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Planetary Boundary layer (PBL) Final Report

A. B. Milstein

17 March 2022

Lincoln Laboratory
MASSACHUSETTS INSTITUTE OF TECHNOLOGY
LEXINGTON, MASSACHUSETTS

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FINAL REPORT
Planetary Boundary Layer (PBL)

17 March 2022

SUBMITTED BY:

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Contents

1. INTRODUCTION

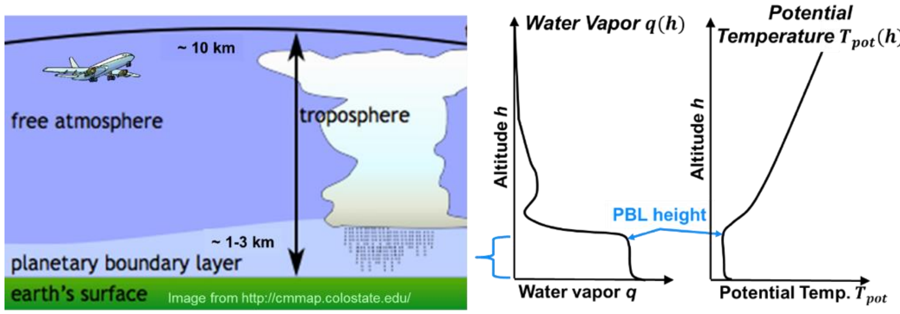

Figure 1: Planetary boundary layer (PBL) illustration, and illustrated water vapor and potential temperature profiles showing sharp gradient at the top of the PBL

Improved understanding of thermodynamics within the Planetary Boundary Layer (PBL), including its structure and PBL height (PBLH) over land and water as a function of time of day, is of great importance to NASA, as recommended by the National Academy of Sciences in the 2017 Decadal Survey for Earth Science and Applications from Space ("ESAS 2017") [1, 2] and subsequently by the NASA PBL Incubation Study Team Report (STR; [3]). During the ESAS 2017 process, improved PBL monitoring from space was identified as a high priority across multiple interdisciplinary panels and science and application questions, leading to the current NASA PBL Decadal Survey Incubation (DSI) program that will invest in future spaceborne PBL mission development.

In recent decades, spaceborne microwave and hyperspectral infrared (HIR) sounding instruments on Aqua, Suomi NPP, and JPSS have significantly improved weather forecasting [4, 5]. However, existing retrievals of lower troposphere temperature T and water vapor q profiles from HIR and microwave sounders have limitations in vertical resolution, and often cannot accurately represent key features such as the mixed layer thermodynamic structure and the inversion at the PBL top, the latter of which appears as a sharp gradient in q or potential temperature T_{pot} as illustrated in Figure 1. With the mixed layer itself being ~1-3 km thick, previously reported AIRS T and q profile resolution (and resultant PBLH) errors on the order of ~1-2 km [6] are not sufficient, and, alone, fall well short of the ESAS recommendation of ~100-300 m vertical resolution for new PBL observing systems. **Because of the existing limitations in PBL remote sensing from space, there is an urgent need to improve routine, global observations of the PBL and enable advances in scientific understanding and weather and climate prediction.** In addition, existing program of record (POR) satellite measurements such as those from HIR have not been the focus of targeted PBL retrieval assessment or development to date, which is particularly critical as NASA considers what next-generation sensors or observing systems will needed to address PBL needs. With the HIR sensor record continuing beyond the next decade with SNPP, JPSS, IASI, and planned GEO sounders, new methodologies that improve sounding capability will yield benefit for a long time to come. We therefore summarize the key questions we investigate as follows:

- What is the upper limit of HIR vertical sounding capability in the PBL?
- How can both AI and physics be used to constrain retrieval estimates in an explainable way, and improve upon current state-of-the-art retrieval approaches?

In this report, we describe how some of our recent efforts have made progress toward addressing these questions.

