# Guidance for SBG Project and Science Teams: Uncertainty Quantification for L2A and L2+ Products

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## 1 Introduction

The purpose of this document is to provide guidance for producers of L2A and L2+ data products for the SBG Mission. SBG will have independent processing streams corresponding to the two platforms, SBG-VSWIR and SBG-TIR. Each will downlink its own observed spectra, but in both cases those spectra will serve as input to algorithms that estimate "intermediate" surface state vectors. For SBG-VSWIR, the intermediate state vectors are vectors of surface and water-leaving reflectances, which we denote by $\mathbf{X}_\mathrm{V}$. These comprise the L2A VSWIR product. For SBG-TIR, the intermediate state vectors are vectors containing temperature and emissivities, which we denote by $\mathbf{X}_\mathrm{T}$. These comprise the L2A TIR product. There is also a third instrument and processing stream for the VNIR, but we will not address it since VNIR products are the responsibility of the Italian Space Agency.

The VSWIR and TIR intermediate surface state vectors will be used to estimate geophysical state vectors, denoted by $\boldsymbol{\Theta}$ and described in detail in Table 1, that are derived from intermediate states through a second round of algorithms. These are referred to here as L2+. The L2+ outputs will be provided to the science and applications communities for analysis. In general, the L2+ products listed under the VSWIR processing stream depend on L2A surface and water-leaving reflectances, $\mathbf{X}_\mathrm{V}$; the L2+ products listed under the TIR processing stream depend on L2A temperatures and emissivities, $\mathbf{X}_\mathrm{T}$. However, this is not universally true– there are a few cross-stream dependencies, dependencies on external data sources and, in some cases on the TIR side, L2+ products are derived directly from L1 radiances. We will continue to refer to them as L2+ products nevertheless.

Figure 1 provides an overview of dependencies among these quantities of interest, with a focus on L1 and L2A. The hand-off to L2+ algorithms is represented by the green box in the upper-left and the blue box in the lower-right, both labeled "To L2+". L2+ details for

VSWIR products are given in Figure 2 and for TIR products in Figure 3. In all the figures, the true (but unknown) geophysical surface state is represented by $\mathbf{\Theta}$, a multidimensional vector of the form, $(\theta_1, \theta_2, \ldots, \theta_K)'$ where $K = 22$ is the total number of geophysical variables (at the time of this writing). For now, we specify $\mathbf{\Theta}$ as a column vector with several components corresponding to groups of geophysical states which belong to same science domain: aquatics (AQ), geology (Geo), snow and ice (SnI), and terrestrial ecology (TE). That is, the vector $\boldsymbol{\theta}_{\mathrm{AQ}}$ is a vector containing four elements (benthic properties, chlorophyll, phytoplankton, and water temperature (SST)); $\boldsymbol{\theta}_{\mathrm{Geo}}$ contains five elements, and so on. Subscript codes are shown in Table 1. The four vectors, $\boldsymbol{\theta}_{\mathrm{AQ}}$, $\boldsymbol{\theta}_{\mathrm{Geo}}$, $\boldsymbol{\theta}_{\mathrm{SnI}}$, and $\boldsymbol{\theta}_{\mathrm{TE}}$ are concatenated to form the grand geophysical state vector, $\mathbf{\Theta}$. Prime indicates vector transpose.

$$
\begin{aligned}
\boldsymbol{\theta}_{\mathrm{AQ}} &= \left(\boldsymbol{\theta}'_{\mathrm{Ben}}, \boldsymbol{\theta}'_{\mathrm{ChlA}}, \boldsymbol{\theta}'_{\mathrm{Phyt}}, \boldsymbol{\theta}'_{\mathrm{SST}}\right)', \\
\boldsymbol{\theta}_{\mathrm{Geo}} &= \left(\boldsymbol{\theta}'_{\mathrm{Etemp}}, \boldsymbol{\theta}'_{\mathrm{MA}}, \boldsymbol{\theta}'_{\mathrm{TSM}}, \boldsymbol{\theta}'_{\mathrm{VA}}, \boldsymbol{\theta}'_{\mathrm{VSM}}\right)', \\
\boldsymbol{\theta}_{\mathrm{SnI}} &= \left(\boldsymbol{\theta}'_{\mathrm{SnA}}, \boldsymbol{\theta}'_{\mathrm{SnFC}}, \boldsymbol{\theta}'_{\mathrm{SnGS}}, \boldsymbol{\theta}'_{\mathrm{SnST}}\right)' \\
\boldsymbol{\theta}_{\mathrm{TE}} &= \left(\boldsymbol{\theta}'_{\mathrm{Alb}}, \boldsymbol{\theta}'_{\mathrm{ChlC}}, \boldsymbol{\theta}'_{\mathrm{LMAC}}, \boldsymbol{\theta}'_{\mathrm{NC}}, \boldsymbol{\theta}'_{\mathrm{ESI}}, \boldsymbol{\theta}'_{\mathrm{ET}}, \boldsymbol{\theta}'_{\mathrm{EWT}}, \boldsymbol{\theta}'_{\mathrm{FC}}, \boldsymbol{\theta}'_{\mathrm{WUE}}\right)', \\
\mathbf{\Theta} &= \left(\boldsymbol{\theta}'_{\mathrm{AQ}}, \boldsymbol{\theta}'_{\mathrm{Geo}}, \boldsymbol{\theta}'_{\mathrm{SnI}} \boldsymbol{\theta}'_{\mathrm{TE}}\right)'.
\end{aligned}
$$

The intermediate surface state vectors, $\mathbf{X}_{\mathrm{V}}$ and $\mathbf{X}_{\mathrm{T}}$ are physically connected to $\mathbf{\Theta}$, and embody the radiative characteristics of the surface, separate from the effects of the atmosphere. L1 radiance derives from these surface characteristics (as shown in Figure 1) after accounting for the atmosphere. Indeed, the inferential problem we face at L2A is to recover these intermediate state vectors.

Radiances are input to L2A algorithms, which yield L2A products: surface and water-leaving reflectances for VSWIR, $\hat{\mathbf{X}}_{\mathrm{V}}$, and temperature and emissivities for TIR, $\hat{\mathbf{X}}_{\mathrm{T}}$. These are fed to L2+ algorithms for estimation of surface geophysical characteristics in $\mathbf{\Theta}$. There are, however, a couple of exceptions. First, as the diagram shows, two important TIR-derived data sets are actually obtained directly from TIR radiances. They are the Elevated Temperature Product and the Sea-surface Temperature (SST; i.e., water temperature) Product. Second, an additional processing algorithm exists for L2A VSWIR– the production of pixel-by-pixel fractional cover characteristics. Denoted by $\boldsymbol{\rho}$, this is a four-dimensional vector with components adding to one, that describes the fractional portion of a pixel that is deemed to be of four constituent types: vegetation, barren, liquid water, and snow/ice. The L2A Fractional Cover Product is important in its own right, but also plays a crucial role in subsequent L2+ processing for VSWIR radiances because this fractional pixel composition will determine which L2+ algorithms a given pixel feeds. For the TIR processing stream, the ocean mask determines which pixels are routed to processing to

