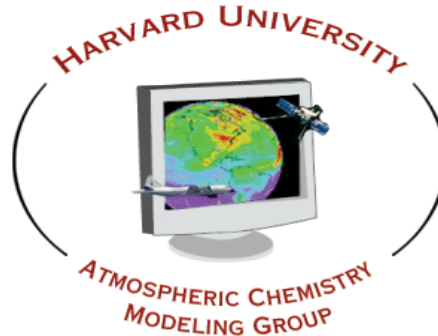


Integrated Methane Inversion (IMI) on the AWS cloud: a tool to infer greenhouse gas fluxes from satellite observations

Daniel Varon, Lucas Estrada, Melissa Sulprizio, Daniel Jacob



ExxonMobil project managers: Cynthia Randles, Felipe Cardoso Saldaña, Bryan Mignone

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.

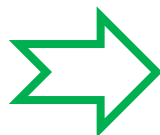
A highly productive 8-year relationship with ExxonMobil

- 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

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

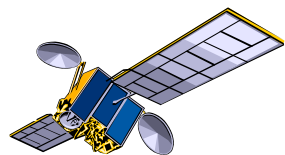
- enable global inversions
- increase spatial resolution
- Integrate point source data
- enable real-time monitoring



Longer-term vision

- Extend to multi-satellite fleet and to CO₂
- 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



Satellites

Different platforms have complementary attributes of continuity, coverage, precision



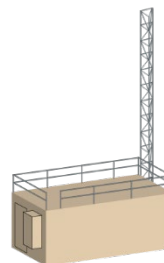
Aircraft



On-road vehicles



Transport model and other analytics to infer surface fluxes (inversions)



Ground stations

in space
scheduled
canceled

MethaneSAT

GOSAT-GW

TROPOMI

GOSAT

Sentinel-5

Area flux
mappers

Regional/global mapping
0.1-10 km pixels
high precision

GeoCarb

CO2M

MERLIN

Carbon
Mapper

EnMAP

EMIT

Individual plumes
< 60 m pixels

PRISMA

GHGSat

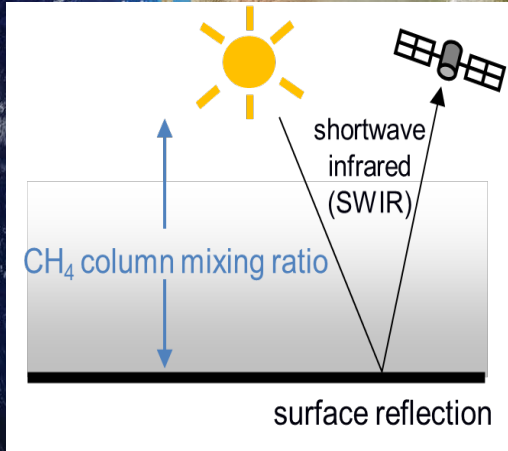
Point source
imagers

Methane Observations from Space

Sentinel-2

WorldView-3

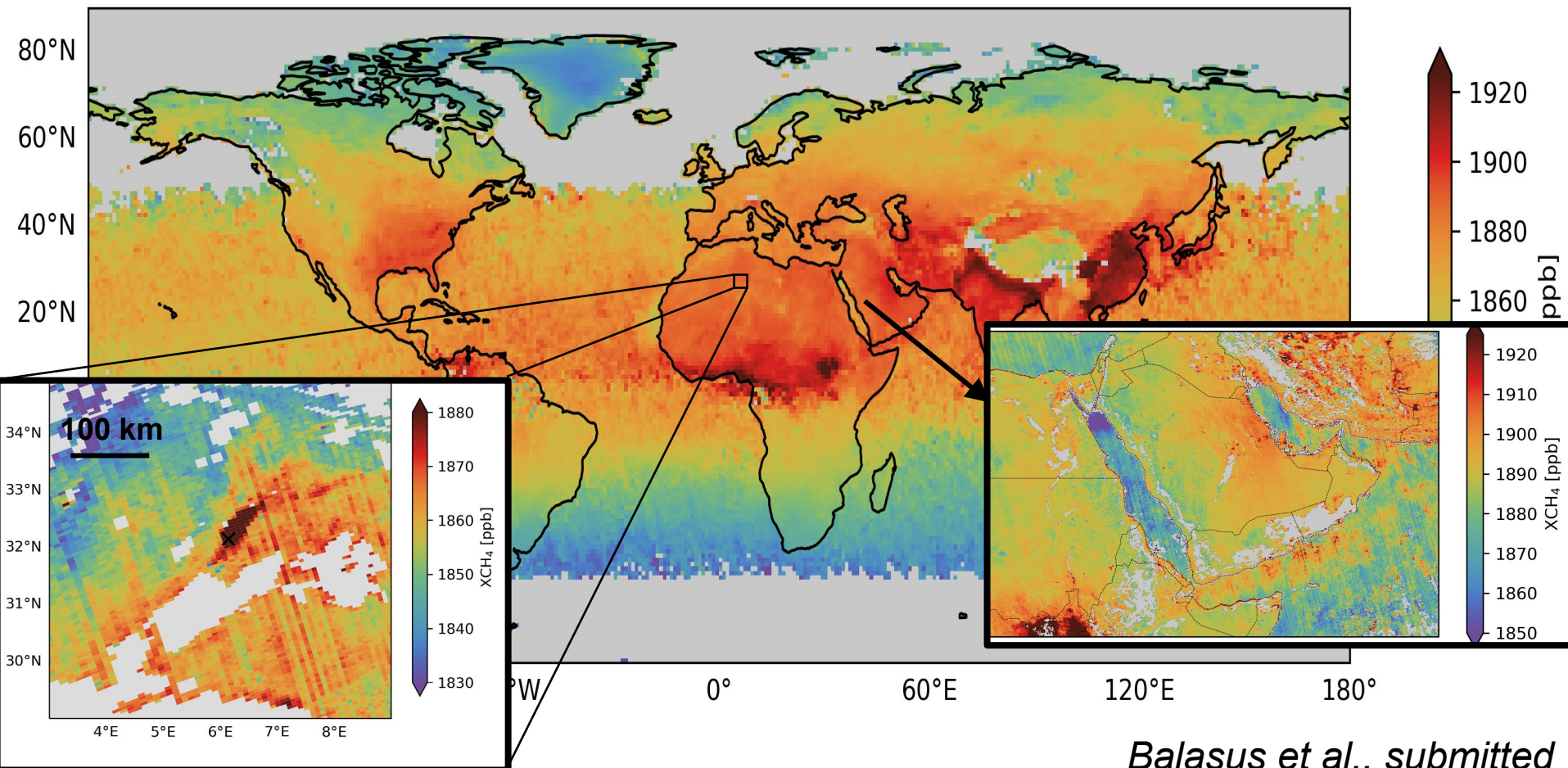
Landsat



TROPOMI (2018-): global daily mapping
with $5.5 \times 7 \text{ km}^2$ pixels, 0.6% precision

