Bayesian Source Identification with Dual Hierarchical Neural Networks for Urban Air Pollution

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Healthy People and Healthy Planet: AI for Decarbonized, Healthy, Inspiring, and Energy Positive Cities

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Introduction

- Air pollution is a growing concern with many negative impact on public health and the environment.
- Identifying the sources of pollution can help address air quality issues and inform policies and regulations for reducing harmful emissions.
- We propose a novel hierarchical framework for urban air pollution source identification, leveraging deep learning (DL) within an efficient Bayesian inference framework.

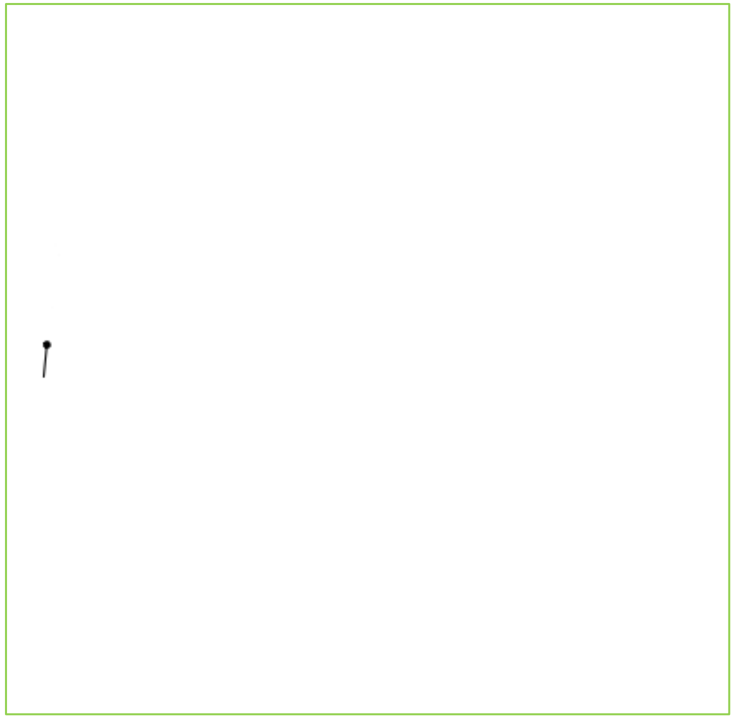
Bayesian Inference

- Baye's rule

$$\pi(M|D) \propto \pi(M)\pi(D|M)$$

Posterior probability ∝ prior probability × likelihood probability

- Advantages:
    - Incorporating prior knowledge
    - Adapting to new information
    - Uncertainty quantification
- Requirement: stochastic sampling tools → Monte Carlo Markov Chain (MCMC) family



Metropolis Hastings-MCMC Algorithm

1. Sample a candidate point from the posterior distribution.
2. Run the forward model.
3. Compute the model-data discrepancy, and the likelihood.
4. Accept or reject to build the corresponding chain.

MH-MCMC in Air Pollution Source Identification

Inverting for 4 parameters (M)

- Longitude (x)
- Latitude (y)
- Emission Rate (q)
- Emission Duration (d)

Uniform prior distribution $\pi(M)$

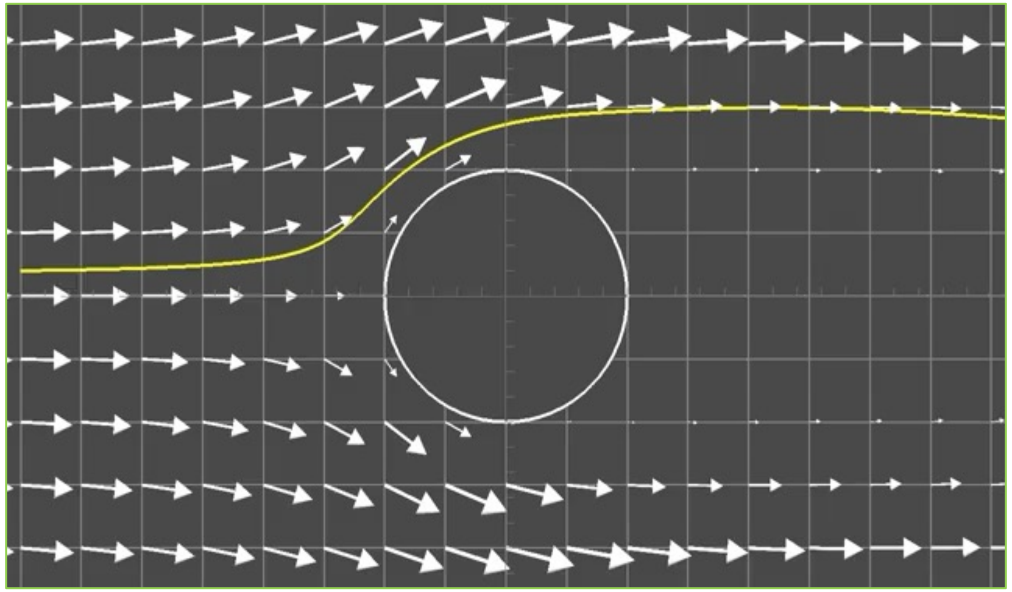
MH-MCMC in Air Pollution Source Identification

- Available environmental monitoring techniques:
  - Sensors
  - Satellite images
  - Remote sensing techniques
- Two forms of pollution observations:
  - Discrete point-wise concentration values
  - Concentration fields

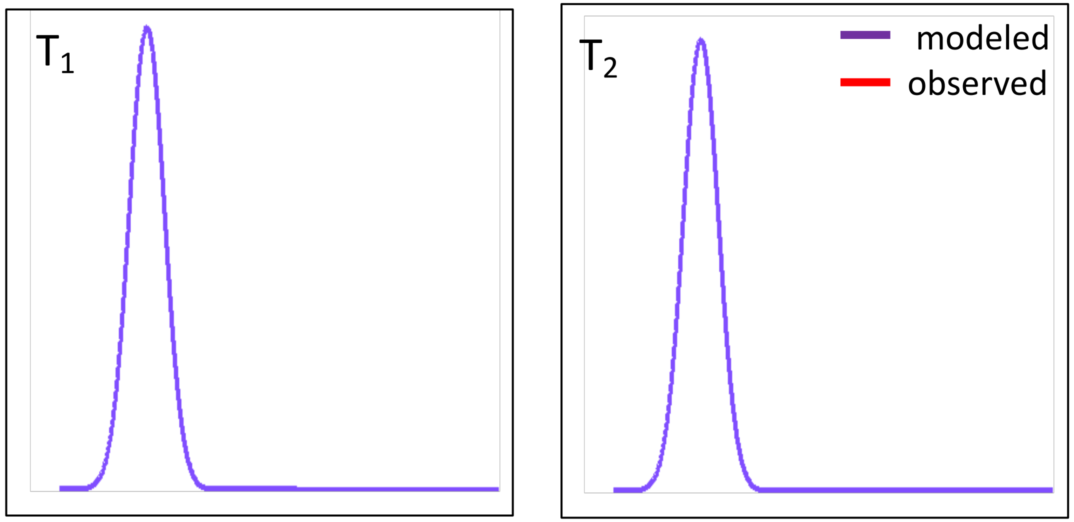
Al Aawar, et al, (2023). Bayesian source identification of urban–scale air pollution from point and field concentration measurements. Computational Geosciences. (in production).