2. CURRENT RETRIEVAL APPROACHES

Sounding retrieval algorithms reconstruct a vertical distribution of atmospheric temperature and water vapor from the observations, which consist of thermal IR and microwave radiation emitted by layers of the atmosphere and measured by a sounder instrument on orbit [7]. The objective is to estimate the state of the atmosphere (represented by unknown parameter vector x, a vertical profile of $T(p)$ or $q(p)$, given spaceborne spectral radiance observations (represented by a radiance vector y). The IR observations used in y are typically a cloud-cleared spectrum derived from a 3 by 3 group of neighboring cloudy spectra beforehand (though single-FOV retrievals have recently advanced [8] as well). This inverse problem is ill-posed, lacking a single unique solution, with vertical details beyond a certain (scene- and data-dependent) vertical resolution limit not directly observable from the spectral measurements, including in the lower troposphere and the PBL. As highlighted below, this limitation in PBL information content from the instrument motivates the need for the new, AI-informed techniques described herein.

Two approaches to sounding retrievals are described in Figure 2: physical retrievals and statistical regression retrievals. The physical retrieval approach uses a forward model (the radiative transfer model) to calculate the expected measurements $f(x)$ given a specific atmospheric state x. The estimate $\hat{x}$ is iteratively adjusted to reduce the squared difference between the observations y and prediction $f(\hat{x})$. Due to ill-posedness, an additional regularization term is required to stabilize the retrieval, often taking a form similar to what is shown in Figure 2, in which a penalty for deviations from a first guess x_{prior} is imposed. Statistical regression approaches, including neural networks, learn an empirical relationship $\hat{x} = z(y)$ between an ensemble of measurements $y_{ensemble}$ and collocated ground truth datasets $x_{ensemble}$ [9]. For a neural network, $z(\cdot)$ is a nonlinear function composed of simple, interconnected computational elements, or nodes, defined by learned weight parameters and an activation function. A key advantage for neural networks over physical approaches is that they are fast and accurate, and, as universal function approximators [10], they can empirically learn complex, often indirect and nonlinear dependencies embedded in the data that may be difficult to physically model[9]. A key advantage of physical retrievals over statistical retrievals is that they are directly explainable, meaning that it is clear what part of the solution is introduced from the instrument radiances versus propagated from the first guess. Neural networks have attracted increasing wide from the sounding community in recent years [11-14]

In recent years, the Level 2 retrieval algorithm for Aqua's Advanced Microwave Sounding Unit (AMSU) has combined both of these approaches by using MIT-LL's Stochastic Cloud Clearing/Neural Network (SCC/NN) retrieval [15, 16] as first guess for NASA GSFC's physical retrieval. The introduction of SCC/NN as the first guess has led to improved accuracy and yield in down to the surface, including the PBL, versus previous versions with a different regression first guess[17]. In the current retrievals, PBL phenomenology is, to a significant degree, introduced via the SCC/NN first guess. This combination of neural networks and physical retrieval to improve operational science products resulted from over a decade of investment by NASA, long predating the recent intensified focus on AI from the larger science and technology community.

Physical Retrieval	**Neural Network Retrieval**
$\hat{\boldsymbol{x}} = \text{argmin}_{\boldsymbol{x}} \left\{ \lVert \boldsymbol{y} - \boldsymbol{f}(\boldsymbol{x}) \rVert_{\boldsymbol{\Lambda}}^2 + \lVert \boldsymbol{x} - \boldsymbol{x}_{\text{prior}} \rVert_{\boldsymbol{B}}^2 \right\}$	$\hat{\boldsymbol{x}} = \boldsymbol{z}(\boldsymbol{y})$, where $\boldsymbol{z}(\cdot)$ is a neural network, trained using:
$\boldsymbol{x}$ Unknown *T(p)* or *q(p)* profile	
$\boldsymbol{y}$ Spectrum measurements	
$\boldsymbol{f}(\cdot)$ Forward model	$\text{argmin}_{\boldsymbol{z}(\cdot)} \{ \lVert \boldsymbol{x}_{\text{ensemble}} - \boldsymbol{z}(\boldsymbol{y}_{\text{ensemble}}) \rVert^2 \}$
$\boldsymbol{\Lambda}, \boldsymbol{B}$ Meas. and prior inverse covariances	
$\boldsymbol{x}_{\text{prior}}$ First guess of *T(p)* or *q(p)*	

