Integrated Methane Inversion (IMI) on the AWS cloud: a tool to infer greenhouse gas fluxes from satellite observations

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Varon, D.J., D.J. Jacob, M. Sulprizio, L.A. Estrada, W.B. Downs, L. Shen, S.E. Hancock, H. Nesser, Z. Qu, E. Penn, Z. Chen, X. Lu, A. Lorente, A. Tewari, and C.A. Randles, Integrated Methane Inversion (IMI 1.0): a user-friendly, cloud-based facility for inferring high-resolution methane emissions from TROPOMI satellite observations, Geosci. Model Dev., 15, 5787–5805, https://doi.org/10.5194/gmd-15-5787-2022, 2022.

A highly productive 8-year relationship with ExxonMobil

- Review of methane observations from space and their utility to infer methane emissions [Jacob et al., 2016]
- Requirements for satellites to detect methane super-emitters [Cusworth et al., 2018; Turner et al., 2018]
- Discovery of the capability of land surface imagers to detect super-emitters [Cusworth et al., 2019, 2021]
- High-resolution continental-scale inversion of methane emissions in North America [Nesser et al, to be submitted soon]
- Boundary conditions for regional inversions [Nesser, ongoing]
- Integrated Methane Inversion (IMI) on the AWS cloud [Varon et al., 2022; ongoing]

Our vision for the IMI: enable stakeholders to infer greenhouse gas fluxes from satellite data in real time with an easy-to-use, cutting-edge inversion capability on the cloud bringing compute to data

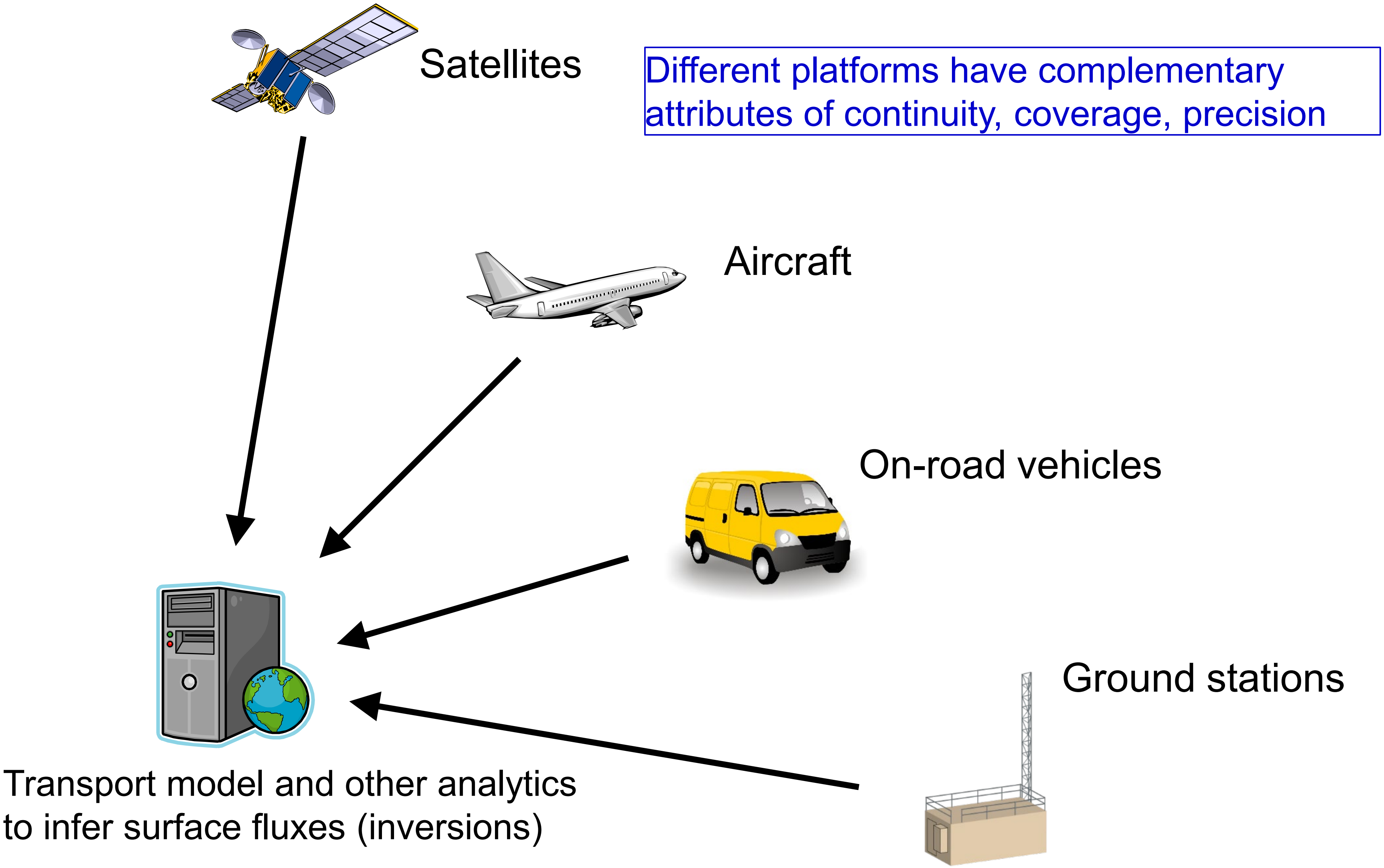
[redacted]

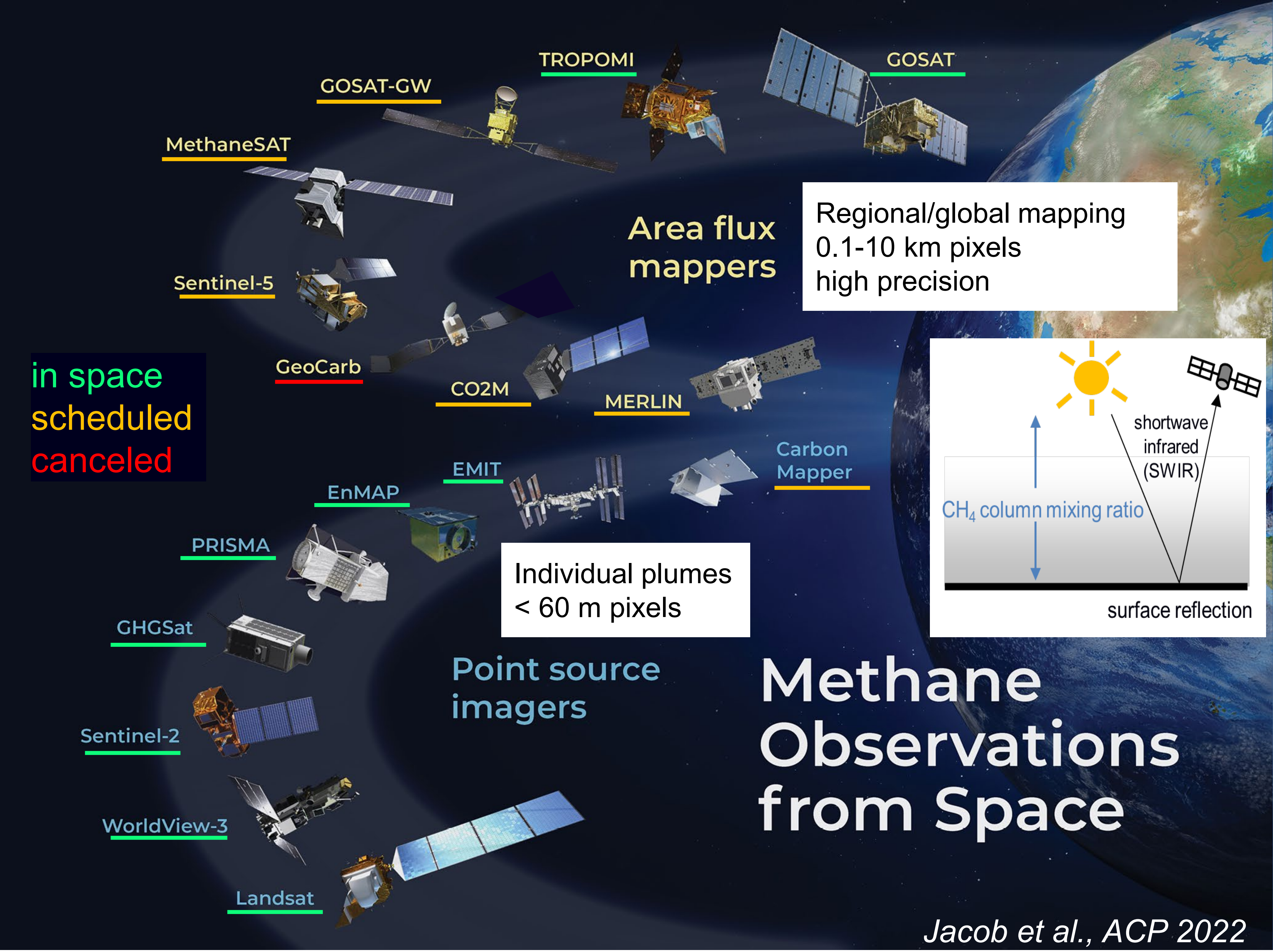
The current prototype
- exploits TROPOMI satellite data to infer methane emissions at 25-km resolution over regional (~1000 km) domains
- uses research-grade inversion analytics with open-access code documented in literature
- circumvents difficulties in working with satellite data
- has over 50 users, is endorsed by International Methane Emissions Observatory (IMEO)

Current development
- enable global inversions
- increase spatial resolution
- Integrate point source data
- enable real-time monitoring

Longer-term vision
- Extend to multi-satellite fleet and to CO_2
- Couple with independent tools for automated plume detection
- Provide reference top-down flux tool to support LDAR programs, climate policy, cloud-based Earth Information System

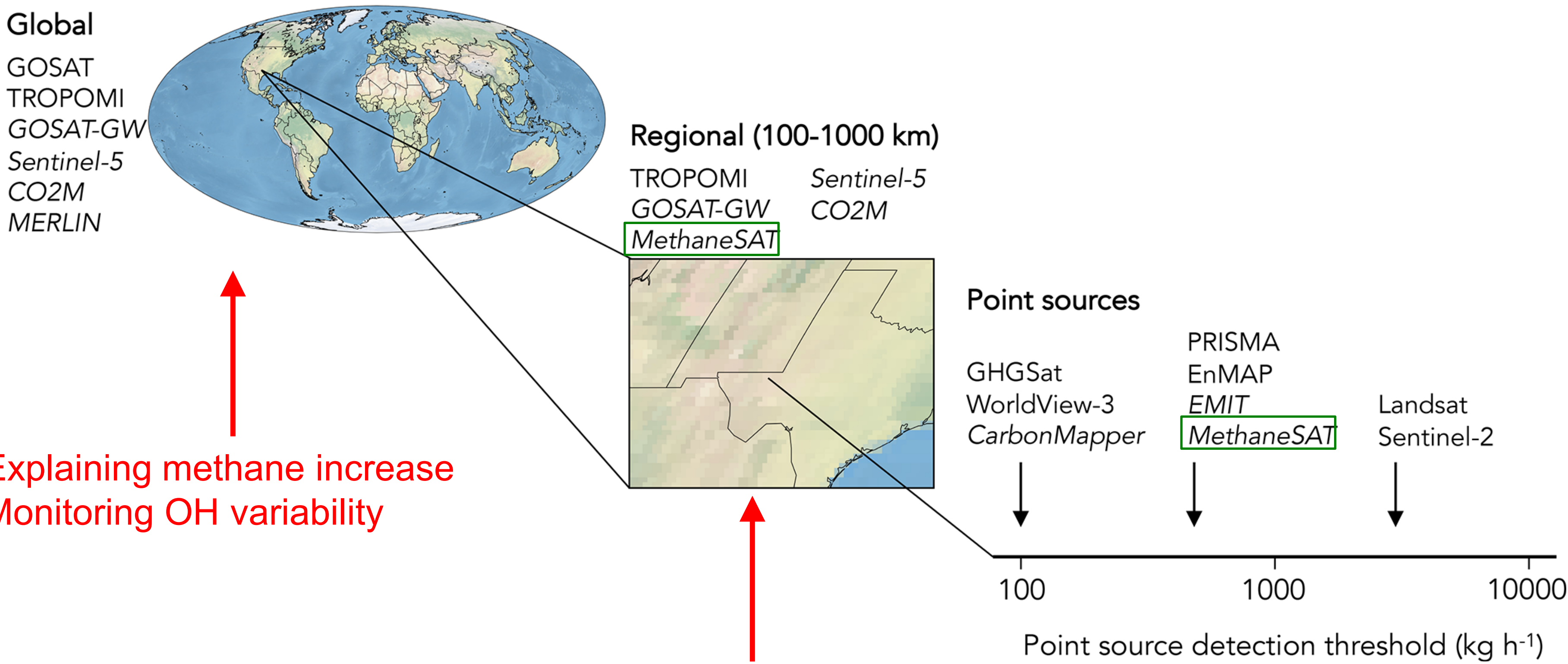
Multitiered observing system for greenhouse gases





TROPOMI
GOSAT
GOSAT-GW
MethaneSAT
Sentinel-5
GeoCarb
CO2M
MERLIN
Area flux mappers
Regional/global mapping
0.1-10 km pixels
high precision
in space
scheduled
canceled
shortwave infrared (SWIR)
CH_4 column mixing ratio
surface reflection
Carbon Mapper
EMIT
EnMAP
PRISMA
GHGSat
Sentinel-2
WorldView-3
Landsat
Individual plumes
< 60 m pixels
Point source imagers
Methane Observations from Space
Jacob et al., ACP 2022

