CLIMATE-SPACE - THEME II: CROSS-ECV ACTIVITIES

ARCFRESH (ARCTIC FRESHWATER BUDGET)

Uncertainty Propagation Strategy (UPS)

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Change Log

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0.5	D. Fantin, S&T	All	Document created	
1.0	E. Woolliams	All	V 1.0 consolidated	Released to ESA

Acronyms and Abbreviations

CCI	Climate Change Initiative
CMEMS	Copernicus Marine Environment Monitoring Services
CPS	Climate Processes Section
CRD	Climate Research Division
DTU	Technical University of Denmark
ECCC	Environment and Climate Change Canada
ECV	Essential Climate Variable
ENVEO	ENVironmental Earth Observation
EO	Earth Observation
ESA	European Space Agency
FWF	Freshwater flux
GCOS	Global Climate Observing System
GIS	Greenland Ice Sheet
GIS	Greenland Ice Sheet
GRACE	Gravity Recovery and Climate Experiment
IPCC	Intergovernmental Panel on Climate Change
IV	Ice Velocity
METNO	Norwegian Meteorological Institute
MFID	Mass Flux Ice Discharge
NERSC	Nansen Environmental and Remote Sensing Center
NORCE	Norwegian Research Centre
NPL	National Physical Laboratory
OBP	Ocean Bottom Pressure
RCM	RADARSAT Constellation Mission
S1	Sentinel-1
SAR	Synthetic Aperture RADAR

SEC	Surface Elevation Change
SIM	Sea Ice Motion
SMB	Surface Mass Balance
SMHI	Swedish Meteorological and Hydrological Institute
SoW	Statement-of-Work
SSH	Sea Surface Heights
SSS	Sea Surface Salinity
TBA	To be announced
TOPAZ	Towards an Operational Prediction system of the North Atlantic and the coastal Zone.
UBO	Université de Bretagne-Occidentale

1 Introduction

1.1 Applicable Document

This document contains the Uncertainty Propagation Strategy (UPS) for the ARCFRESH project for CLIMATE-SPACE - THEME II: CROSS-ECV ACTIVITIES, in accordance with the contract [AD1], SoW [AD2] and proposal [AD3-AD10].

The purpose of this document is to document an approach to uncertainty assessment for the ARCFRESH project. Here, we outline how the project approaches identifying, quantifying, propagating and disseminating uncertainty information. Our main focus is on the observational datasets. However, we also consider uncertainties in the models.

At this stage (version 1.0) of the document, the analysis here is limited and has some aspects that are as yet unclear. In this, it has the role of highlighting potential issues and unknowns to be considered more thoroughly in the next phase of the project.

1.2 Applicable Document Contents

This document is structured as follows:

- Chapter 1 introduces this document.
- Chapter 2 describes the QA4EO Five Steps approach to uncertainty assessment that has been developed for observational datasets.
- Chapters 3 - 7 go through each of the Five Steps in turn, considering how they apply to the datasets.
- Chapter 8 finishes the section on observational datasets by considering validation approaches.
- Chapter 9 extends the analysis to consider the modelling activity and the information available from closing the freshwater budget.

1.3 Applicable Document

No	Doc. Id	Doc. Title	Date	Issue/ Revision/ Version
AD-1	4000145884/24/I-LR	ESA Contract No. 4000145884/24/I-LR	27/09/2024	NA
AD-2	ESA-EOP-SC-AMT-2023-21	Statement of Work and Annexes and Appendexes	01/12/2023	1.0
AD-3	DTU-ESA-ARCFRESH-CL-001	ARCFRESH Cover Letter	22/02/2024	1.0
AD-4	DTU-ESA-ARCFRESH-TPROP-001	ARCFRESH Technical Proposal	22/02/2024	1.0
AD-5	DTU-ESA-ARCFRESH-IPROP-001	ARCFRESH Implementation Proposal	22/02/2024	1.0
AD-6	DTU-ESA-ARCFRESH-MPROP-001	ARCFRESH Management Proposal	22/02/2024	1.0
AD-7	DTU-ESA-ARCFRESH-FPROP-001	ARCFRESH Financial Proposal	22/02/2024	1.0
AD-8	DTU-ESA-ARCFRESH-CPROP-001	ARCFRESH Contractual Proposal	22/02/2024	1.0
AD-9	DTU-ESA-ARCFRESH-BF-001	ARCFRESH Background and Facilities	22/02/2024	1.0
AD-10	DTU-ESA-ARCFRESH-CV-001	ARCFRESH Curricula Vitae	22/02/2024	1.0

Note: If not provided, the reference applies to the latest released Issue/Revision/Version

2 Observational datasets: the QA4EO Five Steps

Uncertainty assessment for this project's observational datasets is based on the QA4EO Five Steps approach (www.qa4eo.org). A recent paper describes the theoretical background [Woolliams, 2025, to be published] and how the Five Steps are rooted in metrological principles for uncertainty analysis and particularly the Joint Committee for Guides in Metrology (JCGM) Guide to the Expression of Uncertainty in Measurement (GUM). The principles build on work in earlier projects such as FIDUCEO (https://research.reading.ac.uk/fiduceo/) and GAIA-CLIM (https://www.gaia-clim.eu/), as described originally in [Mittaz et al 2019]. QA4EO is the Quality Assurance framework for Earth Observation and is a set of principles endorsed by the Committee on Earth Observation Satellites (CEOS) and the Global Satellite Intercomparison System (GSICS). The QA4EO approach has also been highlighted in the Global Climate Observing System (GCOS) 2022 Implementation Plan (GCOS, 2022).

The metrological approach involves the following aspects (quote from Woolliams et al., 2025):

- Consistent terminology, including a clear distinction between 'error' and 'uncertainty',
- Well-defined measurand (or, for multivariate quantities, measurands), defined through an associated measurement model,
- Measurement model incorporating in its input quantities all known effects, including correction terms relating to known biases.
- Propagation of uncertainties (and covariances) through the same measurement model that is used to calculate the measured value (the estimate of the measurand).

It is clear from this list that the availability of a suitable measurement model is central to a metrological approach. The measurement model describes how the measurand — the quantity intended to be measured — is calculated from input quantities. It is often written by an analytic (algebraic) expression, but measurement models may also be defined through code, particularly where iterative processes and inverse problem solution methods are used, or when there are classification or similar steps in the processing. Note that the measurement model does not necessarily describe a pure 'measurement', indeed it is common for the measurand to be calculated from the input quantities through some appropriate model. In real measurement scenarios, the measurement model is also usually a 'multi-stage measurement model', in that the input quantities to the calculation of the final 'measurand' are themselves calculated from their own measurement models.

Another core aspect of a metrological uncertainty assessment is the clear distinction between 'uncertainty' and 'error'. The International Vocabulary of Metrology (VIM), in its current (third) edition (JCGM 200) defines measurement error as 'measured quantity value minus a reference quantity value' and measurement uncertainty as 'non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used'. The error is almost always unknown (because if it were known, it would be corrected for, to create a 'measurement model incorporating all known effects'). It is the unknown difference between the measured value and the true value. The standard uncertainty is the standard deviation of the distribution around the measured value in which the true value is expected to lie. In most cases, where the distribution is symmetrical, the uncertainty also describes the distribution of possible errors.

The Five Steps approach is summarised in Figure 2.1.

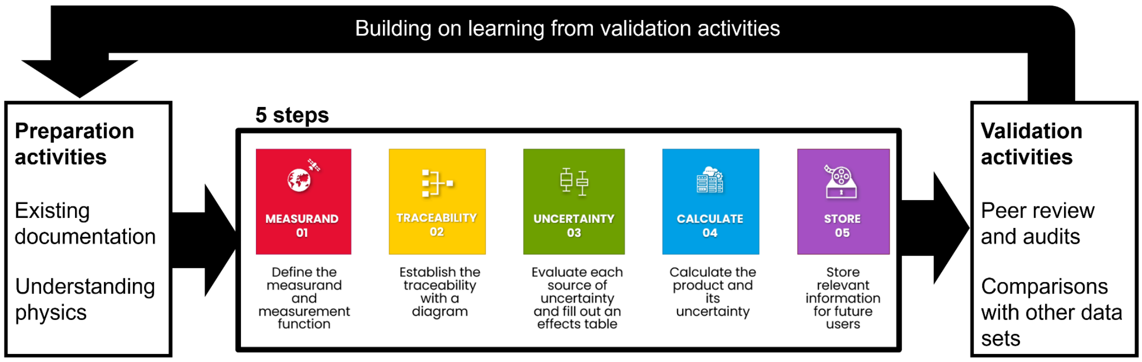

Figure 2.1: The QA4EO Five Steps to uncertainty analysis. Further details are available on (www.qa4eo.org). The Five Steps are given within the central box and are placed within an external iteration loop that represents how such analyses are informed by preparation activities and refined through validation activities.

The Five Steps are as follows:

- Step 1: Define the measurand and measurement model
- Step 2: Establish traceability with a diagram
- Step 3: Evaluate each source of uncertainty and fill out an effects table
- Step 4: Calculate the product and its uncertainty
- Step 5: Store relevant information for future users.

The Five Steps are shown in Figure XX as being within an iterative feedback loop that is informed by validation activities involving both peer review and comparisons across datasets.

Each step is described in its own chapter below, including application to each of the observational datasets in the project. Chapter 8 considers the iteration step.

3 Observational datasets, step 1: Define the measurand

3.1 What do we mean by 'Step 1: Define the measurand'?

The most important of the QA4EO Five Steps is the first: providing a clear definition of the measurand. In metrology, the measurand is the quantity intended to be measured, specified without ambiguity in terms of its physical basis, system boundaries, and conditions. This clarity underpins traceability and uncertainty analysis. Without it, subsequent steps—such as uncertainty quantification—lack robustness. This need is described in the GUM-6, section 6.2 as:

> "Taking account of any given target measurement uncertainty, the measurand should be specified sufficiently well so that its value is unique for all practical purposes related to the measurement." **JCGM GUM-6:2020**

Within this project, the scientific aim is to close the budget of *freshwater flux in the Arctic Ocean*. Freshwater flux is not a directly observable property. It is a derived quantity, dependent on assumptions such as reference salinity, spatial boundaries, and time averaging. These choices affect both interpretation and comparability. The concept of freshwater is used because of its practical utility. There are limited inputs of salt into the global ocean, and therefore changes in salinity are caused either by water (or sea ice) transport from one part of the ocean to another of different salinity, or by the input of freshwater from rivers or glaciers, or by the relative difference of precipitation and evaporation. In the Arctic Ocean, these quantities can be independently assessed.

Defining the measurand must start by asking three questions: What is freshwater? What is flux? What is the Arctic Ocean? To determine freshwater flux in the Arctic, we also work with different input quantities: sea ice flux, river discharge, glacier discharge, evaporation/precipitation, and ocean gateway fluxes. We compare the sum of these input quantities to a direct freshwater estimate based on ocean salinity and sea surface height. These terms are considered in the subsections below.