Over 100 million
observations per year

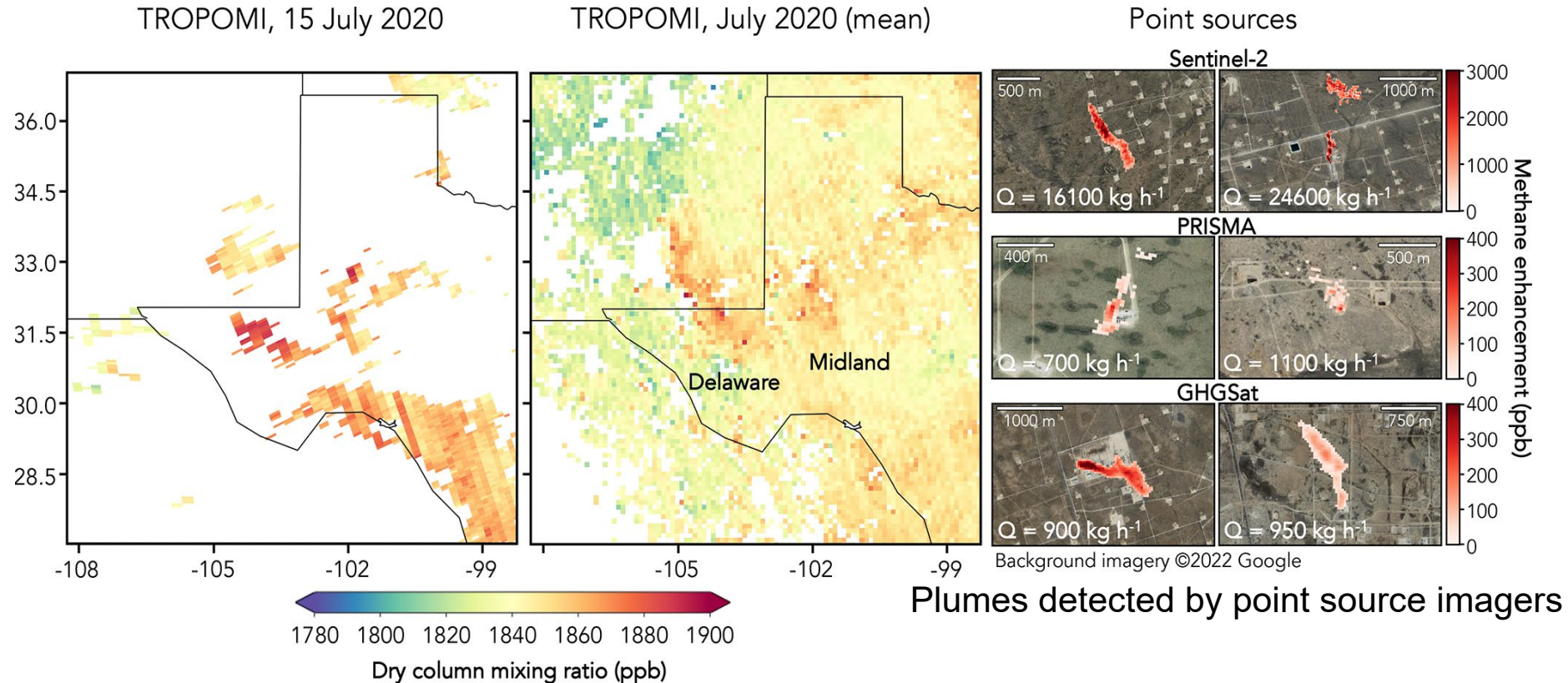
Annual mean TROPOMI observations, 2021



Balusus et al., submitted

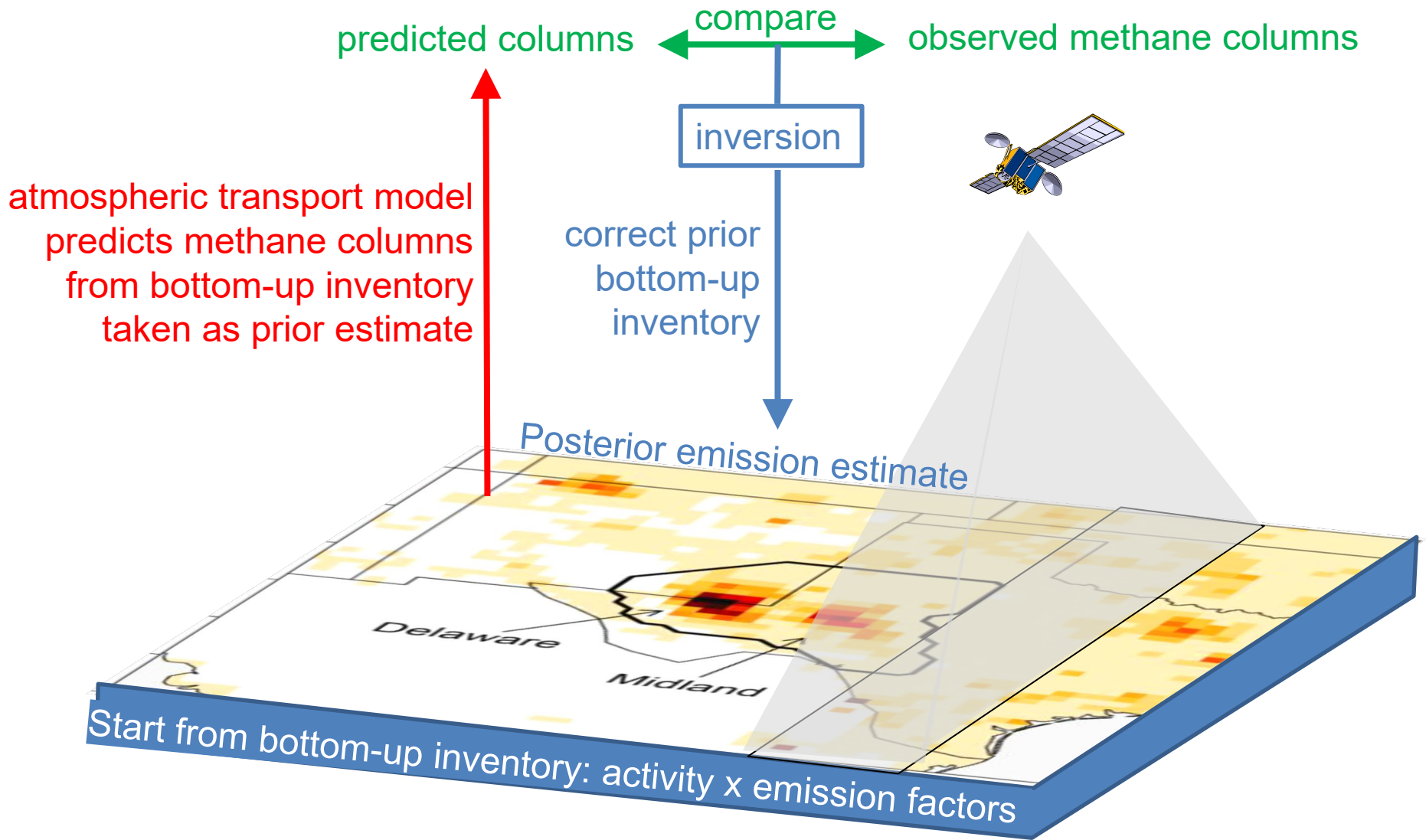
Complementarity of TROPOMI and point source observations to quantify basin-scale emissions

Observations over Permian Basin



- Point source imagers detect large point sources (200-25000 kg h⁻¹)
- TROPOMI observes total emissions

Inversion procedure to infer methane emissions



Inversion uses Bayes' probability theorem:

$$p(\text{true emissions} \mid \text{observations}) \sim p(\text{bottom-up emissions}) \times p(\text{observations} \mid \text{true emissions})$$

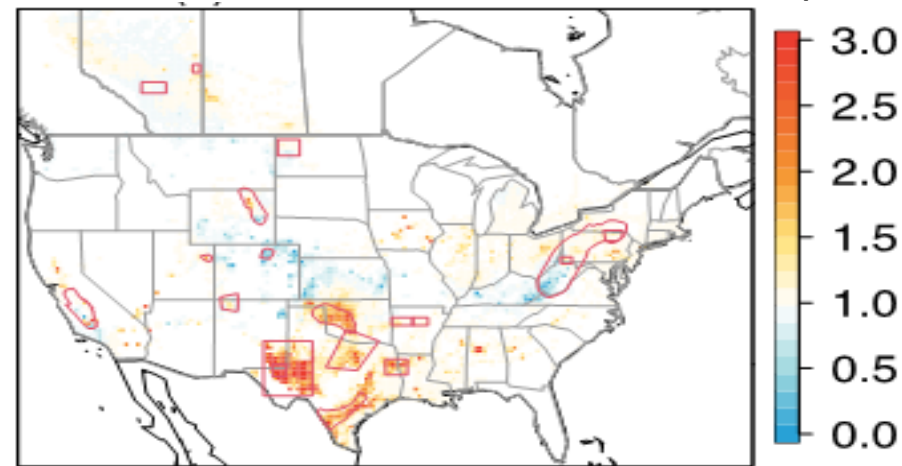
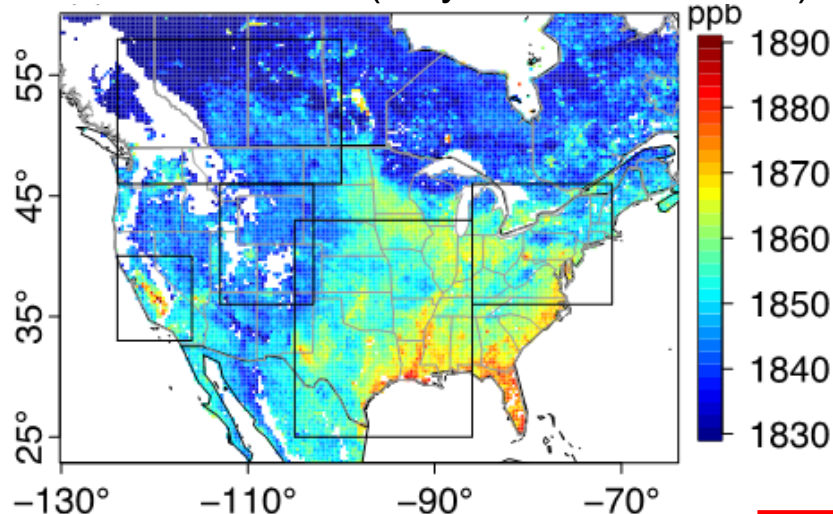
posterior

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



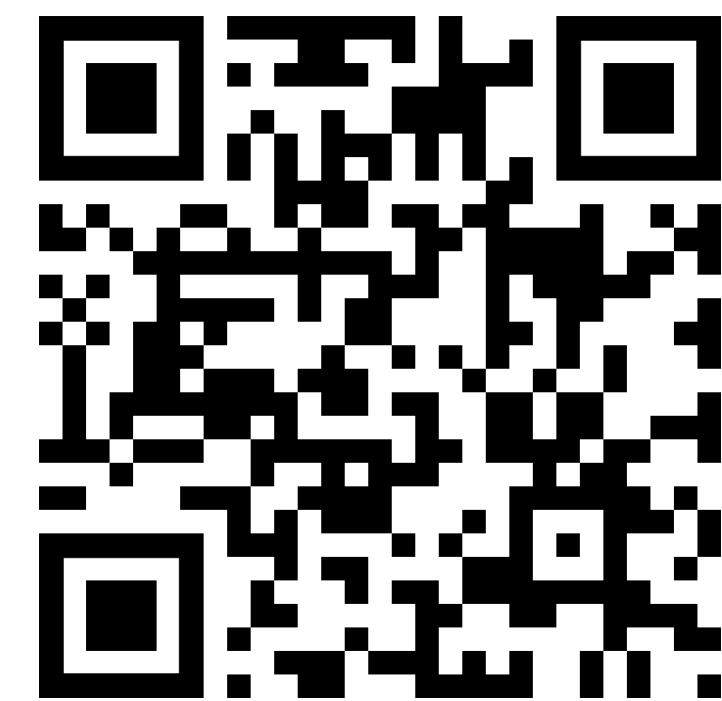
Integrated Methane Inversion (IMI) on the AWS cloud

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

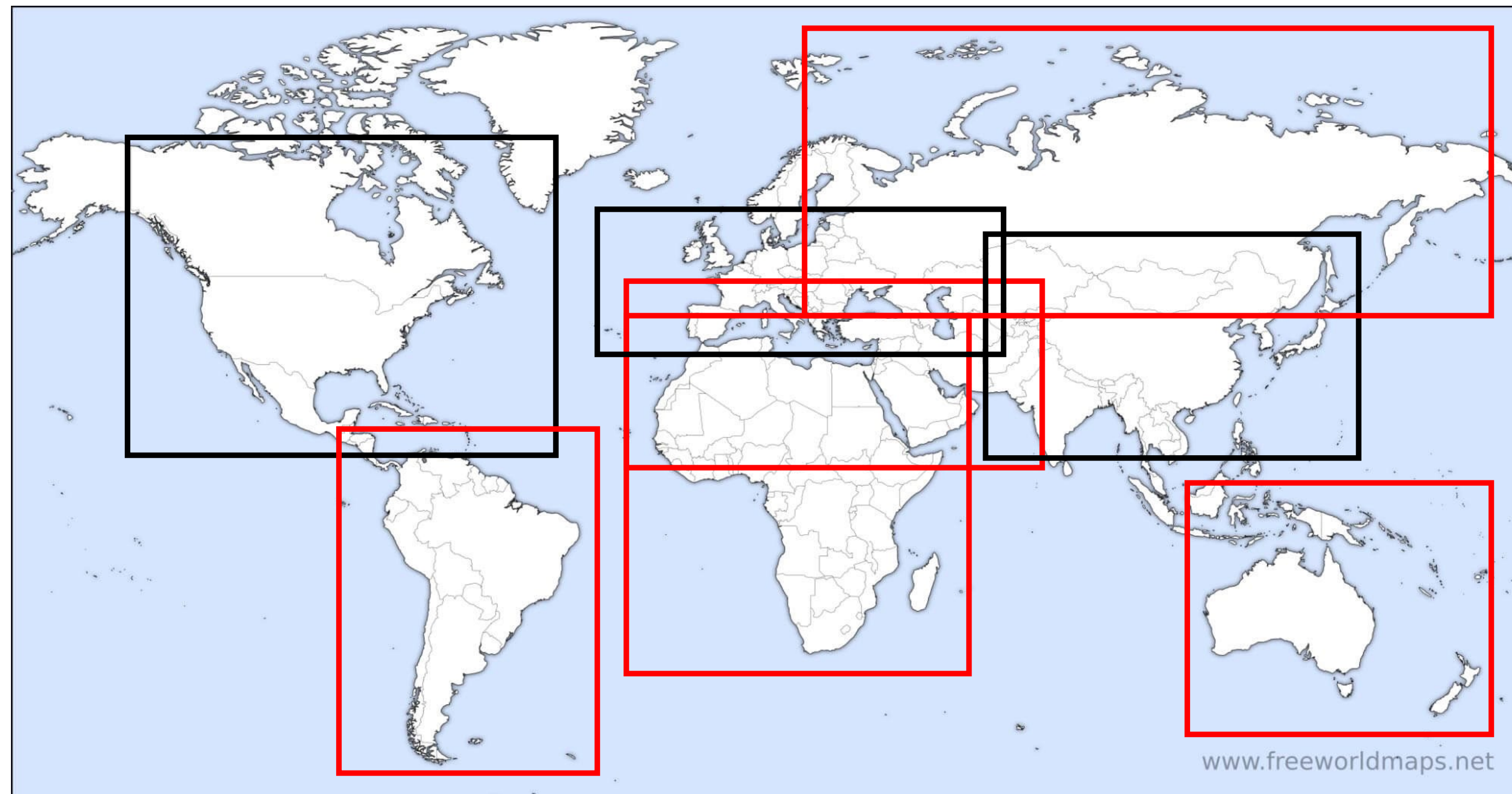
Integrated Methane Inversion (IMI) on the AWS cloud

The IMI...

