National Aeronautics and Space Administration

Retrieve Methane from IR sounder measurements Using Machine Learning-Enhanced Physical Inversion

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Introduction

- IR sounders including CrIS, AIRS, and IASI provide mid-wave IR spectral measurements in the 7.7 μm region, providing important complementary information to other sensors (e.g. TANSO-FTS, TROPOMI, EMIT …)

- Resolving weak CH_4 signals from sounder observations is challenging due to the limited information provided by the measurement and the complexity of isolating CH_4 signals from other trace gases. CH_4 products have been developed for current sounders. However, the retrieval accuracy, especially at the daily temporal scale, may need to be further improved.

- A novel CH_4 retrieval methodology based on the "spectral fingerprinting" approach has been explored. Implementation study on CrIS L1B data has been carried out.

- Initial results and validation

The role of hyper-spectral IR sounders in global CH_4 monitoring

- With a heat-trapping capability more than 25 times greater than CO_2, CH_4 accounts for 4–9% to the greenhouse effect. Satellite-based measurements play a crucial role in assessing the geographical distribution of CH_4 in a global scale.

IR hyperspectral sensors provide

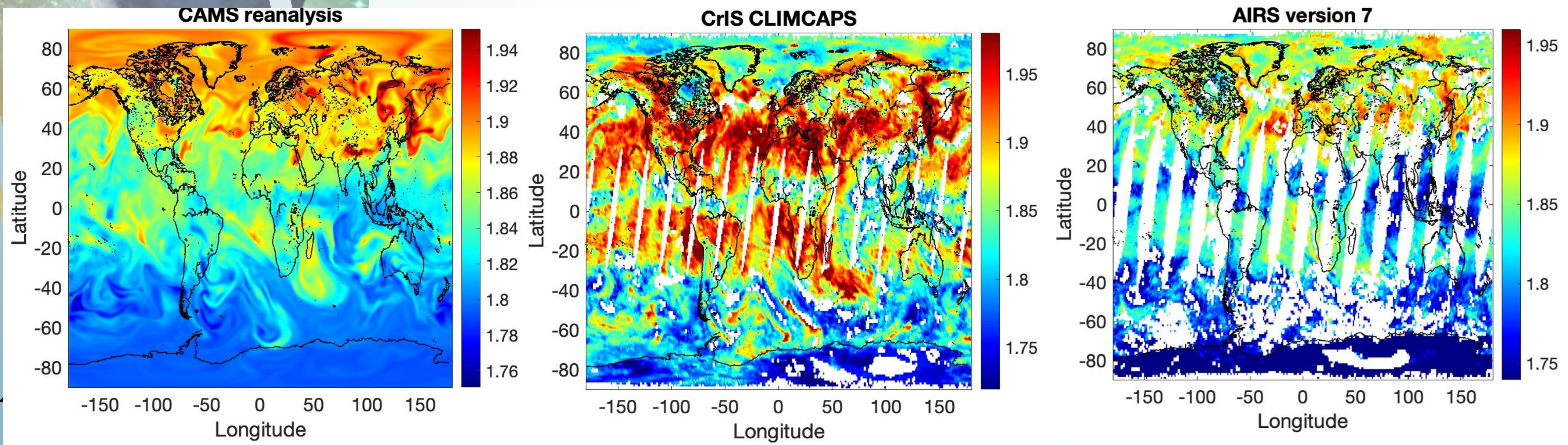
- ❖ **Nighttime observation**
- ❖ **More sensitive to mid to upper tropospheric CH_4**