<table>
<tr><th rowspan="2">Level</th><th rowspan="2">Domain</th><th colspan="5">Processing stream</th></tr>
<tr><th>VSWIR</th><th>State variable</th><th>TIR</th><th>State variable</th><th>NIR</th></tr>
<tr><td colspan="2">L2A</td><td>Surface reflectance<br>Water-leaving reflectance<br>Fractional Cover</td><td>$\mathbf{X}_{\mathrm{V}}$<br><br>$\boldsymbol{\rho}$</td><td>Temperature<br>Emissivity</td><td>$\mathbf{X}_{\mathrm{T}}$</td><td>Surface reflectance</td></tr>
<tr><td rowspan="4">L2+</td><td>Aquatics</td><td>Benthic composition<br>Chlorophyll<br>Phytoplankton</td><td>$\boldsymbol{\theta}_{\mathrm{Ben}}$<br>$\boldsymbol{\theta}_{\mathrm{ChlA}}$<br>$\boldsymbol{\theta}_{\mathrm{Phyt}}$</td><td>Water temperature*</td><td>$\boldsymbol{\theta}_{\mathrm{SST}}$</td><td>NDVI</td></tr>
<tr><td>Geology</td><td>Mineral abundance<br>Surface mineralogy</td><td>$\boldsymbol{\theta}_{\mathrm{MA}}$<br>$\boldsymbol{\theta}_{\mathrm{VSM}}$</td><td>Elevated temperature*<br>Surface mineralogy<br>Volcanic activity</td><td>$\boldsymbol{\theta}_{\mathrm{Etemp}}$<br>$\boldsymbol{\theta}_{\mathrm{TSM}}$<br>$\boldsymbol{\theta}_{\mathrm{VA}}$</td><td></td></tr>
<tr><td>Snow and ice</td><td>Snow albedo<br>Snow fraction<br>Snow grain size</td><td>$\boldsymbol{\theta}_{\mathrm{SnA}}$<br>$\boldsymbol{\theta}_{\mathrm{SnFC}}$<br>$\boldsymbol{\theta}_{\mathrm{SnGS}}$</td><td>Surface temperature</td><td>$\boldsymbol{\theta}_{\mathrm{SnST}}$</td><td></td></tr>
<tr><td>Terrestrial ecology</td><td>Albedo<br>Canopy chlorophyll<br>Canopy leaf-mass area<br>Canopy nitrogen<br>Equiv. water thickness<br>Fractional cover</td><td>$\boldsymbol{\theta}_{\mathrm{Alb}}$<br>$\boldsymbol{\theta}_{\mathrm{ChlC}}$<br>$\boldsymbol{\theta}_{\mathrm{LMAC}}$<br>$\boldsymbol{\theta}_{\mathrm{NC}}$<br>$\boldsymbol{\theta}_{\mathrm{EWT}}$<br>$\boldsymbol{\theta}_{\mathrm{FC}}$</td><td>Evapotranspiration<br>Evap. stress index<br>Water-use efficiency</td><td>$\boldsymbol{\theta}_{\mathrm{ET}}$<br>$\boldsymbol{\theta}_{\mathrm{ESI}}$<br>$\boldsymbol{\theta}_{\mathrm{WUE}}$</td><td></td></tr>
<tr><td colspan="7">* Derived directly from L1 radiances.</td></tr>
</table>

Table 1: Table of SBG data products. Intermediate surface states are denoted by $\mathbf{X}_{\mathrm{V}}$ and $\mathbf{X}_{\mathrm{T}}$ for VSWIR and TIR respectively. Fractional Cover, $\boldsymbol{\rho}$, is a four-dimensional vector with components summing to one, that describes pixels' fractional cover by relative contribution of four categories: vegetated, barren, liquid water, and snow/ice. Geophysical state variables are denoted by $\boldsymbol{\theta}$ with identifying subscripts (including "V" and "T" where necessary to distinguish between VSWIR and TIR versions.). Colors indicate families of L2+ products by science domain.

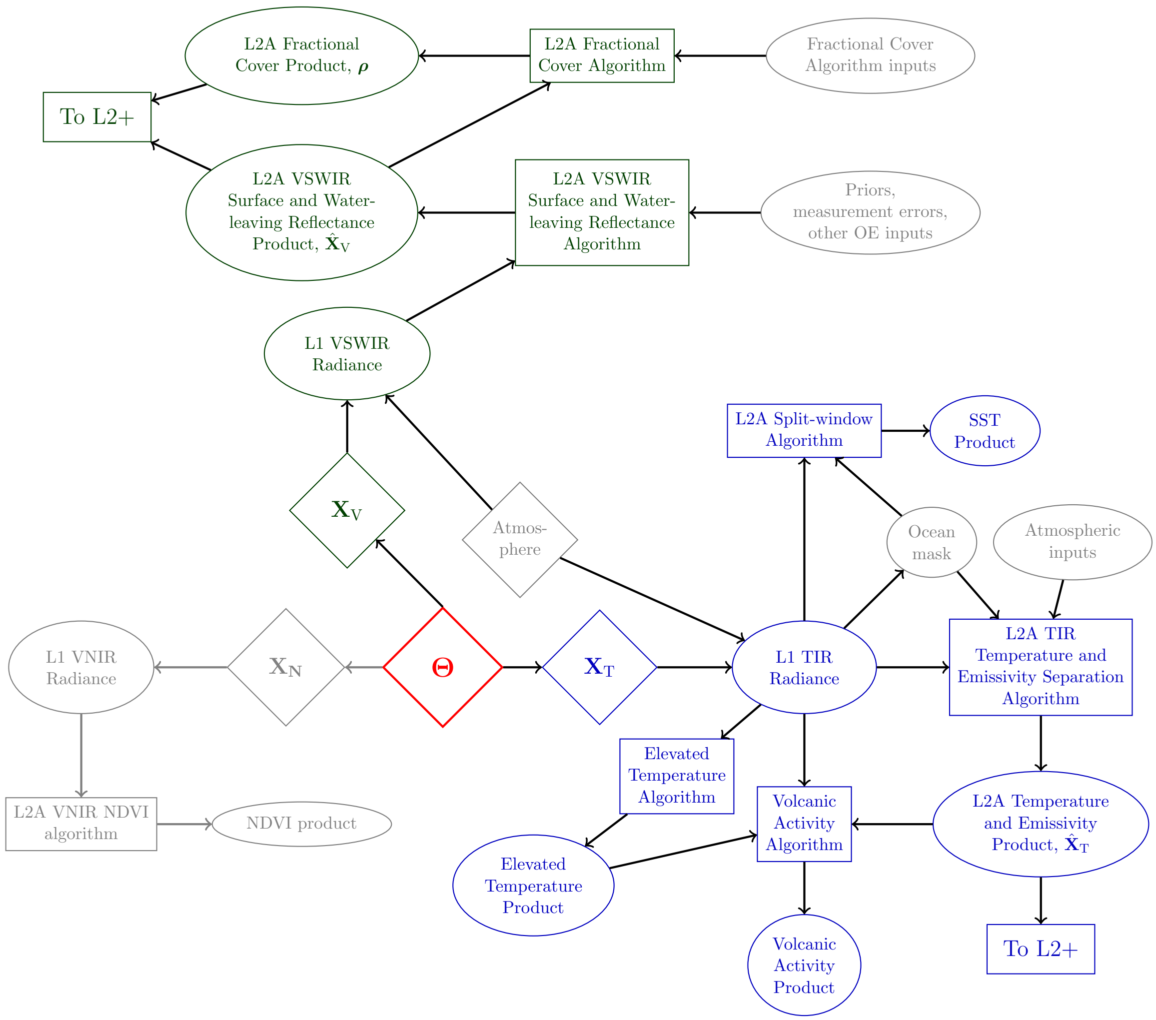


Figure 1: Overview of data processing dependencies for L1 and L2A products. Rectangles indicate algorithms, and ellipses are data sets. $\boldsymbol{\Theta}$ represents the underlying geophysical state. $\mathbf{X}_\mathrm{V}$ and $\mathbf{X}_\mathrm{T}$ are intermediate state vectors: surface and water-leaving reflectances for VSWIR, and surface temperature and emissivities for TIR. Conceptually, these are informed by $\boldsymbol{\Theta}$ and, along with atmospheric state, they subsequently inform their respective observed radiances. VSWIR radiances, along with ancillary inputs such as prior distributions, are ingested by the L2A VSWIR Surface and Water-leaving Reflecance Algorithm to produce the L2A VSWIR Surface and Water-leaving Reflectance Product. Reflectances are then input to the Fractional Cover Algorithm, which determines the L2+ VSWIR processing route for individual pixels at L2+. On the TIR side, an ocean mask sorts pixels into ocean and land surface cases. For L2+, ocean cases are processed by the L2A Split-window Algorithm to directly provide the SST product. Land cases are sent to the L2A TIR Temperature and Emissivity Separation Algorithm, which yields input for L2+ TIR algorithms.

