National-extent Groundwater Quality Prediction Project
National Integrated Water Availability Assessment Program

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U.S. Geological Survey

National Groundwater Quality Prediction Project

Objectives and Methods

- **National IWAA Program requires:**
  - ***Reliable predictions of GW quality conditions***
  - ***Understanding of factors affecting GW quality conditions***
  - ***Strategies for representing GW loading to streams***

- **Direct Simulation of GW Quality and Age at the National Scale with Continuous-Domain, Process-based Models is Computationally Impractical**
  - ***Data-driven (machine learning) methods have proven effective for predicting GW quality and age from large, complex datasets through the process of statistical learning***

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Outline

1. **Groundwater Quality**
   - *Nitrate Concentrations in GW*

2. **Groundwater Characteristics**
   - *Major-Ion Composition of GW*

3. **Loading of contaminants from GW to streams**
   - *The travel time distribution (TTD) of baseflow is a critical link between GW & SW*

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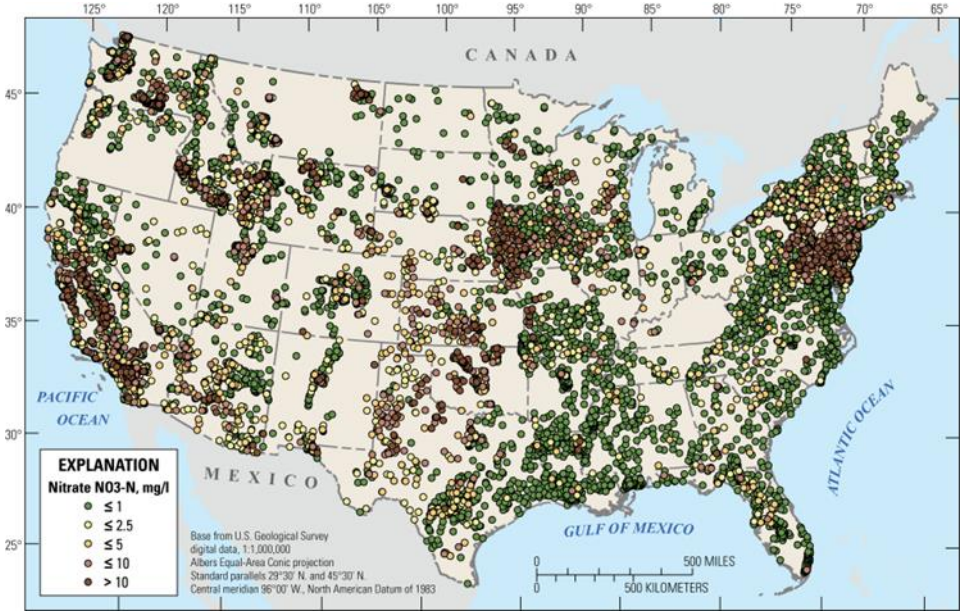
Groundwater Quality – nitrate

1. *Nitrate measurements at >12K locations*
2. *Attribute model features (predictor variables) to sample locations*
3. *Develop machine learning model*
   - *80% training; 20% hold out*
4. *Predict nitrate at selected depths at 1km resolution*



Ransom et al., 2022, https://doi.org/10.1016/j.scitotenv.2021.151065

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Groundwater Quality – nitrate

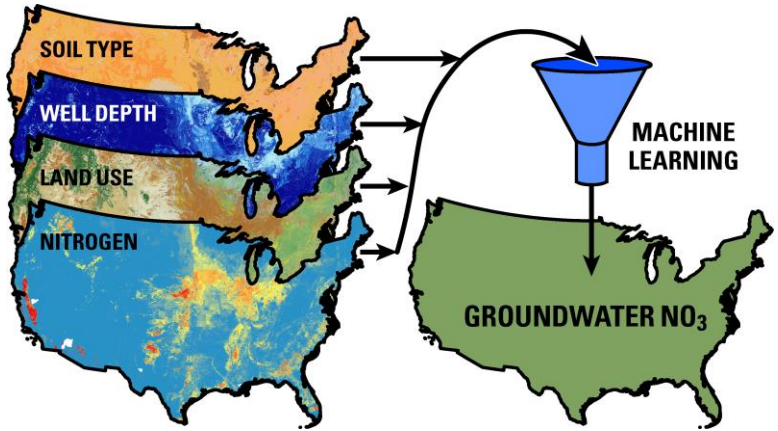
Features that are available “wall-to-wall”

