

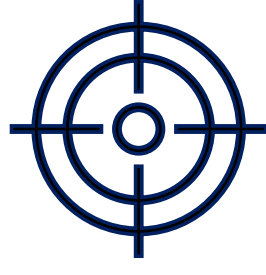
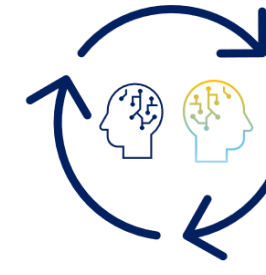
Parametric Physics-Informed Neural Networks (pPINNs) for Air Quality (AQ) Modelling and Inference

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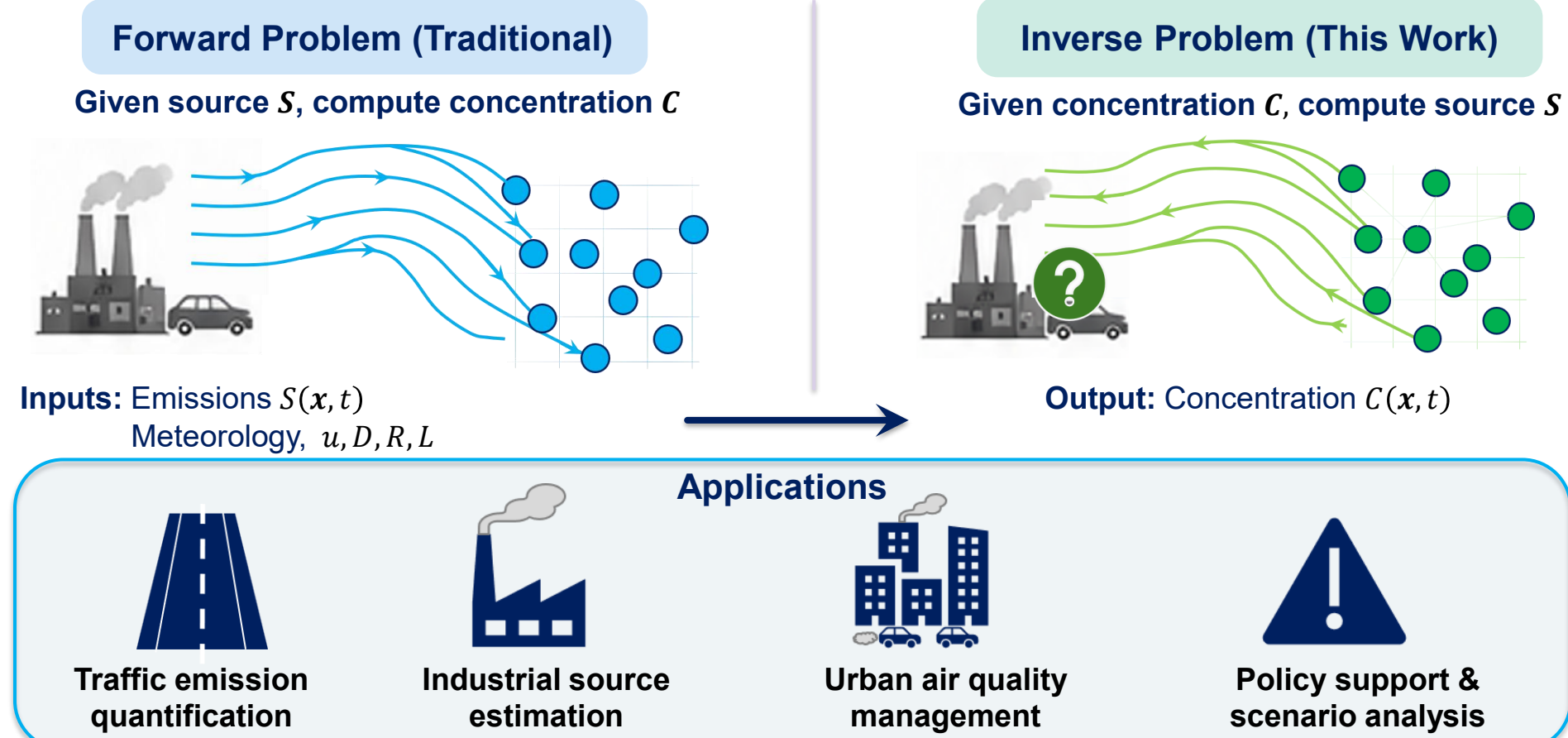
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Combining Data, Physics and Machine Learning for Cleaner Air