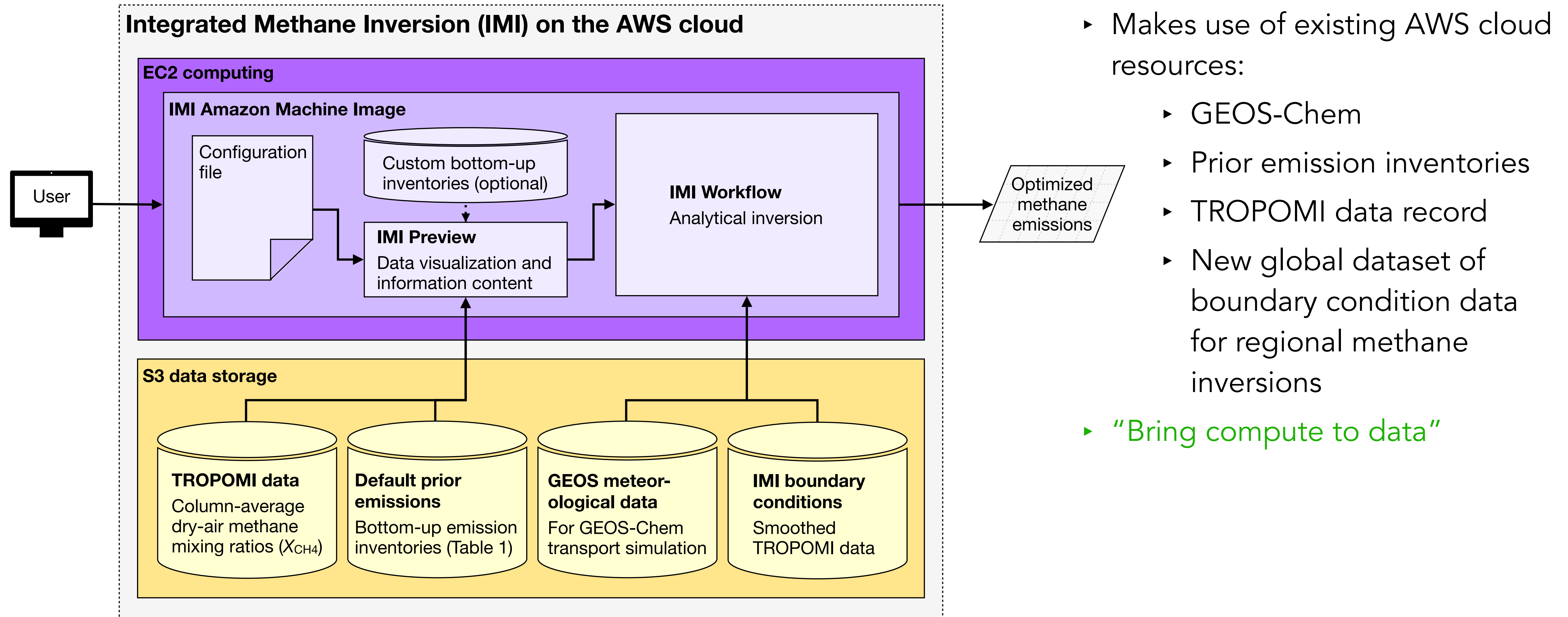
- ▶ Uses TROPOMI observations to infer methane emissions on a 25-km or 50-km grid;
- ▶ Performs regional methane inversions anywhere in the world;
- ▶ Provides an analytical solution to the Bayesian optimization of emissions.

