time/location of  
 122 data acquisition is built into the majority of these climatologies and other existing Arctic  
 123 model-data syntheses. These products are constructed using statistical methods such  
 124 as optimal interpolation (e.g., PHC, WOA), 3D-Var, or sequential 4D-Var with short as-  
 125 similation windows (Stammer et al., 2016; Uotila et al., 2019; Mu et al., 2018; Carton  
 126 et al., 2019). The advantage of these methods is that the synthesis ensures a local fit to  
 127 available observations (Fig. 1, Carton et al., 2019). Away from observed locations, how-  
 128 ever, the interpolator relies on incomplete, unavailable or unobtainable information. Miss-  
 129 ing values are, for example, determined via spatial/temporal correlations, potentially de-  
 130 rived from regions/times of very different dynamics. By construction, high frequency vari-  
 131 ability cannot be fully accounted for and as a result spectral agreement with observa-  
 132 tions can be poor (Verdy et al., 2017). Importantly, this type of interpolation – and that  
 133 used in 3D-Var or sequential 4D-Var – can introduce artificial sources/sinks (e.g., of mass  
 134 and enthalpy, Wunsch & Heimbach, 2013), making the resultant product unsuitable for  
 135 robust identification and attribution of change (Stammer et al., 2016).

136 To provide additional support to studies of the Arctic ocean-sea ice system on decadal  
 137 time scales we have developed a new model-data synthesis utilizing the non-linear in-  
 138 verse modeling framework developed within the consortium for Estimating the Circu-  
 139 lation and Climate of the Ocean (ECCO, Stammer et al., 2002; Wunsch & Heimbach,  
 140 2007; Heimbach et al., 2019). The use of the primitive equations as a dynamical inter-  
 141 polator distinguishes our effort from purely statistical approaches. The inversion con-



**Figure 2.** 2002–2015 mean circulation in the Arctic at depth 250 m as represented in ECCOv4r3 (left) and *ASTER1* (right). The color scale shows temperature at the same depth from the two solutions. Vector arrows are grouped into speed ranges of [0–1.5] cm/s (light gray), [1.5–10] cm/s (dark gray) and >[10–20] cm/s (black), with the vector length scales provided for 1.5 cm, 5 cm, and 20 cm.

142 consists of an iterative, gradient-based minimization of a least-squares model-data misfit func-  
 143 tion. Unlike most reanalysis products that are based on sequential data assimilation, only  
 144 independent, uncertain input variables, i.e. initial conditions, surface boundary condi-  
 145 tions and model parameters are adjusted. No periodic analysis increments during the  
 146 estimation period that would incur artificial sources or sinks are permitted. Through strict  
 147 adherence to conservation laws, all sources and sinks within the state estimate can be  
 148 accounted for over the full estimation period, permitting meaningful analysis of closed  
 149 budgets (Buckley et al., 2014; Piecuch & Ponte, 2012).

150 Our work builds upon extensive prior efforts of the ECCO community to produce  
 151 the best kinematically- and dynamically-consistent data-constrained estimates of the ocean  
 152 state across the globe and in various regional domains. Among the publicly available ECCO  
 153 state estimates is ECCO Version 4 Release 3 (ECCOv4r3, Forget, Campin, et al., 2015;  
 154 Fukumori et al., 2018), which has been constrained to satellite and Argo data outside  
 155 of the Arctic, ITP data in the Arctic, and other mooring data at important Arctic gate-  
 156 ways. The ECCOv4 releases have been widely used, with applications including inves-  
 157 tigation of global vertical heat and salt redistribution (Liang et al., 2017; Liu et al., 2019),  
 158 heat budgets in the North Atlantic (Buckley et al., 2014, 2015; Piecuch et al., 2017; Foukal  
 159 & Lozier, 2018) and the Nordic Seas (Asbjørnsen et al., 2019), high-latitude freshwater  
 160 budgets (Tesdal & Haine, 2020), and sea level change (Piecuch & Ponte, 2013).

161 The state-estimation procedure entails reducing the total time- and space-integrated  
 162 model-data misfit. Since ECCOv4r3 is a global solution, reduction of the relatively well-  
 163 sampled misfit at lower latitudes dominates the production of this solution. As a result,  
 164 ECCOv4r3 possesses notable biases in the Arctic (Carton et al., 2019; Tesdal & Haine,  
 165 2020), including a strong anticyclonic circumpolar circulation of Atlantic Water (Fig. 2).  
 166 Furthermore, the ECCOv4r3 horizontal grid spacing of 40–45 km is well above the Rossby  
 167 deformation radius in the Arctic and Nordic Seas (Nurser & Bacon, 2014). This has mo-

168 tivated a dedicated effort to build a higher resolution regional state estimate covering  
 169 the 21st century for use in Arctic decadal climate research, culminating in the Arctic Sub-  
 170 polar gyre sTate Estimate (ASTE).

171 Here we describe the first release of ASTE (*ASTE\_R1*), providing an estimate of  
 172 the ocean-sea ice state for the period 2002–2017. We describe the model configuration,  
 173 observational constraints and the state estimation machinery (section 2) and present the  
 174 model-data misfit reduction (section 3). We then compare our estimates of volume, heat  
 175 and freshwater transports through important Arctic gateways with those in the exist-  
 176 ing literature as well as present an analysis of *ASTE\_R1* heat and freshwater budgets  
 177 for the Arctic Ocean, Greenland-Iceland-Norwegian (GIN) Seas and subpolar North At-  
 178 lantic (section 4). In section 5 we examine how an improved fit is achieved, identifying  
 179 key adjustments of our independent control variables, and review remaining issues in *ASTE\_R1*  
 180 . In section 6 we summarize key findings and discuss future directions.

## 181 2 Methodology

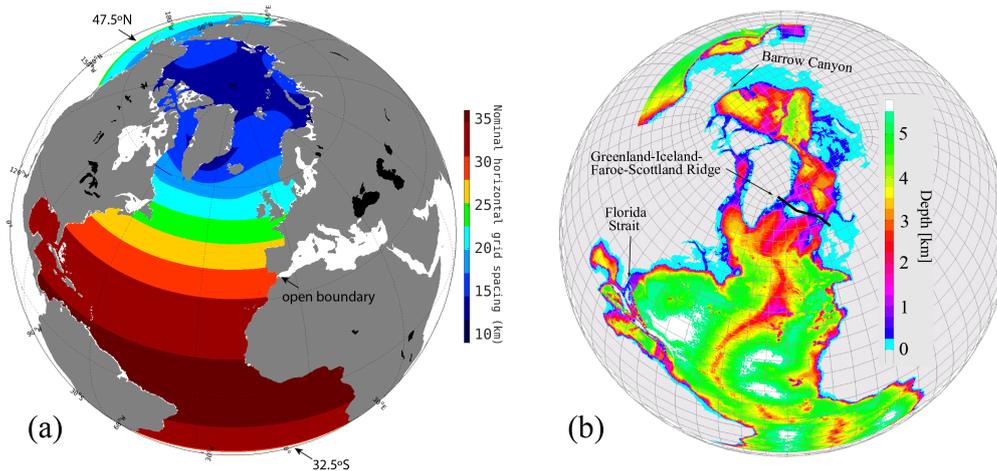
### 182 2.1 Model Description

183 The coupled ocean-sea ice model underlying the estimation framework is an evolved  
 184 version of the Massachusetts Institute of Technology general circulation model (MIT-  
 185 gcm; Marshall et al., 1997; Adcroft et al., 2018). The model solves the primitive equa-  
 186 tions in rescaled  $z^*$  coordinates (Adcroft & Campin, 2004) with a full non-linear free sur-  
 187 face (Campin et al., 2004). The dynamic-thermodynamic sea ice model is an evolved ver-  
 188 sion of Menemenlis et al. (2005); Losch et al. (2010); Heimbach et al. (2010). Eddy-induced  
 189 tracer mixing and transports along isopycnal surfaces are parameterized following Redi  
 190 (1982); Gent and McWilliams (1990).

191 The model uses a finite-volume discretization in a so-called “latitude-longitude-polar-  
 192 cap” grid configuration (LLC grid, Forget, Campin, et al., 2015). The LLC grid is topo-  
 193 logically equivalent to a cubed-sphere grid (Adcroft et al., 2004), but reverts to a reg-  
 194 ular latitude-longitude grid equatorward of  $\sim 57^\circ\text{N}$ . The computational cost associated  
 195 with solving the non-linear optimization problem for eddy-resolving simulations, which  
 196 would need to require resolutions well below 4–15 km for the Arctic Mediterranean (Nurser  
 197 & Bacon, 2014), is prohibitively high. As a compromise, ASTE is based on the medium-  
 198 resolution LLC-270 grid, providing a nominal grid spacing of  $1/3^\circ$ , which corresponds  
 199 to  $\sim 22$  km in the North Atlantic,  $\sim 16$  km in the Nordic Seas, and  $\sim 14$  km in the high  
 200 Arctic interior (Fig 3).

201 The ASTE domain covers the entire Atlantic northward of  $32.5^\circ\text{S}$ , the entire Arc-  
 202 tic and its surrounding seas (Labrador, Nordic, Barents, Bering north of  $47.5^\circ\text{N}$ ) and the  
 203 Canadian Archipelago. The model has 50 unevenly spaced vertical height levels; thick-  
 204 nesses range from 10 m at the surface to 500 m at 5000 m depth. Partial cells (Adcroft  
 205 et al., 1997) are used to improve the representation of topography. The domain has bound-  
 206 aries at  $35^\circ\text{S}$  in the South Atlantic,  $48.6^\circ\text{N}$  in the Pacific, and at the Gibraltar Strait.  
 207 Rationales for choosing a full Atlantic-Arctic domain for ASTE – rather than limiting  
 208 it to the Arctic Mediterranean – are to extend the applicability of the solution to inves-  
 209 tigation of latitudinal connectivity between Atlantic and Arctic variability on decadal  
 210 timescales, and to displace the imposed open boundary conditions far from the region  
 211 of key interest.

212 We prescribe lateral open boundary conditions from the global ECCOV4r3 solu-  
 213 tion, which has been shown to be in good agreement with large-scale constraints from  
 214 Argo and satellites. The bathymetry is a merged version of W. H. F. Smith and Sandwell  
 215 (1997), version 14.1, below  $60^\circ\text{N}$  and the international bathymetric chart of the Arctic  
 216 Ocean (IBCAO, Jakobsson et al., 2012) above  $60^\circ\text{N}$ , blended over a range of  $\pm 100$  km  
 217 about this latitude. Special attention was paid to remove abrupt jumps over the merged



**Figure 3.** (a) Nominal horizontal grid spacing (km) and (b) the bathymetry in ASTE. The lateral open boundaries of the ASTE domain are at  $47.5^{\circ}\text{N}$  in the North Pacific,  $32.5^{\circ}\text{S}$  in the South Atlantic, and at the Gibraltar Strait. White areas in (a), which include the Hudson Bay, Baltic Sea, White Sea, Gulf of St. Lawrence, and all channels in the Canadian Arctic Archipelago except Nares and Barrow Straits, are masked. Depths of several important channels, including the Barrow Canyon, Greenland-Iceland-Faroe-Scotland Ridge and the Florida Strait, were carefully inspected to ensure transports consistent with published observations.

218 region. Model depths within important canyons (e.g. Barrow) and across important gate-  
 219 ways (e.g., Florida Straits, Greenland-Iceland-Faroe-Scotland ridge, Aleutian islands chain,  
 220 Gibraltar Strait) were enforced to be consistent with observations in order to realisti-  
 221 cally simulate key transports and regional circulations.

222 Atmospheric forcing is applied via bulk formulae (Large & Yeager, 2008) over the  
 223 open ocean, with the initial estimate of the atmospheric state variables from JRA-55 (Kobayashi  
 224 et al., 2015). We considered taking ERA-Interim (Dee et al., 2011) – employed by EC-  
 225 COv4r3 (Forget, Campin, et al., 2015; Fukumori et al., 2018) – as our first guess. How-  
 226 ever, this product has a well documented warm bias of up to  $2^{\circ}\text{C}$  in the Arctic (Beesley  
 227 et al., 2000; Freville et al., 2014; Jakobson et al., 2012; Lupkes et al., 2010) that causes  
 228 excessive sea ice melt. ECCOv4r3 accommodated this warm bias through increased sea  
 229 ice and snow wet albedos. Nguyen et al. (2011) showed reasonable modeled sea ice con-  
 230 centration and thickness using the Japanese Reanalysis (JRA-25) without the need to  
 231 increase sea ice albedos above their observed values. For this reason, the updated three-  
 232 hourly, higher-resolution JRA-55 was chosen as the initial surface boundary forcing. Monthly-  
 233 mean estuarine fluxes of freshwater are based on the Regional, Electronic, Hydrographic  
 234 Data Network for the Arctic Region (R-ArcticNET) dataset (Lammers & Shiklomanov,  
 235 2001; A. I. Shiklomanov et al., 2006).

236 As shown in Fig. 2 the ECCOv4r3 solution does not exhibit the anticyclonic cir-  
 237 culation of Atlantic water in the Arctic that is inferred from hydrographic observations  
 238 (Rudels, 2012). For this reason, we elected to initialize from alternative products. Ta-  
 239 ble 1 summarizes our first-guess model input parameters for sea ice, ocean mixing and  
 240 momentum dissipation, along with our choice of ocean-sea ice state to initialize the un-  
 241 constrained simulation. This run serves as iteration 0 of the optimization and will be re-  
 242 ferred to as *it0* for the remainder of the paper. Our selection is informed by existing observation/model-  
 243 based estimates. Importantly, sea ice albedos and drag coefficients are chosen within the  
 244 range of observed and previously optimized estimates Nguyen et al. (2011).

245 The three-dimensional parametric horizontal stirring fields for temperature and salin-  
 246 ity are based on typical values used in the literature (Pradal & Gnanadesikan, 2014), Campin,  
 247 2014 (*pers. comm.*) with consideration for where the ASTE grid resolves the baroclinic  
 248 deformation radius as follows. The vertical background diffusivity  $\mathcal{K}_d$  was set based on  
 249 typical values at latitudes below 79°N of  $\sim 10^{-5}$  m<sup>2</sup>/s and limited observed and mod-  
 250 elled ranges of  $10^{-7}$  to  $10^{-6}$  m<sup>2</sup>/s at high latitudes (Padman & Dillon, 1988; Zhang &  
 251 Steele, 2007; Nguyen et al., 2011; Fer, 2014; Sirevaag & Fer, 2012; Cole et al., 2014). Ver-  
 252 tical diffusivities are enhanced by factor of 10 near the sea floor to mimic lee wave-driven  
 253 mixing (Toole, 2007; Mashayek et al., 2017). Horizontal dissipation is applied as a com-  
 254 bination of biharmonic Leith and Laplacian viscosity (Griffies, 2004; Fox-Kemper & Men-  
 255 emenlis, 2008). At lower latitudes, where eddy effects are better resolved, we follow the  
 256 formulation of Leith (1996) to represent the direct enstrophy cascade at mesoscales. Within  
 257 the attached Gulf Stream, a higher Laplacian viscosity is initially required to reduce the  
 258 Reynolds number and prevent premature separation (Dengg, 1993; Chassignet & Gar-  
 259 rraffo, 2001; Chassignet & Marshall, 2013). In the Arctic Mediterranean, where the de-  
 260 formation radius is 4–10 km, an ad-hoc combination of biharmonic Leith and Laplacian  
 261 viscosity is used to ensure consistency of inflow velocity at the Fram Strait and an ap-  
 262 proximate cyclonic circumpolar AW circulation inside the Arctic (Jochum et al., 2008,  
 263 see Table. 1). The model is spun up for 6 years using repeated year 2002 atmospheric  
 264 forcing and open boundary conditions (Table 1). The ocean, sea ice and snow states at  
 265 the end of this 6 year spin up became the initial condition for the unconstrained *it0* in  
 266 the optimization procedure described next.

## 267 2.2 State Estimation Framework

268 ASTE is formally fit to observations through a gradient-based iterative least-square  
 269 minimization of the model-data misfit function that takes into account data and model  
 270 parameter uncertainties (Nguyen et al., 2017). The gradient with respect to a high-dimensional  
 271 space of uncertain input variables, the “controls”, is obtained via the adjoint of the model,  
 272 derived by means of algorithmic differentiation (AD; Giering et al., 2005; Heimbach et  
 273 al., 2005). The model-data misfit (or “cost”) function is defined as:

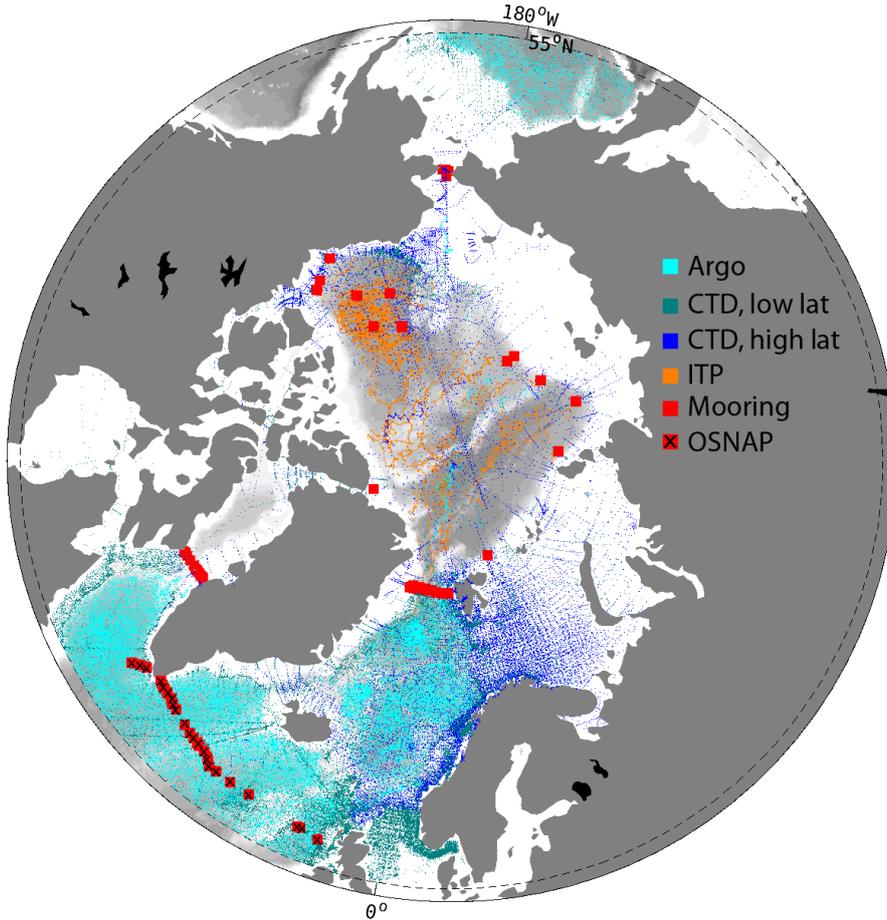
$$\begin{aligned}
 J &= [\mathbf{y}(t) - \mathbf{E}(t)\mathbf{x}(t)]^T \mathbf{R}(t)^{-1} [\mathbf{y}(t) - \mathbf{E}(t)\mathbf{x}(t)] \\
 &+ [\mathbf{x}_0 - \mathbf{x}(0)]^T \mathbf{B}(0)^{-1} [\mathbf{x}_0 - \mathbf{x}(0)] \\
 &+ \sum_{t=0}^{t_f-1} \mathbf{u}(t)^T \mathbf{Q}(t)^{-1} \mathbf{u}(t)
 \end{aligned} \tag{1}$$

274 where  $\mathbf{y}(t)$  is the observation vector and  $\mathbf{x}(t)$  the combined ocean and sea ice state vec-  
 275 tor. The combined initial model state  $\mathbf{x}_0$  and input parameters  $\mathbf{u}(t)$  collectively com-  
 276 prise the control vector  $\boldsymbol{\Omega} \ni \{\mathbf{x}_0, \mathbf{u}(t)\}$ .  $\mathbf{E}$  is the operator mapping the state variables  
 277 to the observations. The model-data misfit  $\mathbf{y}(t) - \mathbf{E}(t)\mathbf{x}(t)$  is weighted by the inverse  
 278 error covariance matrix  $\mathbf{R}(t)$ . This accounts for both observational uncertainty and model  
 279 representation error, where the latter considers the extent to which real variability can-  
 280 not be represented at the chosen model resolution (Nguyen, Heimbach, et al., 2020).  $\mathbf{B}(0)$   
 281 and  $\mathbf{Q}(t)$  are error covariances of  $\mathbf{x}_0$  and  $\mathbf{u}(t)$ , respectively. Full knowledge of  $\mathbf{R}$ ,  $\mathbf{B}$ , and  
 282  $\mathbf{Q}$  is often unattainable (Wunsch & Heimbach, 2007). As a result, the misfit  $\mathbf{y}(t) - \mathbf{E}(t)\mathbf{x}(t)$   
 283 and variables  $\delta\mathbf{x}_0 = \mathbf{x}_0 - \mathbf{x}(0)$  and  $\mathbf{u}(t)$  are often assumed Gaussian, with zero means  
 284 and standard deviations whose squares fill the diagonal entries of their respective covari-  
 285 ance matrices (Wunsch & Heimbach, 2007).

286 There are three distinct contributions to the misfit cost function, eqn. (1). The first  
 287 term describes the normalized model-data squared misfit to be minimized. This term  
 288 sums weighted contributions from all observational data considered. The second term

Field	Value	Reference	Note
<b>Unconstrained run (<i>it0</i>)</b>			
<b>Ocean-sea ice state for Jan/2002 obtained after 6-yr spin up from:</b>			
$\theta_0$	WOA09	Locarnini et al. (2010)	Temperature
$S_0$	WOA09	Antonov et al. (2010)	Salinity
$\mathbf{u}_0$	0.0	–	Ocean velocity
$A_{SI_0}$	PIOMAS	Zhang and Rothrock (2003)	Sea ice concentration
$h_{SI_0}$	PIOMAS	Zhang and Rothrock (2003)	Sea ice thickness
$\mathbf{u}_{SI_0}$	0.0	–	Sea ice velocity
<b>Sea ice parameters:</b>			
$\alpha_{SI_{wet,dry}}$	0.7, 0.68	Johnson et al. (2007)	sea ice albedo
$\alpha_{sn_{wet,dry}}$	0.84, 0.77	Johnson et al. (2007)	snow albedo
$C_{da,dw}$	0.00114, 0.0054	Nguyen et al. (2011)	sea ice-[air,ocean] drag
<b>Mixing and dissipation parameters:</b>			
		Nguyen et al. (2011)	Below 50 m in
	–6.5 to –6.0	Zhang and Steele (2007)	eastern Arctic &
		Padman and Dillon (1988)	below 75 m
$\log_{10}(\mathcal{K}_z)$		Sirevaag and Fer (2012); Fer (2014)	in western Arctic
	–5	Munk (1966)	Outside the Arctic & near
	value plus 1	Mashayek et al. (2017)	surface in the Arctic
$\mathcal{K}_\sigma$	50	Pradal and Gnanadesikan (2014)	Grid points next to land
	17		South of 60°N
			North of 60°N
$\mathcal{K}_{gm}$	50	Pradal and Gnanadesikan (2014)	South of 60°N
	50		North of 60°N
	Leith	Leith (1968)	Ocean interior
$\nu$	Ah=0.0005	Forget, Campin, et al. (2015)	Coastal south of 40.5°N
	Ah=0.003		Coastal north of 40.5°N
<b>Optimized run (<i>ASTER1</i>)</b>			
$\theta_0, S_0, \mathcal{K}_\sigma, \mathcal{K}_{gm}, \log_{10}(\mathcal{K}_z)$ : optimized.			
$\alpha_{SI_{wet,dry}}, \alpha_{sn_{wet,dry}}, C_{da,dw}, \mathbf{u}_0, A_{SI_0}, h_{SI_0}, \mathbf{u}_{SI_0}$ : same as <i>it0</i>			
	Leith	Leith (1968)	South of [70,73]°N in
$\nu$			[Pacific, Atlantic] sector
	Ah=0.0054	Griffies (2004)	North of [70,73]°N in
			[Pacific, Atlantic] sector

**Table 1.** Values of initial ocean and sea ice state, sea ice parameters, and ocean mixing and dissipation for the unconstrained run *it0* and optimized *ASTER1* solution.  $\nu$  is either the biharmonic ( $\text{m}^4/\text{s}$ ) or harmonic ( $\text{m}^2/\text{s}$ ) viscosity, and Ah is the harmonic viscosity coefficient (Griffies, 2004). Units for the mixing coefficients  $\mathcal{K}_{[\sigma, gm, z]}$  are  $\text{m}^2/\text{s}$



**Figure 4.** In situ observations used to constrain ASTE. Red squares with “x” are additional OSNAP mooring data, used for independent evaluation but not part of the cost function.

