Continuous Water Quality Monitoring using Field Deployable NMR and Explainable AI

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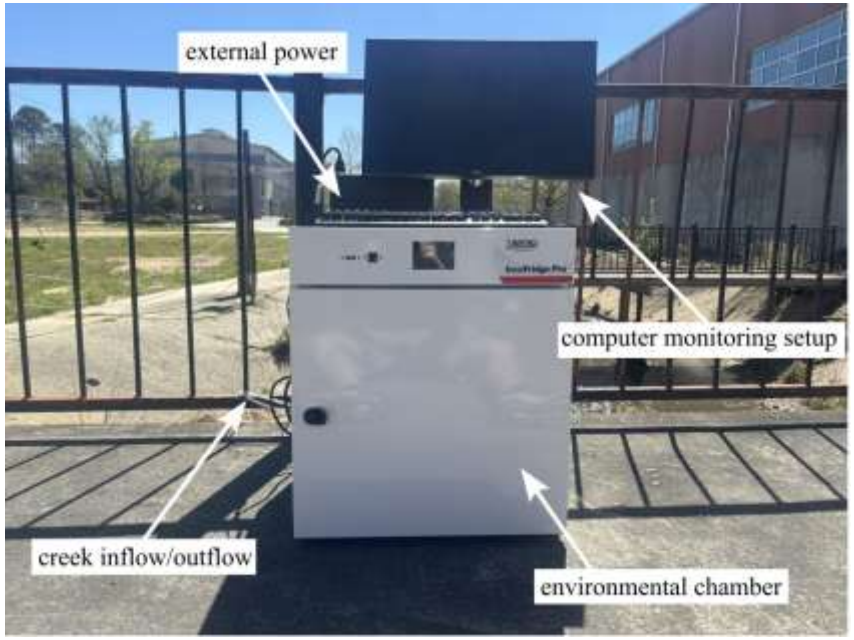
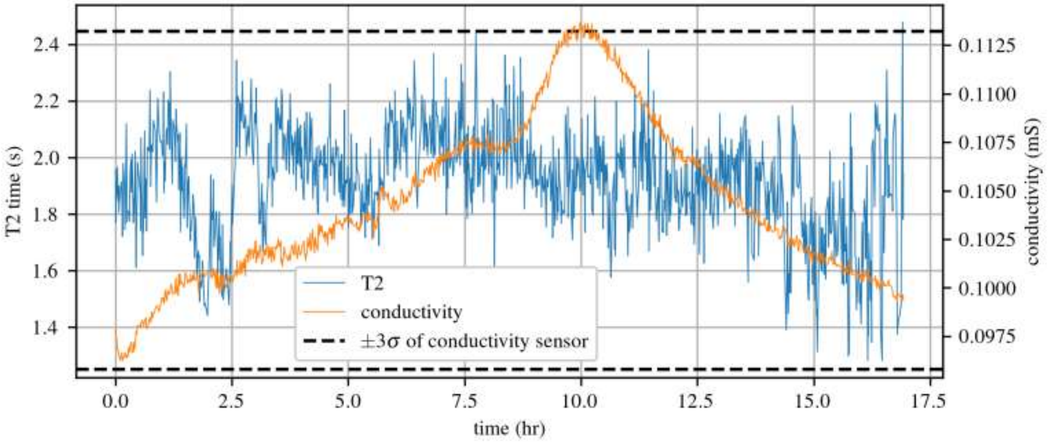
Outline

- Proposed NMR-based Water Quality Monitoring System
- Open-source NMR Hardware
- The Quantum Physics of Precession
- Use Case: Wildfire Ash
- ML-based Contaminant Monitoring
- Lab Data Collection for Model Training
- Field Deployment of In Situ NMR system

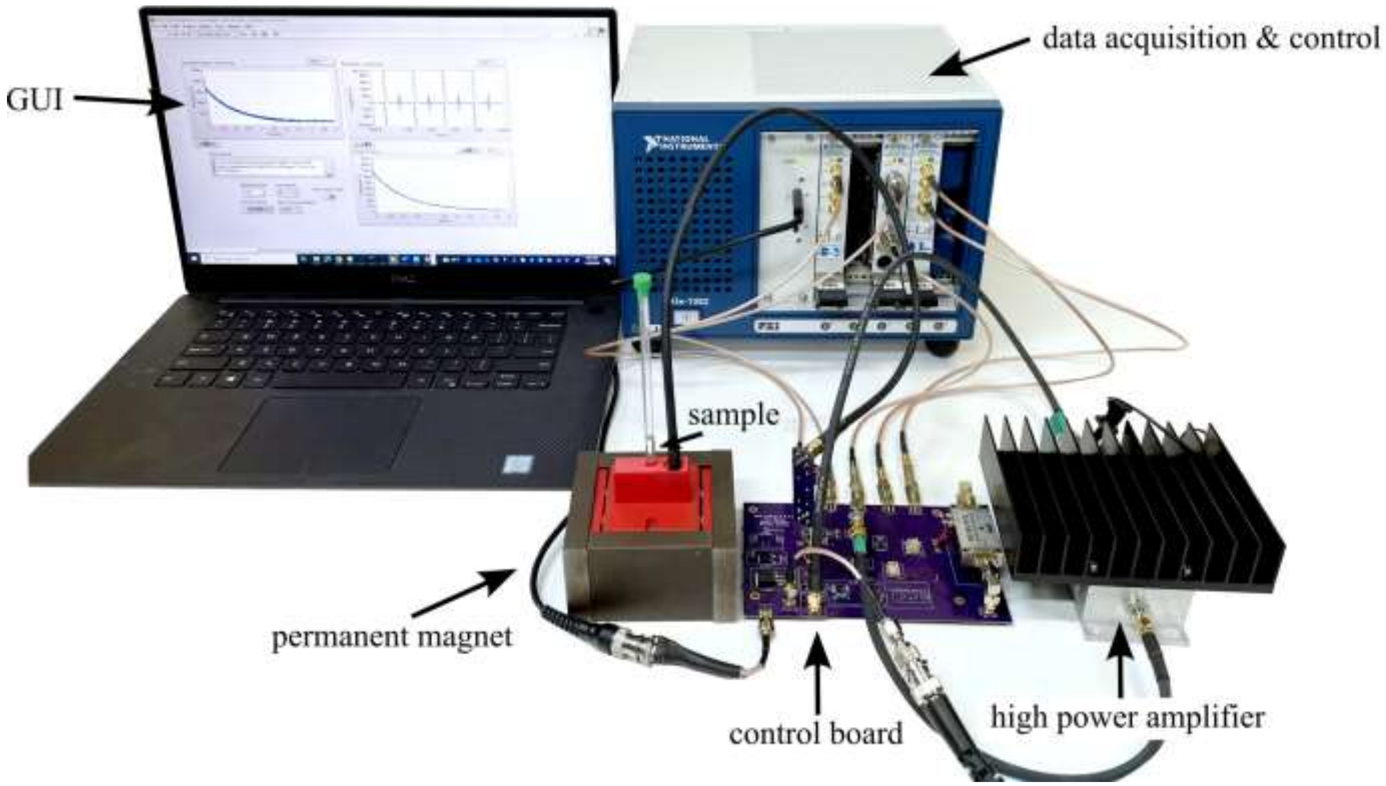




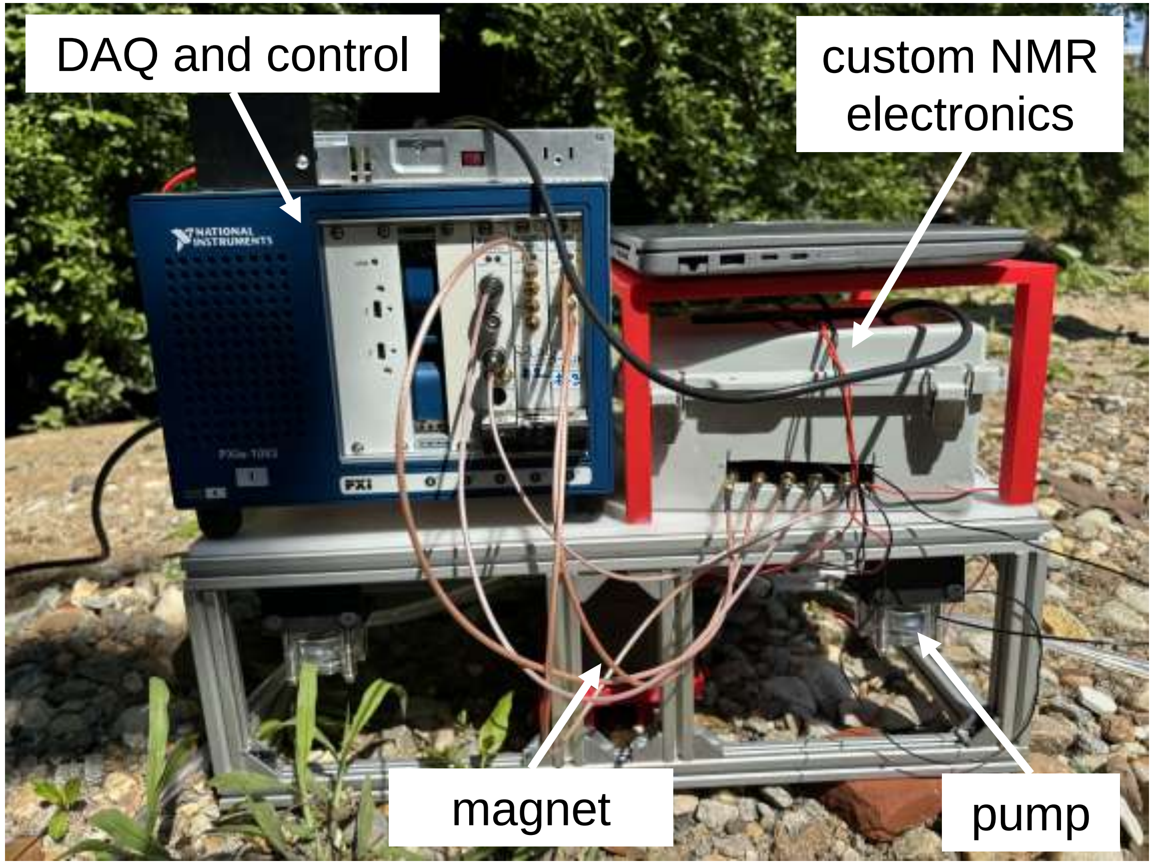
Proposed NMR-based Water Quality Monitoring System