Figure 2: Physical versus neural network retrieval approaches for atmospheric sounding

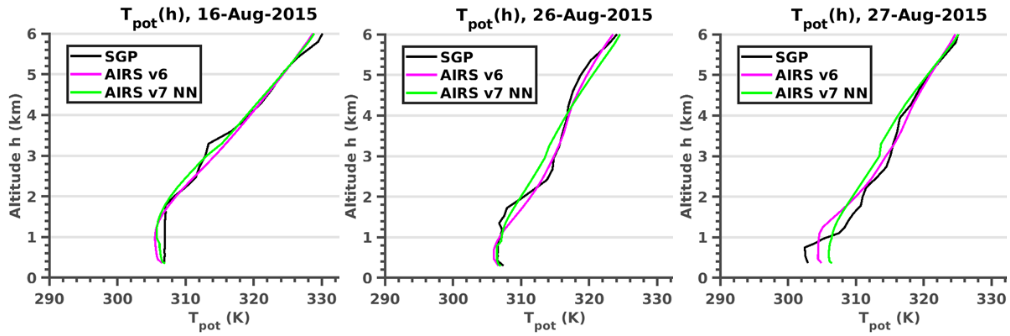

Figure 3: PBL T_{pot} profiles for ARM-SGP, AIRSv6, AIRSv7 NN

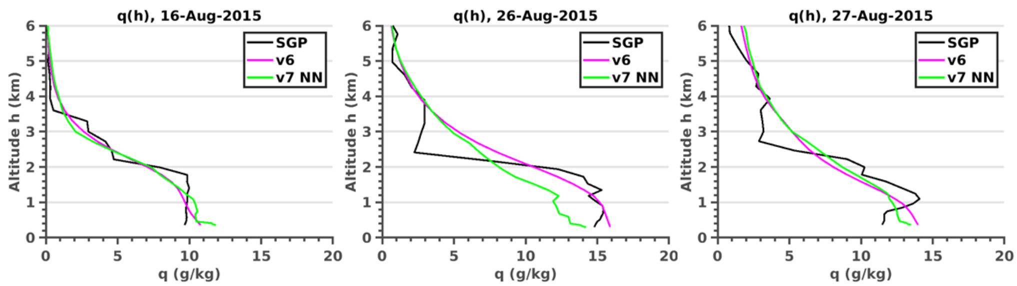

Figure 4: PBL q profiles for ARM-SGP, AIRSv6, AIRSv7 NN

Despite these recent improvements, further efforts are needed to both understand and improve performance in the PBL. Figure 3 shows three example afternoon T_{pot} retrievals from AIRS/AMSU compared collocated radiosonde truth profiles at the Southern Great Plains (SGP) site in Oklahoma operated by the Atmospheric Radiation Measurement (ARM) facility in 2015[18]. The AIRS/AMSU retrievals include the version 6 ("AIRS v6") product, and the NN first guess for the new v7 product ("AIRS v7 NN") which aimed for PBL improvements. Figure 4 shows an analogous set of plots for q profiles. The collocations used the nearest profiles flagged as high quality down to the surface, and are therefore best-case matchups. Nevertheless, the examples illustrate limitations in current capability addressed by this proposal. Profiles tend to be overly smooth, with relatively weak vertical gradients compared to the sonde profiles due to limited information in the lower troposphere. As a result, distinguishing between the well-mixed layer and the PBL top inversion is difficult, as is accurate determination of PBLH. This problem is especially apparent for q, where we have noted significant room for improvement.