Sensor	Satellite	CH_4 Meas. Band (μm)	Spectral Resolution	Footprint Size (km)	Swath Width (km)
SCIAMACHY	ENVISAT	~ 1.65	~ 0.48 nm	30 x 60	1000
TROPOMI	Sentinel-5P	~ 0.76 & 2.3 ~ 2.4	~ 0.25 nm	7 x 3.5 & 7 x 7	2600
TANSO-FTS	GOSAT	~ 1.65 ~ 7.7	~ 0.2 cm^{-1}	10.5 x 10.5	790
CrIS	SNPP, JPSS	~ 7.7	~ 0.625 cm^{-1}	14 x 14	2200
IASI	METOP	~ 7.7 & ~3.7	~ 0.5 cm^{-1}	12 x 12	2200
IASI-NG	EPS-SG	~ 7.7 & ~3.7	~ 0.25 cm^{-1}	25 x 25	2000
AIRS	AQUA	~ 7.7	1200 ($\lambda/\Delta\lambda$)	13.5 x 13.5	1800

Challenge of retrieving CH_4 profiles from IR sounder observations

- Strong absorption lines of H_2O and N_2O exist in the spectral region of CH_4 absorption.
- IR sounders have limited measurement sensitivity and instrument spectral resolution.
- Cloud contamination.

Daily global distribution of these CH_4 need more validation (e.g. July 9, 2017 results)



A spectral fingerprinting methodology-based retrieval algorithm

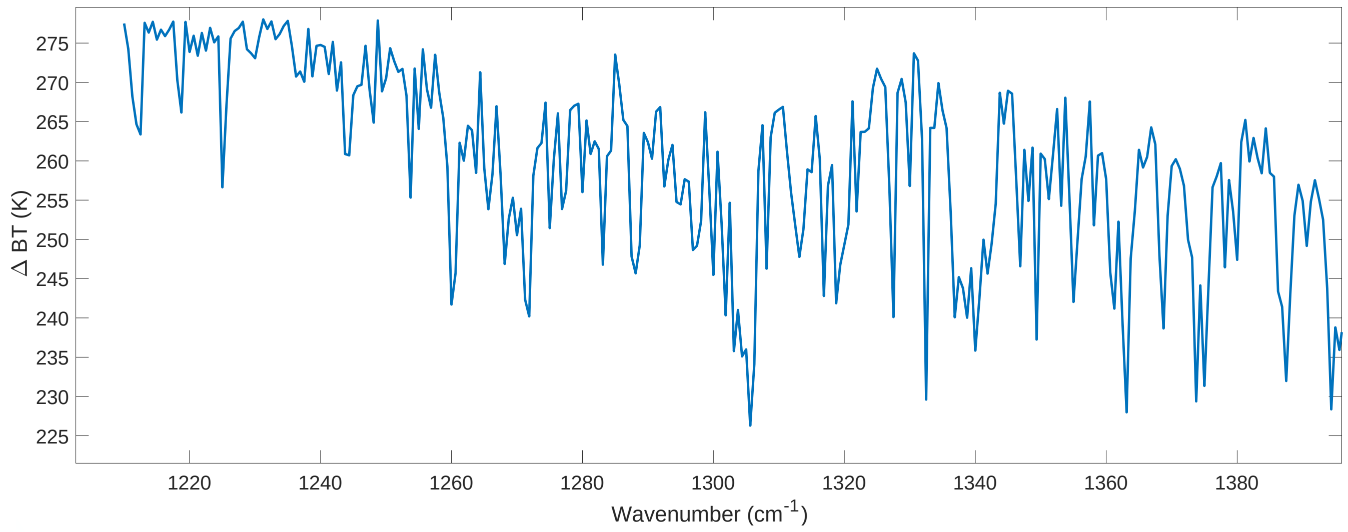
$$\Delta r = \mathrm{K}\Delta x + \varepsilon$$

$$\Delta x = \left(\mathrm{K}^T\Sigma^{-1}\mathrm{K} + S_a^{-1}\right)^{-1}\mathrm{K}^T\Sigma^{-1}\Delta r,$$

$$x = x_0 + \left(\mathrm{K}^T\Sigma^{-1}\mathrm{K} + S_a^{-1}\right)^{-1}\mathrm{K}^T\Sigma^{-1}(r - r_0),$$

$$\mathrm{K} = {}^{dr}/_{dx}\big|_{x=x_0}$$

Standard Optimal Estimation Methodology based Formula,
Identify reference state x_0 and r_0 is the key