The Lagrangian Transport Model

- The Graz Lagrangian model **GRAL**:
  - Microscale wind field computations.
  - Lagrangian particle tracking.
- Navier-Stokes equation along with the k-ϵ turbulence closure model.
- Inputs: topography, land use, buildings, meteorological conditions and emission sources.

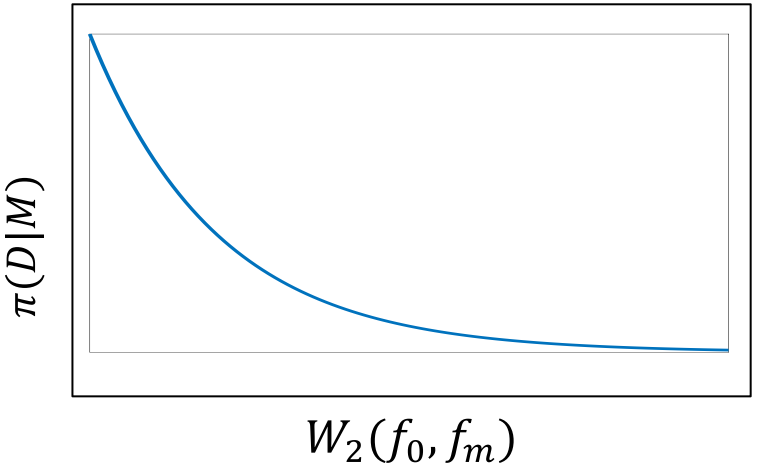


Modeling the Likelihood



- Each concentration field is considered as a distribution that could be displaced.
- The Wasserstein distance is the cost of displacing the predicted model output to the observation.
- This cost physically represents the required work as the product of the mass to be moved and the distance to be traveled.