IMI 1.0

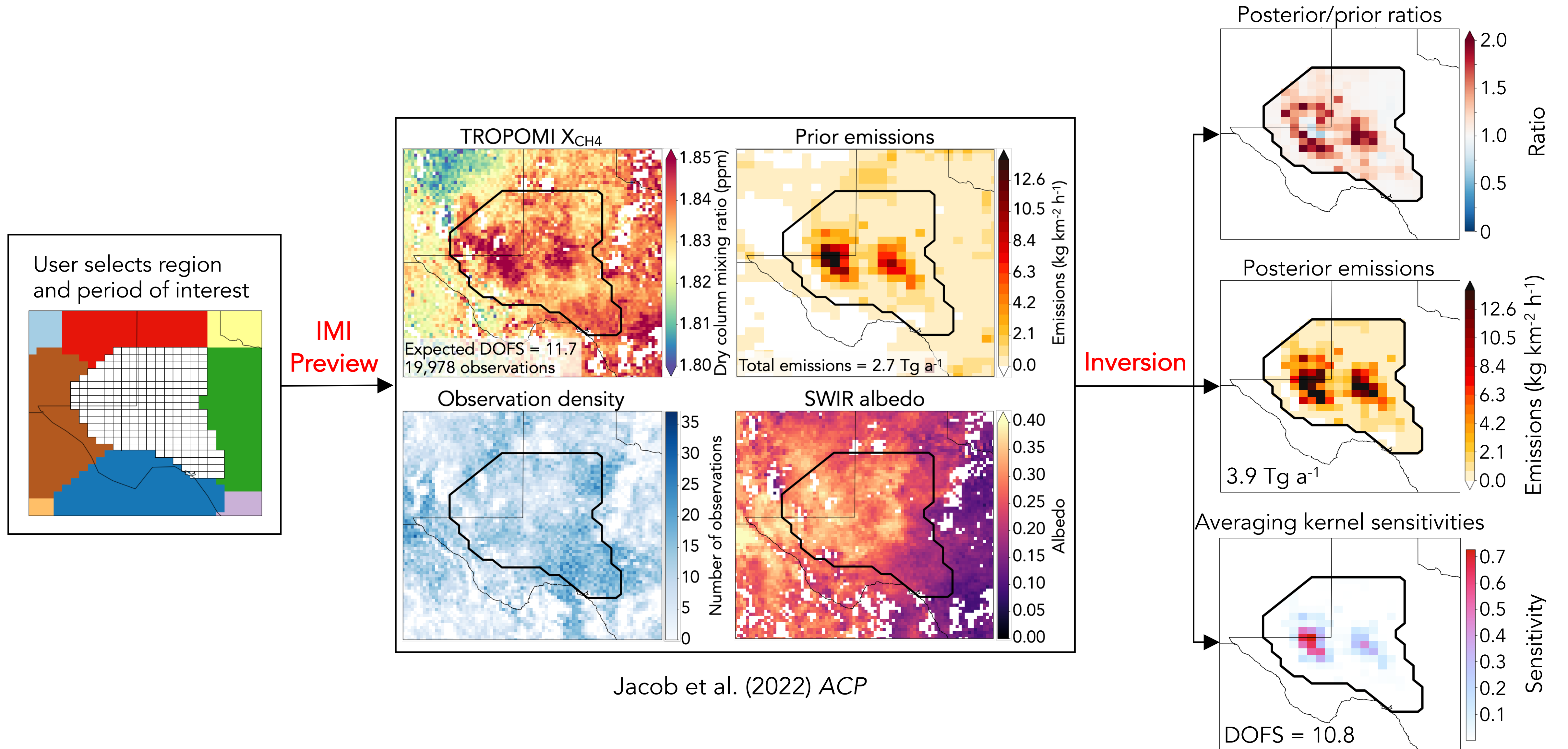
IMI 1.1



Architecture of the IMI on the AWS cloud



Integrated Methane Inversion (IMI) on the AWS cloud



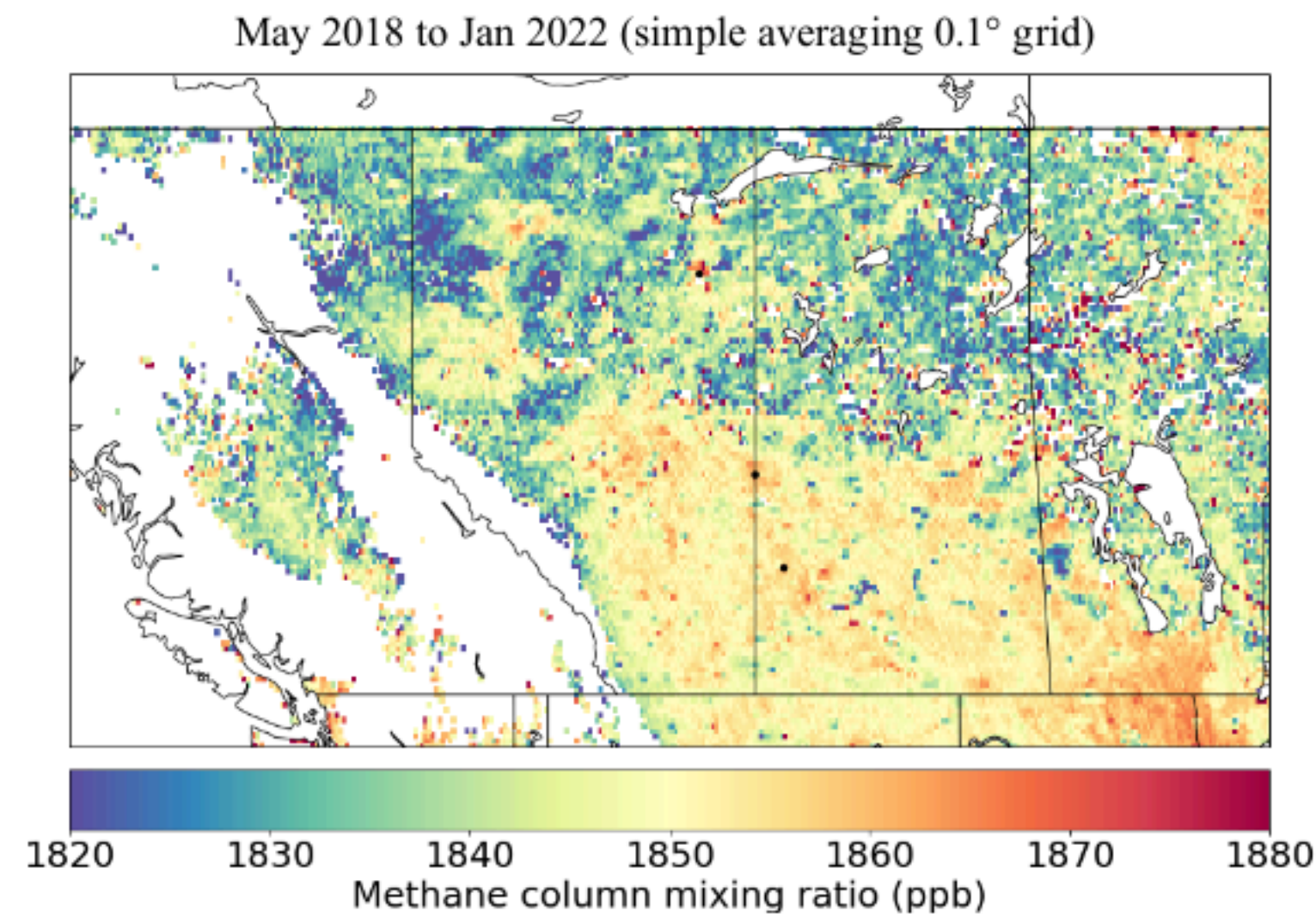
Example applications of the IMI

Some known community applications

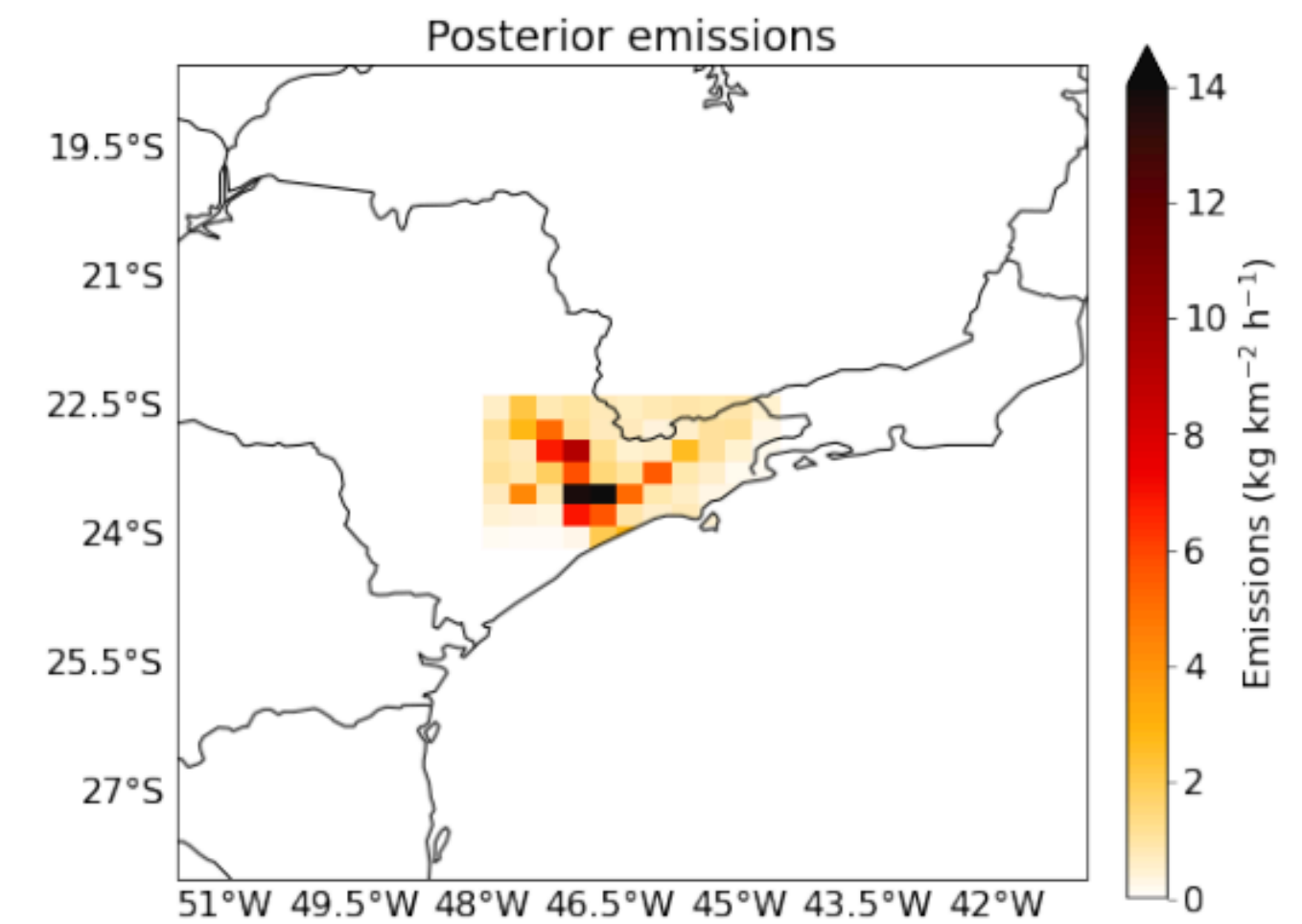
- ▶ Canadian oil/gas production regions (Environment & Climate Change Canada)
- ▶ Large Canadian cities (C-CORE, Inc.)
- ▶ São Paulo, Brazil (University of São Paulo)
- ▶ Venezuela (SRON Netherlands Institute for Space Research → Now IMI development partners)

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

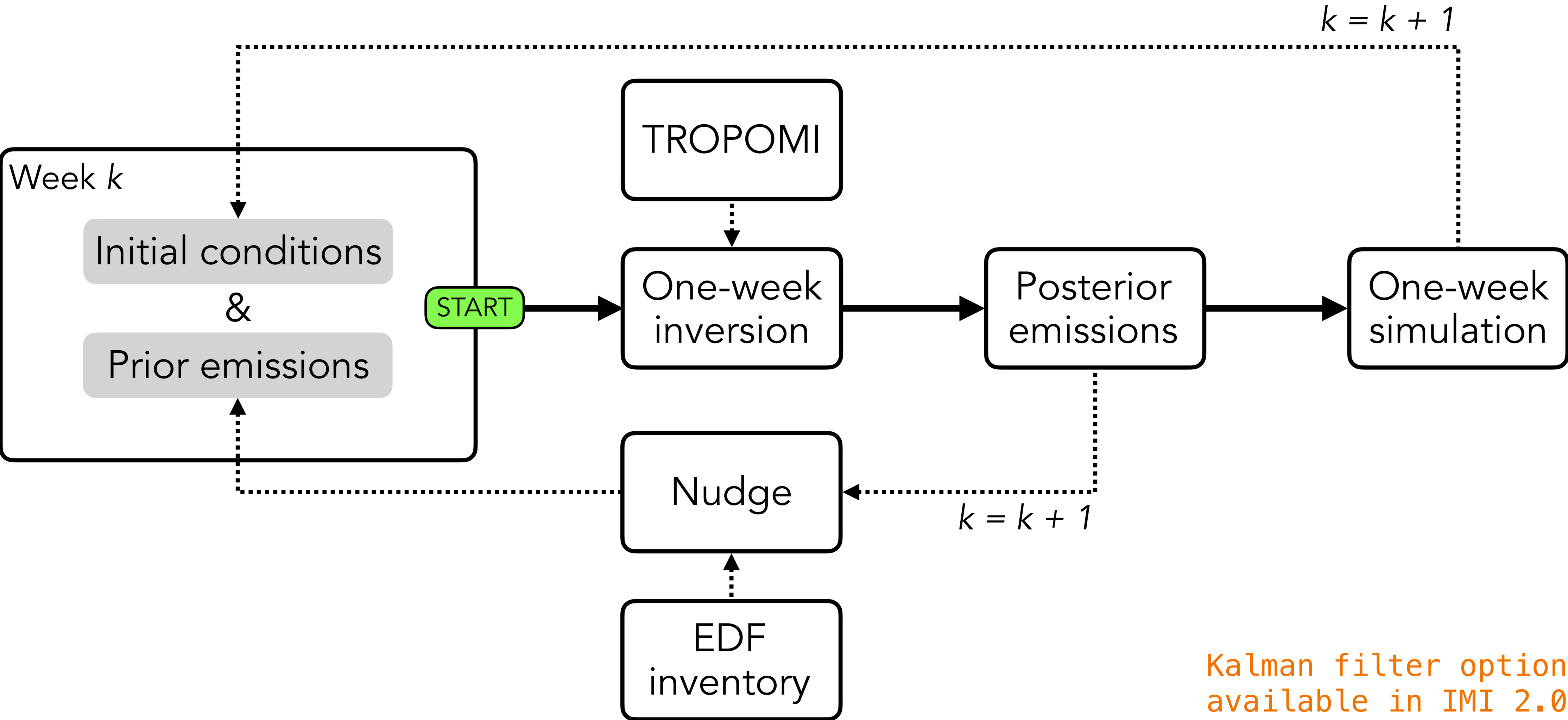
Roadmap to IMI 2.0

- ▶ 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?