Satellites can provide the backbone of an observing system for monitoring methane emissions from the global scale down to point sources



- Explaining methane increase
- Monitoring OH variability

- Quantifying national/regional emissions
- Improving bottom-up inventories

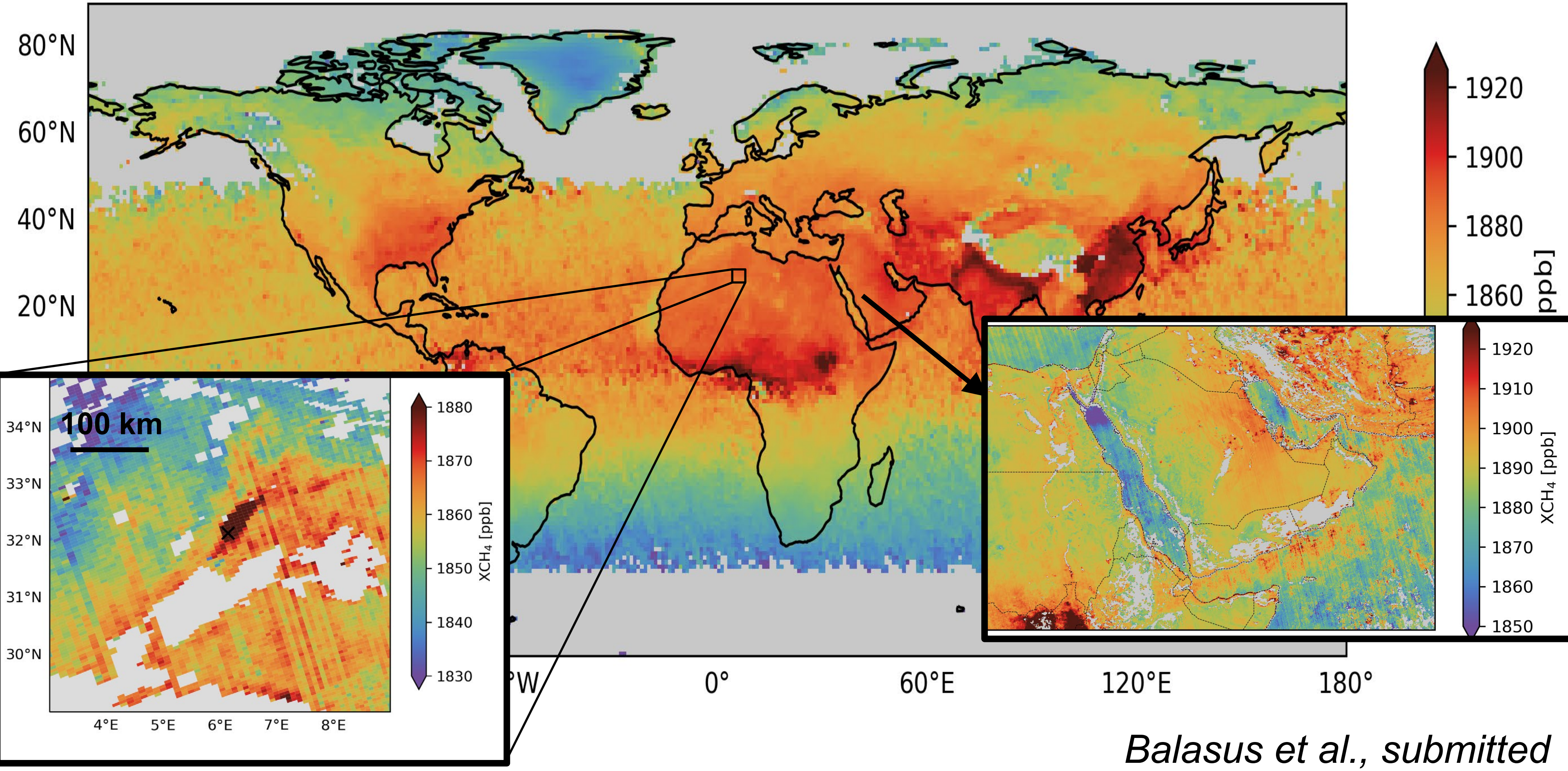
- Detecting large point sources
- Enabling quick mitigation

Jacob et al., ACP 2022

TROPOMI (2018-): global daily mapping with 5.5x7 km^2 pixels, 0.6% precision

Over 100 million observations per year

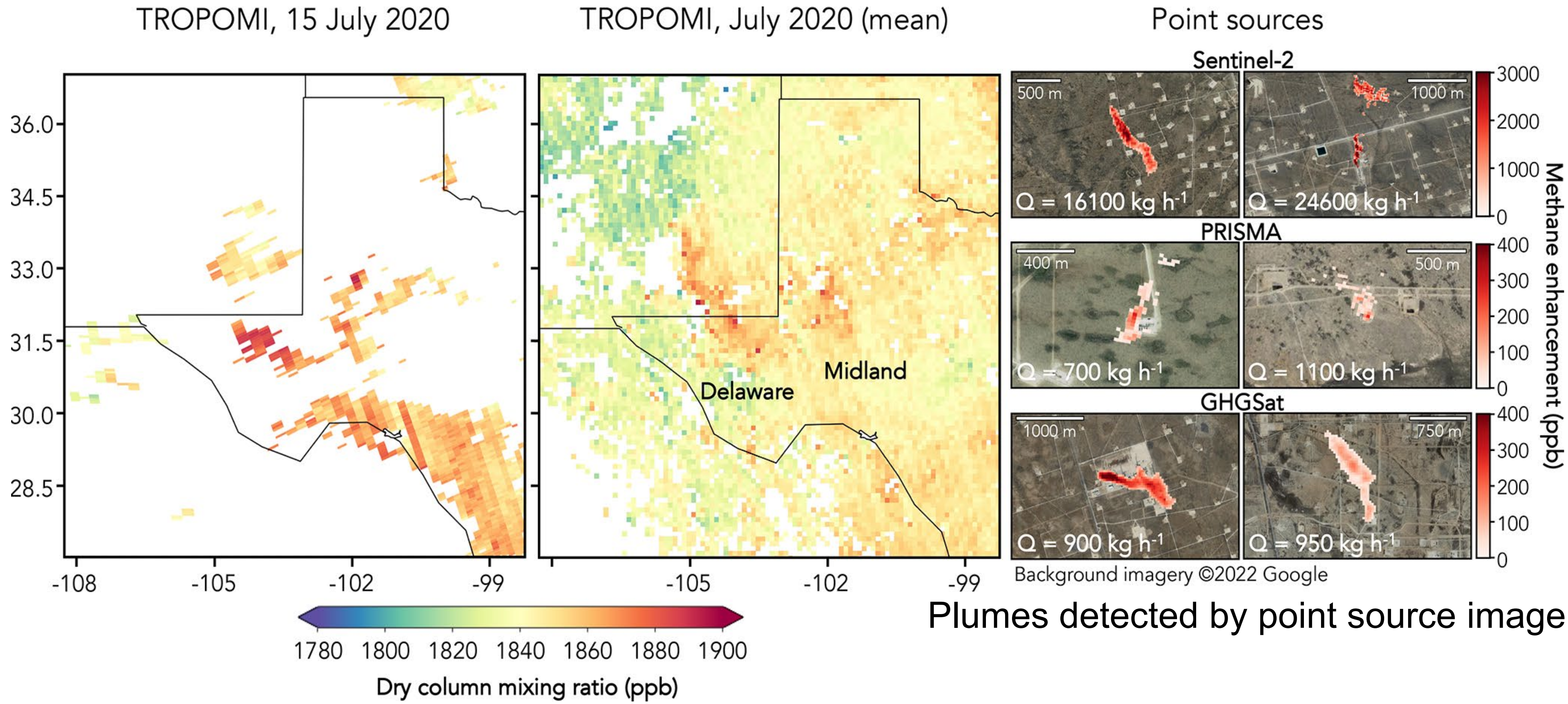
Annual mean TROPOMI observations, 2021



Balasus et al., submitted

Complementarity of TROPOMI and point source observations to quantify basin-scale emissions

Observations over Permian Basin

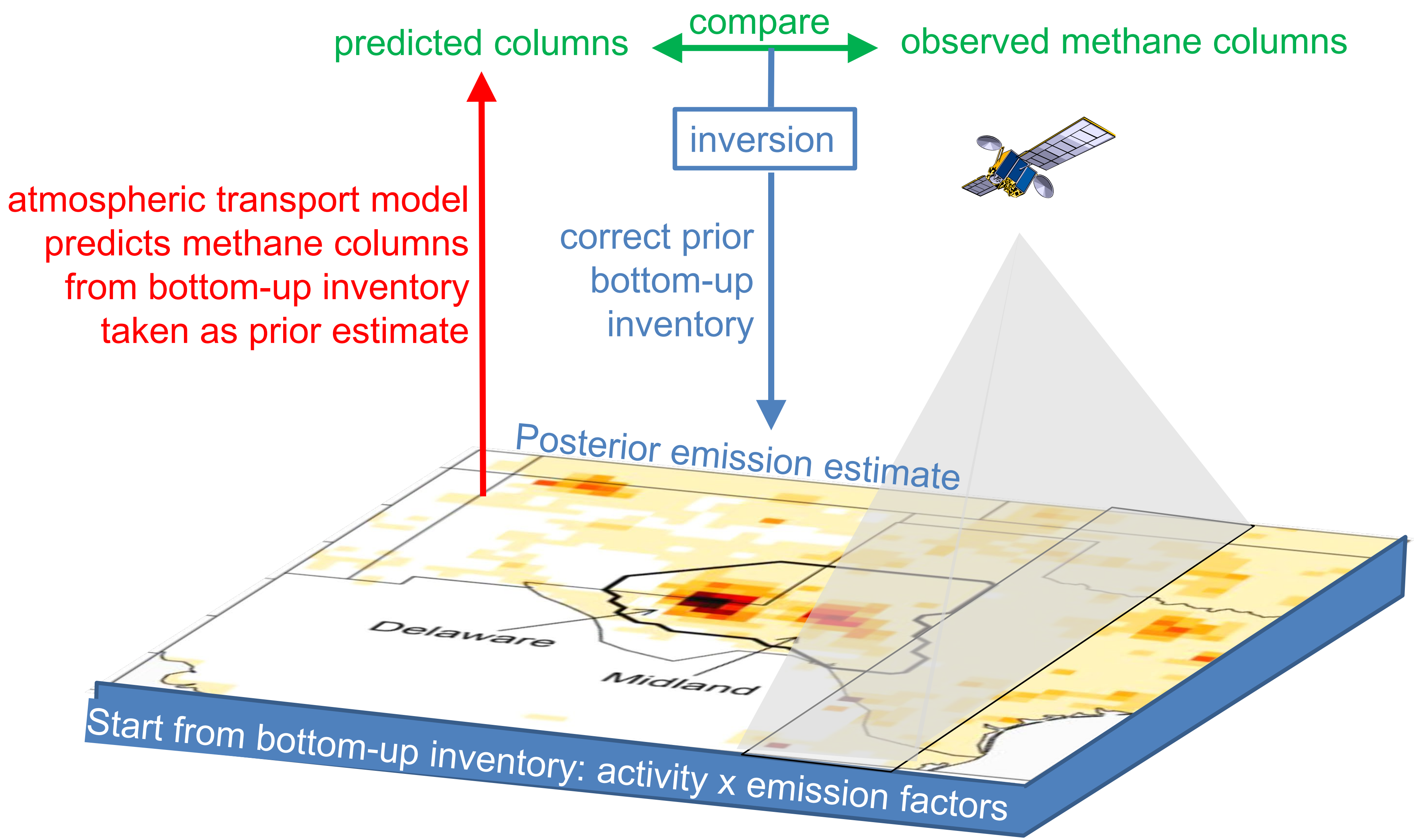


Plumes detected by point source imagers

- Point source imagers detect large point sources (200-25000 kg h^{-1})
- TROPOMI observes <u>total</u> emissions

Jacob et al., ACP 2022

Inversion procedure to infer methane emissions



Inversion uses Bayes' probability theorem:

p (true emissions | observations) ~ p (bottom-up emissions) x p (observations | true emissions)