**PHYSICALLY CONSISTENT**
Respects governing laws of nature**DATA EFFICIENT**
Works with sparse and noisy measurement**INVERSE CAPABILITY**
Infer emissions from concentration field observations**REAL-TIME (RT) DIGITAL TWIN (DT)**
Update emissions & AQ in real-time w/ bidirectional parameter exchange

1. The Problem

Accurate AQ prediction requires reliable emissions estimates
Monitoring data are sparse, while emissions are uncertain
PINNs integrate physical laws with data to predict concentration fields & infer unknown emissions



2. Governing Equations

Atmospheric transport of a pollutant (e.g. PM_x or NO_x) is commonly described by the advection-diffusion-reaction (ADR) equation:

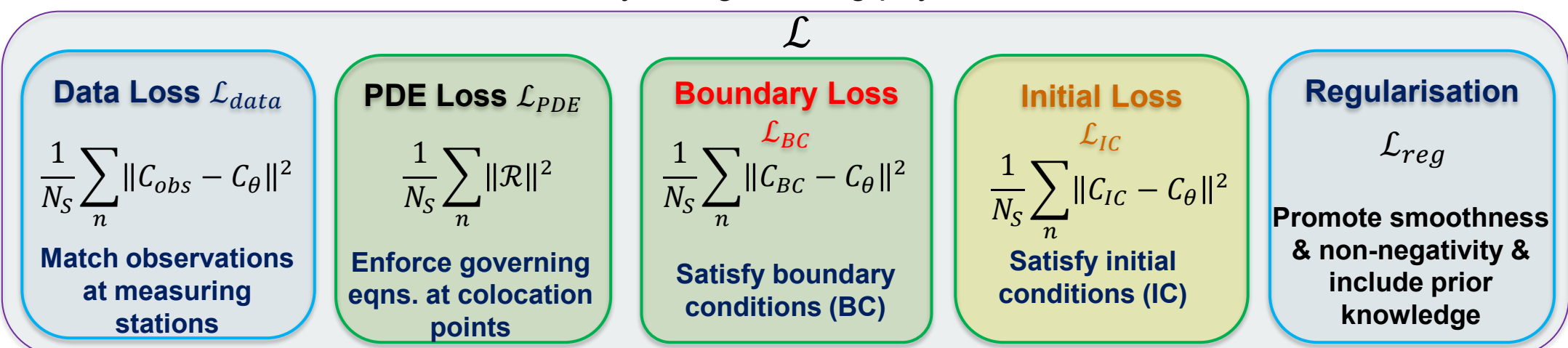
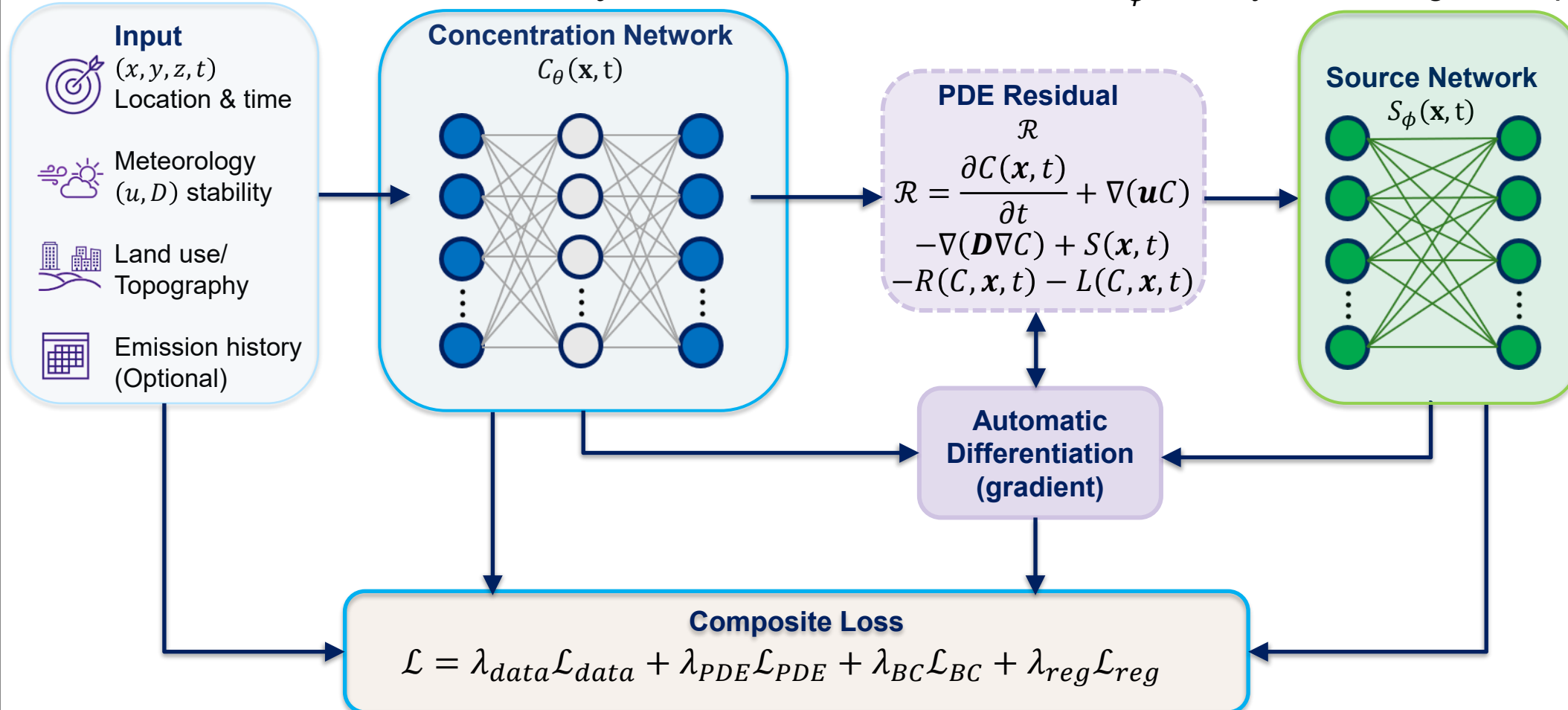
$$\frac{\partial C(x, t)}{\partial t} + \nabla(uC) = \nabla(D\nabla C) + S(x, t) - R(C, x, t) - L(C, x, t)$$

 $x = (x, y, z)$ - 3D spatial coordinates [m] t = time [s] $C(x, t)$ pollutant concentration [kgm^{-3}] $u(x, t)$ flow velocity vector [ms^{-1}] D diffusion tensor $S(x, t)$ source term (emissions per unit volume) [$kgm^{-3}s^{-1}$] $R(C, x, t)$ reaction/chemical transformation term (mass removed/mass produced) [$kgm^{-3}s^{-1}$] $L(C, x, t)$ losses due to deposition, settling, wet scavenging, ... [$kgm^{-3}s^{-1}$]