Note that the step *defines the measurand* is always more complicated than it first appears in any metrological uncertainty analysis. In the case of freshwater flux, this is particularly so. A valuable paper in this space (Schauer and Losch, 2019) is entitled *"Freshwater in the ocean is not a useful parameter in climate research"*. At this stage in the project, our measurand is not well defined. The pre-work described here sets out many of the challenges in defining "freshwater flux in the Arctic Ocean", and efforts early in the second year of the project will explore this further.

To understand these challenges, we first examine the building blocks of the measurand: salinity and freshwater.

3.2 Freshwater flux in the Arctic Ocean

3.2.1 What is salinity?

Since freshwater is defined relative to salinity, we begin by clarifying what salinity means in oceanography and how it is measured. At a basic level, salinity relates to the amount of salts dissolved in seawater. There are two different types of salinity commonly used:

- Absolute Salinity (usually written as SA) is the mass of dissolved salts per unit mass of seawater, expressed typically in grams of salt per kilogram of water [g kg^{-1}]. Note that this definition includes a built-in factor of 10^{-3} compared to using the coherent SI units directly [kg kg^{-1}].
- Practical Salinity (usually written as SP), which is derived from the conductivity ratio of seawater to a standard KCl solution, following the Practical Salinity Scale of 1978. Corrections are made for the major ions (Na^+, Cl^-, etc.), but it does not account for minor constituents, broader sea water composition (that varies regionally) or non-ionic solutes. Practical salinity is unitless, but in practice, it is numerically close to the absolute salinity in [g kg^{-1}]. This leads to the common, though technically incorrect, practice of treating it as though it were a measure of [g kg^{-1}].

For typical ocean salinities, the difference between SA and SP is small, around 0.01 g kg^{-1} to 0.05 g kg^{-1}. In regions with unusual seawater composition (including the Arctic shelf seas), the difference can be as much as 0.1 g kg^{-1}.

Satellite measurements add further complexity. Microwave radiometers measure brightness temperature, which is sensitive to the dielectric properties of the sea surface—strongly influenced by salinity—as well as temperature, surface roughness, wind speed, and atmospheric conditions. The retrieved sea surface salinity is derived through complex inversion algorithms and empirical models, without a direct link to either SP or SA. The uncertainties inherent in this retrieval process—combined with natural variability across the satellite's spatial footprint—are much larger than the typical SA–SP difference. For this project, we will not be concerned about this distinction but note it for future consideration.

3.2.2 What is freshwater?

With salinity defined, we can now consider freshwater. Here, ambiguity arises because freshwater is not a distinct tracer but a conceptual quantity derived from salinity. There are several mutually ambiguous ways that 'freshwater' can be defined.

As previously presented in the SRD, the most obvious definition of freshwater would be given by:

$$F_{\mathrm{FW}}^{\mathrm{abs}} = 1 - S^{\mathrm{SA}}/1000. \quad (1)$$

That definition, based on absolute salinity, is unique. However, it is difficult to assess in terms of flux.

More commonly, freshwater fraction is defined by contrast with salinity in the water body of interest relative to a reference salinity, using practical salinity measurements:

$$F_{\mathrm{FW}} = \frac{S_{\mathrm{ref}}^{\mathrm{SP}} - S_{\mathrm{FW}}^{\mathrm{SP}}}{S_{\mathrm{ref}}^{\mathrm{SP}}} \quad (2)$$

As discussed in the SRD, and explained in detail in Schauer and Losch (2019), the practical application of this in the literature is not sufficiently unique because of different values of $S_{\mathrm{ref}}^{\mathrm{SP}}$ used in different studies. and because it is extremely sensitive to that value when mass is not conserved. Moreover, this definition is extremely sensitive to the reference value when mass is not conserved. Schauer and Losch emphasise that because of the non-linear nature of this equation, the sensitivity to reference is far more than a change in unit. They illustrate that while length units (metre, yard, cubit) differ by simple scaling, and temperature scales differ by linear transformations, freshwater flux defined as in equation (2) is so non-linear that no straightforward comparison can be made across studies.

These definitions form the conceptual basis for expressing freshwater flux, which we address next. However, as this discussion shows, the choice of reference salinity introduces non-linear behaviour that complicates interpretation and comparability: a key challenge for defining the measurand in a metrological sense.

3.2.2.1 Freshwater volume and mass

At present, there is no consensus within the project on whether fluxes should be expressed in terms of mass fluxes or volume fluxes. Volume fluxes ($m^3\ s^{-1}$ in coherent SI units) are often written in sverdrups (Sv) (1 Sv = $10^6\ m^3/s$) or km^3 per year (1 mSv ≈31.5 km^3/year), although the latter is ambiguous through the definition of ‘year’ (albeit that the definitional uncertainty in year may be insignificant compared to other uncertainties. Mass fluxes (kg s^{-1} in coherent SI units) may be written in gigatonnes per year (Gt/year).

Salinity is defined per unit mass, which suggests a mass-based approach, yet volume fluxes are often used because sea surface height changes are observed directly. Converting between the two requires density, which depends on both salinity and temperature. A simplistic linear model would be:

$$\rho = \rho_0\left[1 - \alpha(T - T_0) + \beta(S - S_0)\right] \quad (3)$$

Where,

ρ is the sea water density in kg m^{-3}

ρ_0 is the reference density

T, T_0 are the temperature and reference temperatures (in kelvin or degrees Celsius)

S, S_0 are the salinity and reference salinity in g kg^{-1}

α is the thermal expansion coefficient, which is $\sim 2 \times 10^{-4}$ °C^{-1}.

β is the haline contraction coefficient, which is $\sim 8 \times 10^{-4}\ (\mathrm{g\ kg}^{-1})^{-1}$.

In principle, temperature influences density through the thermal expansion coefficient α, but in the Arctic, this effect is small compared to salinity because (a) the haline contraction coefficient β is larger than α, and (b) salinity anomalies are much greater than temperature anomalies. For this reason, temperature changes are often considered negligible in practical flux calculations. However, this assumption needs careful review to ensure it does not introduce hidden biases when comparing methods or closing budgets. As with the freshwater flux more generally, it requires reference temperatures and salinities. Furthermore, even if there was a desire to take the temperature sensitivity into account, this may be difficult to do practically, because of limited information about the temperature and salinity column profiles in the Arctic Ocean. Surface observations from satellites are insufficient to separate the two steric effects without more information about profiles.

A further conceptual issue is the assumption of mass conservation within the Arctic Ocean: that freshwater inputs displace saline water exported through gateways. This assumption simplifies budget closure and underpins many indirect flux estimates, but its validity is uncertain. The Arctic can store freshwater in the halocline or as sea ice, and export pathways vary, so displacement is neither instantaneous nor complete. How much this matters for our uncertainty analysis remains an open question. If the assumption is too strong, it risks circular reasoning—interpreting salinity changes as freshwater flux while assuming those fluxes explain salinity changes.

Related to this is the distinction between steric and barystatic freshwater fluxes, which the community often defines separately. Steric changes refer to volume changes driven by density variations (e.g., salinity and temperature effects), while barystatic changes reflect actual mass addition or removal (e.g., river discharge, glacial melt). Both influence sea level and ocean dynamics, but they are not interchangeable. In practice, many studies conflate these concepts when interpreting salinity anomalies as freshwater flux, which further complicates metrological clarity.

These questions remain unclear at this stage of the project.

3.2.2.2 Freshwater fluxes from a sum of components (Le Bras and Timmermans)

In the SRD, we propose using the definitions of freshwater flux given in the Le Bras and Timmermans (2025) paper, which is given as a mass flux as:

$$\frac{d}{dt}(\rho V) = \Phi_m^{\mathrm{OCE}} + \Phi_m^{\mathrm{FW}} + \Phi_m^{\mathrm{SI}}. \quad (3)$$

Here, we have re-written Equation (1) of Le Bras and Timmermans (2025) in more (metrologically) robust notation, namely:

$\frac{d}{dt}(\rho V)$ is the rate of change of density times volume (i.e. mass), and this is given as the sum of Φ_m^{OCE} the mass flux (rate of change) of the ocean Φ_m^{FW}, the mass flux (rate of change) of freshwater inputs and Φ_m^{SI} the mass flux of sea ice.

In the SRD, we recommend using the further conversion done by Le Bras to get to a volume flux:

$$\frac{d}{dt}(V) = \Phi_V^{\mathrm{OCE}} + \Phi_V^{\mathrm{FW}} + \frac{\rho_{\mathrm{SI}}}{\rho_{\mathrm{ML}}} \cdot \Phi_V^{\mathrm{SIF}} + 0.8 \cdot \left(\frac{\rho_{\mathrm{SI}}}{\rho_{\mathrm{ML}}} - 1\right) \cdot \Phi_V^{\mathrm{SIM}} \quad (4)$$

Here,

$\frac{d}{dt}(V)$ is the volume rate of change.

Φ_V^{OCE} is the volume change of the ocean.

Φ_V^{FW} is the volume change of freshwater given as $\Phi_V^{\mathrm{FW}} = \Phi_V^{\mathrm{rivers}} + \Phi_V^{\mathrm{glacier}} + \Phi_V^{\mathrm{P-E}}$, i.e. the sum of the volume flux from rivers, glaciers and precipitation minus evaporation.

The sea ice volume has two components. The first, $\frac{\rho_{\mathrm{SI}}}{\rho_{\mathrm{ML}}} \cdot \Phi_V^{\mathrm{SIF}}$ represents the movement of solid sea ice into or out of the defined region, and is given by a scale of sea ice density and mixed layer density. The paper describes this as being corrected to account for the displaced sea water. The second term, $0.8 \cdot \left(\frac{\rho_{\mathrm{SI}}}{\rho_{\mathrm{ML}}} - 1\right) \cdot \Phi_V^{\mathrm{SIM}}$ relates to the flux of sea ice melting, where melted sea ice is of lower density than the water it is replacing. A scaling factor of 0.8 is included 'to account for the fact that there is a correction required in order to account for the heat required to melt sea ice.' that comes from Jenkins and Holland (2007). Within our project team, there is still debate about whether a melt term is needed and, if it is, whether the value 0.8 is justified by the evidence in the Jenkins and Holland paper. If sea ice melt is to be considered, we would also need to consider sea ice formation.

This gives us our first project measurement model for freshwater volume flux of:

$$\frac{d}{dt}(V) = \Phi_V^{\mathrm{OCE}} + \Phi_V^{\mathrm{rivers}} + \Phi_V^{\mathrm{glacier}} + \Phi_V^{\mathrm{P-E}} + \left[\frac{\rho_{\mathrm{SI}}}{\rho_{\mathrm{ML}}} \cdot \Phi_V^{\mathrm{SIF}} + 0.8 \cdot \left(\frac{\rho_{\mathrm{SI}}}{\rho_{\mathrm{ML}}} - 1\right) \cdot \Phi_V^{\mathrm{SIM}}\right] \quad (5)$$

To perform this calculation, we have to define the volume fluxes associated with the ocean transport, river discharge, glacier discharge, precipitation minus evaporation and the sea ice-related quantities. These are discussed separately in the subsection on dataset conversion, below.