289 penalizes deviation of the initial state  $\mathbf{x}(0)$  from the initial guess  $\mathbf{x}_0$  (Table. 1). Similarly,  
 290 the third term describes moderation of input parameter adjustments  $\mathbf{u}(t)$  so that the ad-  
 291 justment amplitude does not far exceed the uncertainties. The adjoint (or Lagrange mul-  
 292 tiplier) method consists of augmenting the the cost function (eqn. (1)) with an additional  
 293 term that enforces the strict adherence of the model to the underlying physics along the  
 294 model full trajectory. Once the cost function  $J$  is defined, beneficial control adjustments  
 295 that reduce the misfit are informed by the gradient  $\nabla_{\Omega} J$ . This gradient can be efficiently  
 296 computed for very high-dimensional control spaces using the adjoint model (Wunsch &  
 297 Heimbach, 2007). Control vector adjustments are determined iteratively using a quasi-  
 298 Newton method. Control variable updates are used in a consecutive iteration, in which  
 299 model, model-data misfit, and gradient are recomputed. This iteration is continued un-  
 300 til little further misfit reduction is achieved between successive iterations. This is expected  
 301 when  $J \approx 1$ , i.e., when the state estimate is in agreement with the observations to within  
 302 the error  $\mathbf{R}(t)$ .

303 The ASTE control space  $\{\mathbf{x}_0, \mathbf{u}\} \in \Omega$  comprises the 3D hydrographic initial condi-  
 304 tions, potential temperature and salinity ( $\theta_0, S_0$ ), the time-varying 2D surface atmo-  
 305 spheric state variables, spatially-varying but temporally invariant model coefficients of  
 306 vertical diffusivity ( $\mathcal{K}_z$ ) and parameterized eddy activity ( $\mathcal{K}_\sigma, \mathcal{K}_{gm}$ ), denoting the strength  
 307 of eddy-induced isopycnal diffusivity and potential energy transfer, respectively (Forget,  
 308 Ferreira, & Liang, 2015). The atmospheric state control variables are 2m air tempera-

309 ture,  $T_{air}$ , specific humidity,  $q_{air}$ , downward short- and long-wave radiation,  $R_{sw}$ ,  $R_{lw}$ ,  
 310 precipitation,  $P$ , and 10 m winds  $u_w, v_w$ . Although runoff and evaporation are not part  
 311 of the control space, in practice they project onto the precipitation sensitivities, inter-  
 312 preted as linear combination of net freshwater fluxes (evaporation minus precipitation  
 313 minus runoff, E-P-R). To ensure the adjustments are physically reasonable, *a-priori* un-  
 314 certainties (i.e. the square-roots of the diagonal terms of  $\mathbf{B}$  and  $\mathbf{Q}$ ) are estimated fol-  
 315 lowing Forget and Wunsch (2007) and Fenty and Heimbach (2013a) for oceanic hydrog-  
 316 raphy and Chaudhuri et al. (2013, 2014) for atmospheric forcing.

317 The vector  $\mathbf{y}(t)$  contains as many available ocean and sea ice observations as prac-  
 318 tical. They include the standard suite of in-situ and remotely-sensed ocean and sea-ice  
 319 data used in ECCOV4r3 (Fukumori et al., 2018), augmented by updated high latitude  
 320 in-situ data at important Arctic gateways and in the Arctic interior. The estimation pe-  
 321 riod chosen for ASTE, 2002–2017, leverages the increase in satellite (GRACE, ICESat-  
 322 1/2, CryoSat-2) and in situ (ITP) observations in the Arctic. In total, approximately  $1.2 \times 10^9$   
 323 observations were employed to constrain distinct aspects of the modeled ocean and sea-  
 324 ice state, culminating in the optimized *ASTE.R1* solution. Distinct datasets are sum-  
 325 marized in Table 2. Key among these are satellite-based observations of sea level anoma-  
 326 lies (SLA) to aid removal of the precipitation bias in JRA-55, Argo and lower latitude  
 327 CTD to improve surface and sub-surface hydrography in the North Atlantic and Nordic  
 328 Seas, and a suite of moorings in the Arctic. This suite includes the Fram Strait moor-  
 329 ing array to constrain the boundary current strength and heat flux from the Nordic-Seas  
 330 into the Arctic, and the combined ITP and Beaufort Gyre moorings to constrain the Canada  
 331 Basin hydrography. Finally, OSSISaf daily sea ice concentration was essential for con-  
 332 straining the ice edge and upper ocean hydrography in the Arctic and its surrounding  
 333 marginal seas.

334 The practical implementation of eqn. (1) follows that described in Forget, Campin,  
 335 et al. (2015). Several approximations to parameterization in the adjoint model were made  
 336 to ensure stable behaviour. Maximum isopycnal slopes are limited in the GM/Redi pa-  
 337 rameterization, the vertical mixing scheme (K-Profile Parameterization, Large et al., 1994)  
 338 is omitted in the adjoint, and increased horizontal and vertical momentum dissipation  
 339 are employed in the adjoint to suppress fast growth of unstable sensitivity.

340 The full sea ice adjoint, as described in Fenty and Heimbach (2013a); Fenty et al.  
 341 (2015), was not used in this study (nor in ECCOV4), due to persistent instability issues.  
 342 In its place, the sea ice concentration model-data misfit is used to relate air-sea fluxes  
 343 to the enthalpy of the integrated surface ocean-sea ice system as follows. Where the model  
 344 has an *excess/deficiency* of sea ice, extra heat is added to/removed from the system to  
 345 bring the sea surface to above/below the freezing temperature. In these two cases, the  
 346 pseudo-sea ice cost function contributions  $J_{\text{seaice\_conc\_}[ex,de]}$  are in enthalpy units rather  
 347 than normalized model-data misfits. Normalization is chosen to obtain amplitudes com-  
 348 parable to other model-data misfits  $J_i$  contributing to the total cost function  $J$ , so that  
 349 these terms play an active role in the optimization. Lastly, convergence – if achievable  
 350 for these two pseudo-sea ice costs – is when they approach zero and not unity.

351 After 62 iterations, adjustments are obtained for the initial conditions, 3D inter-  
 352 nal mixing fields, and surface atmospheric state. The initial conditions of the optimized  
 353 state, ASTE Release 1 (*ASTE.R1*), are derived by adding the adjustments  $[\Delta\theta, \Delta S]_{i62}$   
 354 to the first guess fields  $[\theta, S]_{i0}$ . The same holds for the optimized mixing fields and sur-  
 355 face atmospheric state (see Table 1).

356 The full monthly mean state of *ASTE.R1* is distributed via the ECCO & ASTE  
 357 data portal at the Texas Advanced Computing Center (TACC). In addition, the model  
 358 configuration, required input fields and code are distributed to enable reruns (see Ap-  
 359 pendix A). Since the focus of ASTE is on the North Atlantic and the Arctic Ocean, we  
 360 restrict both the discussion presented below and the distributed *ASTE.R1* fields to lat-

itudes above  $10^{\circ}\text{N}$ . As for ECCOv4r3, the mass, salt, and heat budgets in *ASTE\_R1* are fully closed when computed using the distributed standard ECCO diagnostics that we provide. In Appendix B, we show how lateral transports may be accurately computed and provide estimates for the errors incurred in offline calculations using the *ASTE\_R1* monthly mean diagnostics.

### 2.3 Making Meaningful Model-Observation Comparisons

A meaningful assessment of *ASTE\_R1* through comparison with observations is non-trivial and requires careful consideration. One of the biggest challenges is properly accounting for the sparse spatio-temporal sampling and the potential for aliasing. For example, measurements might only be taken at a discrete location (e.g. a mooring) or along-track (i.e., with high along-track coverage and drastically lower resolution in the cross-track direction) or only during summer months (e.g., ship-based CTD). “Averages” of these measurements (e.g., average Argo or ITP data over 1 month or 1 year) incurs aliasing in both space and time as well as potential spatial or seasonal biases. “Averages” of *ASTE\_R1* outputs at the smallest spatial scale (grid cell size), on the other hand, are over a spatial area of  $\sim 200 \text{ km}^2$ . Unless observations are well sampled over this grid-area, a direct comparison between observations and *ASTE\_R1* can be problematic. Furthermore, *ASTE\_R1* does not resolve eddies in the Arctic and GIN Seas. As a result, we should neither expect nor demand a perfect fit to discrete (in space/time) measurements. The ECCO framework utilizes “representation errors” in the weighting of the model-data misfits, eqn. (1), to safeguard against over-fitting and facilitate more meaningful model-data comparison (Wunsch & Heimbach, 2007). However, these representation errors are themselves highly unconstrained often relying on unconstrained high-resolution model runs for their derivation (see Nguyen, Heimbach, et al., 2020, for a more detail discussion).

In Section 3 we present both normalized misfit reductions as well as comparisons of dimensional transports and heat/freshwater contents. For the dimensional quantities, several potential challenges can emerge related to resolution and bias issues, which we briefly discuss in the following. A serious challenge stems from the need to compare watermasses in the presence of hydrographic biases. From observations, watermasses are often defined in temperature, salinity, and density ( $T, S, \sigma$ ) space with tight thresholds/bounds reflecting the measurement precision (e.g. to the first or second decimal place). These definitions can be problematic to adopt in *ASTE\_R1*, where we are averaging over grid-cell areas of  $\sim 200 \text{ km}^2$  and thicknesses of 10–500 m. Furthermore, in some regions the model representation errors may be up to an order of magnitude larger than measurement precision. In these regions, the normalized misfit can be within acceptable range but *ASTE\_R1* can still possess notable absolute ( $T, S, \sigma$ ) biases if the representation errors are large. For this reason, a watermass is likely to exist in *ASTE\_R1* but with modified thresholds/bounds. Where appropriate, we analyzed *ASTE\_R1* carefully in ( $T, S, \sigma$ ) space to identify suitable classifications for calculation of watermass transports. Details on the modified bounds are provided in Appendix C.

A second challenge is related to the region over which derived quantities are computed. In cases where these regions are defined with geographic bounds based on availability of observations rather than dynamical regimes, the equivalent derived quantities in *ASTE\_R1* can be highly sensitive to small shifts in bounding region, especially when the grid resolution and uncertainties in the control input parameters (e.g., forcing, internal mixing) are taken into account. For this reason, we also explore the sensitivity of area/volume integrals to choice of geographical bounds in Appendix C.

Lastly, comparison of (dimensional) integrated transports can be problematic due to spatial sampling issues and representation error, preventing precise estimation of narrow boundary currents in *ASTE\_R1*. An example is at the Fram Strait, where the *ASTE\_R1* grid cannot resolve the e-folding scale of the West Spitsbergen Current (Beszczynska-

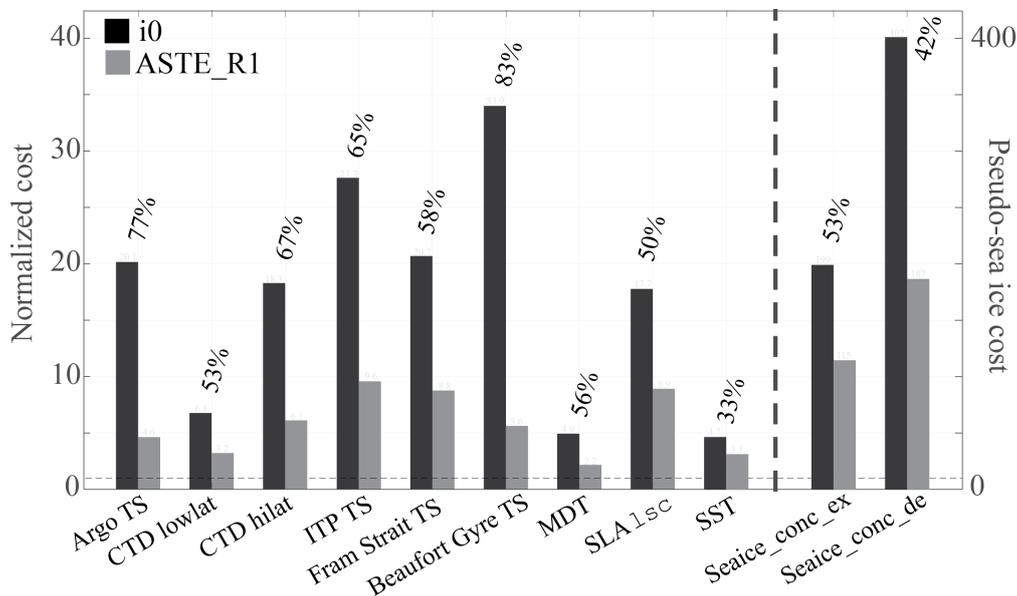
Data Type	Spatial coverage	Temporal coverage	Description	Source
<b>Sea ice</b>				
Velocity <sup>1</sup>	N.Hemis	2002–2012	passive microwave & AVHRR & IABP	<a href="http://rkwok.jpl.nasa.gov/radarsat/3dayGr_table.html">rkwok.jpl.nasa.gov/radarsat/3dayGr_table.html</a> <a href="http://nsidc.org/data/docs/daac/nsidc0116_icemotion.gd.html">nsidc.org/data/docs/daac/nsidc0116_icemotion.gd.html</a> Kwok and Cunningham (2008), Fowler et al. (2013)
	N.Hemis	2012–2015	ASCAT & SSMI	<a href="http://ftp.ifremer.fr/ifremer/cersat/products/gridded/psi-drift">ftp.ifremer.fr/ifremer/cersat/products/gridded/psi-drift</a>
Thickness <sup>1</sup>	N.Hemis	2011–2017	CryoSat-2	<a href="http://www.meereisportal.de/datenportal.html">www.meereisportal.de/datenportal.html</a> & Ricker et al. (2017)
	N.Hemis	2010–2017	SMOS	<a href="http://icdc.zmaw.de/l3c-smos_sit.html">icdc.zmaw.de/l3c-smos_sit.html</a> & Tian-Kunze et al. (2014)
	N.Hemis	2003–2008	ICESat	<a href="http://rkwok.jpl.nasa.gov/icesat/index.html">rkwok.jpl.nasa.gov/icesat/index.html</a> & Kwok and Cunningham (2008); Kwok et al. (2009)
Concentration	N.Hemis	2002–2017	SSMI & OSISaf	<a href="http://osisaf.met.no/p/ice/index.html">osisaf.met.no/p/ice/index.html</a> & Lavergne et al. (2019)
<b>Ocean</b>				
ITP (T,S)	Arctic	2004–2017	Profilers	<a href="http://www.whoi.edu/itp/data/">www.whoi.edu/itp/data/</a> Krishfield et al. (2008), Toole et al. (2011); Krishfield (2020),
Hydrographic Survey (T,S)	GINs	2002–2006	ASOF	<a href="http://www.pangaea.de/">www.pangaea.de/</a>
	Beaufort Sea	2003–2017	BGOS	<a href="http://www.whoi.edu/beaufortgyre/home/">www.whoi.edu/beaufortgyre/home/</a> <a href="https://doi.org/10.1594/PANGAEA.761766">doi.pangaea.de/10.1594/PANGAEA.761766</a> & Bauch et al. (2009)
	Laptev Sea	2002–2003		<a href="https://doi.org/10.1594/PANGAEA.763451">doi.pangaea.de/10.1594/PANGAEA.763451</a> & Bauch et al. (2011)
	East Arctic	2007		<a href="https://doi.org/10.1594/PANGAEA.763451">doi.pangaea.de/10.1594/PANGAEA.763451</a> & Bauch et al. (2011)
Mooring (T,S,currents)	GINs	2002–2013		Våge et al. (2015)
	Fram Strait	2002–2017	ASOF	Fahrbach et al. (2001), Beszczynska-Möller et al. (2012)
	East Arctic	2002–2015	NABOS	<a href="http://nabos.iarc.uaf.edu/">nabos.iarc.uaf.edu/</a> , Pnyushkov et al. (2013) and
	West Arctic	2002–2015	CABOS	Polyakov et al. (2012)
	Beaufort Gyre	2004–2017	BGOS	<a href="http://www.whoi.edu/website/beaufortgyre/data">www.whoi.edu/website/beaufortgyre/data</a>
	Bering Strait	2002–2017		<a href="http://psc.apl.washington.edu/HLD/Bstrait/Data/">psc.apl.washington.edu/HLD/Bstrait/Data/</a> & Woodgate (2018)
Transports <sup>1</sup> of Vol & Heat & Freshwater	Davis Strait	2004–2015		<a href="http://iop.apl.washington.edu/data.html">iop.apl.washington.edu/data.html</a> , Curry et al. (2011)
	Fram Strait	2002–2017	ASOF	Schauer and Fahrbach (2004) & Beszczynska-Möller et al. (2012)
T,S	Bering Strait	2002–2017	mooring	Woodgate (2018)
	High Latitude	2002–2015	IARC	<a href="http://oregon.iarc.uaf.edu/dbaccess.html">oregon.iarc.uaf.edu/dbaccess.html</a>
			IARC	<a href="http://climate.iarc.uaf.edu/geonetwork/srv/en/main.home">climate.iarc.uaf.edu/geonetwork/srv/en/main.home</a>
			ICES	<a href="http://ocean.ices.dk/HydChem/HydChem.aspx?plot=yes">ocean.ices.dk/HydChem/HydChem.aspx?plot=yes</a>
	CAA	2002–2015	SBI	<a href="http://www.eol.ucar.edu/projects/sbi/">www.eol.ucar.edu/projects/sbi/</a>
Arctic	2002–2015	BIO	<a href="http://www.bio.gc.ca/science/data-donnees/base/run-courir-en.php">www.bio.gc.ca/science/data-donnees/base/run-courir-en.php</a>	
Arctic	2002–2015	ACADIS	<a href="http://www.aoncadis.org/home.htm">www.aoncadis.org/home.htm</a>	
Arctic	2002–2015	WHOI	(Krishfield, 2020)	

**Table 2.** Satellite and *in situ* data currently used to constrain or assess ASTE in addition to the standard ECCOv4r3 set. <sup>1</sup>datasets that are used only for assessment and not part of the cost function.

413 Möller et al., 2012). Enforcing fit to the observed mooring velocity would likely result  
 414 in an overestimation of the net inflow volume transport here. In *ASTE\_R1*, velocities  
 415 at gateways were not employed as active constraints but were used for offline assessment  
 416 of the derived transports. Ultimately, however, the spacing between discrete moorings  
 417 offers incomplete information on the total volume transports across a given gateway, and  
 418 existing observation-based estimates generally require various assumptions on spatial/temporal  
 419 correlations in order to interpolate between the mooring measurements. As a result, our  
 420 direct comparisons of *ASTE\_R1* and observation-based transports presented below seeks  
 421 consistency in terms of sign and order of magnitude rather than exact agreement of am-  
 422 plitude. This is especially true for assessment of *ASTE\_R1* heat/freshwater transports,  
 423 computed relative to the wide range of reference values used in the literature.

### 424 3 Model-data misfit reduction and residuals

425 We begin by assessing the *ASTE\_R1* solution in context of existing observation-  
 426 based estimates of the circulation and hydrography in the Arctic. We summarize the re-  
 427 duction in the integrated model-data misfits and costs achieved in the production of *ASTE\_R1*  
 428 . We then expand this discussion, considering the *ASTE\_R1* fit to constraints in the Ar-  
 429 ctic, GIN Seas, and Subpolar North Atlantic in turn (sections 3.1-3.3). Note that assim-  
 430 ilation aids – but by no means guarantees – model-data consistency due to errors and/or  
 431 deficiencies in the data, model, and/or state estimation framework. This point will be  
 432 revisited in our discussion in section 5. We refer to “misfit” as the dimensional model  
 433 minus data difference, “normalized misfit” as misfit scaled by the respective uncertainty  
 434 (dimensionless), and “normalized cost” or “cost” as the square of the normalized mis-  
 435 fit (dimensionless). The overall cost reductions in *ASTE\_R1* have been grouped into sev-  
 436 eral categories as shown in Fig. 5 and summarized in Table 3.



**Figure 5.** Individual costs calculated from key data sets that were used in the optimization. The numbers listed above each data set are the percentage of cost reduction in *ASTE\_R1* compared to *it0*. The magnitudes of the two pseudo-sea ice costs are indicated on the right y-axis.

Cost name	Normalized cost		Percentage reduction (%)
	<i>it0</i>	<i>ASTE_R1</i>	
$J_{\text{Argo\_TS}}$	20.1	4.6	77
$J_{\text{CTD\_lowlat}}$	6.8	3.2	53
$J_{\text{CTD\_hilat}}$	18.3	6.1	67
$J_{\text{ITP}_{\text{TS}}}$	27.7	9.6	65
$J_{\text{FramStrait}_{\text{TS}}}$	20.7	8.8	58
$J_{\text{BeaufortGyre\_TS}}$	33.9	5.6	83
$J_{\text{BeringStrait\_TS}}$	6.3	4.2	33
$J_{\text{DavisStrait\_TS}}$	3.8	4.3	-11
$J_{\text{NABOS\_TS}}$	43.1	25.3	41
$J_{\text{StAnnaTrough\_TS}}$	22.9	7.2	69
$J_{\text{seaice\_conc\_ex}}$	402	187	53
$J_{\text{seaice\_conc\_de}}$	199	115	42
$J_{\text{SST}_{\text{[Reynolds+TMI/AMSRE]}}}$	4.7	3.1	33
$J_{\text{MDT}}$	4.9	2.2	56
$J_{\text{SLA}_{\text{[gfo+ers+tp]}}}$	2.7	1.4	49
$J_{\text{SLA}_{\text{lsc}}}$	17.7	8.9	50
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$J_{\text{seaice\_area15}}^{(o)}$	1.0	0.36	64
$J_{\text{seaice\_extent15}}^{(o)}$	1.0	0.17	83
$J_{\text{seaice\_thickness}}^{(o)}$	22.0	25.8	-17
$J_{\text{seaice\_UV}}^{(o)}$	2.1	1.6	23
$J_{\text{FramStrait\_vNorth}}^{(o)}$	1.3	1.0	26
$J_{\text{NABOS\_mmpUV}}^{(o)}$	2.0	1.6	23
$J_{\text{OSNAP\_TS}}^{(o)}$	6.3	3.5	44
$J_{\text{lineW\_TS}}^{(o)}$	3.3	2.5	26

**Table 3.** Active and offline costs and reductions in *ASTE\_R1* compared to *it0*. The quantities listed above the triple horizontal lines contribute directly to the total  $J$  in Eqn 1, while those listed below the triple horizontal lines ( $J^{(o)}$ ) are used only for offline assessment and do not influence the optimization. The offline sea ice area and extent (both defined using the common 15% cutoff threshold) costs are normalized by the Arctic Mediterranean’s area.

