An information content approach to diagnosing and improving CLIMCAPS retrieval consistency across instruments and satellites

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Abstract. The Community Long-term Infrared Microwave Combined Atmospheric Product System (CLIMCAPS) characterizes the atmospheric state as vertical profiles of temperature, water vapor, CO_2, CO, CH_4, O_3, HNO_3 and N_2O, together with a suite of Earth surface and cloud properties. The CLIMCAPS record spans more than two decades (2002–present) because it utilizes measurements from a series of hyperspectral infrared sounders on different satellite platforms. In this paper, we take a step-wise approach to diagnosing the CLIMCAPS V2 system with the goal of identifying which Bayesian retrieval components to improve for a future V3 release. CLIMCAPS is based on the NASA (National Aeronautics and Space Administration) heritage retrieval approach, and is the first system to extend the Aqua record with sounders on next-generation platforms in the same orbit. With the baseline quality of CLIMCAPS V2 soundings well-established, the objective of a V3 upgrade is to improve retrieval consistency across the different instruments and platforms for the sake of a seamless global record of atmospheric soundings. We demonstrate how the retrieval averaging kernels (AKs) are key metrics in diagnosing a multi-instrument system such as CLIMCAPS, and we conclude with the recommendation to upgrade the channel subsets and radiative transfer model error spectrum used in defining the Bayesian measurement error covariance matrix.

1 Introduction

The launch of Aqua on 4 May 2002 heralded in a new era for satellite sounding of the Earth atmosphere with the hyperspectral Atmospheric Infrared Sounder (AIRS) (Aumann et al., 2003; Chahine et al., 2006). AIRS was the first of its kind in space, and measures emitted infrared (IR) radiance with hundreds of spectrally narrow channels and low instrument noise. Its high spectral resolution allows AIRS to measure a wide range of parameters about the thermodynamic structure *and* chemical composition of the atmosphere (Susskind et al., 2003). More than 21 years later and still in operational orbit, Aqua continues to contribute important Earth system measurements (Parkinson, 2022). But, with only a few years before the spacecraft is decommissioned, our focus switch to ways that would see the Aqua record continue with next-generation instruments and platforms.

The Community Long-term Infrared Microwave Combined Atmospheric Product System (CLIMCAPS) retrieves atmospheric soundings from hyperspectral infrared (IR) measurements, like those made by AIRS. CLIMCAPS soundings are profiles of

30   temperature, water vapor and a host of minor gases (CO_2, CO, CH_4, O_3, N_2O, HNO_3) as well as cloud and Earth surface properties (Smith and Barnet, 2023a). CLIMCAPS augments measurements from AIRS with those from AMSU (Advanced Microwave Sounding Unit), also on the Aqua spacecraft, to help distinguish whether a retrieval scene is uniformly clear or uniformly cloudy. CLIMCAPS builds on decades of investment in sounding science to extend the Aqua retrieval record with CrIS (Cross-track Infrared Sounder) and ATMS (Advanced Technology Microwave Sounder) on the Suomi National Polar-

35   orbiting Partnership (SNPP) and Joint Polar Satellite System series (JPSS-1 to JPSS-4). CLIMCAPS is the first system to explicitly address instrument differences in its retrieval approach for the sake of a continuous record between AIRS+AMSU and CrIS+ATMS (Smith and Barnet, 2023a). We use the term "continuous" to mean a data record that is consistent in its characterization of natural variation despite changes in source instrumentation.

40   The CLIMCAPS retrieval approach has its origin in the NASA sounder retrieval method (Susskind et al., 2003), which deviates from traditional Bayesian Optimal Estimation (OE, Rodgers 2000) most notably in its dynamic, scene-dependent regularization approach that applies singular value decomposition (SVD) to the signal-to-noise ratio (SNR) matrix (see Smith and Barnet, 2020 for details). Our focus in this paper is on the CLIMCAPS V2 product suite released by GES DISC in 2020, which is the only data record to date that spans the combined lifetimes of AIRS+AMSU and CrIS+ATMS with a consistent retrieval

45   approach.

CLIMCAPS has, to date, been supported by a series of competitive NASA grants, each funding, at most, the full-time-equivalent (FTE) of one expert for three years. Product roll-out, evaluation and improvement, therefore, have to manifest within a collaborative community. Each CLIMCAPS sounding is made up of many Earth system parameters (See Table 1 in

50   Smith and Barnet, 2023a) and collectively characterize the global atmosphere twice daily. With such a data load that already spans more than two decades, typical validation studies (Nalli et al., 2018a, b; Wang et al., 2020; Yue et al., 2022) are not only resource-intensive, but fall far short of providing a comprehensive analysis of the overall retrieval quality, especially within an ever-changing climate system. For CLIMCAPS to meaningfully support its wide range of science applications (e.g., Gaudel et al., 2024; Ouyed et al., 2023; Prange et al., 2023), end-users need to be equipped with the diagnostic metrics and

55   documentation to enable correct interpretation within data applications (e.g., Smith et al., 2021; Smith and Barnet, 2023b). The work described in this paper is testimony to the value of such an interactive science community that fosters dialogue between Developer and Stakeholder. What we learned is that a future CLIMCAPS V3 release should, first and foremost, improve upon the baseline consistency we established in V2 (Smith and Barnet, 2020) for the sake of higher product accuracy in support of long-term, large-scale studies.

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The format of this paper is unconventional in that we do not simply list our experimental methodology, but instead discuss how we arrived at the methodology in the first place. CLIMCAPS is a complex retrieval system with many component parts, so it is not straightforward to identify which components to address first, given our goals for a V3 upgrade. We, therefore,

include a discussion of the systematic approach we took to diagnosing and improving retrieval consistency to help foster confidence in the product and promote accurate interpretation. So, in Section 2 we summarize the CLIMCAPS components that afford us a diagnostic evaluation of its retrieval products. In Section 3, we first justify then outline our experimental design, and in Section 4 discuss results. Section 5 summarizes our conclusions for future system improvements. The analysis presented in this paper uses CLIMCAPS retrievals from Suomi-NPP CrIS+ATMS and Aqua AIRS+ATMS measurements made in 2016 when both instrument suites were in operational orbit at full spectral resolution. Henceforth, we distinguish these two systems as "CLIMCAPS-Aqua" and "CLIMCAPS-SNPP". Note that a demonstration of continuity between CLIMCAPS-Aqua and CLIMCAPS-SNPP implies continuity with CLIMCAPS-JPSS+, since all four JPSS platforms, JPSS-1 through JPSS-4, have the same CrIS+ATMS instruments. This means that the CLIMCAPS sounding record has potential to span at least four decades, 2002 to ~2040.

2 CLIMCAPS retrieval approach

The full CLIMCAPS record was made publicly available for the first time in 2020 as Version 2 (Table S1). Where the initial development of CLIMCAPS drew on decades of stove-piped efforts at NASA and NOAA (National Oceanic and Atmospheric Administration), the full CLIMCAPS V2 record, now in public domain, allows us to make targeted upgrades using diagnostic criteria suited to known product applications. This section describes the algorithm elements we employed to address systematic instrument differences in the CLIMCAPS V2 record. Detailed descriptions of the CLIMCAPS retrieval approach can be found elsewhere (Smith and Barnet, 2019, 2020, 2023a, 2023b). Of interest here is the fact that CLIMCAPS generate myriad quantitative metrics for in-depth evaluation of the retrieval system and a sounder science approach to algorithm upgrades.

2.1 Instrument-specific algorithm components

CLIMCAPS is instrument agnostic at its core, which enables the same code to run all configurations, eliminating many potential discontinuities due to version control. Instrument design directly affects measurement information content, and therefore retrieval quality. For example, spectral coverage determines which atmospheric gases can be retrieved, while spectral resolution affects their retrieval quality. Many of the Level-1 product differences are addressed and neutralized in the CLIMCAPS pre-processor, but fundamental instrument differences that affect measurement SNR propagate systematically into the retrieved quantities. As a result, instrument biases can disrupt the geophysical consistency of a long-term data record even if a retrieval system is instrument agnostic. AIRS is a grating spectrometer (Aumann et al., 2003; Chahine et al., 2006) and CrIS an interferometer (Glumb et al., 2002; Strow et al., 2013). Smith and Barnet (2019) summarized these two instruments from a retrieval perspective and elaborate on a few key aspects in Table S1 of this paper. Given these fundamental instrument differences, one has to consider AIRS and CrIS spectral resolution and how their instrument design affects the fecundity of spectral channels. But IR spectra do not provide the only source of information. CLIMCAPS additionally harvests spatial information from the 3 x 3 cluster of instrument fields-of-view (FOVs) making up each retrieval field-of-regard (FOR), as well

as spectral information from the collocated microwave (MW) sounders, AMSU on Aqua and ATMS on SNPP and JPSS+. The reason for this is that retrieval parameters can be mathematically degenerate within a single source of measurement. Adding other sources can help break this degeneracy to allow the retrieval of discrete parameters (see Table 1 in Smith and Barnet, 2023a for a full list). A good example is the degeneracy of cloud and surface parameters within the IR radiances. Adding MW and spatial information to the retrieval process helps CLIMCAPS distinguish between cloud tops and Earth surface. While the IR sounders provide the primary source of spectral information, one should always keep in mind that the spatial arrangement of IR FOVs and the quality of collocated MW measurements also affect CLIMCAPS retrieval quality.

AIRS and CrIS each have hundreds of spectral channels measuring IR radiation in narrow intervals. In CLIMCAPS, we do not use all the available IR channels for each parameter retrieval because there is no reason to include channels insensitive to the target parameter that would be filtered out during dynamic SVD regularization anyway. So, for the sake of retrieval speed and improved SNR, we pre-select subsets of channels for each target variable as discussed in Gambacorta and Barnet (2013). The channel subsets we implemented in CLIMCAPS V2 for AIRS and CrIS reflect best practices currently at NASA and NOAA for each instrument configuration (Table S2). But persistent differences in AKs between CLIMCAPS-Aqua and CLIMCAPS-SNPP (Smith and Barnet, 2020), reflect systematic effects in SNR that could be traced back to CLIMCAPS V2 channel subsets. We, therefore, revisit the V2 channel sets in this paper and make recommendations for upgrades to improve the consistency in CLIMCAPS retrieval quality across AIRS+AMSU and CrIS+ATMS. Note that we select the CLIMCAPS channel sets from the full range that is available for CrIS (2211 in total). For AIRS, however, the full channel set (2378 in total) is first reduced into a "pristine" list (less than 1600 after sub-setting) ahead of channel selection to remove channels with measurable noise effects due to, for example, large thermal cycles in orbit or on Earth (Manning et al., 2020).