Finally, Le Bras and Timmermans separate the steric freshwater volume flux from the barystatic volume flux. Their equation (4) describes this, in our notation, as:

$$\frac{d}{dt}(V) - \frac{d}{dt}\left(\frac{\rho V}{\rho_0}\right) = \left(\Phi_V^{\mathrm{OCE}} - \Phi_m^{\mathrm{OCE}}/\rho_0\right) + \left(1 - \frac{\rho_{\mathrm{FW}}}{\rho_0}\right)\Phi_V^{\mathrm{FW}} + 0.8\left(\frac{\rho_{\mathrm{ML}}}{\rho_{\mathrm{SI}}} - 1\right) \cdot \Phi_V^{\mathrm{SIM}} + \left(\frac{\rho_{\mathrm{SI}}}{\rho_{\mathrm{ML}}} - \frac{\rho_{\mathrm{SI}}}{\rho_0}\right) \cdot \Phi_V^{\mathrm{SIM}} \quad (6)$$

Where most terms have the same meaning as above, and additionally, ρ_0 is the mean density of the full Arctic Ocean, a reference density for the Arctic (adding more ambiguity?).

3.2.2.3 Direct measurements of freshwater fluxes

Within this project, we want to compare an estimate of freshwater flux determined as described above (equation (5)) with one that is measured from sea surface salinity, sea surface height and gravimetric changes.

In [Solomon et al, 2021], the authors provide a definition of freshwater flux that is based on this definition and is given, in their notation, as:

$$\Delta FWC = \frac{S_2 - S_1}{S_2} \cdot A\Delta \sum h_i$$

And

$$\Delta h = \eta\left(1 + \frac{\rho_1}{\rho_2 - \rho_1}\right) - \frac{\Delta m}{\rho_2 - \rho_1}.$$

Where,

A is the grid cell area, h_i is the freshwater layer thickness within each grid cell (as measured by the satellite). Their equation assumes an ocean of two layers: a salty lower layer (2) with salinity S_2, and density ρ_2, and a freshwater upper layer (1) with salinity S_1 and density ρ_1.

The second equation provides a way of distinguishing mass change in the water from a steric density change (due, e.g., to salinity). Interpreting this requires an understanding of the concept of a two-layer exchange model. As freshwater enters the Arctic Ocean—via river runoff, precipitation, or ice melt—it is assumed to displace an equivalent volume of saltier ocean water, rather than simply adding mass to the system. This is a simplifying assumption that allows the change in thickness of the upper freshwater-influenced layer to be isolated, rather than tracking total mass changes. The second term, $\Delta m/(\rho_2 - \rho_1)$, subtracts the height difference due to any change in mass. Note that this is not in the summation over grid cells, because of the mismatch between altimetry (10s of km) and gravimetry (100s of km), so for the Arctic Ocean, a single mass change is assumed. The steric sea level rise (after the mass change has been removed) is multiplied by a steric amplification factor $(1 + \rho_{\mathrm{FW}}/(\rho_{\mathrm{ref}} - \rho_{\mathrm{FW}}))$, which translates what is seen for the ocean as a whole to a change in thickness of the top layer of freshwater. That steric amplification factor is needed to account for the buoyancy-driven effect (simplistically: heavier water pushes down the water underneath it, and thus the rise is not accounted for purely by the expansion of water).

The equation provides a freshwater flux in units of [m^3], i.e., as a freshwater volume flux, calculated from masses and densities. It is valid under the assumption that the freshwater replaces more salty sea water.

In order to clarify the definitions, we propose rewriting the Solomon equation as:

$$\Delta V_{\mathrm{FW}} = \frac{S_{\mathrm{ref}} - S_{\mathrm{FW}}}{S_{\mathrm{ref}}} \cdot (A \cdot \Delta h_{\mathrm{sum}} - \Delta V_{\mathrm{bary}}) \tag{7}$$

where,

ΔV_{FW} is the steric volume freshwater change, and $\dfrac{S_{\mathrm{ref}} - S_{\mathrm{FW}}}{S_{\mathrm{ref}}}$ is the freshwater fraction.

A is the area of the grid cell over which freshwater layer thickness changes are measured, Δh_{sum} is the grid-integrated change in freshwater layer thickness, and ΔV_{bary} is the barystatic sea volume change caused by the addition or removal of water mass.

The grid-integrated change in freshwater layer thickness can be written as:

$$\Delta h_{\mathrm{sum}} = \sum_{i=1}^{N} h_i(t) - \sum_{i=1}^{N} h_i(t_{\mathrm{ref}}) \tag{8}$$

Where the time change for the flux difference is from time t_{ref} to time t, and h_i is the measured freshwater layer thickness for the grid cell i. In turn, this freshwater layer thickness can be calculated from the freshwater layer measured height (sea surface height), η_i in a grid cell i, as:

$$h_i(t) = \eta_i(t) \cdot \left(1 + \frac{\rho_{\mathrm{FW}}}{\rho_{\mathrm{ref}} - \rho_{\mathrm{FW}}}\right). \tag{9}$$

And the barystatic sea volume change is given by:

$$\Delta V_{\mathrm{bary}} = \frac{\Delta m}{\rho_{\mathrm{ref}} - \rho_{\mathrm{FW}}} = \frac{m(t) - m(t_{\mathrm{ref}})}{\rho_{\mathrm{ref}} - \rho_{\mathrm{FW}}}, \tag{10}$$

where Δm is the mass change across the full Arctic Ocean. If the gravimetry data were on the same grid as the surface height data, this could also be brought into the grid summation.

Note the following points:

- This is a practical definition based on volume (not mass) and on what can be measured (surface heights).
- This definition makes several assumptions about this being a two-layer system with only two densities.
- It assumes that the water volume is not changed by the freshwater addition, instead the freshwater displaces sea water.
- It assumes that the mass change should be removed from the definition.
- It makes no attempt to correct for temperature variations of the water during the time from t_{ref} to t

3.2.2.4 Comparing flux summation with direct measurements

In the project, we wish to close the freshwater flux budget. For that, we need to compare the freshwater flux estimate in the first of these subsections (sum of inputs) with the freshwater flux budget from the second of these (direct measure). It is important to determine whether these are measuring the same measurand before such a comparison is meaningful.

To do this, we have to use volume flux versions of both equations. Furthermore, we have to decide whether to use a steric-only freshwater flux (e.g., equations (6) and (7)) or a total volume freshwater flux (e.g., equations (5) and a version of (7) without the mass term subtracted).

Figure 3.1 shows diagrammatically a possible balance for the fluxes. This will need further analysis in later stages of the project.

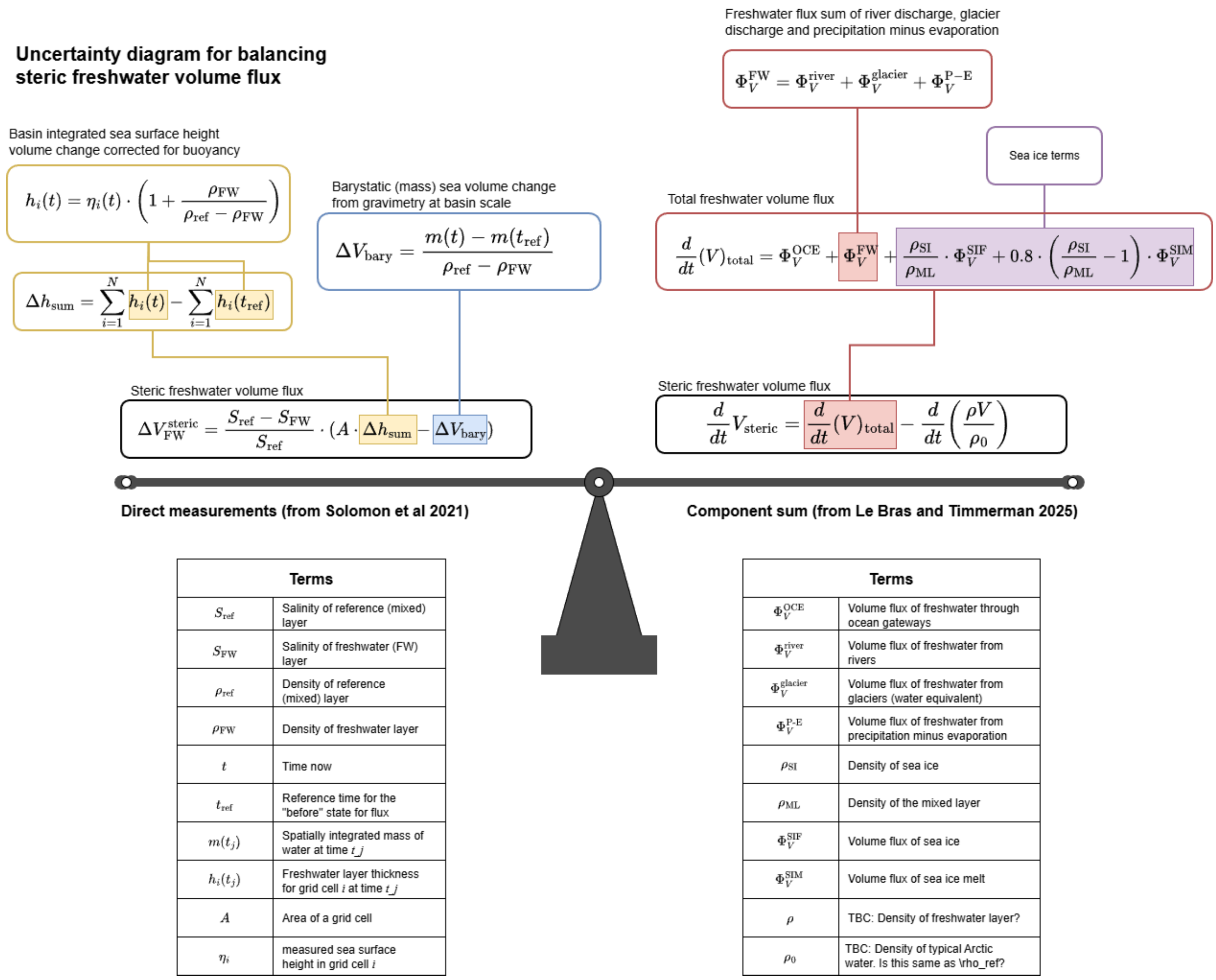

Figure 3.1: Possible conceptual framework for balancing the freshwater flux budget.

3.2.3 What is the Arctic Ocean?

As well as defining freshwater flux, we have to consider what is meant by the Arctic Ocean. This topic has been discussed in Section 2.2 of the Science Methodology Strategy and is justified in the discussions in Section 2.6 of the Science Requirements Document.