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### 3.1 Arctic

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#### 3.1.1 Sea ice

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Improved representation of sea ice extent in *ASTER1* (compared to the unconstrained simulation) is indicated by a significant reduction of  $J_{\text{seaiceconc}[ex,dec]}$  by 53% and 42%, respectively (Table 3, Fig. 5). Fenty and Heimbach (2013b) showed that these improvements can be effectively achieved through small adjustments of atmospheric controls, within their uncertainty range. These improvements are independently confirmed by the reduction in passive misfits for sea ice area ( $J_{\text{seaice\_area15}}$ , 64%) and extent ( $J_{\text{seaice\_extent15}}$ , 83%) (Table 3). The largest improvements occur in the seasonal ice zones e.g., Greenland and Barents Seas and Southern Beaufort Gyre (Fig. 6a) associated with a systematic decrease in total simulated area/extent without alteration of the seasonal cycle (Fig. 6b).

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The improved sea ice edge representation in *ASTER1* (Fig. 6e,h) is accompanied by a reduction in the passive misfits for sea ice velocities ( $J_{\text{seaice\_vel}}$ , Table 3), primarily in locations where nonzero ice velocities in *it0* were accompanied by observations of zero ice concentration and vice versa. Unlike velocity, however, the sea ice thickness costs  $J_{\text{seaice\_thickness}}$  did not decrease (Table 3), primarily because the pseudo-sea ice adjoint does not contain physics relating ice thickness to the atmospheric forcing or ocean interaction from below. We will return to this in section 6.

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#### 3.1.2 Fram Strait

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The dynamics in the vicinity of the Fram Strait are highly complex, governed by strong air-ice-ocean interaction, vigorous generation of eddies associated with highly sheared boundary currents and their recirculations in the presence of significant topographic steering (Beszczynska-Möller et al., 2012; de Steur et al., 2014; von Appen, Schauer, Hattermann, & Beszczynska-Möller, 2015; von Appen, Schauer, Somavilla Cabrillo, et al., 2015; Hattermann et al., 2016). Due to this complexity, correct simulation of Atlantic Water inflow from the Nordic Seas is non-trivial (e.g., Nguyen et al., 2011; Ilicak et al., 2016; Docquier et al., 2019) and the local moorings provide an important constraint.

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Daily-average moored velocity for the years 2002–2011 at various depths along the entire array (Beszczynska-Möller et al., 2011, 2012) were used to constrain the *ASTER1* velocity across the strait. The mooring temperature and salinity constrain the inflow and outflow of AW. Additional data available for the years 2012–2017 (von Appen, Schauer, Somavilla Cabrillo, et al., 2015) were withheld from the optimization and used instead for offline evaluation. We find that optimizing the circulation to the 2002–2011 data yields AW properties which are also consistent with the 2012–2017 data withheld.

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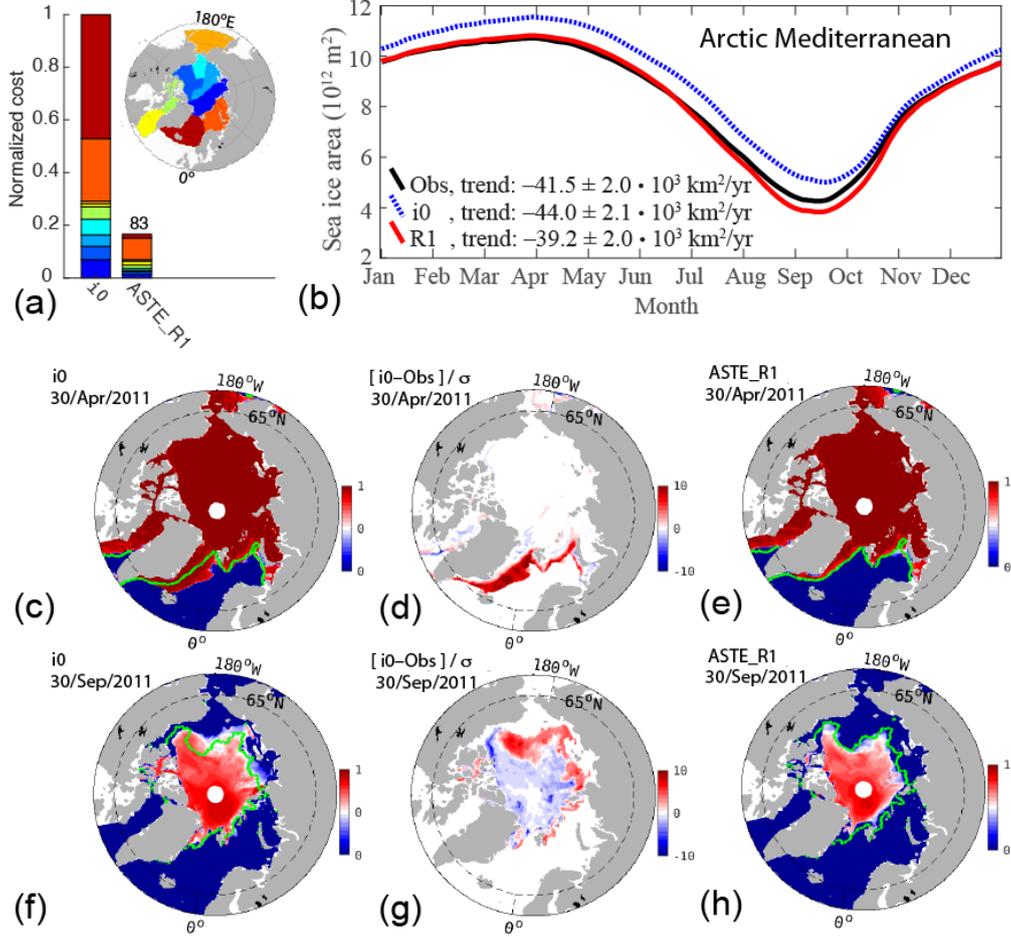
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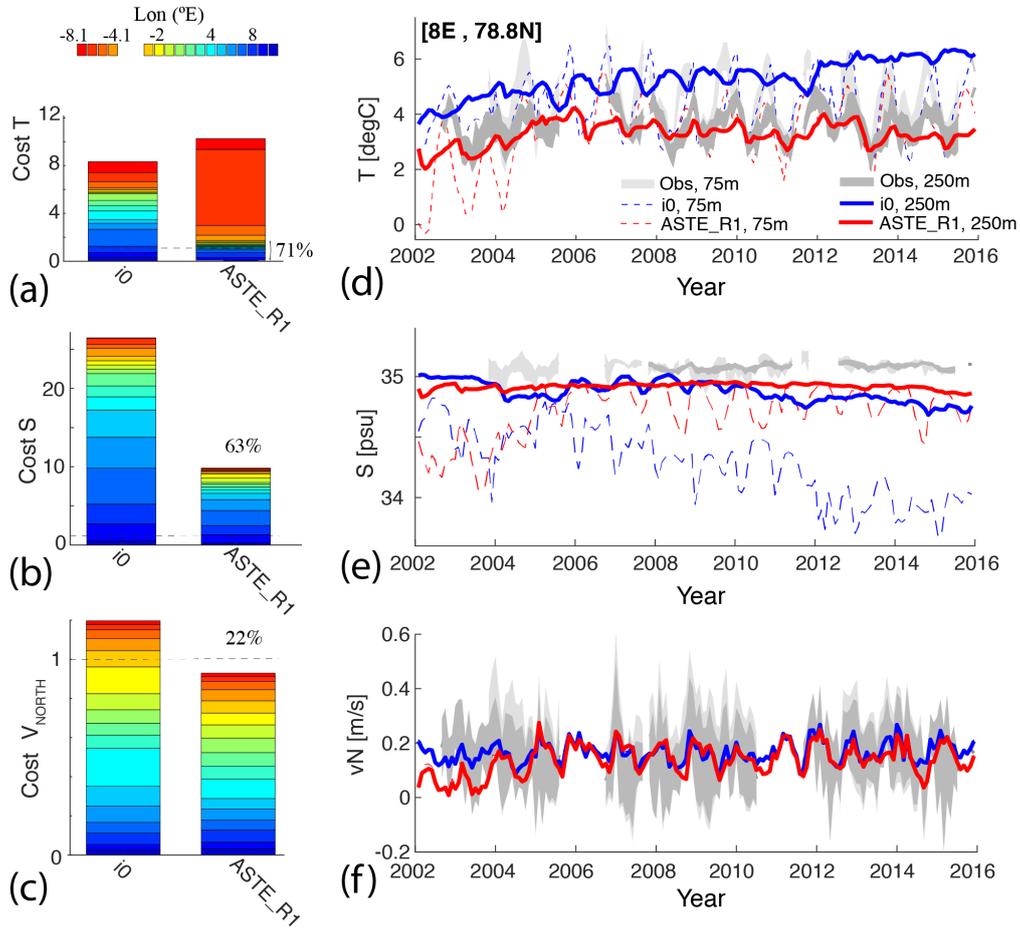
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Fig. 7 shows the unconstrained *it0* and *ASTER1* misfits to moored  $T$ ,  $S$ , and northward velocity. The normalized misfit in temperature as a function of longitude is reduced by 71% compared to the unconstrained *it0* simulation (Fig. 7a). On the shelf west of  $4^\circ\text{W}$ , *ASTER1* has a warm bias compared to the observations, which resulted in higher misfits here (red bar between longitude  $8.1^\circ\text{W}$  and  $4.1^\circ\text{W}$  in Fig. 7a). The reduction in misfits for inflow of the AW, however, is more important for the large-scale Arctic hydrography, as AW passing through this important gateway propagates along the entire boundary of the Eastern Arctic and into the Canada Basin. Here its properties can be compared to ITP data, which serve as the main constraint on subsurface  $T/S$  over the entire pathway from the Fram Strait (see section 3.2.3). The misfit reduction can be seen for one example mooring at approximately  $8^\circ\text{E}$  (Fig. 7d–f) at multiple depths. The significant improvement in salinity at the surface (dashed blue in Fig. 7e) is related to the improved ice edge (see also Fig. 6c–e). Another significant improvement is in the AW core temperature at depth  $\sim 250$  m (solid blue and red lines in Fig. 7d).



**Figure 6.** Comparison of sea ice misfits in the Arctic Mediterranean, for the unconstrained *it0* and fully optimized *ASTE\_R1* solution, assuming the standard 15% cutoff threshold for both total ice area and extent. Comparison of (a) cost (misfit squared) to observed sea ice extent,  $J_{\text{seaice\_extent15}}^{(o)}$ , showing contributions from individual basins. Comparison of (b) 12-month climatology of sea ice area, also showing observation-based climatology from OSSISaf (black). The climatology and the trends listed in the legend were derived from the 01/Jan/2002–31/Dec/2017 time-series. Comparison of daily sea ice concentration between (c,f) *it0* and (e,h) *ASTE\_R1* for days selected at times of (c,e) maximum and (f,h) minimum ice extent. The green contour in panels (c,e,f,h) delineates the observed sea ice concentration from OSSISaf at the indicated dates. The optimization acts to reduce concentration at the ice margin where notable biases exist in *it0*. These biases are shown normalized by uncertainty in the OSSISaf observations for (d) 30/Apr/2011 and (g) 30/Sep/2011.



**Figure 7.** Normalized cost at Fram Strait for (a) temperature, (b) salinity, and (c) northward velocity between moored observations and unconstrained *it0* and *ASTE\_R1* solutions, plotted as a function of longitude. Time series of (d) temperature, (e) salinity, and (f) northward velocity at one example mooring at [8°E,78.8°N] for depths 75 m and 250 m show that these properties are improved over the entire observed record. Grey envelopes in (d,e,f) show observed monthly-mean  $\pm$  monthly-std values, with monthly values derived from the daily-mean values for each observed variable.

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### 3.1.3 Canada Basin hydrography

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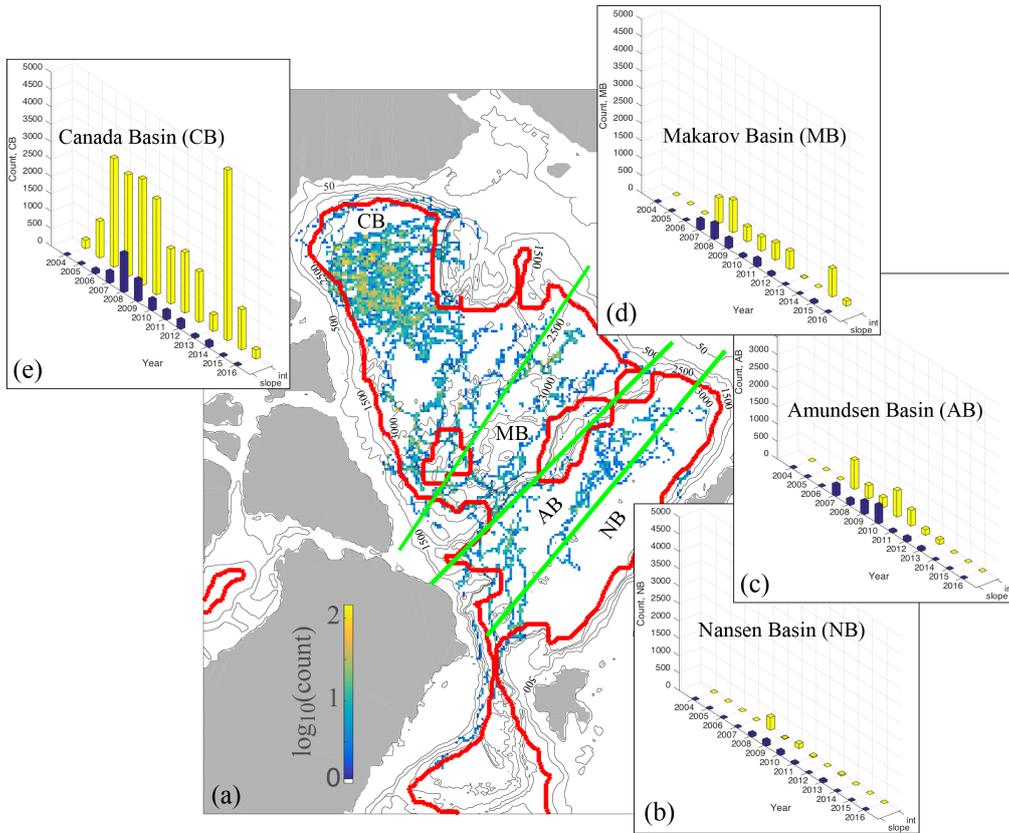
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Once the AW, via the West Spitsbergen Current, crosses the Fram Strait and traverses the Eastern Arctic along the continental slope (Rudels, 2015; Pnyushkov et al., 2018; Polyakov et al., 2017), the watermass properties (e.g., current strength and direction, density, temperature) are not as well constrained due extreme data paucity in the Eastern Arctic. In particular, along the boundary current path (shore-ward of the red contour in Fig. 8a), only 1% of the total 2004–2016 ITP data are acquired within the Nansen Basin; only 4.5% are acquired in the combined Amundsen and Makarov Basins. The majority of the ITP data (71%) are from within the Canada Basin. It is important to note that any bias may be relatively well-sampled here, but may result from weak sub-surface constraint throughout the entire eastern Arctic. Fig. 9 shows the reduction of misfits between the unconstrained *it0* and *ASTE\_R1* as a function of basins and depths. The reduction is throughout the upper 800 m of the water column. Seawater density in



**Figure 8.** Distribution of ITP data as a function of year and geography. In (a), the red contour serves as a proxy for the separation between the continental shelf/slope (slope) and basin interior (int) regions. It is defined as  $\sim 100$  km offshore of the 300 m depth contour. The thick green lines approximately separate the Nansen Basin (NB), Amundsen Basin (AB), Makarov Basin (MB) and Canada Basin (CB). In (b)–(e), histograms of the number of ITP profiles for the continental shelf/slope (dark blue) and Arctic interior (yellow) are normalized by the maximum number available for the Canada Basin (5000). There are a total of 39,904 ITP profiles.

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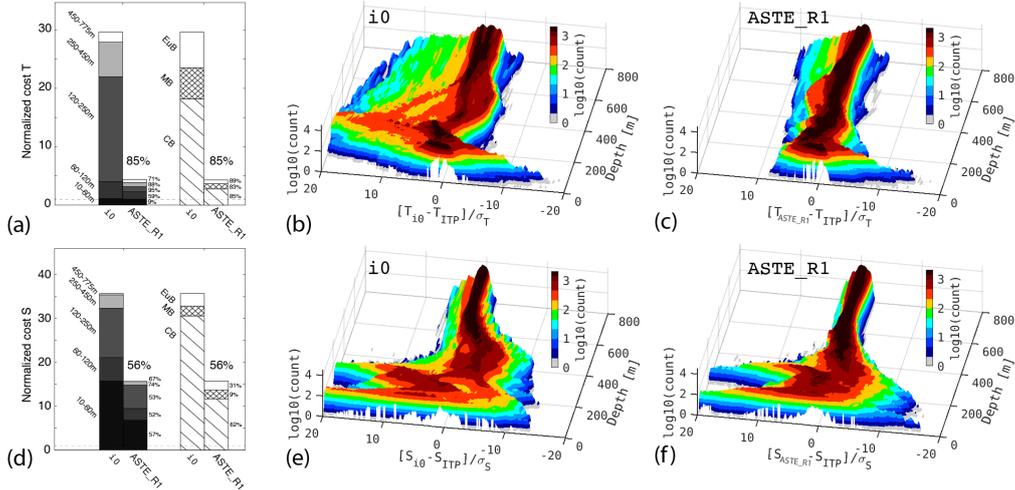
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the Arctic is primarily controlled by salinity, whereas temperature behaves more like a passive tracer and can be more flexibly impacted by the optimization procedure. As a result, the reduction in *ASTE\_R1* temperature misfits greatly exceeds the reduction in

501 salinity misfits in the Arctic. For salinity, the highest remaining misfits in *ASTE\_R1* are  
 502 at depths occupied by the mixed layer and halocline (Fig. 9e–f).

503 Fig. 10 shows an example of how temperature misfits are reduced in the water col-  
 504 umn for ITP #55 whose trajectory began in the Canada Basin interior (red circle in Fig. 10a)  
 505 and ended at the slopes of the Chukchi Plateau (green square). In the observations sev-  
 506 eral watermasses can be seen, including the surface cold layer above  $\sim 30$  m, warm Pa-  
 507 cific Summer Water (PSW) at  $\sim 40$ – $100$  m, Cold Halocline Waters at  $\sim 110$ – $250$  m, and  
 508 the Atlantic Water core at depths  $\sim 300$ – $750$  m (Fig. 10b). In the unconstrained *it0*, both  
 509 the AW boundary current and the halocline are too warm, the AW layer is too thick,  
 510 and the PSW is too cold. In *ASTE\_R1*, closer consistency is obtained with tempera-  
 511 ture observations for all watermasses. We emphasize that we have not applied direct ad-  
 512 justments to the time-varying ocean hydrography to achieve this fit. Instead, it is through  
 513 adjustments of the control variables, i.e., the initial hydrography in 2002, time-averaged  
 514 internal mixing parameters, and surface atmospheric forcing. As a result, a “near-perfect”  
 515 fit, such as that of the WOA18 hydrography to the mean ITP data seen in Fig. 1, is not  
 516 possible for this under-determined problem. The fit is, nevertheless, within the spec-  
 517 ified temperature and salinity uncertainties, with improved watermass representation for  
 518 all ITP data (e.g., Fig. 10), Beaufort Gyre Moorings, NABOS moorings, and Fram Strait  
 519 moorings.

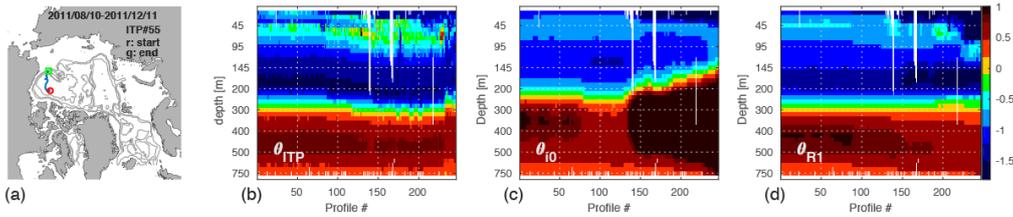


**Figure 9.** Normalized cost for ITP (a–c) temperature and (d–f) salinity. Costs to all ITP data are grouped by depth range and basin in (a) and (d). For the Canada Basin, histograms as a function of depths (b–c, e–f) show a narrowing of the misfit distributions for both temperature and salinity, especially in the AW layer below 250 m.

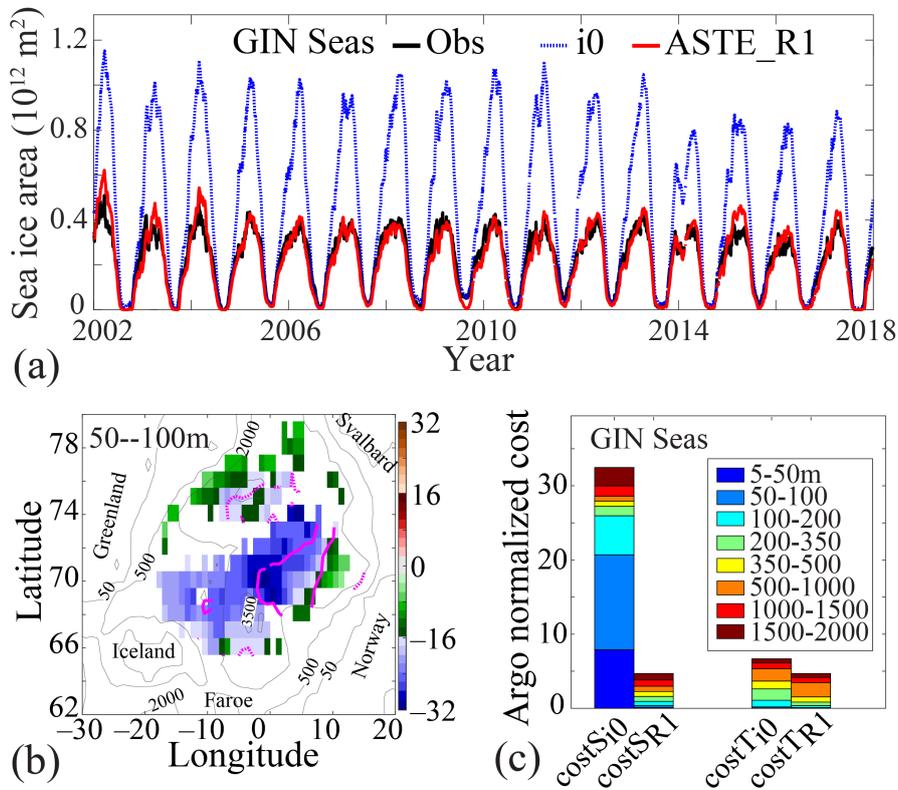
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### 521 3.2 The Greenland Iceland Norwegian Seas

522 The Greenland-Iceland-Norwegian (GIN) Seas are defined here as bounded to the  
 523 south by the the Greenland-Scotland Ridge (GSR) and to the north and north east by  
 524 the Barents Sea Opening and the Fram Strait, respectively (see Fig. 11b). The sea ice  
 525 near Fram Strait and along the East Greenland coast is seasonal and the largest mis-  
 526 fits in *it0* were due to excessive ice here, including the Odden ice tongue (Wadhams et  
 527 al., 1996) reaching further to the east during winter months (Fig. 6c–d and Fig. 11a).  
 528 Surface winds and air temperature have been found to play an important role in con-



**Figure 10.** ITP #55 (a) trajectory, (b) potential temperature  $\theta$  for all observed profiles along the trajectory, and the model equivalent for (c) *it0* and (d) *ASTE\_R1*. In (a), the red circle and green square mark the first and last profile positions.

