Forecasting Groundwater Levels and Optimizing Monitoring Networks for Remediation Design Using Diffusion Models

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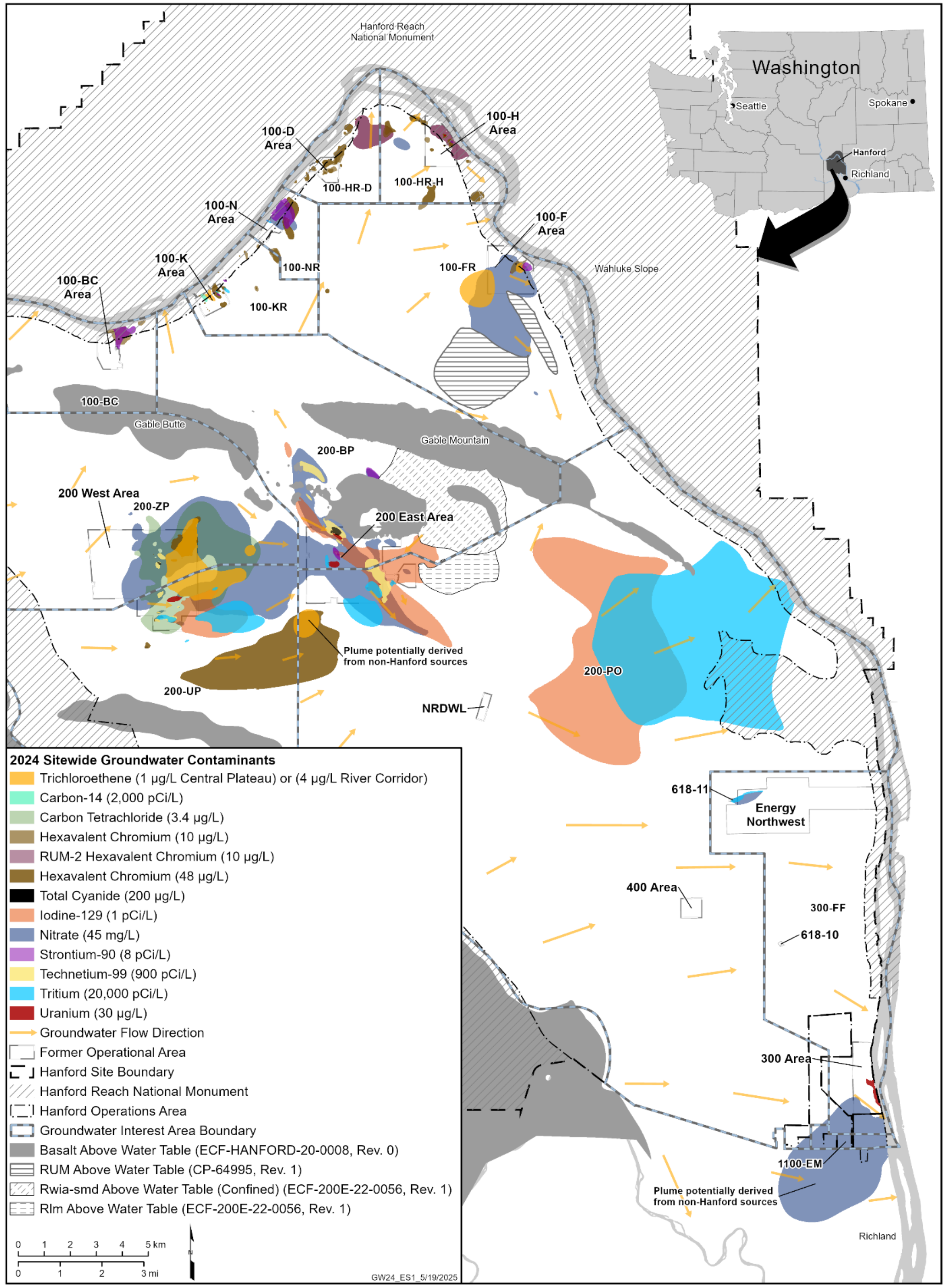
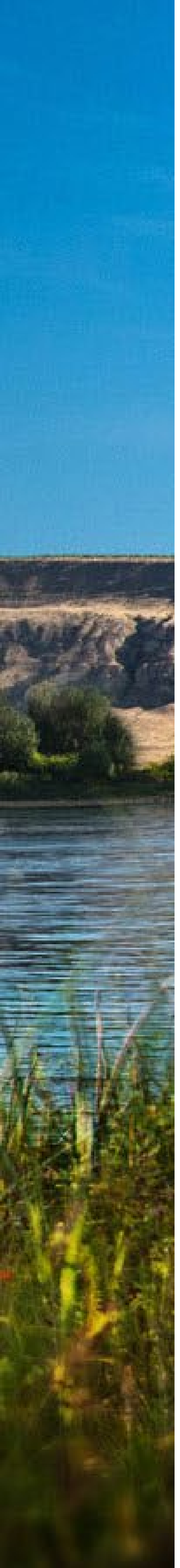
Motivation: Optimize the Groundwater-Level Monitoring Network

- Continuous groundwater-level (GWL) mapping is essential to anticipate plume migration and inform remedy decisions.
- Traditional workflows are periodic, manual and static; they don't include per-well information-value metrics.
- Need: a method that generates uncertainty-aware, time-resolved GWL maps to **optimize monitoring-network design**—prioritizing wells and setting measurement-frequency targets.