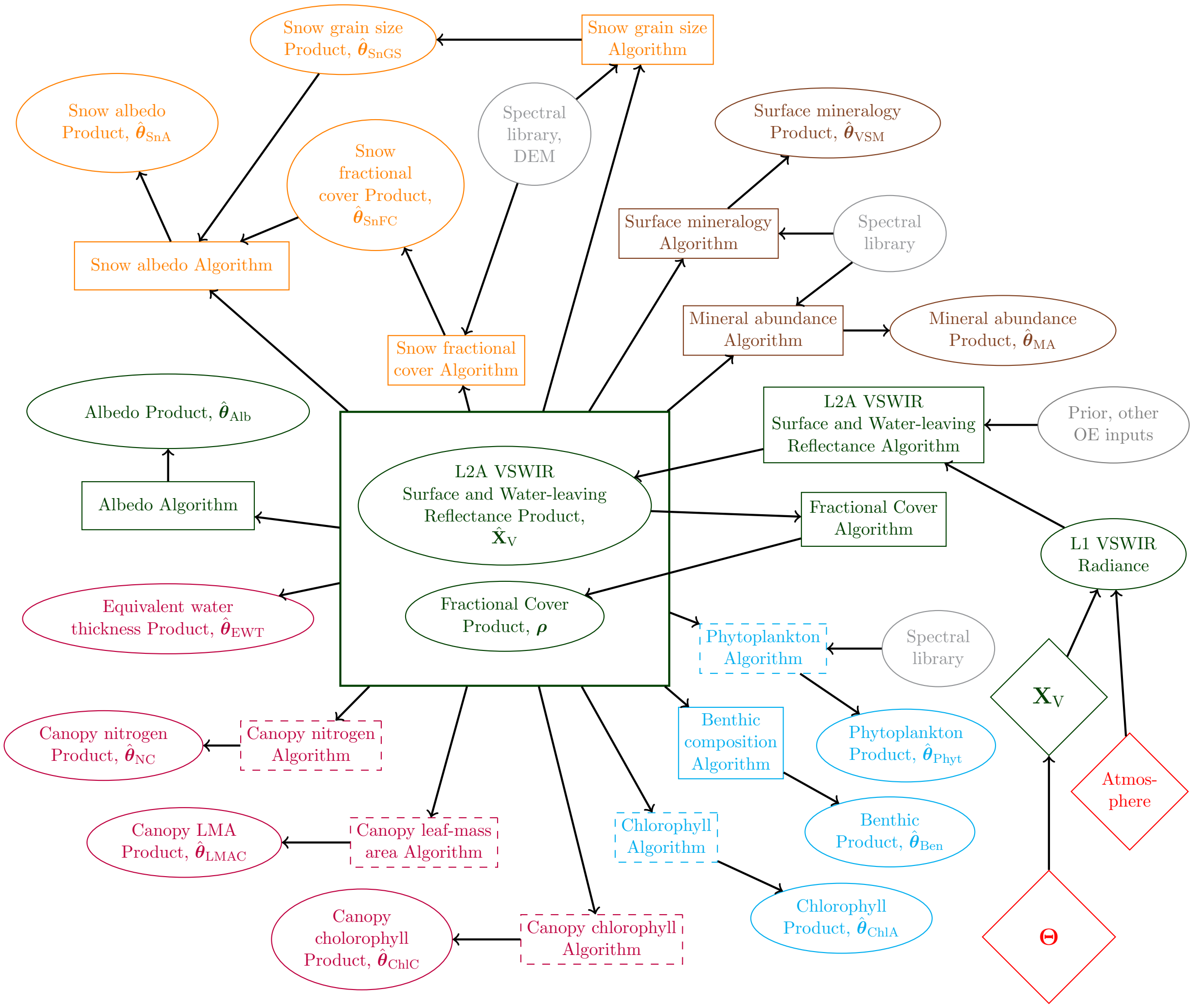


Figure 2: Schematic diagram of L1, L2A, and L2+ processing and data dependencies for SBG-VSWIR. Rectangular boxes are algorithms, and products (or other data sets) are in ellipses. Solid-boundary rectangles indicate physical algorithms, while dashed-boundary rectangles indicate empirical algorithms. Colors indicate families of products. External data sources are shown in gray. The red diamond labeled $\boldsymbol{\Theta}$ represents unknown geophysical quantities of interest, the red diamond labeled "Atmosphere" represents atmospheric state, and $\mathbf{X}_{\text{V}}$ represents intermediate surface states (surface and water-leaving reflectances). $\boldsymbol{\Theta}$ and the atmospheric state influence the observed L1 radiances through a true forward function (not shown). The L2+ output products are identified as estimates of corresponding components of $\boldsymbol{\Theta}$. The box in the center containing the L2A VSWIR Surface and Water-leaving Reflectance and the Fractional Cover Products reflects the fact that both these products are inputs to all L2+ algorithms.


Figure 3: Schematic diagram of L1, L2A, and L2+ processing and data dependencies for SBG-TIR. Rectangular boxes are algorithms, and products (or other outputs) are in ellipses. Solid-boundary rectangles indicate physical algorithms, while dashed-boundary rectangles indicate empirical algorithms. External data sources are shown in gray ellipses. The red diamond labeled $\boldsymbol{\Theta}$ represents unknown geophysical quantities of interest, the red diamond labeled "Atmosphere" represents atmospheric state, and $\mathbf{X}_{\mathrm{T}}$ represents intermediate surface states (temperature and emissivities). $\boldsymbol{\Theta}$ and the atmospheric state influence the observed L1 radiances through a true forward function (not shown). Each output product is identified as the estimate of a corresponding component of $\boldsymbol{\Theta}$.

produce SST, while pixels deemed to be land are all fed to the L2A TIR Temperature and Emissivity Separation Algorithm.

All algorithms impart uncertainties to their outputs by 1) deforming the uncertainties of their inputs in various ways, and 2) incorporating additional inputs that are uncertain (e.g., spectroscopy information, digital elevation models, (DEM's), etc.). For example, processing L1 radiance to generate L2A water-leaving reflectance creates uncertainty by deforming the L1 radiance uncertainty, and then the Benthic Composition Algorithm magnifies this uncertainty again. The result is a compounding effect that is difficult to anticipate and to characterize analytically through error propagation methods. Instead, we use an approach based on Monte Carlo simulation.

We think of $\mathbf{\Theta}$ as generated by a complex probability distribution that evolves in space and time, and that represents natural variability. If an appropriate distribution for $\mathbf{\Theta}$ could be asserted, then in principle, uncertainties associated with the outputs of all L2+ products could be estimated using Monte Carlo simulation: members of an ensemble of $\mathbf{\Theta}$'s would be processed through L1, L2A, and L2+ algorithms radiating through Figures 1, 2, and 3 resulting in distributions not only for the outputs of L2+, but also for those of L2A and L1, and (importantly) the joint distributions of combinations of these. Of course, such an enterprise is not computationally feasible in its totality, but conceptually this forms the basis of our approach to uncertainty quantification.

This guidance document spells out various options for executing Monte Carlo experiments within this framework to obtain robust estimates of uncertainties on L2A and L2+ products. Some options are more comprehensive and expensive than others. The technical prescription for carrying out these experiments was articulated in the SBG Uncertainty Quantification Plan, and will not be repeated here. Guidance is split into two sections: one intended for the projects teams creating L2A products and the the other for the project teams creating L2+ products. In the future we will add guidance for those creating new L2+ products through a competed Science Team, and eventually for other community-members-at-large.