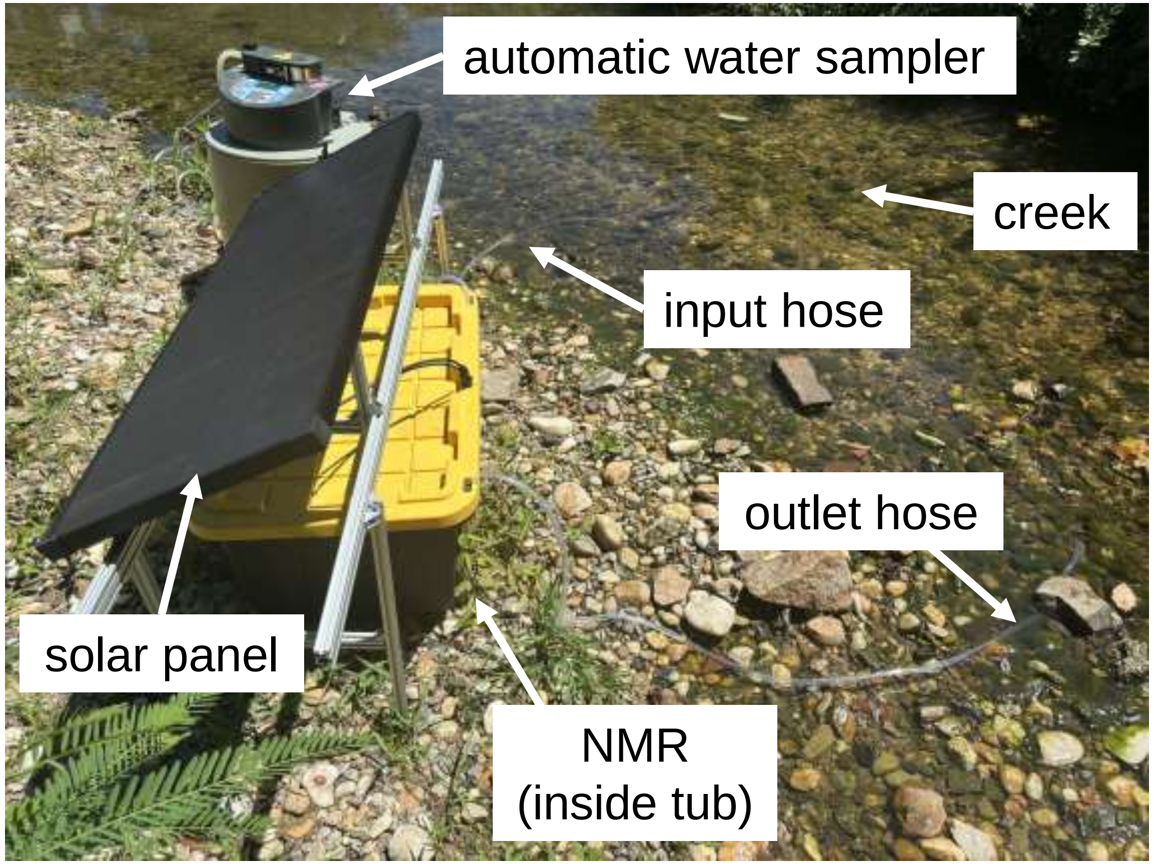
ARTS-Lab Desktop NMR System

- Control handled by LabVIEW program and NI-PXI chassis
- All electronics (barring two amplifiers) housed on a single PCB
- GUI developed for easy data acquisition and export



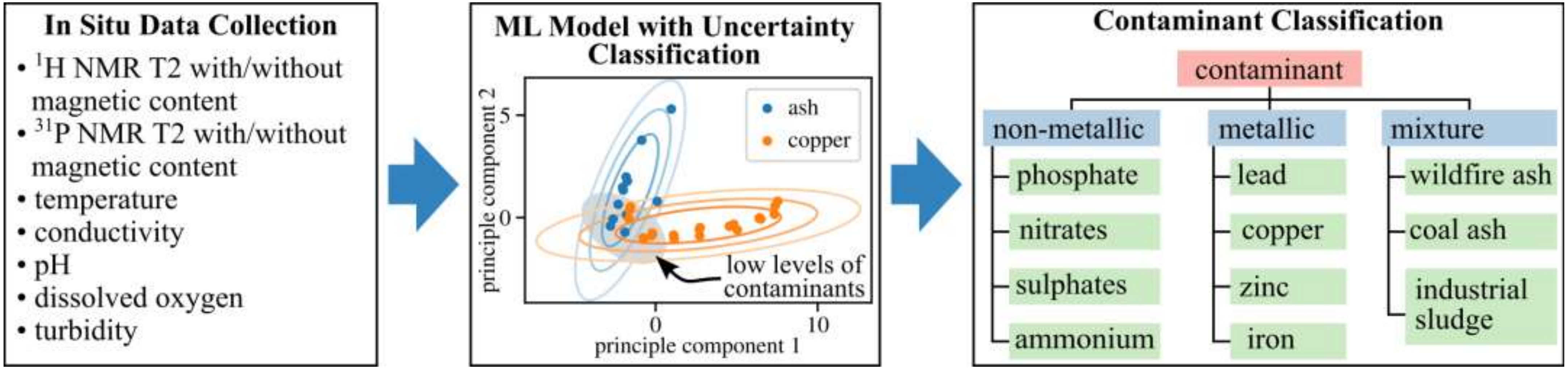
Flow-through NMR





Future Goal: Distinguish Contaminants

- Provide data for multiple contaminants
- Incorporate a ML model with physics-based understanding on magnetic behavior
- Identify and quantify different contaminants using ML based on T2, water quality, and time series data



Open-source NMR Hardware

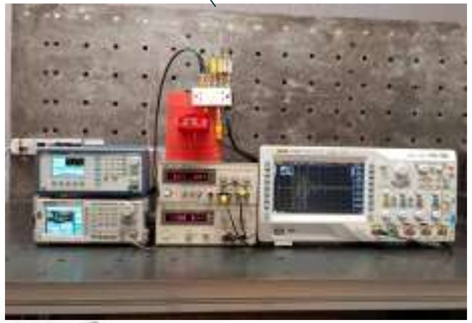
Our NMR Development Path

	2019	2020	2021	2022	2023	2024	2025
Funding	Downey/San Hee		Army	USC	NSF CA		

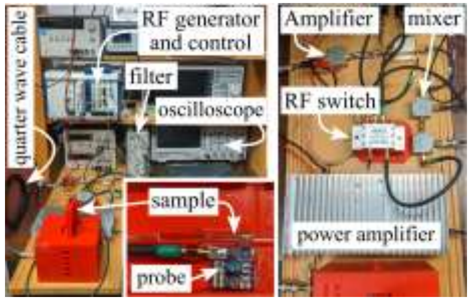
Hardware

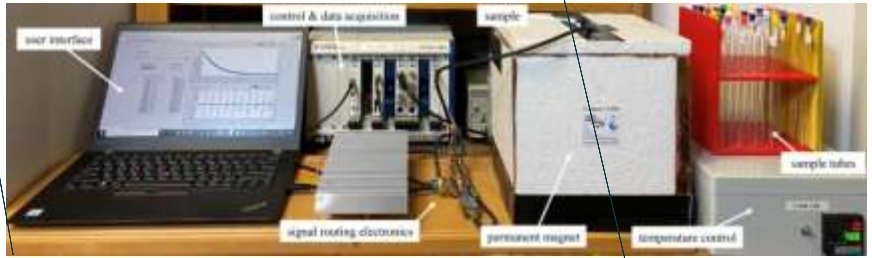
Collogue asks if it can be done?

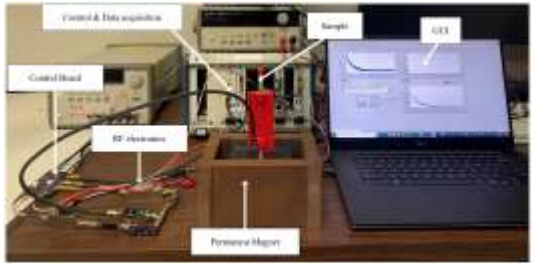
Tracking down specialized hardware, magnets cost 10-20k

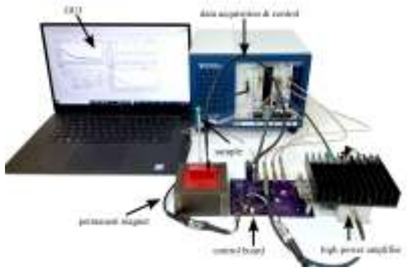


Coil magnet design





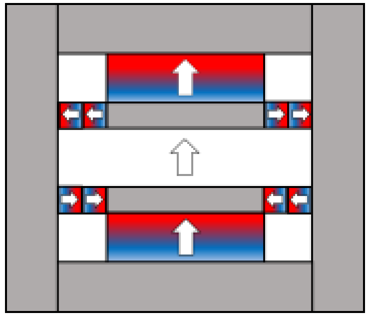




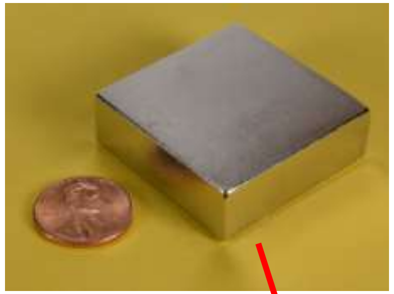
Open-source Design

Permanent Magnet Array

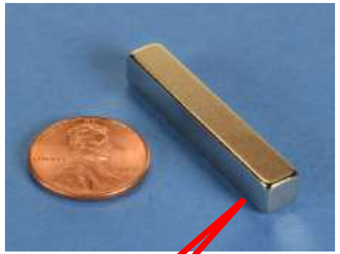
- **0.565 T** strength at 23ºC
  - -800 ppm/K gradient
- Larmor (operating) frequency:
  - $f_{Larmor} = \gamma B = \left(42.58\,\frac{MHz}{T}\right)(0.565\ T) \approx \mathbf{24\ MHz}$
- 150 ppm homogeneity
- 4.4 lbs