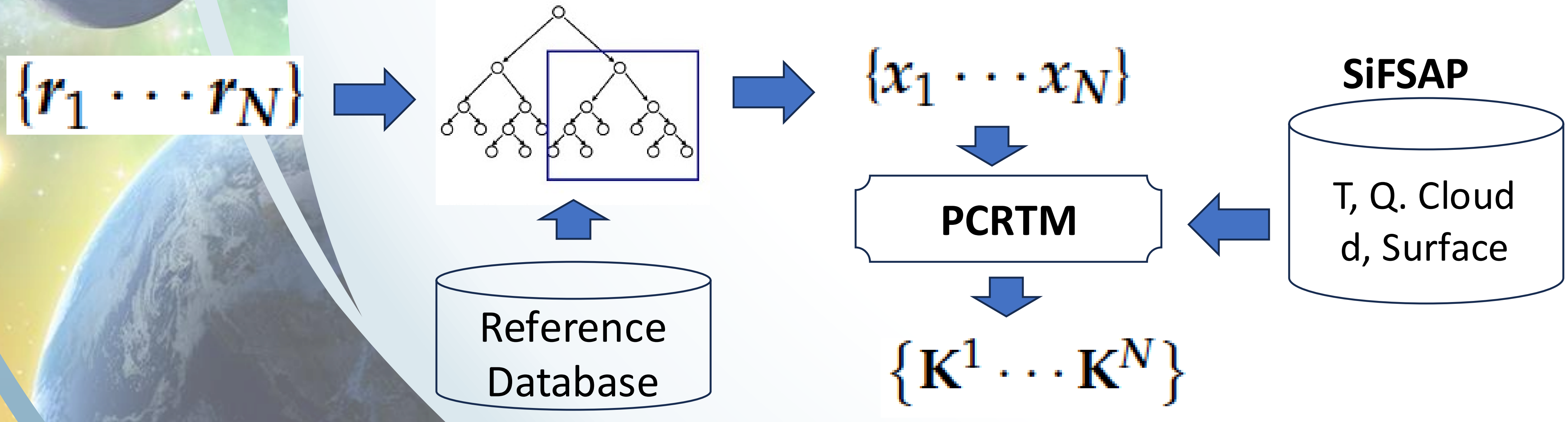


- Spectral Feature based pattern matching
- Kernel (Jacobian) based physical inversion

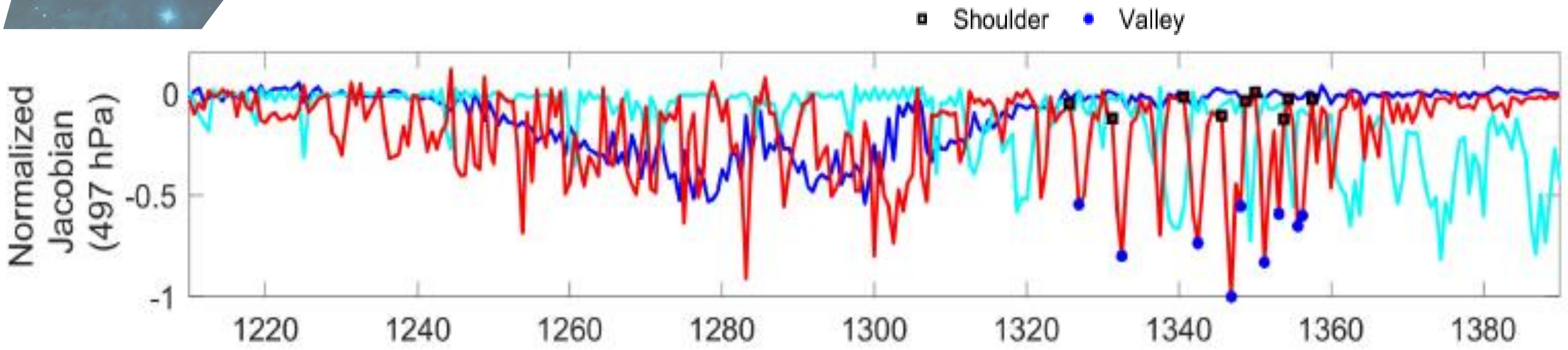
Using classification to provide scene-dependent a priori