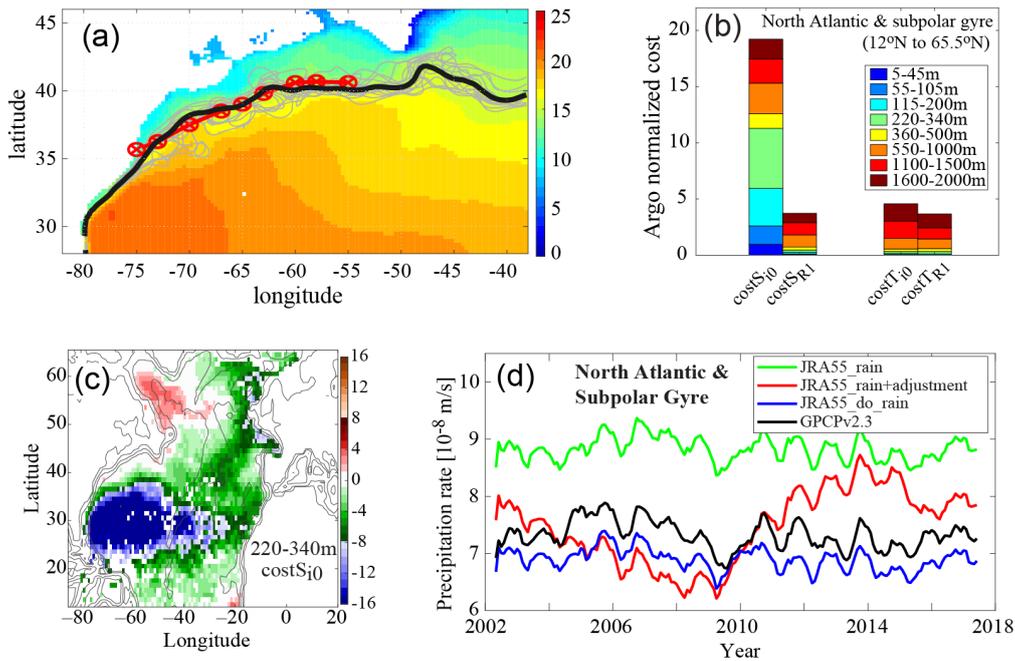


**Figure 11.** Improvements in GIN Seas sea ice and hydrography in *ASTE\_R1* compared to *it0*. (a) Time-series of sea ice area for OSSISaf observations (black), *it0* (blue) and *ASTE\_R1* (red). (b) Normalized misfits in salinity at depths 50–100m, defined as  $(S_m - S_o)/\sigma_S$  where “m” and “o” are model and observed Argo, for *it0* in the GIN Seas (color scale, unitless). The magenta solid and dashed contours indicate *ASTE\_R1* normalized misfits of magnitude  $\pm 4$  and  $\pm 1$ ; overlaying the contours on top of the colorscale thus show the misfits decrease from magnitudes 16–32 in *it0* to 1–4 in *ASTE\_R1*. The breakdown of cost reductions for all other depth ranges are shown in (c) for the GIN Seas, with overall reductions of costs of 81% and 19% in salinity and temperature relative to Argo data.

529 trolling the eastern extent of the ice edge in this region (Germe et al., 2011; Moore et  
 530 al., 2014). Adjustments of these atmospheric forcing variables during the optimization,  
 531 within their specified uncertainties, drove a reduction in sea ice area (Fig. 11a) to im-  
 532 prove the model-data fit.

533 The Nordic Seas host the interaction of several important watermasses. Warm and  
 534 salty Atlantic water enters across the GSR along three major branches, meeting locally  
 535 modified water recirculating in the Lofoten, Greenland and Iceland Basins, and the south-  
 536 ward flowing cold, fresh East Greenland Coastal Current (Hansen & Østerhus, 2000).  
 537 This region is characterized by very weak stratification, resulting in a very small defor-  
 538 mation radius of 4–7 km throughout the region (Nurser & Bacon, 2014) which further  
 539 challenges realistic representation of watermass distribution in models (Drange et al., 2005;  
 540 Heuzé & Årthun, 2019) and *ASTE\_R1*. Nevertheless, the improvements obtained in *ASTE\_R1*  
 541 are significant, with overall reductions of  $\sim 85\%$  and  $30\%$  for salinity and temperature  
 542 costs, respectively, through the 2000 m water column (Fig. 11c). The largest improve-  
 543 ments are associated with reduction of a fresh bias in the upper 100 m (Fig. 11b–c), across  
 544 the Lofoten, Iceland, and Greenland basins, which are important regions for deep wa-  
 545 ter formation.

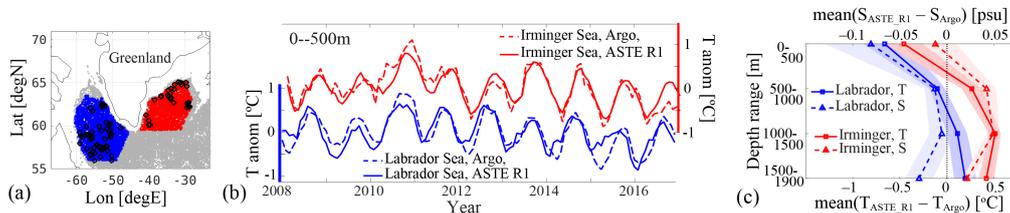
### 546 3.3 The Subpolar Gyre and North Atlantic



**Figure 12.** (a) The 2002–2017 mean proxy path of the Gulf Stream in *ASTE\_R1* (black) and the World Ocean Atlas 2009 mean 15°C isotherm at 200 m depth (red, Wolfe et al. (2019)). The gray lines are the paths in *ASTE\_R1* for all the years. (b) Normalized cost for salinity and temperature in the North Atlantic and subpolar gyre region (latitudes 12°N–65.5°N) for *it0* and *ASTE\_R1* as a function of depth range. (c) Normalized misfits in *it0* (relative to observed Argo salinity) in the water column at depth range 220–340 m. (d) Net precipitation into the North Atlantic and subpolar Gyre from JRA55 (Kobayashi et al., 2015), JRA55-do (Tsujino et al., 2018), observational based product GPCPv2.3 (Adler et al., 2018), and adjusted rain used to force *ASTE\_R1*.

547 Although the primary focus of the study is on the assessment of *ASTER1* in the  
 548 Arctic Mediterranean, the North Atlantic ocean serves as both the source of near sur-  
 549 face heat and salt to the Arctic and the sink of dense deep water and surface freshwa-  
 550 ter from the Arctic Mediterranean, and so will be briefly assessed here.

551 One of the greatest challenges in modeling the North Atlantic is to correctly sim-  
 552 ulate the observed Gulf Stream pathway. Capturing a realistic Gulf Stream separation  
 553 is non-trivial in  $z$ -level numerical models (Ezer, 2016; Chassignet & Xu, 2017). In *ASTE*,  
 554 a combination of coastal biharmonic and off-shore Leith viscosity as described in Sec-  
 555 tion 2.1 was used to achieve an observationally-consistent mean Florida Strait transport  
 556 of  $\approx 32 Sv$  (Baringer & Larsen, 2001; Johns et al., 2002) and a separation near Cape  
 557 Hatteras. After separation, the Gulf Stream path can be approximately tracked using  
 558 a proxy of the  $15^\circ\text{C}$  isotherm at 200 m depth (from the WOA13, Wolfe et al., 2019). Fig. 12a  
 559 shows this proxy of the Gulf Stream path for the years 2002–2017 in *ASTER1* compared  
 560 to that derived from WOA13.



**Figure 13.** (a) Distribution of Argo data in the Irminger Sea (red dots) and Labrador Sea (blue dots) for the full period 2002–2017. To provide an impression of temporal coverage, black circles show data acquired within the month of January 2016. (b) Upper 500 m ocean mean temperature anomalies for the Labrador Sea (blue) and Irminger Sea (red) from Argo observations (dashed) and *ASTER1*. Anomalies are defined as the full time-series minus its respective mean, showing that *ASTER1* captures both the seasonal and interannual ocean temperature variability in both the Irminger and Labrador Seas. The biases are shown in (c) for mean temperature and salinity at various depth ranges sampled by Argo.

561 The dynamical mechanisms underlying the transports of warm AW from the Gulf  
 562 Stream extension to the subpolar North Atlantic (SPNA) and into the GIN Seas across  
 563 the GSR is poorly understood and its representation in state-of-the-art models remains  
 564 a great challenge (Heuzé & Årthun, 2019). Compared with Argo data, the eastern SPNA  
 565 hydrography (south of the GSR) contains large biases in *it0* (Fig. 12b–c) but is signif-  
 566 icantly improved in *ASTER1*, with a net reduction of misfit over the entire North At-  
 567 lantic (north of  $12^\circ\text{N}$ ) of  $\sim 80\%$  and  $\sim 21\%$  in salinity and temperature, respectively (Fig. 12b).  
 568 Closer inspection reveals that, just south of the GSR, in the Irminger and Labrador Seas,  
 569 *ASTER1* can reliably reproduce the observed hydrographic variability (Fig. 13a–b). How-  
 570 ever, the solution exhibits a systematic warm ( $0.1$ – $0.7^\circ\text{C}$ ) and salty ( $0.01$ – $0.08$  psu) bias  
 571 throughout the upper 2000 m (Fig. 13c).

572 In the subtropical North Atlantic, a large fraction of the salinity misfit in *it0* is due  
 573 to excess freshwater flux from the atmosphere. Comparison to the Global Precipitation  
 574 climatology Project version 2.3 product (GPCPv2.3, Adler et al., 2018) reveals an ex-  
 575 cess precipitation bias in JRA-55, that is most pronounced in the North Atlantic and  
 576 subpolar gyre region of the *ASTE* domain (Fig. 12d), and that resulted in a large fresh  
 577 bias in the upper  $\sim 500$  m of the unconstrained *it0* solution (Fig. 12c). The adjoint-based  
 578 optimization provided a systematic approach for removing this excess precipitation bias,

579 such that after approximately 12 iterations the misfits to Argo salinity in the upper ocean  
580 reduced to within the observed uncertainty (Fig. 12c).

## 581 4 Transports through Key Oceanic Gateways and Regional Storage

582 Here we summarize the volume, heat, and freshwater transports across important  
583 Arctic and GIN Seas gateways (Table 4, Fig. 14–16) and provide comparison to all known  
584 observation-based estimates (Skagseth et al., 2008; Schauer & Beszczynska-Möller, 2009;  
585 de Steur et al., 2009; Beszczynska-Möller et al., 2011; Curry et al., 2011, 2014; Hansen  
586 et al., 2015; Woodgate, 2018; Rossby et al., 2018; Østerhus et al., 2019). Where avail-  
587 able, we also assess *ASTER1* transports against previously published estimates from  
588 coordinated modeling studies (Q. Wang et al., 2016b, 2016a; Ilicak et al., 2016; Heuzé  
589 & Årthun, 2019), ocean reanalyses (Uotila et al., 2019), and an independent inverse es-  
590 timate (Tsubouchi et al., 2018).

591 The published literature offers notable differences in tracer reference values employed  
592 in the computation of reported heat, freshwater and volumetric watermass fluxes. These  
593 range from regional basin means (Smedsrud et al., 2010; Beszczynska-Möller et al., 2012;  
594 de Steur et al., 2018; Tesdal & Haine, 2020) to gateway and surface means (Tsubouchi  
595 et al., 2018) to freezing temperature in the Arctic (Beszczynska-Möller et al., 2012; Woodgate,  
596 2018). In some cases, transports were computed along a particular range of isopycnals  
597 (Tsubouchi et al., 2018). Heat transport computed in *ASTER1* assumes a reference tem-  
598 perature  $\theta_r = 0^\circ\text{C}$  (most accurate numerically, see Appendix B). For the Bering Strait,  
599 we also compute heat transport referenced to the freezing temperature of seawater  $\theta_r =$   
600  $-1.9^\circ\text{C}$  to facilitate comparison with published estimates. For the computation of fresh-  
601 water transports, we assume a reference salinity  $S_r = 34.8$  psu and integrate from the  
602 surface down to the reference isohaline. We refer the reader to Appendix B for details  
603 on potential errors incurred when computing transports using non-zero reference values.  
604 Due to the difference in reference values employed here and in some of the studies listed  
605 above, we seek consistency in terms of comparable transport magnitudes as opposed to  
606 exact agreement.

607 To provide a useful comparison of *ASTER1* mean transports with those reported  
608 in the literature, it is important to note whether published estimates are based on his-  
609 toric data or more recent acquisitions, given how fast the high latitudes are observed to  
610 be changing. In the first four years of the *ASTER1* period, 2002–2005, transports in  
611 both the North Atlantic and the Arctic exhibit distinctly different characteristics com-  
612 pared to the period 2006–2017. This transition of hydrographic properties and circula-  
613 tion patterns around 2005–2006 has been extensively discussed, with studies noting a  
614 strong increase in volume and heat transports into the Barents Sea (Skagseth et al., 2008),  
615 increased salinity and density in the lower halocline in the Eastern Arctic (Dmitrenko  
616 et al., 2011), abrupt changes in North Atlantic heat (Piecuch et al., 2017; Foukal & Lozier,  
617 2018) and freshwater (Dukhovskoy et al., 2019) content, and rapid freshening of the Nordic  
618 Seas (Tesdal & Haine, 2020). To avoid averaging over these two apparently distinct regimes,  
619 we chose to report all mean transports for the most recent period, following the abrupt  
620 transition. Reported associated standard deviations to the 2006–2017 mean transports  
621 are computed based on the monthly values after the seasonal cycle has been removed.  
622 Details of the calculation of *ASTER1* transports are given in Appendix B, and water-  
623 mass definitions are given in Appendix C.

### 624 4.1 Volume Transports

625 Østerhus et al. (2019) summarized existing estimates of volume transports across  
626 all the important Arctic–Nordic Seas gateways including the Bering Strait (BS), Davis  
627 Strait (DaS), and the Greenland-Scotland Ridge (GSR). The latter comprises the Den-  
628 mark Strait (DS), Iceland-Faroe channel (IF) and Faroe-Shetland channel (FSh). Time-

<i>Transports</i>				
Gate	Volume [Sv]	Heat [TW]	FW [mSv]	
(1)Bering Strait	1.11 ± 0.35	4.70 ± 7.25	54.24 ± 20.62	
(2)CAA	-1.72 ± 0.39	7.95 ± 2.99	-94.19 ± 31.60	
(3)Fram Strait	-1.50 ± 0.66	54.15 ± 13.24	-84.83 ± 23.29	
(4)Svalbard-FJL <sup>1</sup> -SZ <sup>2</sup>	2.04 ± 0.64	-0.85 ± 8.03	45.23 ± 31.14	
(5)Barents Sea Opening	1.98 ± 0.66	62.33 ± 15.06	-3.25 ± 3.30	
(6)Davis Strait	-1.72 ± 0.39	25.40 ± 4.71	-103.32 ± 19.59	
(7)Denmark Strait	-2.00 ± 0.76	11.92 ± 7.81	-42.61 ± 12.21	
(8)Iceland-Faroe	2.26 ± 0.90	119.11 ± 24.09	-0.29 ± 0.69	
(9)Faroe-Shetland	0.71 ± 1.30	95.00 ± 38.12	6.25 ± 4.29	
(10)Newfoundland-Gr	-1.74 ± 0.38	67.30 ± 17.41	-110.67 ± 23.44	
(11)48.3°N	-1.39 ± 0.36	449.66 ± 75.75	-111.60 ± 22.80	

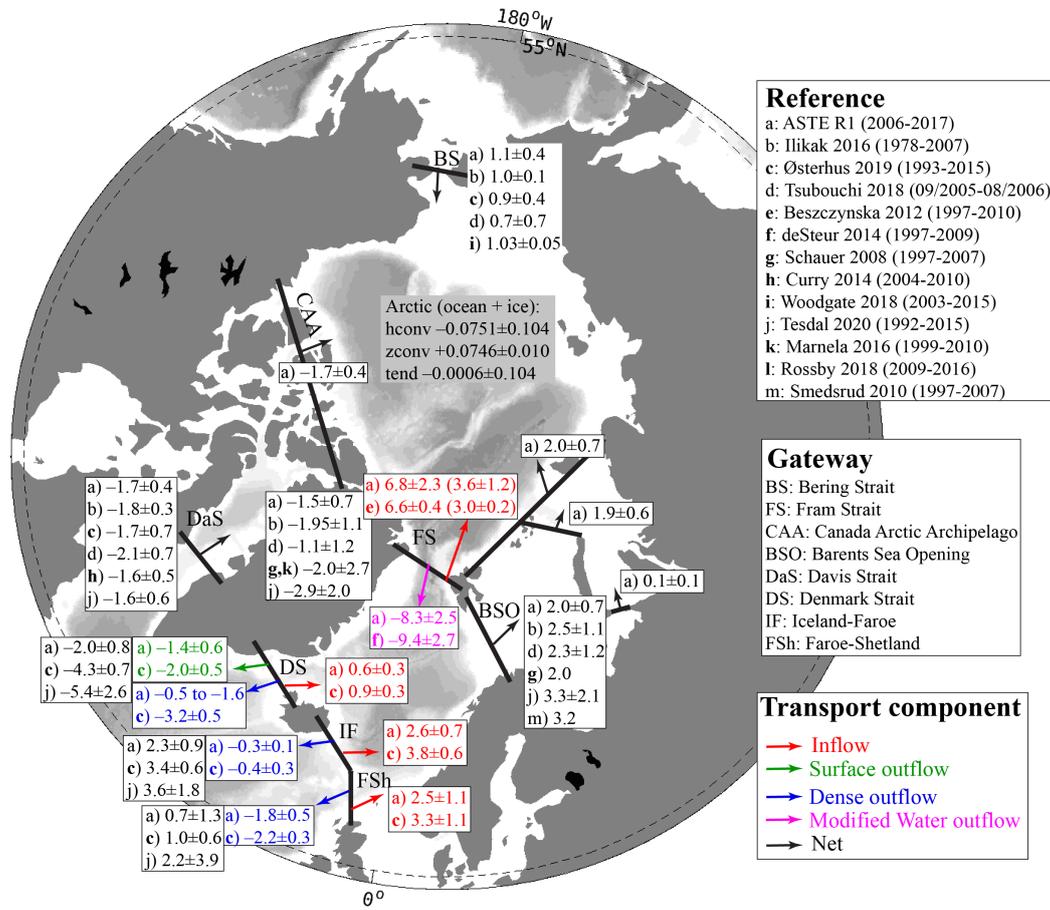
  

<i>Heat Budget [TW]</i>				
Domain	Lateral conv	Vertical conv	Tendency	Bounded Gates
Arctic	65.95 ± 13.57	-39.53 ± 39.48	26.39 ± 41.34	1,2,3,4
CAA	17.46 ± 5.84	-18.08 ± 12.55	-0.63 ± 15.60	2,6
Barents	63.18 ± 19.94	-63.63 ± 37.27	-0.45 ± 47.98	4,5
GINs	109.55 ± 34.28	-110.06 ± 60.55	2.19 ± 78.36	3,5,7,8,9
Labrador Sea	41.90 ± 16.81	-49.40 ± 39.83	-7.50 ± 47.30	6,10
East SPNA	156.33 ± 96.91	-146.97 ± 92.94	6.65 ± 165.61	7,8,9,10,11

<i>FW Budget [mSv]</i>				
Domain	Lateral conv	Vertical conv <sup>a</sup>	Tendency	Bounded Gates
Arctic	-79.55 ± 40.31	74.57 ± 10.28	-9.45 ± 35.83	1,2,3,4
CAA	-9.13 ± 26.29	5.78 ± 2.86	-0.51 ± 22.68	2,6
Barents	-48.48 ± 30.96	57.54 ± 7.89	-4.17 ± 30.29	4,5
GINs	51.43 ± 23.16	34.52 ± 17.74	1.20 ± 16.89	3,5,7,8,9
Labrador Sea	-7.35 ± 23.15	20.55 ± 9.58	4.56 ± 22.35	6,10
East SPNA	35.72 ± 16.92	93.94 ± 26.42	2.41 ± 20.32	7,8,9,10,11

**Table 4.** *ASTER1* budgets of volume, heat ( $\theta_r = 0^\circ\text{C}$ ), and FW ( $S_r = 34.8\text{psu}$ ) for the combined ocean and ice system for the period 2006–2017. Standard deviation are computed from monthly mean values after the seasonal cycle has been removed. FW transport is computed using Eqn B3.2 from Appendix B. <sup>a</sup>The vertical convergence of FW, from air-ice-sea fluxes, is the same as that for volume and is exact. Lateral convergence and tendency of FW, however, are approximate. As a result, the budget for FW is not fully closed (see Appendix B). <sup>1</sup> Franz Josef Land, <sup>2</sup> Severnaya Zemlya.



**Figure 14.** Volume transports across important Arctic and Nordic Seas gateways listed for (a) *ASTER1* and (b-m) published estimates referenced in the legend. Net transports across the full width and depth of each section are written in black; transport component contributions to this total are written in color for (red) total inflow, (green) surface outflow, (blue) dense outflow, and (magenta) modified water outflow, where arrows show the direction ascribed to in/outflow. Positive (negative) transport indicates Northward and Eastward (Southward and Westward). Quantities listed are 2006–2017 mean and standard deviation after the seasonal cycle has been removed. All net transports in *ASTER1* are diagnosed online, while separate transport components through FS, DS, IF, and FSh are diagnosed offline using archived monthly advection terms. See text and Appendix C for further discussion on watermass identification used in determining the in/outflow transport components. For the Fram Strait inflow, the two provided estimates are for the West Spitsbergen current only, and we give both the total current transport and, in parenthesis, the fraction above 2°C (Beszczynska-Möller et al., 2011). Numbers in parenthesis in Reference legend refer to the period covered by the respective studies.

629 mean values of these transports in *ASTER1* are given in Table 4 and Fig. 14, listed along-  
 630 side previously published estimates from observations (Beszczynska-Möller et al., 2012;  
 631 de Steur et al., 2014; Beszczynska-Möller et al., 2011; Woodgate, 2018; Curry et al., 2014;  
 632 Skagseth et al., 2008; Hansen et al., 2015), and modeling studies (Tsubouchi et al., 2018;  
 633 Heuzé & Årthun, 2019; Ilicak et al., 2016). In addition to net transports, we also pro-  
 634 vide estimates of transports of important watermasses at Fram Strait (as defined in Beszczynska-  
 635 Möller et al., 2011) and through the GSR (as defined in Hansen & Østerhus, 2000; Øster-  
 636 hus et al., 2019). For the in/outflow transport estimates given in Fig. 14, we follow wa-  
 637 termass definitions of Beszczynska-Möller et al. (2012) for the Fram Strait and Østerhus  
 638 et al. (2019) for the GSR.