Hanford Sitewide Plumes, 2024
(Source: DOE/HFO-2024-41, Rev. 0)



From 15 to nearly 1,200 Wells — Evolving Coverage Across 75 Years

- The Hanford Environmental Information System (HEIS) archives 187,000+ GWL measurements from 2,151 wells (1948–2024).
- Sampling remains uneven—half of wells have fewer than 57 readings, while a small subset exceeds 200 measurements.
- This irregular space-time coverage complicates interpolation and uncertainty quantification, motivating approaches that account for monitoring network coverage and measurement frequency explicitly.

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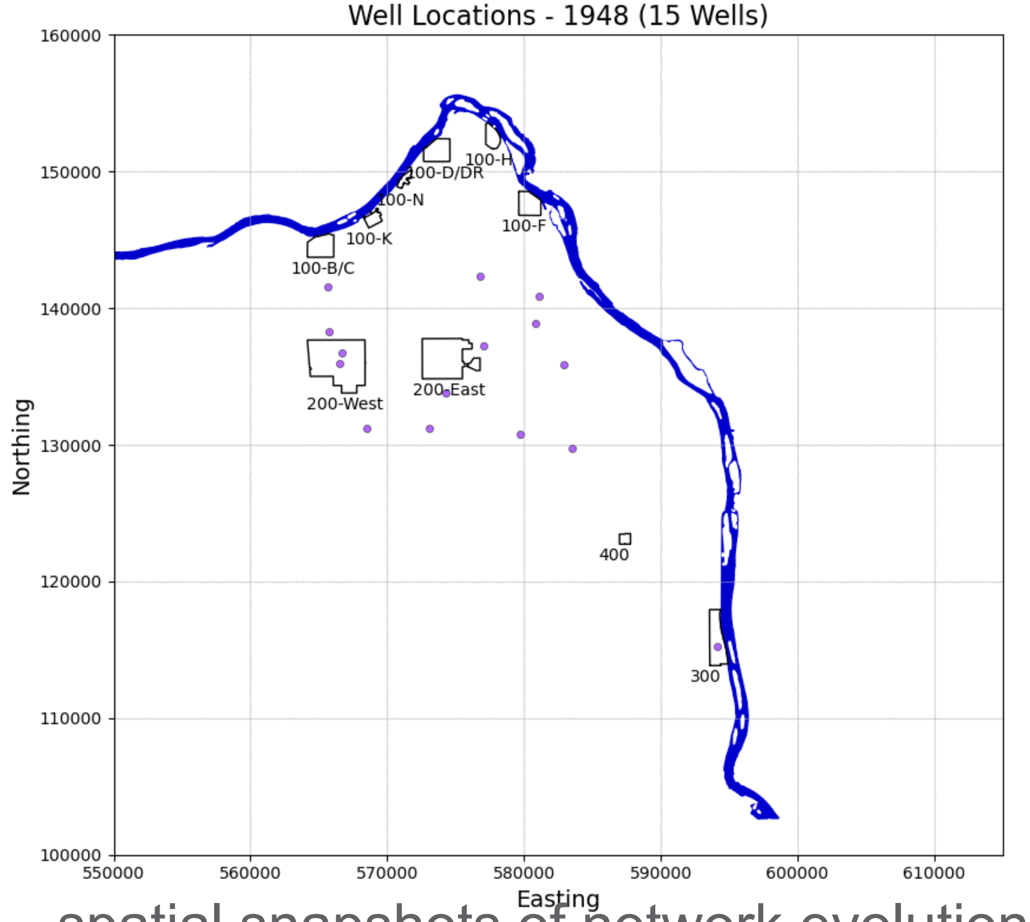
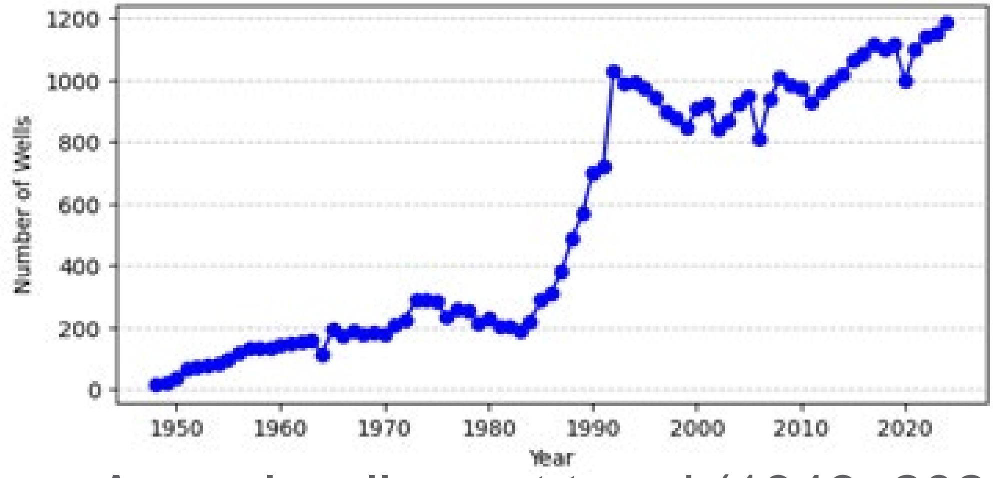