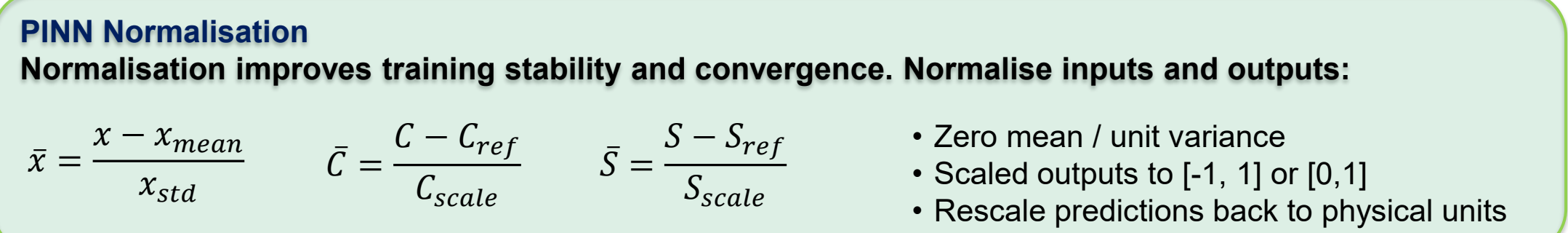
Boundary conditions (inflow, outflow, ground, top) and initial conditions (IC, $C(x, 0) = C_0$) complete the model

3. PINN Formulation

PINNs learn the concentration field $C_\theta(x, t)$ and the emissions source $S_\phi(x, t)$ by minimising a composition loss which enforces both data fidelity and governing physics

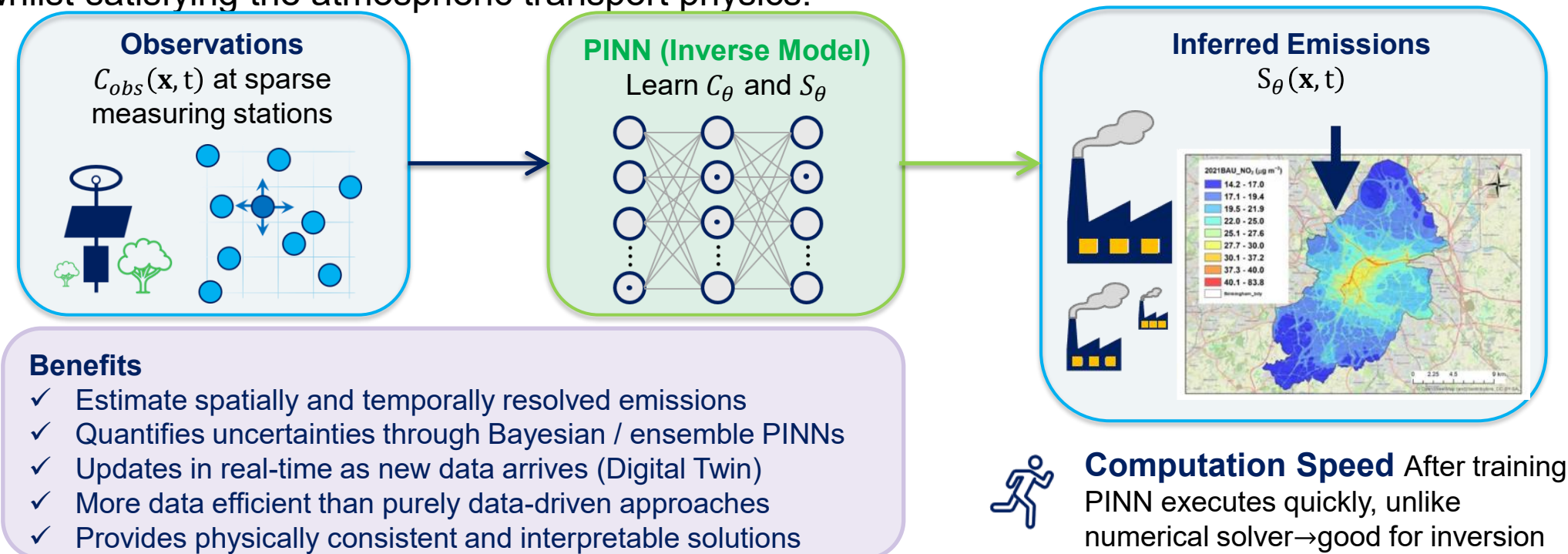


Optimised with Adam / L-BFGS to learn $\theta, \phi \rightarrow$ physical consistent C and S