- Use sample CH_4 data from CAM reanalysis and Carbon Tracker matched to Satellite based sounder observations to construct the reference training data set.
- Use Single Field-of-view Atmospheric Sounder Product (SiFSAP) to provide the supplement information (T, Q, Cloud, Surface)
- The principal Component based radiative transfer model (PCRTM) is used to derive Jacobian

nearest neighbor (k-NN) algorithm



Optimization of Spectral Information



$$r = \frac{r_{valley} - r_{shoulder}}{r_{window}}$$

The choice of CrIS channels is made to avoid the N_2O absorption region and minimize the interference due to water vapor absorption.

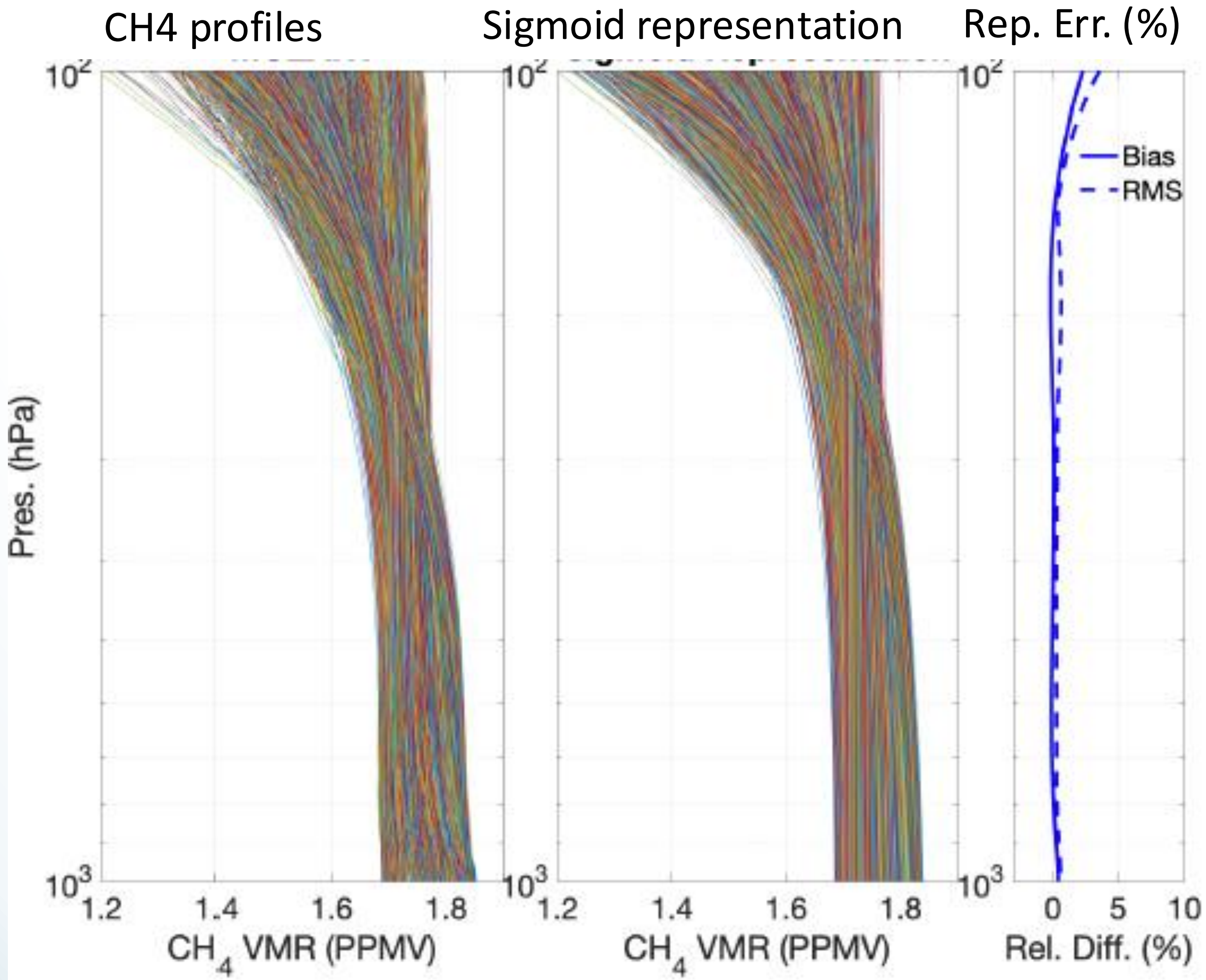
Vertical profile distribution constraint