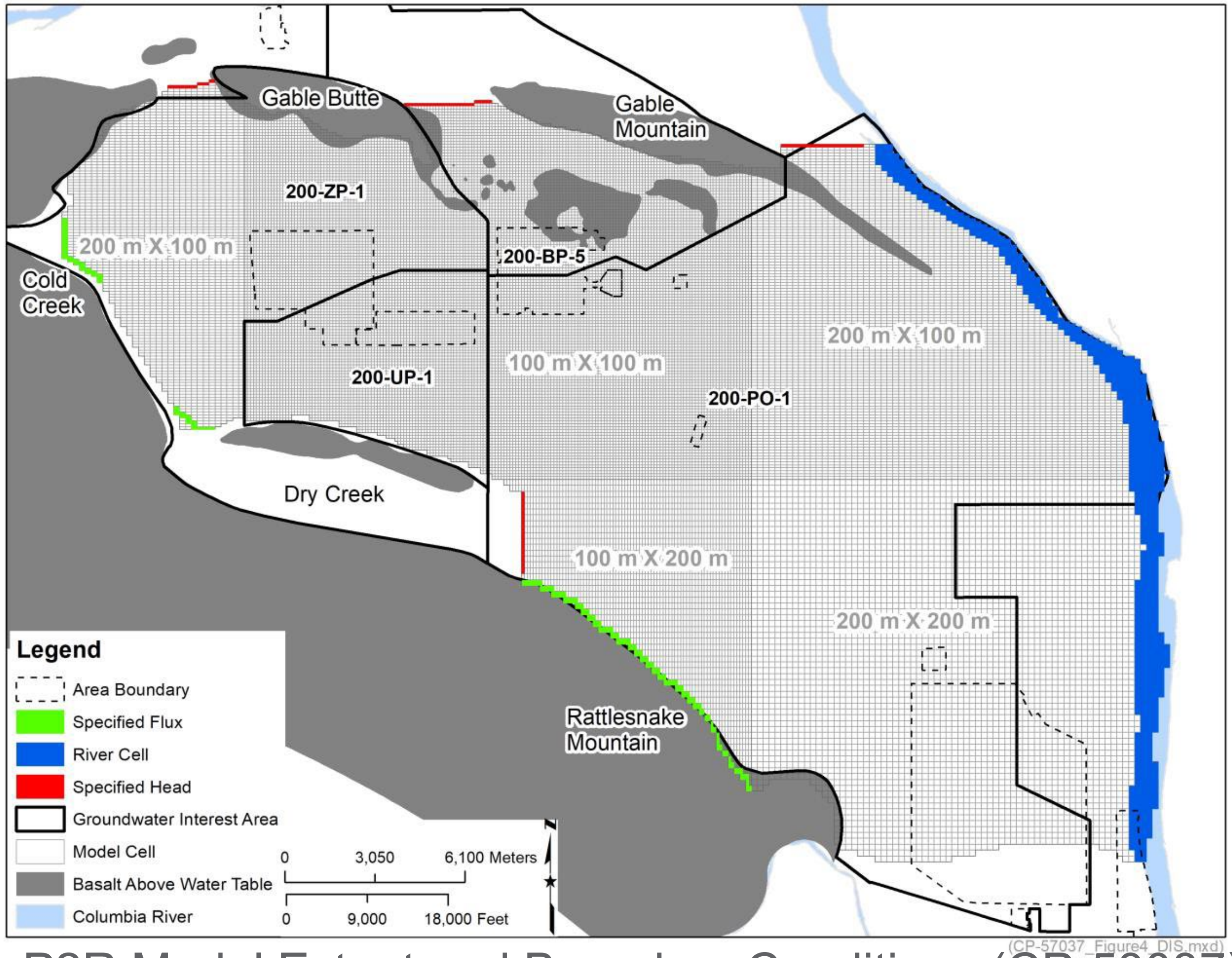
spatial snapshots of network evolution



Annual well count trend (1948–2024)

Physics Simulations Provide Spatiotemporal Patterns for Learning

- The Hanford Plateau-to-River (P2R) model, calibrated to historical wells, outputs GWL fields over a 1943–2018 history-matching period and extending through a projection interval to 2137.
- These physics-consistent sequences capture regional gradients, barrier effects, capture/low-flow zones—the site-scale spatiotemporal patterns we can learn from.



P2R Model Extent and Boundary Conditions (CP-53037)

- Simulation fields define reference patterns; HEIS data later anchor the mapping to actual observations.

Diffusion + Score-Based Data Assimilation for Observation-Consistent GWL Mapping

- **Diffusion prior (learns physics patterns):** 1) forward stochastic differential equation (SDE) perturbs from P2R GWL sequences $\mathbf{x}$, inducing a family of noisy densities $p_s(\mathbf{x})$ over diffusion time/step s; 2) The model then learns the score $\nabla_x \log p_s(\mathbf{x})$ and uses the reverse SDE to denoise, generating physically coherent GWL fields.

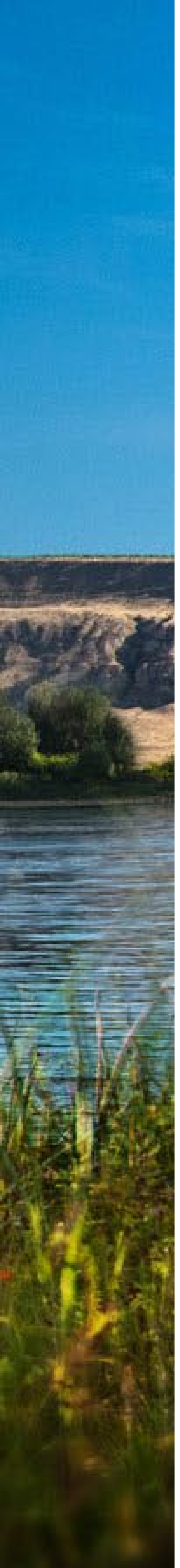
- **Score-Based Data Assimilation (SDA) :** conditions on well observations by, at each reverse step s and observed time t, the observation operator H_t maps gridded GWL field $\mathbf{x}_t$ to HEIS GWL measurements $\mathbf{y}_t$ with Gaussian observation errors R_t.

$$\nabla_{x_t} \log p\left(\mathbf{y}_t \middle| \mathbf{x}_t\right) = H_t^T R_t^{-1} (\mathbf{y}_t - H_t \mathbf{x}_t)$$

- **Joint update (physics prior + data):** balances physics patterns and field measurement under sparse, irregular sampling.