2.2 Diagnostic metrics

CLIMCAPS yields a number of diagnostic metrics that can be used to evaluate its data record. For this study, we predominantly employ three types of metrics to analyse the degree to which retrievals from the two different instrument suites, AIRS+AMSU and CrIS+ATMS, are consistent in space and time. These are (i) cloud clearing metrics that quantify the random and systematic error introduced by clouds, (ii) AKs and DOFS that quantify measurement SNR, and (iii) the difference between the final retrieval and a-priori estimate, which we will refer to as ADIFF from here on. AKs quantify the degree to which a solution depends on the measurement. It is a unitless quantity where *zero* means that the solution is equal to the a-priori estimate, and *one* means that the solution is entirely derived from the measurements without any contribution from the a-priori. A metric that complements the AKs, is the degree to which the solution deviates from the a-priori, i.e., ADIFF. This is an especially informative metric in CLIMCAPS where *all the a-priori estimates are independent of the instrument measurements* (Smith and Barnet, 2019). For temperature, water vapor and O_3 the CLIMCAPS a-priori is dynamically defined by the reanalysis model, MERRA-2 (Gelaro et al., 2017; GMAO, 2015), that is interpolated in time and space to each instrument footprint ahead of retrieval. For the well-mixed gases, CO_2, N_2O, and CH_4, we use estimates of their long-term trends across seasons and

hemispheres. The CLIMCAPS CO a-priori is a seasonal and inter-hemispheric climatology, and for HNO_3 and SO_2 we have a single static profile at this time. As knowledge of these gases grows, we can consider developing new climatologies and/or employing other chemistry or reanalysis models. Having a-priori estimates that are instrument independent is one of the key aspects that enable continuity in the CLIMCAPS record since they help avoid abrupt changes when new instrument measurements are introduced or when SNR is low. A CLIMCAPS retrieval typically deviates from its a-priori estimate when the measurements add new information about the true state of the atmosphere within the FOR. On rare occasions, however, a retrieval can be dominated by noise when SNR is very low. One can diagnose CLIMCAPS retrievals to better understand the reasons for |ADIFF| > 0 values using the AK matrices that are reported for every retrieval parameter at every FOR in the Level 2 product. These are discussed in detail in Smith and Barnet (2020) but is worth summarizing here:

(1) High AK, high ADIFF: measurement sensitivity is high and updates the a-priori estimate with new information about the target variable. This is by far the largest category defining ~79% of all retrievals on any given day of measurements. These retrievals are typically flagged "successful" in that they pass all CLIMCAPS quality control (QC) thresholds.

(2) High AK, low ADIFF: measurement sensitivity is high and agrees with the a-priori representation of the target variable. This is the second largest category (~17%) of CLIMCAPS retrievals.

(3) Low AK, low ADIFF: measurement sensitivity is low, so the retrieval predominantly resembles the a-priori estimate. This is the smallest category, defining only ~1% of retrievals on any given day.

(4) Low AK, high ADIFF: measurement sensitivity to the target variable is low and the spurious effects visible in ADIFF is predominantly error. The CLIMCAPS QC filters typically flag retrievals in this category as "failed.

When we evaluate retrieval continuity between CLIMCAPS-Aqua and CLIMCAPS-SNPP, we typically want to see similar space-time patterns in these metrics as it would mean that CLIMCAPS maintains consistency in retrieval SNR despite changes in instrumentation.

3 Methodology

3.1 Background and rationale

CLIMCAPS retrieves its large suite of atmospheric state parameters sequentially in a series of steps (Smith and Barnet, 2023a). This step-wise approach holds many advantages, not least because it helps minimize the size of the a-priori error covariance matrix employed during retrieval for the sake of a computationally efficient algorithm that can support both real-time and full mission applications. Of primary concern to the CLIMCAPS V2 data record, however, is how such a sequential approach enables step-wise, targeted updates to the measurement error covariance matrix as knowledge of the true state and retrieval uncertainty grows (Smith and Barnet, 2019). The CLIMCAPS measurement error covariance matrix, S_m, is the sum of the radiance error covariance matrix, $\delta R \delta R^T$, and radiance uncertainty due to the background atmospheric state, $K^T S_b K$, where K

160   is the Jacobian and $\mathbf{S}_b$ the background state error covariance matrix (Smith and Barnet 2019, 2020). All atmospheric state parameters held constant during any given retrieval step are considered "background" parameters. CLIMCAPS retrieves clouds first, followed by temperature [air_temp] and water vapor [h2o_vap] in that order (Smith and Barnet 2023a). Being first, the cloud properties are retrieved using only a-priori, not retrieved, estimates of the clear atmospheric state. Similarly, $\mathbf{S}_m$ is, at first, defined only by a-priori estimates of radiance and background state uncertainty. After retrieval of the cloud parameters,

165   the IR radiance measurements are cloud cleared (Smith and Barnet, 2023b) to allow sounding retrievals of the full, clear atmospheric column (i.e., characterization of atmospheric state past, not through, clouds). During this step (and each subsequent step), retrieval uncertainty is quantified, then propagated to the next step. Note that cloud clearing is the only step that updates the radiance uncertainty directly. In all subsequent steps, $\mathbf{S}_m$ will incorporate the cloud-cleared radiance uncertainty $\delta\mathbf{R}_{cc}\delta\mathbf{R}_{cc}^{\mathrm{T}}$ instead of the a-priori measurement uncertainty $\delta\mathbf{R}\delta\mathbf{R}^{\mathrm{T}}$ (see Eq. 5 in Smith and Barnet, 2023b). Once

170   [air_temp] is retrieved, $\mathbf{K}^{\mathrm{T}}\mathbf{S}_b\mathbf{K}$ is updated with the retrieved uncertainty of [air_temp]. More generally, a CLIMCAPS retrieval at step x+3 uses a background state with a-priori estimates replaced by the retrieved parameters from steps x, x+1 and x+2. In other words, the step-wise CLIMCAPS approach uses scene-specific signal *and* noise estimates as soon as they become available so that the a-priori state is gradually updated to represent retrieved conditions within the FOR. The main purpose of this step-wise retrieval approach is to improve the efficiency with which the radiance measurement can be decomposed into

175   discrete signals (Smith and Barnet, 2019).

The sequence and number of CLIMCAPS retrieval steps are not fixed but can be arranged to suit target applications. The CLIMCAPS V2 sequence broadly progresses as follows. (i) Clouds are by far the largest spectral signature and affects most of the measured spectral range, so cloud-cleared radiances are retrieved first. (ii) [air_temp] is spectrally the most linear of

180   all sounding parameters and it is important to have a stable, accurate representation of [air_temp] before attempting [h2o_vap] and trace gas retrievals, so [air_temp] is retrieved ahead of all trace gases. (iii) [h2o_vap] is the largest perturbation after clouds and [air_temp]. Water vapor is also pervasive in the whole spectrum. This is why we retrieve [h2o_vap] after the first [air_temp] retrieval and why it precedes all the other gases. (iv) O_3 is somewhat non-linear but has second order effects on [air_temp] and [h2o_vap], so it is retrieved next. (v) CO is highly linear with negligible

185   impacts on other parameters. (vi) HNO_3 is linear and impacts [air_temp] in polar regions. (vii) [air_temp] is then retrieved a second time from the same MERRA-2 a-priori to capture non-linearities due to retrieved (not a-priori) knowledge of the value and error in [h2o_vap] and O_3. (viii) Finally, CO_2, N_2O and S_2O are retrieved in this sequence. Their spectral signals are mostly linear but the measurement information content for these gases is very low so we do not consider the retrievals of sufficient quality to affect the final [air_temp] retrieval. In future, we may change the order of these retrieval

190   steps as we develop more accurate a-priori estimates.

Of primary importance in the CLIMCAPS product suite are the atmospheric profile retrievals from cloud-cleared radiances, so our experiment will start with an evaluation of cloud clearing uncertainty metrics that propagate and affect measurement SNR in all subsequent steps. Cloud clearing is a well-established method for addressing the way clouds affect IR radiation through the atmosphere (Chahine, 1977; Susskind et al., 1998) and is implemented in CLIMCAPS V2 as discussed in Smith and Barnet (2023b). In short, cloud clearing aggregates the clear-sky radiance signal from each cluster of 3 x 3 FOVs (~15 km at nadir) to retrieve a single cloud-cleared radiance spectrum that represents the atmosphere within the larger FOR (~45 km at nadir). Figure 1 depicts the key uncertainty metrics CLIMCAPS generates during its cloud clearing step, namely `etarej` and `ampl_eta`. The former quantifies the bias in retrieved cloud-cleared radiance and the latter the degree to which random instrument noise is affected within the aggregated FOR. If there are differences in the degree to which instruments measure atmospheric clouds, we expect to see them amplified in these uncertainty metrics. The swath width of CLIMCAPS-SNPP (Figures 1a and 1c) is slightly wider than CLIMCAPS-Aqua (Figures 1b and 1d), hence the smaller data gaps at lower latitudes. Otherwise, we see that `etarej` and `ampl_eta` are largely consistent between CLIMCAPS-SNPP (Figures 1a and 1c) and CLIMCAPS-Aqua (Figures 1b and 1d) when aggregated onto a 1° equal-angle grid. Note similarities in the range of values as well as the absence of any view angle effects (i.e., uncertainty does not increase with view angle). Cloud clearing introduces systematic uncertainty (`etarej` > 0) and amplifies random instrument noise (`ampl_eta` > 1) wherever clouds are present. However, cloud clearing reduces random instrument noise (`ampl_eta` < 1) when clouds are absent and a cluster of measurement FOVs are simply averaged into a single FOR radiance spectrum (Smith and Barnet, 2023b). Figures 1c and 1d show that `ampl_eta` < 1 for much of the globe on any given day.