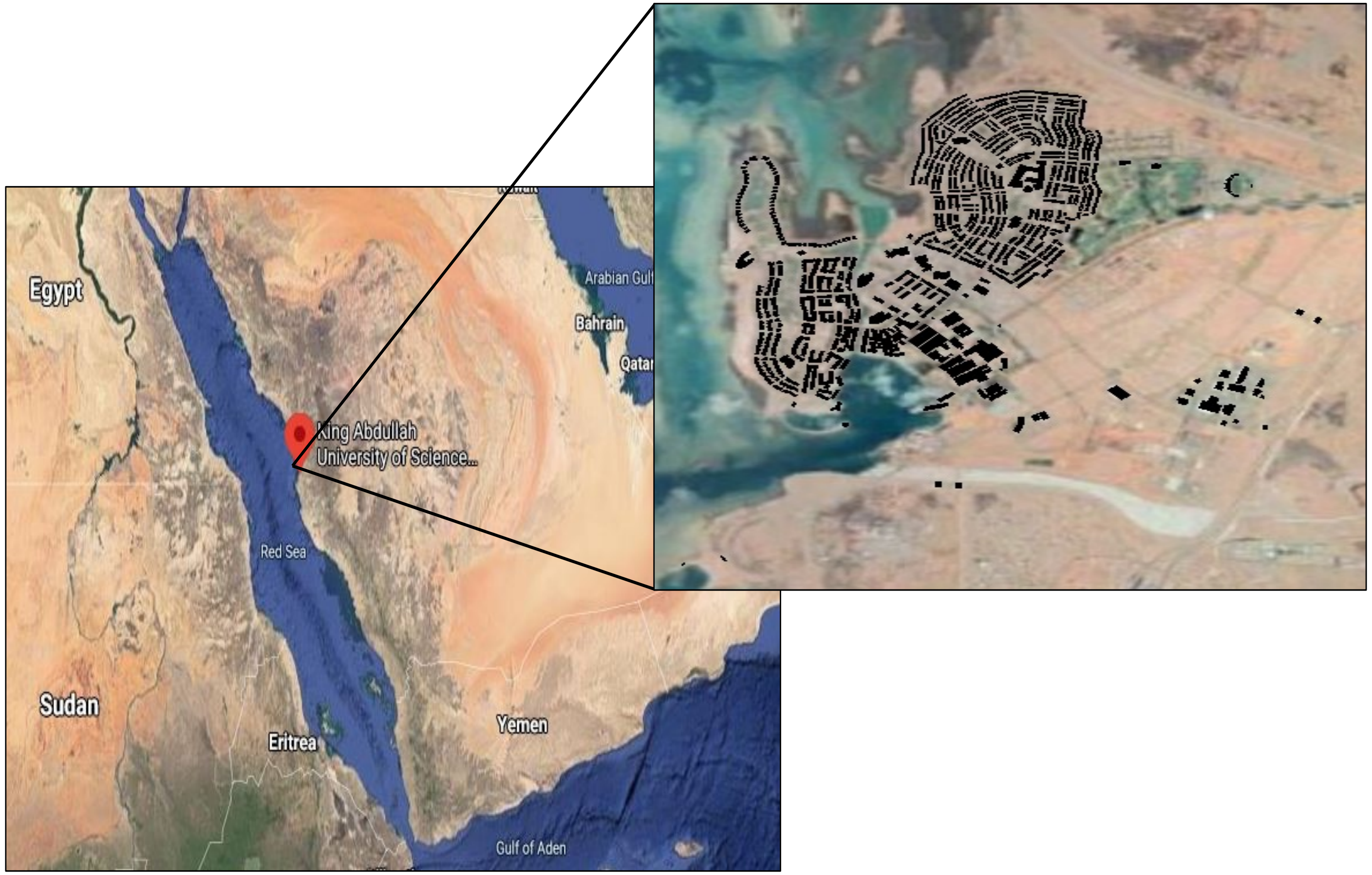
Exponential likelihood

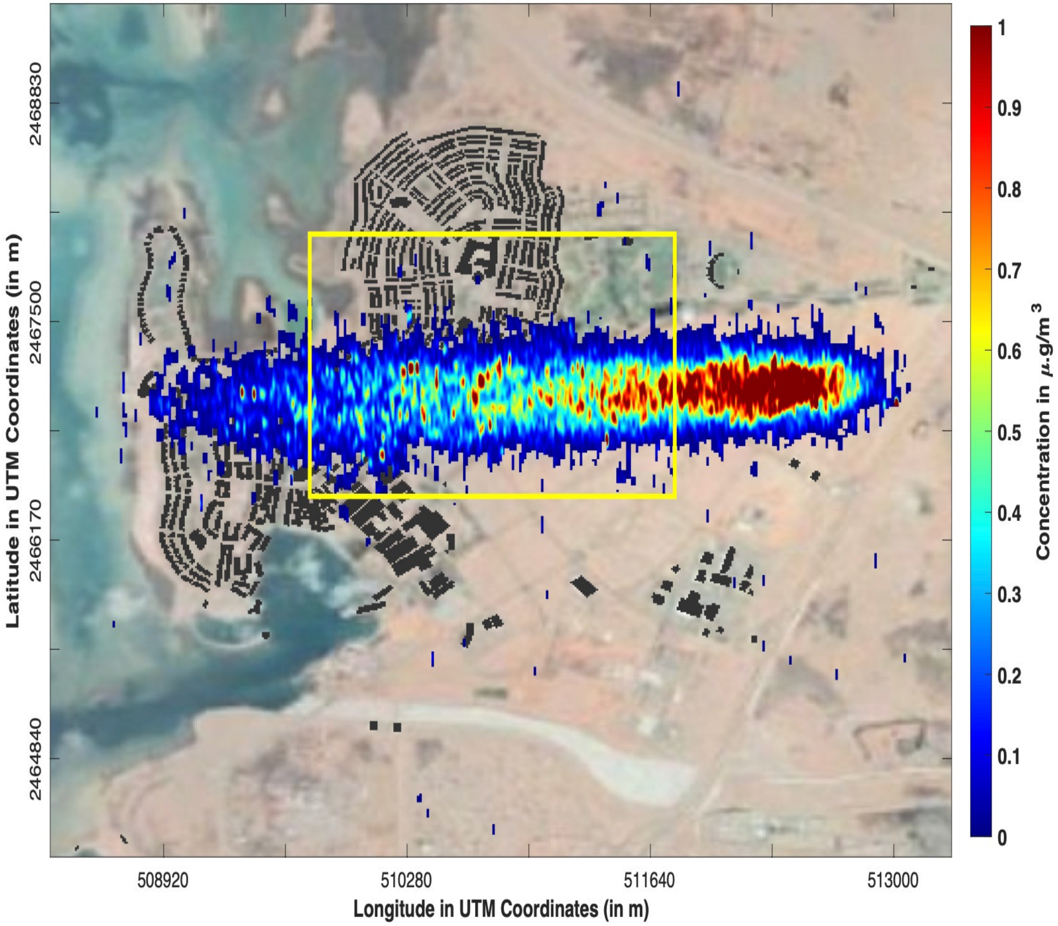


$$W_2(f_0, f_m) = \min_{T^* \in \mathcal{T}(f_0, f_1)} \mathcal{L}(u, v) f_0(u)$$

- f_0 and f_m: observed and modeled concentration fields, respectively.
- $\mathcal{T}$: set of regular bijections mapping f_0 to f_m.
- $\mathcal{L}(u, v)$: Euclidean distance from point u to point $v = T(u)$.

Case Study: KAUST Synthetic Scenario





Al Aawar, E., El Mohtar, S., Lakkis, I., Alduwais, A. K., & Hoteit, I. (2023). Bayesian source identification of urban-scale air pollution from point and field concentration measurements. Computational Geosciences, 27(4), 605-626.

Results and Challenges

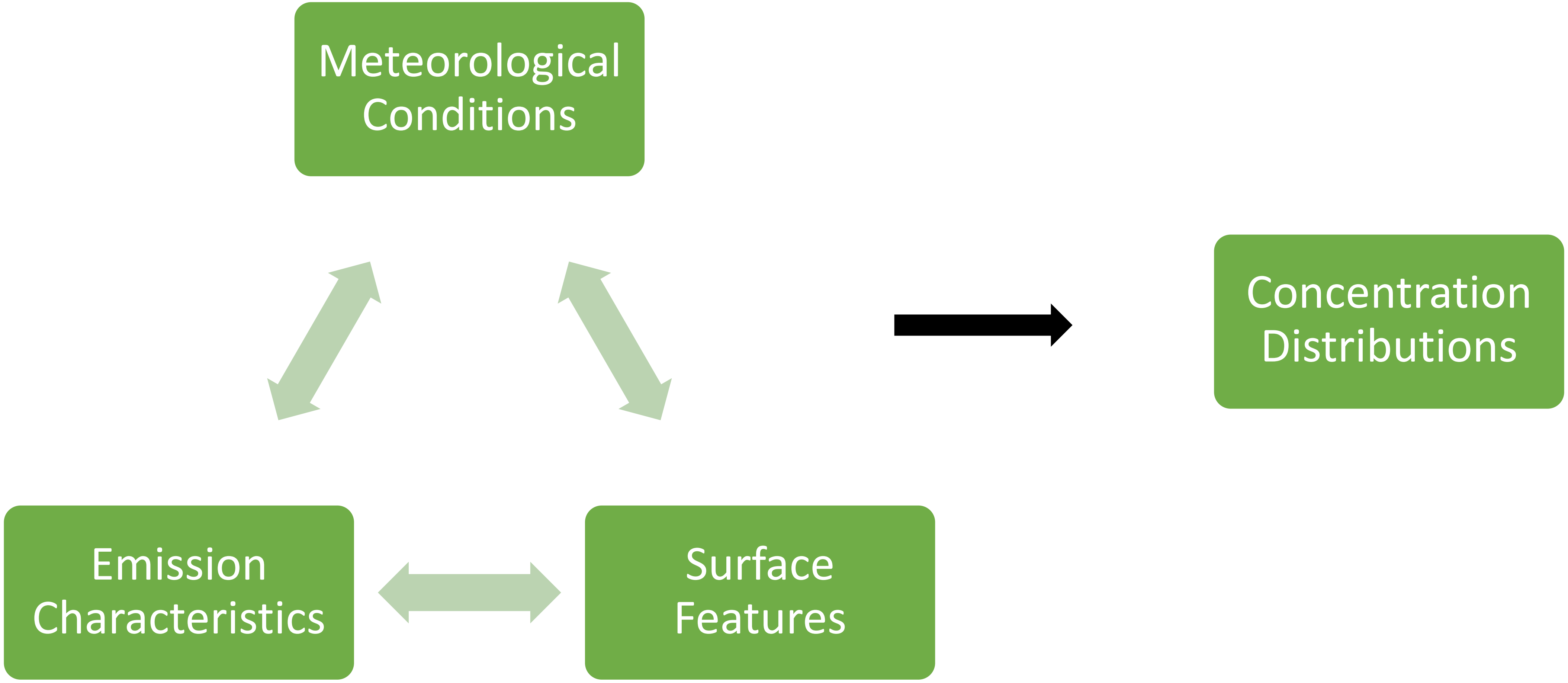
- Excellent solutions are obtained with the global W_2 dissimilarity metric.