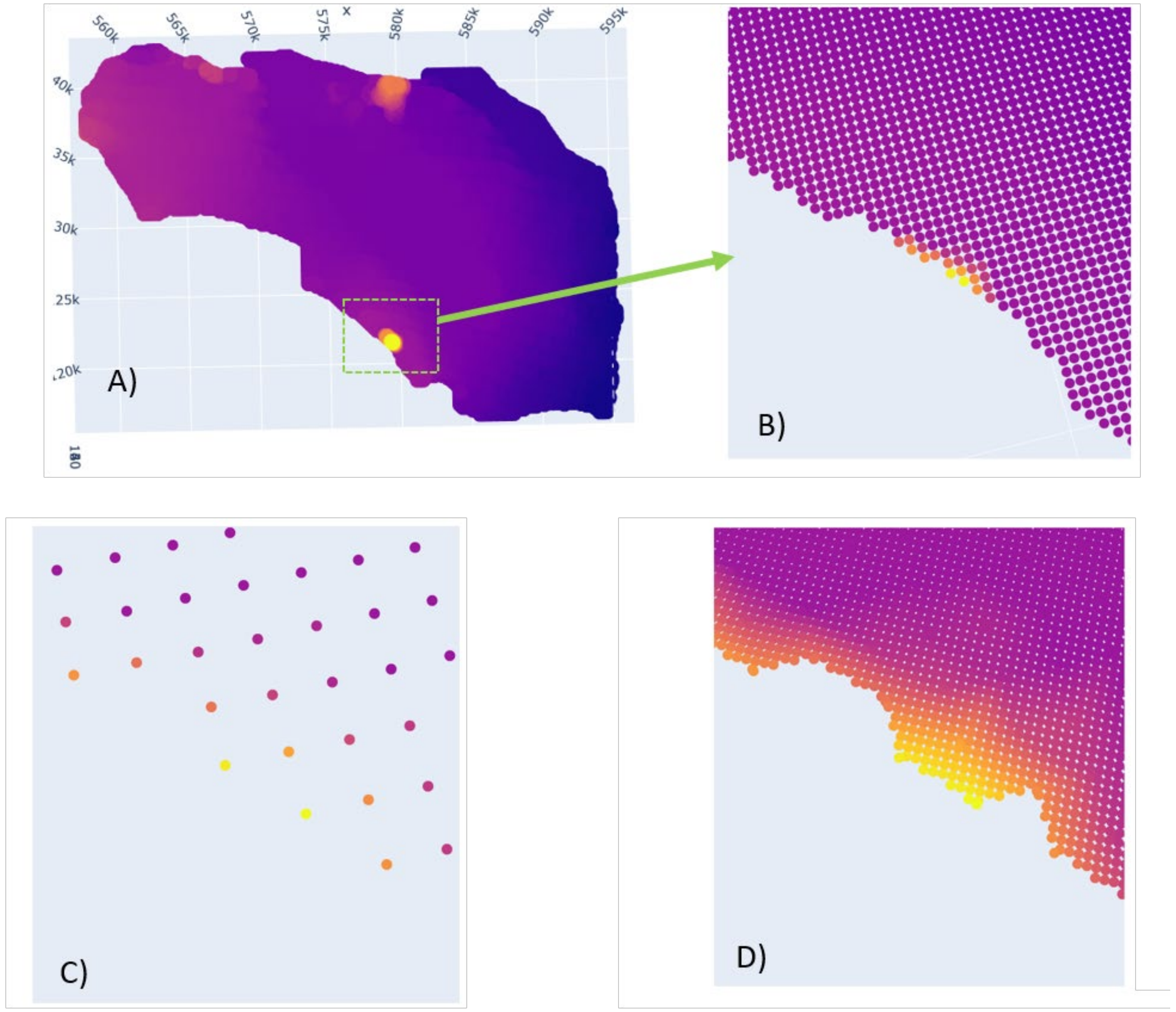
$$\Delta \mathbf{x}_t = \alpha_s \nabla_{x_t} \log p_s(\mathbf{x}_t) + \beta_s \nabla_{x_t} \log p\left(\mathbf{y}_t \middle| \mathbf{x}_t\right)$$

where $\alpha_s, \beta_s > 0$ are step/weight schedules as functions of diffusion time.



Geosamplerite: Consistent Sampling for Model Grid and Irregular Well Locations

- A lightweight Python toolkit with CUDA acceleration for fast rasterization and easy loading of model and field data
- Samples HEIS well locations on the same grid (the H_t operator), enabling observation conditioning in SDA.
- Supports super-sampling near boundaries and GPU-friendly I/O for long time series.
- Produces model-ready tensors for diffusion/SDA with reproducible preprocessing.



Geosamplerite harmonizes unstructured P2R outputs and irregular well data onto a common grid, preserving boundary features and enabling consistent grid-to-well mapping for diffusion–SDA training and conditioning.