## 2 Guidance for L2A Project Teams

L2A VSWIR surface and water-leaving reflectances derive from L1 VSWIR radiances, and L2A TIR temperature and emissivity derive from L1 TIR radiances. It is possible to treat uncertainty quantification for these L2A products in isolation from the full scenario depicted in Figures 1, 2 and 3 by focusing only on the central portion of Figure 1, and starting not from $\mathbf{\Theta}$, but rather from intermediate surface states. Starting from the intermediate states rather than underlying geophysical states is advantageous for two reasons. First, it is more straightforward to execute than is the full uncertainty quantification framework encompassed by Figures 2 and 3, and it aligns well with previous applications of this approach to uncertainty quantification for other missions. Second, it enables the simplest possible (baseline) approach to uncertainty quantification (UQ) for L2+: forward uncertainty propagation, which will be the approach we need to take for at least some L2+ products.

In the following subsections we introduce our conceptual model for L2A uncertainty quantification, and then provide specific guidance that should be considered by the L2A VSWIR and TIR Teams as they move forward in their planning.

## 2.1 Conceptual Uncertainty Model

The general starting point for our L2A uncertainty quantification model is Figure 4; a pruned and modified version of Figure 1. Figure 4 focuses on relationships only among L1 and L2A algorithms, inputs, and products. The placement of some nodes in this graph have been adjusted (relative to Figure 1) to make room to explicitly show the role of additional entities, including $\mathrm{F}_{\mathbf{Y}\mathrm{V}}$, and $\mathrm{F}_{\mathbf{Y}\mathrm{T}}$. These are notional forward functions, representing nature, that convert intermediate surface states ($\mathbf{X}_\mathrm{V}$ and $\mathbf{X}_\mathrm{T}$) into radiance vectors, denoted by $\mathbf{Y}_\mathrm{V}$ (VSWIR) and $\mathbf{Y}_\mathrm{T}$ (TIR). We have also shown the roles of the atmospheric state, and instrument measurement errors, $\boldsymbol{\epsilon}_\mathrm{V}$ and $\boldsymbol{\epsilon}_\mathrm{T}$ for the VSWIR and TIR instruments. These quantities were omitted from Figure 1 in order to save space.

Suppose we could model $\mathbf{X}_\mathrm{V}$ and $\mathbf{X}_\mathrm{T}$ as separate, spatially and temporally evolving probability distributions[1]. If appropriate distributions could be asserted, then in principle, uncertainties associated with the VSWIR and TIR radiance vectors, $\mathbf{Y}_\mathrm{V}$, $\mathbf{Y}_\mathrm{T}$, and estimates of the VSWIR and TIR intermediate states, $\hat{\mathbf{X}}_\mathrm{V}$ and $\hat{\mathbf{X}}_\mathrm{T}$, could be simulated. (Note that we use "hat" to indicate when a variable is an estimate.) The VSWIR simulation starts from the assumed distribution of $\mathbf{X}_\mathrm{V}$ which generates realizations that are transformed by $\mathrm{F}_{\mathbf{Y}\mathrm{V}}$ into radiances observed with measurement error $\boldsymbol{\epsilon}_\mathrm{V}$ by the SBG VSWIR instrument. These noisy radiances are input to the L2A VSWIR Surface and Water-leaving Reflectance Algorithm, which gives an estimate, $\hat{\mathbf{X}}_\mathrm{V}$, of the original realization of $\mathbf{X}_\mathrm{V}$. The TIR experiment is similar, but with a distribution of temperature and emissivities, $\mathbf{X}_\mathrm{T}$, generating radiances, and the L2A TIR Temperature and Emissivity Algorithm providing estimates, $\hat{\mathbf{X}}_\mathrm{T}$. *The basis for quantifying uncertainties in* $\hat{\mathbf{X}}_\mathrm{V}$ *as an estimate of* $\mathbf{X}_\mathrm{V}$*, and in* $\hat{\mathbf{X}}_\mathrm{T}$ *as an estimate of* $\mathbf{X}_\mathrm{T}$*, is a quantitative description of the statistical relationships between* $\hat{\mathbf{X}}_\mathrm{V}$ *and* $\mathbf{X}_\mathrm{V}$ *for the VSWIR and between* $\hat{\mathbf{X}}_\mathrm{T}$ *and* $\mathbf{X}_\mathrm{T}$ *for the TIR.*

### 2.1.1 Quantifying the Relationship Between Truth and Estimate

The statistical relationship between a state variable, $\mathbf{X}$ and its estimate $\hat{\mathbf{X}}$ is described by the joint probability distribution of the two: $\mathrm{P}(\mathbf{X}, \hat{\mathbf{X}})$. As is, this is not practically

[1]In theory, $\mathbf{X}_\mathrm{V}$ and $\mathbf{X}_\mathrm{T}$ are not separate because they both derive from $\boldsymbol{\Theta}$. However, for simplicity, we treat them separately here.

useful for consumers of uncertainty information or for L2A Teams because we will only get to see the estimate. The true state will remain unknown. In fact, the description of uncertainty we seek is the conditional distribution of the true state given the estimate because this is the uncertainty that remains about the true state after we see the estimate. This conditional distribution is $\mathrm{P}(\mathbf{X}|\hat{\mathbf{X}})$ (read the bar as "given"), and it is derived from $\mathrm{P}(\mathbf{X}, \hat{\mathbf{X}})$ with some additional information provided by a simulation experiment.

The simulation experiment will provide information about the statistical parameters of $\mathrm{P}(\mathbf{X}|\hat{\mathbf{X}})$. The best analogy is simple linear regression. One acquires a training set of pairs of variable values, say X (dependent variable or "predictand") and $\hat{\mathrm{X}}$ (the independent variable or "predictor"), and fits a linear model to obtain estimates of regression line coefficients, slope $b$ and intercept $a$. The conditional distribution of the dependent variable given a value of the predictor variable, is Gaussian with mean $\mathrm{E}(\mathrm{X}|\hat{\mathrm{X}}) = b\hat{\mathrm{X}} + a$, and variance $\mathrm{Var}(\mathrm{X}|\hat{\mathrm{X}}) = \sigma^2_{\mathrm{X}|\hat{\mathrm{X}}}$, where best estimates of $b$, $a$, and $\sigma^2_{\mathrm{X}|\hat{\mathrm{X}}}$ are all functions of the training data:

$$\hat{b} = \bar{\hat{\mathrm{X}}}\left(1 - \hat{r}\frac{s_{\hat{\mathrm{X}}}}{s_{\mathrm{X}}}\right), \quad \hat{a} = \bar{\mathrm{X}} - \hat{b}\bar{\hat{\mathrm{X}}}, \quad \hat{\sigma}^2_{\mathrm{X}|\hat{\mathrm{X}}} = s^2_{\mathrm{X}}(1 - \hat{r}^2). \tag{1}$$

Here, $\bar{\hat{\mathrm{X}}}$ is the mean of the training set predictors, $\bar{\mathrm{X}}$ is the mean of the training set predictands, $s_{\hat{\mathrm{X}}}$ and $s_{\mathrm{X}}$ are the standard deviations of the training set predictors and predictands, and $\hat{r}$ is the training set correlation coefficient between the predictor and predictand. For some new instance of $\hat{\mathrm{X}}$, say $\hat{\mathrm{X}}^*$, the probability distribution of the corresponding true value, $\mathrm{X}^*$, is

$$\mathrm{X}^* \sim \mathrm{P}(\mathrm{X}^*|\hat{\mathrm{X}}^*) = \mathrm{Gau}\left(\hat{b}\hat{\mathrm{X}}^* + \hat{a}, s^2_{\mathrm{X}}\left(1 - \hat{r}^2\right)\right). \tag{2}$$

In our problem, the probability model is a Gaussian mixture model rather than a simple Gaussian, and the simulation experiment provides the training data. The latter is the motivating idea behind the guidance we assert for the L2A teams: the teams should provide data for a simulation experiment generating the training set (or training sets) for learning the parameters of the model $\mathrm{P}(\mathbf{X}|\hat{\mathbf{X}})$.