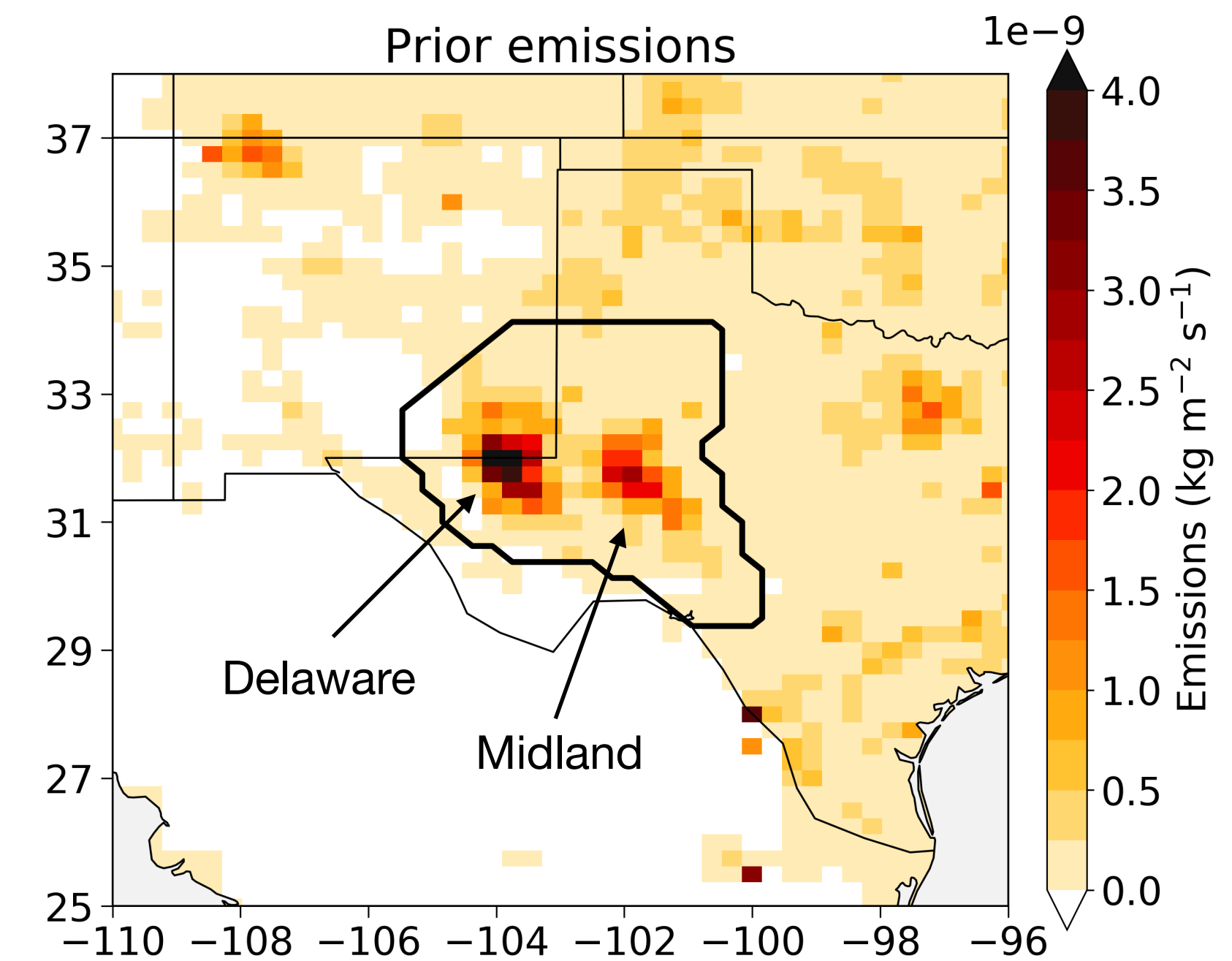
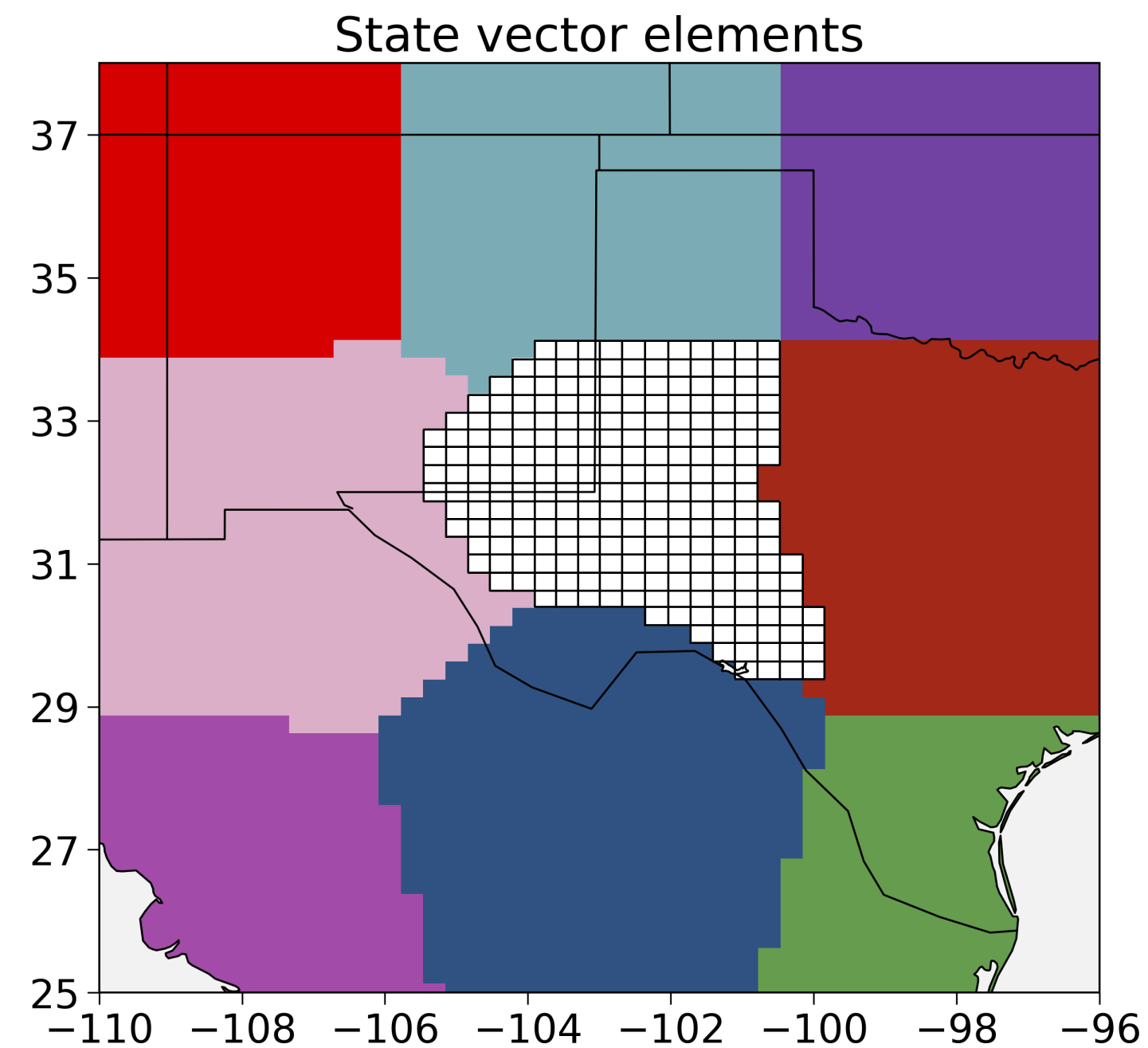
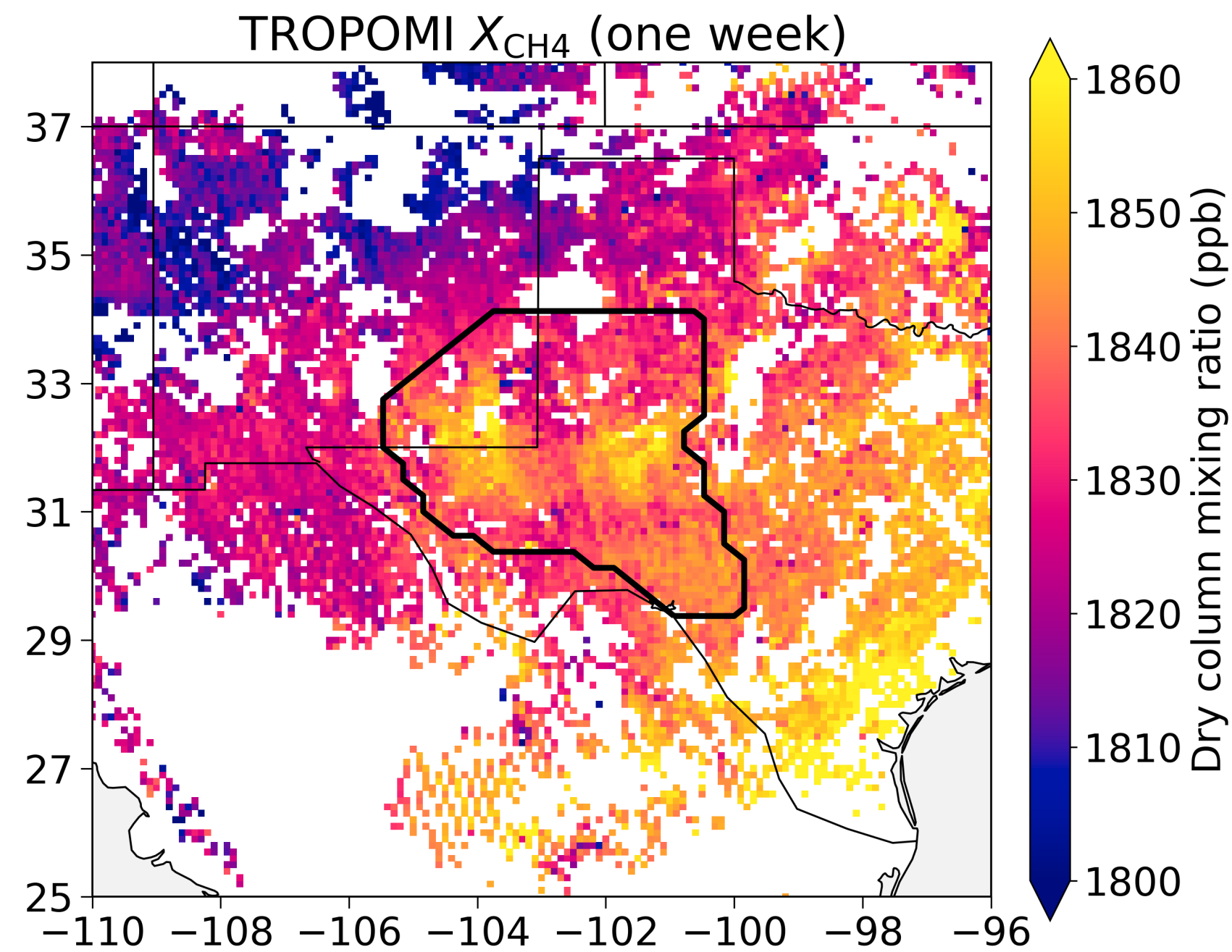
Kalman filter for weekly methane emissions