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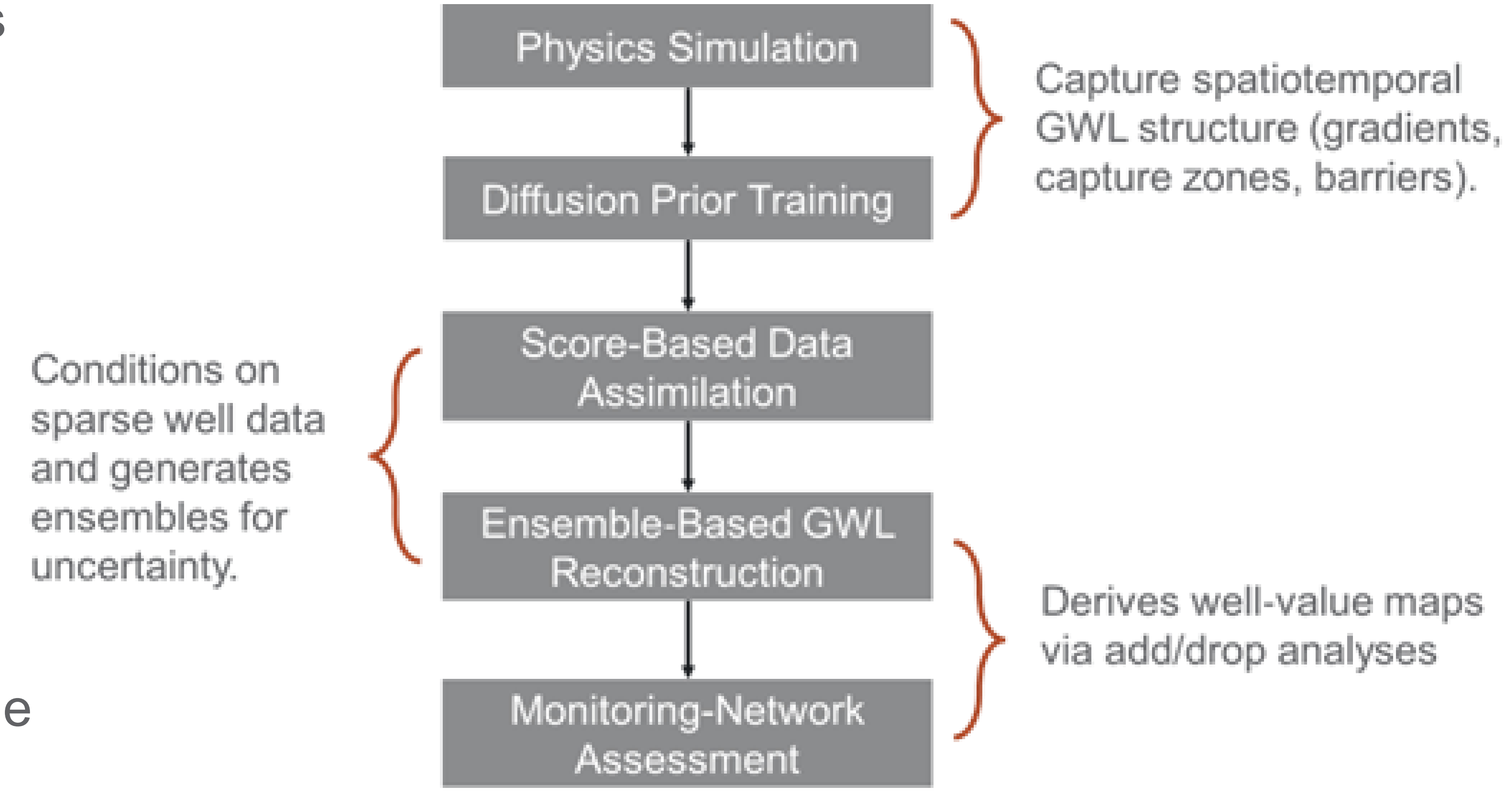
End-to-End Workflow: From Physics to Monitoring Design

- **Physics simulation:** captures gradients, capture zones, and barriers.
- **Diffusion prior:** learns spatiotemporal GWL structure.
- **SDA + ensemble reconstruction:** conditions on sparse well data, quantifies uncertainty.
- **Monitoring-network assessment:** derives well-value maps through add/drop analysis



Integrated workflow connecting physics, data assimilation, and monitoring-network evaluation.

