Towards emulated Lagrangian particle dispersion model footprints for satellite observations

Elena Fillola[1], Raul Santos-Rodriguez[1], Matt Rigby[2]
1. Department of Engineering Mathematics, University of Bristol
2. Atmospheric Chemistry Research Group, University of Bristol
elena.fillolamayoral@bristol.ac.uk

Background: Atmospheric Transport Models

- Inverse modelling systems for **greenhouse gas (GHG) flux quantification** require an atmospheric transport model and a statistical inversion framework to produce spatial estimates of methane
- Backwards running Lagrangian particle dispersion models (LPDMs) produce ***footprints:*** sensitivity of a measurement to emissions in the area around it
- The computational cost of the LPDMs means that the growing volume of satellite GHG measurements is underutilized
- The small number of existing methods to efficiently approximate LPDM footprints use interpolation in time and space, or smoothing of low-resolution runs

Goal: Met-only Emulator

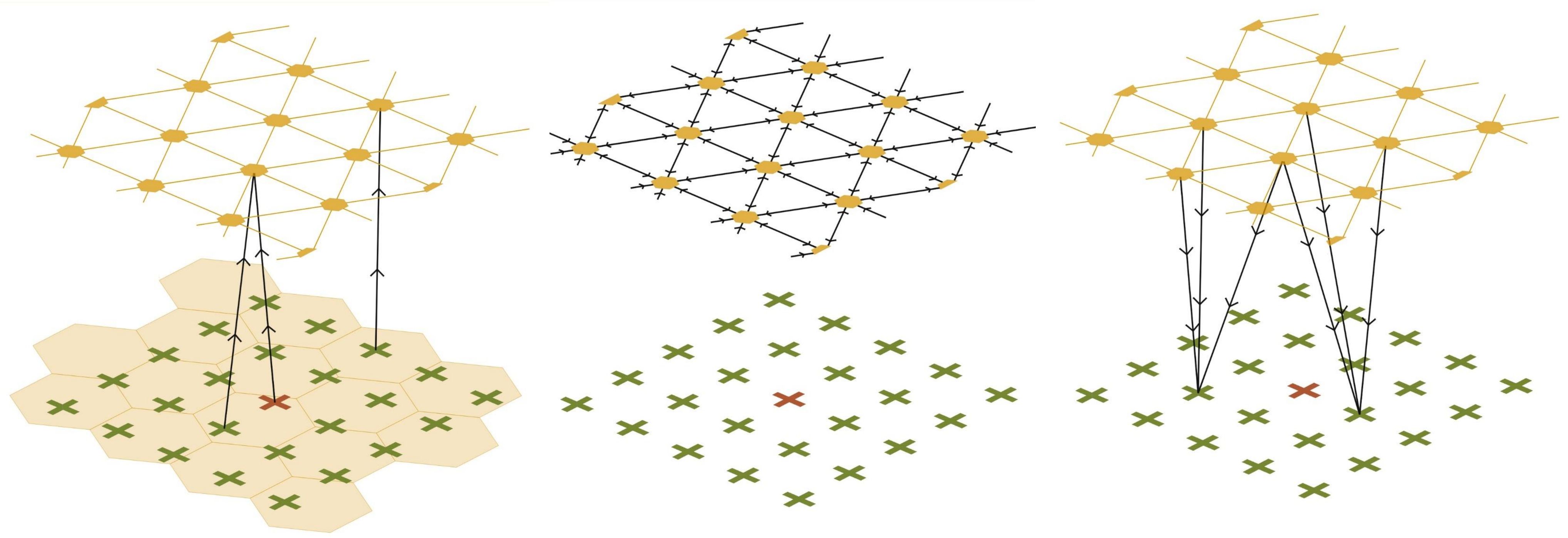
To develop a machine learning LPDM emulator, which can output full-domain footprints for satellite measurements using only meteorological and geographical inputs

Proof of Concept: Simple Emulator for In Situ Data (Fillola et al., 2023)

- Proof-of-concept model with simpler task and simpler design – **footprints for tower site data**
- Footprint value at each cell modelled with independent gradient-boosted regression trees, for a grid centered around the measurement point.
- One model trained per site, using 2-hourly meteorological fields from 2014-2015
- Prediction speed-up of five orders of magnitude
- R^2 scores for CH_4 concentration prediction across sites of 0.69 for 2016
- Limitations: not scalable with domain size

Graph Networks to Emulate Satellite Data

The emulator consists of Graph Networks in a **Encode-Process-Decode** architecture that combines the native data space, a latitude-longitude grid, with an abstract icosahedron mesh. The two grids are always centered around the measurement point and therefore the physical location of the lat-lon grid changes for every sample. Black arrows indicate the flow of information between nodes.