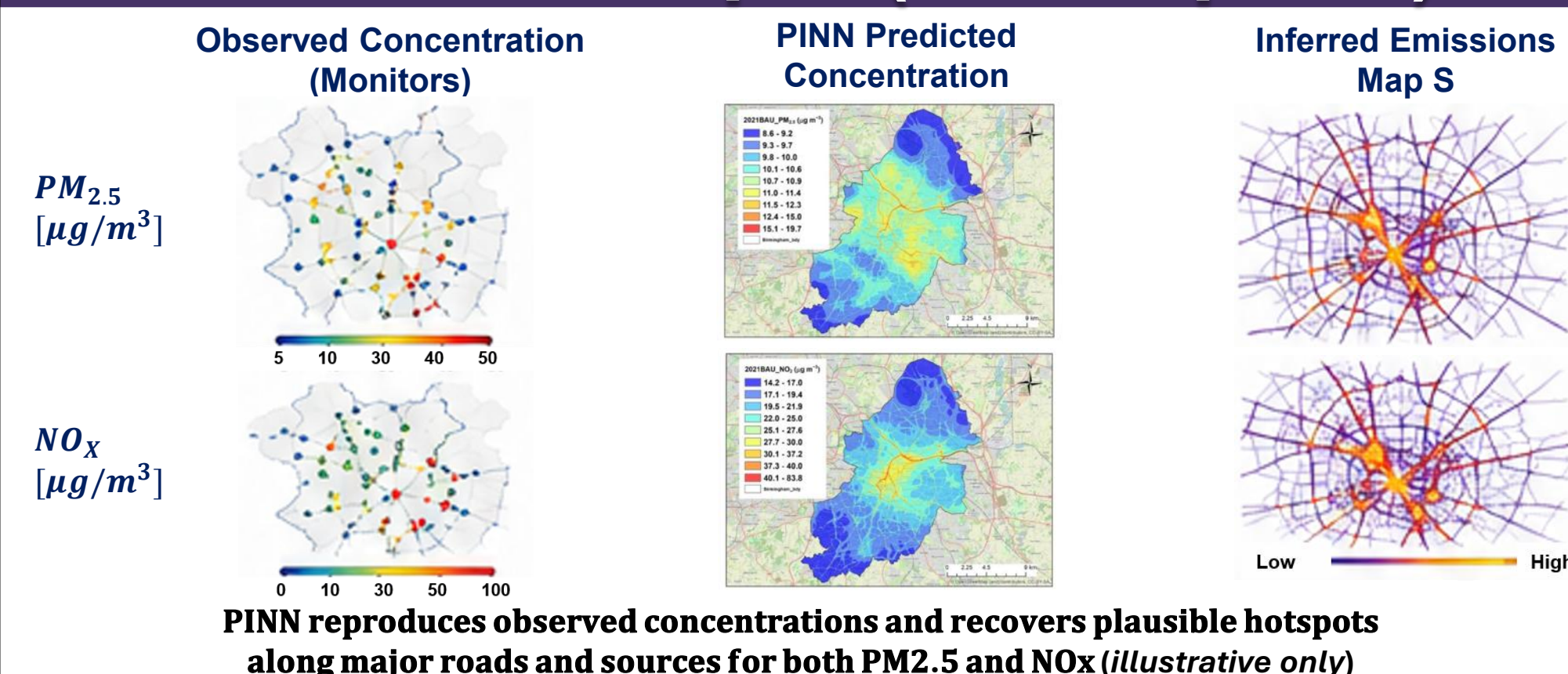


4. Inverse Emissions Inference

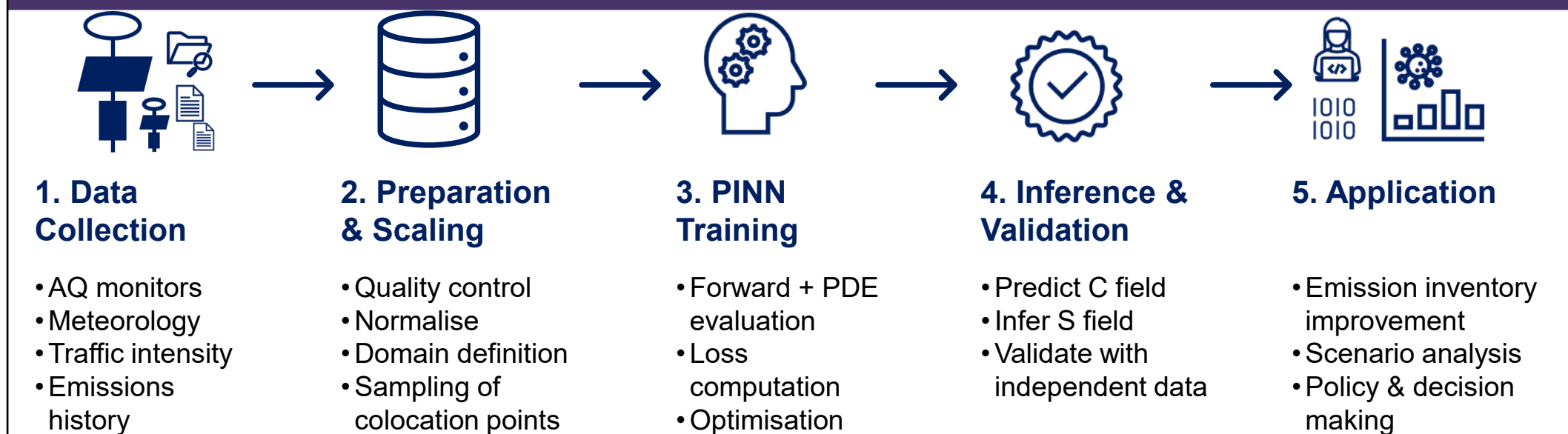
Given concentration observations, PINNs infer emissions sources which best explain the data whilst satisfying the atmospheric transport physics.



6. Results Example (Conceptual)



5. Implementation Overview



pPINN (Parametrised PINN)

Instead of inferring $S_\phi(x, t)$ at every point, emissions are **parametrised** using known drivers α (traffic flow Q , speed V , fleet mix F , road type R , etc.):

$$S_\phi(x, t) = f(Q, V, F, R, \dots, \phi)$$

The PINN learns the parameters α (e.g. emissions factors, scaling factors by road type, time, season, etc.)

- Reduces dimensionality
- Ensures physical plausibility
- Simpler uncertainty quantification

Parametric studies can be performed.

Additional parameters are introduced into the PINN as additional network inputs, expanding the dimensionality of the PINN and increasing the collocation point dimension for training (improved training)

7. Why PINNs for Air Quality?

**Physics-aware**
Built on transport equations $\rightarrow$ physically consistent predictions**Data-efficient**
Works with sparse, noisy, irregular monitoring data**Inverse capability**
Retrieve source emissions from concentration observations**Generalisable**
Robust across space, time and scenarios**R-T DT**
Continuously update emissions and AQ**Decision support**
For policy makers, regulatory authorities, public health, city planners

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CORE TAKEAWAY

PINNs uniquely combine atmospheric science, data & machine learning to predict air quality & infer emissions in a physically consistent, data-efficient & interpretable way $\rightarrow$ **enabling next generation AQ management & cleaner air FOR ALL.**

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