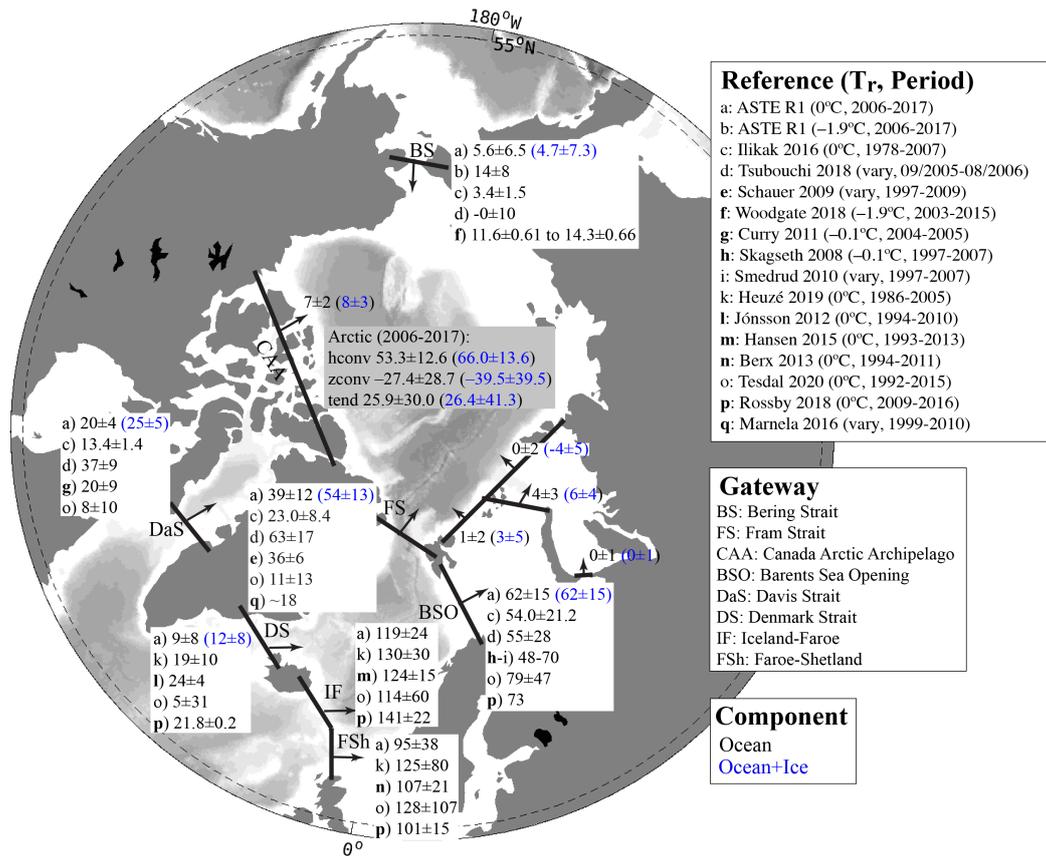
639 The net volume transport across the Bering Strait is northward into the Arctic and  
 640 approximately  $1.1 \pm 0.4$  Sv. Across the Davis Strait, there is a southward transport of  
 641 freshwater near the surface and northward transport of warm water from the Irminger  
 642 Current (Curry et al., 2014). At this gate, *ASTER1* estimates a net volume transport  
 643 of  $1.7 \pm 0.4$  Sv, consistent with observed values of  $1.6 \pm 0.5$  and  $1.7 \pm 0.7$  from Curry  
 644 et al. (2014) and Østerhus et al. (2019). Across the GSR, there is a net near-surface north-  
 645 ward transport of AW across the Denmark Strait (DS), Iceland-Faroe (IF) and Faroe-  
 646 Shetland (FSh) channels (shown in red in Fig. 14), southward surface flow of freshwa-  
 647 ter across DS and dense overflow across the entire ridge (green and blue color in Fig. 14).

648 Watermass definitions for surface outflow, dense outflow, modified water, and in-  
 649 flow AW in *ASTER1* can differ from Østerhus et al. (2019) and Hansen and Østerhus  
 650 (2000) for the reasons outlined in Section 2.3. Our choice for  $\sigma_\theta$  is justified in Appendix  
 651 C. For the overflow through DS, the range of  $27.4 \leq \sigma_\theta \leq 27.8$  used in *ASTER1* is  
 652 associated with southward transports of  $-1.6 \pm 0.9$  to  $-0.5 \pm 0.3$  Sv (shown in blue  
 653 in Fig. 14), corresponding to 16%–50% of the observed estimate using  $\sigma_\theta = 27.8$  from  
 654 Østerhus et al. (2019). Similar considerations for  $\sigma_\theta$  of dense overflow water across the  
 655 IF and FSh ridges (Appendix C) yield  $-0.3 \pm 0.1$  Sv and  $-1.8 \pm 0.5$  Sv, respectively,  
 656 in *ASTER1*, compared to  $-0.4 \pm 0.3$  Sv and  $-2.2 \pm 0.3$  Sv of water with  $\sigma_\theta \geq 27.8$   
 657 in Østerhus et al. (2019). For surface outflow, *ASTER1* underestimates the observed  
 658 estimate at the DS by approximately 30%. In total, the net volume transport across DS  
 659 in *ASTER1* is about 47% of that reported by Østerhus et al. (2019).

660 For the Arctic Ocean and GIN Seas heat and freshwater budgets, transports through  
 661 the Fram Strait (FS) and the Barents Sea Opening (BSO) are also important. Across  
 662 the FS, the inflow of warm AW along the West Spitsbergen Current (red color in Fig. 14)  
 663 is  $6 \pm 1$  Sv in *ASTER1*, with  $3.4 \pm 1.1$  Sv carrying the core AW water warmer than  
 664  $2^\circ\text{C}$ . This is consistent with corresponding estimates of  $6.6 \pm 0.4$  and  $3.0 \pm 0.2$  from  
 665 Beszczynska-Möller et al. (2012) based on observations from an earlier period of 1997–  
 666 2010. The outflow across FS includes freshwater carried by the East Greenland Current  
 667 at the surface and return of modified AW at depth (magenta color in Fig. 14, Beszczynska-  
 668 Möller et al., 2011). For the southward return of modified AW, *ASTER1* estimates a  
 669 flux of of  $-8.3 \pm 2.5$  Sv over the period 2006–2017, consistent with  $-9.4 \pm 2.7$  Sv from  
 670 de Steur et al. (2014) for the period 1997–2009. Across the BSO, volume transport is  
 671 dominated by the eastward Norwegian Coastal Current and the Atlantic inflow which  
 672 carries warm AW into the Barents Sea (Smedsrud et al., 2010). The net eastward vol-  
 673 ume transport in *ASTER1* of  $2.0 \pm 0.7$  Sv is consistent with observation-based esti-  
 674 mate of  $\sim 2.0$  Sv from Smedsrud et al. (2010).

## 675 4.2 Heat Transports

676 All *ASTER1* net heat transports are poleward from lower latitudes into the Arc-  
 677 tic Mediterranean and further north into the Arctic Basin. We find that time-mean pole-  
 678 ward transports across key gateways are consistent with observation-based estimates,



**Figure 15.** As for Fig. 14 but showing net ocean heat transport across important Arctic and Nordic Seas gateways. For select gateways the combined ocean+ice heat transport is also given (in blue). *ASTER1* transports (listed under (a)) are computed assuming a reference temperature  $T_r=0^\circ\text{C}$ . For the Bering Strait we also provide *ASTER1* transports computed using  $T_r=-1.9^\circ\text{C}$  (listed under (b)). Since previously published estimates (c-q) vary in their choice of  $T_r$  (see main text) we assess agreement between estimates as consistency in order of magnitude. Positive (negative) transport indicates Northward and Eastward (Southward and Westward) flow. Quantities listed are 2006–2017 mean and standard deviation after the seasonal cycle has been removed. Numbers in parenthesis in Reference legend refer to the  $T_r$  used and the period covered by the respective studies.

679 a result that is aided – although by no means guaranteed – by constraining the state estimate using mooring  $T/S$  data (Table 4, Fig. 15).  
680

681 At the Bering Strait *ASTER1* poleward heat transport is  $14 \pm 8$  TW (referenced  
682 to  $T_r=-1.9^\circ\text{C}$ ), consistent with the 11.6 TW to 14.3 TW range determined by Woodgate  
683 (2018). At Davis Strait, the *ASTER1* estimate of  $20 \pm 4$  TW is consistent with  $20 \pm$   
684  $9$  TW obtained by Curry et al. (2011). Across the DSR, heat transports are in good agree-  
685 ment with previous published estimates across the two eastern channels (IF and FS, Fig. 15),  
686 but is underestimated across the Denmark Strait. Here, the total poleward diffusive heat  
687 flux dominates and opposes the equatorward advective term in *ASTER1*. This diffu-  
688 sive dominance has also been suggested using heat budget analyses in ECCOV4 (Buckley  
689 et al., 2015). A more detailed discussion of the full time-series and contributions of ad-  
690 vective and diffusive fluxes to the total transport is given in Appendix B.

691 Further north, at the Fram Strait, *ASTER1* poleward heat transport is  $39 \pm 12$  TW  
 692 (referenced to  $T_r=0^\circ\text{C}$ ), consistent with  $36 \pm 6$  TW from Schauer and Beszczynska-Möller  
 693 (2009) and Beszczynska-Möller et al. (2011). The Fram Strait heat flux is increased by  
 694 approximately one third (15 TW) on accounting for sea ice advection. Heat transport  
 695 into the Barents Sea across BSO of  $62 \pm 15$  TW is consistent with observation-based  
 696 estimates of between 48 TW and 73 TW (Skagseth et al., 2008; Smedsrud et al., 2010;  
 697 Rossby et al., 2018). Most of this heat is lost via air-sea exchange in the Barents and  
 698 Kara Seas (Lind et al., 2018), yielding negligible heat transports from this shallow re-  
 699 gion into the Arctic Basin (Fig. 15). Air-sea exchange also accounts for significant loss  
 700 of heat in the Canadian Arctic Archipelago, such that only  $\sim 35\%$  of the amount trans-  
 701 ported across the Davis Strait reaches the Arctic Basin.

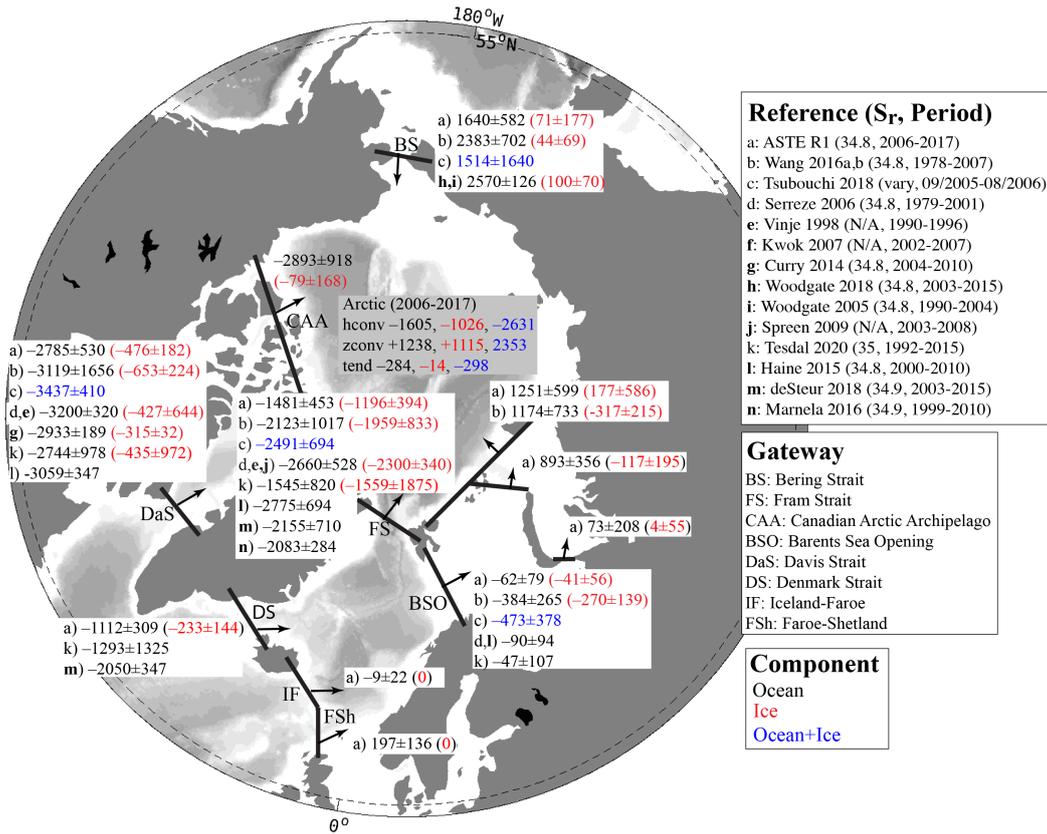
702 We note that there is a large spread amongst existing observation- and model-based  
 703 studies with significant disagreements even after accounting for uncertainty (Fig. 15),  
 704 due in part to the lack of common data period and reference temperature used in the  
 705 calculations. Overall, nevertheless, the poleward heat transports in *ASTER1* are in good  
 706 agreement with previous estimates (Fig. 15).

### 707 4.3 Freshwater Transports

708 The practice of reporting ocean freshwater (FW) transport/content in place of ab-  
 709 solute salt transport/content is ubiquitous in the literature, but plagued by the need to  
 710 specify a reference salinity,  $S_r$  and choose the vertical extent over which the integral is  
 711 computed (i.e., full depth versus to the depth of the reference salinity  $z_{S_r}$ ). No unique  
 712 choice emerges from consideration of seawater physics. Instead,  $S_r$  is selected inconsis-  
 713 tently between studies. As cautioned by Schauer and Losch (2019), this not only com-  
 714 plicates comparisons but can give very different impressions of the changing ocean state,  
 715 due to strong sensitivity to the choice of  $S_r$ . Acknowledging this issue, we nevertheless  
 716 elect to report FW transport below (as did (Tesdal & Haine, 2020) in their recent study  
 717 focusing on the subpolar North Atlantic and Nordic Seas), in an attempt to continue our  
 718 assessment of *ASTER1* hydrography in the context of existing estimates. To the best  
 719 of our knowledge no published observational estimates report Arctic salt transports to  
 720 provide a basis for comparison (the modeling study by Treguier et al., 2014 is one known  
 721 exception). We proceed with caution and flag comparisons for which calculations differ.  
 722 *ASTER1* FW fluxes are reported using a reference salinity of  $S_r=34.8$  psu and integrated  
 723 down to  $z_{S_r}$ . Our calculation uses monthly averages of both the Eulerian velocity and  
 724 salinity. In Appendix B we provide a detailed discussion of the potential errors in FW  
 725 calculations with these choices, along with errors incurred in omitting bolus and diffu-  
 726 sive terms. Salt transport or salt content changes in *ASTER1* will be revisited in fu-  
 727 ture work.

728 Similar to our assessment of volume and heat transports, we start by examining  
 729 FW transports across the gates into the Arctic Mediterranean. At the Bering Strait, *ASTER1*  
 730 combined liquid and solid FW import of  $1711 \pm 608$  km<sup>3</sup>/yr is lower than the  $2670 \pm$   
 731  $144$  km<sup>3</sup>/yr estimated by Woodgate et al. (2015) and Woodgate (2018). At the Davis  
 732 Strait, *ASTER1* liquid and solid FW exports of  $-2785 \pm 530$  km<sup>3</sup>/yr and  $-476 \pm 182$   
 733 km<sup>3</sup>/yr are consistent with estimates of  $-2933 \pm 189$  km<sup>3</sup>/yr and  $-315 \pm 32$  km<sup>3</sup>/yr  
 734 from Curry et al. (2014), on accounting for uncertainty/variability. There is negligible  
 735 FW transports across the Iceland-Faroe and Faroe-Shetland channels. At the Denmark  
 736 Strait, *ASTER1* estimate of  $-1112 \pm 309$  km<sup>3</sup>/yr is approximately half of the value  
 737 reported by Marnela et al. (2016) of  $-2050 \pm 347$  km<sup>3</sup>/yr. This is consistent with the  
 738 50% underestimation of both volume and heat transports in *ASTER1* across this gate  
 739 compared to independent observations.

740 Further north at the Fram Strait, the liquid and solid FW exports of  $-1465 \pm 463$   
 741 km<sup>3</sup>/yr and  $-1195 \pm 394$  km<sup>3</sup>/yr in *ASTER1* are lower than the  $-2050 \pm 710$  km<sup>3</sup>/yr



**Figure 16.** FW flux across important Arctic and Nordic Seas gateways from *ASTE\_R1* and published estimates. Units are in  $\text{km}^3 \text{yr}^{-1}$ .  $S_r=34.8$  psu is used in *ASTE\_R1* calculations for all FW transports and content/tendency terms for the ocean. A fixed salinity  $S_i=4$  psu is used for sea ice transports and tendency terms. Positive (negative) values indicate Northward and Eastward (Southward and Westward) transports. Quantities listed are 2006–2017 mean and standard deviation after the seasonal cycle has been removed. Numbers in parenthesis in Reference legend refer to the  $S_r$  used and the period covered by the respective studies.

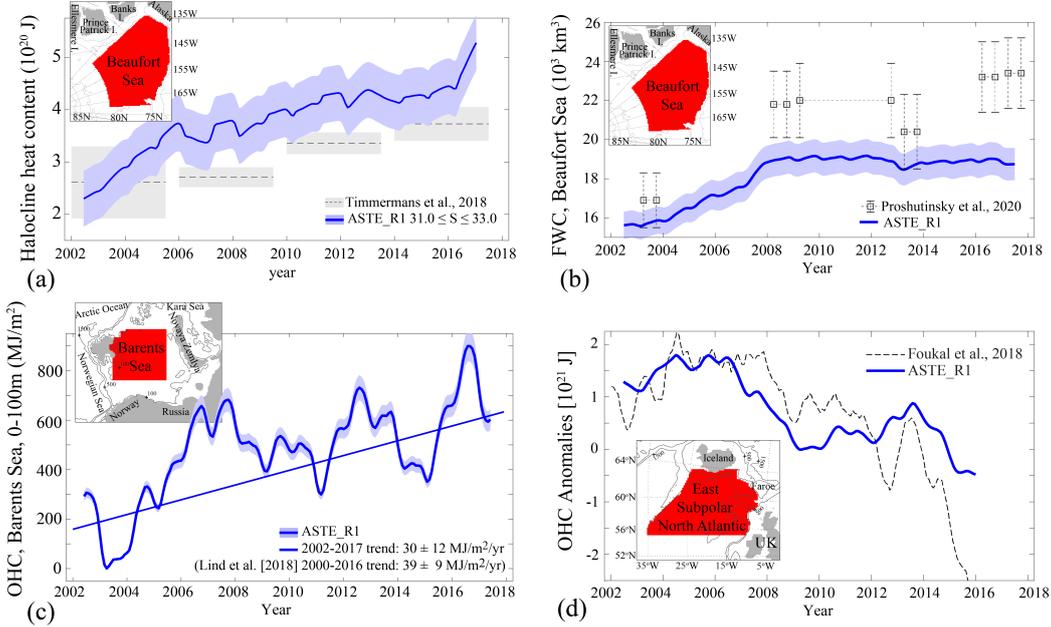
742 and  $-2300 \pm 340 \text{ km}^3/\text{yr}$  estimated by de Steur et al. (2009) and Spreen et al. (2009).  
 743 One main reason for the lower (by  $\sim 1200 \text{ km}^3/\text{yr}$ ) liquid export in *ASTE\_R1* across Fram  
 744 Strait is the lower (by  $\sim 960 \text{ km}^3/\text{yr}$ ) FW import through the Bering Strait relative to  
 745 observations. An additional inconsistency is the use of a runoff climatology in *ASTE\_R1*  
 746, which fails to account for Greenland solid/liquid discharge and its observed recent in-  
 747 crease into the Arctic sector by approximately  $105 \text{ km}^3/\text{yr}$  (Bamber et al., 2012), as well  
 748 as increased river outputs (as reported in Bamber et al., 2012; Proshutinsky et al., 2020).  
 749 With respect to the latter, *ASTE\_R1* has a deficit of  $\sim 220 \text{ km}^3/\text{yr}$ . The climatology  
 750 also does not account for Greenland solid and liquid discharge into the GIN Seas and  
 751 Baffin Bay by nearly  $150 \text{ km}^3/\text{yr}$  and  $250 \text{ km}^3/\text{yr}$ , respectively (Bamber et al., 2012).  
 752 In the Canadian Arctic Archipelago, the product also has a FW flux deficit of  $\sim 226 \text{ km}^3/\text{yr}$   
 753 from land ice (Carmack et al., 2016). These omissions likely contribute to the underes-  
 754 timation of southward FW transports across both the Denmark Strait (by  $\sim 940 \text{ km}^3/\text{yr}$ )  
 755 and Davis Strait (by  $\sim 150 \text{ km}^3/\text{yr}$ ).

756 The net lateral convergence of the combined liquid and solid freshwater flux in *ASTE\_R1*  
 757 of  $-2510 \pm 1272 \text{ km}^3/\text{yr}$  is nearly balanced by the net vertical convergence of  $2353 \pm$

758 324 km<sup>3</sup>/yr, yielding a net tendency of  $-298 \pm 1131$  km<sup>3</sup>/yr. For the liquid flux alone,  
 759 the tendencies are  $-1484 \pm 1123$ ,  $1238 \pm 2478$ , and  $-284 \pm 2169$  km<sup>3</sup>/yr for lateral  
 760 convergence, vertical convergence, and total tendency, respectively.

761 **4.4 Heat and Freshwater Storage**

762 The present assessment focuses on comparisons between *ASTE\_R1* and existing es-  
 763 timates. A full assessment of the mechanisms underlying Arctic Mediterranean and sub-  
 764 polar North Atlantic heat and freshwater content change over the *ASTE\_R1* period will  
 765 be addressed in a separate study. As noted earlier, decisions made in our tracer trans-  
 766 port/budget calculations facilitate these comparisons but are non-unique. For freshwa-  
 767 ter transports/budgets this introduces ambiguity that is best resolved prior to detailed  
 768 dynamical investigation. Here we summarize contributions to the time-mean heat and  
 769 freshwater budgets and 2002–2017 trends.



**Figure 17.** Comparison of *ASTE\_R1* (a) Beaufort Sea halocline (defined as  $31.0 \leq S \leq 33.0$ ) heat content, (b) Beaufort Sea freshwater content above the 34.8 psu isohaline, (c) Barents Sea 0–100m heat content and, (d) East Subpolar North Atlantic full-depth heat content with existing observational-based estimates, as given in the legend of each panel. Insets show the spatial mask defining each region. A 12-month running mean has been applied to filter the seasonal cycle from the *ASTE\_R1* time-series, facilitating comparison with observed trends. Shading in *ASTE\_R1* time-series indicate the sensitivity of the (a,c) heat content to a 5% change in (a) the northern and (c) eastern spatial mask, or the sensitivity of the (b) freshwater content to a 0.5 psu change in the lower limit employed in the halocline watermass definition (see Appendix C).