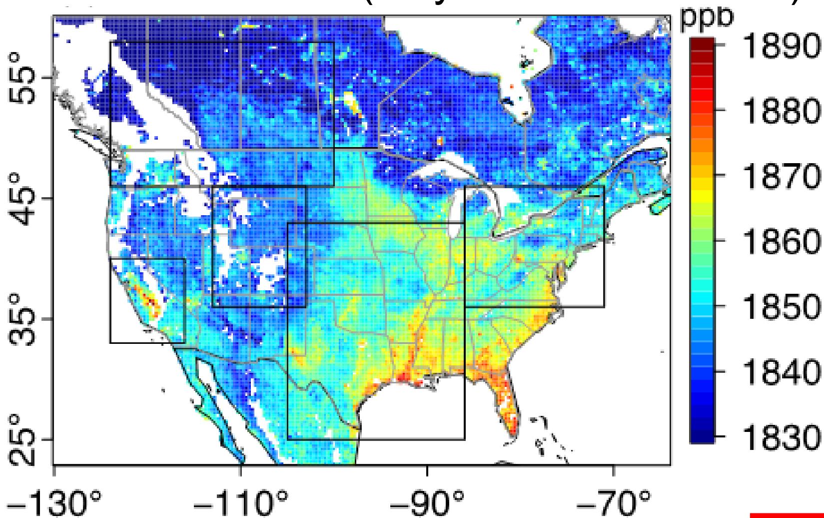
posterior

errors

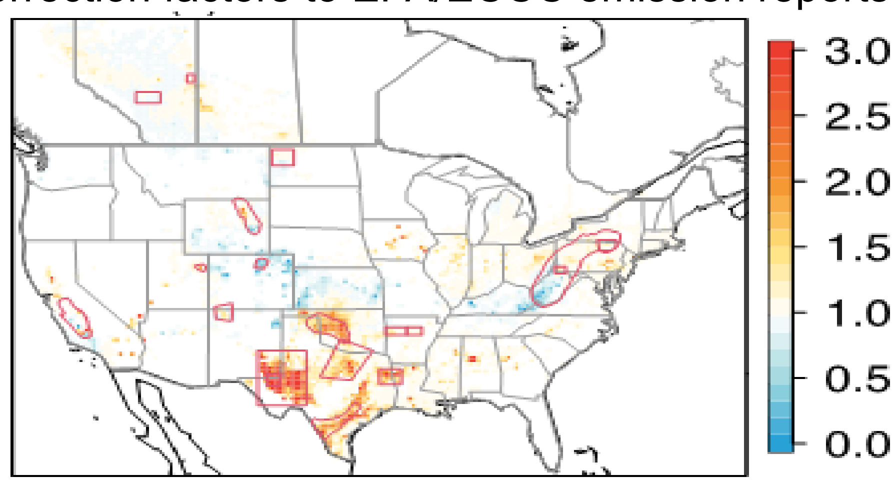
Analytical inversion methodology

- Analytical solution for the Bayesian posterior estimate yields closed-form characterization of posterior errors and information content
- Requires explicit construction of Jacobian matrix for sensitivity of concentrations to emissions; enables inversion ensembles
- Can readily add information from point source observations, ground system networks
- Methods continuously improved by Harvard group members (currently 15 members focusing on methane)

TROPOMI methane (May 2018 – Feb 2020)



Correction factors to EPA/ECCC emission reports



Shen et al., 2022

mature developments feed into the IMI

Integrated Methane Inversion (IMI) on the AWS cloud

Motivation

- Strong interest in quantifying methane emissions with satellites
- TROPOMI data and GEOS-Chem are readily available on the AWS cloud
  → Bring compute to data
- Enable stakeholders to analyze satellite data with advanced inversion algorithms
- Algorithms need to be accessible and transparent

User base

- >50 users in >10 countries
- Growing rapidly
- Endorsed by IMEO and SRON

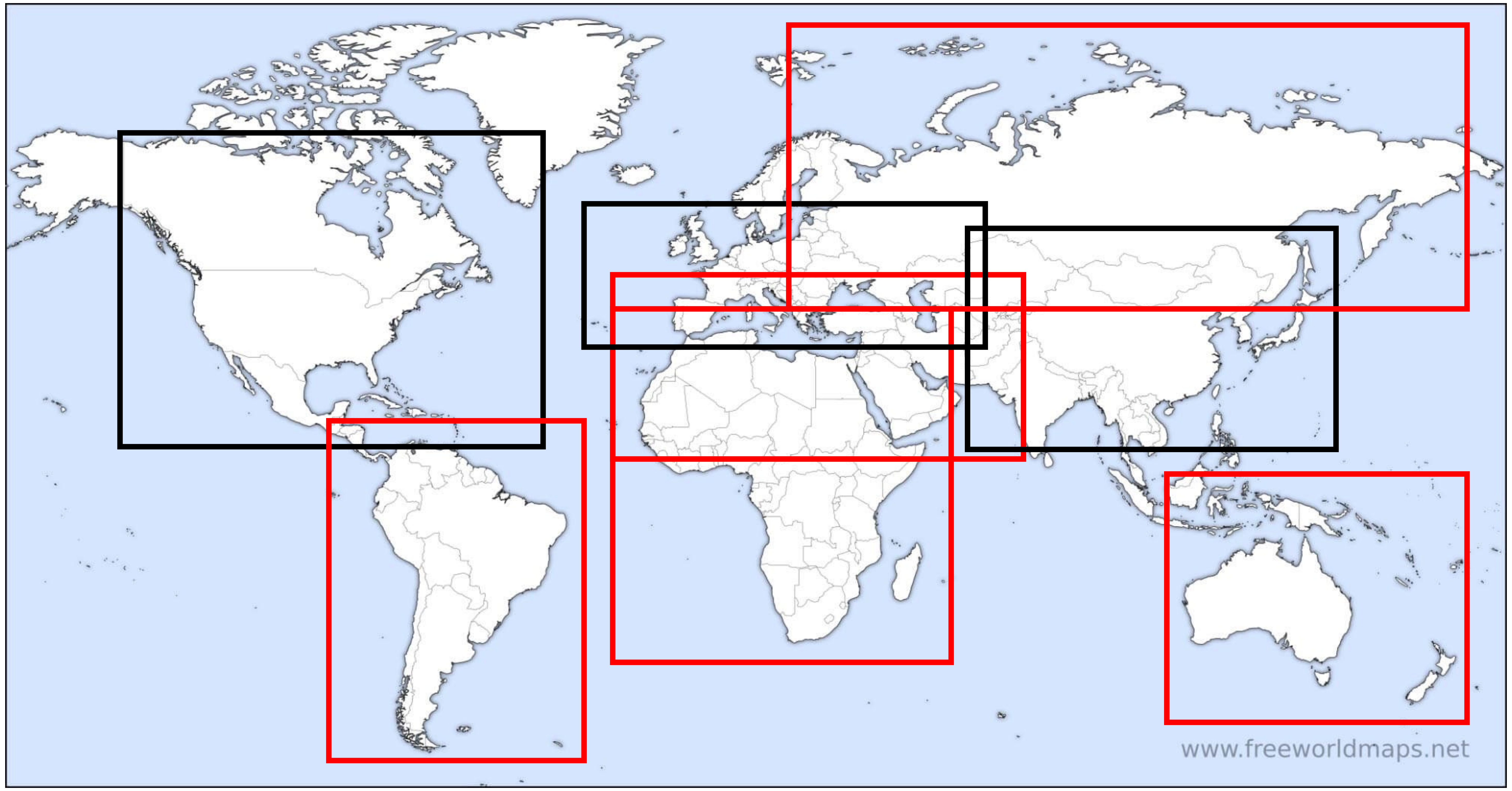
imi.seas.harvard.edu

Integrated Methane Inversion (IMI) on the AWS cloud

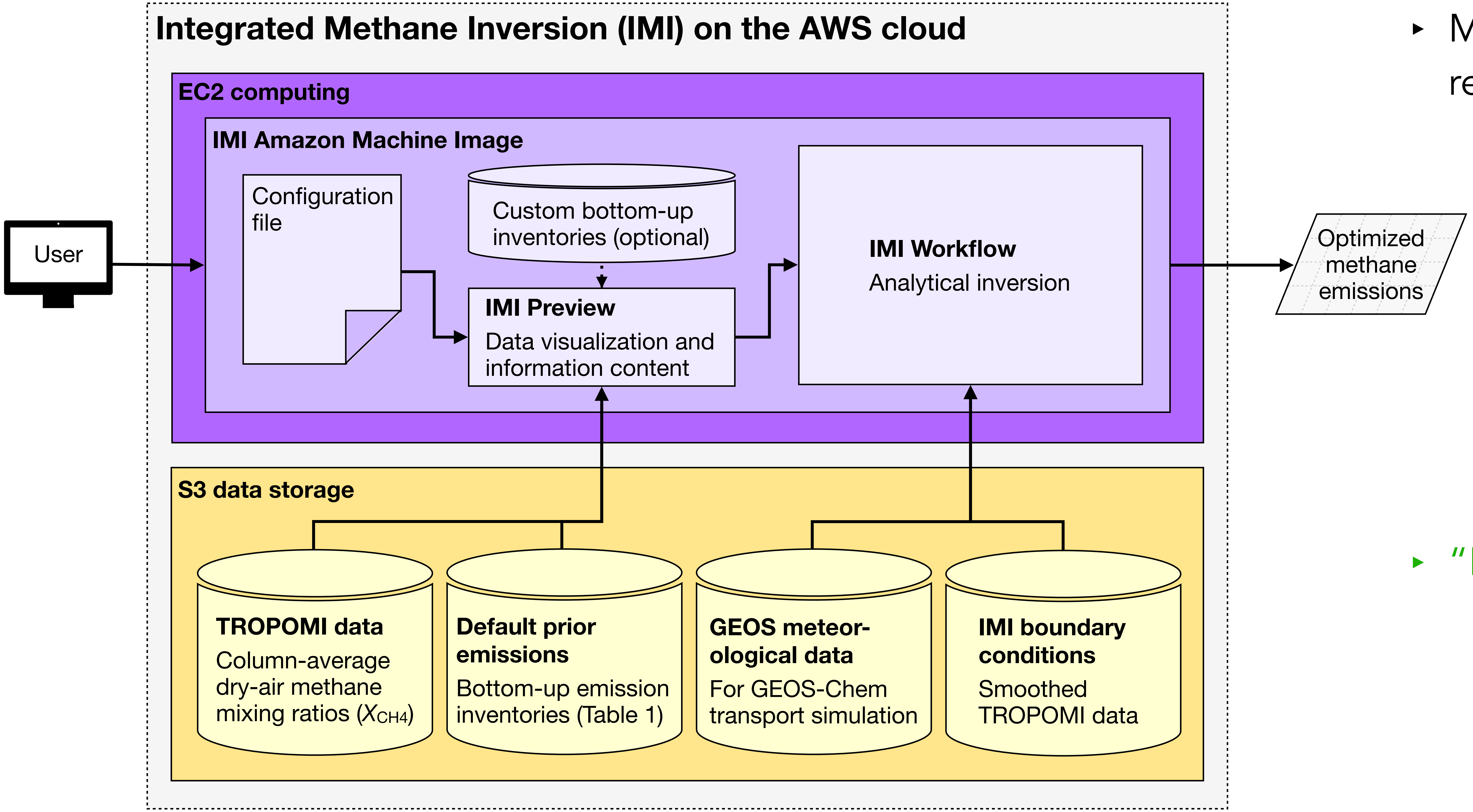
The IMI...

- Uses TROPOMI observations to infer methane emissions on a 25-km or 50-km grid;
- Performs regional methane inversions anywhere in the world;
- Provides an analytical solution to the Bayesian optimization of emissions.

IMI 1.0
IMI 1.1



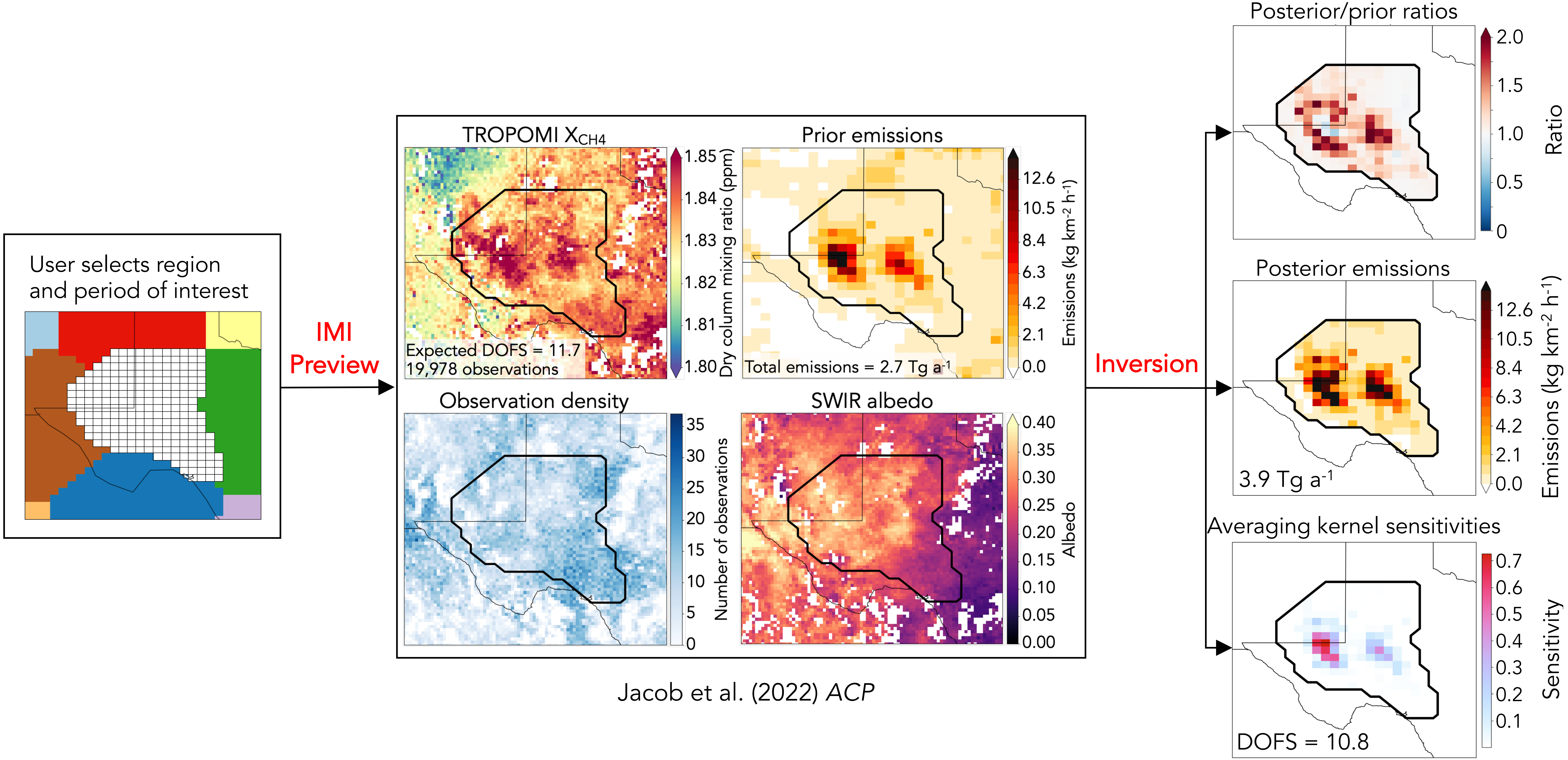
Architecture of the IMI on the AWS cloud