Kalman filter option available in IMI 2.0

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

Sample inversion setup: TROPOMI observations, state vector, & prior emissions

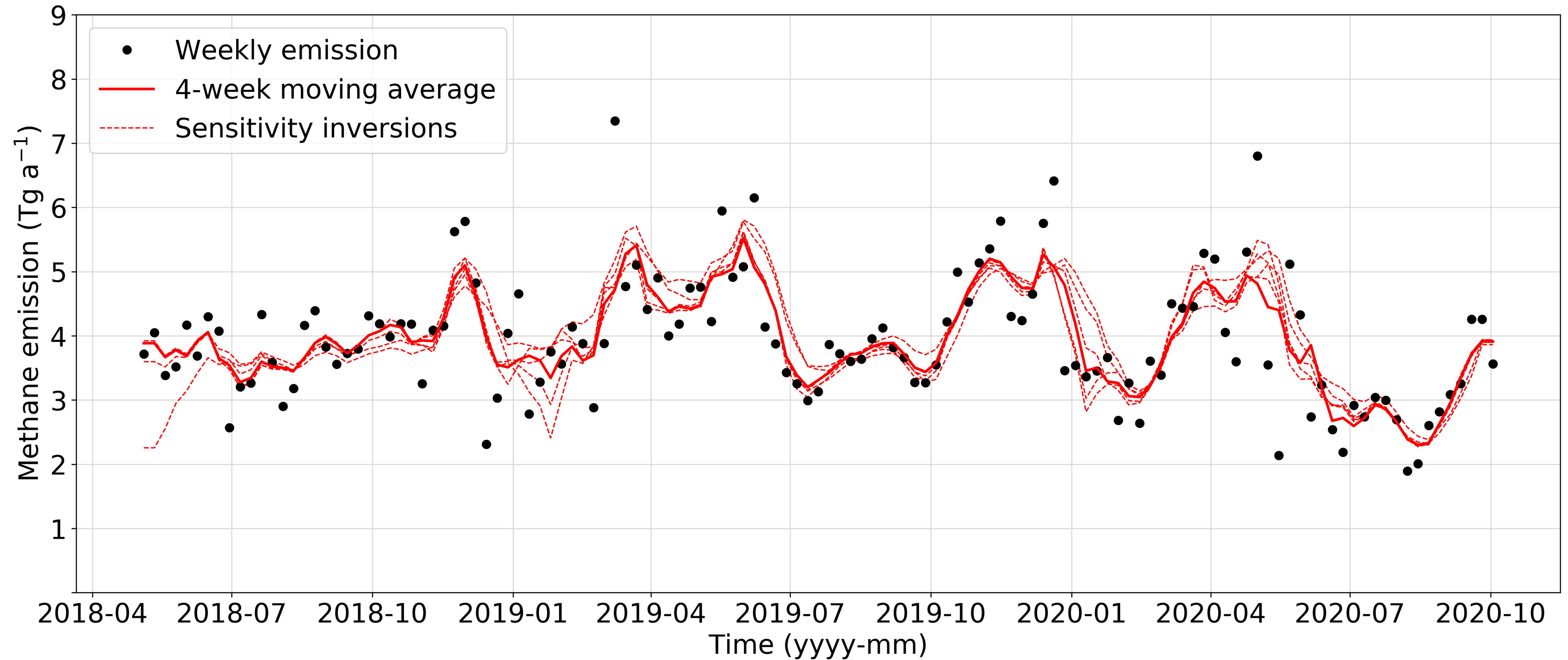


- ▶ ~2.5 years of data
- ▶ May 2018 – October 2020

- ▶ 243 emission elements
- ▶ 235 at $0.25^\circ \times 0.3125^\circ$ 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)

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

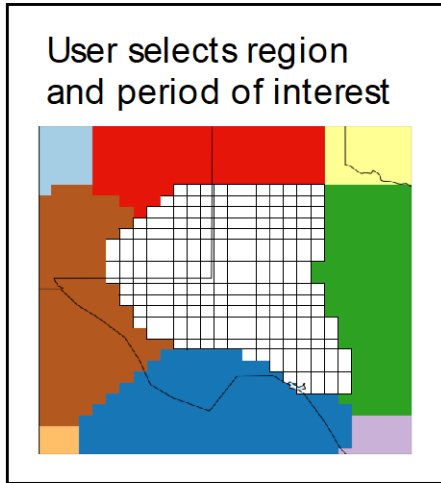
Future development plans

Beyond IMI 2.0

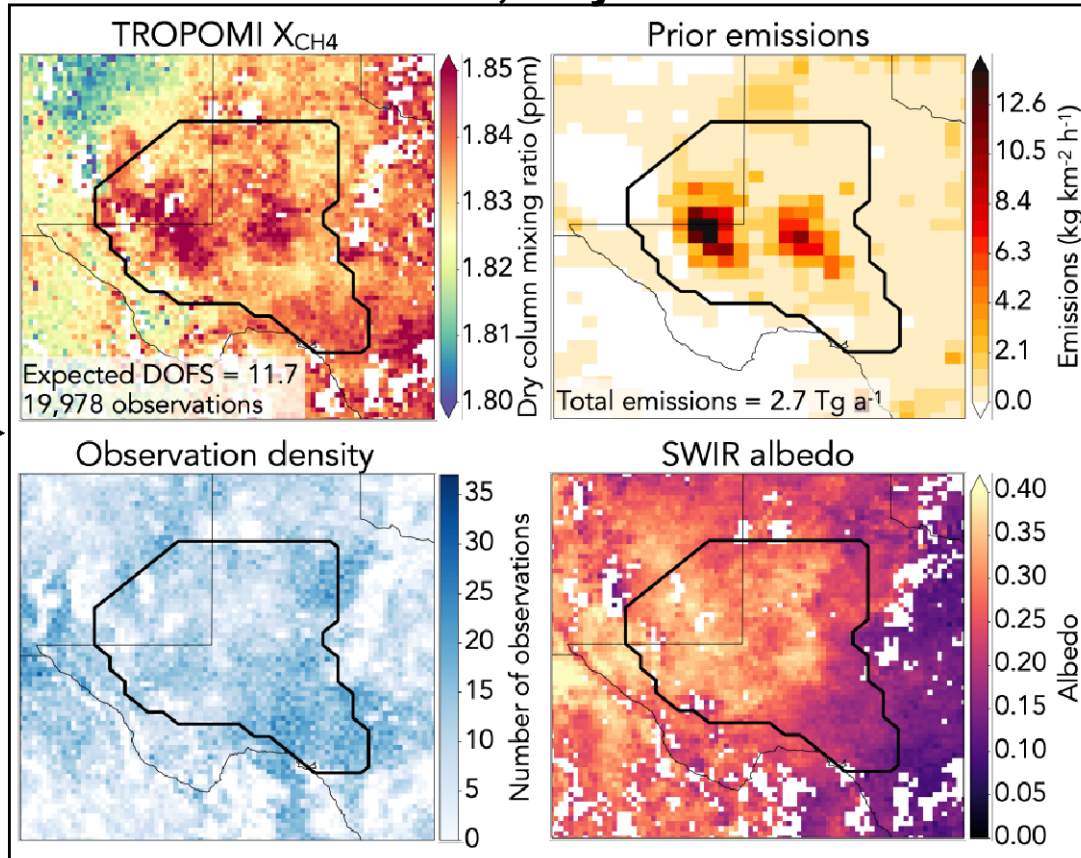
- ▶ Extend to CO₂ fluxes: CH₄ → CO₂
 - ▶ NASA Earth Information System – Greenhouse Gases (EIS-GHG)
 - ▶ IMI + CO₂ = **ICI** could serve as a platform for the EIS-GHG
- ▶ Expand to new satellite instruments (e.g., GOSAT-GW, CO2M)
 - ▶ Future instruments will enable CO₂ inversions & denser CH₄ coverage
- ▶ 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

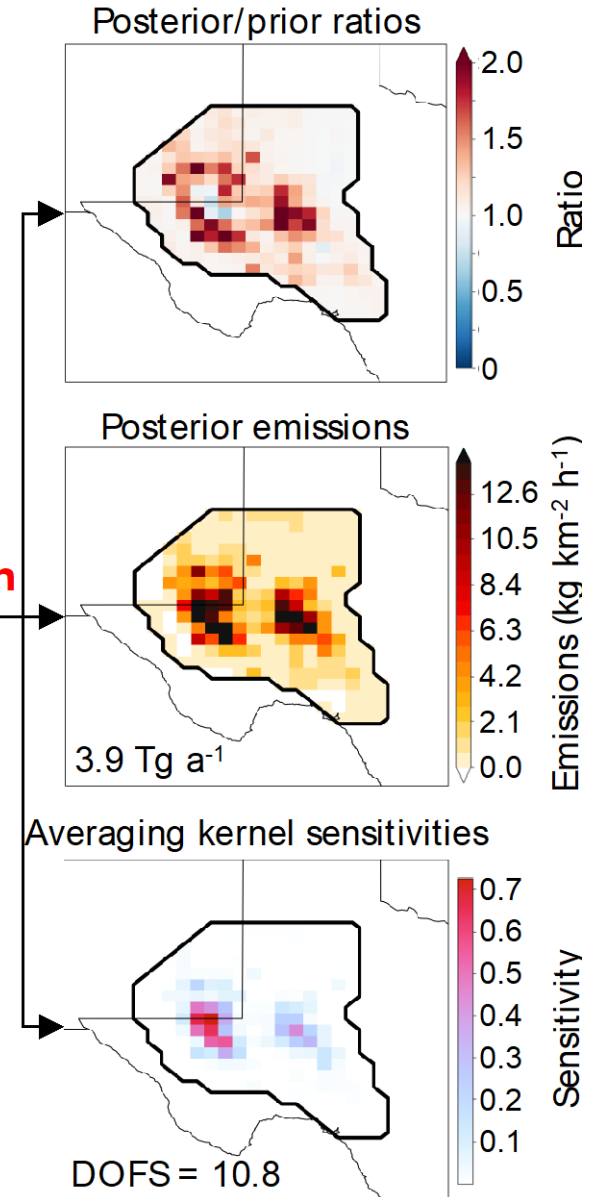
1-Month, May 2018



IMI
Preview



Inversion



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

Our documentation walks through the setup

IMI
latest

Search docs

GETTING STARTED

Quick start guide

1. Create an Amazon Web Services (AWS) account
2. Add S3 user permissions
3. Launch an instance with the IMI
4. Login to your instance
5. Configure the IMI
6. Run the IMI
7. Visualize results with Python
8. Shut down the instance
9. Store data on S3

IMI configuration file

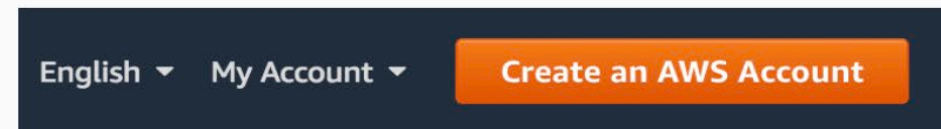
Docs » Quick start guide

[Edit on GitHub](#)

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

EC2 > Instances > Launch an instance > AMIs

Cancel

Choose an Amazon Machine Image (AMI)

An AMI is a template that contains the software configuration (operating system, application server, and applications) required to launch your instance. You can select an AMI provided by AWS, our user community, or the AWS Marketplace; or you can select one of your own AMIs.

imi

Quickstart AMIs (1)
Commonly used AMIs

My AMIs (2)
Created by me

AWS Marketplace AMIs (1)
AWS & trusted third-party AMIs

Community AMIs (500)
Published by anyone

Refine results

Categories

Infrastructure
Software (1)

Publisher

Atmospheric
Chemistry Modeling
Group (1)

imi (1 result) showing 1 - 1

Did you mean [imd](#), [ipi](#)?