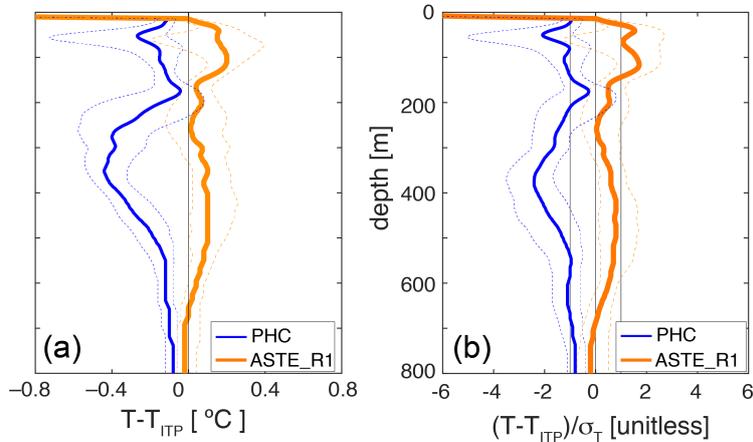
770 **4.4.1 Heat Content**

771 Considering the Arctic region of *ASTE\_R1* in its entirety, the net heat input from  
 772 convergence of horizontal (ocean plus ice) heat transports ( $53.3 \pm 12.0$  TW) exceeds  
 773 the net heat loss due to local air-ice-sea fluxes ( $-27.4 \pm 28.7$  TW) by a factor  $\sim 2$ , yield-  
 774 ing a net heating rate of  $25.9 \pm 30.0$  TW when averaged over the period 2006–2017 (Ta-

775 ble 4). Relative to horizontal convergence, vertical exchange at the air-ice-sea interface  
 776 is significantly less well constrained due to large uncertainties in atmospheric reanaly-  
 777 ses at high northern latitudes (Beesley et al., 2000; Chaudhuri et al., 2014; C. Wang et  
 778 al., 2019). Partitioned by basins, similar enthalpy gains are estimated for both the west-  
 779 ern ( $14.0 \pm 24.3$  TW) and eastern ( $12.5 \pm 14.0$  TW) Arctic region. In the water col-  
 780 umn, heat gain is concentrated mainly in the AW layer (240–1000 m) in both the west-  
 781 ern ( $9.3 \pm 2.7$  TW) and eastern ( $6.4 \pm 4.6$  TW) Arctic. In the upper 60 m of the wa-  
 782 ter column, the tendency is negligible but with large variability ( $0.2 \pm 25.3$  TW) due  
 783 to mixed layer processes and exchange with the atmosphere.

784 Warming since the early 2000s has been reported in the Arctic, documented along-  
 785 side enhanced “Atlantification” in the Eastern Arctic (Polyakov et al., 2017, 2020) and  
 786 a fivefold increase in solar absorption by near surface waters in the Western Arctic (Jackson  
 787 et al., 2010; Timmermans et al., 2018). This warming proceeds at a sustained rate, with  
 788 recent studies suggesting a doubling of OHC in the Beaufort Gyre halocline between 2003  
 789 and 2013 (Timmermans et al., 2018).

790 Fig. 17a shows a comparison of the time-series of the halocline heat content in *ASTE\_R1*  
 791 and estimates based on ITP and mooring data in the Beaufort Sea. As discussed in Sec-  
 792 tion 2.3, adopting exact watermass classifications from observational studies may be in-  
 793 appropriate for model analysis, due to representation error of subgrid scales. Thus in ad-  
 794 dition to the salinity limits used to identify the upper halocline layer of  $31.0 \leq S \leq$   
 795  $33.0$  in Timmermans et al. (2018), we also compute the heat content sensitivity to the  
 796 salinity bounds. By changing the near-surface lower salinity bound within the range 31–  
 797 31.5 psu, the mean halocline heat content changes by 2–3% per 0.1 psu increment, but  
 798 the variability and trend remain unchanged. This confirms that despite the systematic  
 799 warm bias, the positive trend in halocline heat content is well-captured in the *ASTE\_R1*  
 800 solution.



**Figure 18.** Comparison between all ITP-derived temperature profiles in the Canada Basin and PHC (blue) and *ASTE\_R1* (orange). Panel (a) shows the normalized 50th percentile difference (dimensionless) and (b) the 50-percentile difference (°C). The two vertical black lines in (b) at  $\pm 1$  indicate the limits within which the difference is within the uncertainty  $\sigma_T$ . The dotted lines show the 30th and 70th percentile differences.

801 In the Canada Basin, *ASTE\_R1* exhibits a warming rate of  $9.3 \pm 2.7$  TW for the  
 802 period 2006–2017 (Fig. 15). There are insufficient observations to validate this directly,  
 803 but we can corroborate our estimate with a back of the envelope calculation as follows.

804 Recent ITP acquisitions report core AW temperatures in this region  $\sim 0.5^\circ\text{C}$  warmer than  
 805 the PHC climatology (Fig. 18a), where the latter is representative of the second half of  
 806 the 20th century. Since ITPs only measure to  $\sim 800$  m depth, we conservatively assume  
 807 a depth-average warming of  $0.20\text{--}0.25^\circ\text{C}$  over the  $170\text{--}1000$  m range in the Western Arc-  
 808 tic basin interior (area  $4400 \times 10^3 \text{ km}^2$ ), yielding a warming rate of  $\sim 5.7\text{--}7.2$  TW, about  
 809 two thirds of the rate estimated in *ASTER1*. Compared to ITP data, *ASTER1* shows  
 810 a positive bias of  $\sim 0.15^\circ\text{C}$  in the core AW temperature in the Western Arctic basin, which  
 811 accounts for the higher tendency here. However, we note that this *ASTER1* bias is within  
 812 the combined data and representative error  $\sigma_T$ , which is not the case for the PHC bias  
 813 (Fig. 18b).

814 The Eastern Arctic suffers from an even greater paucity of data, such that even back  
 815 of the envelope estimates of basin-wide heat content (and its tendency) are not possi-  
 816 ble. Instead, we turn to recent observations for evidence of warming in this basin. Pulsed  
 817 injection of AW at the Fram Strait has been documented by Polyakov et al. (2011). A  
 818 notable pulse generated a warm anomaly of  $\sim 1^\circ\text{C}$ , which entered the Arctic in 2004 and  
 819 has subsequently been observed crossing the NABOS section at  $126^\circ\text{E}$ , and recorded fur-  
 820 ther downstream at numerous sections along the eastern basin's rim (Polyakov et al., 2011).  
 821 In addition, the seasonal amplitude within the halocline has been observed to increase  
 822 by  $0.75^\circ\text{C}$  between 2004 and 2015 (Dmitrenko et al., 2009; Polyakov et al., 2017; Bau-  
 823 mann et al., 2018). These observations provide evidence for a warming Eastern Arctic  
 824 and a weakened halocline. The latter is accompanied by shoaling of the AW layer to-  
 825 ward the bottom of the mixed layer and increasing heat ventilation (Polyakov et al., 2020).  
 826 This is a mechanism by which heat along the AW pathway is removed instead of being  
 827 sequestered at depth. To determine the relative importance of these two mechanisms (ven-  
 828 tilation versus sequestration) in contributing to the positive heat content tendency at  
 829 different depths and throughout the Arctic in *ASTER1*, a more detailed analysis of AW  
 830 circulation and ventilation will be needed in future work.

831 In the Barents Sea, Lind et al. (2018) documented pronounced increases in decadal  
 832 mean OHC in the upper 100 m of the water column, which they attributed to an increase  
 833 in AW inflow through the Barents Sea Opening. In Fig. 17c we compare OHC trend (up-  
 834 per 100 m) from Lind et al. (2018) with *ASTER1* illustrating that *ASTER1* captures  
 835 the 2002–2016 positive trend. Further south, Piecuch et al. (2017) and Foukal and Lozier  
 836 (2018) have quantified OHC trends in the SPNA (between  $46^\circ\text{N}$  and  $65^\circ\text{N}$ ) using SST,  
 837 ECCOv4r3 and OHC derived from the Hadley Centre EN4 gridded product. The compar-  
 838 ison between Foukal and Lozier (2018) and *ASTER1* (Fig. 17d) shows good quan-  
 839 titative agreement, with an increase in OHC between 2002–2005, a decrease in OHC be-  
 840 tween 2005–2009, and a hiatus between 2009–2014, followed finally by a further decrease  
 841 in OHC after 2014.

#### 842 **4.4.2 Freshwater Content**

843 Based on observations, principally from satellite altimetry and ITPs in the Beau-  
 844 fort Sea, the liquid freshwater content (FWC) in the Arctic has been increasing (Proshutinsky  
 845 et al., 2019). Proshutinsky et al. (2020) summarized recent works attributing this FWC  
 846 increase to several factors including shifts in atmospheric circulation, increased FW fluxes  
 847 through the Bering Strait, and increased runoff from the MacKenzie river. A compar-  
 848 ison between *ASTER1* and Proshutinsky et al. (2019) estimates for FWC in the Beau-  
 849 fort Gyre shows that *ASTER1* captures the observed increase in FWC between the 2004  
 850 to 2008. With the exception of a small decrease in 2015 – also seen in the observations  
 851 – the Beaufort Gyre FWC in *ASTER1* remains relatively constant for the period 2008–  
 852 2017 (Fig. 17b). Proshutinsky et al. (2019) report an increase from 2015–2017 which is  
 853 likely missing from *ASTER1* due to the omission of both increased river runoff and land  
 854 ice discharge in our forcing climatology and absence of the observed increase in FW im-  
 855 port through the Bering Strait as previously discussed (Fig 16).

856 The connection between the Arctic FWC increase and circulation changes in the  
 857 GIN Seas and North Atlantic has been the subject of several investigations (Dukhovskoy  
 858 et al., 2016; Carmack et al., 2016; Tesdal & Haine, 2020). A recent review by Haine et  
 859 al. (2015) summarized Arctic exchanges with the Canadian Arctic Archipelago (north  
 860 of Davis Strait) and the Barents Sea (east of the Barents Sea Opening). These estimates  
 861 heavily rely upon atmospheric reanalyses (for the provision of surface fluxes) and uncon-  
 862 strained model output (for tracer content change). Further south, Dukhovskoy et al. (2019)  
 863 investigated the redistribution of increased Greenland freshwater discharge (solid and  
 864 liquid) in the Subpolar North Atlantic (SPNA) and the GIN Seas, highlighting large un-  
 865 certainty due both to lack of constraint and acute dependency of transports on model  
 866 resolution (see also Weijer et al., 2012).

## 867 5 Discussion

868 A preliminary discussion of the state estimate focuses on the question of which con-  
 869 trol variables played a dominant role in achieving a reduction in misfit between obser-  
 870 vations and the model (Section 5.1). A second point of discussion highlights known is-  
 871 sues with this first release of ASTE and suggestions on how to improve future releases  
 872 (Section 5.2).

### 873 5.1 Identifying Key Control Adjustments

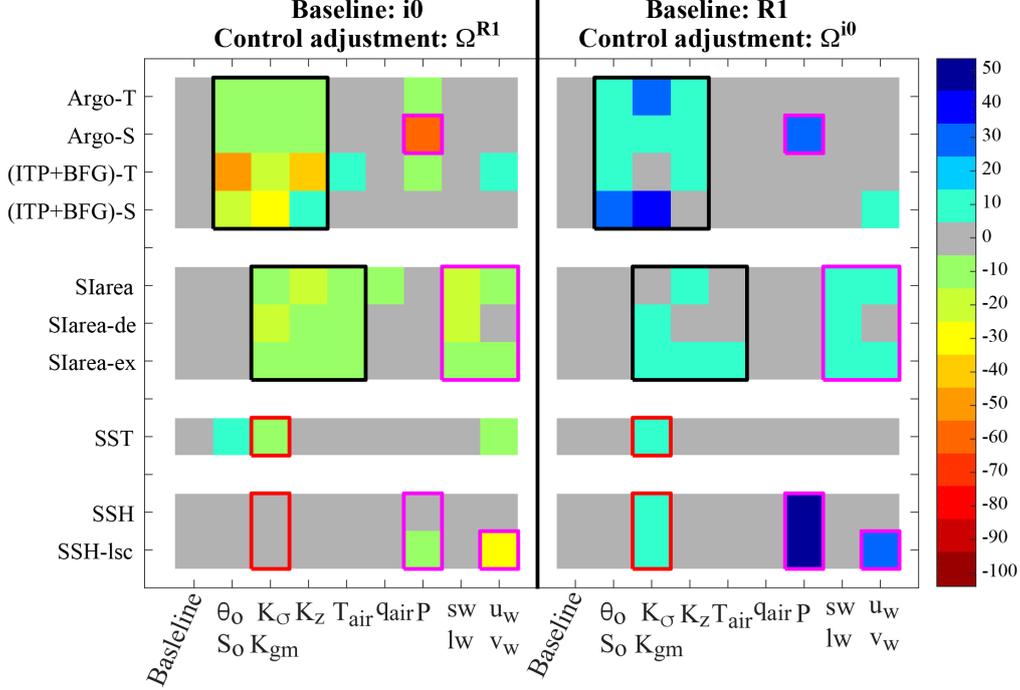
Experiment 1		Experiment 2	
Ensemble Member	optimized control(s) <i>added</i>	Ensemble Member	optimized control(s) <i>withheld</i>
1	$[\theta_0^{R1}, S_0^{R1}]$	1	$[\theta_0^{i0}, S_0^{i0}]$
2	$[\mathcal{K}_\sigma^{R1}, \mathcal{K}_{gm}^{R1}]$	2	$[\mathcal{K}_\sigma^{i0}, \mathcal{K}_{gm}^{i0}]$
3	$\mathcal{K}_z^{R1}$	3	$\mathcal{K}_z^{i0}$
4	$[u_w^{R1}, v_w^{R1}]$	4	$[u_w^{i0}, v_w^{i0}]$
5	$T_{air}^{R1}$	5	$T_{air}^{i0}$
6	$q_{air}^{R1}$	6	$q_{air}^{i0}$
7	$[R_{sw}^{R1}, R_{lw}^{R1}]$	7	$[R_{sw}^{i0}, R_{lw}^{i0}]$
8	$P^{R1}$	8	$P^{i0}$

**Table 5.** Ensemble members for each of the two ensemble experiments. In experiment 1, the control variables listed in column #2 were *added* to *it0*; in experiment 2, the control variables listed in column #4 were *withheld* from *ASTE\_R1*.

874 Optimization of the *ASTE\_R1* solution was achieved by iterative adjustment of a  
 875 set of control variables, as described in Section 2.2. Our control space ( $\Omega$ ) comprises 3D  
 876 fields of initial (i.e., 01/01/2002) temperature and salinity ( $\theta_0, S_0$ ), time-mean ocean mix-  
 877 ing coefficients ( $\mathcal{K}_\sigma, \mathcal{K}_{gm}$ , and  $\mathcal{K}_z$ ), and time-varying 2D fields of near-surface atmospheric  
 878 state variables ( $T_{air}, q_{air}, u_w, v_w, R_{sw}, R_{lw}$ , and  $P$ ). We now seek to identify which of these  
 879 control variable adjustments were key for the reduced model-data misfits in *ASTE\_R1*  
 880 relative to the unoptimized *it0*.

881 To proceed, we performed two additional forward ensemble experiments, each con-  
 882 sisting of eight members. In the first ensemble, optimized controls from *ASTE\_R1* were  
 883 substituted into *it0*, which was then re-run. Each ensemble member is characterized by  
 884 containing one of the *ASTE\_R1* optimized control variables/variable pairs listed in Ta-  
 885 ble 5 (left two columns). Note that there are 4 pairs: the optimized initial conditions ( $\theta_0^{R1}, S_0^{R1}$ ),

886 the optimized diffusivities for the eddy mixing parameterization ( $\mathcal{K}_\sigma^{R1}, \mathcal{K}_{gm}^{R1}$ ), the two com-  
 887 ponents of the wind speed ( $u_w^{R1}, v_w^{R1}$ ), and the net downward radiation ( $R_{sw}^{R1}, R_{lw}^{R1}$ ). For  
 888 any given ensemble member, large reductions in misfit indicate that the substituted opti-  
 889 mized control may play an important role in the *ASTE\_R1* solution. This is further  
 890 supported if misfits are not only reduced but brought close to their *ASTE\_R1* value.



**Figure 19.** Percentage change (color) in cost with respect to the constraint listed on the ordinate, attributable to the control substitutions given on the abscissa. The left group are members of the first ensemble of perturbation experiments, for which optimized controls  $\Omega^{R1}$  are substituted into the *it0* re-runs. The right group are members of the second ensemble, for which non-optimized controls  $\Omega^{i0}$  are substituted into the *ASTE\_R1* re-runs. On the left half of the plot, negative values indicate an improved solution i.e., a cost reduction with respect to *it0*. On the right half, positive values indicate deterioration of the solution i.e., a cost increase with respect to *ASTE\_R1*. Colored rectangular outlines highlight patterns of most impactful control variables (e.g., precipitation is important for the reduction of costs to Argo salinity and SSH).

891 However, a note of caution is needed. Our controls are not fully independent (e.g.,  
 892 some of the atmospheric state variable controls are related via bulk formulae) and as a  
 893 result, it is not possible to determine their full impact in isolation. For this reason, we  
 894 performed a second ensemble experiment, reversing the sense of the substitutions, so that  
 895 the non-optimized controls from *it0* were substituted into *ASTE\_R1*, which was then  
 896 re-run. In this experiment, each member is characterized by containing one of the *it0* non-  
 897 optimized control variables/variable pairs listed in Table 5 (right two columns). This sec-  
 898 ond ensemble lends confidence to our assessment as follows: an optimized control is highly  
 899 likely to be an important ingredient of the *ASTE\_R1* solution if its incorporation notably  
 900 improves the *it0* re-run (first ensemble) while its omission notably degrades the *ASTE\_R1*  
 901 re-run (second ensemble).

902 In Fig. 19 we examine the impact of the control substitutions on the costs in both  
 903 ensemble experiments. We show only normalized costs with respect to the following data

sets: Argo, ITP, Beaufort Gyre moorings, and satellite-based observations of SST, SSH and sea ice concentration. This choice enables a more focused discussion whilst also informing the large-scale quality of the solution near the ocean surface (from SSS and SST data) and throughout the upper ocean in the North Atlantic, GIN Seas, and Labrador Sea interior (from Argo T and S data) and in the western Arctic (from ITP and Beaufort Gyre moorings). Lastly, costs for sea ice concentration indicate performance of modelled air-sea fluxes and mixed layer properties in marginal ice zones (see Fig. 6 and related discussion). Our analysis reveals the importance of precipitation ( $P$ ) adjustments in obtaining realistic subsurface salinity distributions in the North Atlantic (Fig. 19) through the removal of the systematic excess rain bias discussed in Section 3.3 (Fig. 12d). Inclusion of the optimized precipitation  $P^{R1}$  in the *it0* re-run reduced the model cost with respect to Argo salinity by 56%. A 31% increase in this cost was seen on omission of the optimized precipitation in the *ASTE\_R1* re-run. Large improvements in SSH can also be attributed in part to corrected precipitation, as well as surface winds. Amongst other atmospheric forcing variables, surface air temperature, downward radiative forcing, and winds all have important impact on the sea ice cover (collective average of 17% improvement to *it0* and 5% degradation to *ASTE\_R1* ).

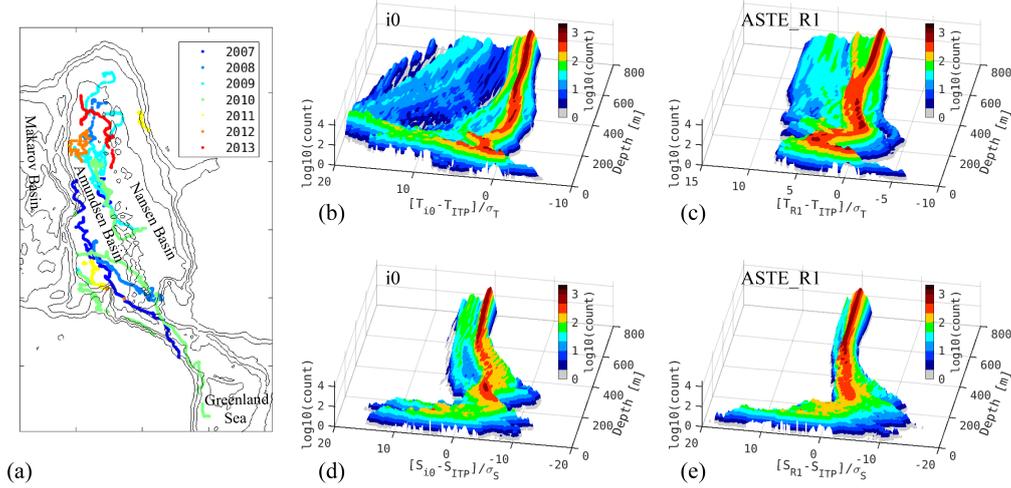
Adjustments to the initial conditions, vertical diffusivity and eddy mixing are also found to be important for improving subsurface hydrography throughout the *ASTE\_R1* domain. Optimized eddy mixing-related controls ( $\mathcal{K}_\sigma^{R1}, \mathcal{K}_{gm}^{R1}$ ) alone result in a 14% improvement (and 14% degradation) of the Arctic hydrography misfit when included (omitted) from the *it0* (*ASTE\_R1*) re-runs, respectively. These adjustments to the eddy mixing parameters also improve SST and SSH, and – in addition to the adjustments made to the vertical diffusivity and atmospheric conditions – are also seen to be critical for improved representation of sea ice cover.

## 5.2 Known Issues and Future Directions

During production of *ASTE\_R1* we have striven to utilize all known constraints that the state estimation machinery could handle. This constraint comprises  $O(10^9)$  observations from the diverse data sources (Table 2). Despite this effort, some systematic biases remain. Here we discuss notable issues in the *ASTE\_R1* solution and possible future directions for developing the next ASTE release.

*Eastern Arctic hydrography:* One of the largest remaining systematic biases is found in the Eurasian Basin, where subsurface constraints comprise sparse ITP sampling of the basin interior alone. Although the inflow is constrained by moorings at the Fram Strait, downstream observation of the circulation, eddy-induced stirring and vertical mixing in the Eurasian Basin along the shelf-basin slope and interior are limited (Fig. 20a). The serious implications of this paucity of data are highlighted by considering that the AW inflow takes  $\sim 6$ -10 years to transit this region without local constraint. As a result the inverse problem is highly under-determined. In practice, under-determination allows non-unique pathways to misfit minimization. For *ASTE\_R1*, we find that the AW layer in the Eastern Arctic, though much improved from *it0*, thickens over time (Fig. 20), a problem common to many state-of-the-art Arctic Ocean models (Holloway et al., 2007; Illicak et al., 2016; Docquier et al., 2019; Uotila et al., 2019).

As it is unlikely that widespread observation of 3-D velocity and mixing will be made in the near future, we anticipate that AW watermass representation in the Eurasian basin will remain an issue for both the next generation of state-of-the-art Arctic Ocean models and the next ASTE release. Although we do not expect large gains from planned changes to the ocean observing system in the near future, we do anticipate improvements in sea ice state, mixed layer representation, and shelf-basin exchanges in the next ASTE release, due to recent improvements to the stability of the adjoint of the sea ice thermodynamics (Bigdeli et al., 2020). This will enable a more complete use of sea ice observations



**Figure 20.** (a) Spatial distribution of ITP data used to constrain *ASTE\_R1* in the Eurasian Basin ; colors distinguish acquisition year. Histograms of normalized misfit to ITP (b,c) temperature and (d,e) salinity as a function of depth in the Eurasian Basin for (b,d) *i0* and (c,e) *ASTE\_R1* .

955 as active contributions to the cost function reduction  $J$  (eqn. (1)). The sensitivity of the  
 956 associated model-data misfits to the control space can then be used to better adjust at-  
 957 mospheric forcings. This will allow us to fully leverage the constraint from satellite-based  
 958 observations of the sea-ice state, which could only be partly exploited in the pseudo sea  
 959 ice adjoint employed for construction of *ASTE\_R1* . Inclusion of the sea ice thermody-  
 960 namics adjoint could potentially improve AW upward ventilation (Ivanov et al., 2012;  
 961 Polyakov et al., 2020) and preserve a more stable AW layer thickness, both in the Eurasian  
 962 Basin and further downstream in the Western Arctic.