#### 2.1.2 Simulation Experiments

Though Figure 4 provides a conceptual map of how these notional experiments might work, it does not tell us how to execute them. Figure 5 replaces certain elements of Figure 4 with proxies in the form of empirical ensembles that *can* be generated in practice via comprehensive simulation experiments. The intermediate geophysical states shown in red

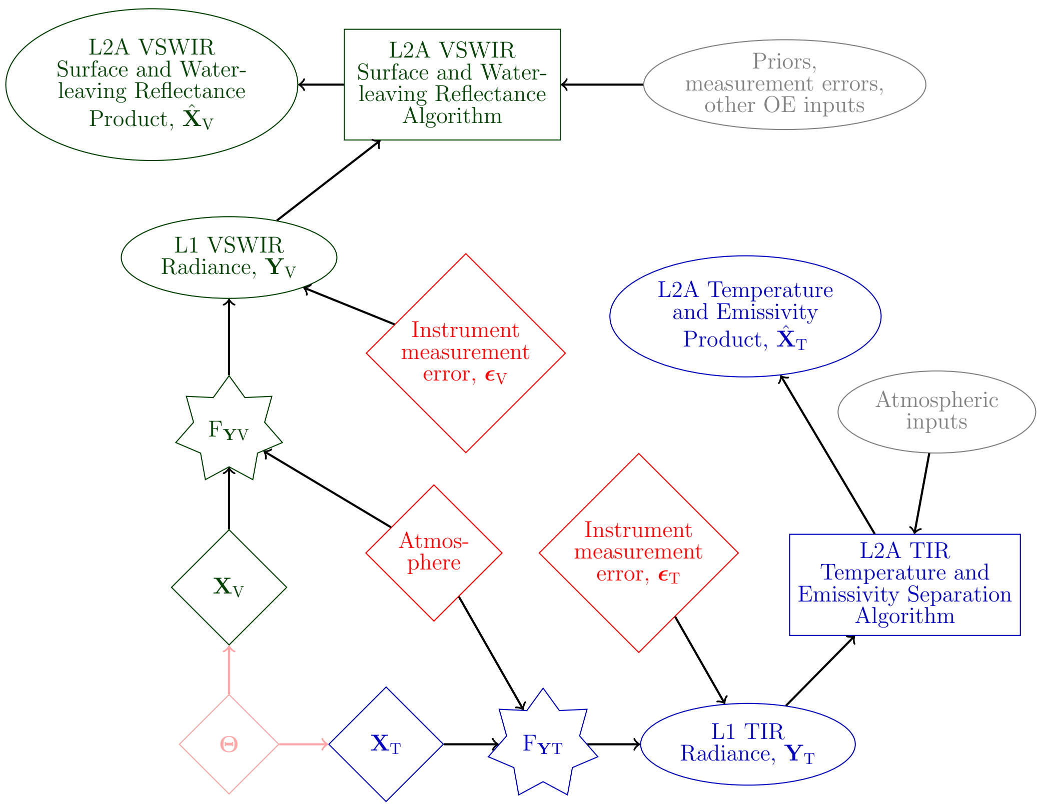


Figure 4: Augmented version of the central portion of Figure 1 highlighting relationships among L1 and L2A algorithms, inputs, and products. The placement of some nodes in this graph have been adjusted to make room to explicitly show the roles of VSWIR and TIR forward functions, $\mathrm{F}_{\mathbf{Y}\mathrm{V}}$ and $\mathrm{F}_{\mathbf{Y}\mathrm{T}}$. These are notional forward functions that convert intermediate surface states ($\mathbf{X}_{\mathrm{V}}$ and $\mathbf{X}_{\mathrm{T}}$) into radiance vectors, now denoted by $\mathbf{Y}_{\mathrm{V}}$ (VSWIR) and $\mathbf{Y}_{\mathrm{T}}$ (TIR). Also new in this figure are the diamonds representing measurement errors $\boldsymbol{\epsilon}_{\mathrm{V}}$ and $\boldsymbol{\epsilon}_{\mathrm{T}}$ for the VSWIR and TIR instruments.

diamonds in Figure 4 are replaced by synthetic ensembles of intermediate state vectors denoted by $\{\mathbf{X}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\mathbf{X}_{\mathrm{T}}^{\mathrm{sim}}\}$. Braces denote ensembles with sizes to be specified later. The superscript "sim" indicates simulated or synthetic quantities. Nature's "true" forward functions are replaced with forward models, $\hat{\mathrm{F}}_{\mathrm{V}}$ and $\hat{\mathrm{F}}_{\mathrm{T}}$. The ensembles $\{\mathbf{A}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\mathbf{A}_{\mathrm{T}}^{\mathrm{sim}}\}$ are ensembles with the same numbers of members as $\{\mathbf{X}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\mathbf{X}_{\mathrm{T}}^{\mathrm{sim}}\}$, which provide simulated atmospheric characteristics required by their respective forward models. $\{\boldsymbol{\epsilon}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\boldsymbol{\epsilon}_{\mathrm{T}}^{\mathrm{sim}}\}$ are synthetic ensembles of additive radiance measurement errors, also with the same numbers of members as $\{\mathbf{X}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\mathbf{X}_{\mathrm{T}}^{\mathrm{sim}}\}$, sampled independently from distributions provided by the instrument teams. All members of the noisy radiance ensembles, $\{\mathbf{Y}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\mathbf{Y}_{\mathrm{T}}^{\mathrm{sim}}\}$, are fed to their appropriate L2A algorithms resulting in output ensembles of estimated intermediate surface states, $\left\{\hat{\mathbf{X}}_{\mathrm{V}}^{\mathrm{sim}}\right\}$ and $\left\{\hat{\mathbf{X}}_{\mathrm{T}}^{\mathrm{sim}}\right\}$, that are in one-to-one correspondence with the elements of $\{\mathbf{X}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\mathbf{X}_{\mathrm{T}}^{\mathrm{sim}}\}$.

The joint ensembles, $\left\{\hat{\mathbf{X}}_{\mathrm{V}}^{\mathrm{sim}}, \mathbf{X}_{\mathrm{V}}^{\mathrm{sim}}\right\}$ and $\left\{\hat{\mathbf{X}}_{\mathrm{T}}^{\mathrm{sim}}, \mathbf{X}_{\mathrm{T}}^{\mathrm{sim}}\right\}$, are empirical (data-driven) representations of the joint probability distributions discussed in Section 2.1.1, $\mathrm{P}(\mathbf{X}, \hat{\mathbf{X}})$. We will learn the statistical parameters of these joint distributions, and the conditional distributions derived from them, from these joint ensembles.

## 2.2 The VSWIR Fractional Cover Algorithm and Product

The L2A VSWIR Fractional Cover Algorithm uses the L2A VSWIR surface and water-leaving reflectance intermediate state vectors to describe the overall composition of individual pixels in terms of four basic sub-pixel constituents: vegetation, barren land, liquid water, and snow and ice. Fractional cover characteristics have significant scientific value in their own right, but the main algorithmic purpose of this product will be to determine which L2+ algorithms will be applied to individual pixels. Like the Surface and Water-leaving Reflectance Product, The Fractional Cover Product is subject to uncertainty that can be quantified using a conditional probability model.