- Makes use of existing AWS cloud resources:
  - GEOS-Chem
  - Prior emission inventories
  - TROPOMI data record
  - New global dataset of boundary condition data for regional methane inversions
- "Bring compute to data"

Varon et al. (2022) *GMD*

Integrated Methane Inversion (IMI) on the AWS cloud



Jacob et al. (2022) *ACP*

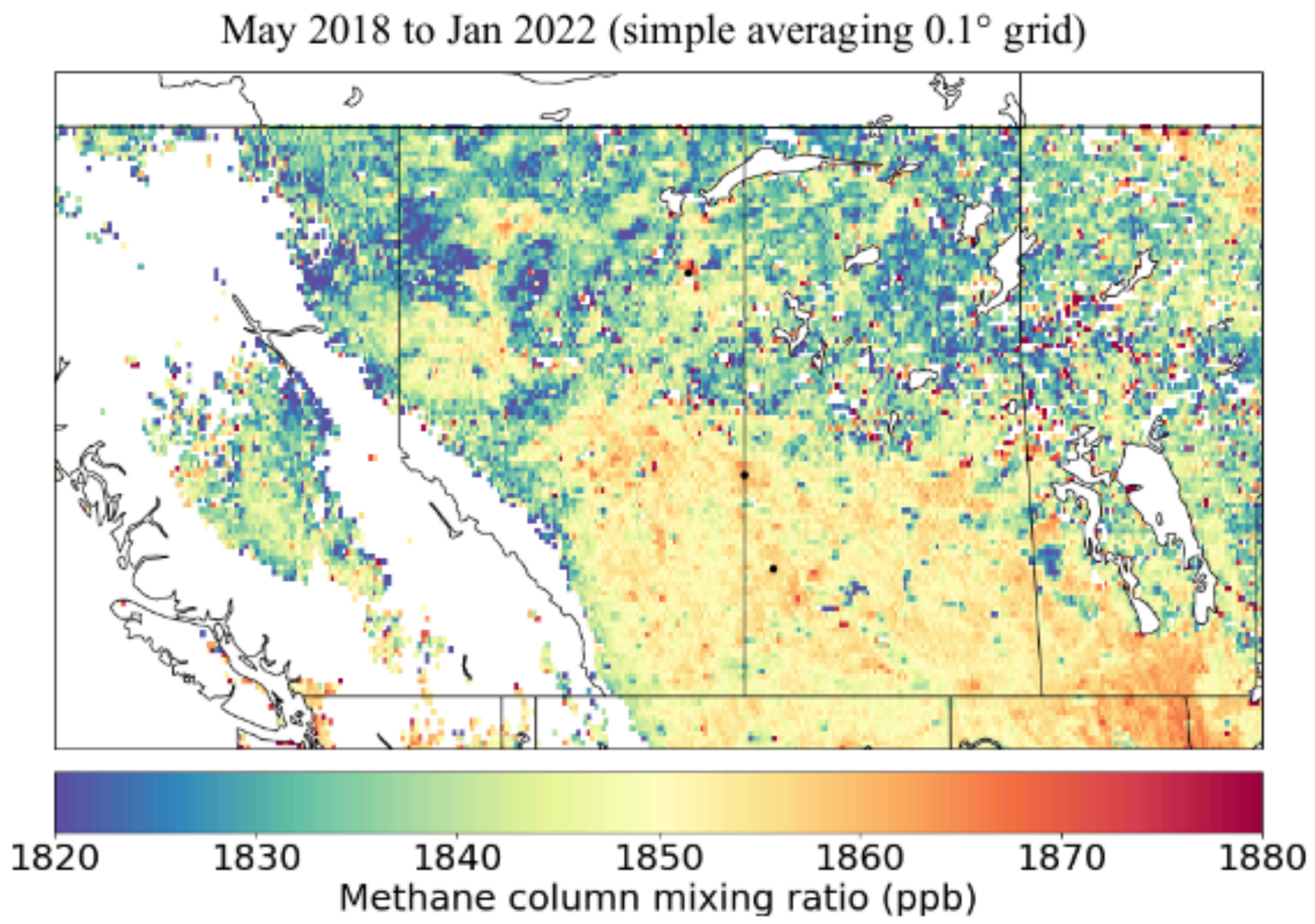
Example applications of the IMI

Some known community applications

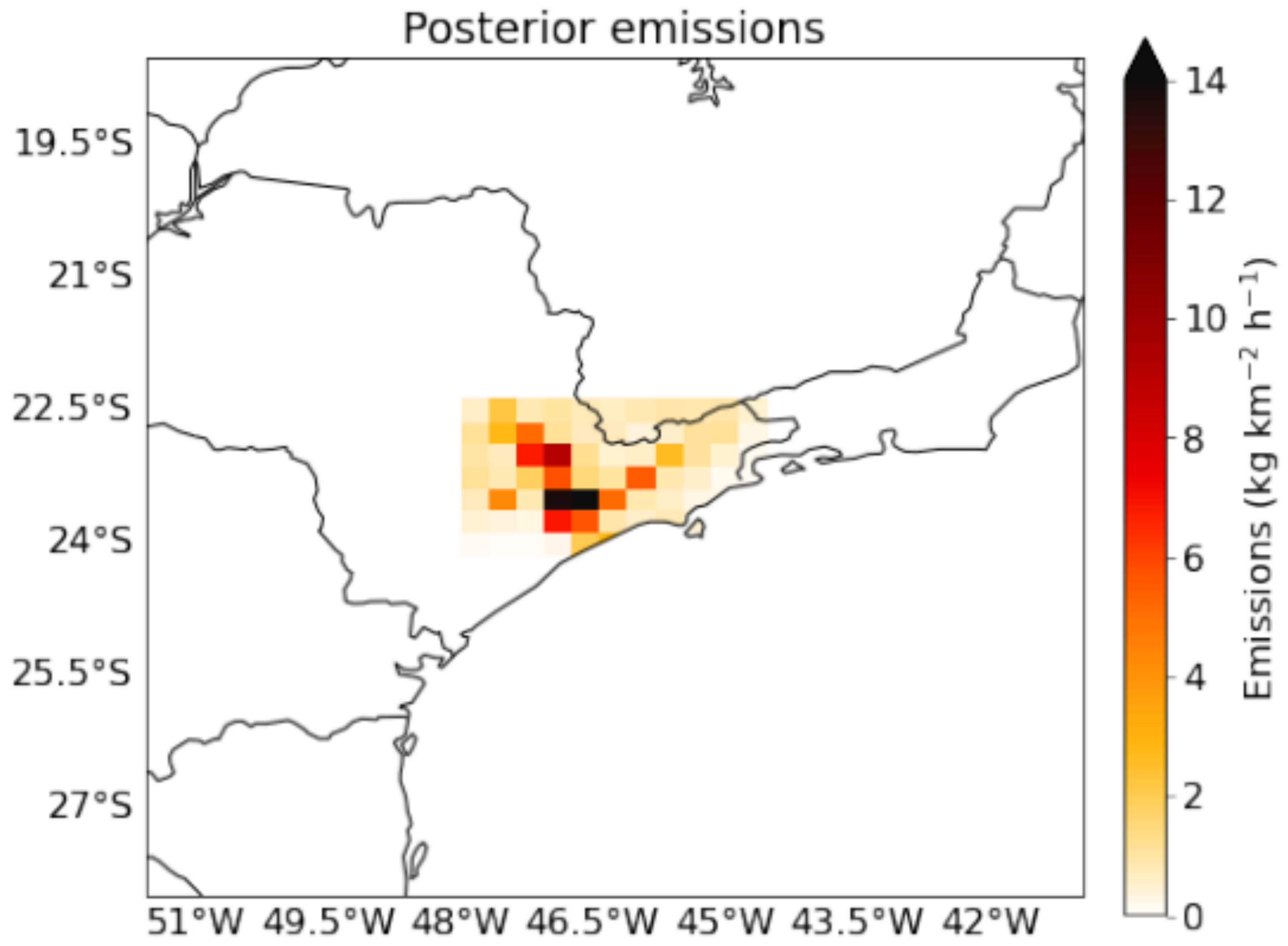
- Canadian oil/gas production regions (Environment & Climate Change Canada)
- Large Canadian cities (C-CORE, Inc.)
- São Paulo, Brazil (University of São Paulo)
- Venezuela (SRON Netherlands Institute for Space Research → Now IMI development partners)

Current applications at Harvard

- Africa (Nick Balasus, Zichong Chen)
- China (Zichong Chen)
- Global Inversions (James East)
- South America (Sarah Hancock)
- Southeast Asia (Haipeng Lin)
- US oil & gas basins (Daniel Varon)



IMI visualization from Sabour Baray (Environment & Climate Change Canada)



IMI visualization from Eduardo Landulfo (University of São Paulo)

IMI development

- **IMI 1.1 - Released**
  - Expand the IMI to new regions
    - Africa, Middle East + North Africa, Oceania, Russia, South America
  - Adoption of TROPOMI super-observations
  - Updates to the latest GEOS-Chem version (14.0.2)
- **IMI 1.2 - In prep.**
  - Smart state-vector clustering for application to large domains
  - Decomposition of source code into discrete components
  - Improved super-observation error characterization
  - Improved representation of offshore emissions
- **IMI 1.X - ongoing development by Harvard/SRON users**
  - Continued development of inversion practices
    - e.g, better representation of prior/observational errors, etc.
  - Continued improvement of prior inventories
    - e.g., incorporate the upcoming gridded EPA inventory for 2018

Future development plans

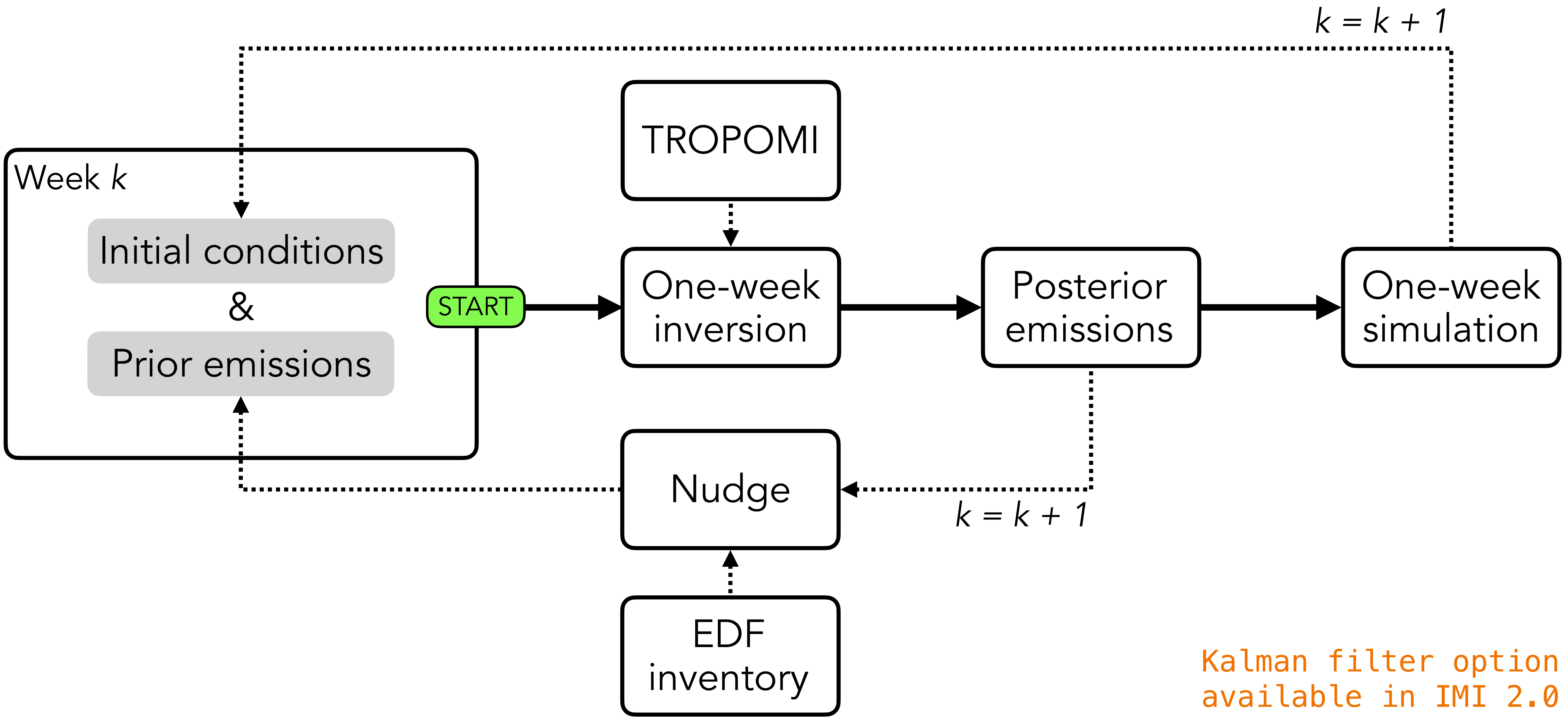
Roadmap to IMI 2.0

- Kalman filter for low-latency monitoring
  - User specifies region/period of interest and desired update frequency (e.g., 1 week, 1 month)
  - IMI performs a series of inversions with chosen update frequency in a Kalman filter framework
- Global inversion capability
  - Including OH optimization
- Incorporate super-emitters into the inversion
  - Super-emitter detections available from SRON (TROPOMI), NASA (EMIT), IMEO (Landsat, S2, PRISMA, etc.)
  - Use those detections for visualization and to define the state vector, prior uncertainties
  - Integrate with weekly Kalman filter capability

Timeline for IMI 2.0 research paper and version release

- **Goal:** Document upgrades from v1.1+ and the three major updates above
- **Submit to:** GMD or JAMES
- **Tentative title:** Integrated Methane Inversion (IMI) 2.0: Continuous near-real-time updates of methane emissions with high resolution by inversion of TROPOMI satellite observations
- **Tentative timeline:**
  - First draft Summer 2023
  - Aim to submit Fall 2023
  - Release IMI 2.0 with submitted paper
  - EMTEC as IMI 2.0 beta testers?