Hydrology

- *Well Depth*
- *Depth to Water*
- *Unsaturated zone travel time*

Nitrogen Sources

- *Land use*
- *Manure & fertilizer*
- *N deposition*



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Soil Characteristics

- *%Sand & Clay*
- *Hydraulic conductivity*
- *Soil drainage*

Climate

- *Precipitation*
- *PET & AET*
- *Temperature*

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76 features were retained in this model

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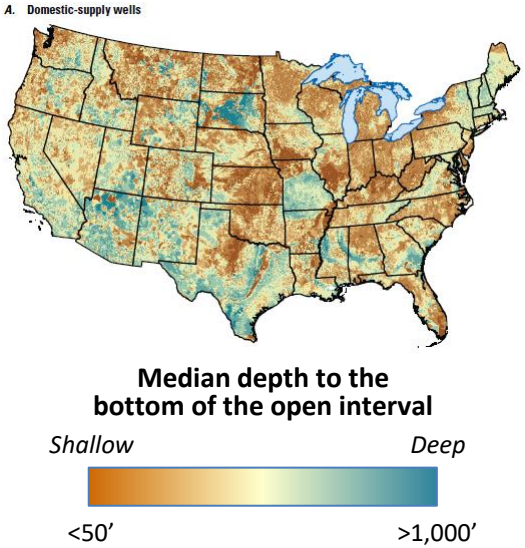
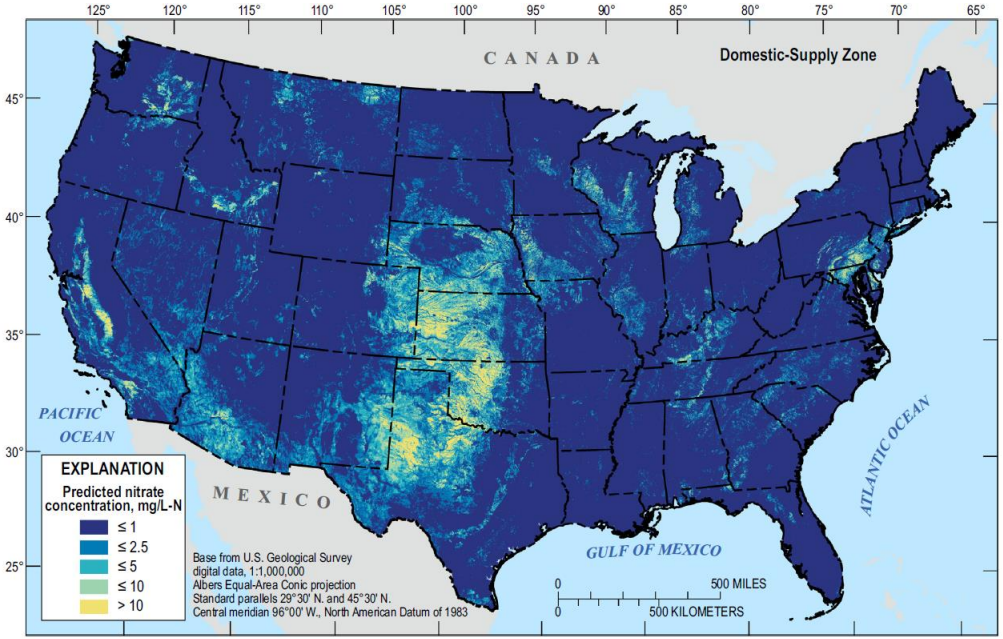
Groundwater Quality – nitrate



Degnan et al., 2021, https://doi.org/ 10.3133/ sir20215069



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Model Predictions are Reliable at the Scale of Hydrogeologic Regions

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Groundwater Quality – nitrate