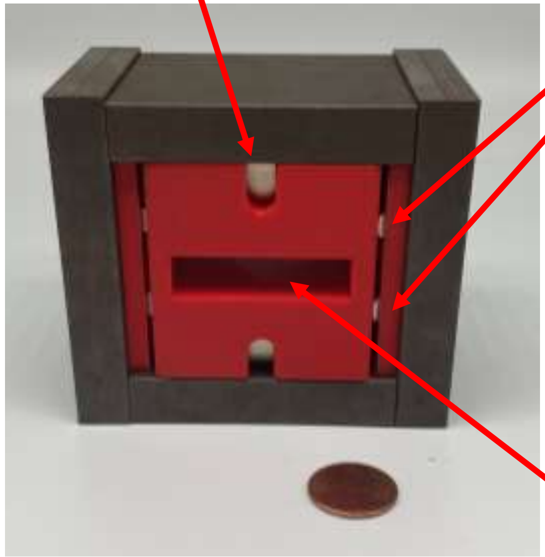


N42 magnet



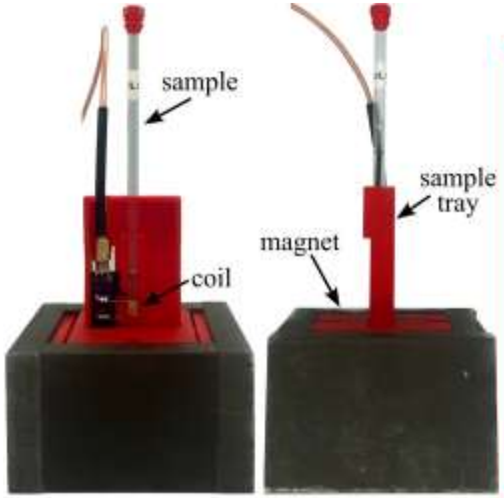
N42 magnet

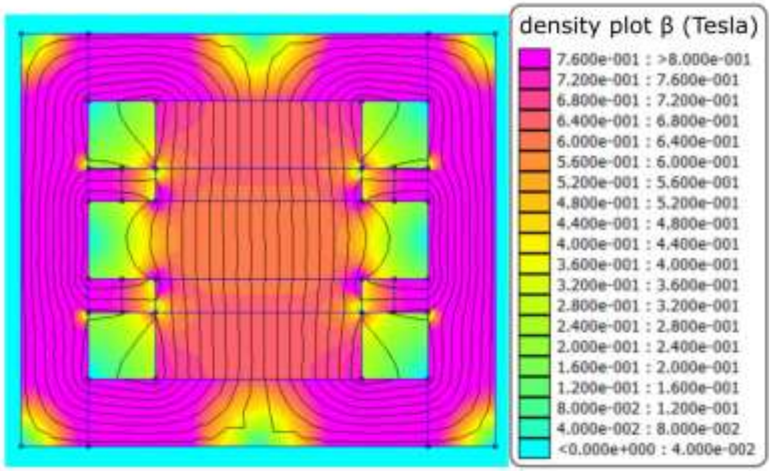




Fully assembled

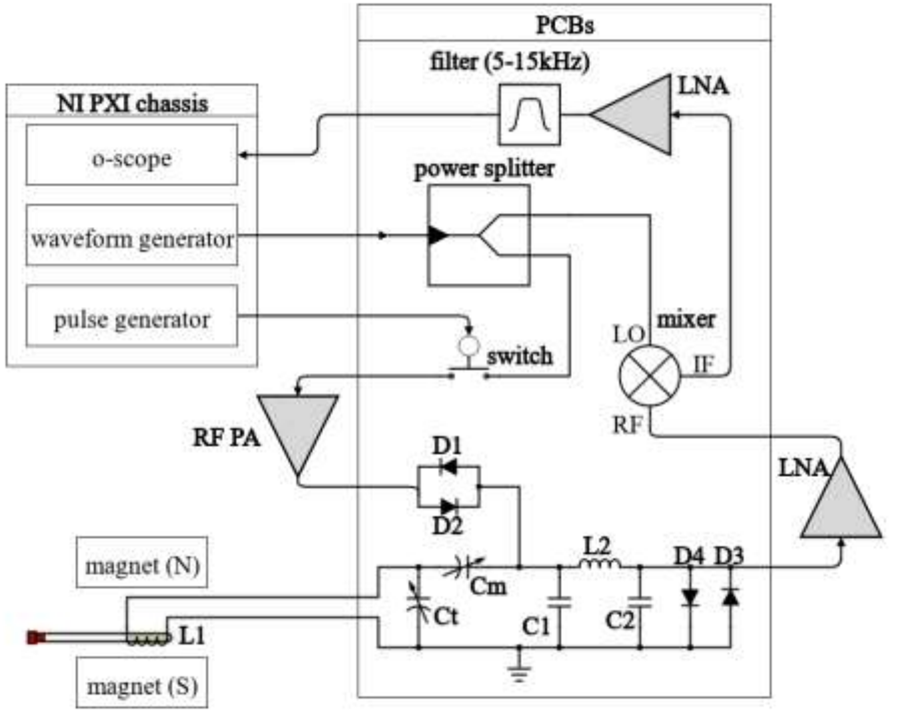
Sample location





RF Electronics

- A single 24 V DC power supply required
- Impedance of all cables and PCB traces matched to 50 Ω
- Waveform generator → sine wave at Larmor frequency
- Pulse generator → follows CPMG pulse train
- Duplexer (crossed diodes) isolates probe and LNA



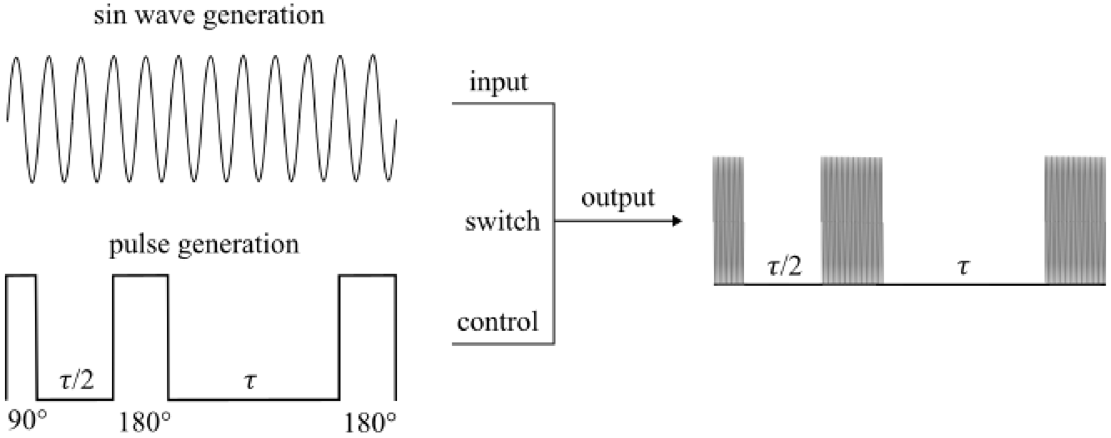
General flow

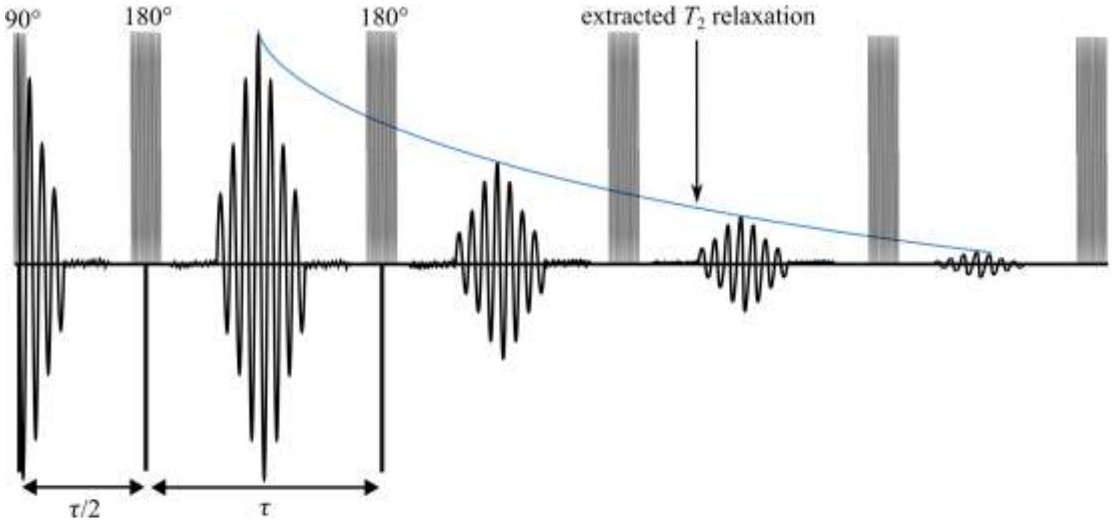
excitation → NMR response → amplification → mixing → filtering

Signal Generation and Control

- NI PXI chassis
  - Arbitrary waveform generator
  - Pulse train generator
  - 16-bit digitizer

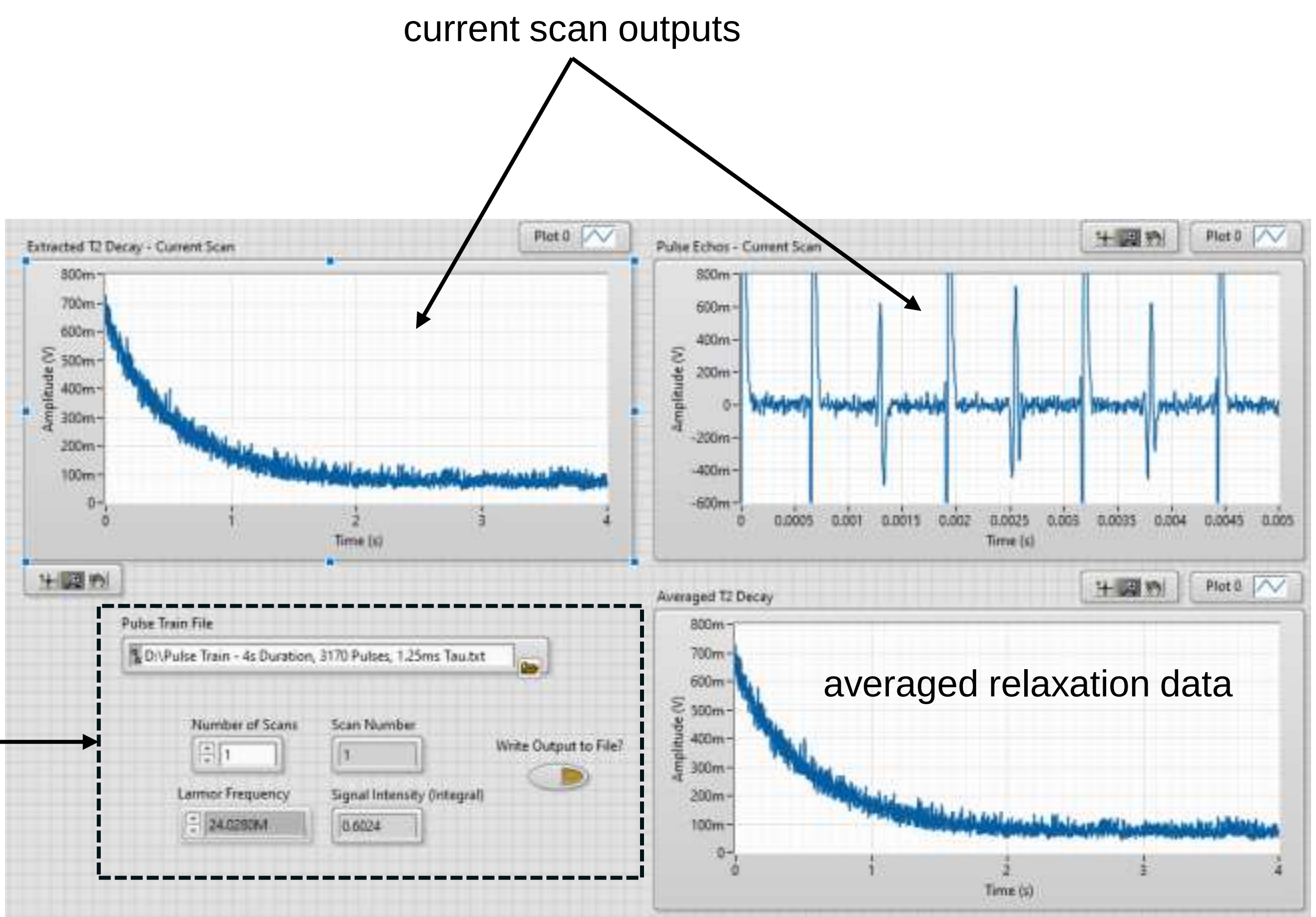
- Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence
  - $90°$ pulse duration is 7 μs
  - $\tau = 1.25$ ms