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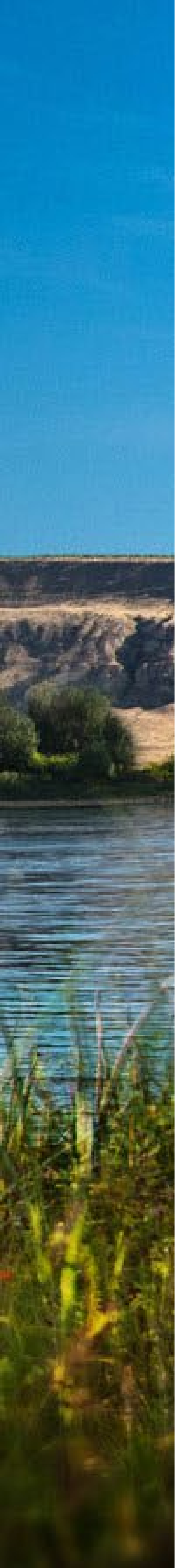
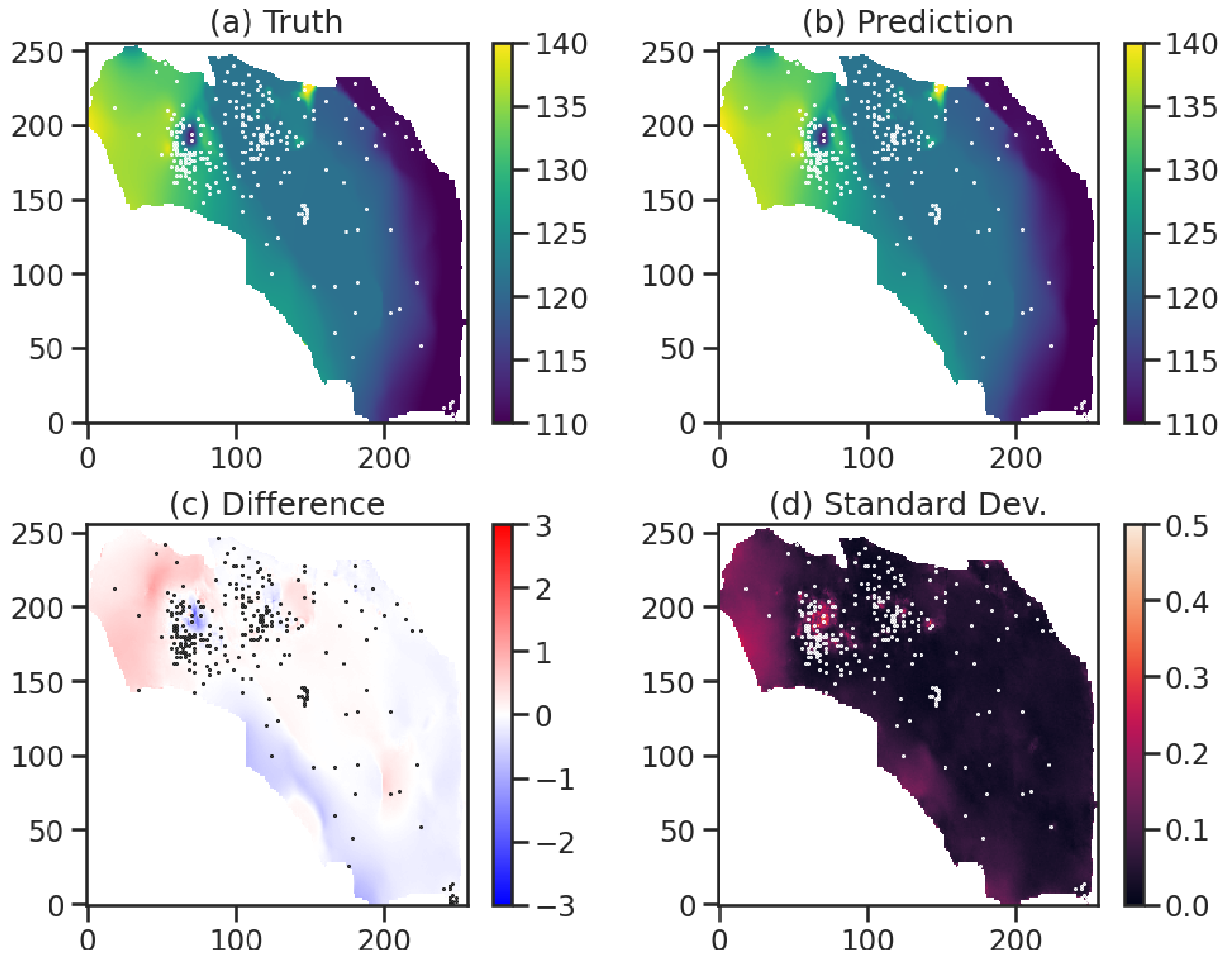


Observation-Conditioned GWL Mapping Results

- March 2023 is randomly chosen as a representative month. Assimilate all available HEIS wells for that date.
- Diffusion–SDA reconstruction agrees closely with the P2R reference (residuals mostly within ±0.5 m)
- Uncertainty (ensemble spread) mirrors residuals.
- Denser well clusters → smaller residuals → lower spread → confidence increases with observation density.



Observation-conditioned GWL maps (meters above sea level, m ASL): (a) Reference (P2R) ,(b) Diffusion–SDA prediction, (c) Residual (m), (d) Ensemble SD (m). Points = assimilated wells.