The differences that do exist between CLIMCAPS-SNPP and CLIMCAPS-Aqua with respect to `ampl_eta` and `etarej` can primarily be attributed to the time difference in observation between the two satellites, as clouds can change significantly over short times. While Aqua and SNPP both have local overpass times of 01:30 am/pm at nadir, the difference in their orbital altitude means their measurements are offset by a few minutes. In addition, there are small spatial shifts in how AIRS and CrIS observe clouds across their field-of-regard FORs since the AIRS and CrIS FOVs are not spatially co-registered. What we mean by this is that the 3 x 3 AIRS FOVs could observe a large radiance gradient compared to CrIS simply because of the sampling differences between the two instruments. Moreover, the CrIS FOVs rotate with respect to each other as a function of view angle, while the AIRS FOVs maintain their alignment with the cross-track scan direction irrespective of view angle. This means that AIRS and CrIS do not necessarily observe the same cloud structure within each FOR. Even if the instruments are exactly the same (such as CrIS on SNPP and JPSS+), one can cannot compare their retrievals directly due to differences in instrument sampling, both spatially and temporally. This is true for all retrieval approaches, whether they employ cloud clearing or not. In CLIMCAPS, we only provide products in the overlap period between satellites (see Table 2) for product evaluation where this aspect is properly accounted for. Overall, the large-scale similarities observed in Figure 1 make sense because cloud clearing does not depend on spectral information content where most of the instrument differences manifest, or

225 any a-priori knowledge of clouds that would amplify sampling differences. Instead, cloud clearing uses *spatial* information content (quantified as measurement variation across a cluster of FOVs) to derive an aggregate cloud-cleared spectrum (Smith and Barnet 2023b). AIRS and CrIS FOVs are ~14 km at nadir, and each instrument has 9 FOVs making up a ~50 km cloud-cleared FOR. Moreover, both instruments have their FOVs arranged in 3 × 3 arrays, so they capture the available spatial information content in similar ways.

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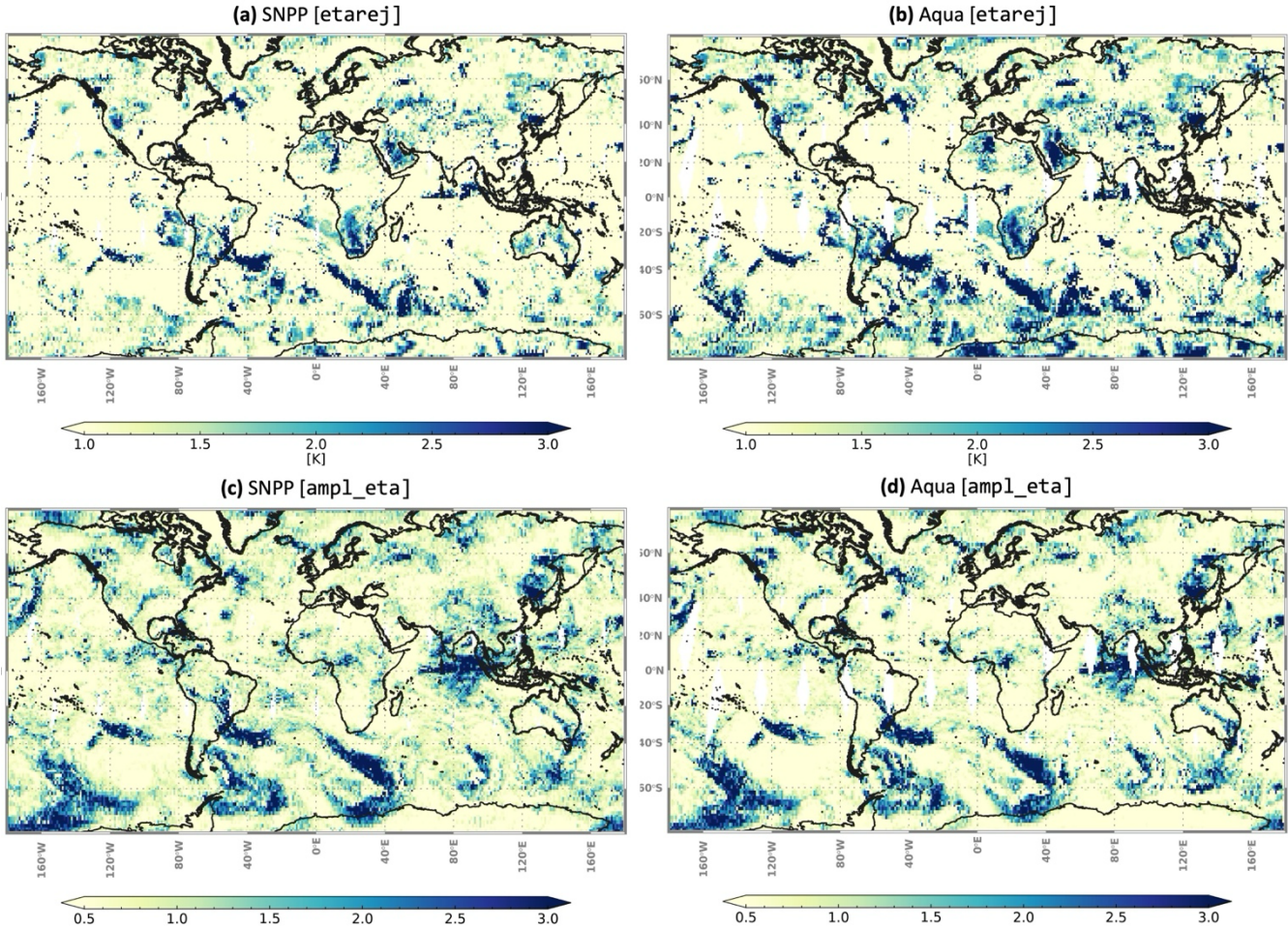
Figure 1: CLIMCAPS V2 cloud clearing error metrics between (a+c) SNPP and (b+d) Aqua Level 2 retrievals on 30 August 2016. These error metrics were binned, then averaged to a uniform 1° equal angle global grid. (Top row) [etarej] represents systematic error due to an incomplete removal of cloud signals from the Level-1B radiances, and (bottom row) [ampl_eta] quantifies the
235 **degree to which random instrument noise is amplified (or reduced) due to cloud clearing.**

For the purpose of this evaluation, there is no need to diagnose differences at finer spatial scales because our objective at this stage is to identify (and address) the large-sale, systematic differences between CLIMCAPS-SNPP and CLIMCAPS-Aqua. Addressing differences at finer scales will be the focus of future work.

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Moving on to the next retrieval step, Figure 2 depicts CLIMCAPS [air_temp] in the lower troposphere for the two instrument configurations. CLIMCAPS employs the Stand-alone AIRS Radiative Transfer Algorithm (SARTA; Strow et al., 2003) to simulate top-of-atmosphere radiances. SARTA was originally developed for AIRS, but later adapted for CrIS. It is possible that SARTA introduces subtle effects into the retrieval product as a result of how it treats differences in instrument spectral correlations. We should note that SARTA is not funded to be maintained consistently for AIRS and CrIS. This means we can expect SARTA to introduce retrieval differences, which we will group under the umbrella of "instrument effects" for the sake of simplicity and clarity of argument in this paper. Another instrument difference that may manifest in the retrievals is the fact that AIRS requires a frequency correction – which is a function of orbital position and season (See Table S1 in the supplement for more details). Figure 2 depicts no significant difference in the spatial pattern of [air_temp] gradients, maxima and minima, between these two CLIMCAPS configurations.
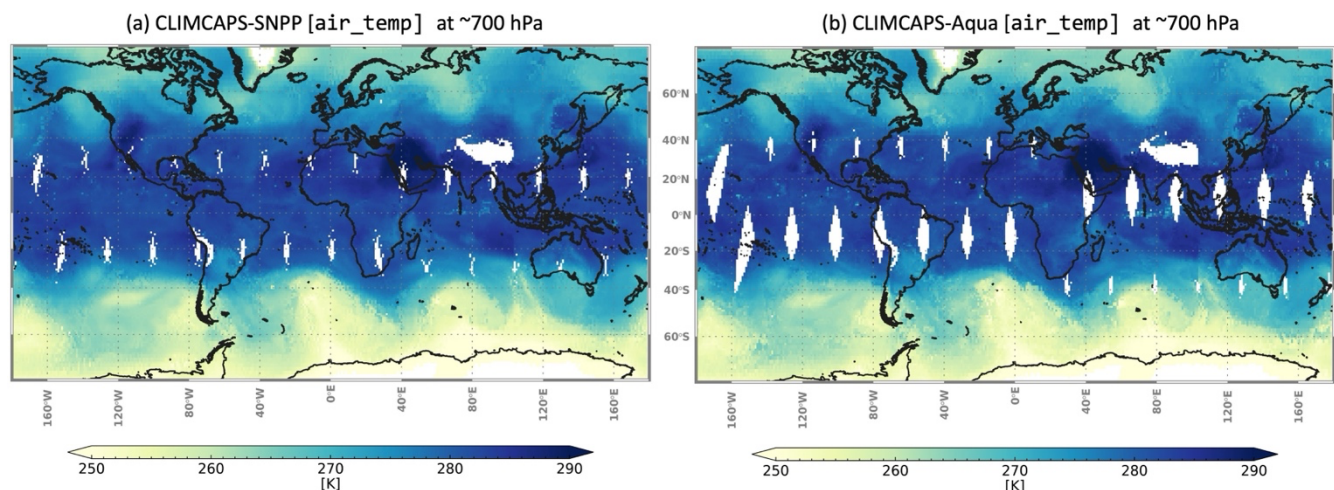
Figure 2: CLIMCAPS V2 [air_temp] retrievals from (a) SNPP and (b) Aqua measurements acquired on 30 August 2016. The CLIMCAPS [air_temp] retrievals are made on 100 pressure levels spanning the vertical atmospheric column from Earth surface to top-of-atmosphere (~0.05 hPa). These figures represent all retrievals that passed quality control [ispare_2=0] and were made at ~700 hPa. For display purposes, the values were binned and averaged to a 1° equal angle global grid.