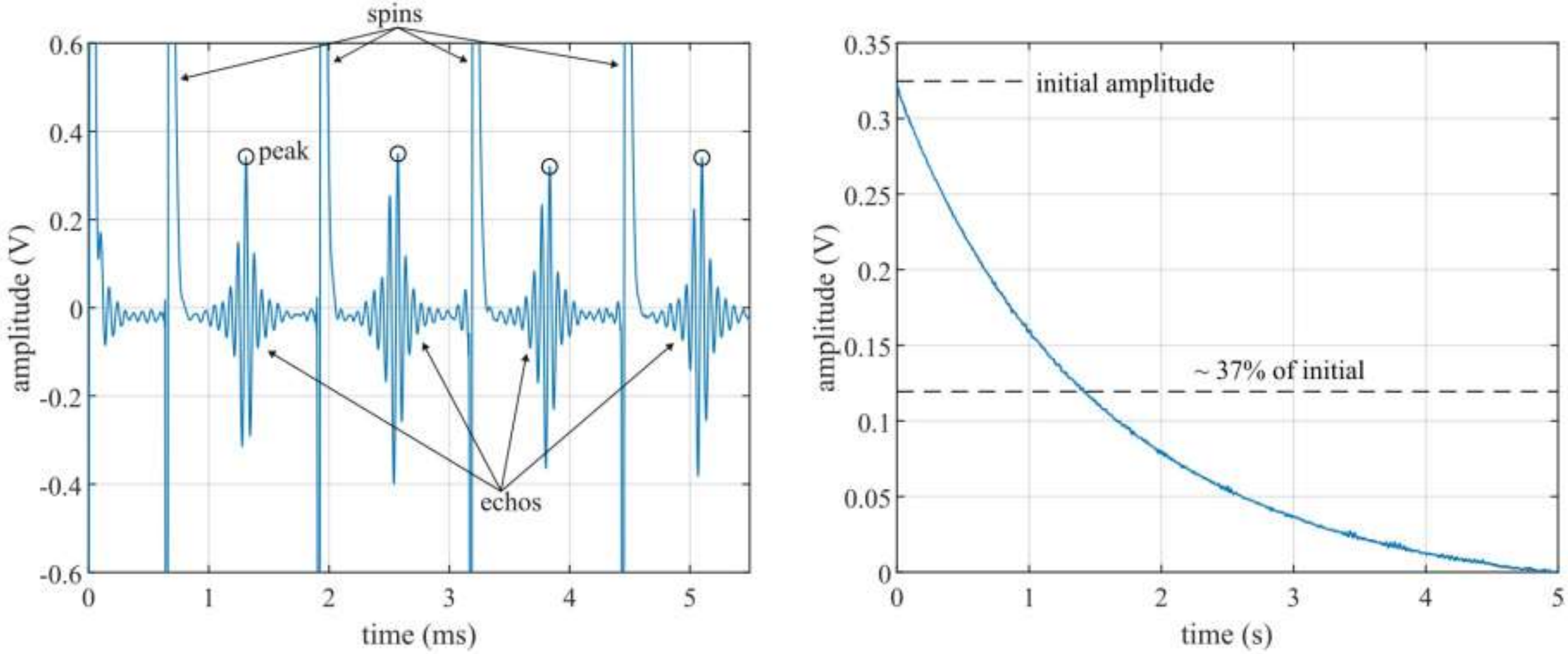
Data Acquisition

- LabVIEW GUI serves as front end
- Each test comprises 5 scans (averages)
- Time for T_2 curve acquisition < 10 seconds
- Thermocouple used for frequency calibration



TD-NMR Signals and MP Content

- T_2 relaxation modeled as $M_{\text{xy}}(t) = M_0 \exp(-t/T_2)$
- Relaxation rate is the reciprocal of relaxation time (i.e., $R_2 = 1/T_2$)
- Linear relationship between R_2 and MP concentration well established



The Quantum Physics of Precession

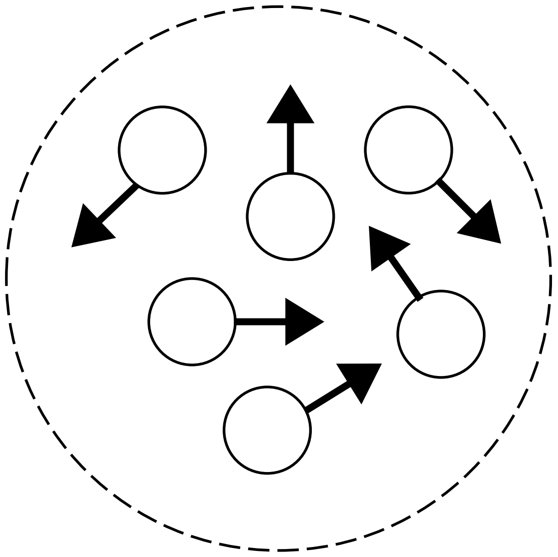
Particles in a magnetic field, B_0

- Start with the population of nuclei in thermal equilibrium

- Degenerate nuclear spin states

- Random orientation

- The microcanonical ensemble perspective tells us that in an unaligned field, there is no net magnetic field.

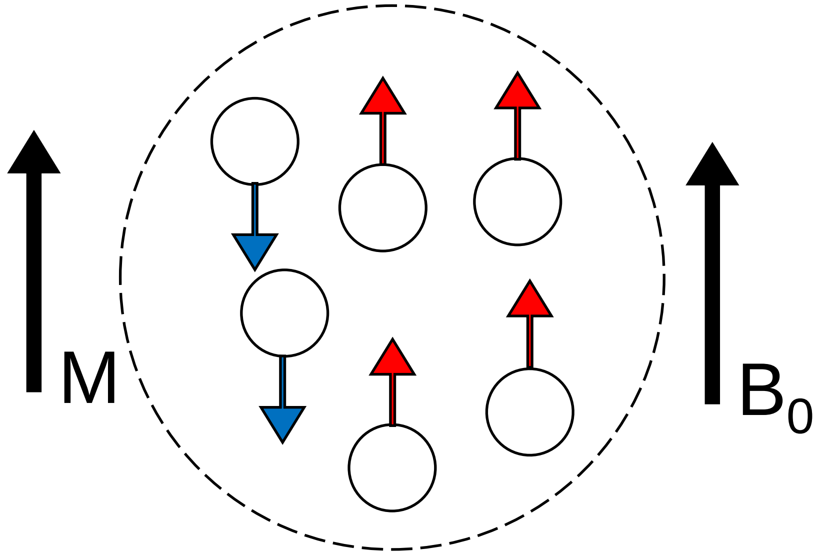


Boltzmann distribution (classical mechanics)

- Higher energy states less likely to be occupied

$$\frac{P_{m=-1/2}}{P_{m=1/2}} = e^{-\Delta E/kT}$$

- More nuclei aligned with B_0 than anti-aligned

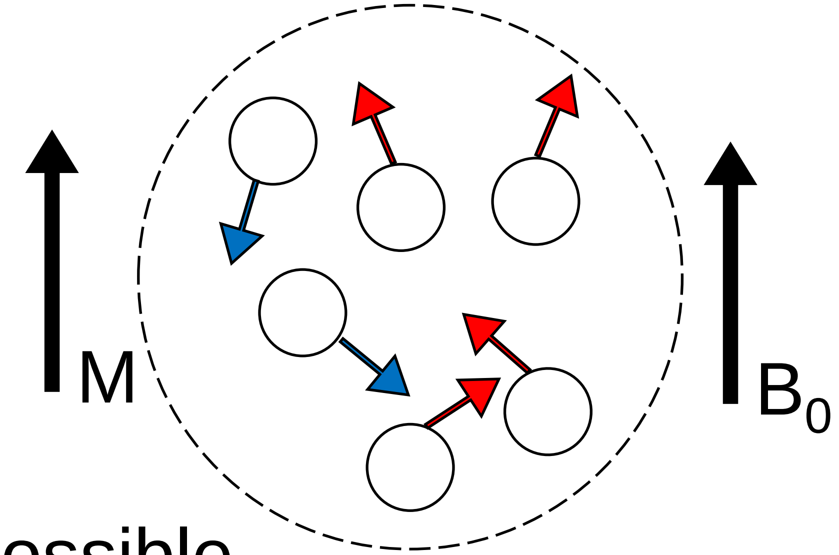


- Results in net magnetization

Quantum mechanics view

- If each magnetic moment's direction is known, S_z is known
  - Knowing S_Z means S_x and S_y are also known
  - Violating uncertainty