- Challenge:
  - Each chain generation with **10,000** samples requires **143** hours.
  - Numerous runs of the expensive physical dispersion model.
  - High Cost of the W_2 Distance: Half of the computational time is spent to calculate the W_2 distance for each sample.

Solution: Use DL

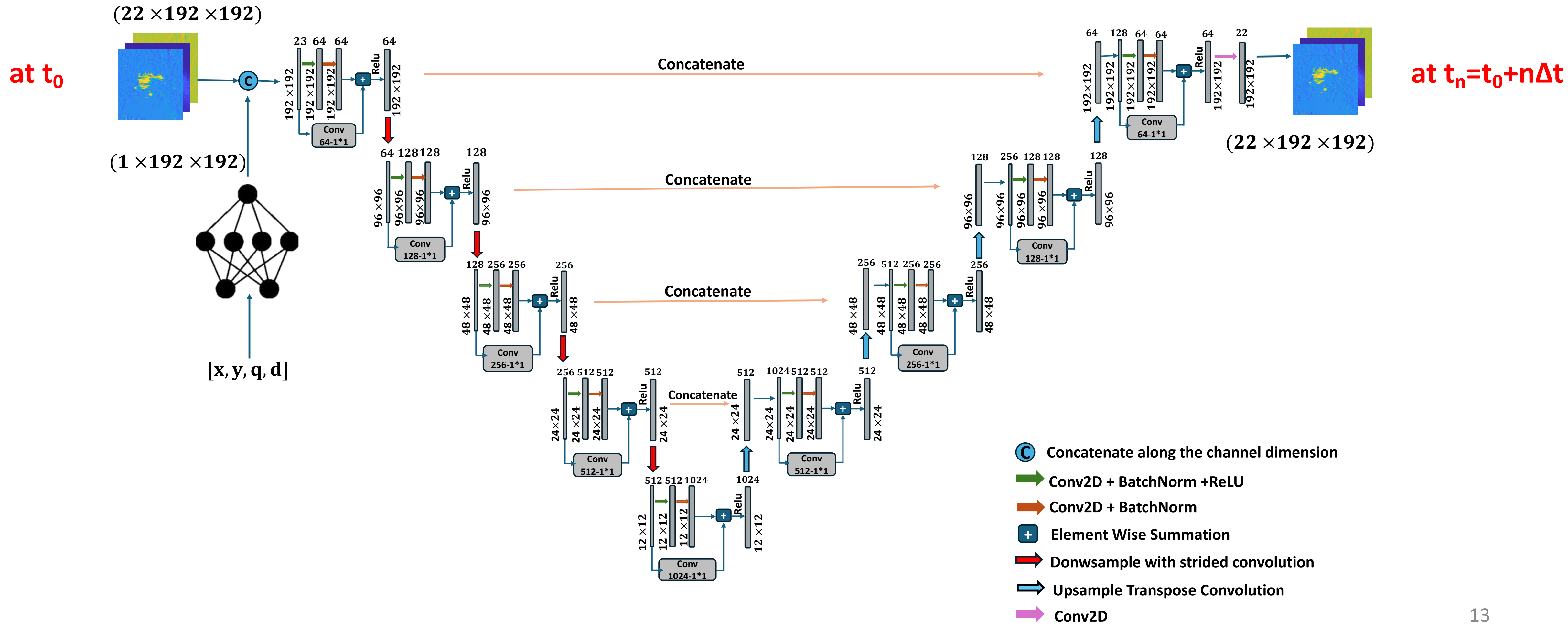
- The acceleration of tradition Bayesian inference by training a NN to predict air pollutant concentrations based on given flow conditions and emission characteristics.
- Coupling this emulator with a NN approximation of the likelihood distribution to synergistically accelerate computations.
- Full operation on GPUs, leveraging parallel computing architectures to expedite computational costs.

The Lagrangian Transport Surrogate Model: Learning Task



Al Aawar, E., Resifi S., Jebari H. & Hoteit I. (2024). Bayesian Source Identification with Dual Hierarchical Neural Networks for Urban Air Pollution. (Under Revision)

The Lagrangian Transport Surrogate Model: Architecture



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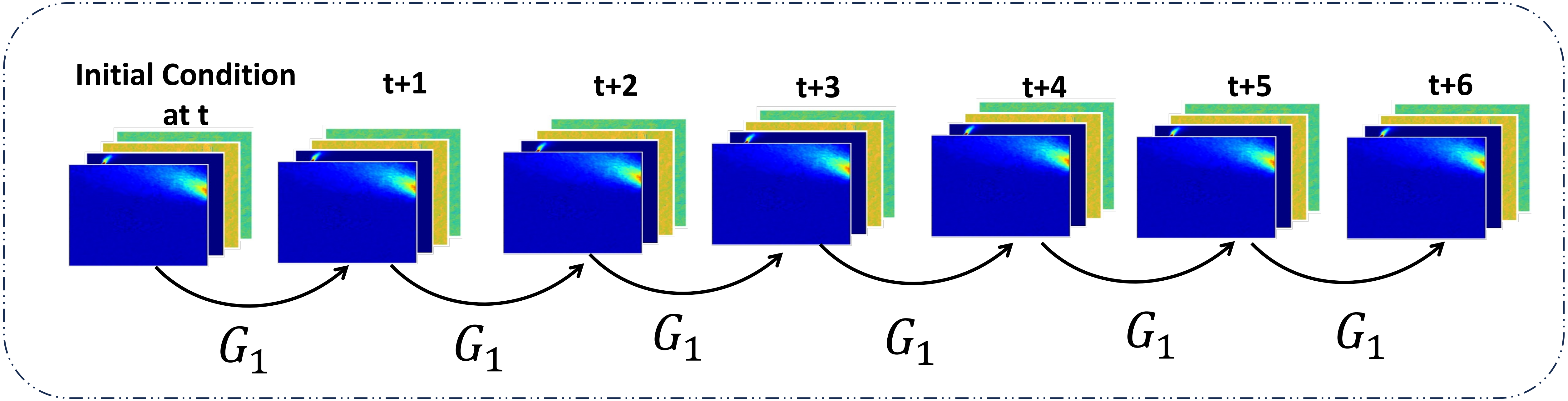
The Lagrangian Transport Surrogate Model: Training

- Prediction in time at each time step.
- Cumulative error growth for each time step.