Conceptually, we think of the L2A Fractional Cover Product data as vectors, one for each pixel, of length four and such that the sum of its elements equals one. Call this vector $\boldsymbol{\rho} = (\rho_1, \rho_2, \rho_3, \rho_4)'$. $\rho_i$ is the proportion of a pixel deemed to be of the $i$-th type, where the types are vegetation ($i = 1$), barren ($i = 2$), liquid water ($i = 3$), and snow/ice ($i = 4$). To quantify uncertainty, an ensemble of simulated "true" fractional cover vectors, $\boldsymbol{\rho}^{\mathrm{sim}}$, will be created in conjunction with elements of $\{\mathbf{X}_{\mathrm{V}}^{\mathrm{sim}}\}$. Just as the purpose of the fractional cover product is to sort pixels in a way that dictates how they will be processed at L2+, that same coarse sorting can inform how to select representative ensembles of surface reflectance vectors. For example, if the fraction cover vectors cluster into groups, then it makes sense to choose members of $\{\mathbf{X}_{\mathrm{V}}^{\mathrm{sim}}\}$ that are representative of those groups both in type and

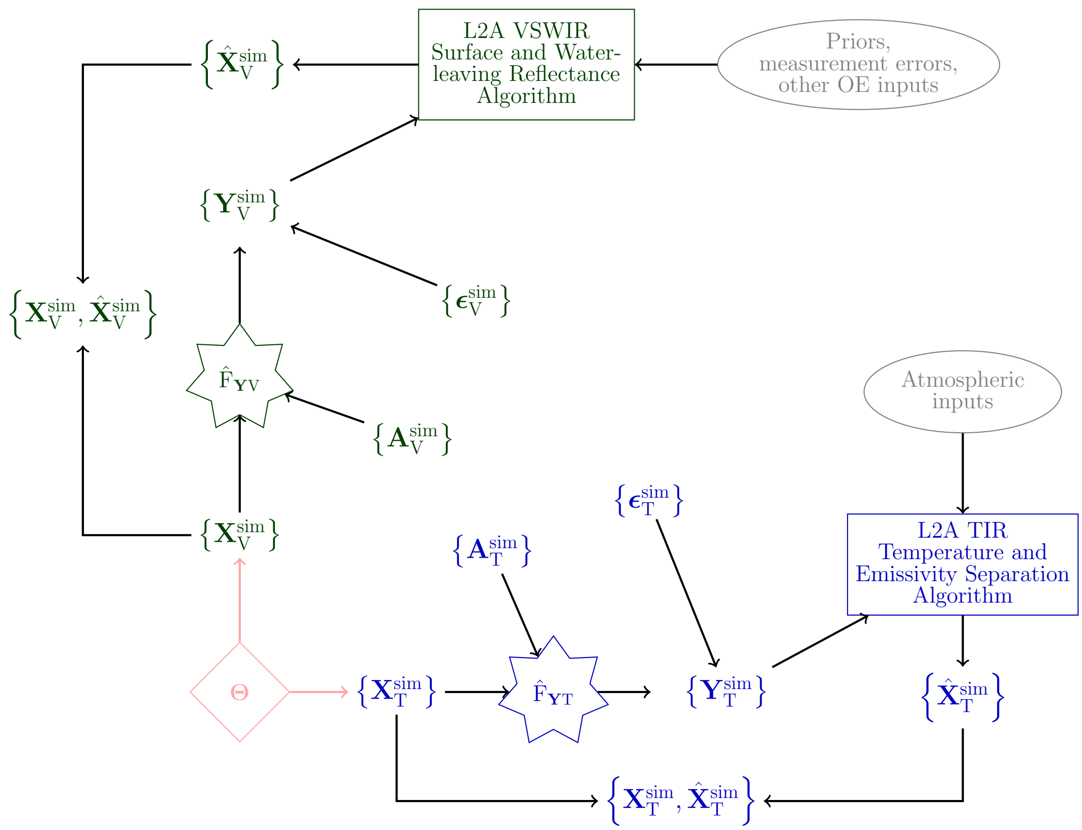


Figure 5: Simulation experiment analog of Figure 4. Two experiments are shown: the VSWIR experiment in green and the TIR experiment in blue. Each starts with an empirical ensemble of simulated intermediate surface state vectors, $\{\mathbf{X}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\mathbf{X}_{\mathrm{T}}^{\mathrm{sim}}\}$. All elements of these ensembles are processed through a forward model, $\hat{\mathrm{F}}_{\mathbf{Y}\mathrm{V}}$ for VSWIR and $\hat{\mathrm{F}}_{\mathbf{Y}\mathrm{T}}$ for TIR, to produce ensembles of simulated radiance vectors, $\{\mathbf{Y}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\mathbf{Y}_{\mathrm{T}}^{\mathrm{sim}}\}$. The ensembles $\{\mathbf{A}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\mathbf{A}_{\mathrm{T}}^{\mathrm{sim}}\}$ provide atmospheric information required by the forward models, and independently-generated instrument measurement errors, $\{\boldsymbol{\epsilon}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\boldsymbol{\epsilon}_{\mathrm{T}}^{\mathrm{sim}}\}$, are added to the radiances. Finally, elements of the ensembles of simulated, noisy radiances are input to their respective L2A algorithms. This yields ensembles of simulated estimates of the intermediate surface states, $\{\hat{\mathbf{X}}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\hat{\mathbf{X}}_{\mathrm{T}}^{\mathrm{sim}}\}$. The elements of these ensembles are in one-to-one correspondence with the elements of $\{\mathbf{X}_{\mathrm{V}}^{\mathrm{sim}}\}$ and $\{\mathbf{X}_{\mathrm{T}}^{\mathrm{sim}}\}$, respectively.

proportion. So members of the ensembles $\{\boldsymbol{\rho}^{\mathrm{sim}}\}$ and $\{\mathbf{X}_{\mathrm{V}}^{\mathrm{sim}}\}$ should be chosen *jointly*.

Figure 6 shows how the joint ensemble of simulated true and estimated fractional cover vectors can be incorporated into the VSWIR simulation experiment. As before, we use this empirical ensemble, $\{\boldsymbol{\rho}^{\mathrm{sim}}, \hat{\boldsymbol{\rho}}^{\mathrm{sim}}\}$ as training data to estimate the parameters of the probability model, $\mathrm{P}(\boldsymbol{\rho}^{\mathrm{sim}}|\hat{\boldsymbol{\rho}}^{\mathrm{sim}})$, and obtain conditional distributions for new instances of $\hat{\boldsymbol{\rho}}^{*}$. However, Figure 6 suggests something more: what is actually being produced is a joint ensemble that includes simulated true and estimated surface and water-leaving reflectance vectors *and* simulated true and estimated fractional cover vectors simultaneously: $\left\{\mathbf{X}_{\mathrm{V}}^{\mathrm{sim}}, \hat{\mathbf{X}}_{\mathrm{V}}^{\mathrm{sim}}, \boldsymbol{\rho}^{\mathrm{sim}}, \hat{\boldsymbol{\rho}}^{\mathrm{sim}}\right\}$. This simulation experiment will tell us a great deal about the properties of the SBG-VSWIR data production system's interdependencies in the form of empirical relationships between the quantities being simulated here.

## 2.3 A Notional TIR Fractional Cover Algorithm and Product

For the same reasons that it is desirable to construct the VSWIR intermediate state vector ensemble jointly with a VSWIR fractional cover ensemble, it is desirable to do so for the TIR as well. Fractional cover provides quantitative information about pixel geophysical composition, and is a logical guide to the construction of the intermediate state vector ensemble, $\{\mathbf{X}_{\mathrm{T}}^{\mathrm{sim}}\}$. Figure 7 is analogous to Figure 6, and uses $\boldsymbol{\omega}$ for TIR fractional cover to distinguish it from VSWIR fractional cover, $\boldsymbol{\rho}$. At the time of this writing, no TIR fractional cover algorithm or product exists and it remains to decide whether and how this could be created.

## 2.4 Specific Guidance for the L2A Teams

The L2A Teams will need to work with the UQ Team to provide:

1. ensembles of simulated training true states along with the concomitant fractional cover or other stratification information used to construct the ensembles
2. forward models and necessary inputs required to run them on the ensembles of simulated training true states in order to produce simulated noisy radiances
3. retrieval algorithms and all inputs required to run them on the ensemble of simulated noisy radiances to produce simulated estimates.