The results in Figure 2 alone, however, do not satisfy the requirement for consistency nor does it demonstrate that we have mitigated the differences between the Aqua and SNPP systems sufficiently. CLIMCAPS employs dynamic regularization, which means that it populates the true null space within each FOR with the a-priori estimate. A measurement with large null space (or low information content and weak sensitivity to the target parameter) will yield a retrieval that approximates the a-

priori estimate, a feature that generally applies to all OE retrieval systems. CLIMCAPS prepares its a-priori for [air_temp] by selecting the two MERRA-2 reanalysis fields on either side of the measurement in space-time, and linearly interpolate them to the exact location. The CLIMCAPS V2 a-priori for [air_temp] provides a good estimate of prevailing conditions even if

265 no new information is contributed by the measurement. At this scale we, thus, expect the MERRA-2 a-priori to neutralize any differences in observing capability between SNPP and Aqua. For an evaluation of retrieval consistency, we instead turn our attention to diagnosing the CLIMCAPS uncertainty metrics that quantify retrieval SNR where Aqua and SNPP instrument would typically manifest. For this reason, all the results discussed in subsequent sections focus on an evaluation of CLIMCAPS V2 uncertainty, not its retrievals. This is a major departure from standard validation techniques that compare geophysical

270 quantities from multiple, independent sources (e.g., Nalli et al., 2018; Wang et al., 2020). It is important to distinguish these two approaches and recognize their divergent end-goals. This said, the evaluation of uncertainty metrics presented in this paper is made possible largely *because* of the CLIMCAPS algorithm and product design. Prior to 2020, we did not have access to 20+ years of AKs from the same system across different instrument suites. Moreover, the fact that CLIMCAPS employs instrument-independent a-priori estimates, means that retrieval AKs and ADIFF can be interpreted in a straightforward manner.

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Having established the target metrics for our evaluation in this paper, Figure 3 addresses questions regarding view angle and time-of-day, both of which potentially affect signal strength and thus continuity across instruments. We use CLIMCAPS-Aqua on 30 August 2016 as illustration but the same holds for CLIMCAPS-SNPP on the same day (not shown). The DOFS of a retrieval system with respect to a target variable is the sum-total of all corresponding AK peaks (or, the trace of the AK matrix).

280 When mapped out, as in Figures 3a and 3b, DOFS provides an efficient way of summarizing information content patterns. It is immediately obvious that the CLIMCAPS-Aqua DOFS for [air_temp] does not increase with view angle, nor does it change dramatically between the AM and PM orbits. We can attribute this consistency in CLIMCAPS DOFS across all view angles and time-of-day to the efficiency with which CLIMCAPS applies dynamic regularization. In a retrieval system without such ability, one may see DOFS increase with view angle because at high angles the measurements observe a larger portion

285 of the atmosphere and has more spectral channels sensitive to conditions in the mid- to lower troposphere. One can think of this as the channels traversing a thicker atmosphere at higher view angles due to a larger slant path, which causes the AK sensitivities to move higher up in the atmosphere. Channel sensitivity to the boundary layer at nadir may be sensitive to the mid-troposphere at edge-of-scan (50˚ for CrIS, 49.5˚ for AIRS). This means that the channels we select for profile retrievals need to have sensitivities that span the full vertical column at all view angles. At nadir, many of the channels may become

290 sensitive to surface conditions where CLIMCAPS error estimates are also high (due to larger errors in cloud, surface skin temperature and emissivity). For such channels, their information contribution may be minimal at nadir. At higher view angles, however, their SNR improve due to decreasing errors in emissivity and surface skin temperature at higher altitudes (lower atmospheric pressure). There is similar variability in channel SNR with changes in atmospheric conditions (e.g., lapse rate) and seasonal cycles. The dynamic regularization approach we adopted in CLIMCAPS allows access to channel information

295 content whenever and wherever it is available. Stated differently, retrieval systems that employ static regularization (e.g.,

Rodgers, 2000) limit instrument spectral information in many cases because their a-priori assumptions and parameterization may be outdated or fail to reflect localized conditions.

The ADIFF for CLIMCAPS temperature at 700 hPa (Figures 3c and 3d) complements the DFS maps (Figures 3a and 3b) and illustrates that the degree to which CLIMCAPS adjusts the MERRA-2 a-priori with information from the measurements, is consistent across land and ocean, night and day, as well as nadir and edge-of-scan. Figure 3e depicts the vertical information content for seven CLIMCAPS retrieval variables: [air_temp], [h$_2$o_vap], O_3, CO, CH_4, CO_2 and HNO_3. These profiles represent the global average of the AK peaks (i.e., diagonal vector of AK matrix), with the error bars depicting the standard deviation of SNR across all types of conditions on a global day. For each of the variables represented in Figure 3e, the AK statistics are reported separately for the 1:30 am and 1:30 pm orbits to demonstrate how time-of-day does not impose significant differences. Therefore, we focus our evaluation for the remainder of this paper on large ensembles of AKs that include all view angles and orbits to optimize continuity in the CLIMCAPS V3 product for all scenes across multiple satellites.
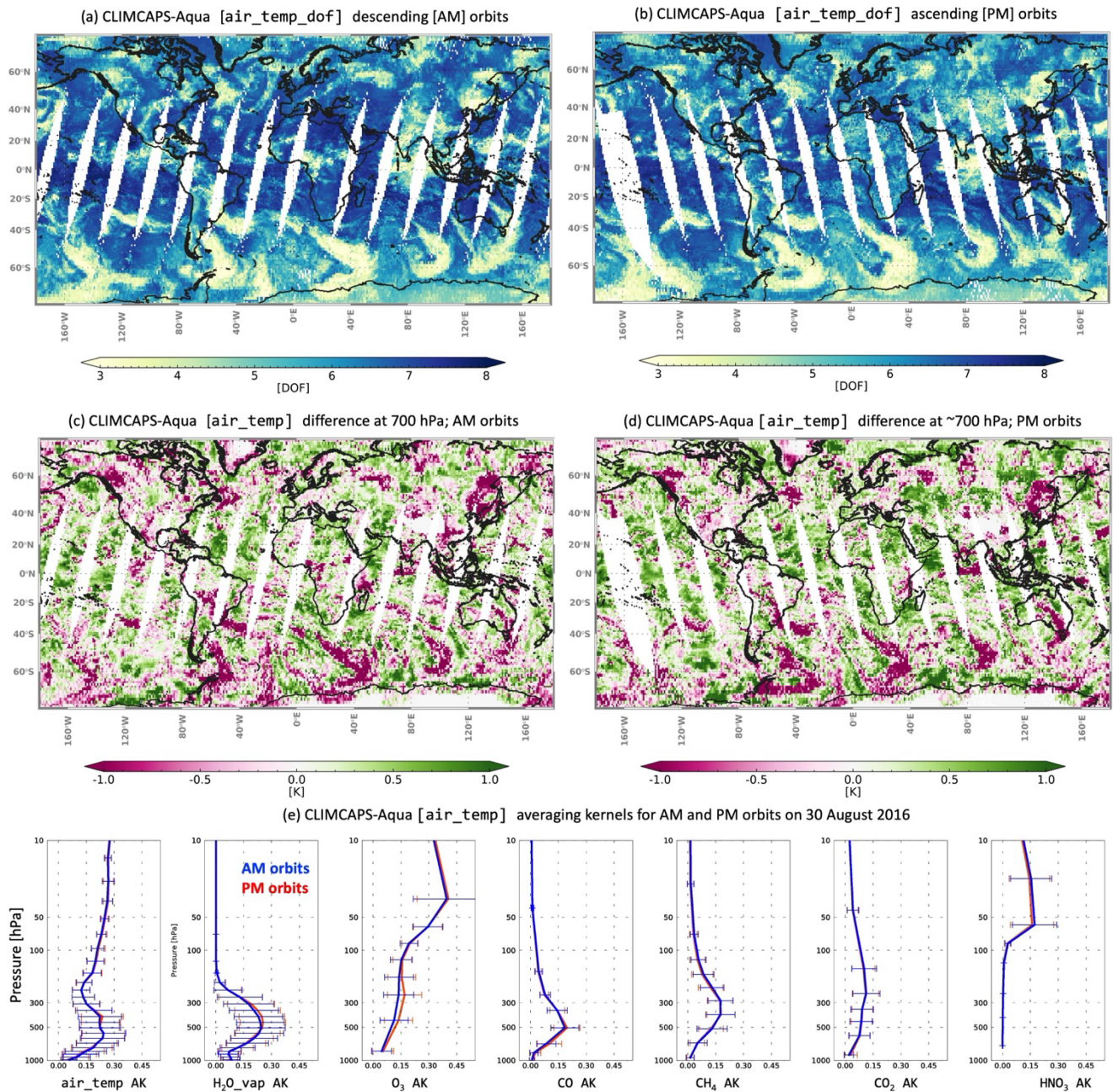
Figure 3: CLIMCAPS information content as a function of (a–d) view angle and (e) time-of day. (a) CLIMCAPS-Aqua degrees of freedom (DOFS) for [air_temp] from all FORs in descending orbits (13h30 LT) on 30 August 2016. (c) CLIMCAPS-Aqua [air_temp] difference between retrieval and a-priori (MERRA-2) at ~700 hPa for all descending orbits. (b+d) Same as (a+c) but for all ascending orbits (01h30 LT). CLIMCAPS DOFs are independent of view angle and time-of-day (e) CLIMCAPS-Aqua [air_temp] AK mean and standard deviation (error bars) from all (red) ascending FORs and (blue) descending FORs. The AKs represent the average (and standard deviation) of the diagonal vectors from the retrieval AK matrices. CLIMCAPS AK structure and variance are independent of time-of-day.

3.2 Experimental design

Table 1 summarizes the algorithm components that we identified as directly affecting retrieval consistency, and specifically that of [air_temp], CO_2 and O_3 where instrument-specific inconsistencies have been reported (Smith and Barnet, 2020). In total, there are six algorithm components (Column 1) reported for the two CLIMCAPS configuration currently implemented for V2 as well as how we propose to change then for a future version V3. The values reported in Columns x1, x2 and x3 represent the experimental configurations we analyse and discuss in Section 4. In summary, the six algorithm components we test in this paper are as follows:

- B_{max} is employed during CLIMCAPS regularization (see Smith and Barnet, 2020 for details). In short, B_{max} is an empirical term that informs the eigenvalue (λ) threshold as follows: $\lambda_c = {}^1/_{B_{max}^2}$. During regularization, CLIMCAPS applies SVD to the measurement SNR matrix, $\widetilde{K}^T S_m^{-1} \widetilde{K}$. All functions with $\lambda \geq \lambda_c$ are used in the retrieval without any regularization. Those functions with $0.05 < \lambda < \lambda_c$ are damped and all with $\lambda < 0.05$ are excluded from the retrieval. A larger B_{max} imposes a lower threshold value (λ_c), which means a greater number of eigen functions pass into the retrieval without any regularization. B_{max} should not be too large because all measurements have noise to filter out, nor should B_{max} be too small because all successful measurements have some information to contribute. Note that when we talk about B_{max} in this paper we mean the B_{max} value employed specifically for [air_temp] retrievals. CLIMCAPS associates a different B_{max} for each retrieval parameter. Our focus in this paper is on [air_temp], so we will therefore not qualify each mention of B_{max} in this paper.