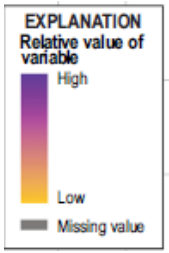
more important

Model Features

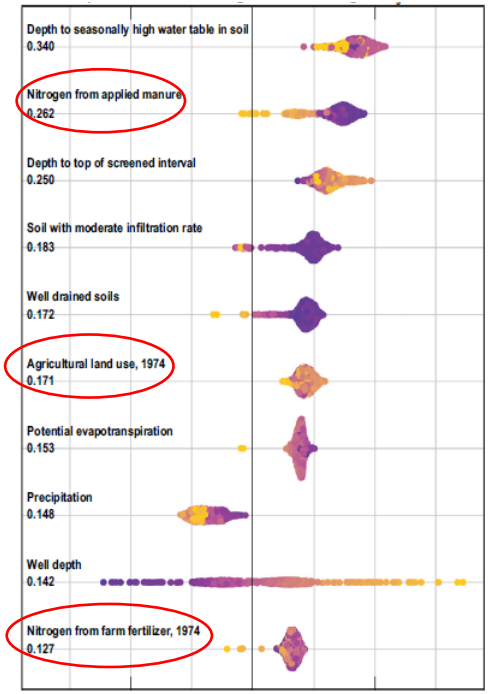
less important

Global Model (training sites)

SHAP value (impact on model prediction)



Predictions > 10 mg/L in Carbonate Aquifers of the Piedmont-Blue Ridge System



SHAP value (impact on model prediction)

Piedmont – Blue Ridge Aquifer System

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Groundwater Characteristics – major-ion composition

The Major-Ion Composition of Groundwater Affects:

- Mobility and aqueous speciation of dissolved constituents
- The potential for galvanic corrosion or encrustation
- The salinity of SW and, in turn, toxicity of metals to aquatic organisms
- Measurements of salinity, TDS, and minimum desalination energy cost

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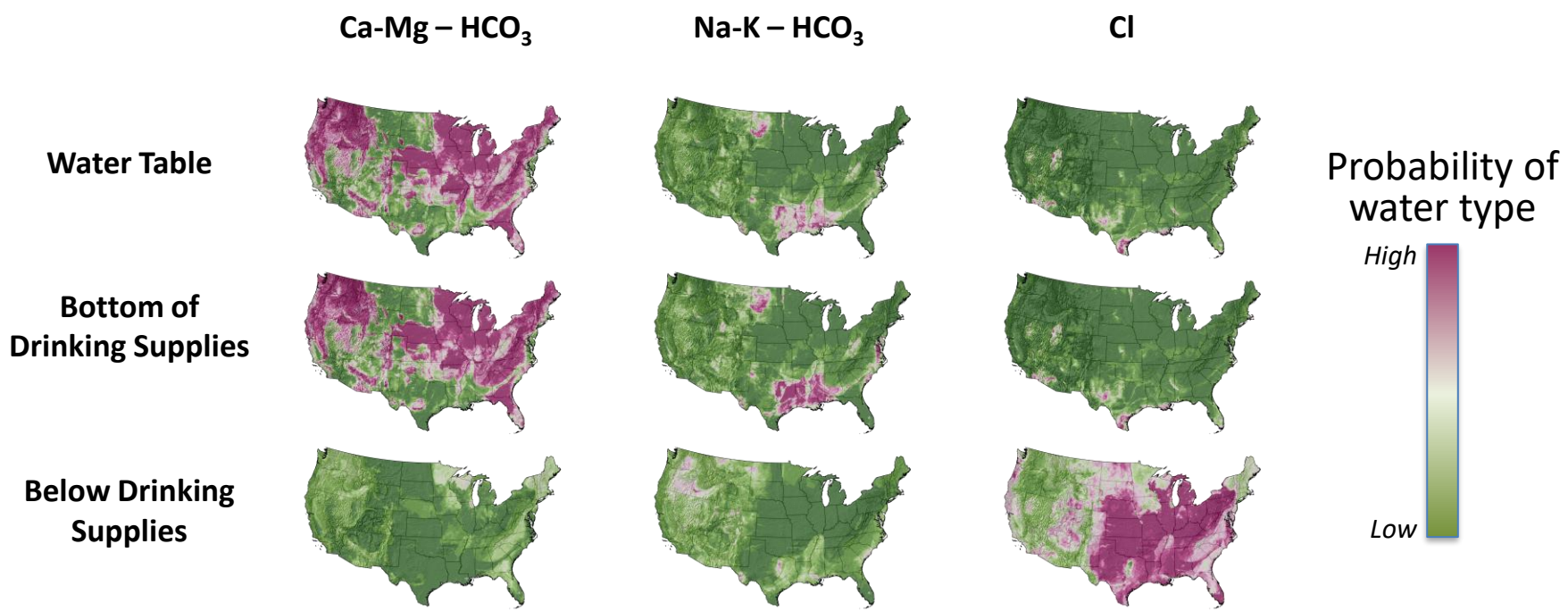
Groundwater Characteristics – major-ion composition