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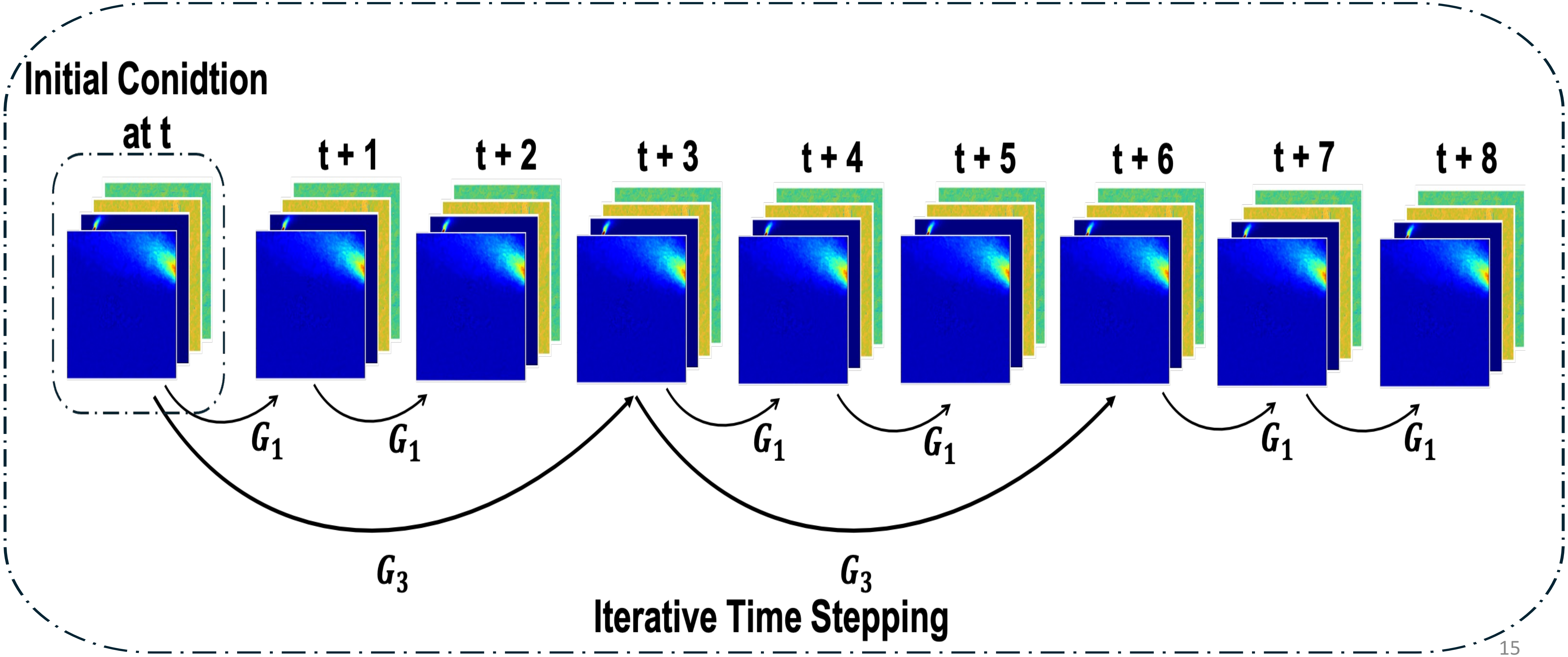
The Lagrangian Transport Surrogate Model: Training