- [RTAerr] quantifies the radiative transfer algorithm (RTA) bias that propagates into CLIMCAPS retrievals, whenever a radiative transfer calculation is made. [RTAerr] applies to each channel individually and varies according to the accuracy of transmittance and radiance calculation within the RTA. The [RTAerr] associated with a specific RTA will typically decrease as the RTA matures. Historically, the [RTAerr] is calculated offline using a large ensemble of data for specific instrument configurations. CLIMCAPS-SNPP uses the NOAA [RTAerr] calculated for CrIS, whereas CLIMCAPS-Aqua uses the NASA [RTAerr] calculated for AIRS. CLIMCAPS-Aqua and CLIMCAPS-SNPP uses different versions of SARTA (due to funding limitations that inhibits synchronized SARTA upgrades across all instrument configurations), so we do not expect the [RTAerr] to be universal for all CLIMCAPS configurations. We list the [RTAerr], averaged across all spectral channels, for CLIMCAPS-SNPP and CLIMCAPS-Aqua in Table 1 below. Note how the V2 [RTAerr] is on average an order of magnitude larger for CLIMCAPS-SNPP (~0.5 K) than CLIMCAPS-Aqua (~0.05 K). We investigate this disparity in Section 4 and demonstrate how a lower [RTAerr] for CLIMCAPS-SNPP improves retrieval quality.

- [apodcor] defines the degree to which adjacent channels are correlated due to apodization of the CrIS interferograms (or, radiance measurements). AIRS is a grating spectrometer (Table A.1) and its measurements, therefore, are naturally apodized. CLIMCAPS applies Hamming apodization to CrIS measurements to impose

localized spectral response function and thus remove a significant portion of the geophysical noise otherwise present in the CrIS interferograms (Barnet et al., 2000, 2023)

350   -   The last three rows summarize the number of channels within each spectral subset that CLIMCAPS uses in the retrieval of [air_temp], CO_2 and O_3 respectively. As with [RTAerr], CLIMCAPS V2 development benefited from existing efforts at NOAA and NASA to inform these channel selections. We critically evaluate these V2 channel sets here and make recommendations for future upgrades.

355 **Table 1: Summary of the CLIMCAPS algorithm configurations discussed in this paper. Each configuration is unique with respect to the six algorithm parameters depicted in Column 1. The "V2" configurations represent the CLIMCAPS V2 record available via NASA GES DISC (Table 2). The x1 , x2 and x3 configurations depict the experiments we performed and V3 is the configuration we propose for the next CLIMCAPS release for AIRS+AMSU and CrIS+ATMS. Since CrIS+ATMS are identical on the SNPP and JPSS platforms, the SNPP-V3 configuration depicted here, also applies to JPSS-V3. The number of [air_temp] channels reported**
360 **here represent those selected from the long-wave (LW) IR band only. As shown in Table S2, CLIMCAPS uses channels from all three bands for [air_temp] retrievals.**

	CLIMCAPS-SNPP					CLIMCAPS-Aqua			
	V2	x1	x2	x3	V3	V2	x1	x2	V3
[air_temp] SNR threshold [B_{max}][*]	0.2	0.8	0.175	0.175	0.175	0.25	0.8	0.15	0.15
SARTA error spectrum [RTAerr][Δ]	~0.5 K	~0.5 K	0	0	0	~0.05 K	~0.05 K	~0.05 K	~0.05 K
Correlation factor for each set of 3 adjacent apodized channels [apodcor]	1.0, 0.625, 0.133	1.0, 0.625, 0.133	1.0, 0.0, 0.0	1.0, 0.625, 0.133	1.0, 0.625, 0.133	N/A	N/A	N/A	N/A
[air_temp] channels in LW band	105	105	225	105	105	134	134	134	134
Total [CO_2] channels[ξ]	54	54	54	54	96	61	61	61	96
Total [O_3] channels[ξ]	77	77	77	77	77	40	40	40	73
[*] (Smith and Barnet, 2020). [Δ]See Fig 4c and Table S1 for more details. [ξ]See Figure 5.									

Figures 4 and 5 provide graphic depictions of the algorithm elements summarized in Table 1. Figure 4a contrasts the V2
365 channel subsets for [air_temp] in CLIMCAPS-SNPP (red) and CLIMCAPS-Aqua (mustard). This is not the full channel set but rather just those channels from the 660–760 cm^{-1} spectral range with sensitivity to temperature at pressure levels from Earth surface to top-of-atmosphere. It is immediately obvious that there are significant differences in the channels sets for or air_temp between SNPP and Aqua. For the CLIMCAPS V2 implementation in 2019, we combined best practices at NOAA and NASA. The goal with all present and future upgrades to CLIMCAPS is to evolve the system to a place where the retrievals
370 represent the observing capability common to all instruments making up the full record. The blue lines in Figure 4a represents

the `x2` configuration we test for CLIMCAPS-SNPP. For a full list of the CLIMCAPS V2 channel sets currently used for all retrieval parameters, see Table S2.

In addition to channel set differences that affect CLIMCAPS SNR, there is also the SARTA forward model error, [`RTAerr`],
375   typically calculated by the respective retrieval teams. Similar to the channel sets, [`RTAerr`] evolved separately for SNPP and Aqua at NOAA and NASA, respectively. Figure 4c illustrates the NOAA [`RTAerr`] for SNPP that we implemented in CLIMCAPS V2. Also, in Figure 4c is the [`RTAerr`] for Aqua, but this spectrum is invisible due to it being orders of magnitude smaller the SNPP [`RTAerr`], and thus off scale in Figure 4c (see Table 1, Row 2). This tells us that [`RTAerr`] is a potential source of discontinuity in CLIMCAPS V2 record and needs to be updated and normalized across both system configurations
380   for the sake of retrieval consistency across instrument suites. Of importance here is the large disparity in [`RTAerr`] across the Aqua and SNPP configurations, not a detailed depiction of each [`RTAerr`] individually.
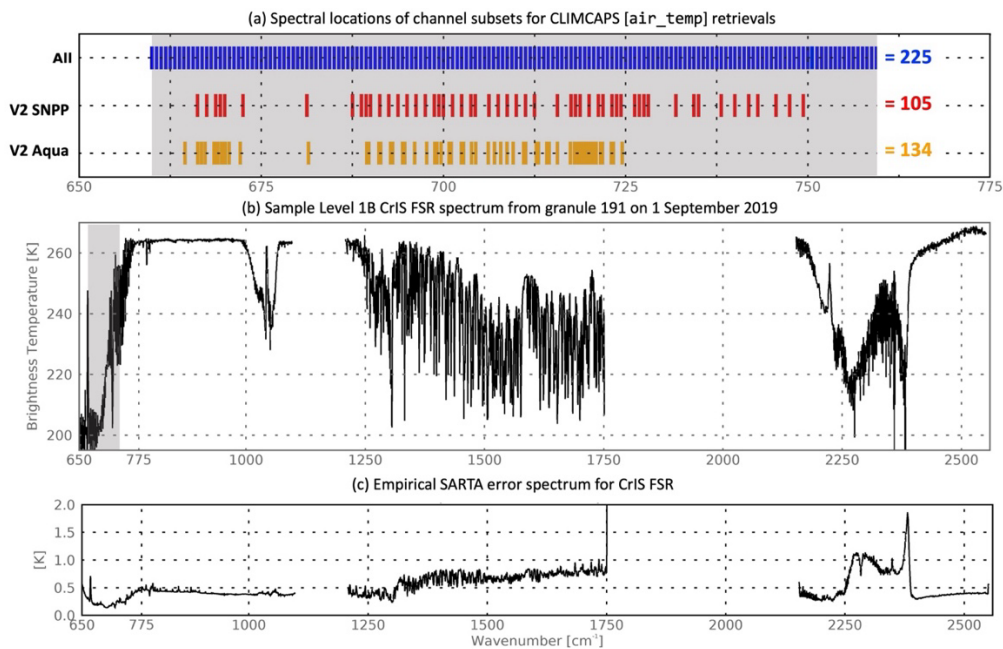
Figure 4: (a) CLIMCAPS V2 spectral channel subsets used in [`air_temp`] retrievals for Aqua (orange) and SNPP (red) in the (grey
385   **area) 1.4 μm CO$_2$ absorption band. An experimental subset of channels used in the CLIMCAPS-SNPP x3 configuration (see   1) is in (blue). (b) Sample of CrIS full spectral resolution (FSR) measurement given by Level 1B product granule 191 on 1 September 2019 to contextualise the location of the 1.4 μm region in the CrIS long-wave band (~650–1100 cm^{-1}). (c) CLIMCAPS V2 empirically derived error spectrum of SARTA forward model bias for CrIS FSR spectra.**

390   Given known differences in CLIMCAPS V2 AKs for SNPP and Aqua (Smith and Barnet, 2020), we additionally diagnose channel subsets for CO_2 and O_3 in this paper. Figure 5 illustrates differences in the SNPP and Aqua V2 channel sets for O_3 and CO_2 (orange), and how we propose to standardize then for a future V3 implementation (blue).
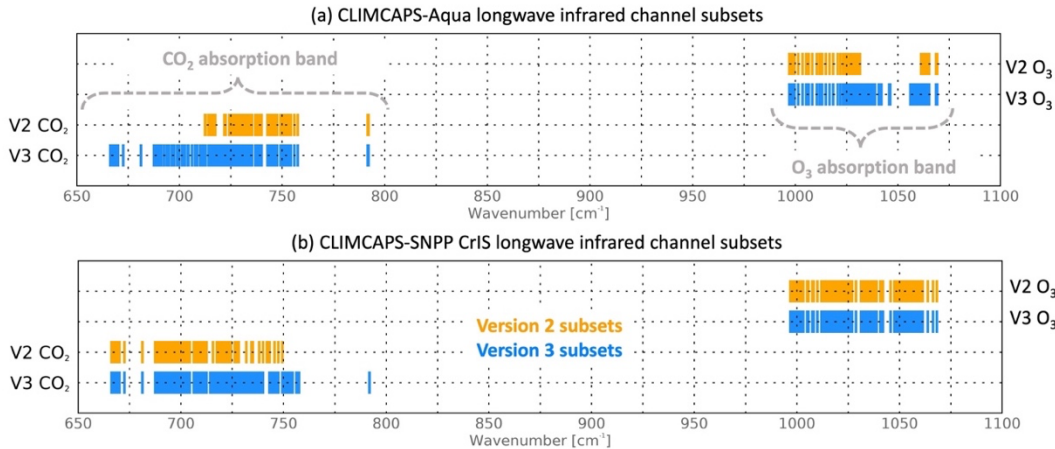
Figure 5: Illustration of the channel subsets used for CO_2 and O_3 retrievals in the (orange) V2 and (blue) proposed V3 configurations for (a) CLIMCAPS-Aqua and (b) CLIMCAPS-SNPP (see Table 1).