3. MAP ESTIMATION AND VARIABLE SPLITTING FRAMEWORK

A traditional approach to solving the physical retrieval problem is known as optimal estimation”[7], or maximum a posteriori (MAP) estimation. Here, we review MAP estimation, and then we use it to motivate a more general framework. We define, again, observations y and unknown atmospheric state x (describing temperature T and humidity q).

$$\begin{aligned}\hat{x} &= \arg\max_x \{\log p(y|x) + \log p(x)\} \\ &= \arg\max_x \{(\text{data fitting term}) + (\text{regularization term})\}\end{aligned} \quad \textbf{(1)}$$

The data likelihood $p(y|x)$ describes how well the observations y match predictions $f(x)$, and is typically assumed normally distributed with inverse measurement covariance as in Figure 2:

$$\log p(y|x) = -\frac{1}{2}\|y - f(x)\|_\Lambda^2 + (\text{const.}) \quad \textbf{(2)}$$

In principle, the prior model $p(x)$ describes how the set of all x should be distributed, including complicated joint dependencies. In practice, a model $p(x)$ is chosen to regularize the MAP solution with certain key properties expected of x, like proximity to a first guess or a resolution limit, that can be captured in a tractable cost function, and it is typically assumed Gaussian, as shown in the example in Figure 2. We define $g(x) = -\log p(y|x)$ and $h(x) = -\log p(x)$, so that

$$\hat{x} = \arg\min_x \{g(x) + h(x)\} \quad \textbf{(3)}$$

For many typical choices of $g(x)$ and $h(x)$, (3) can be solved using nonlinear least squares optimization techniques such as the Levenberg-Marquardt technique[7], or analogous techniques. Here, we use a different approach, known as “variable splitting”, with the aim of enabling the use of a wider variety of options for $h(x)$, including non-Gaussian models [19-21]. Suppose we split x into two different variables, x_1 and x_2, and minimize $g(x_1) + h(x_2)$ such that $x_1 = x_2$ as follows:

$$\begin{aligned}(\hat{x}_1, \hat{x}_2) &= \arg \min_{x_1 = x_2} \{g(x_1) + h(x_2)\} \\ &= \arg \min_{x_1, x_2} \left\{g(x_1) + h(x_2) + \frac{1}{2\sigma^2}\left|\left|x_1 - x_2 + u\right|\right|^2\right\}\end{aligned} \quad \textbf{(4)}$$

where u is an “augmented Lagrangian” to be solved for, similar to a Lagrange multiplier, and σ is a selectable parameter which controls the rate of convergence. This problem can be solved with a series of update steps that alternate among all the unknowns. This scheme, called “Alternating Direction Method of Multipliers” (ADMM)[19, 20], is powerful because it enables solution of a difficult, constrained optimization problem as a sequence of simpler unconstrained steps:

- Initialize $u = 0$
- Repeat until converged:
  - $\hat{x}_1 = \arg \min_{x_1} \left\{g(x_1) + \frac{1}{2\sigma^2}\left|\left|x_1 - \hat{x}_2 + u\right|\right|^2\right\}$ *// Sensor model update step*
  - $\hat{x}_2 = \arg \min_{x_2} \left\{h(x_2) + \frac{1}{2\sigma^2}\left|\left|\hat{x}_1 - x_2 + u\right|\right|^2\right\}$ *// Prior model update step*
  - $u = u + (\hat{x}_1 - \hat{x}_2)$ *// “Augmented Lagrangian”*

We can define the following functions, which are called “proximal maps”, corresponding to the above update steps as follows:

$$G(x) = \arg\min_{v}\left\{g(v) + \frac{1}{2\sigma^2}\left||v-x|\right|^2\right\}$$
$$H(x) = \arg\min_{v}\left\{h(v) + \frac{1}{2\sigma^2}\left||v-x|\right|^2\right\} \quad \textbf{(5)}$$

Informally, we can interpret the proximal map as an "agent" that improves the current estimate:

- "Agent" that improves sensor model fit: $G(x) \approx x\text{-}\alpha\nabla g(x)$
- "Agent" that improves prior model fit: $H(x) \approx x\text{-}\alpha\nabla h(x)$

The above ADMM algorithm is then:

- Initialize $u = 0$
- Repeat until converged:
  - $\hat{x}_1 = G(\hat{x}_2 - u)$ *// Sensor model "agent"*
  - $\hat{x}_2 = H(\hat{x}_1 + u)$ *// Prior model "agent"*
  - $u = u + (\hat{x}_1 - \hat{x}_2)$ *// "Augmented Lagrangian"*

The ADMM alternates successive small improvements to the sensor model fit and prior model fits until convergence to a final result which strikes a balance between fitting both models. The prior model agent, in particular, tends to enhance the current estimate by denoising it or removing artifacts from it, bringing it closer into alignment with expected properties of valid solutions that the sensor model alone may not directly constrain. The convergence conditions are as follows:

$x = G(x-u)$ *// Sensor model agent*

$x = H(x+u)$ *// Prior model agent*

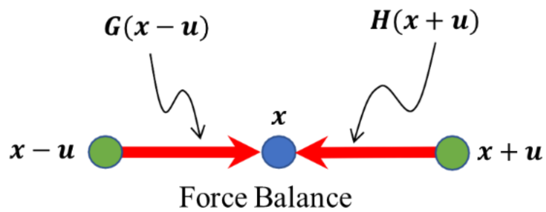

Figure 5: CE force balance illustration

These conditions have been introduced with the name "Consensus Equilibrium" (CE) by Buzzard et al.[21], evoking the idea of a "force balance" or "equilibrium" between multiple agents (in this case, the sensor model agent and the prior mode agent) acting on the estimate, as illustrated in Figure 5.

4. RECENT TARGETED RETRIEVAL WORK AND APPLICATION TO PBL

Drawing on the previous sections, we can describe a sensor model agent as a proximal map, based on (2) and **Error! Reference source not found.**, with cloud cleared observations y and radiative transfer f orward model $f(\cdot)$:

$$G(x) = \arg\min_{v}\left\{\frac{1}{2}\|y - f(v)\|_{\Lambda}^{2} + \frac{1}{2\sigma^{2}}\left||v - x|\right|^{2}\right\} \quad \textbf{(6)}$$

An implementation of (6) for AIRS has already been developed on the existing 2017 TASNPP project, using the v7 SCC/NN retrieval as the clear state for cloud clearing and the Stand-alone Atmospheric Radiative Transfer Algorithm (SARTA) [22] forward model. Under this proposed work, we will draw on the team's experience on the existing AIRS and CrIS Level 2 retrieval algorithms [16, 23] to improve the current sensor agent for both sensors, improving error propagation, cloud clearing, and channel selection. For example, as part of the TASNPP effort AIRS/AMSU Level 2 retrieval performance was evaluated for a selection profiles collocated with a PBL-focused SGP radiosonde measurement campaign. The comparison showed that there is room for improvement in vertical resolution in the PBL via physical retrieval approaches, for q in particular, which subsequently became a subsequent area of focus. As a result, Milstein et al. developed a new approach for retrieving q, with the goal of making better use of the available radiances[24]. The approach starts with the v7 SCC/NN AIRS/AMSU retrieval as first guess accompanied by a newly developed per-retrieval uncertainty covariance estimate predicted using a Mixture Density neural network (described in **Error! Reference source not found.**). This first guess is then used as a clear s tate and first guess for a new physical retrieval approach that differs in important ways from existing retrieval approaches: A total variation (TV) smoothness prior is used to regularize the solution while preserving sharp features. As Karl states in [25], "unlike standard quadratic Tikhonov solutions, total variation regularized answers can contain localized steep gradients, since the regularizer penalizes only the total amount of gradient in the image and not its distribution. As a result, edges are preserved in the reconstructions." In addition, the predicted first guess covariance estimate is employed as a bounds constraint (e.g., "stay within 1-sigma of the first guess"), rather than a Gaussian prior adding a quadratic norm penalty to the cost function. Other bounds constraints from physical realism such as avoiding oversaturation are also enforced. Combined, these priors avoid conventional Gaussian assumptions which tend to oversmooth regularized solutions and are therefore appropriate for PBL-focused q retrievals where a sharp gradient is expected. As illustrated in Figure 6, this approach can be described using the CE framework and alternating optimization approach of 3, with proximal map agents on a profile: a sensor agent similar to (6), a prior model agent that enforces bounds constraints relative to the first guess, and an additional prior agent that enforces the total variation prior model on the profile.