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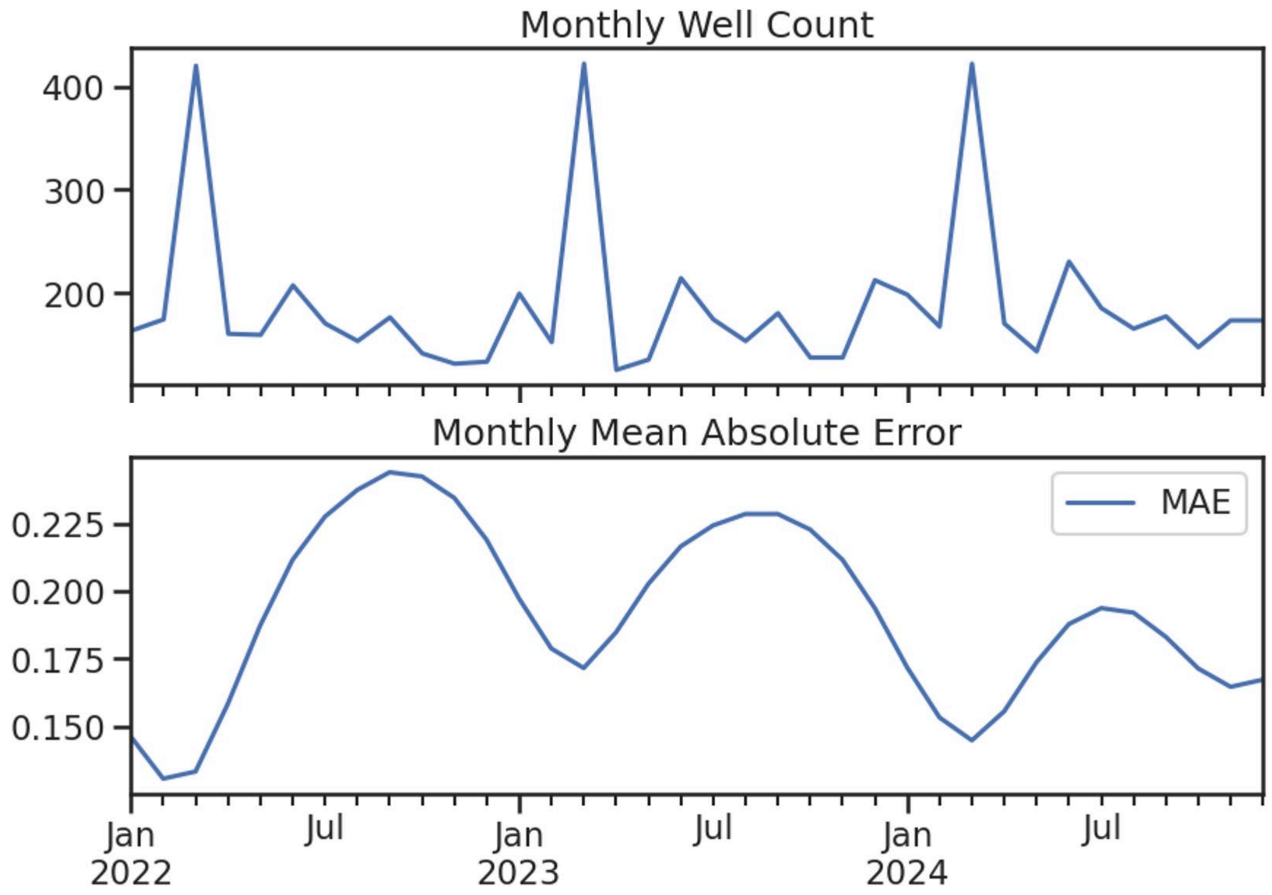
Monitoring Coverage vs. Mapping Accuracy

- Coverage analyzed for January 2022 – December 2024 (24 monthly steps).
- Active well counts per month range from ≈ 300 to > 1000, with domain-wide mean absolute error (MAE) ≈ 0.12–0.24 m across months.
- Higher active-well counts → lower MAE. MAE is computed over all grid cells vs. the reference field, indicating a domain-wide accuracy gain with denser sampling.
- Coverage-sensitive mapping establishes a basis for evaluating well contribution and setting measurement-frequency targets.



Top: Number of wells with measurements each month. Bottom: Monthly MAE (unit, m) between the diffusion–SDA prediction and the reference field

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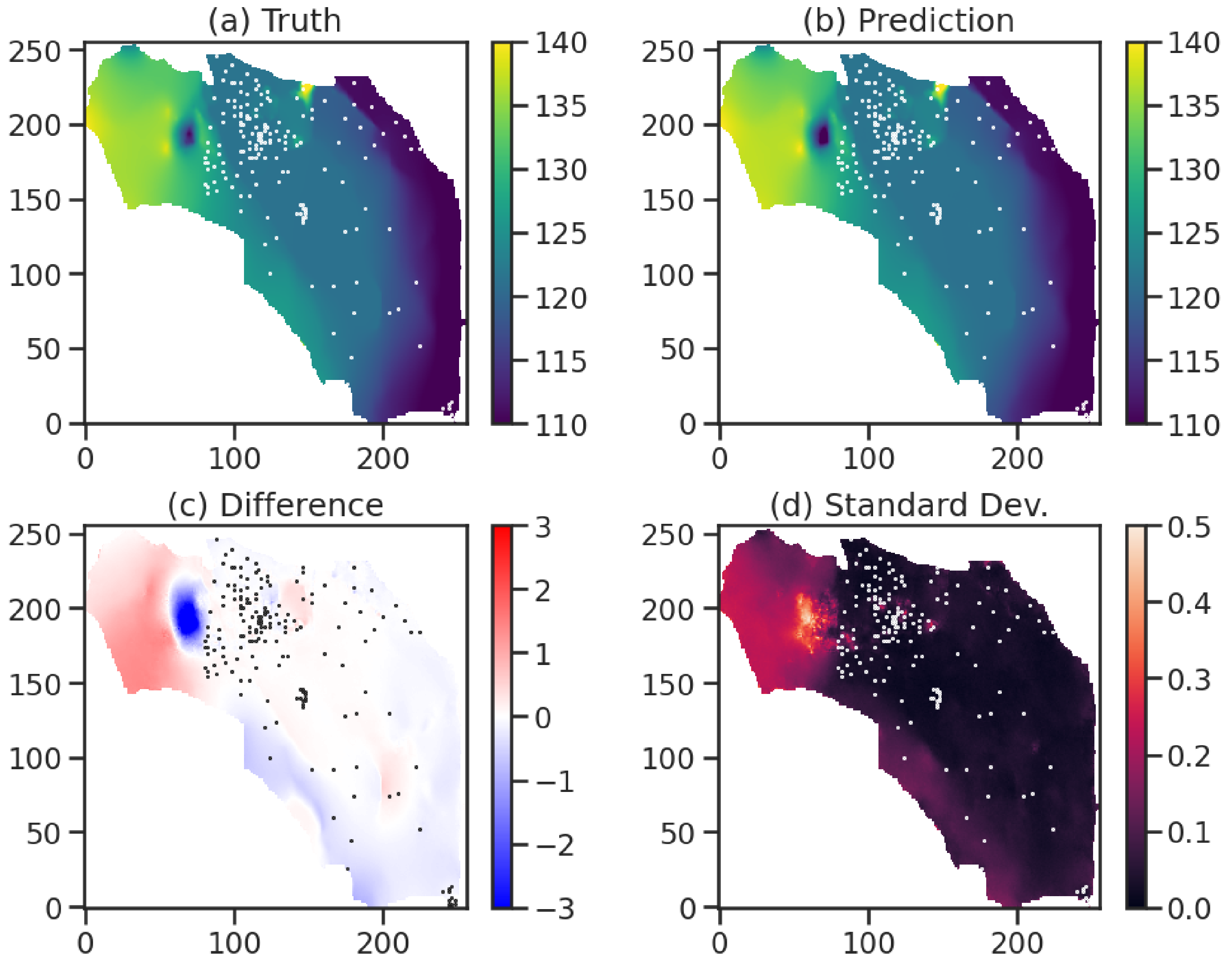
Monitoring-Network Sensitivity (Remove-Well Demonstration)