Kalman filter for weekly methane emissions

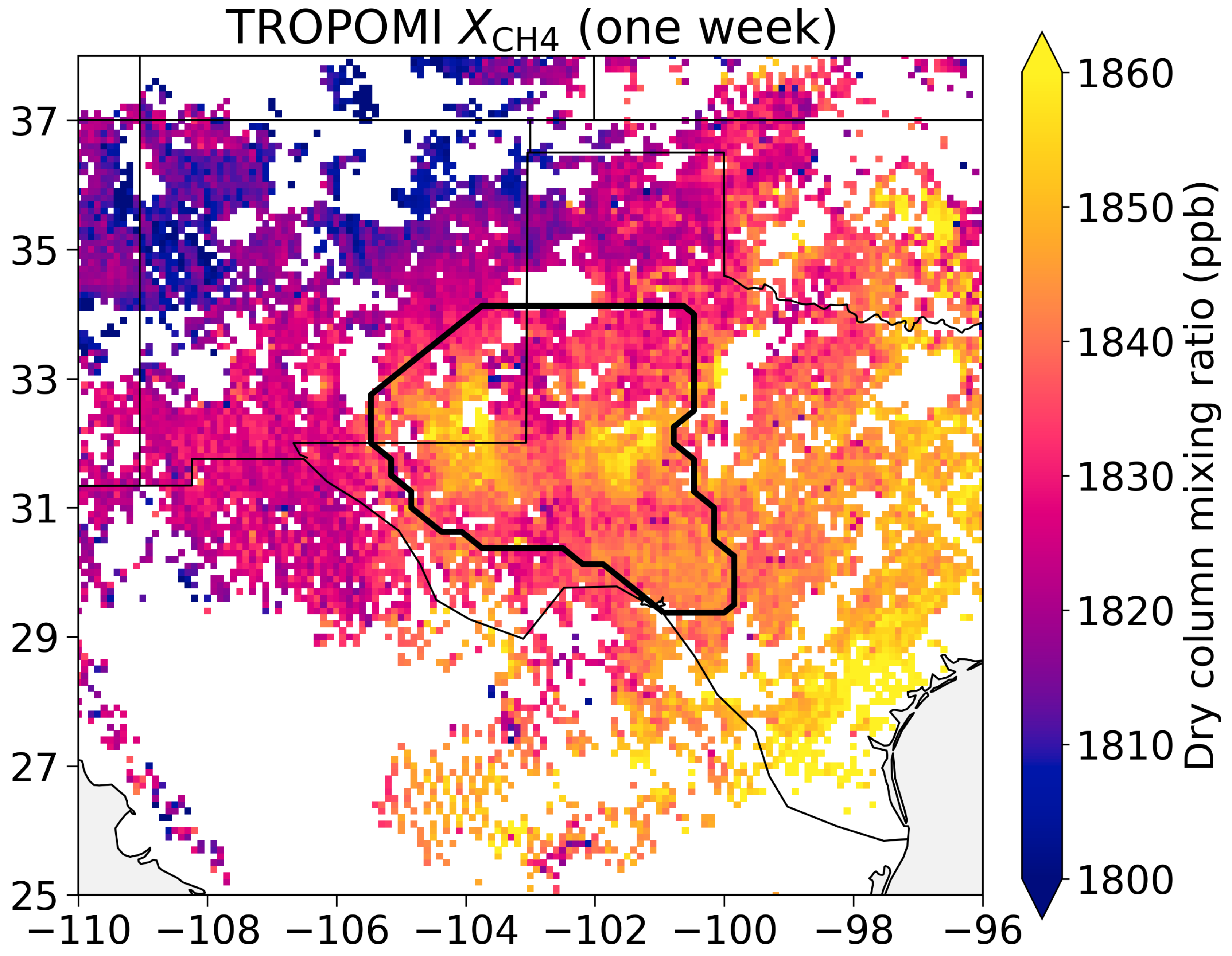


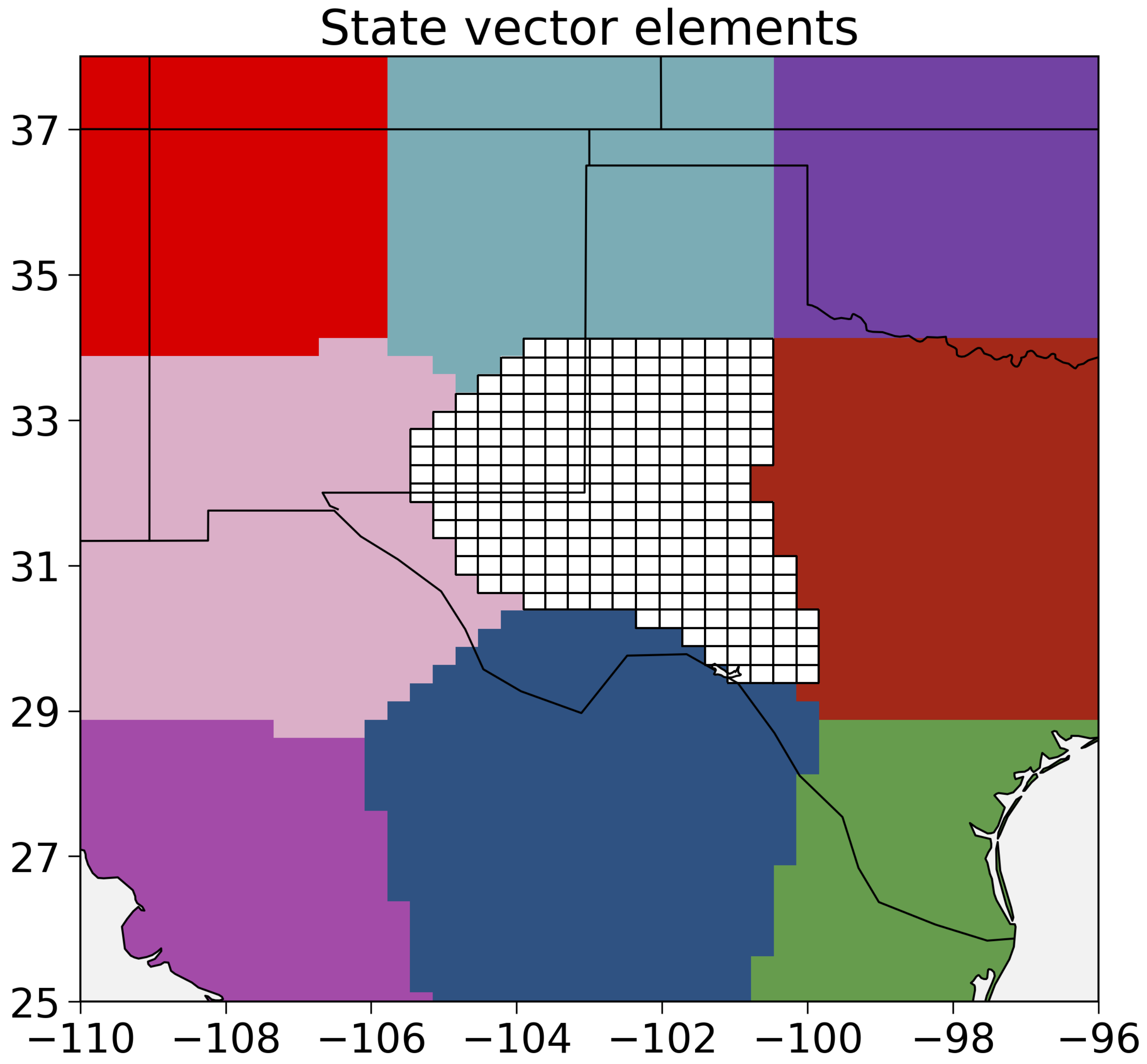
Kalman filter option available in IMI 2.0

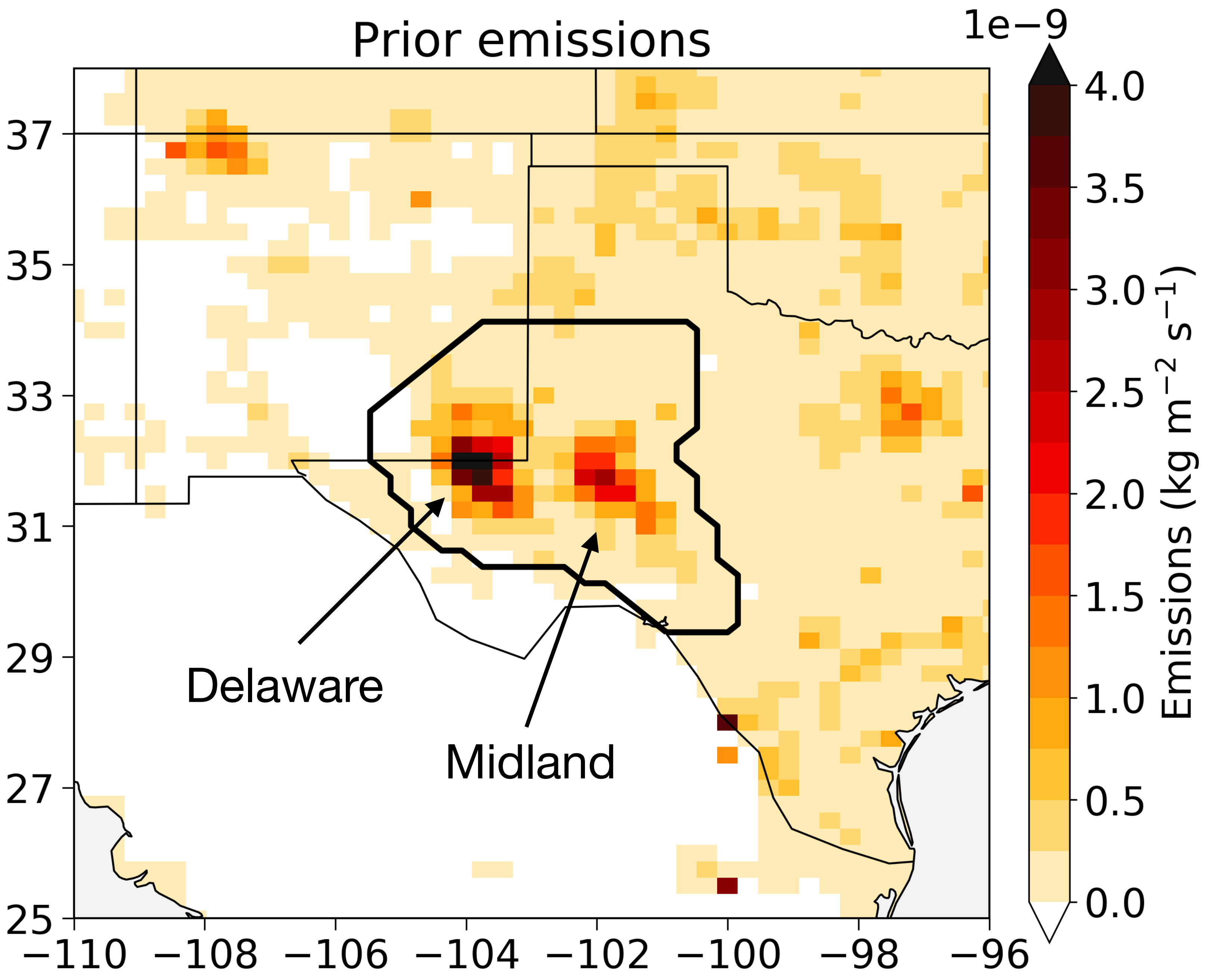
- Fixed prior uncertainty of 50% every week
- 127 weeks from May 2018 to October 2020

Varon et al. (2023) ACP *in review*

Sample inversion setup: TROPOMI observations, state vector, & prior emission estimates