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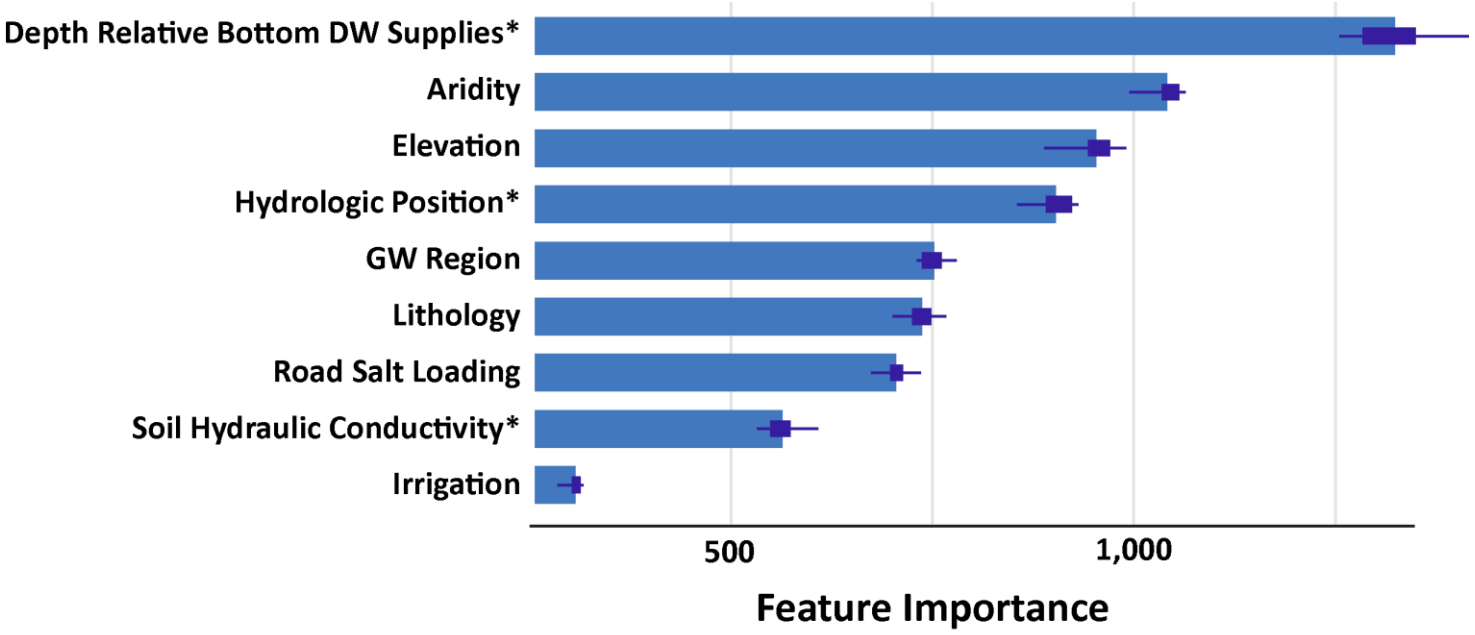
Groundwater Characteristics – major-ion composition

Parsimonious model (9 features) enhances interpretability



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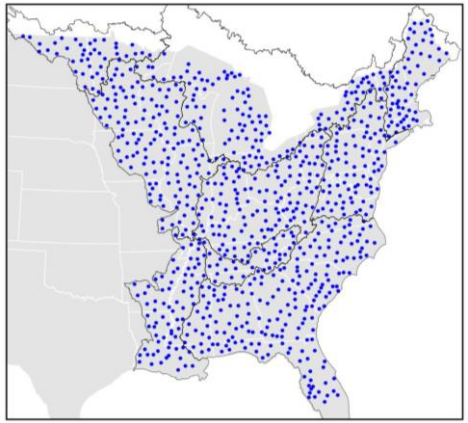
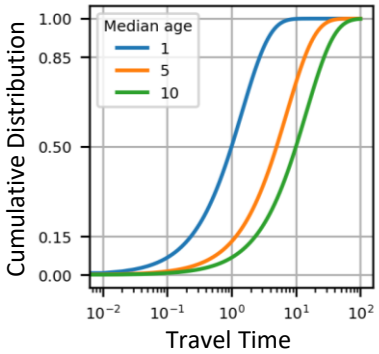
Loading of Contaminants from GW to Streams

- **To Predict GW Loadings to Streams:**
  - Loading history at land surface
  - Travel times from points of recharge to points of discharge along a stream reach
- **MODFLOW/MODPATH can be used to estimate travel time distributions (TTDs)**



● Centroid of HUC12 Watershed

- ~80,000 HUC12 watersheds in CONUS; 843 selected for eastern US
- Develop 843 steady state MF/MP models at 100m resolution



- Generate TTDs for each HUC12 watersheds
- Machine learning used to estimate TTD for remaining eastern US
- Convolve TTDs with loading histories to estimate current and future loadings from GW to streams

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Questions?