- About 5% of the wells (23 total) were withheld for coverage-sensitivity testing.
- Local areas around the removed wells show increased MAE and larger ensemble spread, while the rest of the domain remains stable.
- Spatial ΔMAE and Δspread maps highlight zones most affected by coverage loss, providing a quantitative signal of well's information value.
- The remove-well analysis links well coverage to GWL mapping performance and can be used to guide monitoring-network optimization.



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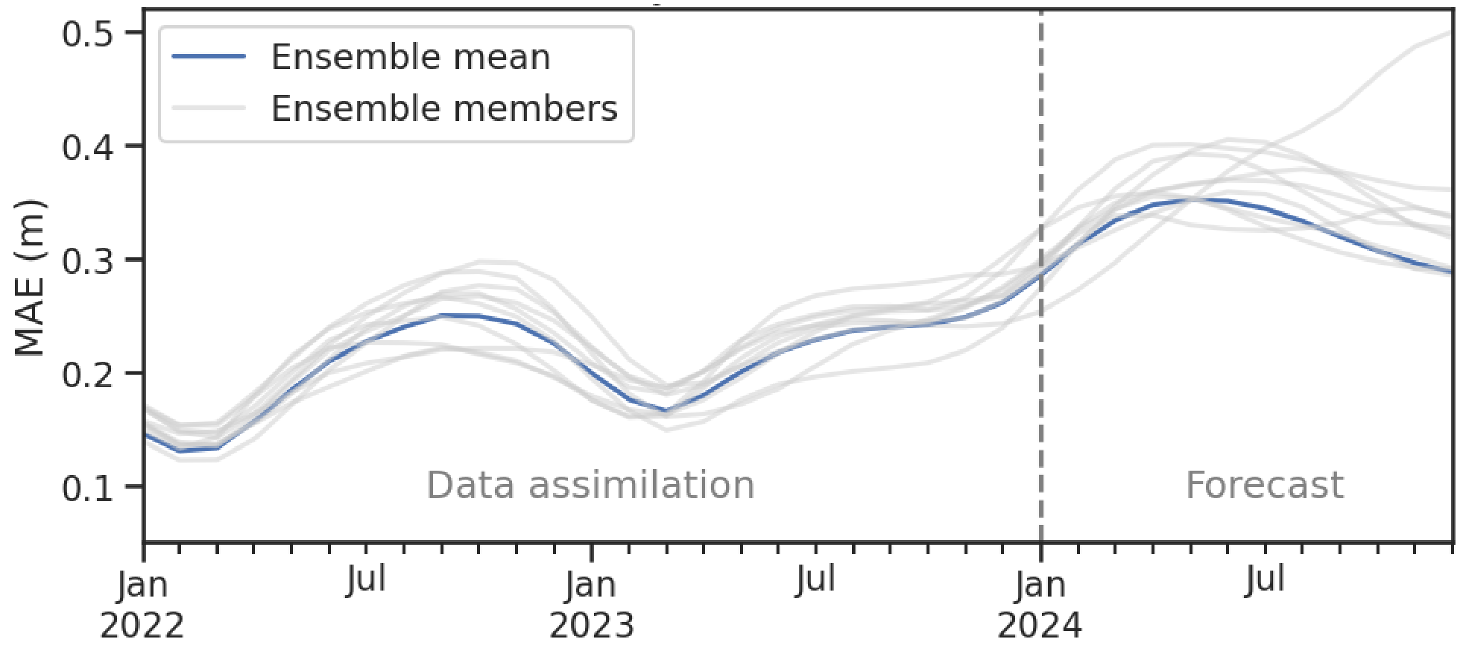
Forecast Baseline without New Observations

- Ensemble initialized from the December 2023 observation-conditioned state and advanced through January–December 2024 with the likelihood term disabled.



- Monthly MAE is low and stable during Jan 2022–Dec 2023, then increases through 2024; the ensemble spread widens in the forecast window.

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- This prior-only run establishes a baseline for error growth and uncertainty in the absence of observation updates, which informs minimum re-anchoring (monitoring) frequency.

Implications and Next Steps

- The diffusion–SDA framework supports time-resolved, uncertainty-aware GWL mapping to optimize monitoring design, set measurement-frequency targets, and evaluate coverage trade-offs.
- For Hanford, this effort supports cost-effective, high-quality GWL mapping to inform remedy activities such as capture-zone monitoring for P&T and plume-migration prediction.
- Next steps
  - **Model tuning**: adjustment of diffusion/noise schedule, network capacity, learning rate, and conditioning weights.
  - **Error model**: refine the observation-error model and the prior–data balance in SDA.
  - **Toolkit**: build an automated add/drop module for well information value (rolling leave-one-out/add-one-in, ΔMAE/Δspread, ranked recommendations).

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Thank you