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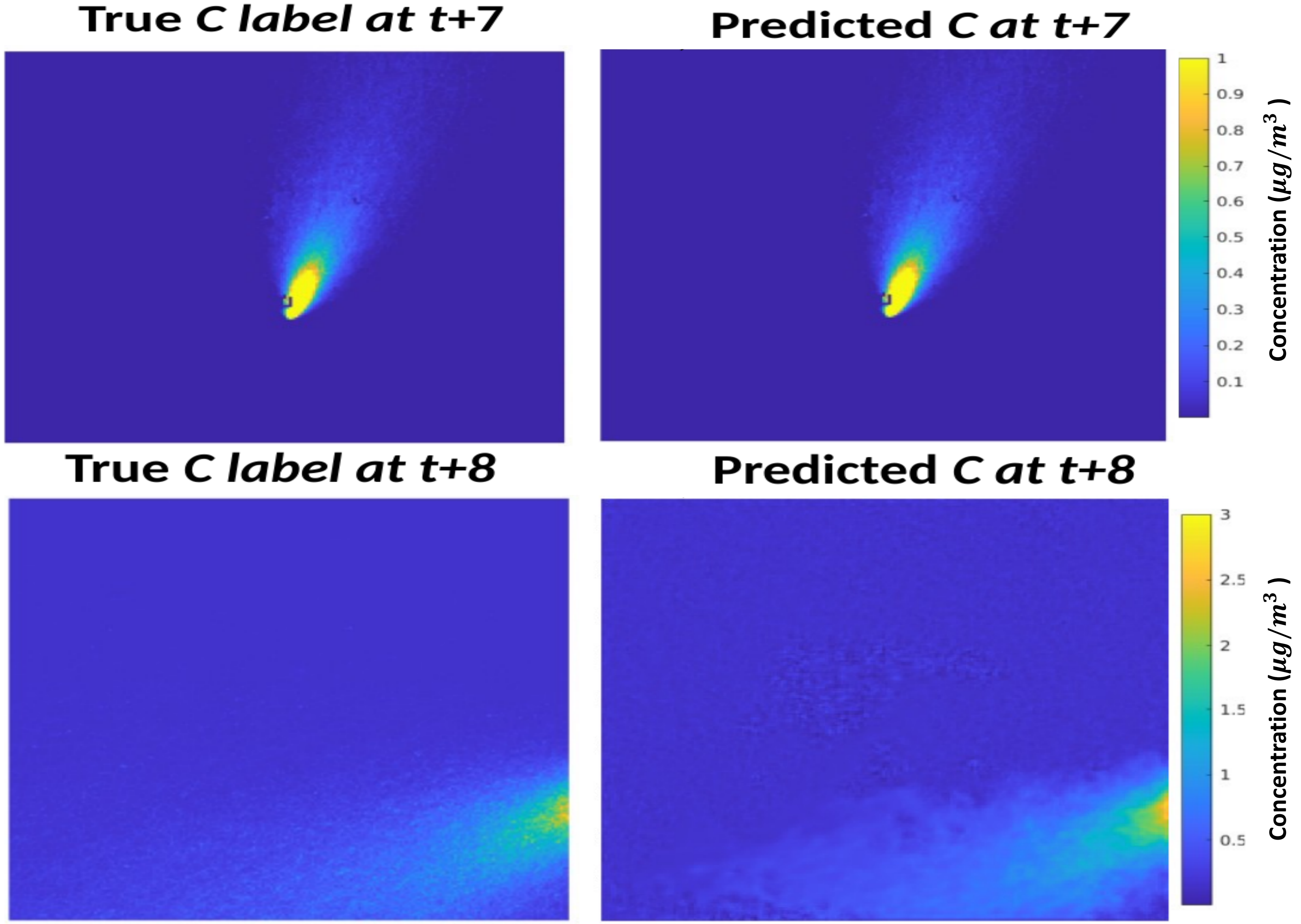
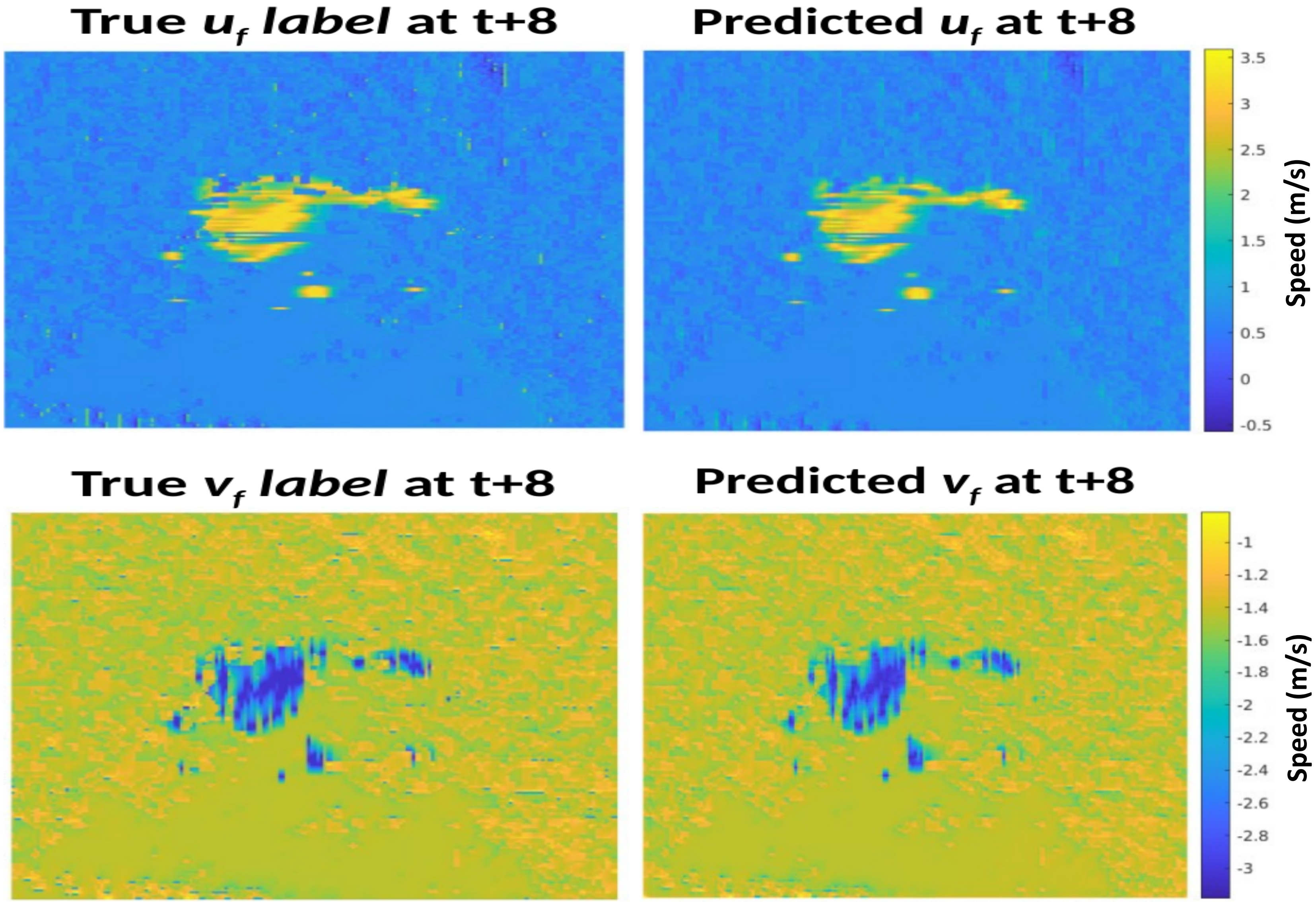
Examples of Predictions



Evaluation Results:

- RRMSE = 3.6%
- MBE = 0.015
- IOA = 98%

Examples of Predictions



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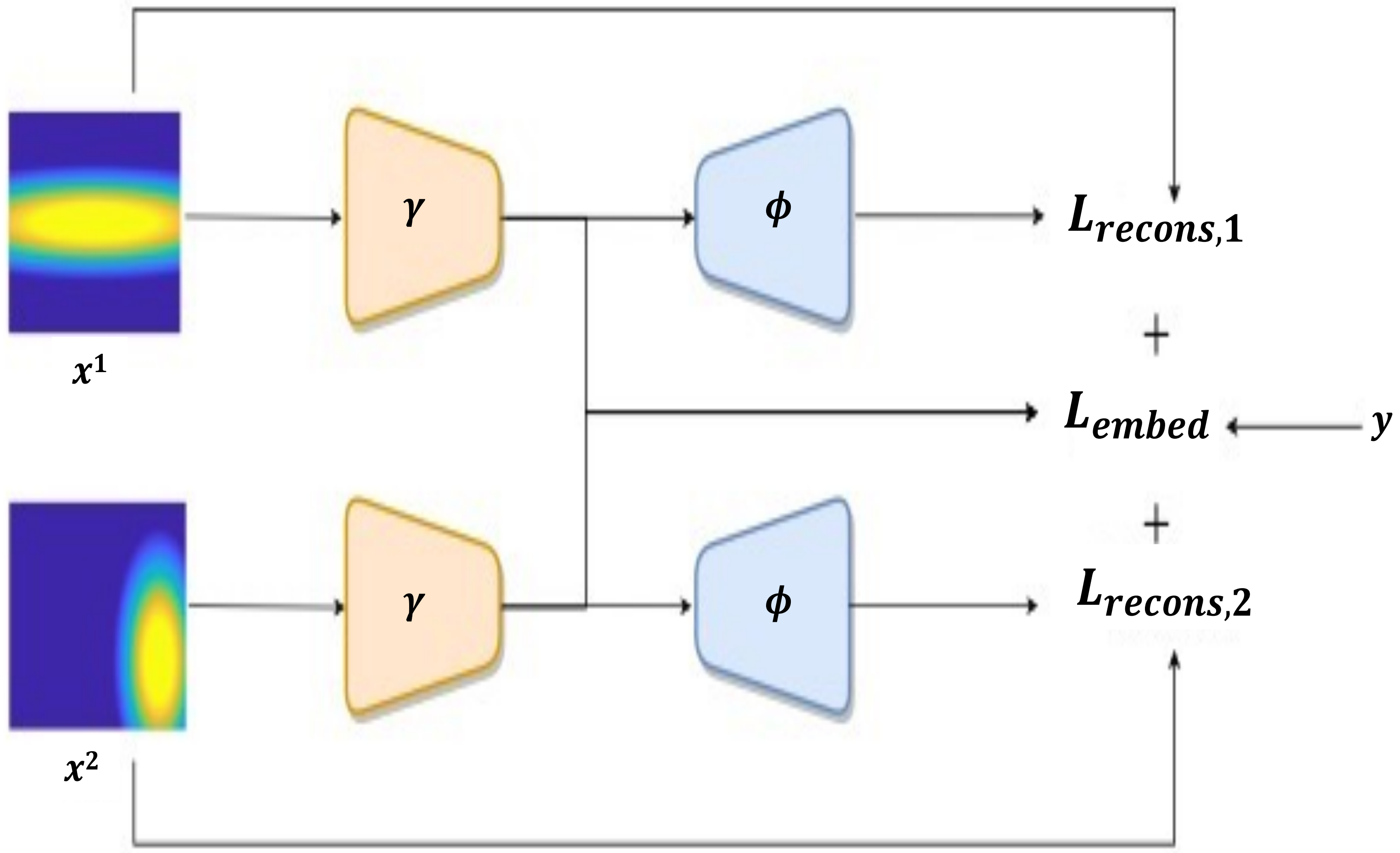
Siamese Network for W_2 Approximation