963 *Arctic Circumpolar Current:* In the Laptev Sea it is thought that the circumpolar  
 964 circulation of AW splits at  $\sim 145^\circ\text{E}$ , with a fraction returning to the Fram Strait along  
 965 the Lomonosov Ridge (Rudels, 2015) and the remainder continuing along the basin’s rim  
 966 into the Western Arctic although the exact partitioning is not well constrained. In the  
 967 Western Arctic it is typically assumed that the AW continues to circulate cyclonically  
 968 along the basin boundary, although both *ASTE\_R1* (Grabon, 2020) and a modeling ef-  
 969 fort informed by observed radionuclide distributions (Karcher et al., 2012) suggest a weak  
 970 anticyclonic circulation during the last decade. Recent work analyzing all available cur-  
 971 rent meters (updated from Baumann et al. (2018)) has yielded velocity probability dis-  
 972 tributions for the Arctic region. This will be investigated as a novel approach to con-  
 973 strain ocean velocities within the AW circulation in the next *ASTE* release. In addition,  
 974 a more detail examination of the momentum and vorticity budgets along the circumpolar  
 975 current will offer insights into the role of viscous dissipation and eddies in maintain-  
 976 ing the cyclonic sense of circulation (Yang, 2005; Spall, 2020).

977 *Arctic river runoff and Greenland discharge:* FW transports and content in the  
 978 late 2010s are low in *ASTE\_R1* relative to independent observations (Section 4.3 and 4.4.2).  
 979 Near the surface in the Arctic and along the Greenland coast, recent increases in river  
 980 (A. Shiklomanov et al., 2020) and tundra runoff (Bamber et al., 2012), surface solid and  
 981 subsurface glacial discharge (Bamber et al., 2012, 2018) have been observed. This increase  
 982 was not included in the *ASTE\_R1* forcing. Meaningful application of these FW fluxes  
 983 as model forcings, especially in the Arctic marginal seas, requires careful consideration  
 984 of the following factors. Sub-glacial discharge is observed to enter the outlet glacier fjord

985 at depths near the grounding line instead of at the surface of the fjord’s exit to the con-  
 986 tinental shelf (Straneo & Cenedese, 2015; Sciascia et al., 2013). Mixing and entrainment  
 987 of this FW with the surroundings creates modified water whose property is prohibitively  
 988 difficult to continuously track downstream from the source using observed  $T/S$  (Beaird  
 989 et al., 2018). Consequently, the pathways of FW redistribution are highly uncertain. Nu-  
 990 merical simulations with Greenland discharge distributed at the surface yield pathways  
 991 from the source into the interior of SPNA and GIN seas that vary substantially with model  
 992 resolution and representation of mean currents (Weijer et al., 2012; Dukhovskoy et al.,  
 993 2016). The depth to which this FW is mixed down also varies highly with resolution (Dukhovskoy  
 994 et al., 2016), causing near surface over-freshening in certain cases and a 30–50% decrease  
 995 in the North Atlantic Meridional Overturning Circulation (AMOC) at time-scales vary-  
 996 ing between 3–50 years (Weijer et al., 2012). Similarly, preliminary sensitivity experi-  
 997 ments in *ASTE\_R1* with observed Greenland discharge applied at the surface show over-  
 998 freshening of the upper ocean in the Greenland Sea and a decrease in the AMOC at 55°N  
 999 by 40% within 5 years, inconsistent with observations (not shown). Prior to the next ASTE  
 1000 release, a dedicated study will be required to implement updated estimates of Greenland  
 1001 discharge as a subsurface freshwater forcing, consistent with observations (Straneo & Cenedese,  
 1002 2015). This will entail incorporation of a melt water plume parameterization into the  
 1003 ASTE framework. Lastly, instead of being absorbed into net  $E-P-R$ , a new control  
 1004 variable for runoff will be introduced to isolate and fully interrogate sensitivity to sub-  
 1005 surface forcing from subglacial discharge.

1006 *Subpolar North Atlantic hydrography:* In the SPNA, a warm bias in *ASTE\_R1*  
 1007 at 1000–2000 m depth (Fig. 13c) is associated with poor representation of transport across  
 1008 the GSR, a common problem in coarse to medium resolution ocean models (Gerdes et  
 1009 al., 2006; Heuzé & Årthun, 2019). Specifically, these models produce lower volume and  
 1010 heat transports across the GSR compared to observations (Heuzé & Årthun, 2019). Since  
 1011 the resolution of *ASTE\_R1* is  $\sim 18$  km in the subpolar gyre, we anticipate incomplete rep-  
 1012 resentation of both eddy/diffusive mechanisms – estimated to be important across the  
 1013 shallow Denmark Strait and Iceland-Faroe Ridge (Buckley et al., 2015) – and watermass  
 1014 transformations in the *ASTE\_R1* solution. Thus, although *ASTE\_R1* can capture the  
 1015 mean transports of volume and heat between Iceland and Scotland (Fig. 14–16), the re-  
 1016 maining warm bias across Denmark Strait and south of the GSR likely impacts our es-  
 1017 timate of heat content in both the eastern SPNA and Nordic Seas and alters the opti-  
 1018 mized air-sea heat flux in both regions. Recent data from the Overturning in the Sub-  
 1019 polar North Atlantic Program (OSNAP) observing system (Lozier et al., 2017, 2019) moor-  
 1020 ing array (deployed in 2014) will provide important information in the subpolar region,  
 1021 and an especially valuable constraint on the boundary currents and overflow waters, not  
 1022 captured by Argo.

## 1023 6 Summary and Outlook

1024 We have presented the first release of the Arctic Subpolar gyre sTate Estimate, *ASTE\_R1*  
 1025 , a data-constrained and dynamically consistent ocean-sea ice synthesis spanning the pe-  
 1026 riod 2002–2017. *ASTE\_R1* is produced using the ECCO adjoint-based state estimation  
 1027 framework, in which an ocean general circulation model, the MITgcm serves as a dynam-  
 1028 ical interpolator, spreading the influence of  $O(10^9)$  incorporated observations through  
 1029 space and time by way of linearized adjustment processes encapsulated in an adjoint model.  
 1030 Importantly, the model-data misfit is reduced via iterative adjustments to the initial hy-  
 1031 drographic conditions, atmospheric forcing and model mixing parameters alone, ensur-  
 1032 ing adherence to the governing equations throughout the entire estimation period. This  
 1033 distinguishes our approach from ocean reanalysis, in which violation of conservation laws  
 1034 complicates application for climate research (Stammer et al., 2016). The ability to as-  
 1035 sess closed tracer and momentum budgets in *ASTE\_R1* is a key strength of the prod-  
 1036 uct. As all sources and sinks are accounted for, full heat, salt and momentum (or vor-

1037 ticity) budgets can be analyzed to identify dominant sources contributing to the observed  
 1038 changes. These closed budget analyses can also be performed in  $T$ ,  $S$ ,  $\sigma$  space follow-  
 1039 ing R. P. Abernathy et al. (2016), enabling diagnosis of watermass evolution and de-  
 1040 struction in the *ASTE\_R1* solution. In addition, the adjoint modeling infrastructure al-  
 1041 lows for linear sensitivity studies using *ASTE\_R1* for investigation of causal mechanisms  
 1042 underlying variability in key quantities of climate interest (e.g., Bigdeli et al., 2020; Nguyen,  
 1043 Woodgate, & Heimbach, 2020; Pillar et al., 2016).

1044 During production of *ASTE\_R1* we have strived to utilize all known constraints that  
 1045 the state estimation machinery can handle. *ASTE\_R1* thus arguably represents the biggest  
 1046 effort undertaken to date with the aim of producing a specialized Arctic ocean-ice es-  
 1047 timate, freely available to the research community. This complements existing global ECCO  
 1048 solutions (Forget, Campin, et al., 2015; Fukumori et al., 2018), the Southern Ocean State  
 1049 Estimation (SOSE, (Mazloff et al., 2010)) and other global and regional ECCO deriva-  
 1050 tives (e.g., Köhl & Stammer, 2008; Gopalakrishnan et al., 2013; Zaba et al., 2018).

1051 For this initial assessment of *ASTE\_R1*, we have focused on comparison to avail-  
 1052 able observational constraints. Many of these were actively employed in the optimiza-  
 1053 tion procedure, but many others (e.g., all volume and tracer transport estimates) were  
 1054 withheld, allowing independent verification. The optimized solution serves as a signif-  
 1055 icant improvement from the unconstrained state, achieving consistency with the major-  
 1056 ity of incorporated observations, including both the set used in the optimization and that  
 1057 retained for post-validation (Table 3).

1058 The most substantial misfit reductions seen in *ASTE\_R1* are sea ice cover in the  
 1059 marginal ice zone, western Arctic hydrography, and subtropical North Atlantic sea level  
 1060 anomaly and subsurface salinity (Table 3, Fig. 5). In the Arctic Mediterranean, using  
 1061 only a proxy sea ice adjoint, *ASTE\_R1* achieves a 83% reduction in misfit to satellite-  
 1062 derived sea ice concentration constraints, mainly via improved representation of the sea-  
 1063 ice edge (Fig. 6). The solution faithfully reproduces both the observed seasonal cycle and  
 1064 low frequency trend of sea-ice extent.

1065 At the Fram Strait, the mooring array is crucial to constraining the important AW  
 1066 inflow and local hydrographic properties. At this important Arctic gateway, *ASTE\_R1*  
 1067 exhibits a 58% misfit reduction through the water column across the strait relative to  
 1068 the unconstrained solution. In the Arctic interior, ITPs provide unique information on  
 1069 the subsurface hydrography. Because 71% of the ITP profiles are located within the up-  
 1070 per 5–800 m in the Canada Basin interior, the most significant misfit reduction was seen  
 1071 here (85% in  $T$  and 62% in  $S$ , Fig. 9). In the remaining Arctic basin, low data coverage,  
 1072 combined with large uncertainty in the mean circulation and mixing parameters, resulted  
 1073 in less notable improvement (reductions of 89% in  $T$  and 31% in  $S$ ), but biases persist,  
 1074 especially at depth below the AW core (Fig. 20).

1075 Accompanying improved fit to hydrographic data used to constrain the solution,  
 1076 we find improvements in basin-scale heat and freshwater content. Interannual variabil-  
 1077 ity and low frequency trends in both heat and FW content are well represented in the  
 1078 Arctic Mediterranean and SPNA of *ASTE\_R1*. In the Beaufort Sea, *ASTE\_R1* captures  
 1079 the observed steady increase in upper halocline heat content from 2004–2017. Both the  
 1080 observed heat content increase in the upper water column within the Barents Sea and  
 1081 the heat content decrease in the east SPNA are also consistently captured (Fig. 17).

1082 We have been careful to clearly outline the notable biases remaining in the *ASTE\_R1*  
 1083 solution. These include a warm bias below the AW core in the eastern Arctic and in the  
 1084 east SPNA. The cause is a combination of lack of constraint here for the hydrography,  
 1085 mean circulation, and the adjustable initial condition and parametric controls. Additional  
 1086 biases exist in FW transports and contents in the Arctic Mediterranean due to the omis-  
 1087 sion of increased runoff from Arctic rivers and Greenland freshwater discharge.

1088 An advantage of our approach is that the use of a dynamical – as opposed to sta-  
1089 tistical – interpolator can improve spectral representation of the estimated state com-  
1090 pared to gridded products produced using statistical interpolations (e.g., Verdy et al.,  
1091 2017). This has not been addressed here, but it is a useful avenue for future ASTE as-  
1092 sessments and ongoing development.

1093 Looking toward the next *ASTER1* release, we expect the greatest progress will  
1094 be made by incorporating new model physics. In particular, improving the stability of  
1095 the sea ice thermodynamic adjoint (Bigdeli et al., 2020) will enable its use in ASTE, pro-  
1096 viding stronger constraint of air-ice-sea exchanges and ocean ventilation. Future efforts  
1097 will target hydrographic improvements along the Arctic shelf-basin slope in the eastern  
1098 Arctic to reduce the *ASTER1* AW layer warm bias. Additionally, updated estimates  
1099 of runoff and calving fluxes and inclusion of a parameterization of sub-glacial discharge  
1100 will enable improved estimate of freshwater redistribution and interbasin exchange. New  
1101 constraints, including datasets from the OSNAP mooring array (Lozier et al., 2017, 2019),  
1102 sea surface salinity (Vinogradova & Ponte, 2012; Fournier et al., 2019), and sea ice thick-  
1103 ness (Tian-Kunze et al., 2014; Ricker et al., 2017) will also be fully utilized in the pro-  
1104 duction of a further improved next ASTE release.

## 1105 Appendix A *ASTE\_R1* Product Distribution

### 1106 A1 Configuration set up

1107 The model configuration and all necessary inputs, including the optimized control  
 1108 adjustments, required for *ASTE\_R1* re-runs are available to the public, as discussed in  
 1109 the next section. The code base employed for *ASTE\_R1* production was MITgcm check-  
 1110 point c65q. *ASTE\_R1* was built using the full state estimation infrastructure, includ-  
 1111 ing specialized packages for misfit and adjustment evaluation, developed for ECCOv4r1  
 1112 (Forget, Campin, et al., 2015). In addition, two code developments specific to *ASTE* in-  
 1113 clude the implementation of a vertical diffusivity power control ( $\log_{10}\mathcal{K}_z$ ) and the ca-  
 1114 pability to switch between daily and monthly SSH costs.

1115 To ensure numerical stability during *ASTE\_R1* production, the following model choices  
 1116 were important: (a) a staggered time-step for momentum advection and Coriolis terms;  
 1117 (b) third-order advection for tracers (scheme code 30 in Table 2.2 in Adcroft et al., 2018),  
 1118 (c) linear free surface approximation, and (d) application of freshwater forcing via a vir-  
 1119 tual salt flux (i.e., no accompanying change in mass). These choices permitted a time-  
 1120 step of 1200 s. After 62 iterations, better model choices were used for the final forward  
 1121 run that produces more accurate physics in the distributed version of *ASTE\_R1*. These  
 1122 include (i) seventh order advection for tracers (scheme code 7 in Table 2.2 in Adcroft et  
 1123 al., 2018); (ii) nonlinear free surface with scaled  $z^*$  coordinates (Adcroft & Campin, 2004),  
 1124 and (iii) application of freshwater forcing via a real freshwater flux (i.e., with accompa-  
 1125 nying change in mass, Campin et al., 2004). These choices required a shorter time-step  
 1126 of 600 s. **The *ASTE\_R1* solution described and assessed in this paper is from**  
 1127 **the re-run of iteration 62 with the model choices (i)–(iii) described above.**

1128 In the distributed code, at compile and run-time, the user has the choice to use the  
 1129 more stable set up with a time-step of 1200 s or employ the more accurate physics with  
 1130 a time-step of 600 s as described above. We found that these small changes in the model  
 1131 configuration for the final forward run did not have a significant impact on the solution.  
 1132 The advantage of their application here is in enabling more accurate physical interpre-  
 1133 tations of mass and freshwater budgets. However, since these options also require a shorter  
 1134 timestep (for the nonlinear free surface) and a larger stencil (for the higher order advec-  
 1135 tion), their use demands significantly more computational resources (twice the walltime).  
 1136 For this reason, it was not feasible to employ these options until the final stages of *ASTE\_R1*  
 1137 development.

### 1138 A2 Distribution of the *ASTE\_R1* solution

1139 The full *ASTE\_R1* solution is publicly available through the UT-Austin ECCO por-  
 1140 tal at: <https://web.corral.tacc.utexas.edu/OceanProjects/ASTE/>, provided by the  
 1141 Texas Advanced Computing Center (TACC). Here we have made available:

- 1142 • time varying fields from *ASTE\_R1* as monthly and climatological averages,
- 1143 • monthly snapshots of the time varying ocean state,
- 1144 • fields representing the underlying grid,
- 1145 • compile time and run time inputs necessary to reproduce these fields with the MIT-  
 1146 gcm,
- 1147 • some MATLAB scripts to help analyze the *ASTE\_R1* fields.

1148 All fields are available here as NetCDF files.

1149 The monthly mean fields are additionally stored in a compressed format on Ama-  
 1150 zon Web Services (AWS) servers, provided by TACC at [https://s3.console.aws.amazon](https://s3.console.aws.amazon.com/s3/buckets/aste-release1/?region=us-east-2)  
 1151 [.com/s3/buckets/aste-release1/?region=us-east-2](https://s3/buckets/aste-release1/?region=us-east-2). These files are meant to be ac-  
 1152 cessed with the `llcreader` module of the open source python package `xmitgcm` (R. Aber-

1153 nathey et al., 2019), which allows users to analyze the data without the need to actu-  
 1154 ally download it. An interactive demonstration of this capability, which shows some sam-  
 1155 ple calculations enabled by `xgcm` (R. Abernathey et al., 2020) and `ECCOV4-py` (`github`  
 1156 `.com/ECCO-GROUP/ECCOV4-py`), is available through the Binder Project (Project Jupyter  
 1157 et al., 2018) at `github.com/crios-ut/aste` (T. Smith, 2020). This repository addition-  
 1158 ally contains environment files so that any user can reproduce the computing environ-  
 1159 ment necessary to analyze *ASTER1*, for instance on their own laptop.

## 1160 Appendix B Transport Calculation with Referenced $\theta/S$

1161 Here we describe heat and freshwater transport calculations used in *ASTER1* with  
 1162 respect to reference values of potential temperature ( $\theta_r$ ) and salinity ( $S_r$ ), respectively.  
 1163 This serves to (1) provide calculation details for comparison to those used by previously  
 1164 published estimates (supplementing results presented in section 4), and (2) expose where  
 1165 calculation differences may prevent meaningful comparisons (following discussion in sec-  
 1166 tion 2.3). For budget calculations, we refer the readers to detailed descriptions provided  
 1167 in Piecuch (2017) and Forget, Campin, et al. (2015).

1168 In the literature, transports are often computed with nonzero referenced values  $\theta_r/S_r$ .  
 1169 In section 4 we also provided online transport estimates for *ASTER1* made using non-  
 1170 zero references (e.g., for the heat flux through the Bering Strait). We caution here, how-  
 1171 ever, that all offline transport calculations made using available diagnostics from *ASTER1*  
 1172 (and all standard configurations of the MITgcm) will be exact only with  $\theta_r = 0$  and  
 1173  $S_r = 0$ , as these are the values used in all online tracer equations. To support users seek-  
 1174 ing to compute *ASTER1* transports offline assuming nonzero references, we now exam-  
 1175 ine the loss of accuracy that will be incurred. This loss of accuracy depends on the am-  
 1176 plitude of various missing terms (e.g., bolus transports and diffusive fluxes) relative to  
 1177 the contributions (e.g., Eulerian advection) contained in the available diagnostics. By  
 1178 deriving these approximations here and comparing their magnitudes with the accurate  
 1179 online values across important Arctic and GIN Seas gateways, we aim to identify which  
 1180 transports reported in Fig. 15-16 are reliable and which ones require caution for inter-  
 1181 pretation.

### 1182 B1 Accurate transport calculations

The horizontal transports of volume, heat, and freshwater (FW) across the Arc-  
 tic Mediteranean gateways are calculated by summing the total horizontal convergence  
 in the mass, heat, and salinity budgets, respectively, (Piecuch, 2017) as follows,

$$F_V = \int_L \int_{-D}^{\eta} \mathbf{u}_E \cdot \hat{\mathbf{n}} \, dz \, dl \quad (\text{B1.0})$$

$$\begin{aligned} F_H &= \rho_0 C_p \int_L \int_{-D}^{\eta} (\theta - \theta_r) (\mathbf{u}_E + \mathbf{u}_b) \cdot \hat{\mathbf{n}} \, dz \, dl + \rho_0 C_p F_{\theta, dif} + F_{H_i, adv} + F_{H_{sn}, adv} \\ &= F_{H_{\theta}, adv} + F_{H_{\theta}, dif} + F_{H_i, adv} + F_{H_{sn}, adv} \end{aligned} \quad (\text{B2.0})$$

$$\begin{aligned} F_{FW} &\approx \int_L \int_{-z_{S_r}}^{\eta} \frac{(S_r - S)}{S_r} (\mathbf{u}_E + \mathbf{u}_b) \cdot \hat{\mathbf{n}} \, dz \, dl + \left(1 + \frac{\eta}{D}\right) \frac{F_{S, dif}}{S_r} + \int_L \left( \frac{S_r - S_i}{S_r} \frac{\rho_i}{\rho_0} h_i \mathbf{u}_i + \frac{\rho_{sn}}{\rho_0} h_{sn} \mathbf{u}_{sn} \right) \cdot \hat{\mathbf{n}} \, dl \\ &= F_{FW_S, adv} + F_{FW_S, dif} + F_{FW_i, adv} + F_{FW_{sn}, adv} \end{aligned} \quad (\text{B3.0})$$

1183 where  $t$  is the time,  $\mathbf{u}_E, \mathbf{u}_b$  the (shaved-cell-weighted) ocean resolved Eulerian and un-  
 1184 resolved bolus velocities, and  $\mathbf{u}_i, \mathbf{u}_{sn}$  the sea ice and snow Eulerian velocities. For each  
 1185 gateway across which the transports are computed,  $\hat{\mathbf{n}}$  is the normal direction at each model  
 1186 grid point along the transport gate and  $L$  the section length along the gate. Vertical in-  
 1187 tegration is between  $\eta$  the sea surface and  $-D$  the ocean floor depth for volume and heat  
 1188 transports. Constants  $\rho_0 = 1029, \rho_i = 910$  and  $\rho_{sn} = 330$  are the seawater, sea ice,  
 1189 and snow densities in  $\text{kg/m}^3$ .  $C_p = 3996 \text{ J}^\circ\text{C}^{-1}\text{kg}^{-1}$  is the specific heat capacity of sea

1190 water,  $\theta_r$  the reference temperature,  $S_r = 34.8$  psu the reference salinity, and  $S_i = 4$  psu  
 1191 the constant sea ice salinity used in ASTE.  $\theta$  and  $S$  are the ocean potential temperature  
 1192 and salinity in  $^{\circ}\text{C}$  and psu, respectively;  $h_i$  and  $h_{sn}$  are the thickness of sea ice and snow  
 1193 in m.  $F_{\theta,dif}$  and  $F_{S,dif}$  are the parameterized diffusive flux of potential temperature and  
 1194 salinity  $\theta_r = 0$  and  $S_r = 0$ . For both advective and diffusive contributions to fresh-  
 1195 water transports (Eqn B3.0), vertical integration is only down to the depth of the refer-  
 1196 ence isohaline  $-z_{S_r}$ .

1197 Exact closure of heat budgets (see equations in Forget, Campin, et al. (2015) and  
 1198 Piecuch (2017)) and exact (to within numerical precision) calculation of heat transports  
 1199 (Eqn B2.0) can be achieved when  $\theta_r = 0$  and all diagnostics terms are computed on-  
 1200 line. Near exact freshwater budgets (see equations in Forget, Campin, et al. (2015) and  
 1201 Tesdal and Haine (2020)) and transports (Eqn B3.0) can be achieved with  $S_r = 0$ . Ad-  
 1202 ditionally the vertical integral must be computed every time step, continuously updat-  
 1203 ing the time-evolving  $z_{S_r}$ .