3.2.4 Dataset Conversion

To use equations (5) or (6), we need to obtain the various fluxes:

- Ocean transport
- Freshwater
  - River discharge
  - Glacier discharge
  - Precipitation minus evaporation
- Sea ice
  - Flux as ice
  - Flux to melt

In each of these cases, this should be converted to a volume flux. These are considered in the subsections below.

3.2.4.1 Ocean transport

Ocean transport is calculated in two steps. First, the geostrophic volume transport through a gateway is estimated from the Dynamic Ocean Topography (DOT), which is derived from satellite altimetry by subtracting the geoid from the observed sea surface height. Second, the freshwater component of this transport is isolated by comparing the salinity of the transported water to that of the reference salinity.

The geostrophic volume transport represents the movement of water through a strait driven by horizontal pressure gradients. It assumes geostrophic balance, where the pressure gradient force (arising from differences in sea surface height or water density) is exactly balanced by the Coriolis force (due to Earth's rotation). This balance typically holds away from the Equator and in regions where wind-driven and eddy effects are limited.

Under geostrophic balance, the flow is perpendicular to and proportional to the cross-strait gradient of dynamic ocean topography. The cross-strait geostrophic velocity is given by:

$$v_{\mathrm{g}} = \frac{g}{f} \cdot \frac{\partial \eta_{\mathrm{DOT}}}{\partial x}, \qquad (11)$$

where g is the gravitational acceleration, f is the Coriolis parameter, and the partial differential is the cross-straight gradient of the dynamic ocean topography. Dynamic ocean topography is defined as:

$$\eta_{\mathrm{DOT}} = h_{\mathrm{SSH}} - N, \qquad (12)$$

where h_{SSH} is the local, instantaneous sea surface height measured relative to the ellipsoid and N is the geoid defined relative to the ellipsoid. This velocity is integrated by the cross-sectional area to give the volume transport through the strait. The volume transport is translated to a freshwater transport by multiplying by a salinity factor.

$$Q_{\mathrm{FW}} = \int_x \int_z \left(\frac{g}{f} \cdot \frac{\partial \eta_{\mathrm{DOT}}}{\partial x} \right) \cdot \left(\frac{S_{\mathrm{ref}} - S(x,z)}{S_{\mathrm{ref}}} \right) dz dx \quad (13)$$

[To discuss in the next version: whether this is the right form following earlier discussions about salinity and freshwater.]

Freshwater flux through ocean gateways is estimated by integrating changes in sea level, ocean bottom pressure (OBP), and sea surface salinity (SSS).

The following are the potential datasets to be used within the ArcFresh project for Ocean gateways flux, with their gridding information:

- Sea level altimetry (Jason 1-3/Sentinel-6MF), along-track altimetry from Radar Altimeter Database System (RADS): 10 days temporal resolution, 7 km spatial resolution.
- Sea level SAR altimetry, along-track altimetry from Sentinel-3: 27 days temporal resolution, 300 m (along track) spatial resolution.
- Salinity, moorings and CTD, Fram Strait Arctic Outflow Observatory: monthly temporal resolution, ~10 km (across strait) / 10 m (depth) spatial resolution.
- Sea level, altimetry, High Latitude Sea Level Anomalies from satellite altimetry (by DTU/TUM): weekly temporal resolution, 0.25 x 0.50 degree spatial resolution.
- Sea level, altimetry, Sea level ESA CCI FCDR v2.0: various times, 6 km spatial resolution (ungridded)
- Sea level, altimetry, High latitude sea level anomalies from Envisat and Saral: weekly temporal resolution, 0.25 x 0.75 degree spatial resolution.
- Sea level budget, altimetry, High Latitude Sea Level Anomalies from satellite altimetry: weekly temporal resolution, 0.25 x 0.50 degree spatial resolution.
- Sea level budget, GRACE and GRACE-FO, ocean bottom pressure: monthly temporal resolution, 0.50 x 0.50 degree spatial resolution.
- Sea Surface Heights, radar altimetry, CryoTempo enhanced Polar Ocean CryoSat-2 dataset: Along-track 250 m spatial resolution.
- Ocean Bottom Pressure, GRACE and GRACE-FO, NASA Goddard Space Flight Center/Jet Propulsion Laboratory: ~ Monthly temporal resolution, ~300 km spatial resolution.
- Sea Surface Salinity, SMOS, SMAP, Aquarius L-Band microwave: ~Monthly temporal resolution, ~45 km spatial resolution.
- Sea Surface Salinity, SMOS Band microwave, CEC CATDS SMOS LOCEAN:~8 days temporal resolution, ~45 km spatial resolution.

3.2.4.2 River discharge

River discharge refers to the total amount of water travelling out of a river to a reservoir (ocean, sea etc.) over a certain timeframe. For the ArcFresh project, this will entail the overall amount of freshwater entering the Arctic Ocean for a certain timeframe and its contribution to the overall Arctic freshwater budget, which can be given as a sum of the discharges of individual rivers:

$$\Delta\Phi_{V,\mathrm{RD,tot}} = \sum_{i=1}^{N} \Delta\Phi_{V,\mathrm{RD,tot},i} \quad (14)$$

The different data sets all directly produce volume flux.

The following are the potential datasets to be used within the ArcFresh project for the evaluation of river discharge, with their gridding information:

- Snow Water Equivalent from passive microwave and in-situ data, 0.10° by 0.10° spatial resolution.
- Snow Cover Extent from optical satellite data, 0.05° by 0.05° and 0.01° by 0.01° spatial resolution.
- River discharge from in-situ stations, with daily and monthly temporal resolution, over 420 different stations providing observations.
- Modelled River Discharge from Arctic-HYPE v3 and v4, daily temporal resolution.

Glacier discharge

Within the ArcFresh project, we must consider the total amount of glacial ice contributing to the total freshwater within the Arctic region from all sources. This can be summarised as a sum of individual glacier fluxes in the following equation:

$$\Delta\Phi_{V,\mathrm{landice}} = \sum_{gl} \Delta\Phi_{V\mathrm{ice},gl} \quad (15)$$

Where the flux from an individual glacier comes from:

- Solid ice discharge (calving from marine-terminating glaciers)
- Surface runoff (surface melt minus retained water by refreezing and local storage)
- Basal runoff (melting and discharge from the base of the ice sheet/glacier)

A large challenge for this ECV is regridding and evaluating the temporal resolution available for each data product for easy summation into the total Arctic freshwater flux. This is of particular concern where no temporal or spatial resolution data is provided.

The following are the potential datasets to be used within the ArcFresh project for evaluation of glacial discharge, with their gridding information:

- Greenland ice sheets and glaciers surface elevation change (SEC and dSEC) from radar altimeter data, given in 5 km spatial resolution with annual and monthly temporal resolution for SEC and dSEC, respectively.

- Greenland ice sheets and glaciers ice velocity given by S-1 SAR altimetry data, provided as monthly, annual or multi-annual data temporal resolution and 100-200 m spatial resolution.
- Greenland ice sheets and glaciers mass flux ice discharge (MFID) data, provided as monthly temporal resolution with 200 m spatial resolution.
- Greenland ice sheets and glaciers inventories and ice sheet outlines from optical and SAR altimetry sensors, provided as 1-18 year temporal resolution with 10-30 m spatial resolution.
- Greenland and ice sheet ice thickness given data from IceBridge Bedmachine for Greenland, based upon airborne radar sounder ice thickness evaluation, with 150 m spatial resolution.
- Greenland ice sheet runoff data, which is modelled,is given at a monthly temporal resolution.
- Greenland and ice sheet basal melt flux, which is modelled data, is provided with a monthly temporal resolution, with spatial resolution provided for individual basins. \

3.2.4.3 Precipitation minus evaporation

Net precipitation minus evaporation represents the **net water flux at the Earth's surface**, which is a critical component of the hydrological cycle. It quantifies the balance between water added to the surface through precipitation (rain, snow, etc.) and water removed through evaporation (and often sublimation or transpiration if included). A positive value indicates a net gain of water at the surface (more precipitation than evaporation), while a negative value indicates a net loss (more evaporation than precipitation).

$$\Delta\Phi_{\mathrm{net}P-E} = P - E$$

The gridding of the input products for precipitation and evaporation is as follows:

- GPCP (precipitation and evaporation) dataset provides daily 1.0° gridded data
- GIRAFE (precipitation) dataset provides daily 1.0° gridded data
- COBRA (precipitation) dataset provides daily 1.0° gridded data
- OAFlux (evaporation) dataset provides daily 1.0° gridded data
- HOAPS (precipitation and evaporation) 6-hourly 0.5° gridded data
- ERA-5 model (precipitation and evaporation) 1-hourly 0.25° gridded data

3.2.4.4 Sea ice

Sea ice volume flux $Q_{x,y}$ from gridded sea ice concentration, thickness and drift, in x and y directions of the projection coordinates, is obtained by the following:

$$Q_{x,y} = G \cdot H \cdot C \cdot D_{x,y}$$

where G is the size of the grid cells, H is the sea ice thickness, C is the ice concentration, and $D_{x,y}$ represents the ice drift in x and y directions respectively (Ricker et al., 2018).

Within the ArcFresh project, we need to consider the direct flow of sea ice out of the defined Arctic area through the gateways. Additionally, we need to consider melting sea ice and how this will contribute to the sea level rise, as well as to the freshwater concentration (for the top level of the Ocean).

The gridding of the input products for Sea Ice Flux is as follows:

- Sea ice concentration dataset: Global sea ice concentration climate data record, provides data on a 12.5 km grid at a daily temporal resolution.
- Sea ice thickness: Global sea ice thickness climate data record provides data on a 25 km grid at a daily temporal resolution.
- Sea ice drift: OSISAF sea ice drift climate data record provides data on a 75 km grid at a daily temporal resolution.
- Sea ice drift: ECCC SAR sea ice drift data, with spatial resolution concentrated to the gates.

4 Observational datasets, step 2: Describe traceability with a diagram

4.1 What is meant by step 2: describe traceability with a diagram

The second step in the QA4EO Five Steps is to describe traceability with a diagram. The concept of 'metrological traceability' usually refers to how a measurement is linked through an unbroken chain of comparisons back to SI standards. Such traceability involves measurement instruments and/or reference standard materials being passed from one laboratory to another. More recently, however, metrologists have begun to expand this concept to also include passing datasets from one community to another through a processing chain (Woolliams, 2025). For traceability to be 'metrological', it is important that, along with the passing of the artefact or data, information is provided about uncertainties and data provenance.

There are different ways in which traceability can be shown. For data processing chains, this is most often done with flow charts showing how datasets are taken through different processes. The QA4EO Five Steps encourage the use of uncertainty tree diagrams that show the measurement models (equations) used in the processing and indicate the origin of different sources of uncertainty.