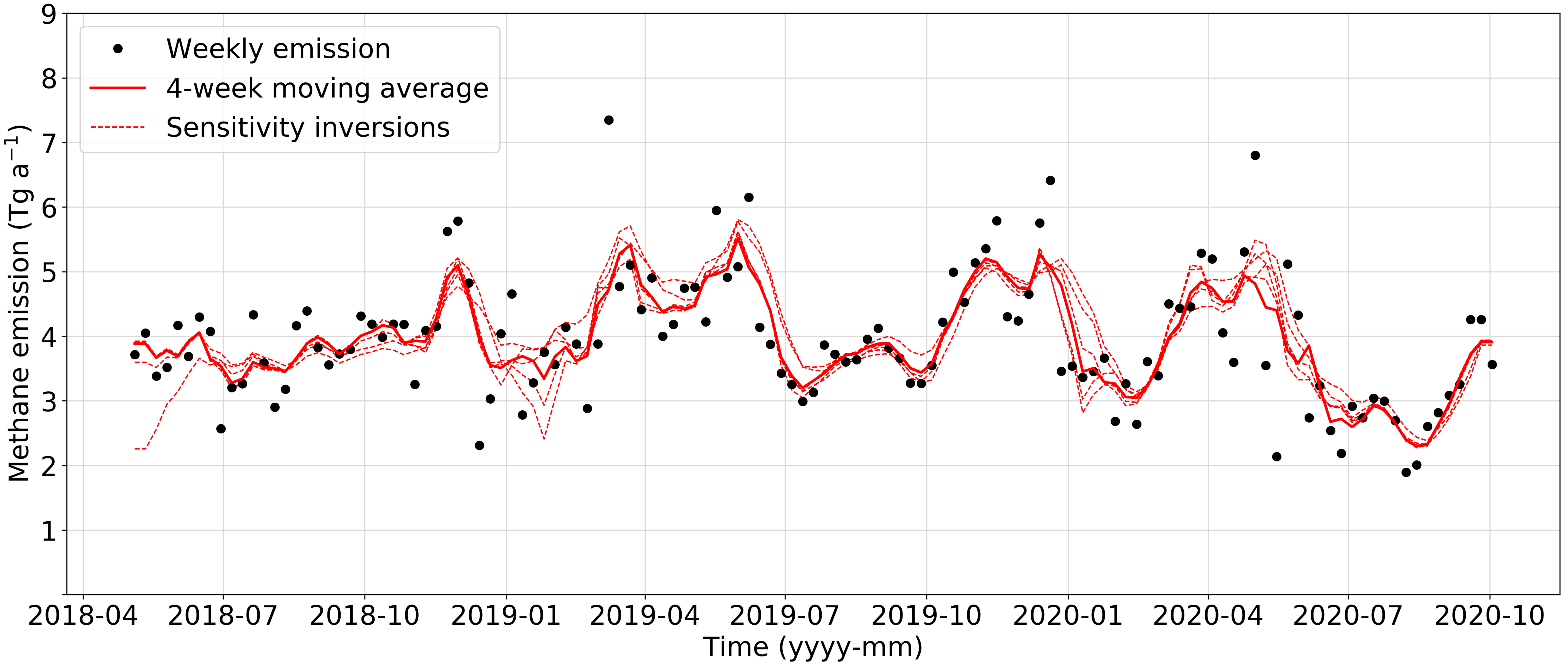
- ~2.5 years of data
- May 2018 – October 2020

- 243 emission elements
- 235 at 0.25°×0.3125° resolution within Permian
- 8 coarse buffer elements

- EDF inventory in basin (2.7 Tg a^{-1})
- Gridded GHGI outside basin (USA)
- GFEI + EDGAR 4.3.2 (Mexico)

Varon et al. (2023) ACP *in review*

Variability of Permian Basin methane emissions from May 2018 to October 2020



- Prototype for national and global near-real-time monitoring of regional methane hotspots

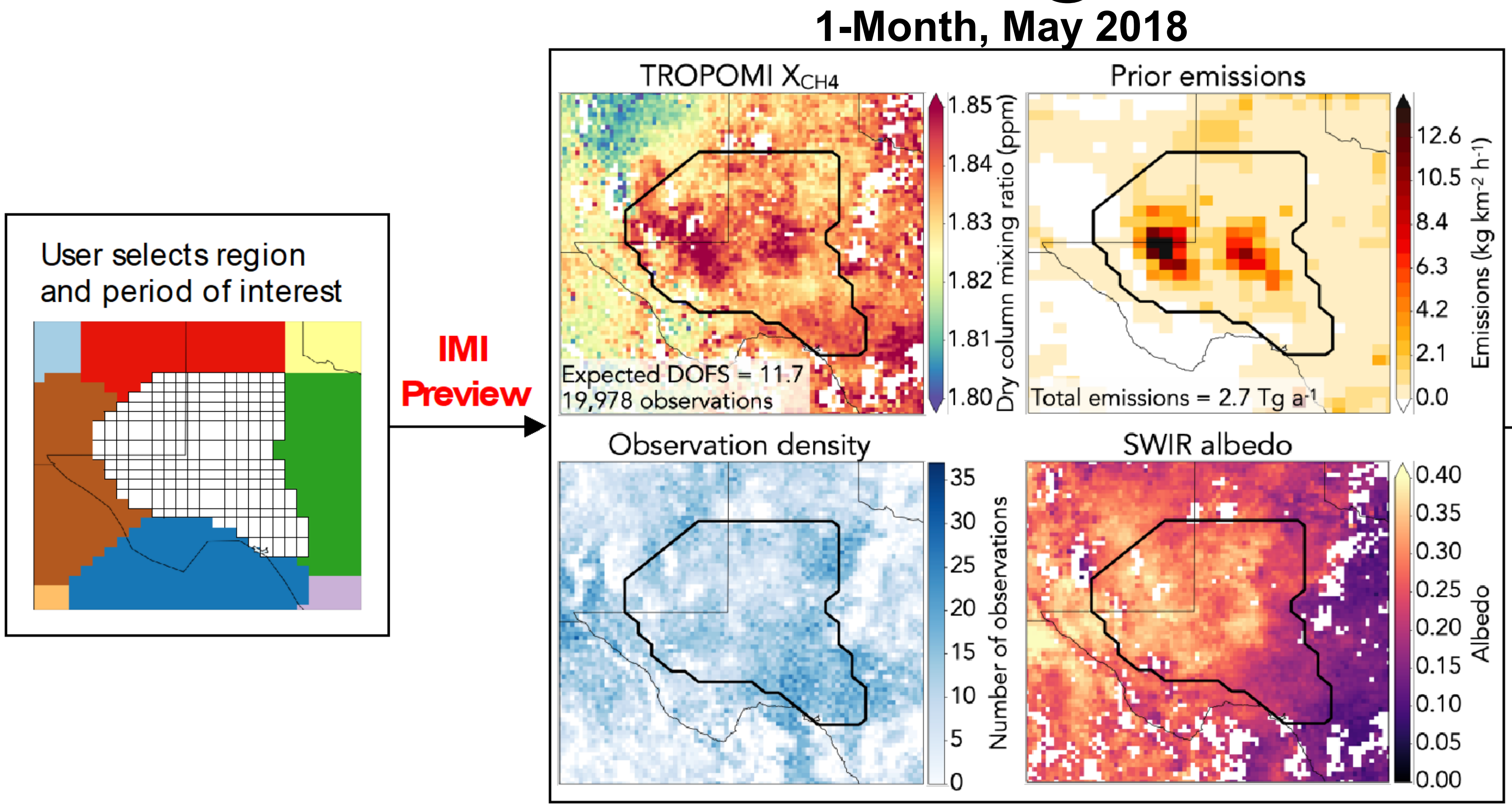
Varon et al. (2023) ACP *in review*

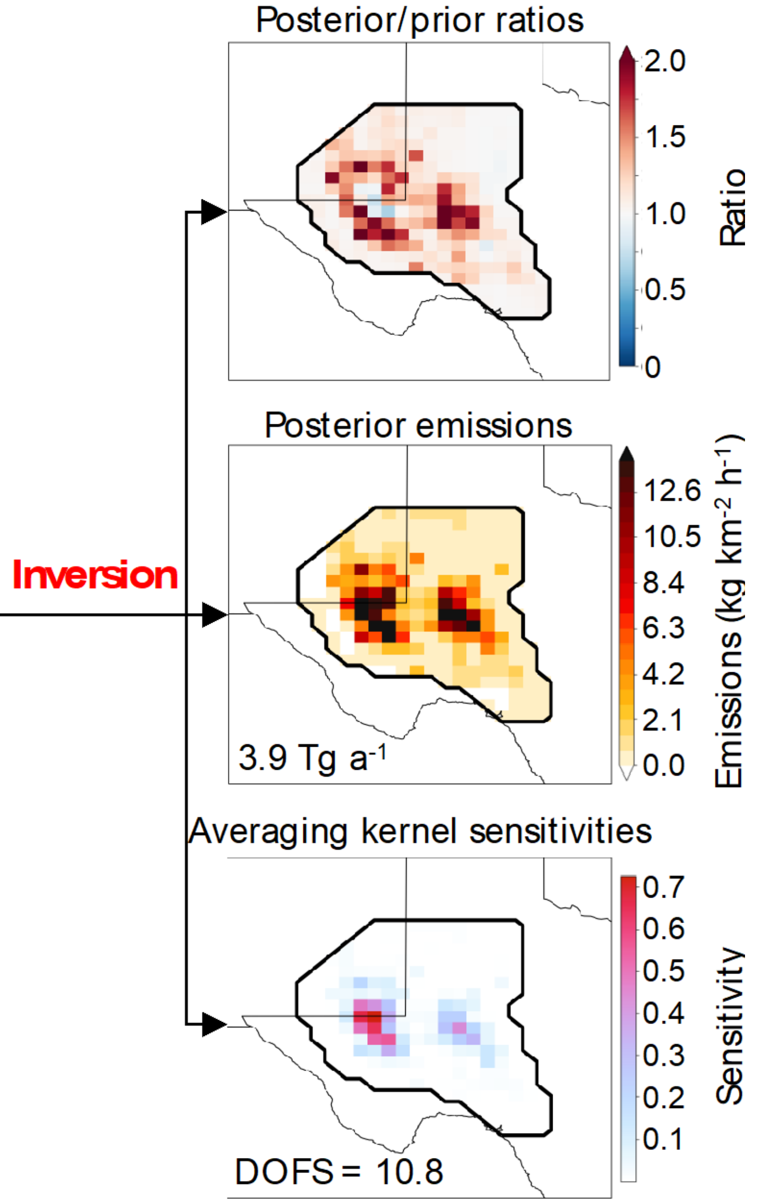
Future development plans

Beyond IMI 2.0

- Extend to CO_2 fluxes: $CH_4 \rightarrow CO_2$
  - NASA Earth Information System – Greenhouse Gases (EIS-GHG)
  - IMI + CO_2 = **ICI** could serve as a platform for the EIS-GHG
- Expand to new satellite instruments (e.g., GOSAT-GW, CO2M)
  - Future instruments will enable CO_2 inversions & denser CH_4 coverage
- Increase inversion resolution
  - Develop a 12-km inversion capability
- Integrate CHEEREIO
  - Would introduce a local ensemble transform Kalman filter (LETKF) capability
- Investigate applications to LDAR
  - Can't detect individual leaks, but could motivate ground/aircraft deployment
- Develop community best practices
  - Guidelines for applying the IMI to different problems

Running the IMI





IMI Preview: User checks data for quality, information content, and estimated cost for full inversion.

Our documentation walks through the setup

Quick start guide

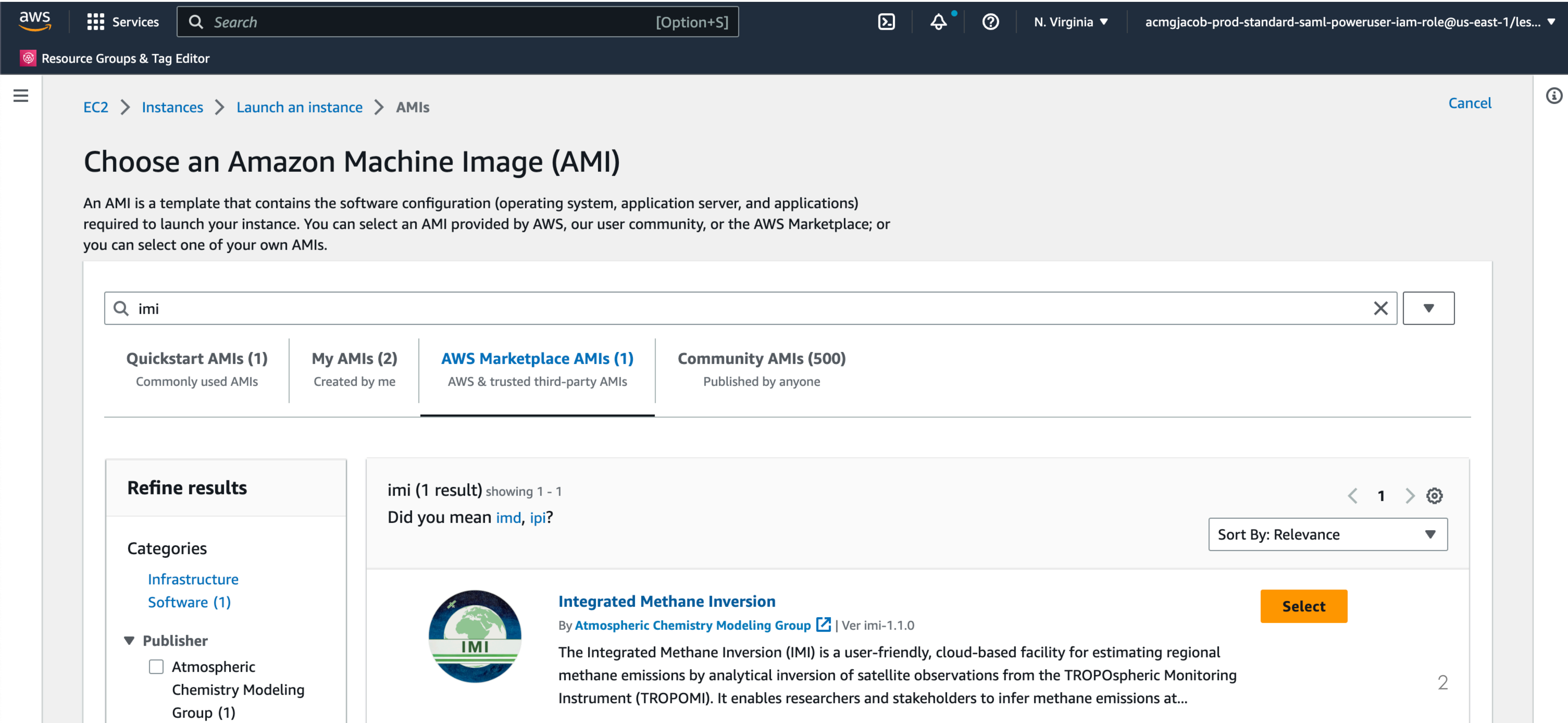
1. Create an Amazon Web Services (AWS) account