Sort By: Relevance



Integrated Methane Inversion

By [Atmospheric Chemistry Modeling Group](#) | Ver imi-1.1.0

The Integrated Methane Inversion (IMI) is a user-friendly, cloud-based facility for estimating regional methane emissions by analytical inversion of satellite observations from the TROPOspheric Monitoring Instrument (TROPOMI). It enables researchers and stakeholders to infer methane emissions at...

Select

Configure Instance Settings

The screenshot shows the AWS Management Console interface for configuring an instance. The top navigation bar includes the AWS logo, 'Services', a search bar, a keyboard shortcut '[Option+S]', and the current region 'N. Virginia'. The breadcrumb trail shows 'Resource Groups & Tag Editor'. The main content area is divided into several sections:

- Key pair (login)**: A section with an 'Info' link. It contains a text input field for 'Key pair name - required' with the value 'imi-testing' and a 'Create new key pair' button.
- Network settings**: A section with an 'Info' link and an 'Edit' button.
- Configure storage**: A section with an 'Info' link and an 'Advanced' link. It features a configuration for the root volume: '1x' [50] GiB [gp2] Root volume (Not encrypted). Below this is a light blue informational box: 'Free tier eligible customers can get up to 30 GB of EBS General Purpose (SSD) or Magnetic storage'. At the bottom is an 'Add new volume' button.
- Summary**: A section with a 'Summary' link. It includes:
 - 'Number of instances' [1]
 - 'Software Image (AMI)' section with 'Integrated Methane Inversion' (ami-080bd7d424290499f).
 - 'Virtual server type (instance type)' section with 'c5.9xlarge'.
 - 'Firewall (security group)' section with 'New security group'.
 - 'Storage (volumes)' section with '1 volume(s) - 50 GiB'.
 - A light blue informational box: 'Free tier: In your first year includes 750 hours of t2.micro (or t3.micro in the Regions in which t2.micro is unavailable)'.
 - At the bottom are 'Cancel' and 'Launch instance' buttons.

Login and edit the IMI config file

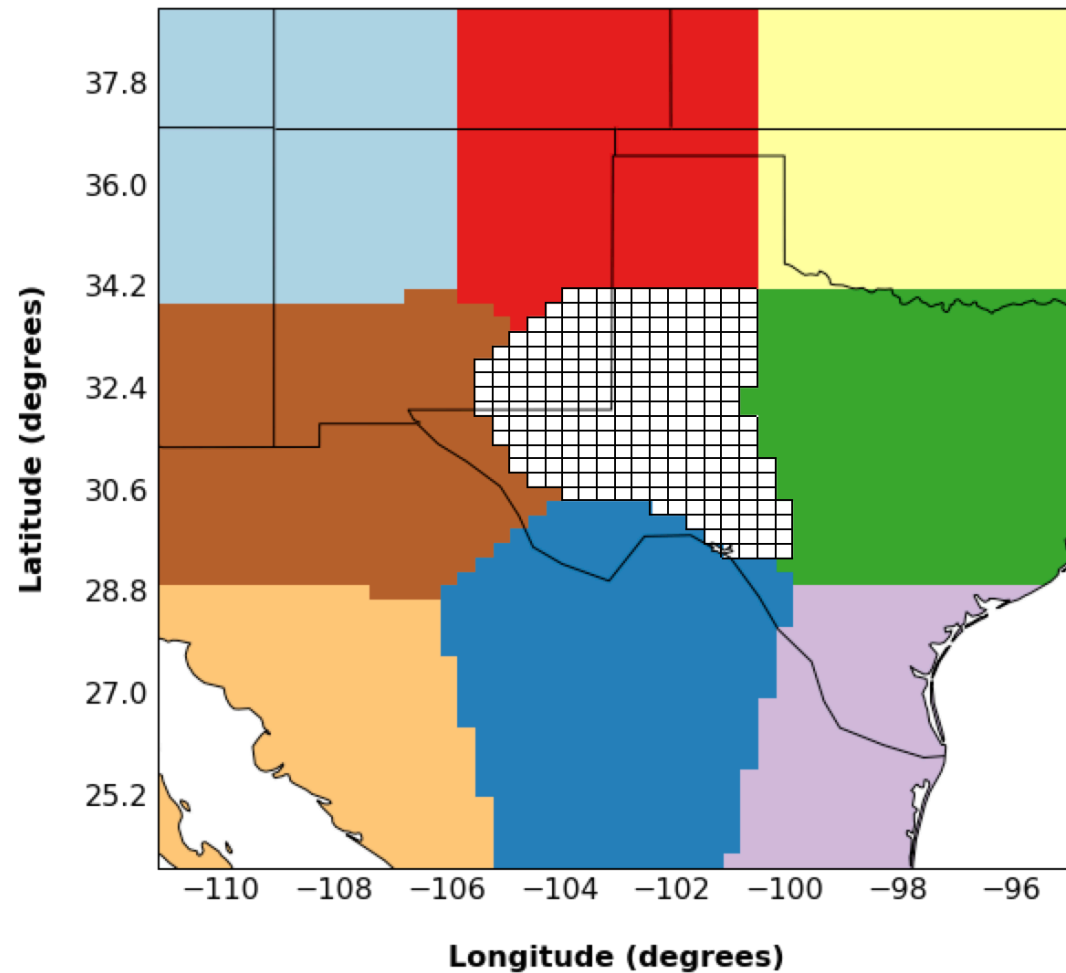
```
## IMI configuration file
## Documentation @ https://imi.readthedocs.io/en/latest/getting-started/imi-config-file.html

## 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

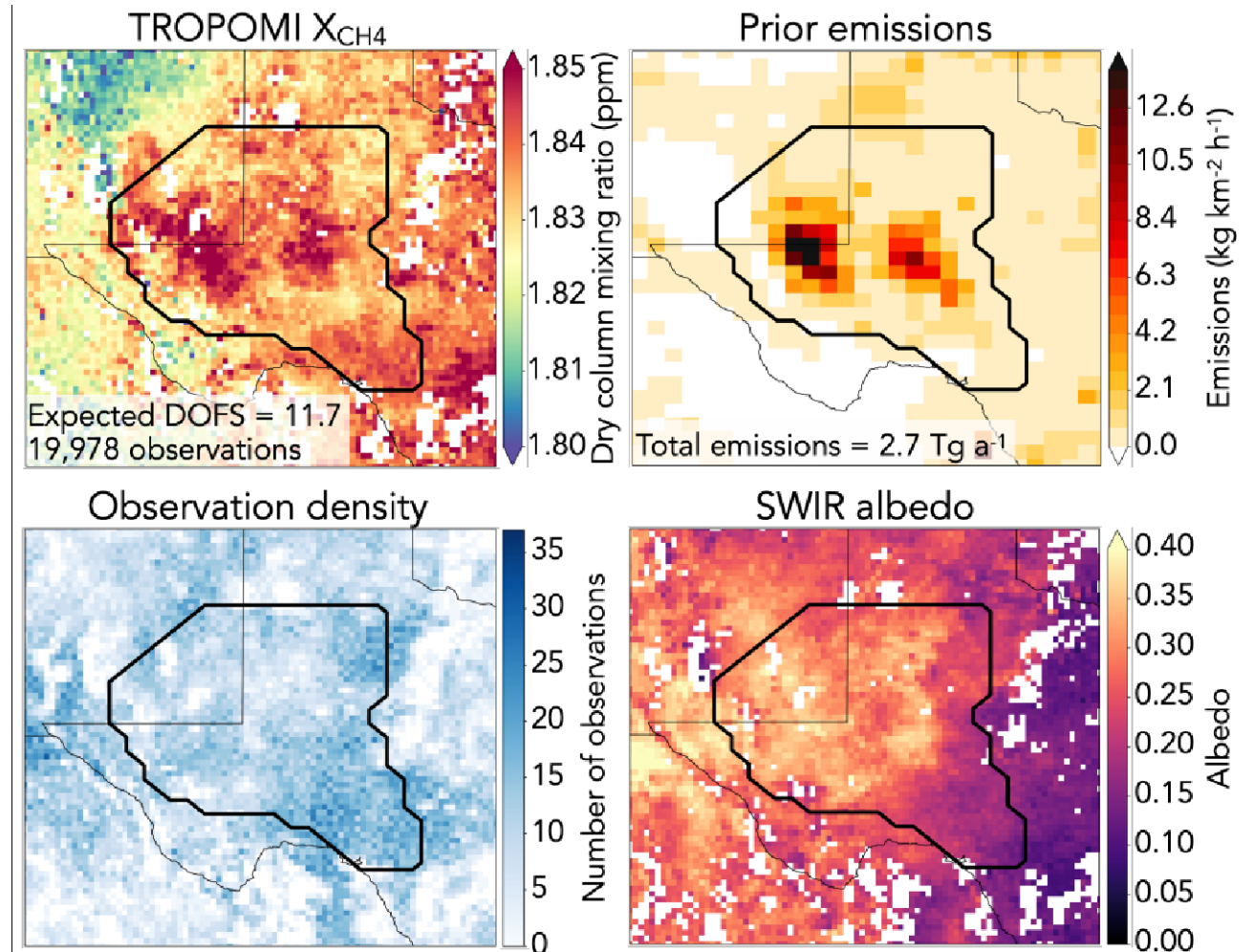


Single command to run the IMI