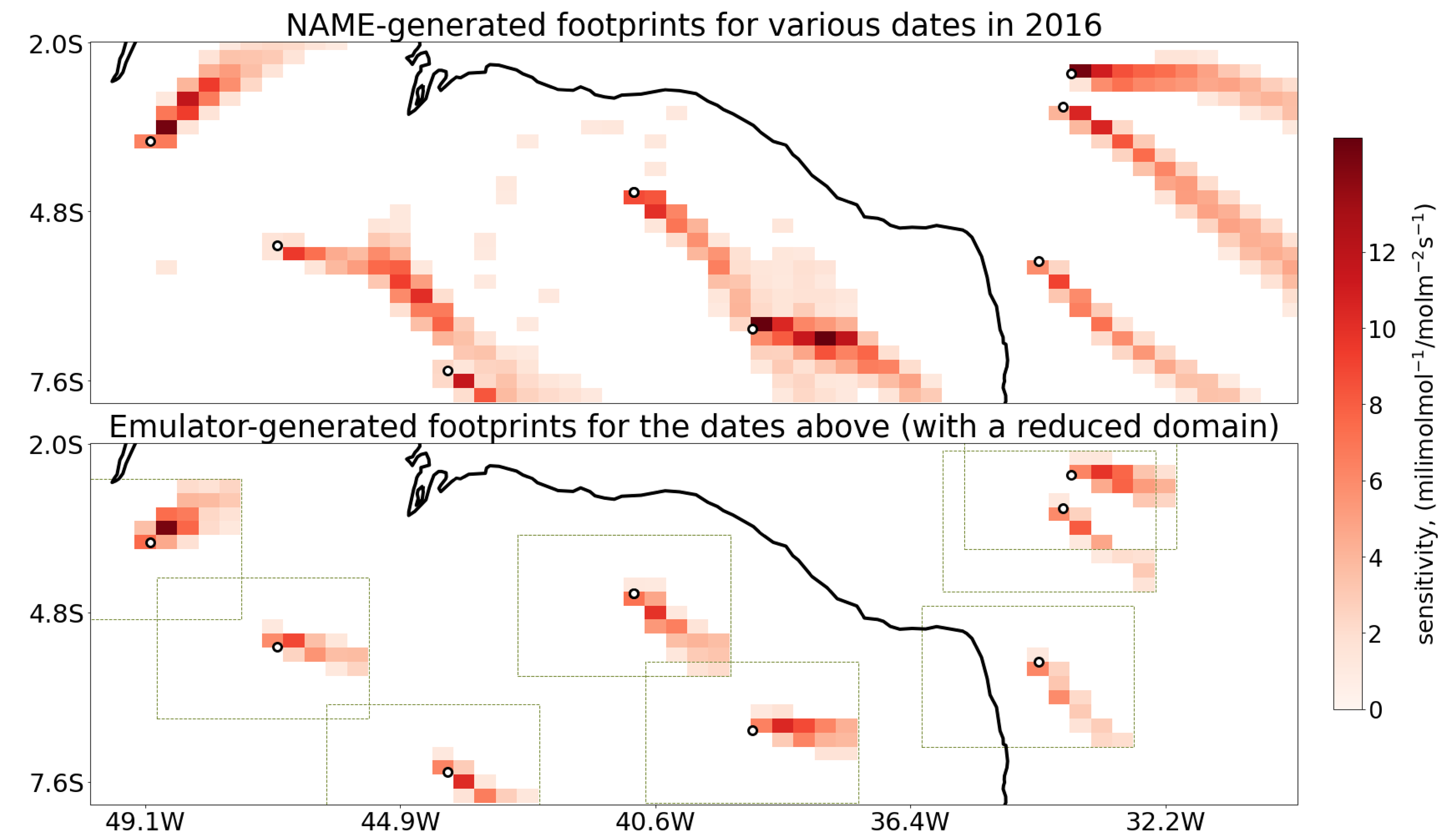
Encoder: meteorology and geographical data at each node in the lat-lon grid is encoded in the closest node of the icosahedron mesh

Processor: a message-passing GNN updates the information in the icosahedron mesh iteratively, spreading the information from each node to its neighbours

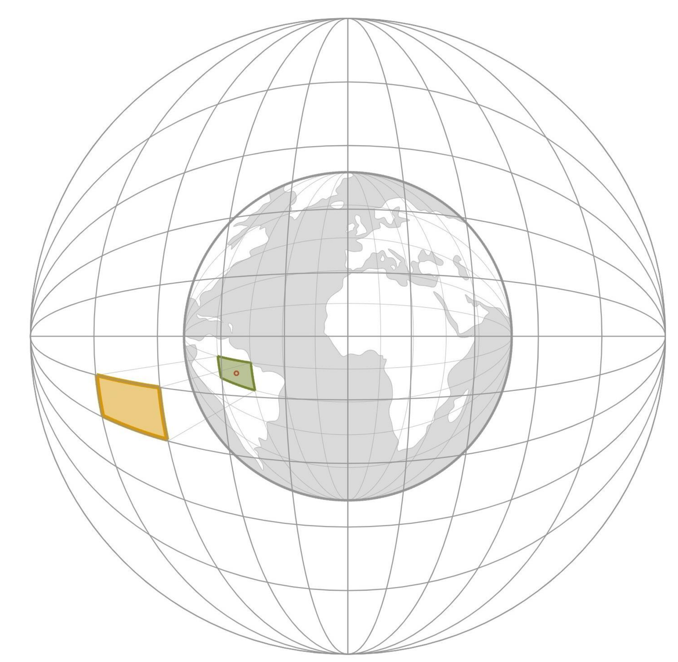
Decoder: the value of the footprint at each point in the lat-lon grid is predicted with the three nearest nodes in the icosahedron mesh

Example Application: GOSAT over Brazil

- Demonstrated for GOSAT measurements over Brazil
- Inputs: Met Office Unified Model fields and geographical information for 2014-2015 to predict NAME satellite footprints
- Reduced domain – 10x10 latitude-longitude grid
- R^2 score for CH_4 concentration prediction over Brazil of 0.60 for 2016



Sample Results: NAME-generated and emulator-generated footprints for GOSAT measurement locations over North-East Brazil at various dates in 2016. Dotted line shows the emulated area around each point



Left - **Diagram of the two data spaces,** centered around the measurement point

Next Steps

- Increase prediction domain
- Analysis of error distribution
- Transfer learning across world regions
- Integration with inverse modelling system to calculate methane fluxes

References and Acknowledgements

Fillola, Elena et al. "A machine learning emulator for Lagrangian particle dispersion model footprints: a case study using NAME." *Geoscientific Model Development* (2023)
Battaglia, Peter et al. "Relational inductive biases, deep learning, and graph networks" arXiv:1806.01261 (2018)

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