Here, we present the first versions of uncertainty tree diagrams for the different observational datasets used in the project. These are still at an early stage and are likely to be developed further over the next few months.

4.2 ESA CCI and supplementary datasets review

In parallel and to inform this uncertainty analysis, there has been a high-level review of all datasets (both ESA CCI and other supplementary) that are relevant to the Arctic freshwater flux, covering the main areas:

- Land Ice flux
- Sea Ice flux
- River Discharge flux
- Net Precipitation Evaporation flux
- Ocean Gate flux

The reviews are built around and answer the following questions:

- What is the chain of measurands?
- Have all aspects of the uncertainty been considered? (i.e. not just measurement uncertainty but all/some other contributions to the uncertainty)
- Are they providing uncertainty that varies according to observational conditions or just a static value? i.e. how specific is the uncertainty to the observations
- Do they consider spatial and temporal correlations?
- Are there any uncertainties provided for representation?

That review is presented in the fitness-for-purpose report.

4.3 Traceability for Arctic freshwater flux

4.3.1 Dataset traceability diagrams

This section includes the individual traceability diagrams for each identified ECV that feeds into the overall Arctic freshwater flux diagram. These diagrams highlight the key uncertainty contributions for the data products along with any approximations and assumptions that have been used in measuring, calculating or modelling the data product. Ideally, the uncertainties highlighted should cover any assumption or approximation being made in the evaluation of the data product. However, key sources are highlighted to be reviewed against expert opinion.

The traceability diagrams will then be expanded based on this opinion and further research in the next phase of the ArcFresh project.

4.2.2.1 Land ice

The application of land ice within the ArcFresh project consists of calculating the total land ice mass change (mostly from the Greenland ice sheet) and then evaluating the impact of this on the total freshwater flux within the Arctic. The total land ice mass change is calculated as a summation from three main sources: surface run-off, basal melt and solid ice change of which have been described in detail within the documents that have been produced alongside this one (the ECV inventory report and the fit-for-purpose report).

Glacial ice run-off is evaluated using a combination of multiple models and various observational datasets. This uses a combination of various inputs, these being: surface melt, firn retention, supraglacial change and subglacial runoff. Basal melt is ice melting on the bottom of the glacier from the presence of geothermal heat. The evaluation of this product is modelled by using the GEUS model. The change in solid ice is evaluated from a combination of surface elevation change measurements and a bedrock model for Greenland to give an estimation of the volume of ice present. The volume is then combined with the ice velocity to give an estimation of the overall solid ice flux. The surface elevation change is measured from radar altimetry measurements of the surface, with radar altimetry in SAR mode used to estimate the ice velocity.

The land ice traceability diagram highlights the uncertainty evaluation present for surface elevation change measurements, ice velocity measurements and the 4D Greenland model, along with key assumptions for these datasets. Further investigation of the 4D Greenland evaluation of ice sheet runoff and the modelled basal melt evaluation will be carried out in the next phase of the project.

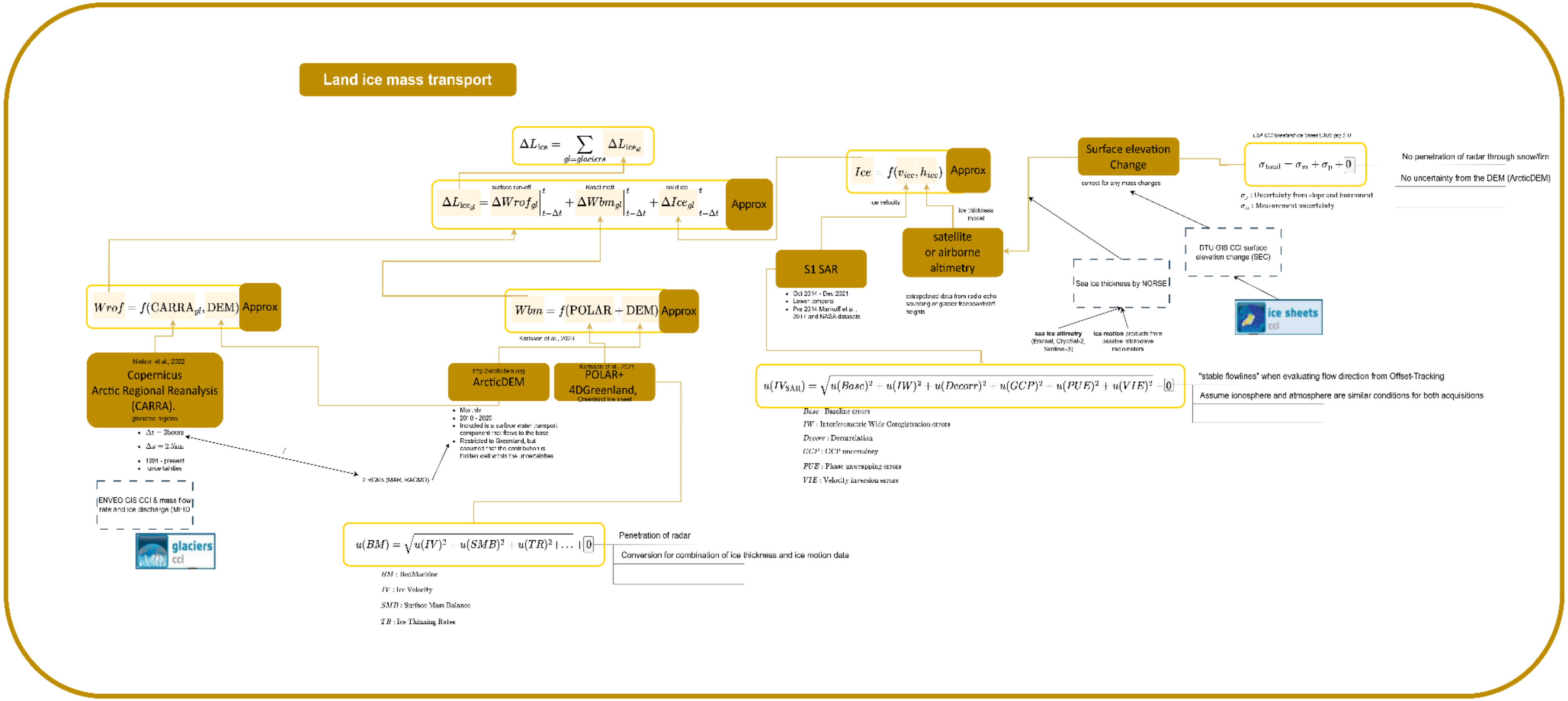

Figure 4.1: Land ice uncertainty tree diagram based on data products highlighted in the EID document.

4.2.2.2 Sea ice

Sea ice plays a critical role in the Arctic freshwater flux and climate system, and its contribution is commonly quantified through sea ice flux, which depends on three key variables (as shown in Sea ice): sea ice concentration, thickness, and drift. Figure 4.2 illustrates the uncertainty pathways for these three components, highlighting both documented uncertainty sources and additional assumptions that may propagate into sea ice flux estimates.

Sea ice concentration is calculated from brightness temperature measurements from passive microwave sensors, which are converted into sea ice concentration using algorithms that rely on the difference in microwave emissivity between open water and ice. The algorithm uses tie points for water and ice to normalise observed brightness temperatures and compute sea ice concentration as a fraction between two extremes. The ice tie point is the brightness temperature signature for 100% sea ice, and the water tie point is the brightness temperature signature for 0% sea ice (open water). These are both derived from satellite brightness temperature data under known surface conditions. The uncertainty calculation method is provided for the dataset, and the assumptions made in creating this dataset, leading to uncharacterised uncertainty found during this review, are presented in Figure 4.3.

Sea ice thickness is evaluated from: freeboard measurements from satellite radar altimeters, snow depth estimated from snow climatological datasets ot auxiliary satellite data, sea ice density and snow density from fixed climatological values based on field observations, and seawater density from oceanographic standards (assumed constant). The details of the uncertainties provided and the assumptions made in creating this dataset, leading to uncharacterised uncertainty found during this review, are presented in Figure 4.4.

Sea ice drift is calculated from: brightness temperature measurements at multiple time steps from passive microwave sensors are passed through an algorithm which finds the best match between images using the maximum correlation of brightness temperature patterns. The displacement between the matched positions gives the drift vector (speed and direction). The details of the uncertainties provided and the assumptions made in creating this dataset, leading to uncharacterised uncertainty found during this review, are presented in Figure 4.5.

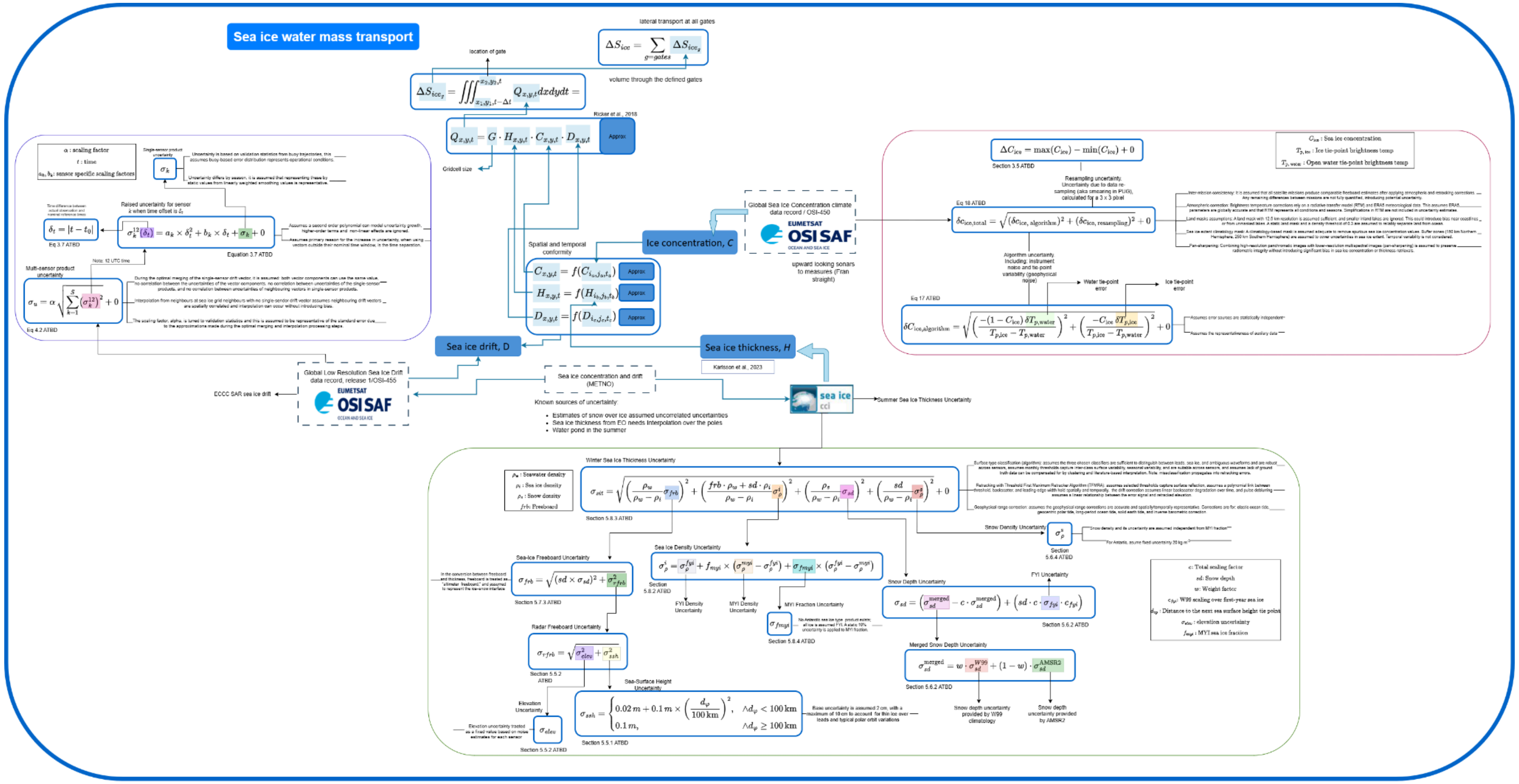

Figure 4.2: ***Sea ice uncertainty tree diagram based on data products highlighted in the EID document. Zoomed-in versions are below.***