```
$ sbatch run_imi.sh
```


Review the IMI Preview

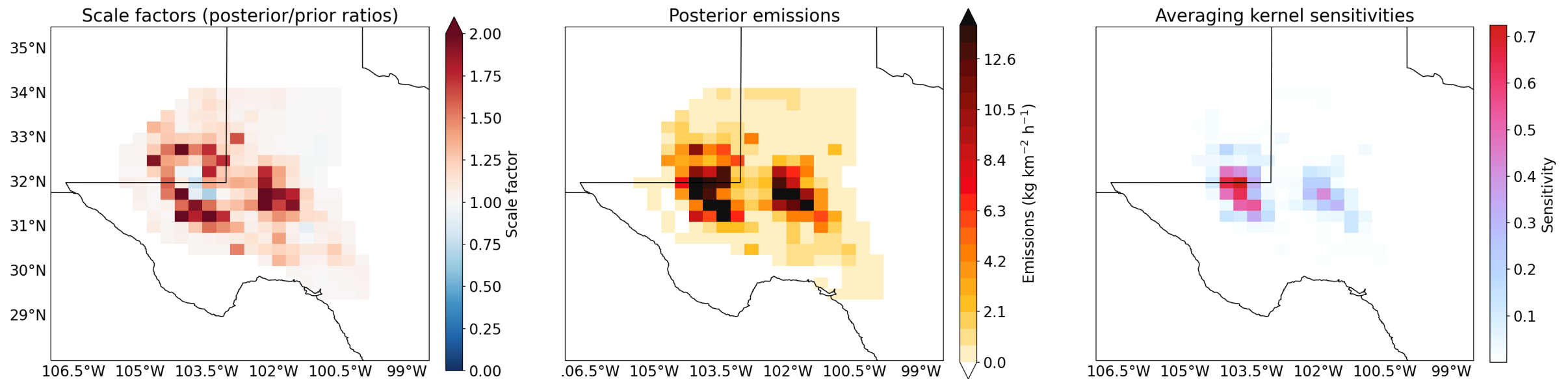
- Check the expected quality of the inversion and cost
- Preview can be run with essentially no cost
- If satisfied, proceed with the inversion



Expected cost of the inversion: ~\$20

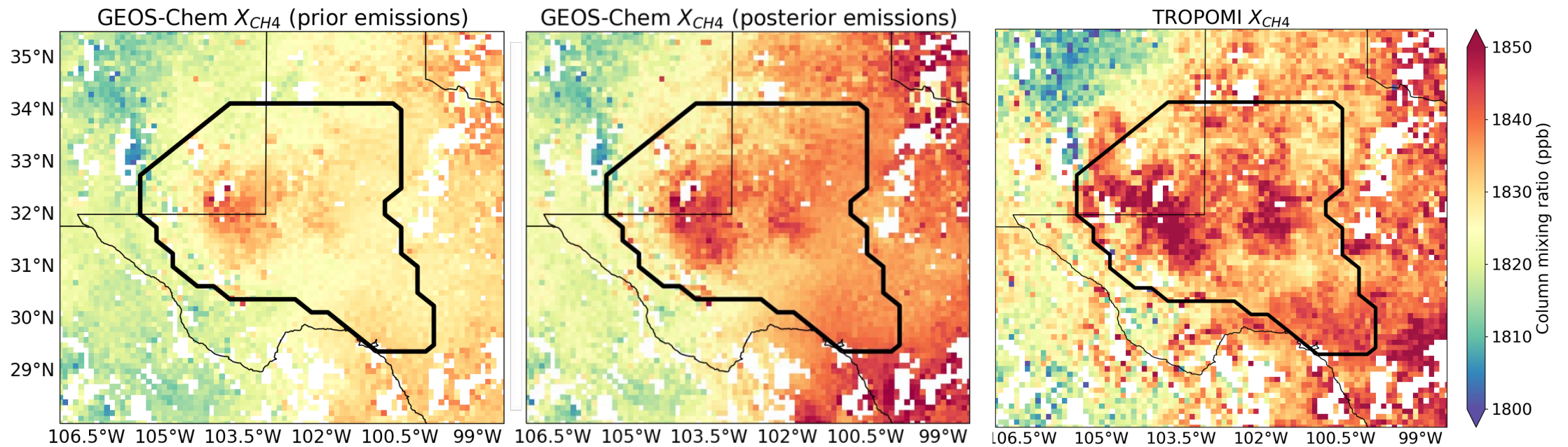
Visualize Inversion Results

- Premade visualization notebook for plotting results



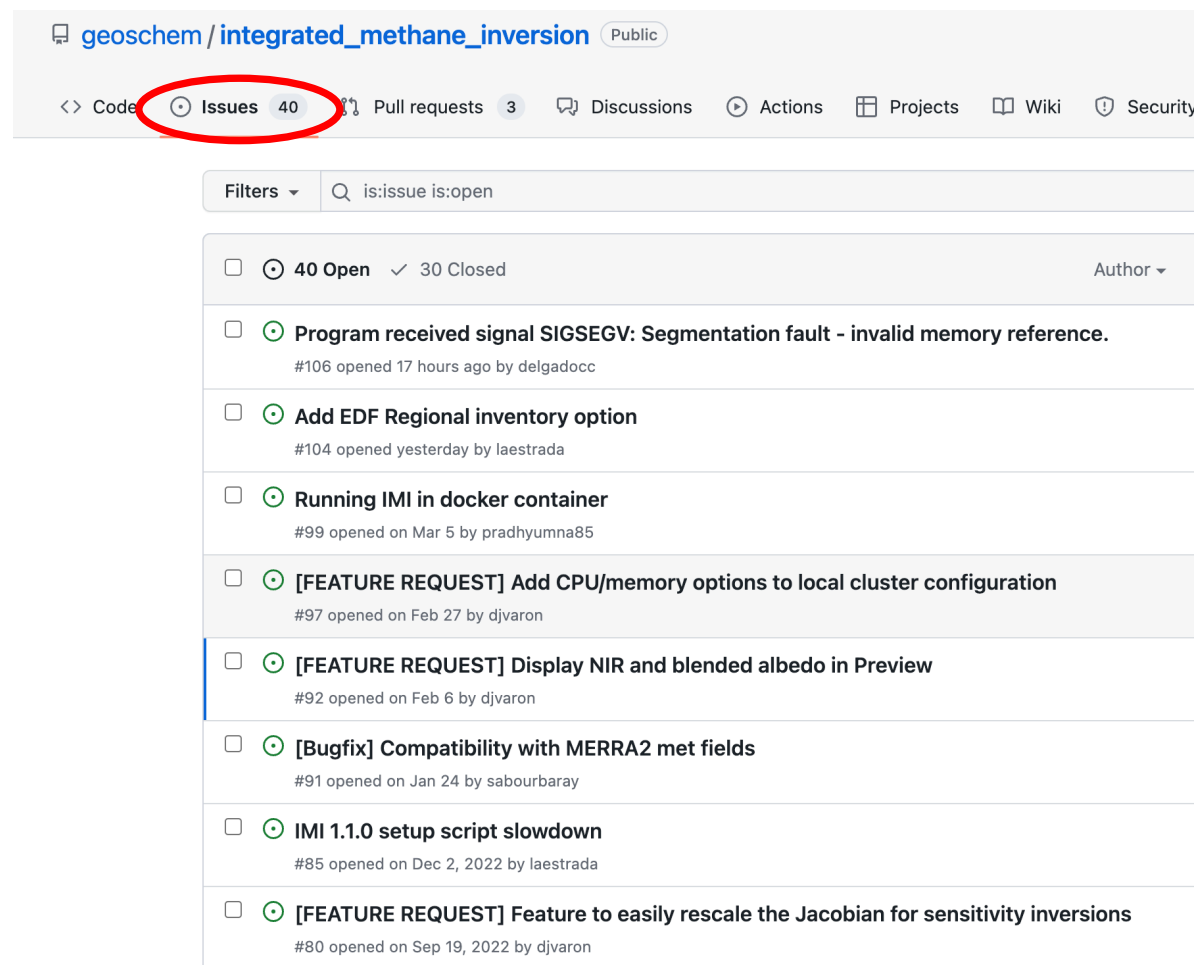
Visualize Inversion Results

- Premade visualization notebook for plotting results



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



The screenshot shows the GitHub repository page for `geoschem/integrated_methane_inversion`. The repository is public. The navigation bar includes links for Code, Issues (40), Pull requests (3), Discussions, Actions, Projects, Wiki, and Security. The Issues section is active, showing a search filter for `is:issue is:open`. The list of issues includes:

- 40 Open, 30 Closed
- Program received signal SIGSEGV: Segmentation fault - invalid memory reference. #106 opened 17 hours ago by delgadocc
- Add EDF Regional inventory option #104 opened yesterday by laestrada
- Running IMI in docker container #99 opened on Mar 5 by pradhymna85
- [FEATURE REQUEST] Add CPU/memory options to local cluster configuration #97 opened on Feb 27 by djvaron
- [FEATURE REQUEST] Display NIR and blended albedo in Preview #92 opened on Feb 6 by djvaron
- [Bugfix] Compatibility with MERRA2 met fields #91 opened on Jan 24 by sabourbaray
- IMI 1.1.0 setup script slowdown #85 opened on Dec 2, 2022 by laestrada
- [FEATURE REQUEST] Feature to easily rescale the Jacobian for sensitivity inversions #80 opened on Sep 19, 2022 by djvaron

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



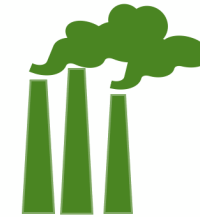
Greenhouse Gases



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



Greenhouse Gases



Fire



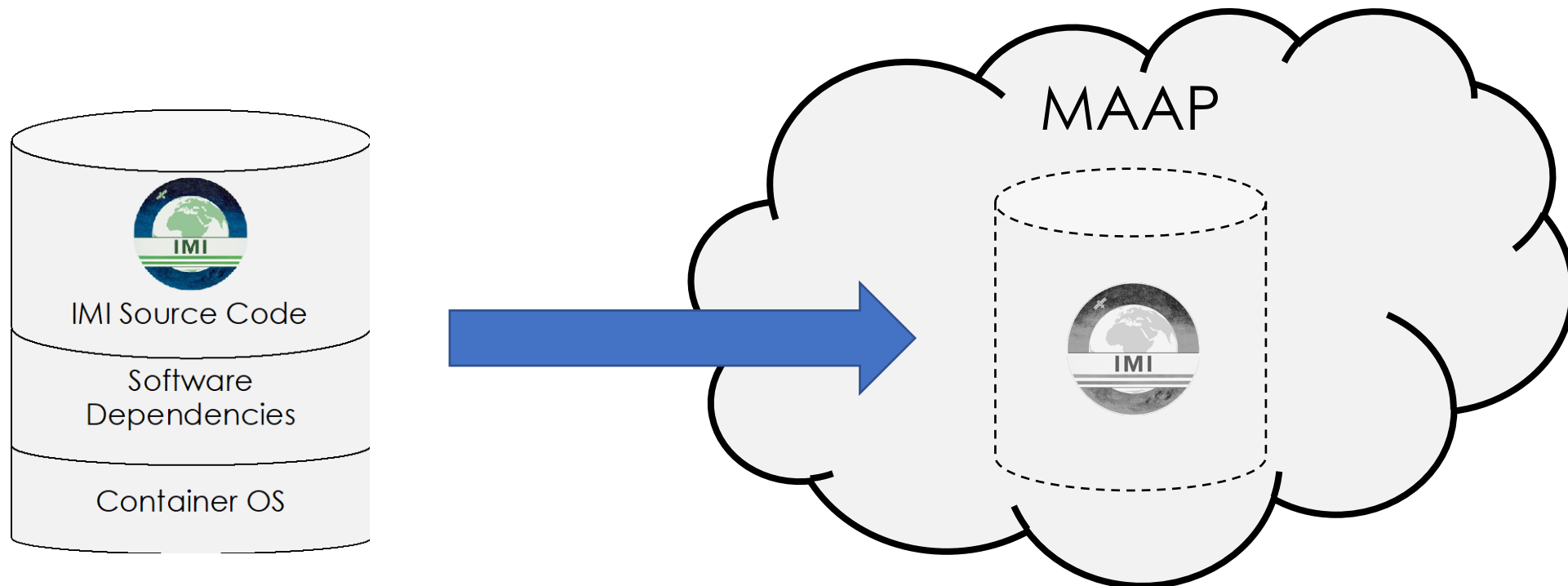
Sea Level Rise



Freshwater

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