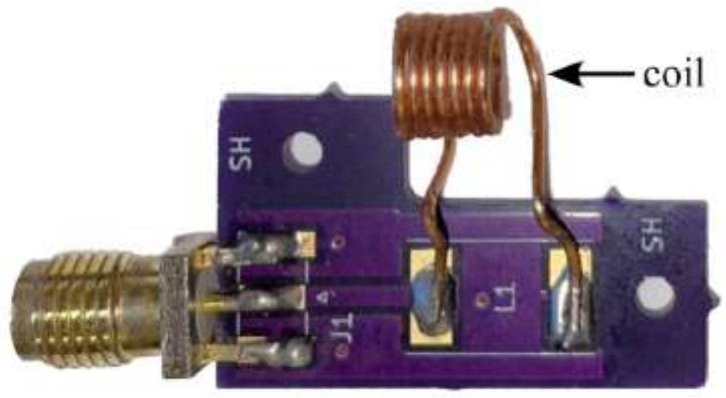
- Each magnetic moment is off-axis



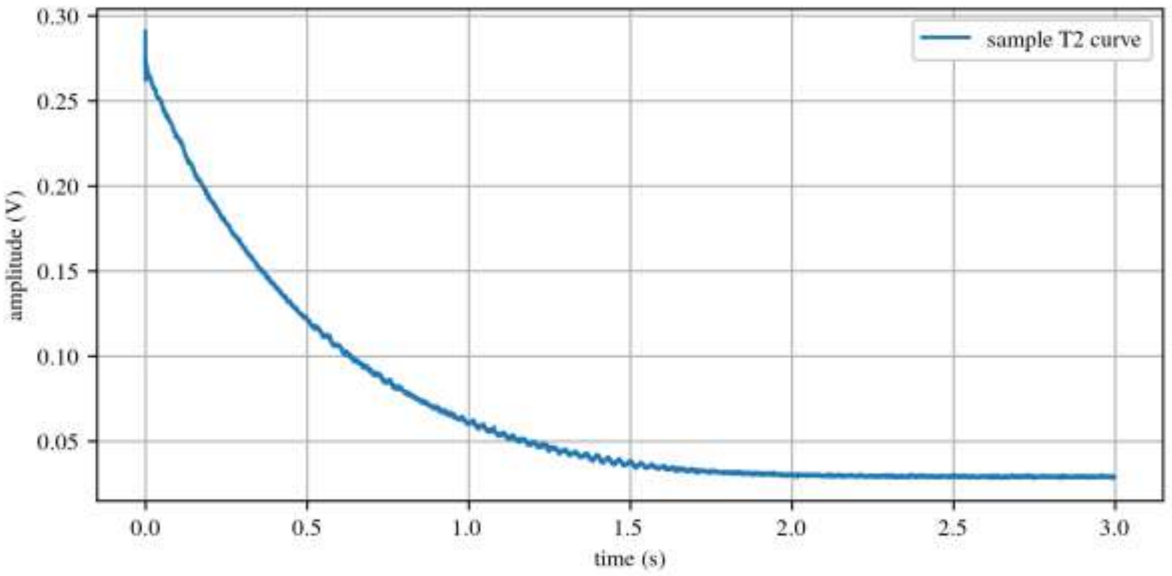
- Resultant net magnetization makes NMR possible

Nuclear Magnetic Resonance (NMR)

- Excites nuclei by applying an oscillating magnetic field via a coil with alternating current
- Measure the diminishing response over time: T2 Curve
- Calculate the exponential decay constant: T2
- Can measure a reference isotope and paramagnetic material in the sample



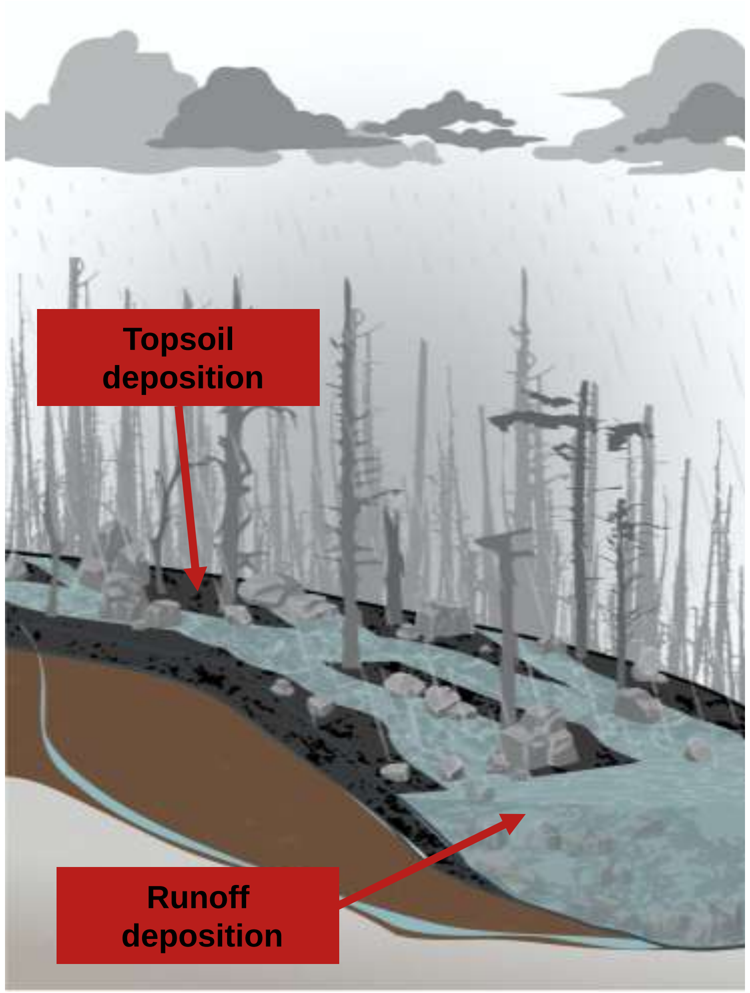
Janvrin et al. Open-Source Compact Time-Domain Hydrogen (1h) NMR System for Field Deployment (2025)



Use Case: Wildfire Ash

Why Monitor Magnetic Contents of Wildfire Ash?

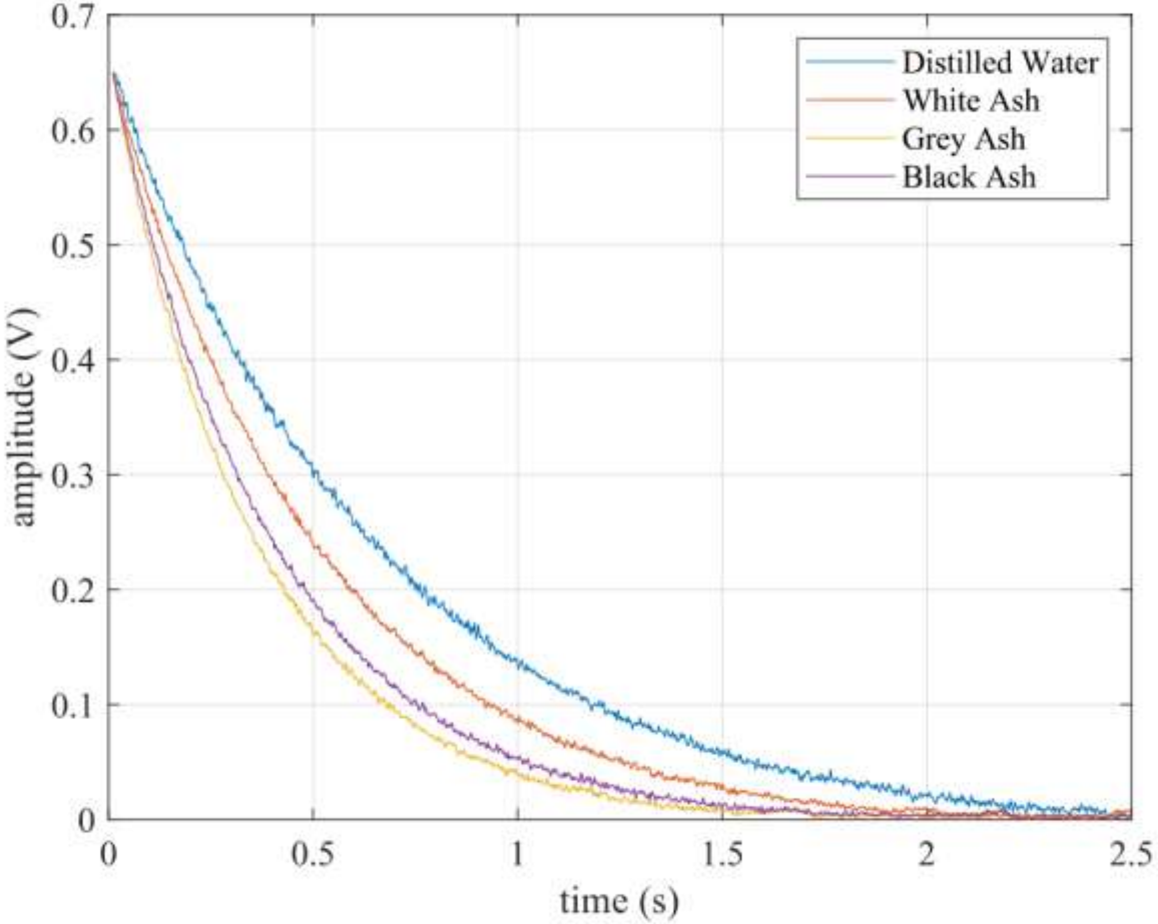
- Effects on topsoil
  - Ash deposits enhance magnetic content in soil
  - Magnetic properties are closely related to climate & rainfall
- Deposition through runoff water
  - Nearby bodies of water accumulate magnetic content
  - Nanoscale magnetite is linked to brain disease
- Understand fire severity and the reaches of magnetic deposition



USGS, "How wildfires threaten U.S. water supplies," Water Data Labs, 06-Nov-2020. [Online]. Available: https://labs.waterdata.usgs.gov/visualizations/fire-hydro/index.html#/. [Accessed: 28-Oct-2022].

NMR Relaxometry with MPs

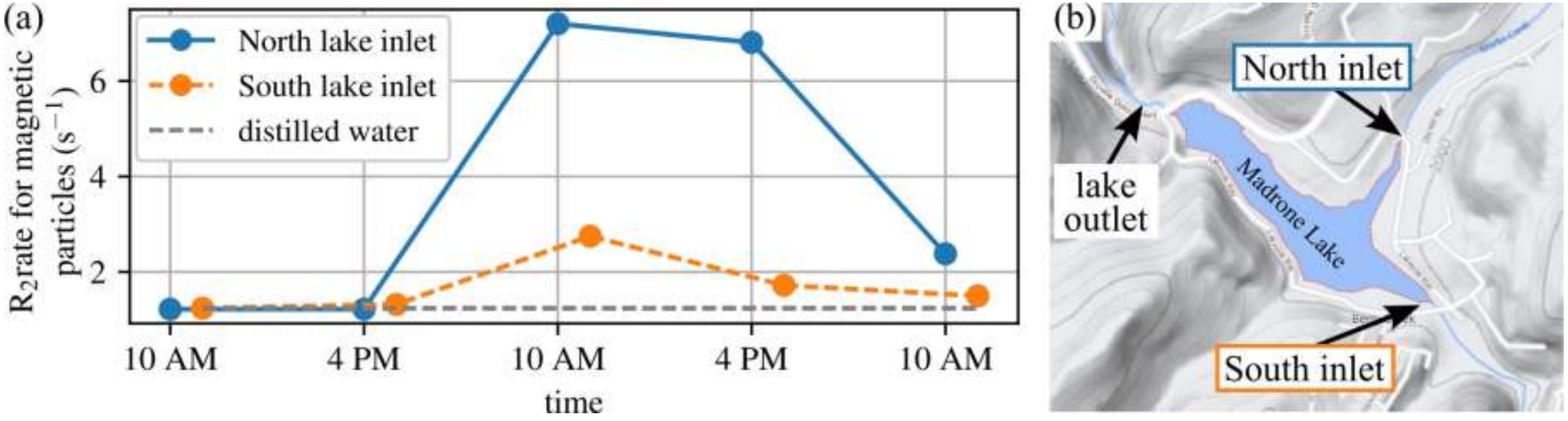
- 10 total ash samples
- 20 mg in 20 mL of water
- Distilled water used as reference
- R_2 extracted via least squares regression
  - $M_{xy} = M_0 \exp(-R_2 t)$