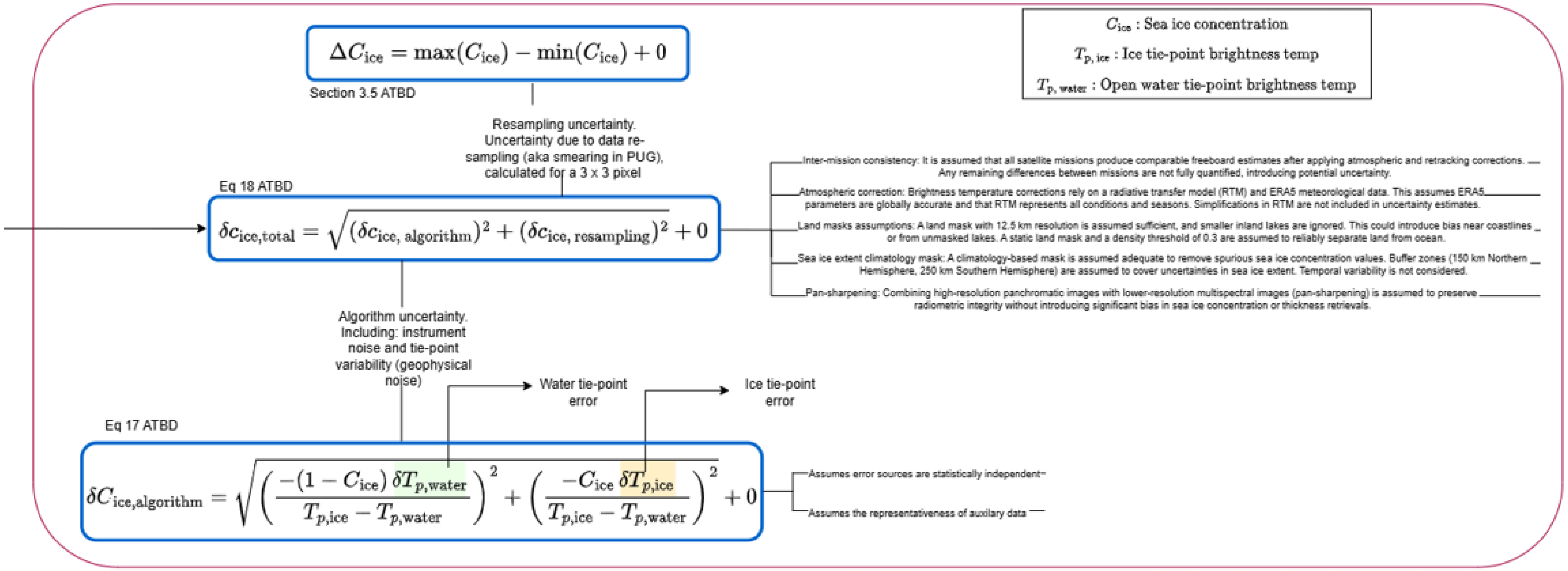

Figure 4.3: *Ice concentration section of the sea ice uncertainty tree diagram in Figure 4.2.*

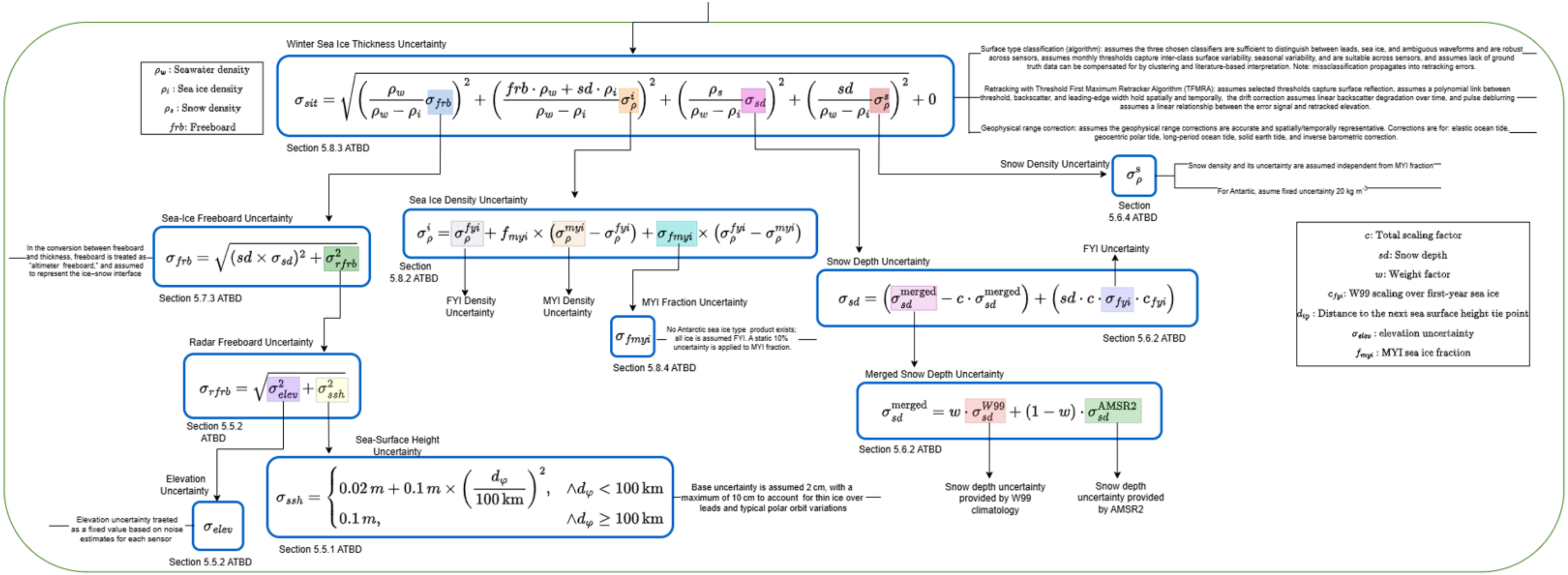

Figure 4.4: Sea ice thickness section of the *sea ice uncertainty tree diagram in Figure 4.2.*

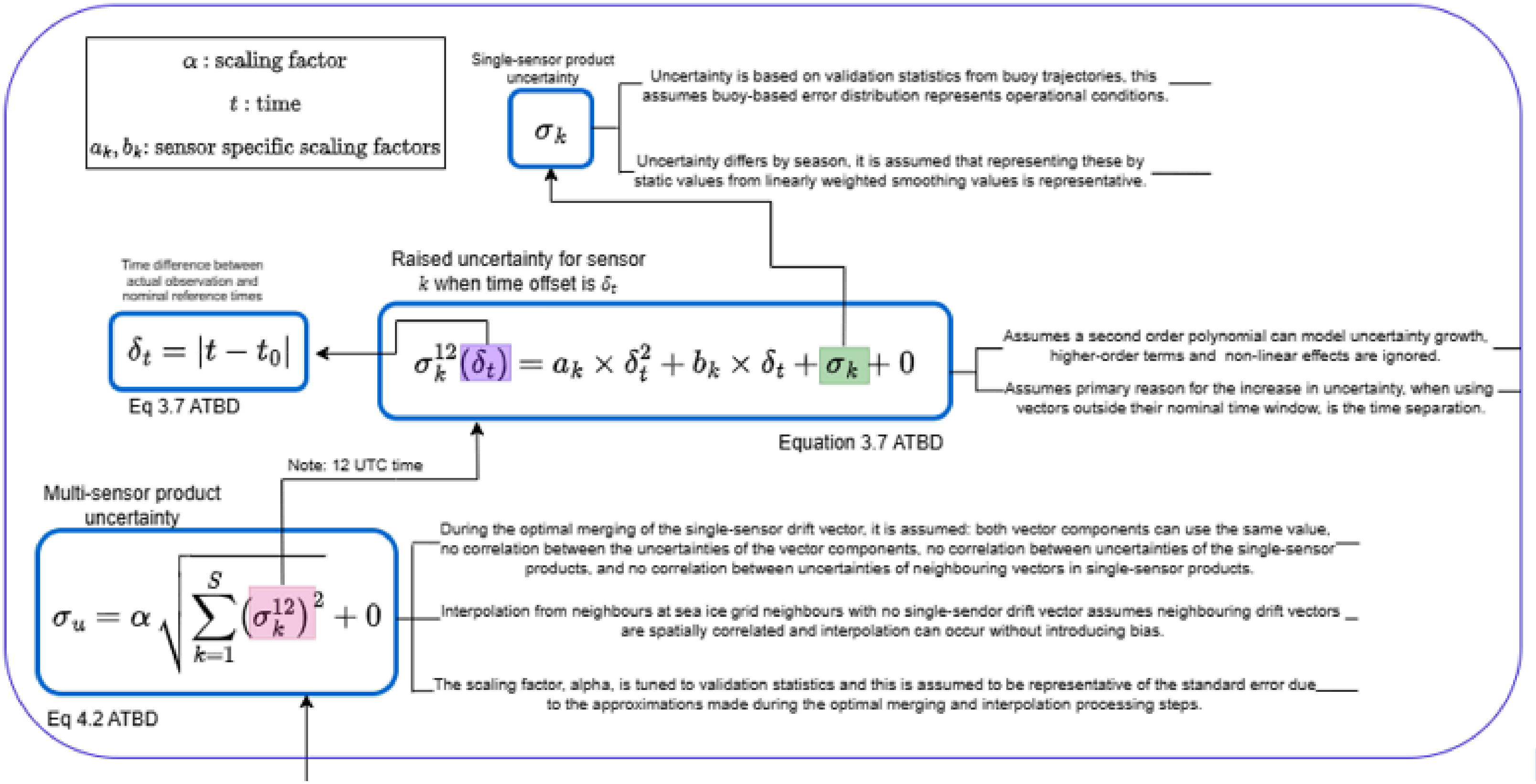

Figure 4.5*: Sea ice drift section of the sea ice uncertainty tree diagram in Figure 4.2.*

4.2.2.3 River discharge

River discharge is a key contributor to the overall Arctic freshwater budget, which in turn will play a role in the overall freshwater flux within the Arctic Ocean. Understanding of river discharge can help to “fill the gap” in understanding how freshwater transitions between precipitation and evaporation within the Arctic area. Additionally, understanding which locations the discharge is occurring can help to understand the further cycles within the Arctic Ocean.