## 1204 B2 Approximations for nonzero $\theta_r/S_r$

1205 When using nonzero reference values (e.g.,  $\theta_r = -0.1^{\circ}\text{C}$  or  $S_r = 34.8$  psu as in  
 1206 Østerhus et al., 2019), neither heat nor freshwater diffusion terms are available in the  
 1207 offline diagnostics. To gauge orders of magnitudes, however, we approximate the diffu-  
 1208 sion term for FW using  $F_{S,dif}$  scaled by the non-linear free-surface factor  $(1 + \frac{\eta}{D})$  fol-  
 1209 lowing Piecuch (2017), then further scale by  $\frac{1}{S_r}$ . For the advection terms, the long-term  
 1210 mean transport can be derived exactly for heat and approximated for FW using a com-  
 1211 bination of readily available offline diagnostics for volume and heat/salt budgets as fol-  
 1212 lows:

$$\begin{aligned} \langle F_{H_{\theta},adv} \rangle &= \rho_0 C_p \left\langle \int_{-D}^{\eta} \int_L \left( (\theta - \theta_r)(\mathbf{u}_E + \mathbf{u}_b) \right) \cdot \hat{\mathbf{n}} \, dz \, dl \right\rangle \\ &= \rho_0 C_p \left\langle \int_{-D}^{\eta} \int_L \theta (\mathbf{u}_E + \mathbf{u}_b) \cdot \hat{\mathbf{n}} \, dz \, dl \right\rangle - \rho_0 C_p \theta_r \left\langle \int_{-D}^{\eta} \int_L \mathbf{u}_E \cdot \hat{\mathbf{n}} \, dz \, dl \right\rangle \end{aligned} \quad (\text{B2.1})$$

$$\begin{aligned} \langle F_{FW_S,adv} \rangle &\approx \left\langle \int_{-z_{S_r}}^{\eta} \int_L \frac{(S_r - S)}{S_r} (\mathbf{u}_E + \mathbf{u}_b) \cdot \hat{\mathbf{n}} \, dz \, dl \right\rangle \\ &\approx \left\langle \int_{-z_{S_r}}^{\eta} \int_L \left( \frac{S_r}{S_r} (\mathbf{u}_E + \mathbf{u}_b) - \frac{S}{S_r} (\mathbf{u}_E + \mathbf{u}_b) \right) \cdot \hat{\mathbf{n}} \, dz \, dl \right\rangle \\ &\approx \left\langle \int_{-z_{S_r}}^{\eta} \int_L \mathbf{u}_E \cdot \hat{\mathbf{n}} \, dz \, dl \right\rangle - \frac{1}{S_r} \left\langle \int_{-z_{S_r}}^{\eta} \int_L S (\mathbf{u}_E + \mathbf{u}_b) \cdot \hat{\mathbf{n}} \, dz \, dl \right\rangle \end{aligned} \quad (\text{B3.1})$$

1213 where the  $\langle \cdot \rangle$  is the multi-year mean which ensures  $\langle \mathbf{u}_b \rangle \equiv 0$  by definition. The approx-  
 1214 imation in  $F_{FW_S,adv}$  is due, again, to the reliance in the offline average of  $\langle S \rangle$  in deter-  
 1215 mining  $-z_{S_r}$ .

## 1216 B3 Approximations using monthly mean $\theta$ , $S$ and $\mathbf{u}_E$ ,

1217 Lastly, we note that due to disk space and I/O restrictions, it is typical for mod-  
 1218 elling studies to save and subsequently provide only monthly-averaged Eulerian veloc-  
 1219 ity  $\langle \mathbf{u}_E \rangle$  and tracers  $\langle \theta \rangle$  and  $\langle S \rangle$  for offline calculations of heat/FW transports and con-  
 1220 tents (e.g., Jahn et al., 2012; Kinney et al., 2014; Q. Wang et al., 2016b, 2016a; Ilicak  
 1221 et al., 2016; Heuzé & Årthun, 2019). In this case, the calculation for the advective terms  
 1222 in heat and FW transports are further approximated due to the cross-terms involving  
 1223 the bolus velocity  $S\mathbf{u}_b$  and  $\theta\mathbf{u}_b$  being excluded:

$$F_{H_{\theta},adv} \approx \rho_0 C_p \int_{-D}^{\eta} \int_L (\theta - \theta_r) \mathbf{u}_E \cdot \hat{\mathbf{n}} dz dl \quad (\text{B2.2})$$

$$F_{FW_S,adv} \approx \int_{-z_{S_r}}^{\eta} \int_L \frac{(S_r - S)}{S_r} \mathbf{u}_E \cdot \hat{\mathbf{n}} dz dl \quad (\text{B3.2})$$

1224 As before, inaccuracies will be incurred when  $z_{S_r}$  is determined using the monthly mean  
 1225  $\langle S \rangle$ . This is the case for all results shown for FW because no diagnostics pertinent to  
 1226 FW, including those of  $S - S_r$  or  $z_{S_r}$ , are available standard MITgcm diagnostic out-  
 1227 puts.

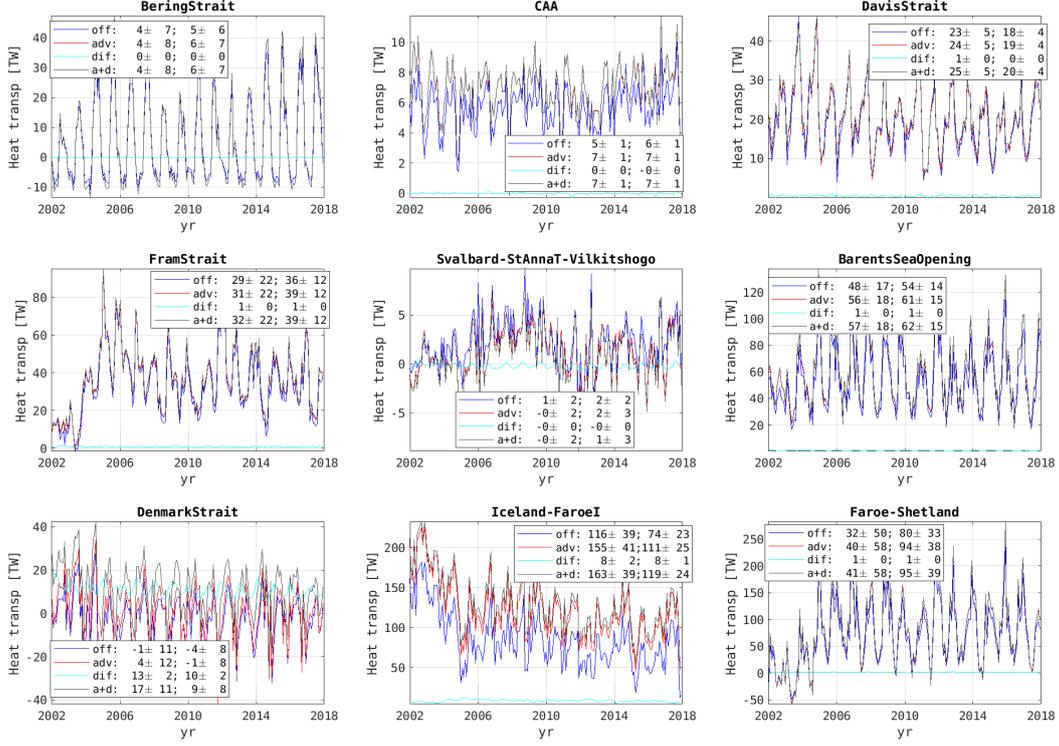
#### 1228 **B4 Interpretation of Transports: Confidence and Caution**

1229 Fig. B1-B2 show time-series of heat and FW transports for key gateways using both  
 1230 the most accurate online method and approximated offline method described above. The  
 1231 diffusion terms for both heat and FW are at least two orders of magnitude smaller than  
 1232 the advection terms and can be ignored almost everywhere. The exception is at the Den-  
 1233 mark Strait and Iceland-Faroe channels where omission of the diffusive contribution to  
 1234 the total heat transport leads to large errors of 30% and 100%, respectively. This shows  
 1235 that the estimates of tracer transports across these two gates should be interpreted with  
 1236 caution when computed offline using only model monthly outputs of the Eulerian veloc-  
 1237 ity and tracer averages.

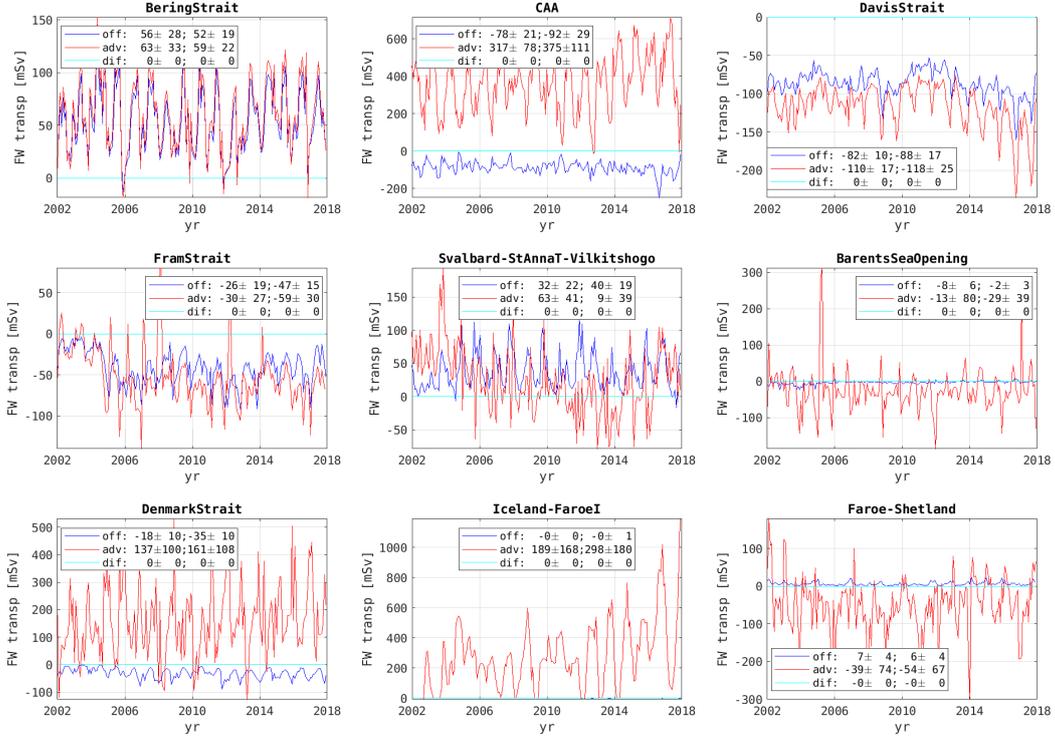
1238 For FW, as all methods are approximated, with the largest error likely due to not  
 1239 tracking the time-evolving depth of the reference isohaline  $z_{S_r}$ . Since there is no exact  
 1240 calculation for comparison, it is not possible to conclude which method, “adv” using the  
 1241 online advective term (Eqn B3.0) or “off” using the monthly mean Eulerian velocity and  
 1242 tracers (Eqn B3.2), is “more” correct in Fig. B2 and Table B1. It is likely that for gates  
 1243 where these two methods provide almost identical estimates (e.g., Bering, Davis and Fram  
 1244 Straits) we have higher confidence in our estimated FW transport. Across the CAA and  
 1245 the GSR the FW transport calculation depends strongly on the method employed and  
 1246 caution should be used in confidently reporting FW fluxes and comparing between dif-  
 1247 ferent studies.

Gate	FW Transports [mSv]	
(1) Bering Strait	<sup>a</sup> 61.32 ± 23.82	<sup>b</sup> 54.24 ± 20.62
(2) CAA	372.06 ± 109.98	-94.19 ± 31.60
(3) Fram Strait	-96.56 ± 34.85	-84.83 ± 23.29
(4) Svalbard-FJL <sup>1</sup> -SZ <sup>2</sup>	14.60 ± 43.37	45.23 ± 31.14
(5) Barents Sea Opening	-30.15 ± 38.18	-3.25 ± 3.30
(6) Davis Strait	-133.47 ± 26.66	-103.32 ± 19.59
(7) Denmark Strait	153.85 ± 106.71	-42.61 ± 12.21
(8) Iceland-Faroe	297.85 ± 178.35	-0.29 ± 0.69
(9) Faroe-Shetland	-53.61 ± 64.84	6.25 ± 4.29
(10) Newfoundland-Gr	-441.55 ± 242.66	-110.67 ± 23.44
(11) 48.3°N	-119.30 ± 38.67	-111.60 ± 22.80

**Table B1.** *ASTER1* Transports of freshwater ( $S_r=34.8$  psu) for the combined ocean and ice system for the period 2006–2017. FW fluxes are estimated using <sup>a</sup>Eqn B3.0 and <sup>b</sup>Eqn B3.2. <sup>1</sup> Franz Josef Land, <sup>2</sup> Severnaya Zemlya.



**Figure B1.** Time series of ocean heat transports (assuming a reference potential temperature  $\theta_r=0$ ) across important Arctic Mediterranean gateways using online (Eqn B2.0) and offline methods (“off”, Eqn B2.2), with the latter using outputs of monthly-averaged Eulerian velocity  $\langle \mathbf{u}_E \rangle$  and potential temperature  $\langle \theta \rangle$ . “adv” and “dif” are online calculations of the advective ( $F_{H\theta,adv}$ ) and diffusive ( $F_{H\theta,dif}$ ) terms for ocean transports on the RHS of Eqn B2.0, and their sum is given by “a+d”. The quantities listed in the legend are the 2002–2006 and 2007–2017 means and month-to-month variability. The variability is computed after the seasonal cycle has been removed. As explained in the main text, statistics are reported separately for these two periods due to large observed changes in the Arctic around 2006/2007.



**Figure B2.** Time series of ocean freshwater transports (assuming a reference salinity  $S_r = 34.8$ ) across important Arctic Mediterranean gateways using online (Eqn B3.0) and of-line (Eqn B3.2) methods. Both methods incur errors due to reliance of the monthly  $\langle S \rangle$  for determining the depth of the reference isohaline  $z_{S_r}$  serving as the integral limit. “off” refers to Eqn B3.2 which computes the transport offline using outputs of monthly-averaged Eulerian velocity  $\langle \mathbf{u}_E \rangle$  and salinity  $\langle S \rangle$ . “adv” and “dif” are the approximated online calculations of advective ( $F_{FW_S,adv}$ ) and diffusive ( $F_{FW_S,dif}$ ) terms on the RHS of Eqn B3.0. The quantities listed in the legend are the 2002–2006 and 2007–2017 means and month-to-month variability. The variability is computed after the seasonal cycle has been removed. Note that “adv” is consistently larger than “off” (and with larger variability), but it is not possible to conclude that the online calculation is superior due to imperfect treatment of  $z_{S_r}$ . Instead, we assume higher confidence in both our FW flux estimation and our FW flux comparisons where “adv” and “off” converge.

## 1248 Appendix C Watermass definition in *ASTE\_R1*

1249 Suitable specification of the characteristic salinity, potential temperature and density  
 1250 ( $S$ ,  $\theta$ ,  $\sigma$ ) defining known watermasses can differ between observations and models  
 1251 due to model biases, as shown in Fig. 13 in the main text for water properties in the Irminger  
 1252 and Labrador Seas. Watermasses can be clearly identified in *ASTE\_R1* as large volumes  
 1253 with a common formation history and distinct properties from surrounding waters, con-  
 1254 sistent with their definition in the literature. However in regions of hydrographic bias,  
 1255 these watermasses will not be identified - or correctly quantified - as their observed coun-  
 1256 terparts if they are tracked following the observed values too strictly. In this appendix,  
 1257 we summarize the choices made in determining watermass and explore the sensitivity  
 1258 to these choices where appropriate.

### 1259 C1 Volume transports of watermass

1260 Table C1 lists the watermass properties at Fram Strait (FS) and across the Greenland-  
 1261 Scotland Ridge (GSR) used to identify the transports reported in Fig. 14 in the main  
 1262 text. At the FS, the mean transports can be decomposed approximately into the West  
 1263 Spitsbergen Current (WSC, east of 5°E, Beszczynska-Möller et al., 2012), recirculated  
 1264 Atlantic Water (AW) (between 3.2°W and 5°E), and the East Greenland Current (EGC,  
 1265 west of 3.2°W,  $S \leq 34$  psu,  $T \leq 1^\circ\text{C}$ ). At the GSR definitions of watermasses such  
 1266 as the surface outflow, dense outflow, modified water, and inflow AW from Østerhus et  
 1267 al. (2019) and Hansen and Østerhus (2000) can be problematic when strictly applied to  
 1268 grid-scale average quantities. For example, the densewater in the outflow through Den-  
 1269 mark Strait (DS) is defined in Østerhus et al. (2019) as having density anomaly  $\sigma_\theta >$   
 1270 27.8, but in *ASTE\_R1* outflow at the lowest depths of the strait are characterized by a  
 1271 lower bound of  $\sigma_\theta$  ranging between 27.28 and 27.81. For this range, the corresponding  
 1272 southward transports are  $-1.6 \pm 0.9$  to  $0.5 \pm 0.3$  Sv (see Fig. 14, blue color text). Sim-  
 1273 ilarly, over the Iceland-Faroe (IF) ridge, the southward transports of densewater defined  
 1274 by  $\sigma_\theta \geq 22.44$  or  $\sigma_\theta \geq 27.55$  in *ASTE\_R1* yield a range of  $-0.4$  to  $-0.3$  Sv, compared  
 1275 to  $-0.4 \pm 0.3$  Sv of water with  $\sigma_\theta \geq 27.8$  in Østerhus et al. (2019). Similar considera-  
 1276 tions applied also to dense water properties at the Faroe-Shetland (FSh) ridge ( $\sigma_\theta \geq$   
 1277 27.81 in *ASTE\_R1* compared to 27.8 in Østerhus et al., 2019). For the northward flow,  
 1278 in addition to salinity thresholds ( $S \geq [34.8, 35, 35.25]$  psu), temperature thresholds of  $\theta \geq$   
 1279  $[5, 4, 5]^\circ\text{C}$  are used in *ASTE\_R1* to identify the warm AW across the DS, IF, and FSh chan-  
 1280 nels.

### 1281 C2 Heat content of upper halocline watermass

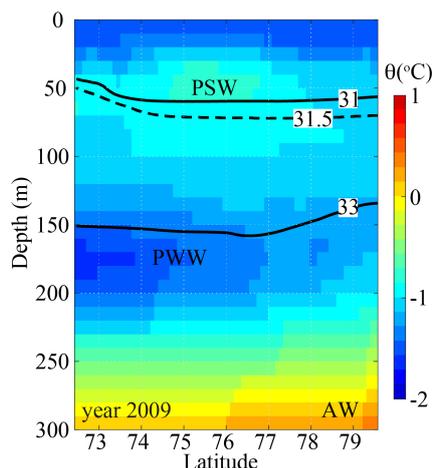
1282 The upper halocline watermass, defined by Timmermans et al. (2018) as a layer  
 1283 within lower and upper salinity bounds of  $S_l=31.0$  psu and  $S_u=33.0$  psu, respectively,  
 1284 was identified based on subsurface in situ observations with fine vertical sampling res-  
 1285 olution. In *ASTE\_R1*, with vertical grid spacing of 15–20 m within the water column  
 1286 depths 50–160 m, average salinity in the water column changes more abruptly than in  
 1287 the observations. For more accurate estimation of halocline-integrated quantities one ap-  
 1288 proach is to “interpolate” the salinity in the vertical to a finer grid to find the exact depths  
 1289 at which salinity fits within the given bounds. Though this is often done during model-  
 1290 data comparisons (e.g., Grabon, 2020), the interpolation introduces additional informa-  
 1291 tion that was not strictly solved for by the model. An alternate approach is to vary the  
 1292 salinity bounds to gauge the sensitivity of the heat content within this watermass to the  
 1293 vertical discretization in the model. As an example, Fig. C1 shows a vertical section in  
 1294 *ASTE\_R1* through the Beaufort Gyre region as defined in Timmermans et al. (2018),  
 1295 with the watermass bounded between a temperature maximum at depths  $\sim 50$ –60 m (Pa-  
 1296 cific Summer Water, PSW,  $S_l=31$  salinity contour) and a temperature minimum at depths  
 1297  $\sim 150$  m (Pacific Winter Water, PWW,  $S_u=33$ ). In *ASTE\_R1*, negligible sensitivity is  
 1298 found with changes to  $S_u$ , but the heat content within the upper halocline in this region

Gate	Watermass	Properties		Reference
		Obs	ASTE	
FS	WSC	$\text{lon} > 5^\circ\text{E}$ , $T \geq 2^\circ\text{C}$ , $\sigma_\theta \sim 27.97 \text{ kg/m}^3$	$\text{lon} \geq 4^\circ\text{E}$ , $T \geq 2^\circ\text{C}$	Beszczynska-Möller et al. (2012), Schauer and Beszczynska-Möller (2009)
	Recirc AW	$-2.5^\circ\text{E} < \text{lon} < 5^\circ\text{E}$	$-3.2^\circ\text{E} < \text{lon} < 4^\circ\text{E}$ , $T \geq 1^\circ\text{C}$ , $S > 34 \text{ psu}$	Beszczynska-Möller et al. (2012)
	deep AW	$\text{lon} < -3^\circ\text{E}$	$-3.2^\circ\text{E} < \text{lon} < 4^\circ\text{E}$ , $T < 1^\circ\text{C}$ , $S > 34 \text{ psu}$	Beszczynska-Möller et al. (2012)
	return flow		$\text{lon} < -3.2^\circ\text{E}$	
	EGC	$\text{lon} < -1^\circ\text{E}$	$S < 34 \text{ psu}$ , $T \leq 1^\circ\text{C}$	de Steur et al. (2014)
DS	inflow AW	–	$S > 34.8 \text{ psu}$ , $T > 5$	
	dense outflow	$\sigma_\theta > 27.8 \text{ kg/m}^3$	$S > 34.5, 34.8 \text{ psu}$ , $T < 3.5^\circ\text{C}$	Østerhus et al. (2019)
	surface outflow	$\sigma_\theta < 27.8 \text{ kg/m}^3$	$\sigma_\theta > 27.44, 27.81 \text{ kg/m}^3$ , $S \leq 34.5 \text{ psu}$	
IF	inflow AW	–	$S > 35 \text{ psu}$ , $T > 5^\circ\text{C}$	
	dense outflow	$\sigma_\theta > 27.8 \text{ kg/m}^3$	$35 \geq S > 34.5, 34.7 \text{ psu}$ , $T \leq 4, 5^\circ\text{C}$ , $\sigma_\theta > 27.44, 27.55 \text{ kg/m}^3$	Østerhus et al. (2019)
FSh	inflow AW	–	$S > 35.25 \text{ psu}$ , $T > 5^\circ\text{C}$ , $\sigma_\theta > 27.87 \text{ kg/m}^3$	Østerhus et al. (2019)
	dense outflow	$\sigma_\theta > 27.8 \text{ kg/m}^3$	$35 \geq S > 34.8 \text{ psu}$ , $T \leq 2^\circ\text{C}$ , $\sigma_\theta > 27.81, 27.97 \text{ kg/m}^3$	

**Table C1.** Watermass at important Arctic Mediterranean gateway defined based on observations and in *ASTE\_R1*.

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changes by approximately 1–2.5% per 0.1 psu change in  $S_l$ . A change in  $S_l$  of  $\sim 0.5$  psu corresponds approximately to one depth level in *ASTE\_R1*, and the heat content change associated with this is shown in shade in Fig. 17 in the main text.



**Figure C1.** Vertical mean temperature for the year 2009 in a section across the Beaufort Gyre. Salinity contours are shown in black with white label, with the upper halocline watermass defined based on Timmermans et al. (2018) as bounded by  $S_l=31$  psu (through the temperature maximum associated with the Pacific Summer Water PSW) and  $S_u=33$  psu (through the temperature minimum associated with the Pacific Winter Water PWW). A change of  $S_l$  by 0.5 psu corresponds approximately to 1 vertical depth level change in *ASTER1*.

### Acknowledgments

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