Real-time In Situ Tracking

- Monitoring Wildland-Urban Interface Fire Ashes and Run off Total iron content collected

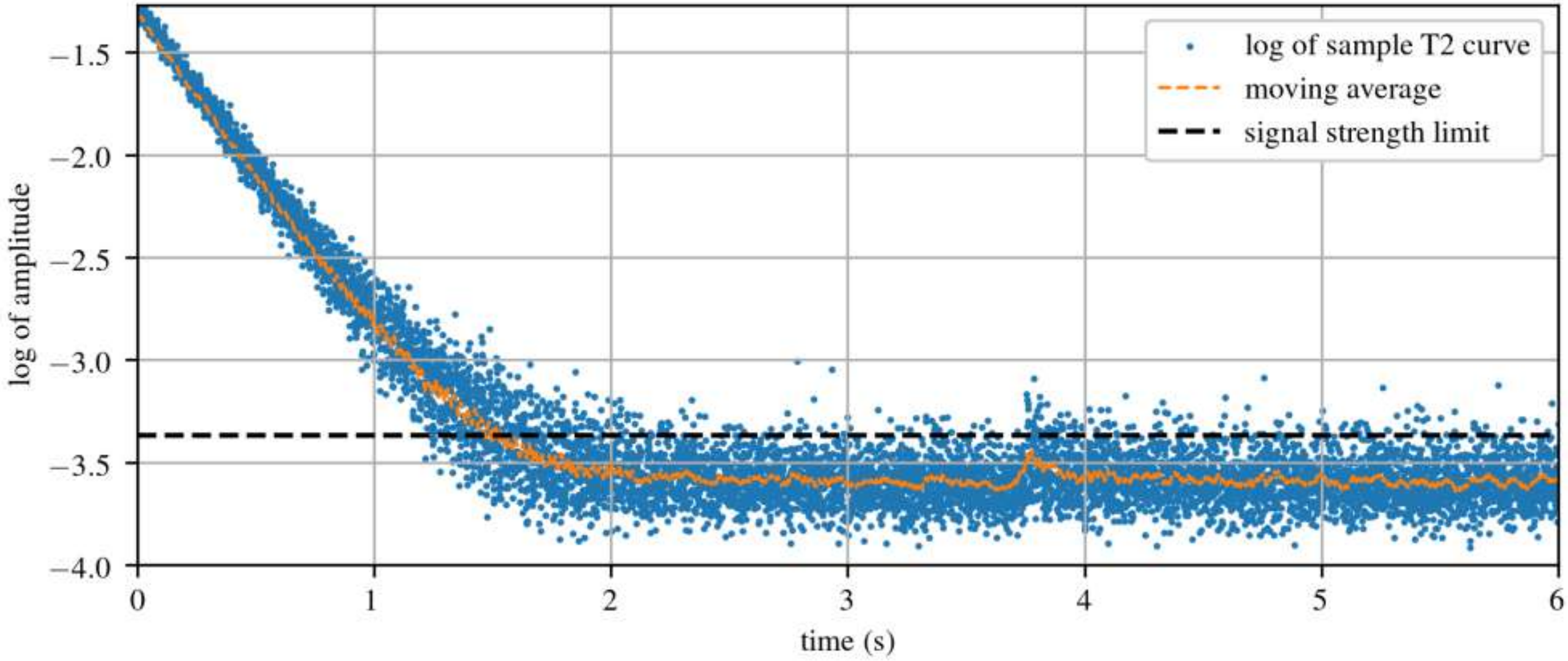
- 10 surface water samples collected from two inlets to Lake Madrone that were subjected to runoff following the North Complex Fire in California



ML-based Contaminant Monitoring

Separating Signal from Noise

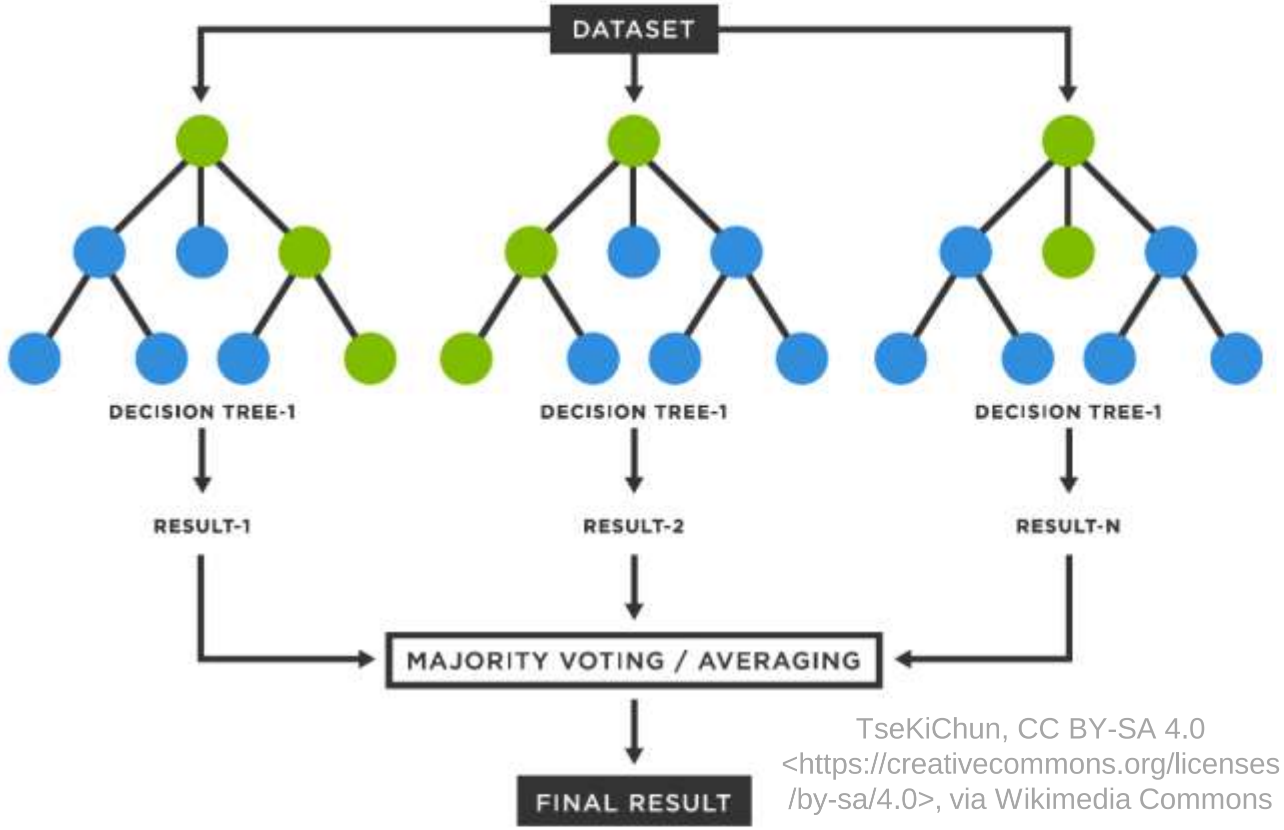
- Natural logarithm of T2 signal allows for the separation of signal and nose



Feature-based Classification using Interpretable Machine Learning

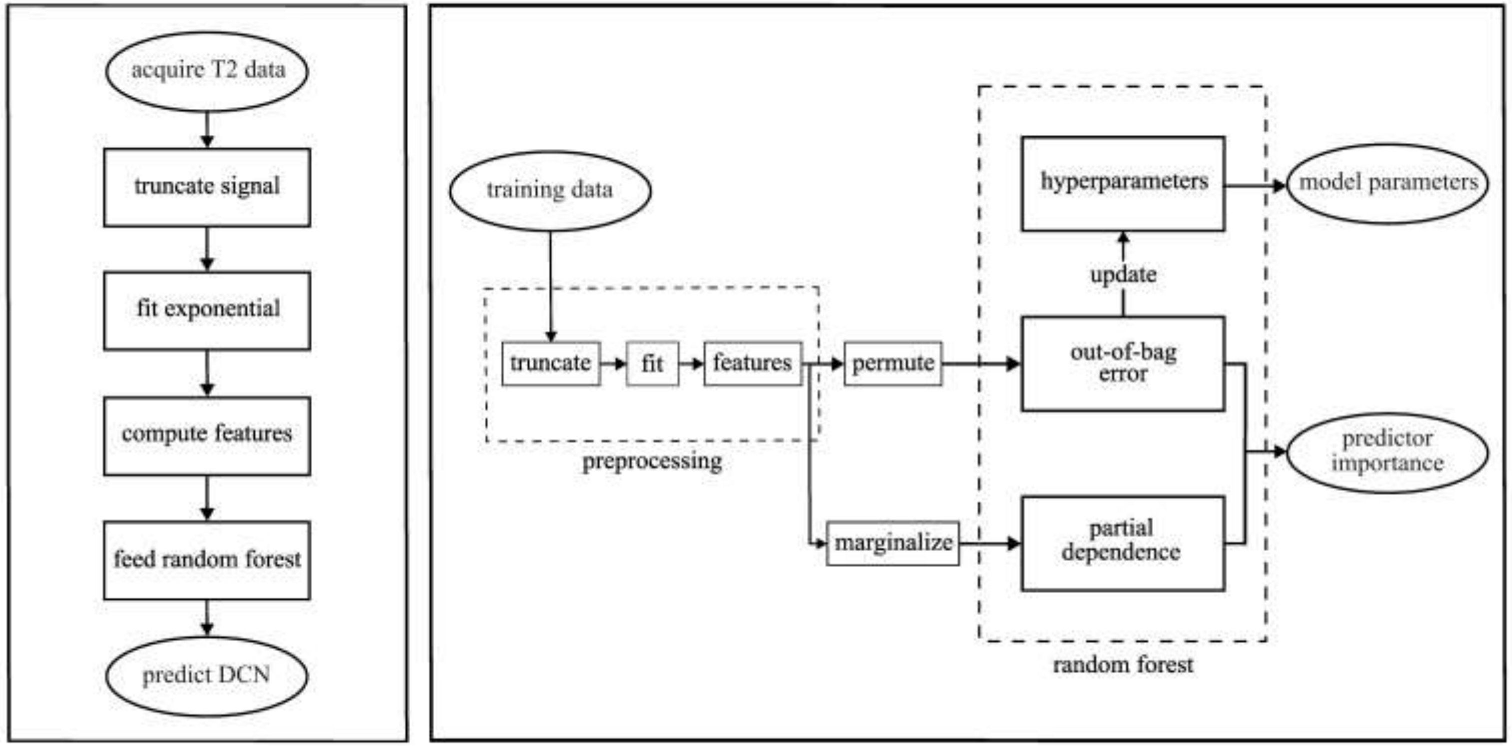
- Visual summary of the interpretable machine learning approach.