There are three main methods in evaluation of river discharge:

1. A combination of radar altimeter measurements of the river surface elevation, in combination with in-situ evaluated discharge time series, is used to create a rating curve. This rating curve characterises a relationship between the discharge data coming from the river and the surface elevation information.
2. Where no in situ data is available, a hydrological model is used in place to go alongside the altimeter data. This is then used to evaluate the rating curve.
3. Finally, where there is no temporal matchup between in-situ or simulated discharge data and altimeter elevation measurements, a rating curve can be evaluated from the distribution of these quantities. This method requires “sufficient” amounts of data for a large time period to encompass data from various different events.

Within the ArcFresh project, each approach can be adopted. The Bayesian approach has been highlighted within the uncertainty tree diagram. Initial investigation of the snow CCI ATBD and E3UB documentation has been performed to inform this tree diagram, looking at snow as an input into the simulated river discharges. Investigation of the SMHI river discharge model is to be carried out in the next phase of the ArcFresh project, alongside further investigation of the snow CCI data product of their contribution to the traceability diagram.

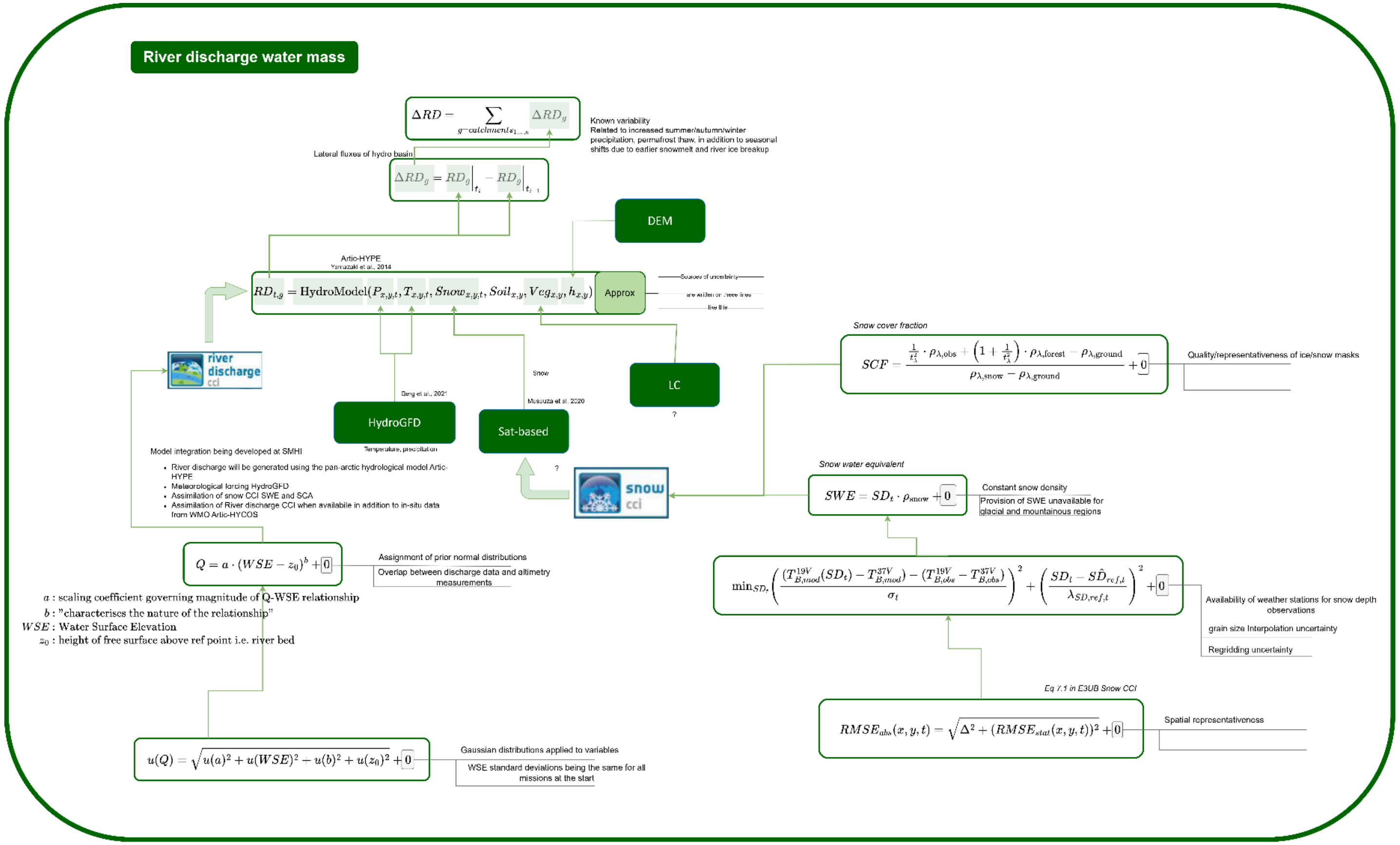

Figure 4.6: *River discharge tree diagram based on data products highlighted in the EID document.*

4.2.2.4 Precipitation-Evaporation

Precipitation and evaporation are fundamental components of the Arctic freshwater flux cycle, representing the exchange of water between the atmosphere and the surface. These processes are expressed as vertical fluxes over the pan-Arctic domain; this means that they describe the net movement of water into, or out of the surface layer per unit area. The balance between them is critical for understanding the Arctic hydrological cycle because it influences surface water storage, river discharge, and sea ice dynamics. A positive indicates that the Arctic system is gaining freshwater from the atmosphere, while a negative value suggests a net loss due to evaporation.

Figure 4.7 illustrates the uncertainty pathways for these variables. The figure highlights both the quantified uncertainty derived from observation errors, model parameterisation and spatial/temporal sampling limitations and assumptions that may propagate uncharacterised uncertainty into P–E flux estimates for each dataset highlighted in the EID document.

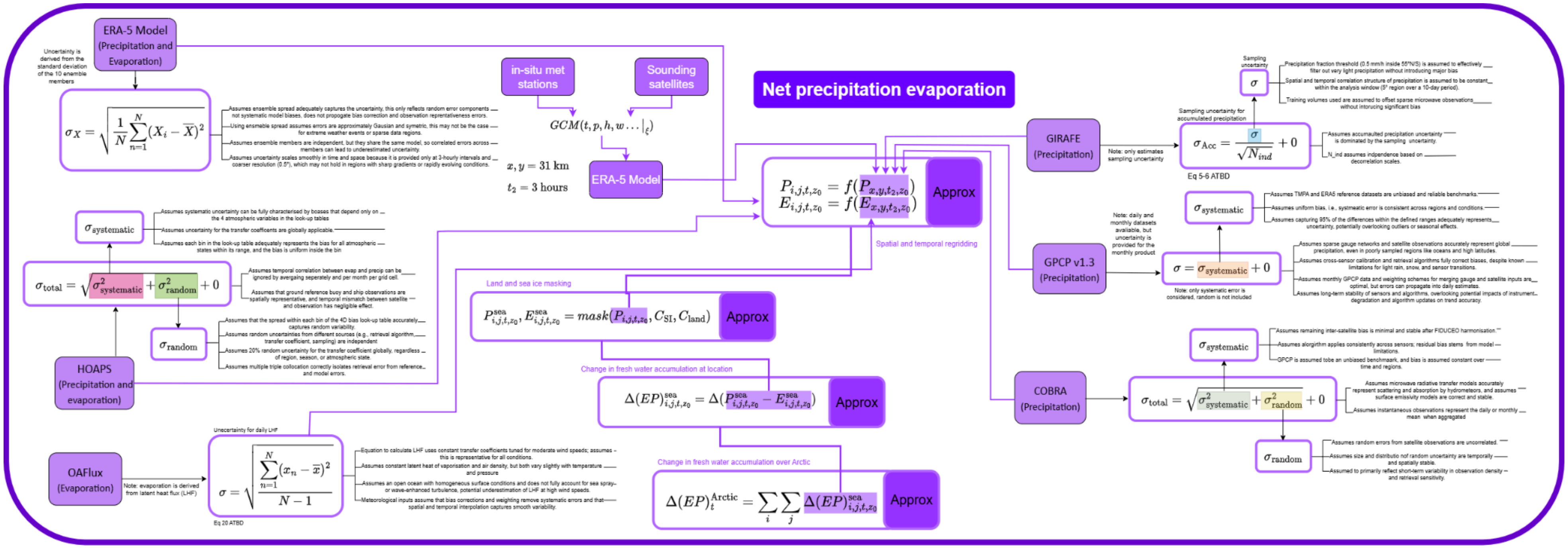

Figure 4.7: ***Net precipitation evaporation uncertainty tree diagram based on data products highlighted in the EID document.***

4.2.2.5 Ocean Gateways, sea level and ocean bottom pressure

There are three main variables that we have investigated, which are used to calculate OBP: sea level, sea surface salinity, and ocean bottom pressure. The uncertainty and assumptions are detailed in Figure 4.8.

Sea Level is the height of the ocean surface relative to a reference point, typically the geoid, and is measured in metres (m). It varies due to thermal expansion, ocean mass changes, and dynamic processes like currents and tides. In the Arctic, freshwater flux from river runoff, precipitation, and ice melt contributes to regional sea level rise by adding mass and reducing salinity, which affects density and circulation.

Ocean Bottom Pressure (OBP) is the hydrostatic pressure at the seafloor caused by the weight of the overlying water column. It is measured in Pascals (Pa) or as equivalent water height (m). OBP is a key indicator of ocean mass changes and circulation, influenced by tides, currents, and large-scale water redistribution. In the Arctic, freshwater flux from river discharge, precipitation, and ice melt alters regional OBP by reducing water density and redistributing mass, which can impact global ocean circulation and sea level patterns.

Sea Surface Salinity (SSS) measures the concentration of dissolved salts in the upper ocean, typically expressed in practical salinity units (psu). It is a key variable for understanding ocean density, stratification, and circulation. In the Arctic, freshwater flux from river discharge, precipitation, and ice melt lowers SSS, enhancing stratification and reducing vertical mixing. These changes influence regional heat exchange and can propagate through global circulation, affecting climate feedback.