In summary, we introduced and explained our experimental design because the evaluation of retrieval consistency across different instrument suites is not straightforward. There is no universal retrieval approach that satisfies the SNR requirements

400   of all applications, nor do we know exactly how instrument differences manifest under all conditions. The fact is that hyperspectral IR instruments measure a large array of atmospheric parameters that together characterize thermodynamic structure (i.e., temperature and water vapor profiles) and chemical composition (e.g., pollutant gas concentrations). But instead of a series of distinct spectral signatures, the result is a convolved IR measurement with complex inter-dependencies of both geophysical signal *and* noise. CLIMCAPS mitigates these complexities to a large degree with its sequential retrieval approach

405   and subsets of channels that maximize the SNR for each target parameter. But even then, the result is not clear-cut because instrument differences can cause spectral effects that are difficult to disassociate from the convolved geophysical signals. This means that one-to-one comparisons with independent datasets can be difficult to interpret. For a transparent evaluation of CLIMCAPS V2 retrieval consistency, we therefore focus on the analysis of CLIMCAPS uncertainty metrics instead. Table 1 summarizes all the algorithm components we tested, the results of which we present and discuss in Section 4 below.

410   **4 Results and Discussion**

In this section, we present results for each experimental configuration (Table 1) using available uncertainty metrics: AKs, DOFS and ADIFF. CLIMCAPS AKs typically have a large dynamic range across a day of retrievals because measurement

SNR varies from scene-to-scene with prevailing conditions and CLIMCAPS regularization minimizes a-priori dependence according to the information content of measurements.

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Figure 6 depicts [air_temp] AKs for the existing V2 record as well as each of the experimental configurations listed in Table 1. The profiles in Figure 6 represent the average of all [air_temp] AKs on 1 September 2019 (321,300 in total), and the error bars the AK standard deviation. It is immediately obvious in Figure 6a that there are systematic SNR differences between CLIMCAPS-SNPP (red) and CLIMCAPS-Aqua V2 (blue). Not only do the SNPP [air_temp] AKs lack vertical
420 structure, they are also much lower in value as well as dynamic range compared to the Aqua [air_temp] AKs. The cause of this disparity is not immediately obvious and could be due to fundamental instrument differences in spectral resolution, over-damping of the measurement within retrieval system, or a combination of both.

We can diagnose the causal factors influencing V2 [air_temp] AK disparities by changing the retrieval configurations as
425 listed in Table 1. Figure 6b contrasts the SNPP V2 [air_temp] AK against three experimental configurations, x1, x2 and x3. When the SNPP B_{max} threshold is increased from 0.2 to 0.8 (i.e., V2 vs. x1) we see a dramatic jump in AK values across all pressure levels as well as a larger dynamic range in the mid-troposphere. As discussed in Section 3, B_{max} is derived empirically and informs the eigenvalue threshold (λ_c) that determines the number of eigen functions CLIMCAPS will damp (or leave undamped) in the retrieval step. B_{max} is considered too large (and its corresponding λ_c too small) when the AKs
430 exhibit spurious effects and retrieval accuracy is low. This happens when CLIMCAPS uses too many eigen functions without any damping. An SVD of the measurement sensitivity matrix, $\widetilde{\mathbf{K}}^T \mathbf{S}_m^{-1} \widetilde{\mathbf{K}}$, results in eigen functions arranged in order of signal strength such that higher order eigen functions are associated with signal and lower order functions are dominated by noise. When lower order eigen functions are not sufficiently damped, then their noise propagates into the retrievals as error. Similarly, a B_{max} value is considered too small (and λ_c too large) when too many higher order eigen functions are damped and not enough
435 measurement information passes on to the retrieval. In such a case, the AKs will be small with a low dynamic range and retrievals will mostly represent the a-priori.
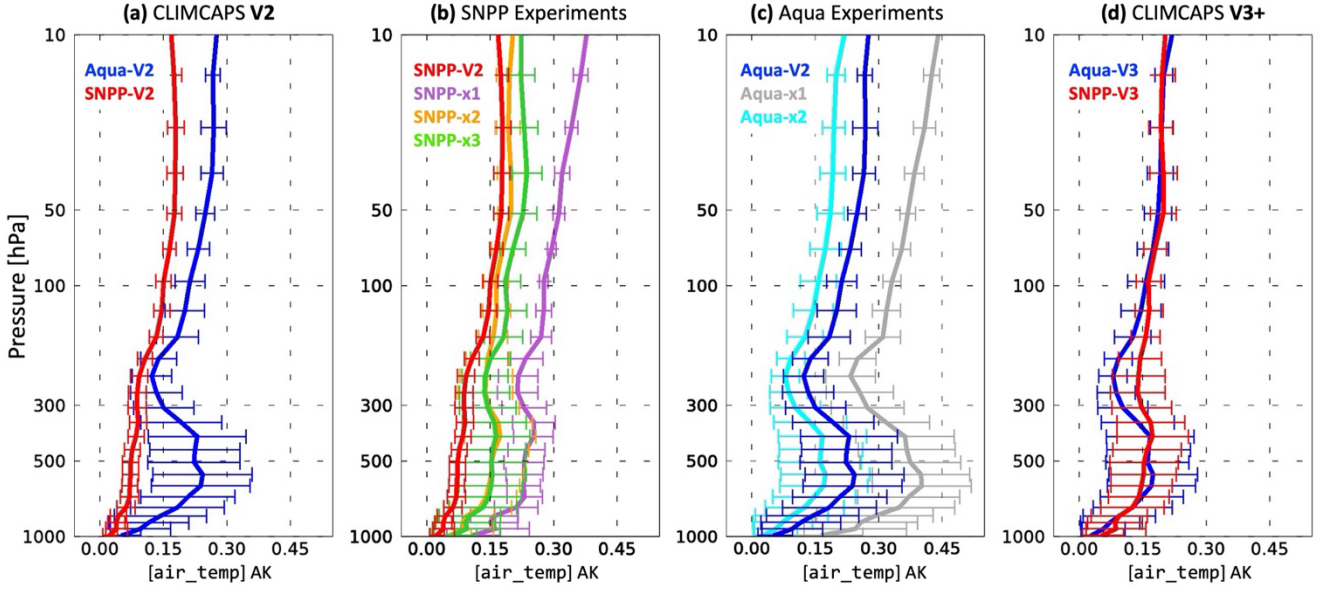
Figure 6: Comparison of AKs to illustrate disparities in [`air_temp`] information content structure and variance for (a) CLIMCAPS V2 (blue) Aqua and (red) SNPP, (b) three CLIMCAPS-SNPP experimental configurations (purple+orange+green) contrasted against the (red) V2 SNPP configuration, (c) two CLIMCAPS-Aqua experimental configurations (cyan+grey) against the (blue) V2 Aqua configuration, and (d) the proposed CLIMCAPS V3 configurations (blue) Aqua and (red) SNPP to improve Level 2 data continuity. (b+c) The experimental configurations referenced here are detailed in Table 1.

What is evident in Figure 6b is that B_{max} alone does not explain the low AK values for CLIMCAPS-SNPP V2 (red). Both the `x2` and `x3` configurations for CLIMCAPS-SNPP (green and orange) have slightly lower B_{max} values (0.175), yet higher AKs with larger variance. This is the oppositive of what we expect for smaller B_{max} values. Using the SNPP-V2 configuration (B_{max} = 0.2) and setting [`RTAerr`] = 0.0 K, we see a significant change in the AK structure, magnitude and variance (not shown). This tells us that the [`RTAerr`] we adopted for CLIMCAPS-SNPP is much too large (Figure 4c). In fact, it is an order of magnitude larger, on average, than the [`RTAerr`] for CLIMCAPS-Aqua (~0.05 K). We, therefore, propose that the [`RTAerr`] should be carefully recomputed for all CLIMCAPS V3 CrIS+ATMS configurations. For the sake of this paper, however, we list [`RTAerr`] = 0 as a placeholder value for future upgrades, since the effort required to achieve an accurate estimate of [`RTAerr`] is out of scope for this paper.

Another question that often arises with regard to CLIMCAPS-SNPP/JPSS+ is the issue of apodization. We will not explain apodization in this paper, nor the reasons for apodizing CrIS radiances ahead of retrievals. Others cover this great detail (Barnet et al., 2000, 2023). What we do wish to illustrate here is how spectral correlation due to apodization has no significant impact on CLIMCAPS AKs and, therefore, retrieval SNR. The SNPP-`x2` and SNPP-`x3` configurations differ only in the number of long-wave (LW) IR channels used in [`air_temp`] retrievals. SNPP-`x2` uses all available CrIS channels in the 660–760 cm^{-1}

460 range (225 channels in total) while SNPP-x3 uses the V2 105 channel subset (Figure 4a). In addition, SNPP-x2 sets [apodcor] = 0 for all adjacent channels to indicate the absence of spectral correlation due to apodization. A comparison of the AKs (Figure 6b) and [air_temp] root-mean-square-error (RMSE, Figure 7a) show no significant difference in retrieval results between SNPP-x2 and SNPP-x3. We, therefore, do not recommend any changes to the apodization of CrIS radiances, nor the V2 [air_temp] channel subsets for future CLIMCAPS upgrades. The SNPP-x1 and Aqua-x1 configurations yielded

465 very high AK values, but because their B_{max} values forced CLIMCAPS to use a large number of eigen functions undamped, their retrieval quality deteriorated relative to the operational V2 product (not shown).