feature	interpretation	formula
amplitude	initial signal strength	x_a
rate	T_2 relaxation rate	x_b
mean	average value	$\frac{1}{N}\sum_{i=1}^{N} x_i$
standard deviation	spread around the mean	$\sqrt{\frac{\sum_{i=1}^{N}(x_i-\bar{x})^2}{N}}$
root mean square	average power	$\sqrt{\frac{1}{N}\sum_{i=1}^{N} x_i^2}$
shape factor	signal shape	$\frac{x_{rms}}{x_{mean}}$
kurtosis	tail length	$\frac{\frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})^4}{[\frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})^2]^2}$
skewness	signal asymmetry	$\frac{\frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})^3}{[\frac{1}{N}\sum_{i=1}^{N}(x_i-\bar{x})^2]^{3/2}}$
impulse factor	ratio of amplitude to mean	$\frac{x_a}{x_{mean}}$
crest factor	ratio of amplitude to RMS	$\frac{x_a}{x_{rms}}$



Interpretable Machine Learning

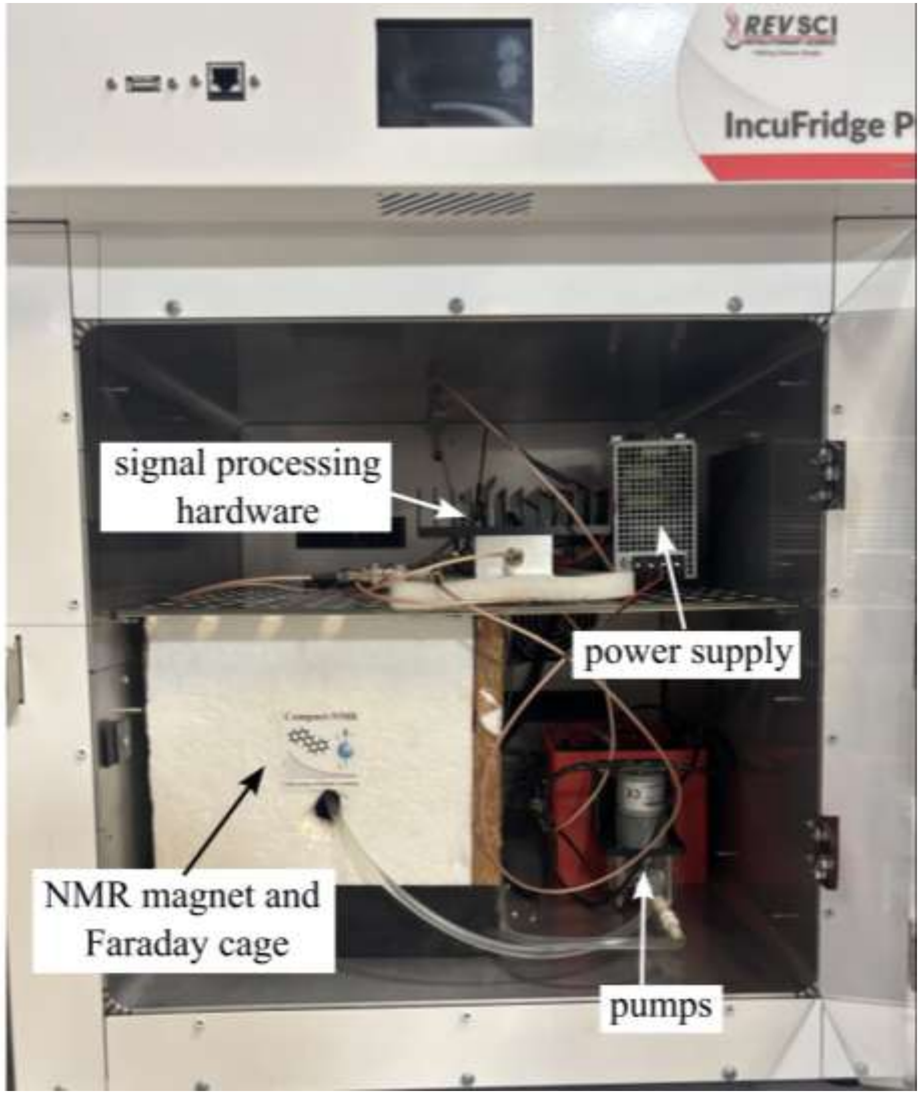
- A random forest model is trained with hyperparameter tuning, generating feature importance scores that highlight which input variables most influence the prediction of DCN.



Lab Data Collection for Model Training

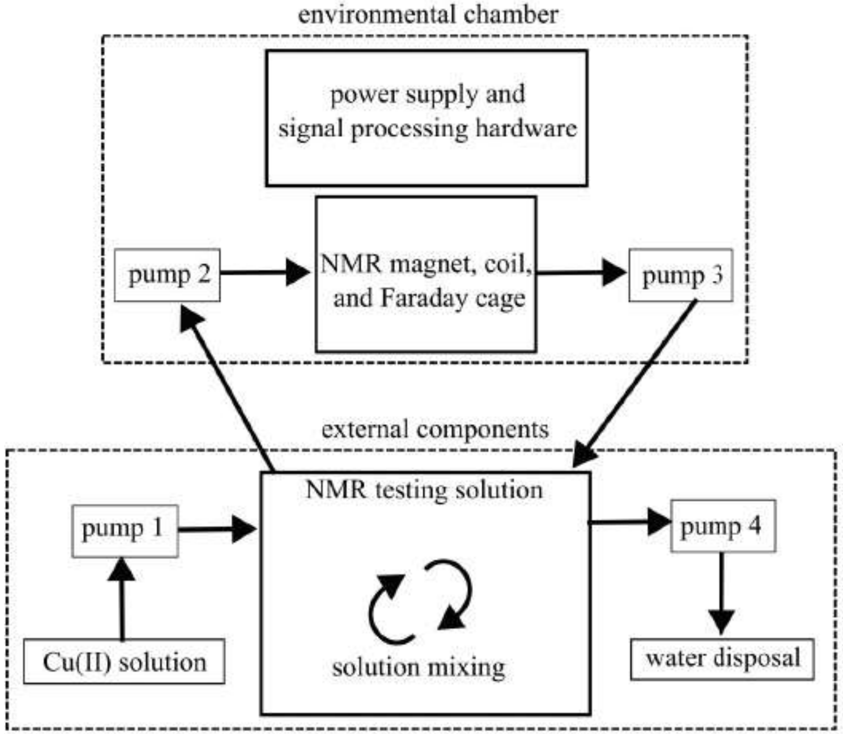
NMR in Environmental Chamber

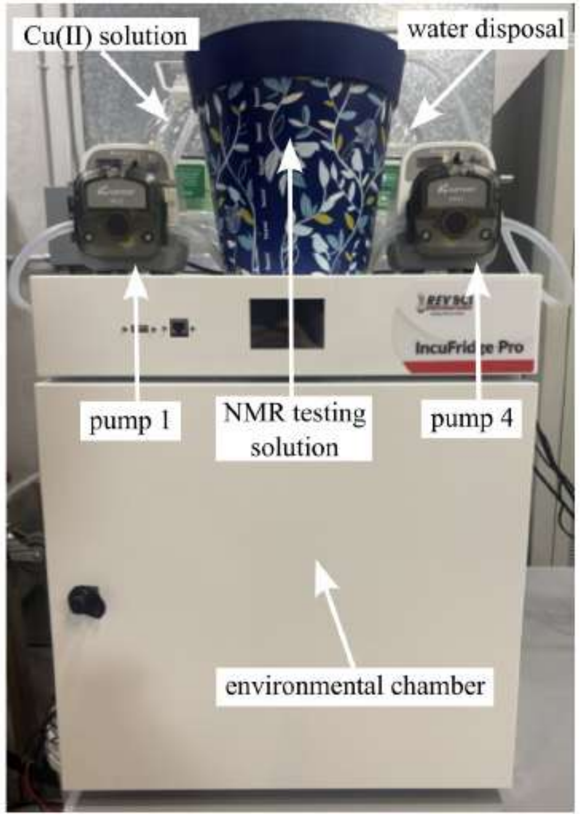
- NMR is placed in an environmental chamber for temperature control.
- Long-term, an environmental chamber would not be easy if the magnet is calibrated over a temperature range.
- Over-sized chamber used for simplicity.



Data Collection for Model Training

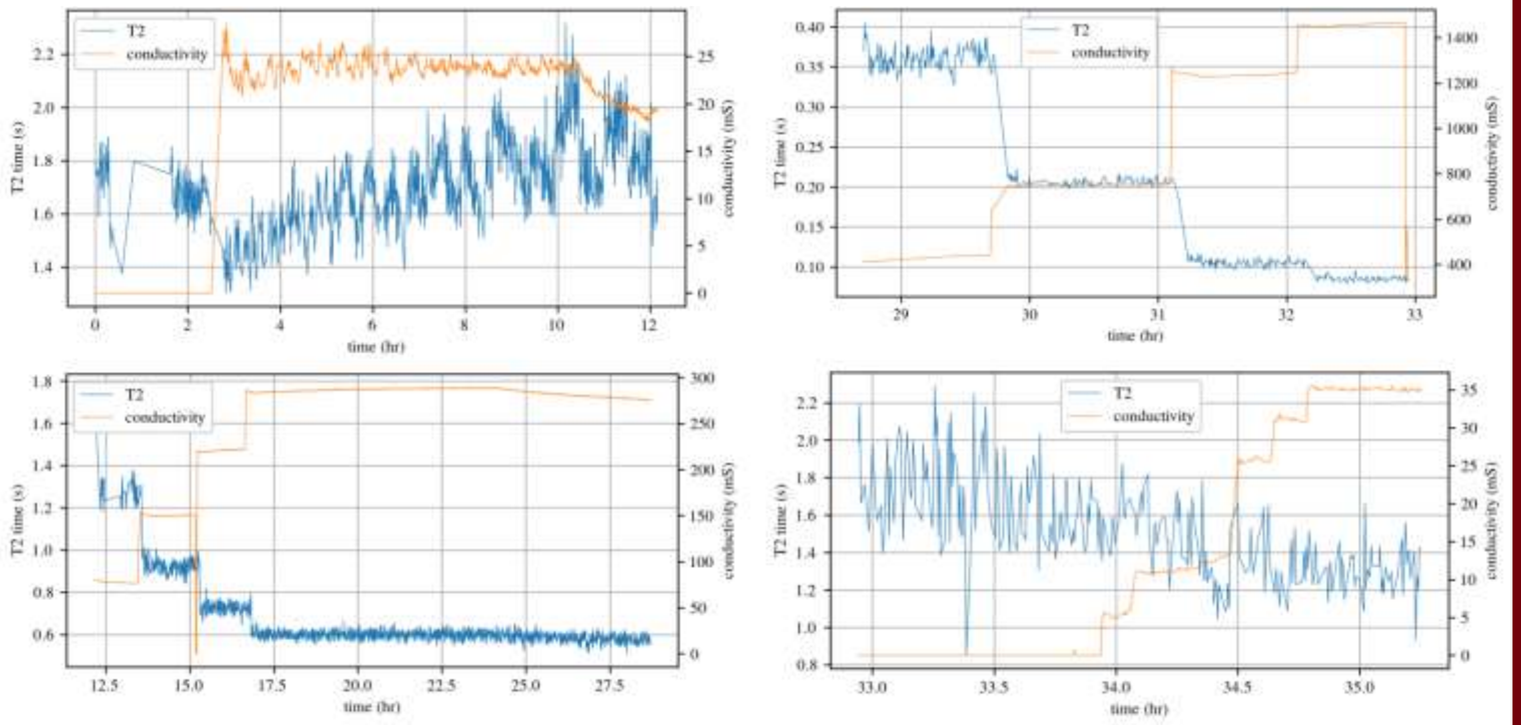
- Data collection method: slowly drip Cu(II) solution into distilled water to provide near-continuous training data
- Remove water at same rate to avoid overflow