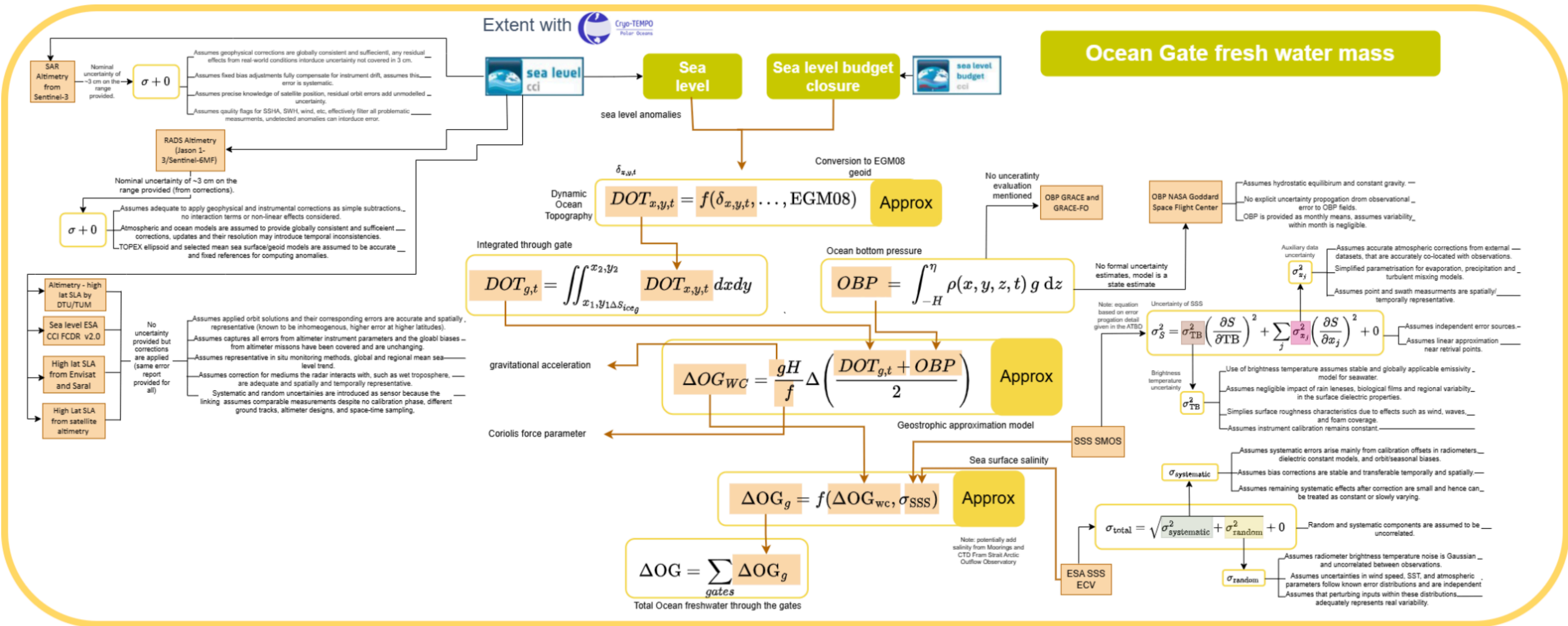

Figure 4.8: ***Ocean gate fresh water mass uncertainty tree diagram based on data products highlighted in the EID document***

4.2.3 Summary of metrological review

This will be provided with a further iteration of the traceability diagrams and initial discussion with the experts to highlight key sources of uncertainty.

5 Observational datasets, step 3: Effects Tables

This section will be completed later in the project when we have a clear understanding of the measurands for each of the input datasets and an understanding of the traceability of the data products (i.e. the variables that are used in the creation of each of the measurands). Once this is completed, the uncertainty information is all summarised within the effects tables.

The purpose of step 3 is to document, for each significant source of uncertainty, what is known about that source of uncertainty. It documents both the magnitude of the uncertainty and the error correlation structure in each dimension that matters.

Within this project, the relevant dimensions are time and space. All the datasets are considered to be time series, and therefore, the temporal dimension relates to the error correlation (that is, whether the unknown error is common or different from one observation to the next) from one time step to the next time step.

In addition, spatial error correlation matters in different ways for each dataset:

- For ocean gateways, there is an integration across the gateway, and therefore, the spatial correlation that matters is that from one location along the gateway to the next.
- For sea ice, the three input quantities (thickness, concentration, velocity) are often determined on different grids. Therefore, the first stage is to understand error correlation in regridding. Secondly, they are integrated across the gateways, and so, as with ocean gateways, the error correlation from one location to the next across the gateway matters.
- For river discharge, there will be three different kinds of river discharge calculations being used: those from hydrological models, those from in-situ river gauge measurements and those from satellite observations. There may be errors that are common to different rivers processed in the same way. In general, we need to consider any river-to-river error correlation structures.
- For land ice, there are three kinds of quantity being considered: solid ice discharge, basal melt and surface runoff. Again, there may be errors that are common to different calculations. In general, we need to consider any glacier-to-glacier error correlation.
- For precipitation minus evaporation, we work with gridded products, so we need to consider error correlation from one grid cell to the next.

5.1 Effects tables for each dataset

This section will be completed during the next phase of the project.

6 Observational datasets, step 4: Propagating Uncertainties

This section will be populated later in the project. It requires the measurand to be evaluated, traceability of data products to be made with uncertainty evaluation being carried out (where applicable) and additionally, all uncertainty contributions to be summarised within the effects tables.

6.1 Overview of LPU and MCM

When considering a method for propagation of uncertainties for a particular measurement model following evaluated traceability, the GUM (Guide to Measurement Uncertainty) suggests two possible methods, the Law of Propagation of Uncertainties (LPU) or the Monte-Carlo method (MCM). The choice of method will largely depend on the characteristics of the measurement or model that is desired to be evaluated, this is due to both methods having distinct strengths and weaknesses for specific situations.

The LPU provides a least linear least squares solution based upon the measurement model and the input values and uncertainties provided for each variable. This method has the form of the following equation:

$$u_c^2 = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + 2\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j} u(x_i, x_j)$$

The first term on the right-hand side accounts for the summation of the individual uncertainty contributions (and their sensitivity) for each variable, and the second term on the right-hand side accounts for the correlations between variables in the equation. This methodology is the least intensive to implement and can provide a reasonable estimation of the total uncertainty for the measurement model with the consideration of correlation contributions.

The limitations for the LPU method arise when the measurement model itself (or an input variable) is particularly non-linear. Due to the LPU providing a least squares estimate localised around the output value, for a non-linear measurement model, if the output deviates, the estimated uncertainty will become less accurate.

The MCM provides an estimation of the output probability density function (PDF) centred around the key output based on best estimates of the input variables and their associated PDFs. This method allows for accurate estimation of the uncertainties on the output for the measurement model, even if that model has non-linear behaviour. An example schematic can be seen in Figure 6.1.

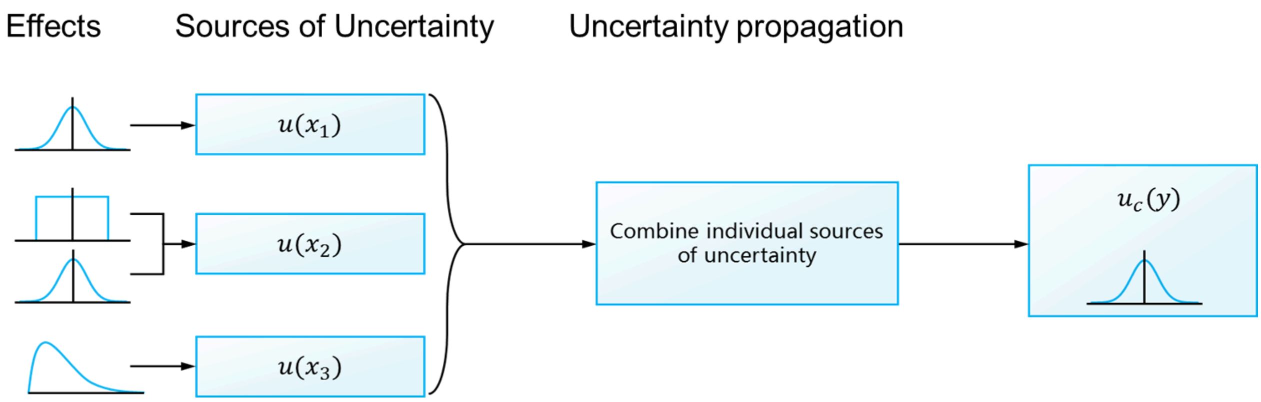

Figure 6.1: ***Example schematic overview of MCM, highlighting both the input uncertainty and possible PDFs for the inputs.***

However, the MCM is significantly more computationally intensive than the LPU due to the quality of the output being limited by the amount of runs being performed, with a greater number of runs increasing quality. Additionally, the MCM is particularly sensitive to the input PDFs provided. These PDFs need to be chosen with care and should not always be normal (Gaussian) distributions. Deciding the appropriate PDF should consider what the input is representing, i.e. is it a natural variable that has physical limits, is it representing a range of values or an individual measurement value, is it more appropriate to use the median instead of the mean in evaluation, etc.

6.2 Application of CoMet to model

This will come later in the project when the data products have been fully defined with characterised uncertainties. Once this is completed, the CoMet toolkit can be applied to the specific data product uncertainties.

7 Observational datasets, step 5: Documenting and disseminating uncertainties

Documentation and dissemination of uncertainties is the final step that will be carried out once the uncertainties have been propagated using the CoMet toolkit (see section 6).

8 Observational datasets, iterations: Validation and review

The observational datasets will be reviewed once full uncertainty analysis has been completed for all steps in the QA4EO five steps to evaluating uncertainty. Ideally, we will use information from comparisons with the model and with the budget closure itself to validate the uncertainty assessment quantitatively.

9 Towards uncertainty analysis for modelling

Numerical models are designed to conserve heat and salt over long integrations, so their freshwater budget is always closed by construction. A numerical ice-ocean model is also a powerful way to propagate uncertainties of input variables based on the Navier-Stokes equations. This can be done by sensitivity experiments like Monte Carlo simulations. On the other hand, ocean and sea ice models are affected by systematic biases caused by the accumulation of various errors over time (from discretisation errors to boundary condition errors), so the model uncertainty is most often underestimated, although qualitatively correct (Xie et al. 2017 for an example with the model proposed in this study).

ARCFRESH has opted for TOPAZ, a regional model of the Arctic, based on a coupled ocean-ice numerical model. The purpose of the modelling experiment is to quantify the effect of changing the system inputs on the quantities of interest. The inputs are affected by both biases and randomly fluctuating errors.

Considerations of uncertainty propagation to models is still at an early stage of development.

10 References

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