Use the sigmoid function to provide a smoothing constrain on vertical variation

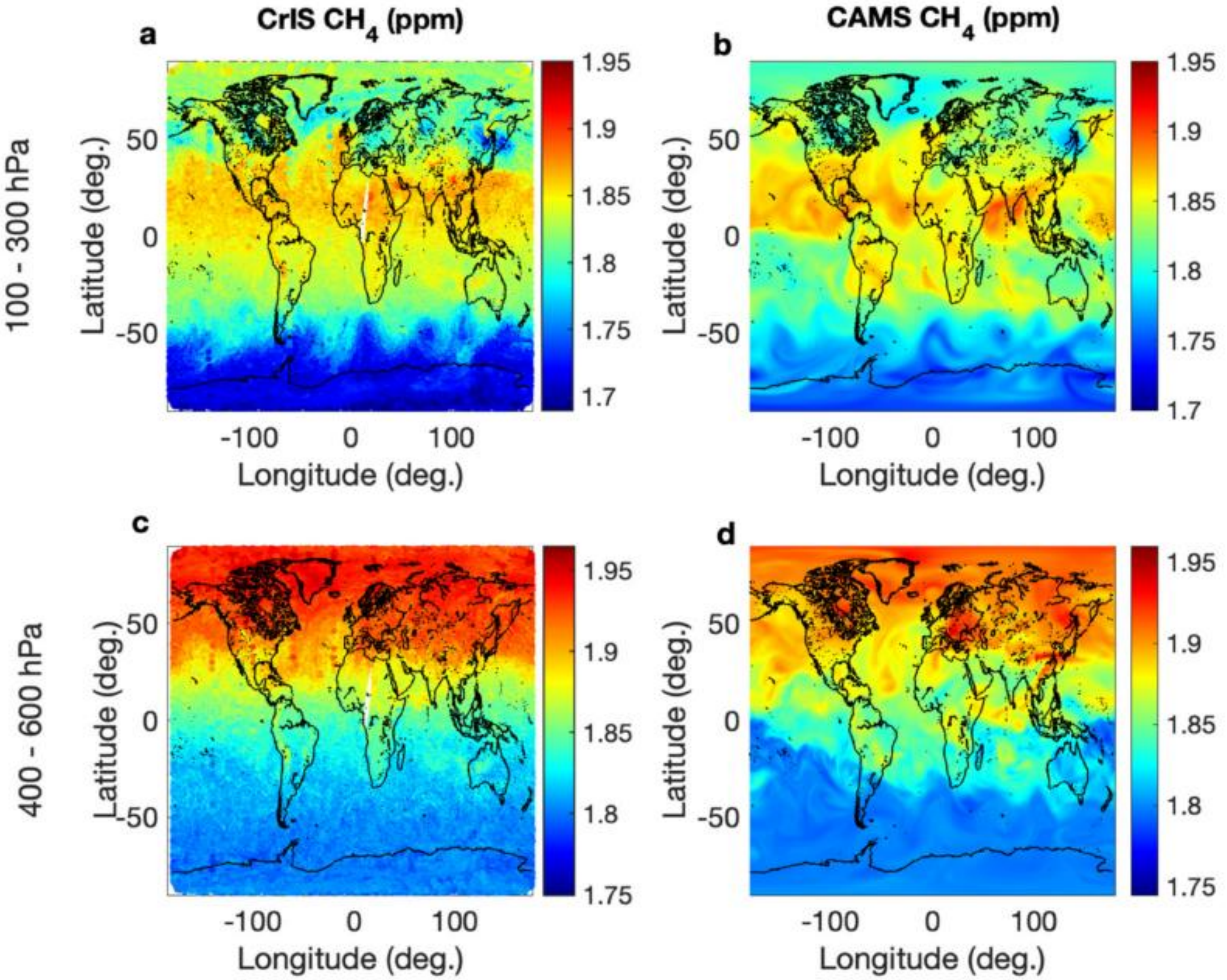
$$f(h) = \frac{S}{1 + e^{-\left(\frac{h-P}{n}\right)}}$$