We can next turn our attention to evaluating ADIFF (Figure 7). As discussed, ADIFF quantifies the difference between retrieval and a-priori. When we look at a global map of ADIFF at a specific pressure level, we can gain insight into the retrieval system.

470 For example, an ADIFF with a consistent speckle pattern across large areas would indicate random retrieval SNR, or an ADIFF with strong latitudinal pattern would indicate systematic bias in retrieval SNR. What we want to see in a global map of ADIFF, instead, is consistency across latitudes with a spatial pattern corresponding to known geophysical features, like clouds.

Figures 7a and 7b depict V2 [air_temp] ADIFF at 700 hPa for the SNPP and Aqua configurations, while Figures 7c and 7d

475 show what ADIFF would look like for a V3 system. It is immediately obvious the CLIMCAPS retrieval SNR is neither truly random nor alarmingly biased. This said, the V2 [air_temp] ADIFF has large differences between the two instrument systems, both in magnitude and dynamic range. This indicates that there are systematic differences in the way CLIMCAPS V2 is configured for CLIMCAPS-SNPP and CLIMCAPS-Aqua, but that these are largely resolved in the proposed V3 [air_temp] configuration. A stronger correlation between CLIMCAPS-SNPP and CLIMCAPS-Aqua in V3 [air_temp]

480 ADIFF tells us that the upgrades we suggest here, will improve continuity in the CLIMCAPS record across CrIS+ATMS and AIRS+AMSU. Even so, we do not expect to fully resolve retrieval continuity across all parameters from CrIS+ATMS and AIRS+AMSU, given the list of known differences in instrumentation (Table S1). Some of the other changes we suggest for a CLIMCAPS V3 upgrade (see Table 1) pertain to the channel subsets for O_3 and CO_2 retrievals, which we illustrate in Figure 8.

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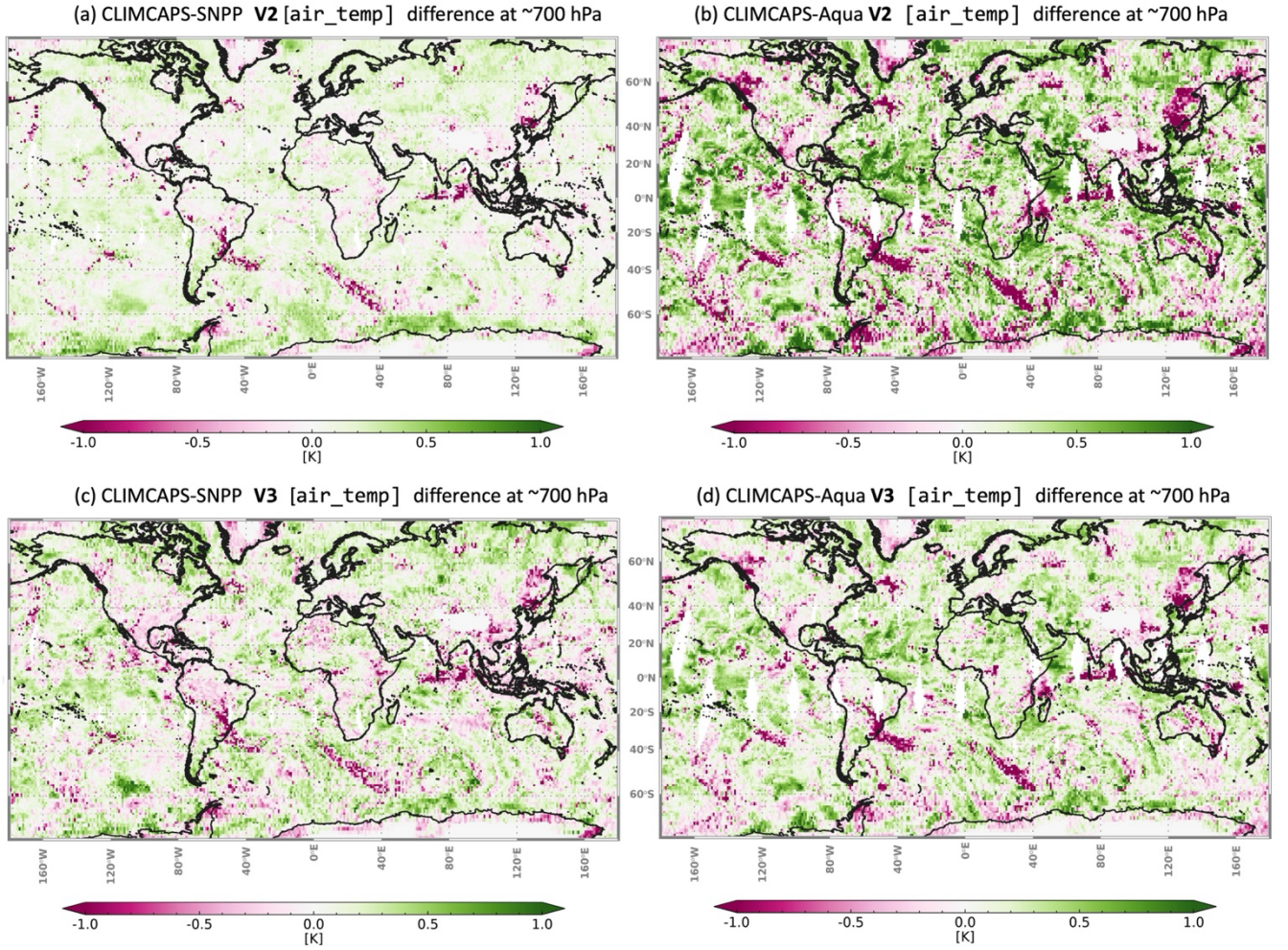
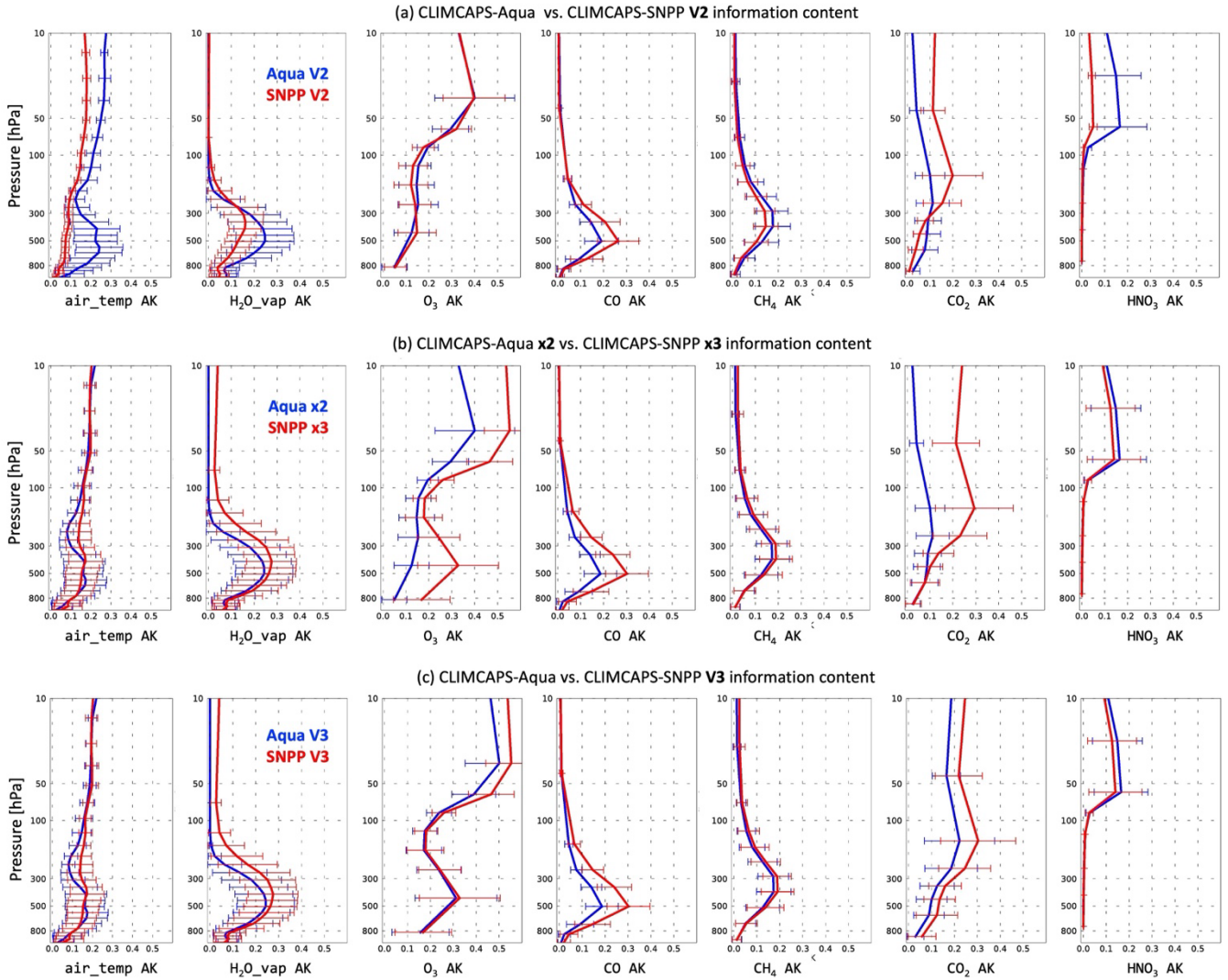


Figure 7: CLIMCAPS [`air_temp`] difference between retrieval and a-priori (MERRA-2) at ~700 hPa on 30 August 2016 for all ascending (13h30 LT) and descending (01h30 LT) orbits aggregated to a uniform 1° equal-angle global grid. Comparison of [`air_temp`] differences, ADIFF, between (a+b) CLIMCAPS V2 and the proposed (c+d) CLIMCAPS V3 configurations for (a+c) SNPP and (b+d) Aqua.