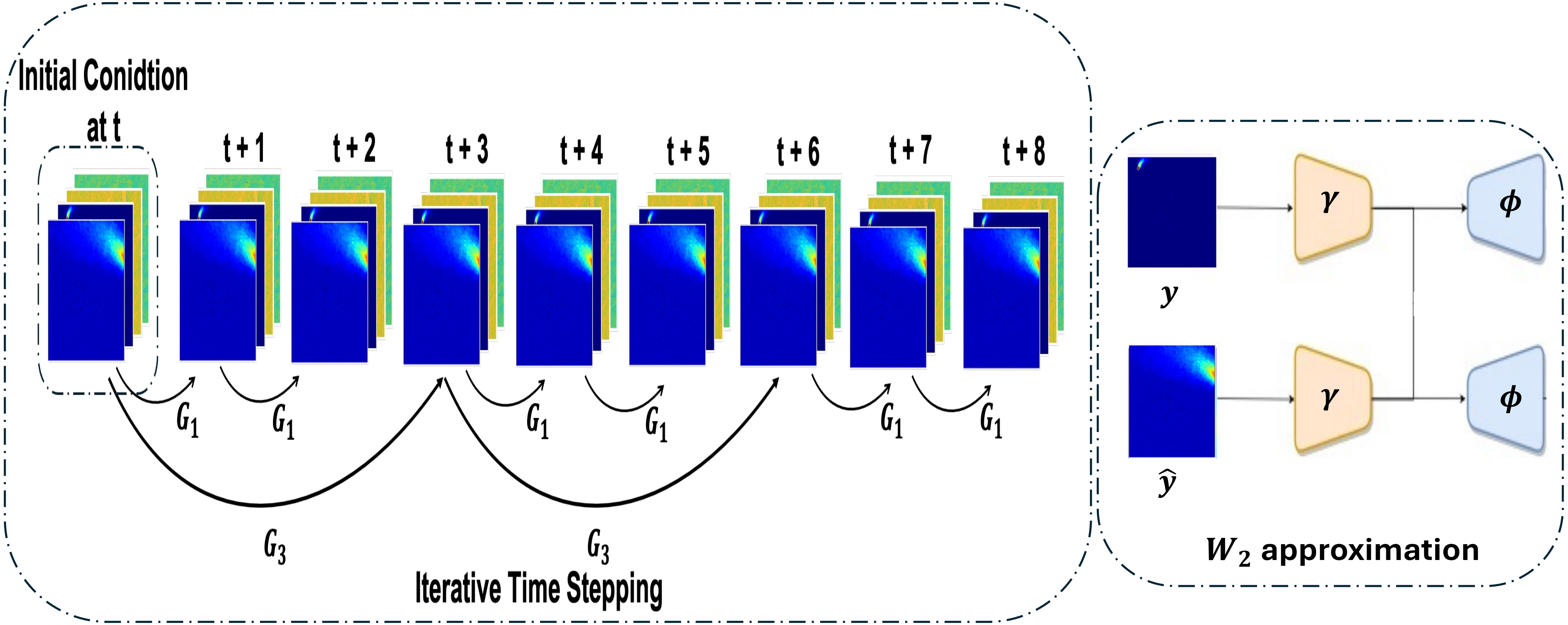


- x^1, x^2: two input fields.
- γ: encoder.
- ϕ: decoder.
- y: the corresponding W_2 distance.
- $L_{recons,1}$ and $L_{recons.2}$: reconstruction loss terms of each input as computed by the KL divergence.
- L_{embed}: L_2 norm of the difference between the Euclidean distance of the embedded features and y.

Normalized L_2 error = 4.35%

Al Aawar, E., Hammoud, M. A. E. R., & Hoteit, I. (2024). Two-step AI-aided Bayesian source identification of urban-scale pollution. Atmospheric Environment, 323, 120388.