$$\Delta f(h) = \frac{\partial f}{\partial S}\Delta S + \frac{\partial f}{\partial P}\Delta P + \frac{\partial f}{\partial n}\Delta n.$$

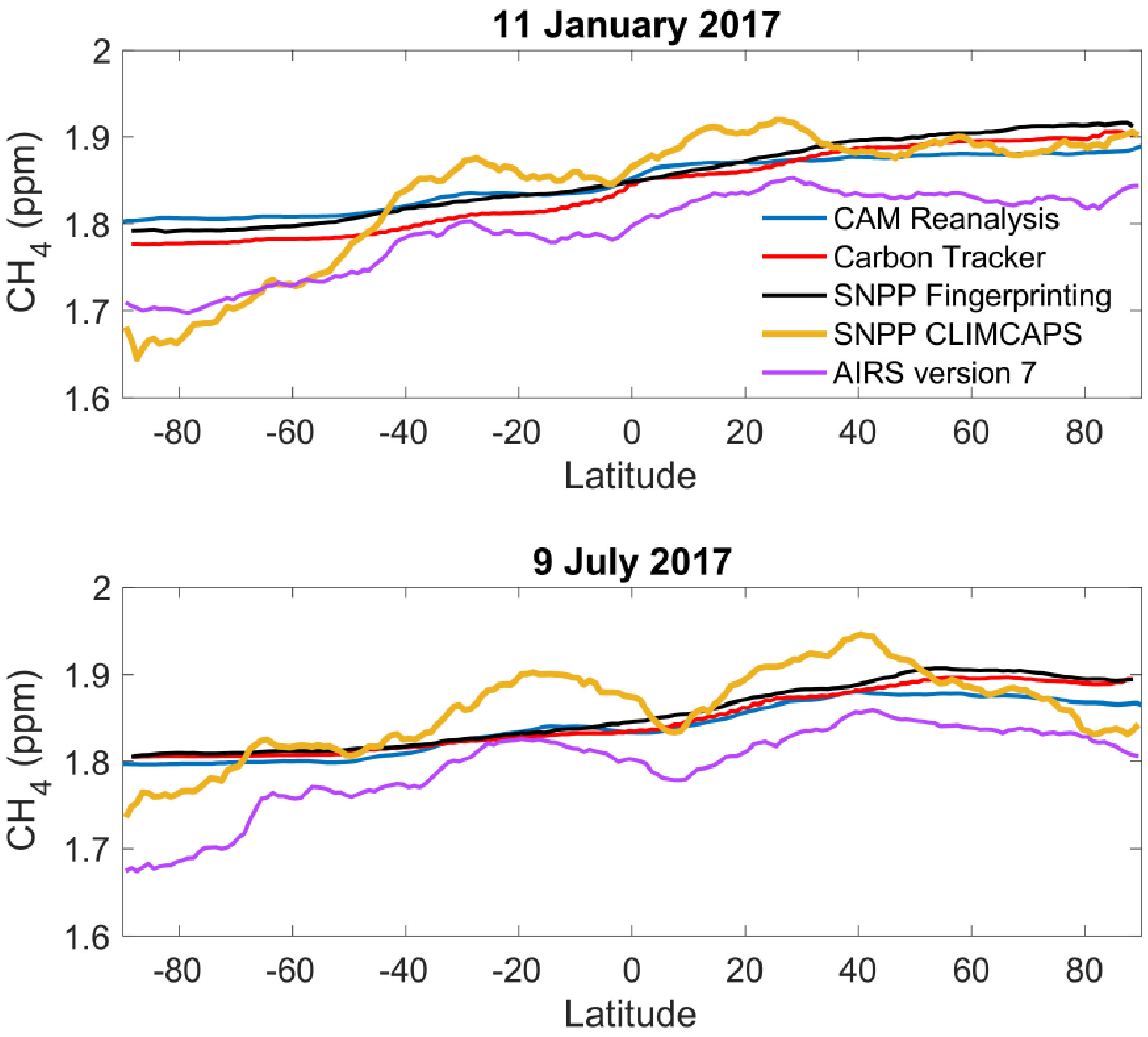
S represents near surface CH4 concentration
P marks the tropopause related vertical profile gradient point
n reflects the rate of CH4 decrement in the stratosphere