The most efficient way to deal with items 2 and 3 (the algorithms and their inputs required to carry out the simulation experiments) is to build into the SDS processing pipeline the ability to ingest simulated data as well as actual data. This is probably necessary for

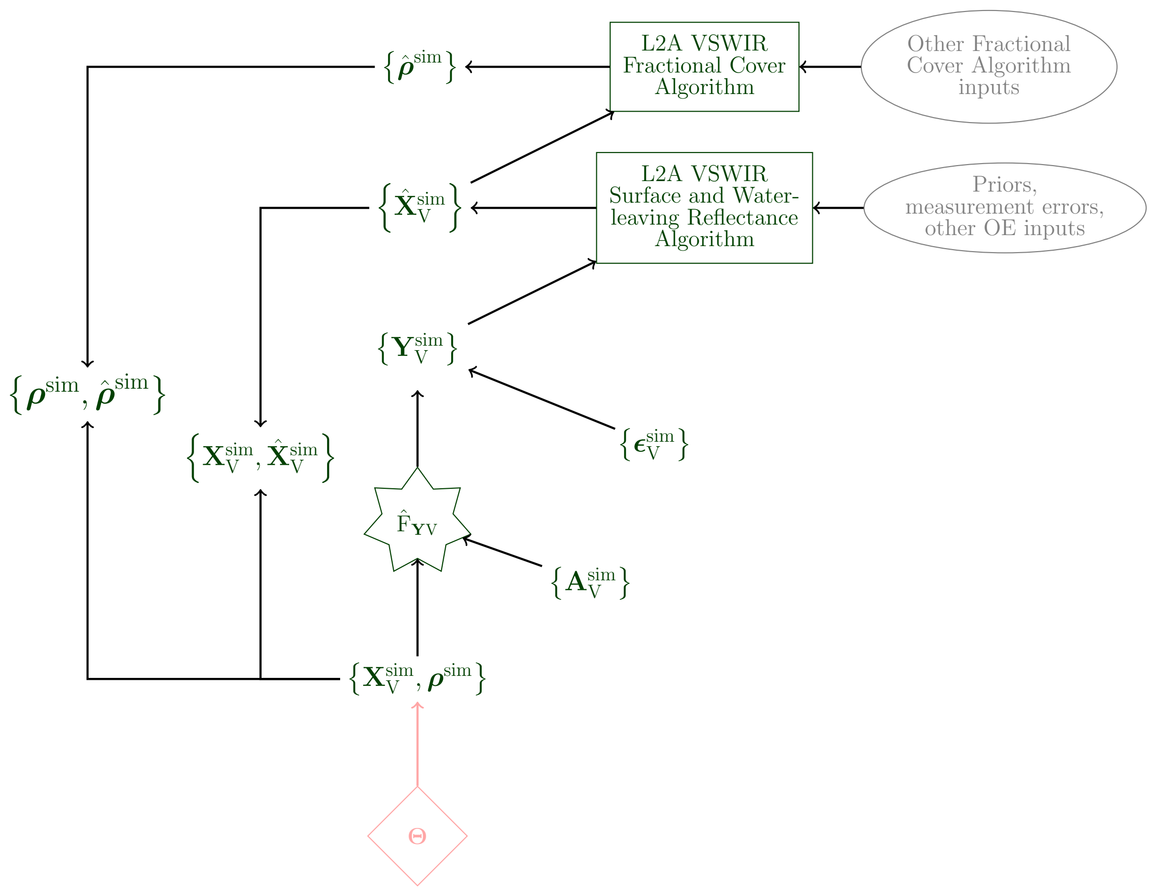


Figure 6: L2A VSWIR simulation experiment augmented to include the Fractional Cover Algorithm and its output, $\{\hat{\boldsymbol{\rho}}^{\text{sim}}\}$. The ensemble of simulated, "true" fractional cover should be created jointly with the ensemble of intermediate state vectors.

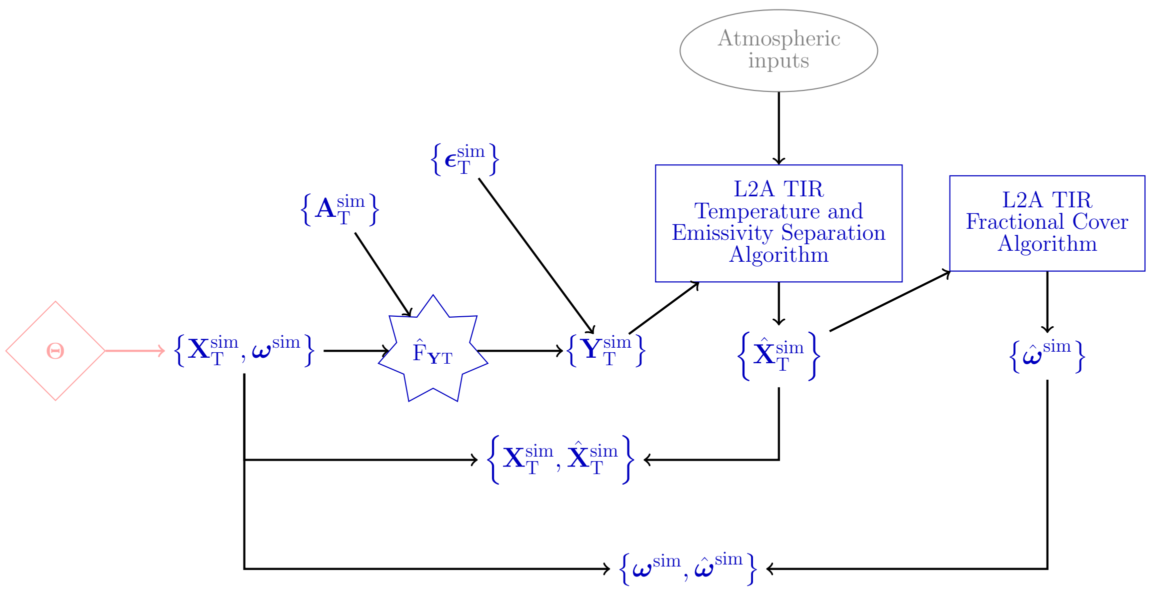


Figure 7: L2A TIR simulation experiment augmented to include a notional Fractional Cover Algorithm and its output, $\{\hat{\boldsymbol{\omega}}^{\mathrm{sim}}\}$. The ensemble of simulated, "true" fractional cover may be created as step on the way to creating the ensemble of intermediate state vectors, $\left\{\hat{\mathbf{X}}_{\mathrm{T}}^{\mathrm{sim}}\right\}$.

algorithm testing anyway, so the L2A Teams should coordinate with the UQ Team when designing these pipelines.

The most complex requirement will be to compile a collection of representative intermediate state vectors (the ensembles $\left\{\mathbf{X}_{\mathrm{V}}^{\mathrm{sim}}, \boldsymbol{\rho}^{\mathrm{sim}}\right\}$ and $\left\{\mathbf{X}_{\mathrm{T}}^{\mathrm{sim}}\right\}$) that will drive the simulation experiments discussed in Section 2.1.2. In order that the probability model derived from the simulation experiments be realistic, the ensembles of representative states must be realistic in the sense that they are generally indicative of the types of scenes that SBG will ultimately see. "Representativeness" of an ensemble is defined here to mean that the ensemble contains instances of intermediate state vectors that satisfy two criteria.

The first criterion is "range representativeness": that the intermediate state vectors are associated with the plausible range of underlying geophysical states that we expect the instruments will see globally in time and space. Range representativeness can be achieved, at least as a first cut, by spatial and temporal stratification. The geophysical states to be considered are defined by the expected range of behavior on quantities output by L2+ algorithms shown in Figure 1.