The Dual Hierarchy



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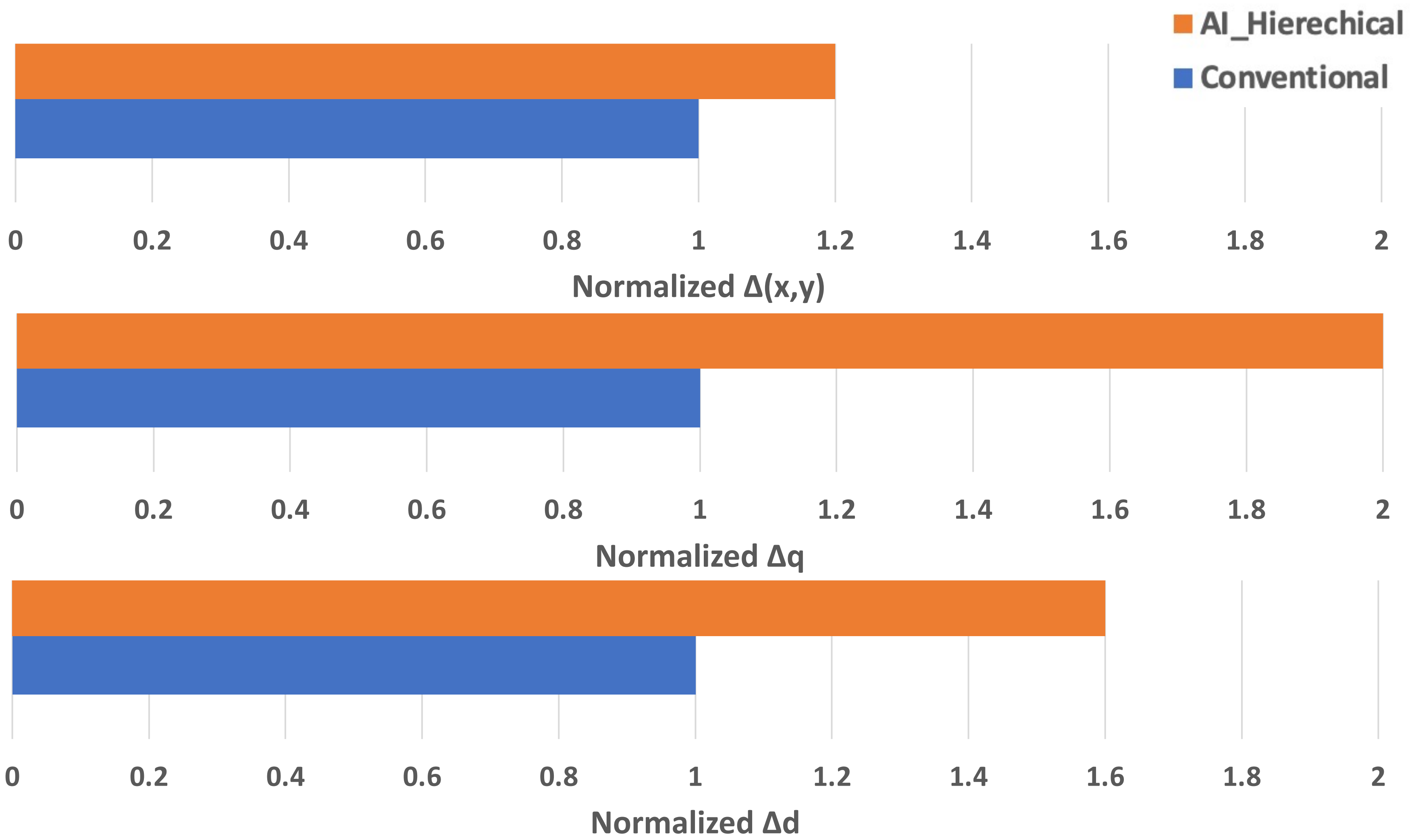
Bayesian Solution-10,000 samples

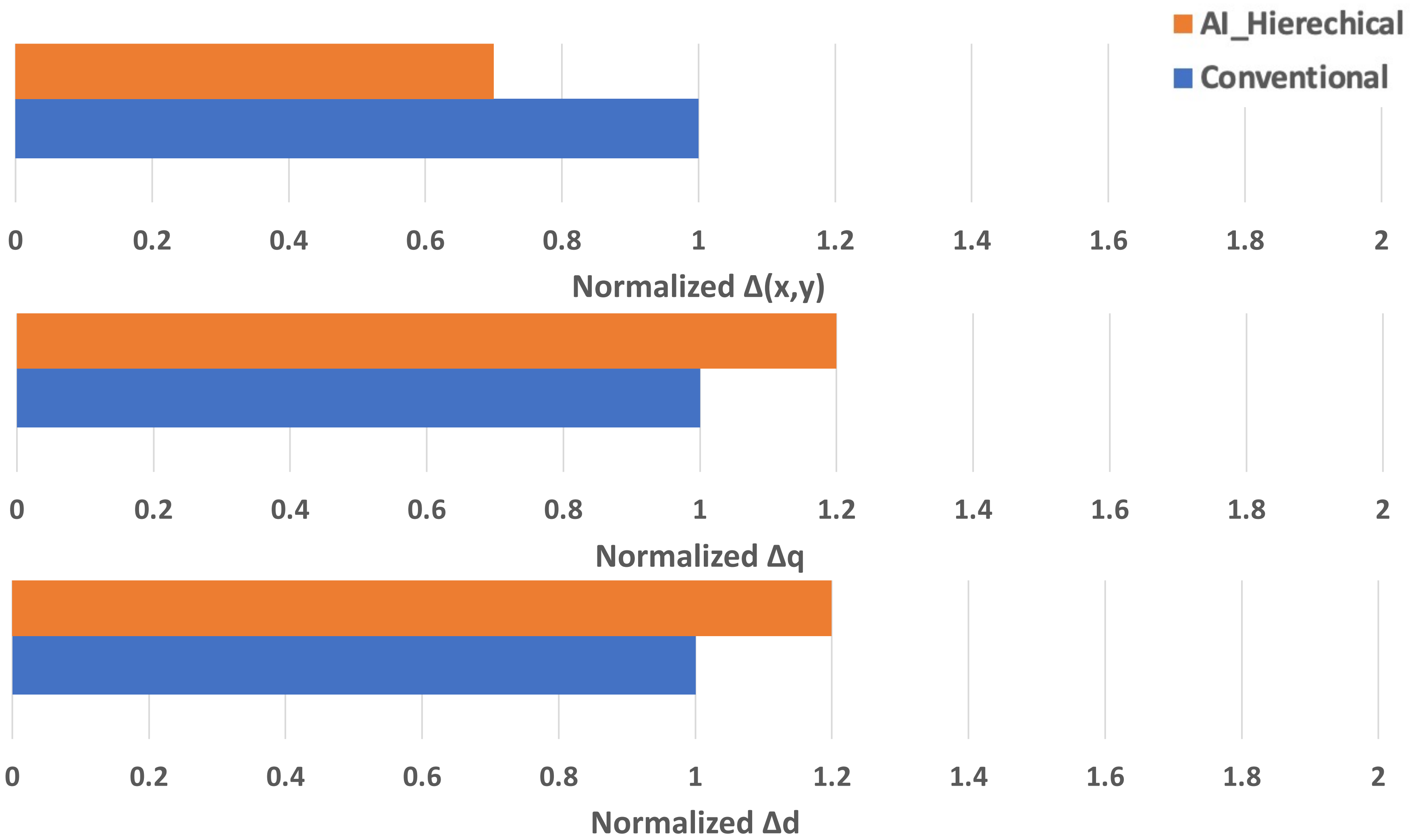


Computational Time

- Conventional: 6days!
- AI-Hierechical: 20minutes

More samples!

Bayesian Solution-100,000 samples



Computational Time

- Conventional: 60days!
- AI-Hierechical: 3.34hours

High Computational Savings
Better Convergence
Higher Confidence

Conclusion

- Successfully developed a NN surrogate model for Lagrangian dispersion, and a NN approximation for the likelihood estimation.
- Bayesian inference framework employs the dual NNs to infer the emission parameters in an urban environment.
- Suggested solutions results in appreciable reduction in computational requirements with minimal loss in performance.
- Our approach can accurately identify sources of air pollution, thus help in responding to harmful emissions and improve overall air quality.

Thank you for your time and attention!

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