Global distribution of CH_4 retrieved from SNPP-CrIS observations (January 11, 2017)



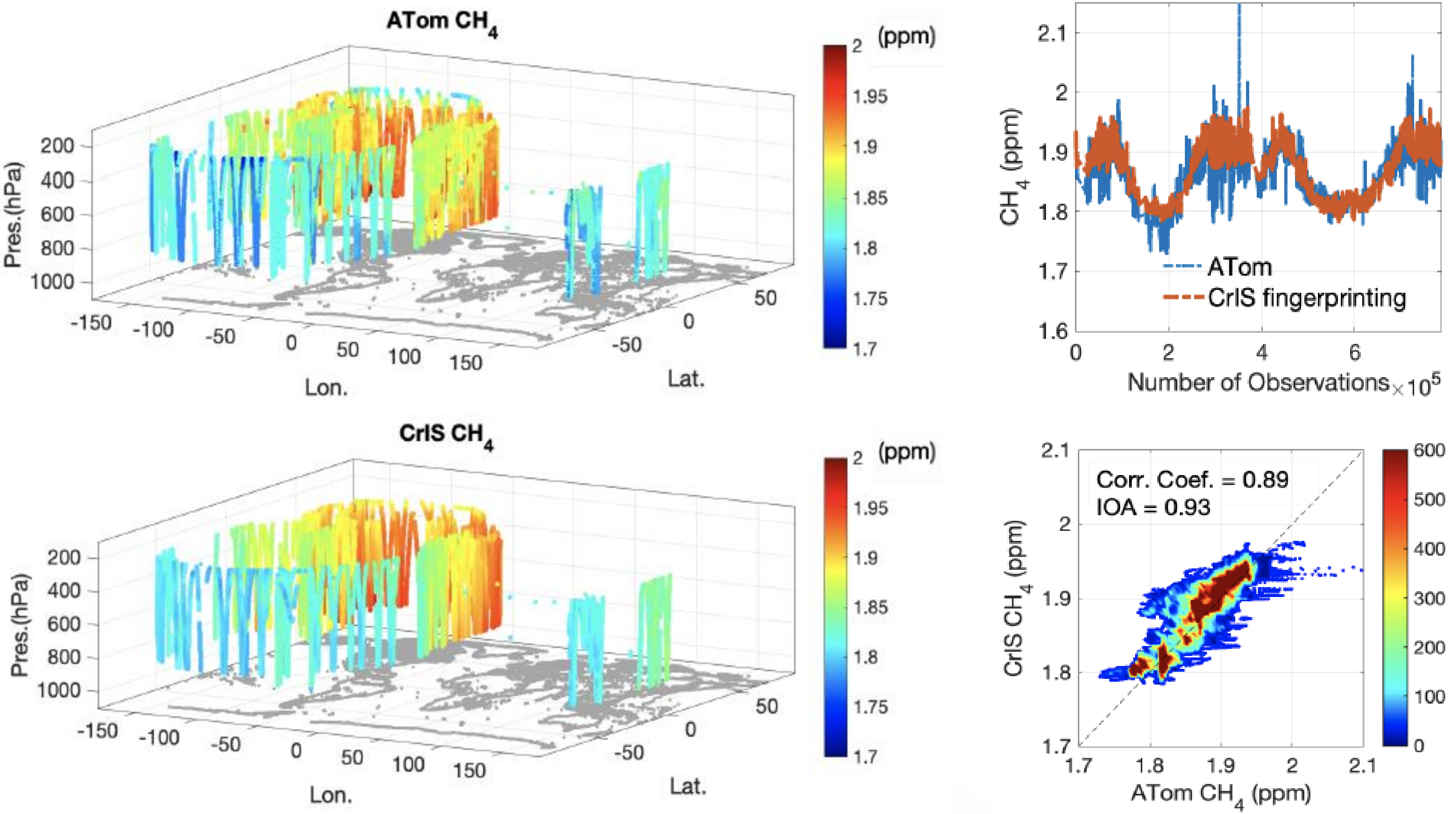
Latitudinal variation mid-tropospheric CH_4



At the daily temporal scale, SNPP CrIS fingerprinting results agree better with the CH_4 reanalysis data than two other NASA sounder CH_4 data products (CLIMCAPS, AIRS V7).

Inter-comparison with in-situ measurements

(Atmospheric Tomography Mission)



Implementation in the updated Single Field-of-View Atmospheric Sounder Product (SiFSAP) algorithm

	Version 1	Version 2
Atmospheric Profile Representation	EOF representation of 98 fix pressure level quantities	EOF representation of 60 sigma pressure level quantities
	Separated as over ocean and over land cases	Unified over ocean and over land cases
Surface emissivity	Classified as land, ocean, coastal, and snow/ice types; Each type has it own EOFs	Classified as land, ocean, coastal, and snow/ice types; Unified EOFs
Cloud parameters	Single layer of cloud for each CrIS FOV	Single or two layers of clouds for each CrIS FOV (ice/water)
Radiance bias and retrieval uncertainty Sy	Scene dependent radiance bias established using linear regression scheme	Scene and viewing angle dependent radiance bias established using a K nearest neighbor scheme
A priori for trace gases O3, CH_4, N_2O	**Preestablished latitude dependent (tropopause dependent) a priori constraint**	**Use sounder spectral radiance as the predictor variable to dynamically generate a prior through a KNN scheme**

SUMMARY

- A spectral fingerprinting scheme has been developed for the CH_4 retrieval using satellite-based IR hyper-spectral sounder measurements.

- It uses a machine learning-based model to initialize the a priori background and an optimized scheme to enhance the spectral fingerprints of CH_4.

- The combination of machine learning and radiative kernel-based inversion has the potential to offer advantages in terms of accuracy and computational efficiency.

- Initial validation against reanalysis results and in-situ measurements looks promising.

Thank you