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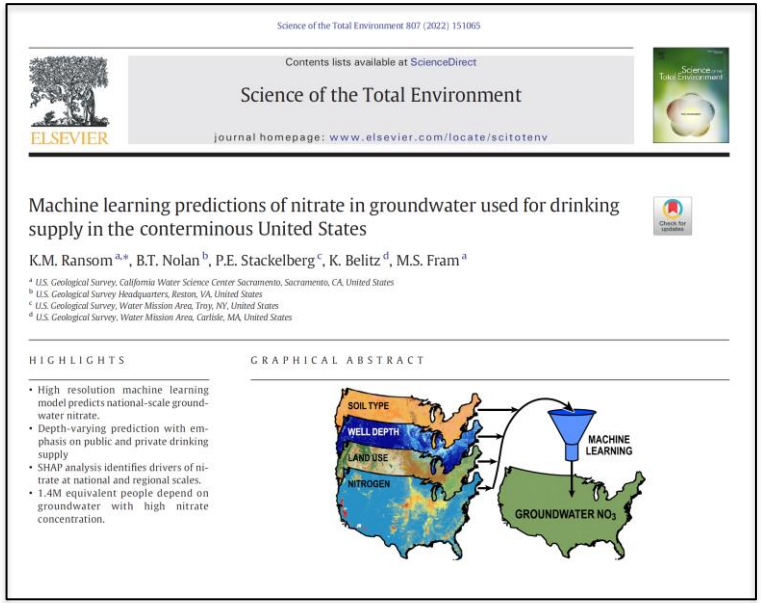
References Cited



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ELSEVIER

Machine learning predictions of nitrate in groundwater used for drinking supply in the conterminous United States

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HIGHLIGHTS

- High resolution machine learning model predicts national-scale groundwater nitrate.
- Depth-varying prediction with emphasis on public and private drinking supply
- SHAP analysis identifies drivers of nitrate at national and regional scales.
- 1.4M equivalent people depend on groundwater with high nitrate concentration.

GRAPHICAL ABSTRACT

Ransom et al., 2022, Science to the Total Environment, v. 807,
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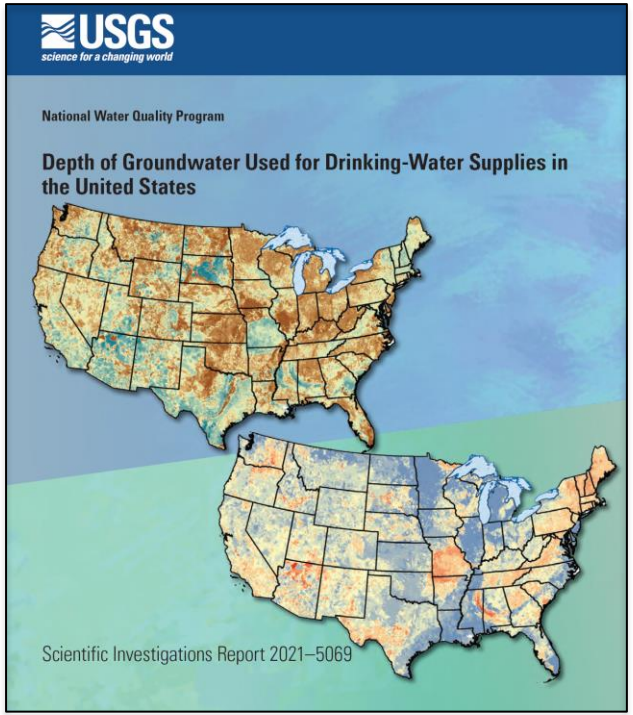

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Depth of Groundwater Used for Drinking-Water Supplies in the United States

Scientific Investigations Report 2021–5069

Degnan, et. al., 2021, Depth of groundwater used for drinking-water supplies in the United States: U.S. Geological Survey Scientific Investigations Report 2021–5069, 69 p.,
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