The second criterion is that the relative frequencies of intermediate state vectors in the ensembles be roughly consistent with relative frequencies of occurrence of their underlying geophysical states. This criterion is "distributional representativeness". To ensure distributional representativeness, we need a quantitative way to characterize frequencies of occurrence of both the underlying geophysical state, and the intermediate states. For instance, if we knew that a certain proportion of future SBG pixels would be of the type that would ultimately be sent to the terrestrial ecology L2+ processing suite, then we would endeavor to include that same proportion of intermediate state vectors having reflectances or temperatures and emissivities similar to what we would expect from vegetation-covered scenes. This is nothing more than relying on some asserted set of fractional cover vectors as a proxy for general conditions. In fact, doing this gives us the desired joint ensemble of surface and water-leaving reflectance vectors and fractional cover vectors shown in Figure 6, for VSWIR. At present, there is no analog on the TIR side, but the same thinking should inform the construction of the ensemble $\left\{\mathbf{X}_{\mathrm{T}}^{\mathrm{sim}}\right\}$.

In practice, limited information is available to achieve range and distributional representativeness in the construction of these ensembles. Initially, the process will have to be guided by domain expertise and prior knowledge gleaned from precursor missions. The specific guidance below is intended help the L2A teams interoperate with the UQ Team in order to achieve the mission's UQ objectives.

### 2.5 Specific Guidance for the L2A VSWIR Team

The L2A VSWIR Team should:

1. Work with the UQ Team to develop an ensemble of representative surface reflectance

and water-leaving reflectance intermediate state vectors coupled with consistent fractional cover vectors, of as large a size as is feasible, but having not less than 100,000 members initially (this may change later). The numbers of surface reflectance and water-leaving reflectance vectors should approximately reflect the relative prevalence of land and water instances that are expected during the mission.

2. Work with the UQ team to ensure that the make-up of the surface reflectance portion of this ensemble approximately reflects the expected proportions of pixels that are expected to be classified as majority-vegetated, majority-barren, and majority-snow/ice examples, and make sure they are consistent with their concomitant fractional cover vectors. Further, within the vegetated, barren, and snow/ice classes, the ensemble should achieve approximate range-representativeness, and distribution-representativeness if possible, over a suitable stratification of sub-types of geophysical conditions within these classes.

3. Work with the UQ Team to ensure that the make-up of the water-leaving reflectance portion of this ensemble achieves approximate range representativeness, and distributional representativeness if possible, over a suitable stratification of types of liquid water geophysical conditions.

4. Work with the UQ Team to develop and apply quantitative criteria for estimating range and distributional representativeness.

5. Work with the UQ Team to ensure that the Surface and Water-leaving Reflectance Algorithm, as implemented, has hooks to allow processing of simulated noisy radiance vectors to produce simulated intermediate state vector estimates.

6. In collaboration with the UQ Team, ensure that existing forward model code and required inputs to convert elements of the simulated intermediate state vector ensemble into simulated noiseless radiance vectors, allows for processing of simulated inputs.

7. Work with the UQ Team to provide either an ensemble of simulated measurement error values or a statistical characterization of such, so that the noiseless radiance vectors can be converted into noisy radiance vectors.

8. Coordinate with the L2A TIR Team to achieve as much commonality (in the sense of characterizing common scenes) as possible between the VSWIR and TIR ensembles of intermediate state vectors. In particular, atmospheric inputs assumed in the L2A VSWIR retrieval should not be inconsistent with those assumed in the L2A TIR retrieval.

### 2.6 Specific Guidance for the L2A TIR Team

The L2A TIR Team should:

1. Work with the UQ Team to develop an ensemble of representative temperature and emissivity intermediate state vectors of as large a size as is feasible, but having not less than 100,000 members initially (this may change later). The character of temperature and emissivity vectors should approximately reflect the relative prevalence of land and water pixels that are expected during the mission.

2. Work with the UQ Team to ensure that the make-up of the land portion of this ensemble approximately reflects the expected character of pixels that are expected to be subjected the various L2+ TIR algorithms. Further, within the terrestrial ecology, geology, and snow/ice domains, the ensemble should achieve approximate range-representativeness, and distribution-representativeness if possible, over a suitable stratification of sub-types of expected geophysical conditions within these classes.

3. Work with the UQ Team to ensure that the make-up of the ocean, coastal, and inland water portion of this ensemble achieves approximate range representativeness, and distributional representativeness if possible, over a suitable stratification of expected types of water-related geophysical conditions.

4. In coordination with the UQ Team, consider creating a fractional cover variable, potentially in concert with the VSWIR Fractional Cover Product, to characterize individual pixels in a way that assists with the construction of the ensemble of representative temperature and emissivity intermediate state vectors.

5. Work with the UQ Team to develop and apply quantitative criteria for estimating range and distributional representativeness.

6. Work with the UQ Team to ensure that the Temperature and Emissivity Separation Algorithm, as implemented, has hooks to allow processing of simulated noisy radiance vectors to produce simulated intermediate state vector estimates.

7. Work with the UQ Team to ensure that the Split-window Algorithm, as implemented, has hooks to allow processing of simulated noisy radiance vectors.

8. In collaboration with the UQ Team, ensure that existing forward model code and required inputs to convert elements of the simulated intermediate state vector ensemble into simulated noiseless radiance vectors, allows for processing of simulated inputs.

9. Work with the UQ Team to provide either an ensemble of simulated measurement error values or a statistical characterization of such, so that the noiseless radiance vectors can be converted into noisy radiance vectors.

10. Coordinate with the L2A VSWIR Team to achieve as much commonality (in the sense of characterizing common scenes) as possible between the VSWIR and TIR ensembles of intermediate state vectors. In particular, atmospheric inputs assumed in the L2A TIR retrieval should not be inconsistent with those assumed in the L2A VSWIR retrieval.

# 3 Guidance for the L2+ Project Teams

At the time of this writing, final decisions have not been made about L2+ algorithms. Planning activities for different algorithms are at different stages of maturity. Under these circumstances it is difficult if not impossible to provide guidance. The subsections below will be filled in over time as the picture crystalizes.

## 3.1 Specific Guidance for VSWIR Aquatics L2+ Teams

TBD.

### 3.1.1 Benthic Product

TBD.

### 3.1.2 Chlorophyll Product

TBD.

### 3.1.3 Phytoplankton Product

TBD.

## 3.2 Specific Guidance for VSWIR Geology L2+ Teams

TBD.

### 3.2.1 Mineral Abundance Product

TBD.

### 3.2.2 Surface Mineralogy Product

TBD.

## 3.3 Specific Guidance for VSWIR Snow/Ice L2+ Teams

TBD.

### 3.3.1 Snow Albedo Product

TBD.

### 3.3.2 Snow Fractional Cover Product

TBD.

### 3.3.3 Snow Grain Size Product

TBD.

## 3.4 Specific Guidance for VSWIR Terrestrial Ecology L2+ Teams

TBD.

### 3.4.1 Albedo Product

TBD.

### 3.4.2 Canopy Chlorophyll Product

TBD.

### 3.4.3 Canopy Leaf-mass Area Product

TBD.

### 3.4.4 Canopy Nitrogen Product

TBD.

### 3.4.5 Equivalent Water Thickness Product

TBD.

### 3.4.6 Fractional Cover Product

TBD.

## 3.5 Specific Guidance for TIR L2+ Teams

TBD.

## 3.6 Specific Guidance for TIR Aquatics L2+ Teams

TBD.

### 3.6.1 Water Temperature (SST) Product

TBD.

## 3.7 Specific Guidance for TIR Geology L2+ Teams

TBD.

### 3.7.1 Elevated Temperature and Volcanic Activity Products

TBD.

### 3.7.2 Surface Mineralogy Product

TBD.

## 3.8 Specific Guidance for TIR Snow/Ice L2+ Teams

TBD.

### 3.8.1 Snow Surface Temperature Product

TBD.

## 3.9 Specific Guidance for TIR Terrestrial Ecology L2+ Teams

TBD.

### 3.9.1 Evapotranspiration, Evaporative Stress Index, and Water-use Efficiency Products

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