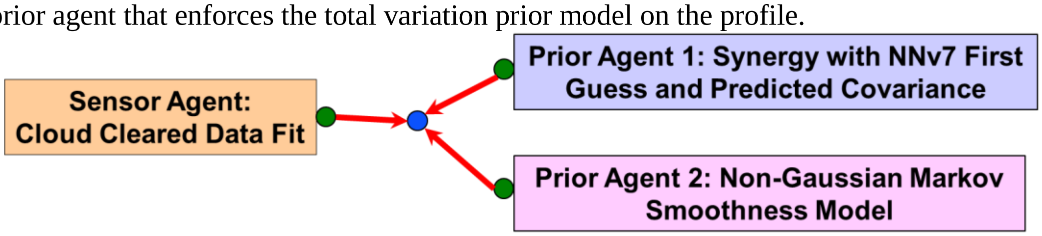

Figure 6: Illustration of the 2017 TASNPP analysis effort as a CE problem

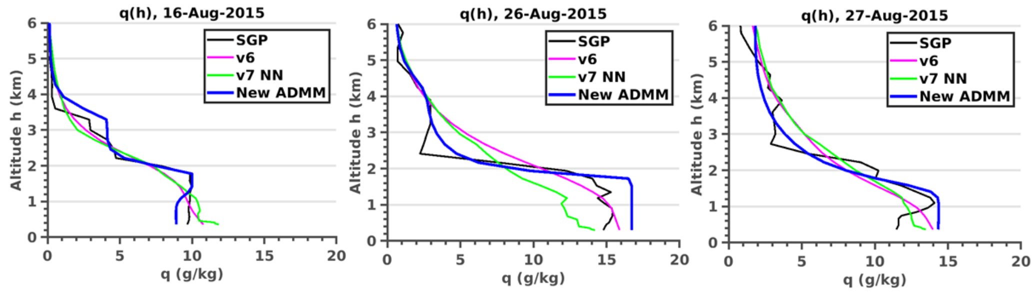

Figure 7: Example PBL *q* profiles for ARM-SGP, AIRSv6, AIRSv7 NN, and new ADMM approach.

To evaluate this approach, these ADMM retrievals were added to those in Figure 4, and the results are shown in Figure 7. The ADMM profiles show more vertical structure, including inversions, near the PBL than the v6 and v7 SCC/NN retrievals. This work illustrates that significant improvement in resolving PBLH is possible using the proposed CE framework, incorporating more machine learning elements (such as first guess error prediction) and nontraditional, non-Gaussian prior models that preserve sharp gradient features of most interest in PBL retrievals.

5. CONCLUSION

We have assessed IR+microwave retrievals from the existing AIRS/AMSU retrieval system and the v7 Stochastic Cloud Clearing/Neural Network (SCC/NN) [15, 16] first guess in comparison to collocated radiosondes.

We first reviewed the current AIRS/AMSU retrieval methodology and how it utilizes a neural network and physical retrieval in combination. We then described the recently introduced consensus equilibrium framework, highlighting how it generalizes traditional Bayesian optimal estimation techniques to include new, powerful prior models. We showed how new moisture retrievals developed under MIT-LL's 2017 TASNPP effort can be viewed as special case of this framework, leading to significant improvements in PBL vertical detail, including sharp gradients at the top of the PB. This new methodology balances sensor physics with a prior model informed by machine learning[24]. While encouraged by this recent progress, we hypothesize that significant further improvement in retrieval of T and q in the PBL is possible by expanding on these approaches. The ESAS 2017 outlines numerous high priority scientific questions that will be addressed with improved observations of the PBL, and our ongoing work, by improving global retrieval accuracy and resolution from POR systems, will offer cross-cutting benefit across all of them.

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