If you do not already have an AWS account, you'll need to sign up for one. Go to http://aws.amazon.com and click on "Create an AWS Account" in the upper-right corner:

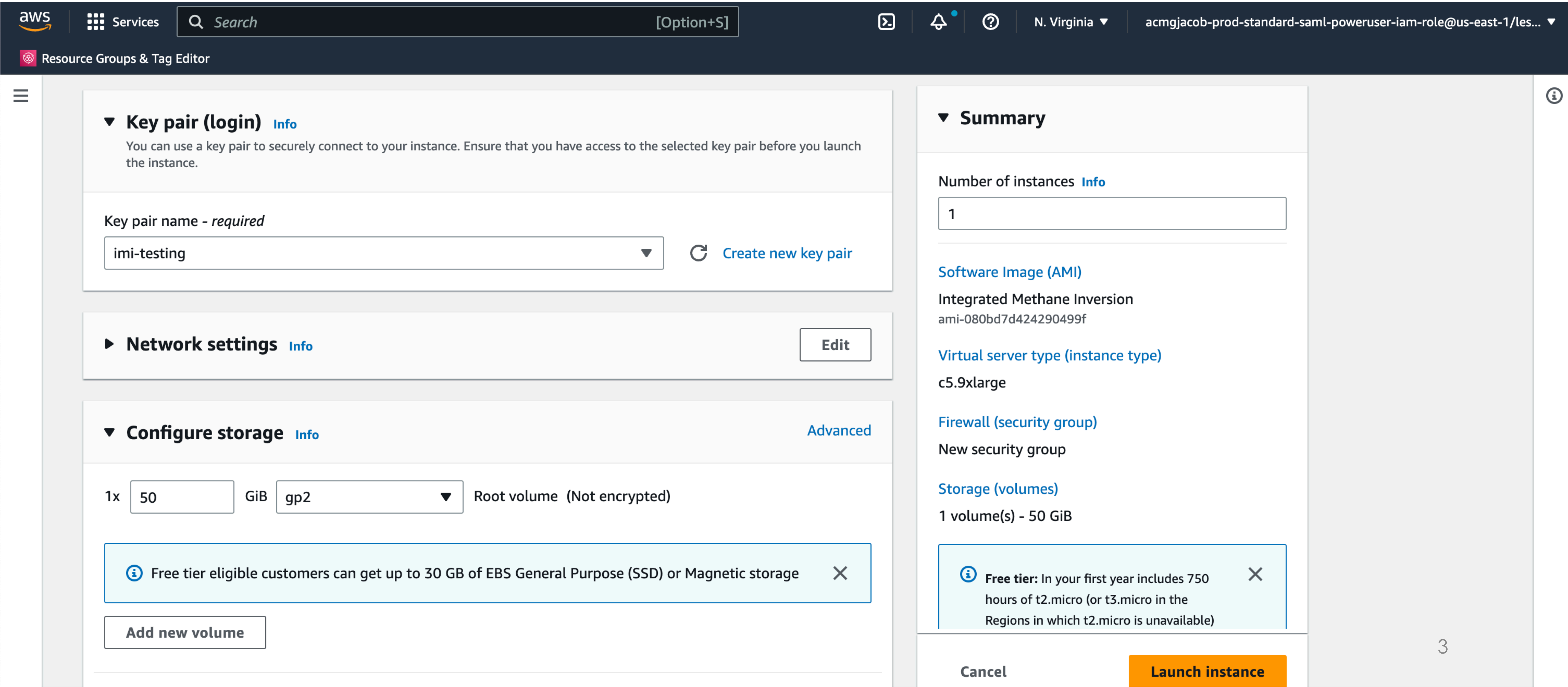
You'll need to enter some basic personal information and a credit card number.

Running the IMI is relatively inexpensive (usually on the order of USD $10-$100). The cost depends on the length of the inversion period, the size of the inversion domain, how long you retain your compute instance after completing the inversion, and how you store the final results.

Launch an IMI Instance



Configure Instance Settings



Login and edit the IMI config file

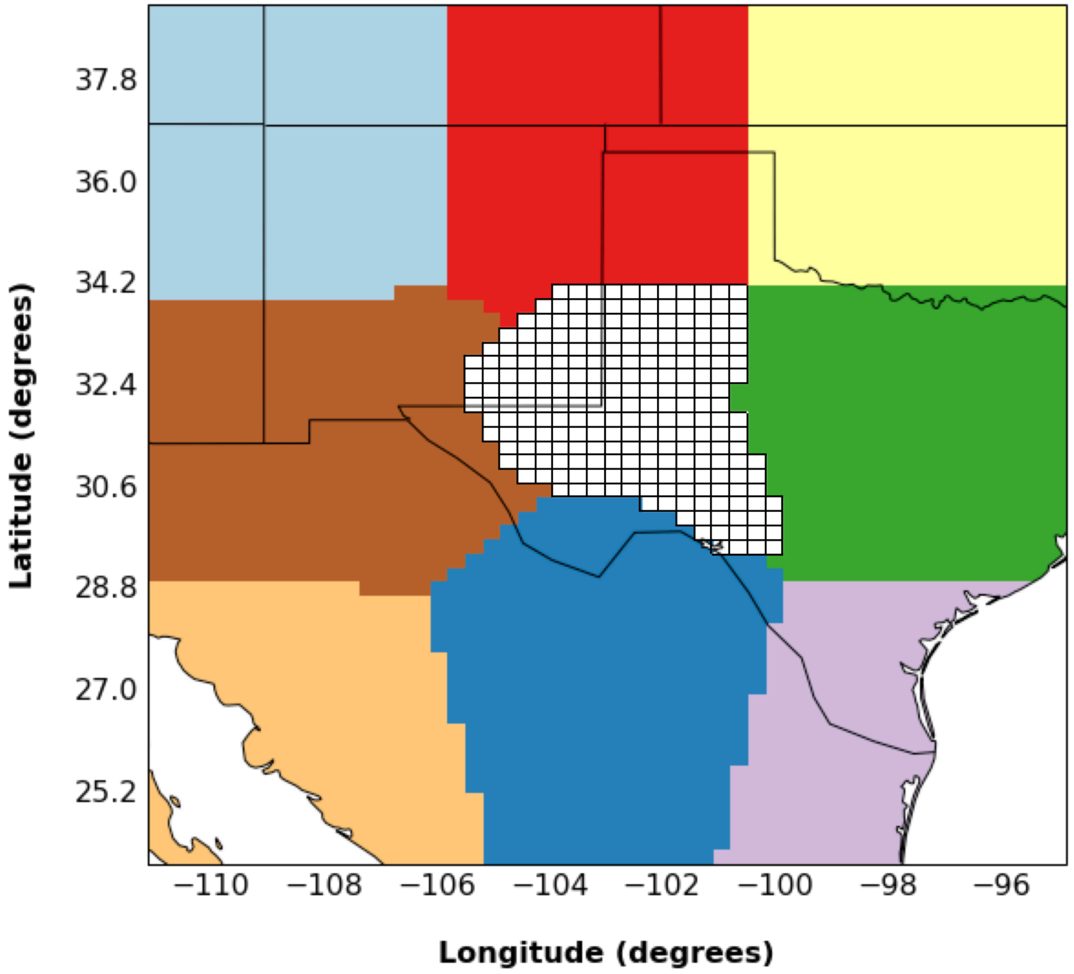
```
## IMI configuration file
## Documentation @ https://imi.readthedocs.io/en/latest/getting-started/imi-config-file.html

## General
RunName: "Test_Permian_1week"
isAWS: true

## Period of interest
StartDate: 20180501
EndDate: 20180508
SpinupMonths: 1

## Region of interest
##   These lat/lon bounds are only used if CreateAutomaticRectilinearStateVectorFile: true
##   Otherwise lat/lon bounds are determined from StateVectorFile
LonMin: -105
LonMax: -103
LatMin: 31
LatMax: 33
```

Select a region of interest

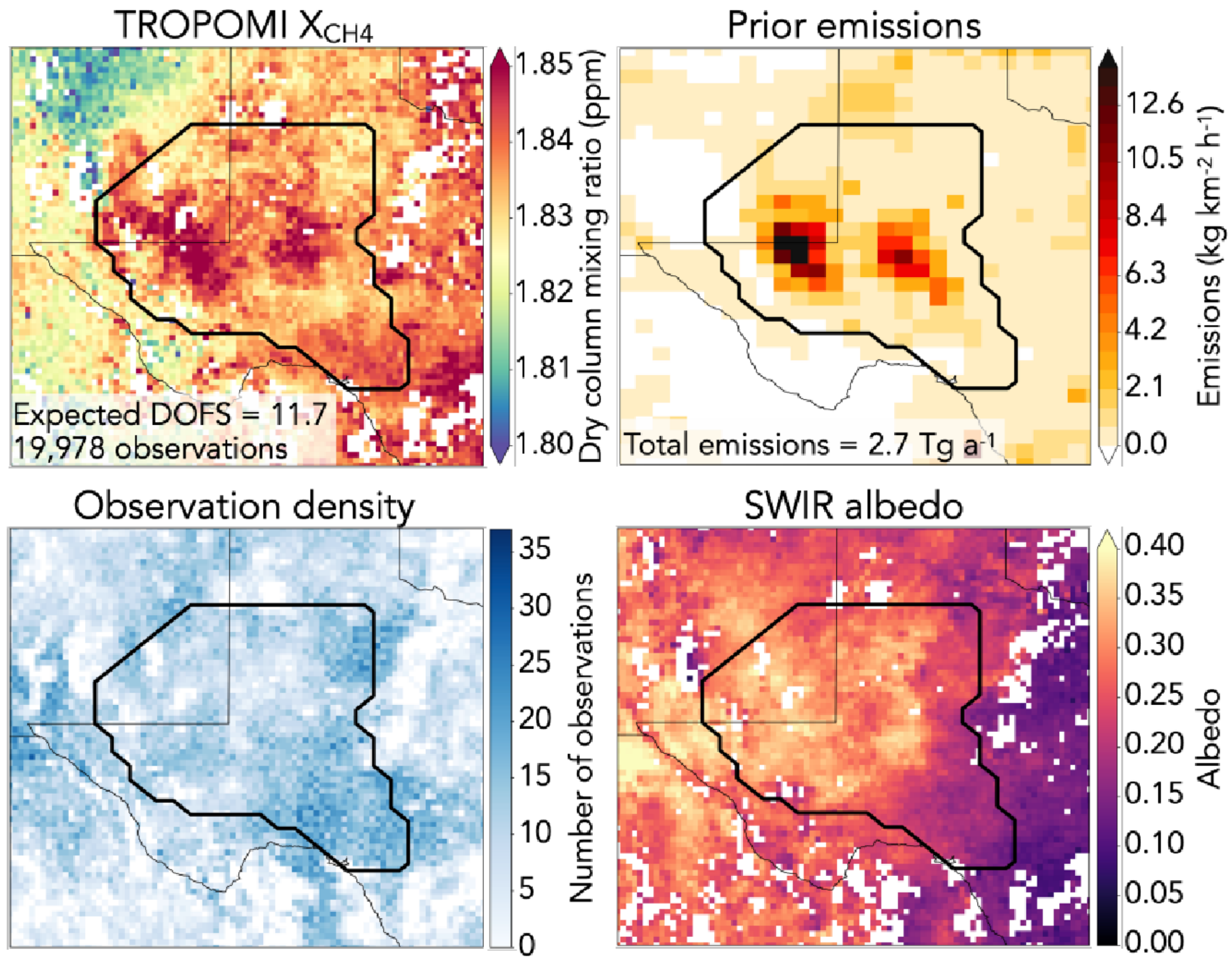


Single command to run the IMI

```
$ sbatch run_imi.sh
```

Review the IMI Preview

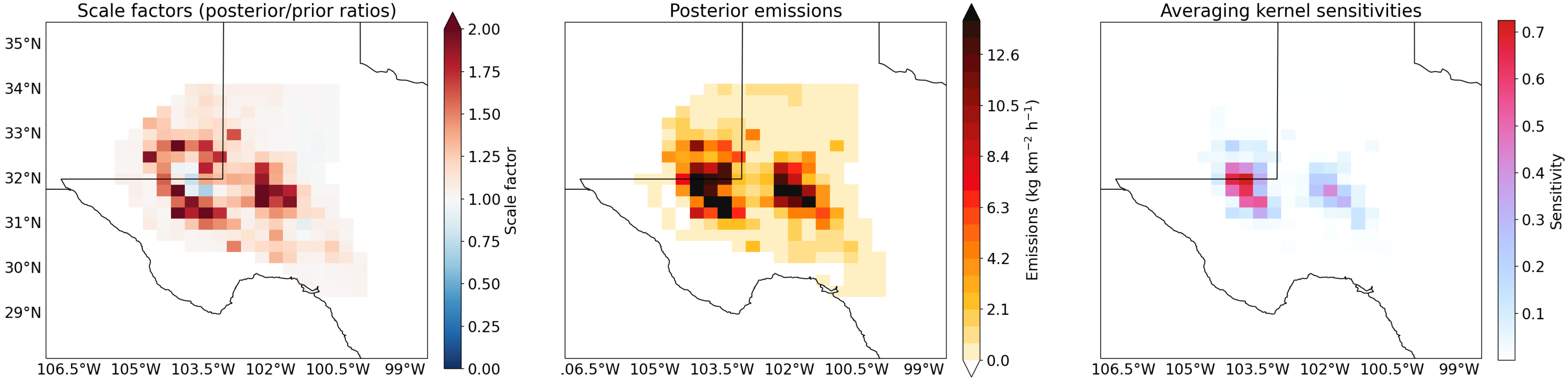
- Check the expected quality of the inversion and cost
- Preview can be run with essentially no cost
- If satisfied, proceed with the inversion