Figure 8 depicts the global average (and standard deviation) of CLIMCAPS AKs for seven retrieval parameters – [`air_temp`], [`h2o_vap`], O_3, CO, CH_4, CO_2 and HNO_3 – for the different configurations evaluated in this paper (Table 1). Figure 8a represents the V2 retrieval capability we discussed in previous work (Smith and Barnet, 2020). Apart from [`air_temp`] and [`h2o_vap`], we also notice disparities in CLIMCAPS V2 AKs for CO_2 and HNO_3. The disparities that exist for the CO AKs across CLIMCAPS-Aqua and CLIMCAPS-SNPP, on the other hand, are predominantly due to known IR instrument differences; the AIRS shortwave (SW) IR band does not cover the full spectral absorption region for CO, while CrIS captures all spectral channels sensitive to CO (Table 1, Smith and Barnet, 2019). There is, thus, a physical limit to the signal that exists for CO in the AIRS sounder. We argue that it is important to capture as much of the CO signal as possible, given the present-day need for information about air quality and fire emissions. We, therefore, propose to make no algorithm

500   changes to CLIMCAPS-SNPP/JPSS+ that would reduce the CO AK for the sake of mimicking CLIMCAPS-Aqua CO capability. This is the only retrieval parameter for which we make this exception. All other retrieval parameters are supported by comparable instrument observing capabilities.

505   **Figure 8: CLIMCAPS AKs for [`air_temp`] as well as six atmospheric gases, [`h2o_vap`], O_3, CO, CH_4, CO_2 and HNO_3, as the mean and standard deviation (error bars) for all retrievals in ascending and descending orbits that passed quality control on 1 September 2016. A comparison of CLIMCAPS AKs from (blue) Aqua and (red) SNPP using three different configurations, (a) V2, (b) experimental SNPP-x3 and Aqua-x2, as well as the proposed (c) V3 for both instrument suites.**

5 Conclusions

With this paper we demonstrated how decadal continuity can be achieved in a Level 2 product using the same retrieval system and measurements from two sounding satellites with different technologies, AIRS and CrIS. Achieving retrieval consistency across instruments is not a trivial task and requires knowledge of instrument design as well as calibration. Like all atmospheric sounding observations, CLIMCAPS retrievals are not direct measurements but, instead, indirect observations derived from inverting the top-of-atmosphere IR and MW spectra. Many signal inversion techniques exist depending on the type of measurement and target application. For CLIMCAPS, we employed the method originally developed by Susskind et al. (2003) for the AIRS instrument. We emphasized how the approach to dynamically regularize each retrieval based on scene-dependent measurement information content, benefits CLIMCAPS retrievals and contrasts with the static, generalized regularization promoted in Rodgers (2000). CLIMCAPS uses a space-time collocated reanalysis model, MERRA-2 (Gelaro et al., 2017), as a-priori estimate for [air_temp], [h2o_vap] and O_3. Not only does this provide a-priori estimates that are largely independent of the measurements, it also allows the calculation of representative a-priori error covariance matrices for use in the Bayesian retrieval steps. In contrast, (Goldberg et al., 2003) and AIRS V7 a neural network retrieval . Statistical a-priori estimates that are derived from the full set of spectral measurements (e.g., Goldberg et al., 2003; Milstein and Blackwell, 2016), confound the analysis of AKs since instrument information is contained in the a-priori estimate as well as the final retrieval. One could argue that reanalysis models, like MERRA-2, already assimilate spectral information from AIRS, CrIS, AMSU and ATMS to derive their model fields. But, as argued in Smith and Barnet (2019), not only do reanalysis models, like MERRA-2, assimilate only a small subsets of spectral channels, they also apply rigorous spatial thinning to avoid any interference from clouds, aerosols or smoke. In addition, a MERRA-2 assimilates spectral information from a large array of sources so the contribution from any individual instrument at a specific space-time location is always low, if not absent. The CLIMCAPS design, with its instrument-independent a-priori and representative error covariance matrices, enables the systematic propagation of error through all retrieval steps to yield accurate retrievals with high yield of successful results across the globe (Smith and Barnet, 2019).

The Level-2 CLIMCAPS V2 product contains the AK matrices for each retrieved parameter, at each instrument FOR, which enables the SNR analysis. The validation of retrieved quantities alone does not advance knowledge of a retrieval system. Instead, the analysis of SNR we presented in this paper offers a more honest, in-depth assessment of the contribution IR measurements make to the retrieved solution. This, in turn, helps promote retrieval consistency since the results can be used to optimize CLIMCAPS to have consistency in measurement contribution (as characterized by the shape, magnitude and variance of the AKs) across a wide range of environmental conditions and despite instrument differences.

We proposed a series of changes that can be implemented in CLIMCAPS V3, should future funding allow, to improve its multi-decadal sounding record. This is especially important for a system, such as CLIMCAPS, that observes the Planetary

Boundary Layer (PBL). The PBL affects human health and well-being first and foremost, so it is one of the primary considerations in CLIMCAPS. Over and above the issues we consider in this paper for V3 upgrades, the CLIMCAPS system allows ample opportunity for targeted upgrades to its PBL observing capability in future. Our paper is additionally relevant to other sounding systems and instruments, such as the NOAA-Unique Combined Atmospheric Processing System (NUCAPS; Barnet et al., 2021). If NOAA optimizes NUCAPS for consistency across all hyperspectral instruments, then their soundings can depict real-time diurnal changes to help inform severe weather forecasts. Moreover, the modern-era approach is to de-aggregate large multi-sensor satellites into smaller IR-only and MW-only satellites, and to merge measurements from low-Earth orbiting and geostationary satellites alike. This means that there is a greater need for the ability to algorithmically handle and evaluate these new dynamic types of "representation" error in retrievals. Also, it is expected that future instruments will have new kinds of instrument errors due to the higher demands on spatial and spectral resolution. The ability to robustly and efficiently account for instrument errors along with the ability to diagnose their impact on the retrieval products is the future of sounding science. The CLIMCAPS system and analysis approach we presented here discusses the type of upgrades that is relevant to sounding science itself and we argue that improvements in one product can translate into the other products in the multi-dimensional sounding space

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670 **Competing interests**

The contact author has declared that none of the authors has any competing interests.

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Author contribution

CB and NS, together, conceptualized this work and designed the experiments. CB is the architect and developer of the CLIMCAPS software. NS performed the formal analysis and generated all graphics. NS wrote the original draft and CB

695 reviewed the original and revised manuscripts with NS editing the final version.

Data Access

Table 2 summarizes the CLIMCAPS V2 product suite that is maintained, archived and distributed by the NASA Goddard Earth Sciences Data and Information Services Centre (GES DISC). CLIMCAPS retrieves atmospheric soundings from

700 AIRS+AMSU on Aqua as well as CrIS+ATMS on SNPP and the JPSS series to form a continuous, long-term record of atmospheric state variables (Table 2, column 3). In addition, CLIMCAPS generates two experimental products that span the full lifetimes of the two early satellites, namely (i) Aqua by predominantly using AIRS channels to overcome the loss of key AMSU channels in 2016 (Table 2, row 3), as well as (ii) SNPP by using CrIS normal (or low) spectral resolution (NSR) radiances (Table 2, row 4). Between 20 January 2012 and to 2 November 2015, the SNPP CrIS measurements were exclusively

705 available in NSR mode, whereafter, a second, "full spectral resolution" (FSR) CrIS Level 1B product was added to better match the spectral information content of AIRS. The CLIMCAPS V2 record includes these two experimental datasets to support sounding science and instrument investigations but will not be released or maintained in future CLIMCAPS versions.

710 **Table 2: Summary of the full CLIMCAPS V2 record that is publicly available via the NASA data and information service centre at the Goddard Spaceflight Centre (or GES DISC). The shaded areas denote experimental products for sounder science and instrument design.**

CLIMCAPS	GES DISC record length	CLIMCAPS L2 continuity product	CLIMCAPS L2 datasets [1]GES DISC shortname (DOI)	Input [2]L1B datasets GES DISC shortname (DOI)
Aqua AIRS+AMSU	2002/08/31– 2016/09/25	**2002/09/01— 2016/08/31**	SNDRAQIML2CCPRET (10.5067/JZMYK5SMYM86)	AIRS: AIRIBRAD (10.5067/YZEXEVN4JGGJ AMSU: AIRABRAD (10.5067/LFUQ1L3IYVQD)

Aqua AIRS-only	2002/08/31– present	N/A	SNDRAQIL2CCPRET (10.5067/ILFPVBTDHTDL)	AIRS: AIRIBRAD (10.5067/YZEXEVN4JGGJ)
[3]**SNPP** CrIS+ATMS NSR	2012/01/20– 2021/05/21	N/A	SNDRSNIML2CCPRETN (10.5067/9HR0XHCH3IGS)	CrIS NSR: SNPPCrISL1BNSR (10.5067/N9J1D8VZVJUX) ATMS: SNPPATMSL1B (10.5067/HFDD6A30MA10)
[4]**SNPP** CrIS+ATMS FSR	2015/11/02– 2021/05/21	**2016/09/01— 2018/01/3**	SNDRSNIML2CCPRET (10.5067/62SPJFQW5Q9B)	CrIS FSR: SNPPCrISL1B (10.5067/9NPOTPIPLMAW) ATMS: SNPPATMSL1B (10.5067/HFDD6A30MA10)
[5]**JPSS-1** CrIS+ATMS	2018/02/17– present	**2018/02/01— present**	SNDRJ1IML2CCPRET (10.5067/LESQUBLWS18H)	CrIS: SNDRJ1CrISL1B (10.5067/EETSCFBDBLX6) ATMS: SNDRJ1ATMSL1B (10.5067/VP66V3OTXOPY)

[1] NASA Goddard Earth Sciences Data and Information Services Center, https://disc.gsfc.nasa.gov/

[2]Level 1B calibrated, geolocated radiance measurements

[3] Suomi National Polar orbiting Partnership (SNPP) Normal Spectral Resolution CrIS mode

[4] SNPP Full Spectral Resolution (FSR) CrIS mode introduced to allow science-quality CO retrievals (Gambacorta et al., 2014)

[5]The first of four Joint Polar Satellite System (JPSS) payloads in space. In operational mode, JPSS-1 is known as NOAA-20