Expected cost of the inversion: ~$20

Visualize Inversion Results

- Premade visualization notebook for plotting results



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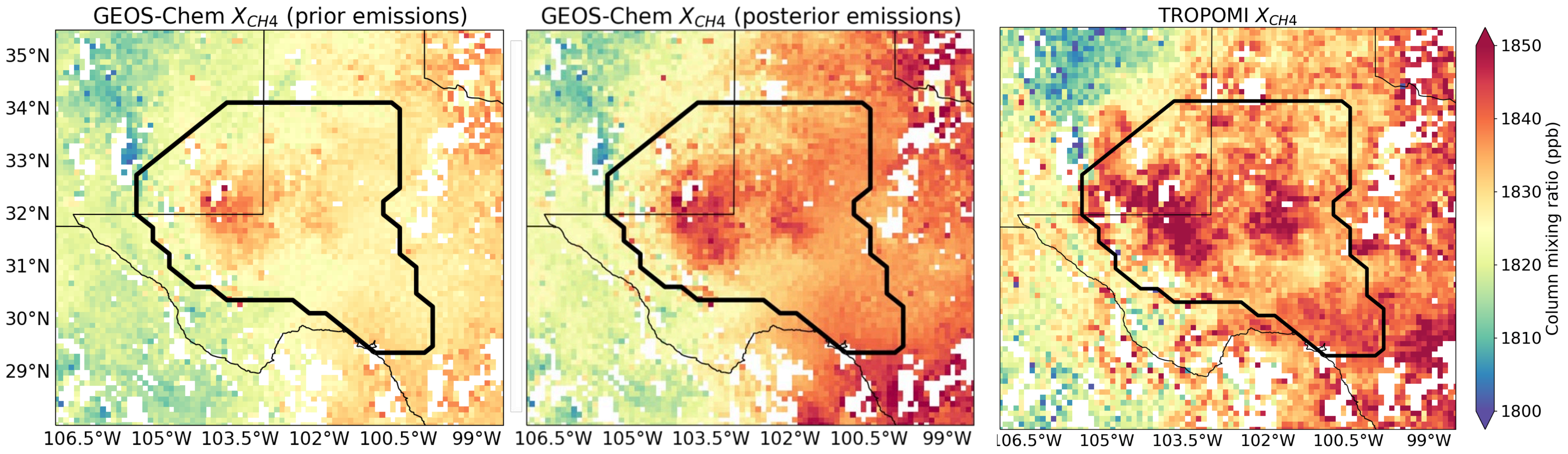
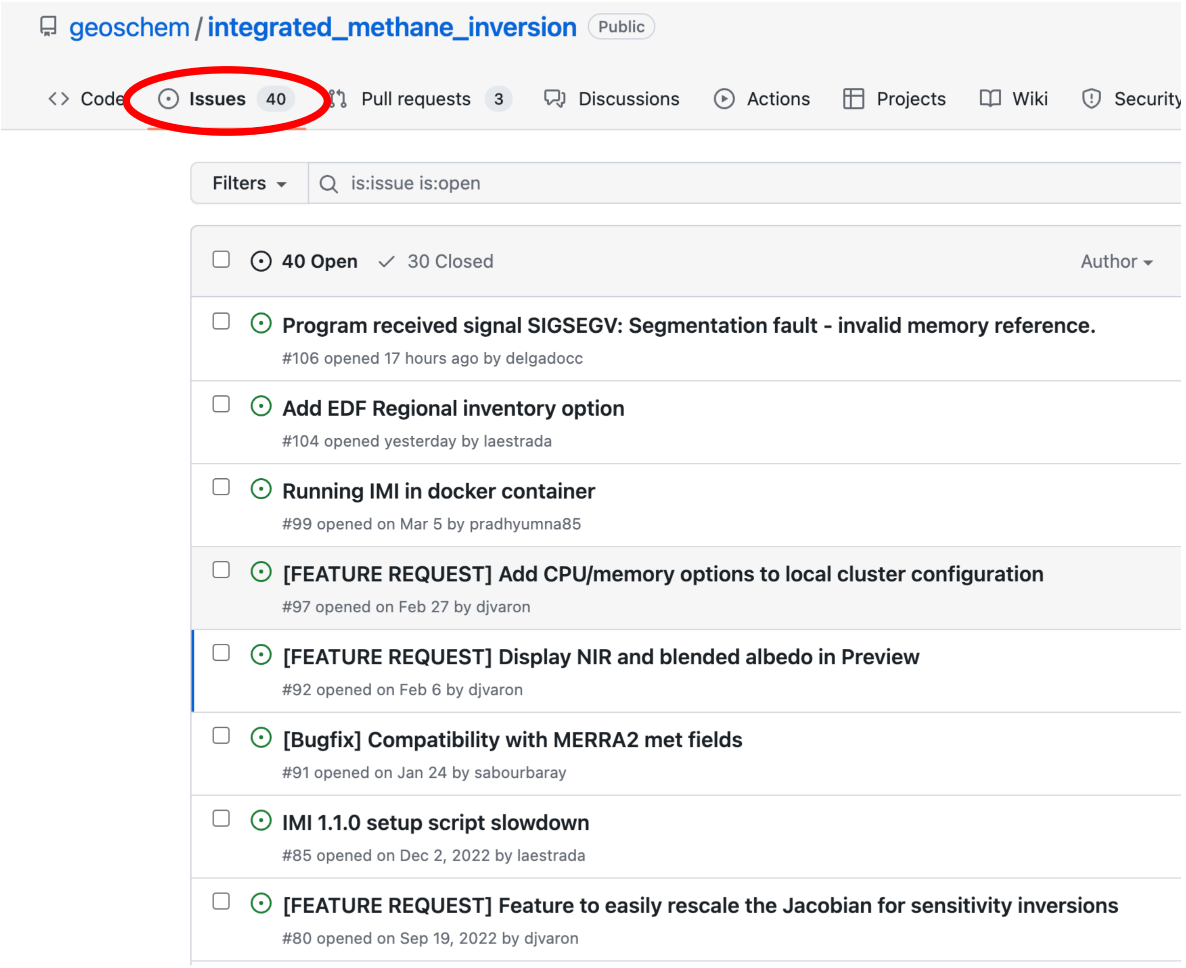


IMI current limitations and future work

- Large domains have high computational expense
- 25 km resolution (hopefully 12 km soon)
- Limited to onshore regions
- Observational data is sparse at high latitudes
- Does not include point source information



NASA's Earth Information System

EIS Mission: To produce and deliver accessible, actionable information on the whole Earth System, powered by NASA's best observations and models

- Integrate NASA's observations and modeling capabilities to produce new science and support decision making in four key areas:

Fire

Freshwater

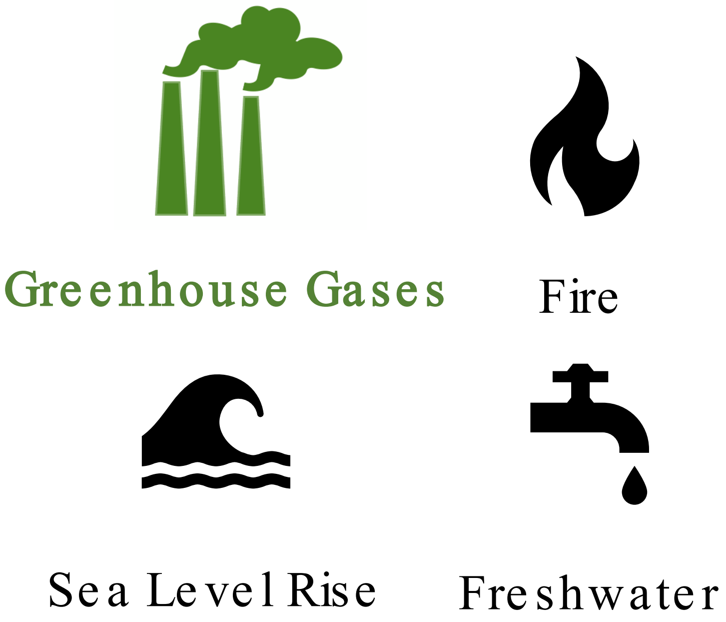
Sea Level Rise

Greenhouse Gases

IMI integration into NASA's Earth Information System

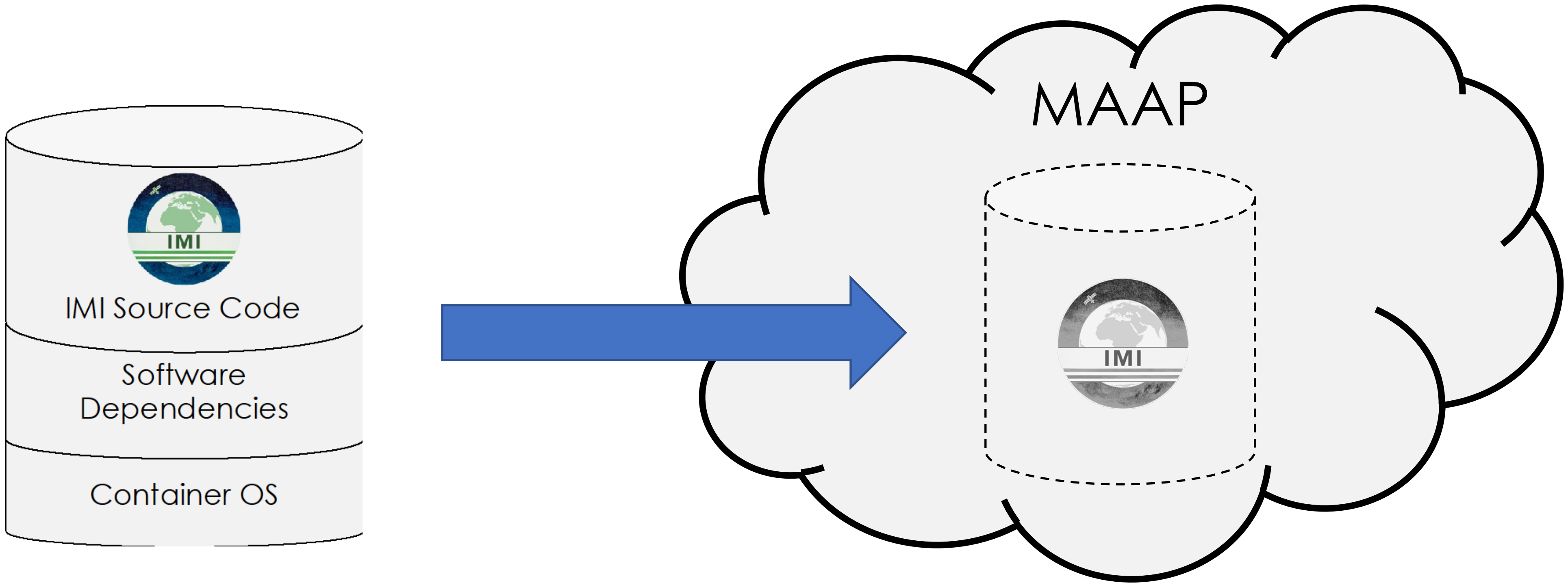
EIS Mission: To produce and deliver accessible, actionable information on the whole Earth System, powered by NASA's best observations and models

- Integrate NASA's observations and modeling capabilities to produce new science and support decision making in four key areas →
- Working with the EIS team to bring the IMI into the EIS cloud framework
- Excitement on the potential for extending the IMI to CO_2



IMI integration into the Earth Information System

- Developing a Dockerized IMI to allow compatibility with EIS and other systems
  - Prepackaged software environment for easy installation and automation



IMI/EIS integration benefits

- Sharing of near real time monitoring of emissions on open access platform
- Opportunities for rapid response to changes in emissions