Model Training Data

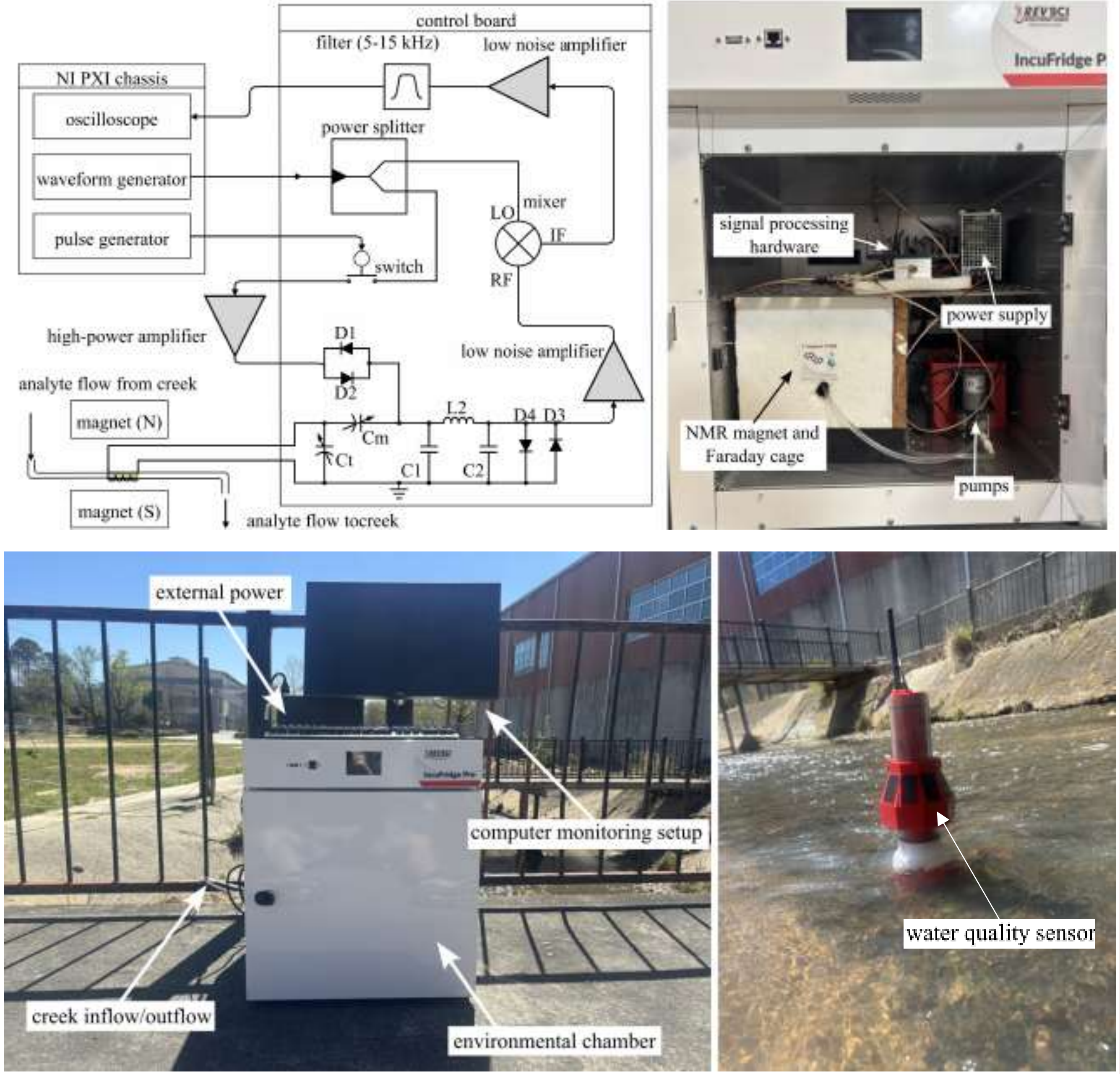
- Consists of Cu(II) contaminated water from 0mg/L to 1000mg/L
- Stair-step concentration increases to provide model with comprehensive ranges
- Slow and steady increase in Cu(II) contamination at low concentrations to provide near-continuous data



Field Deployment of In Situ NMR system

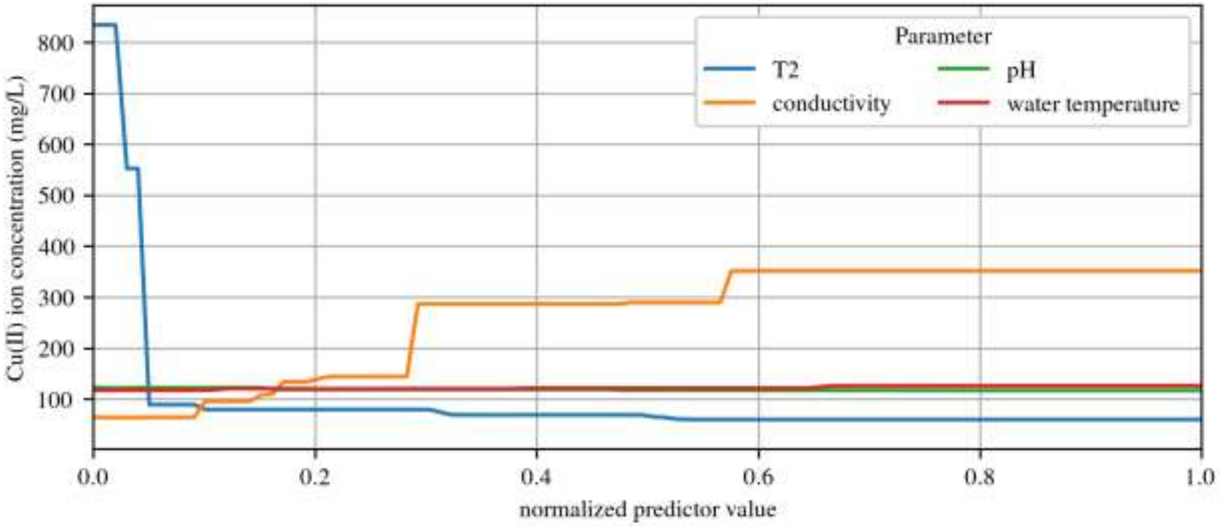
Field Deployed System

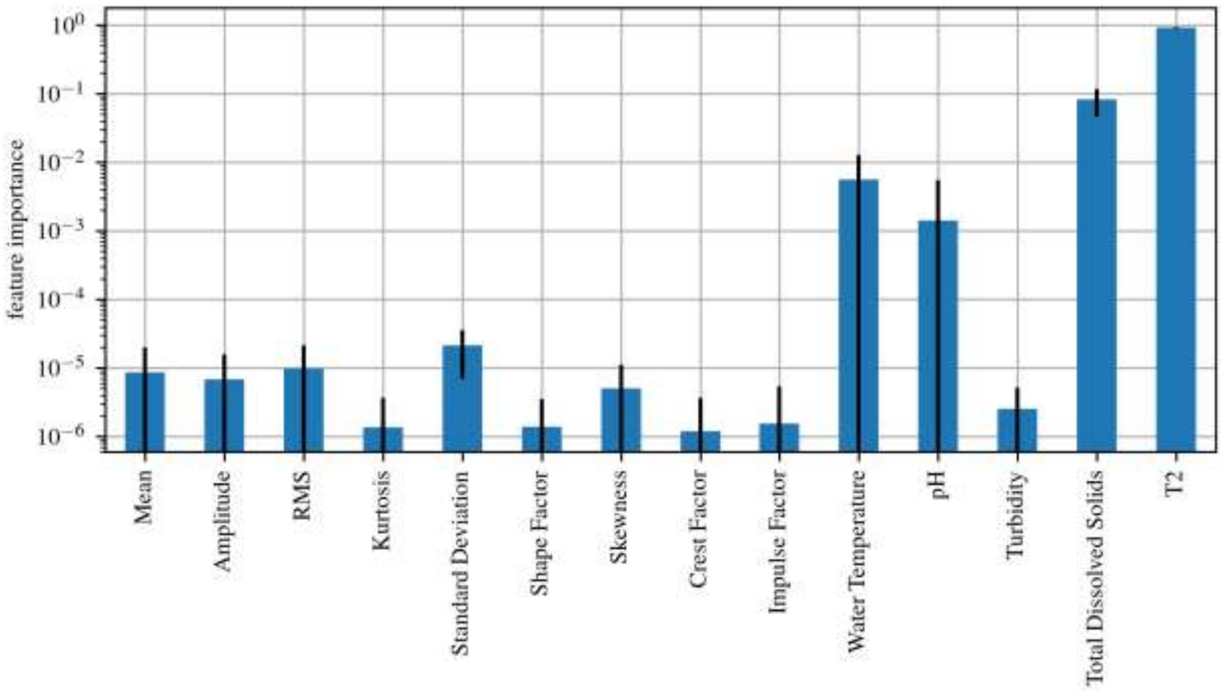
- Environmental chamber: enables temperature control for magnet and RF electronics
- Flow-through pumps: enable automatic sample collection
- NI PXI-8821: enables remote data acquisition with LabVIEW software
- Water quality sensor: measures pH, temperature, turbidity, and conductivity



Machine Learning Model

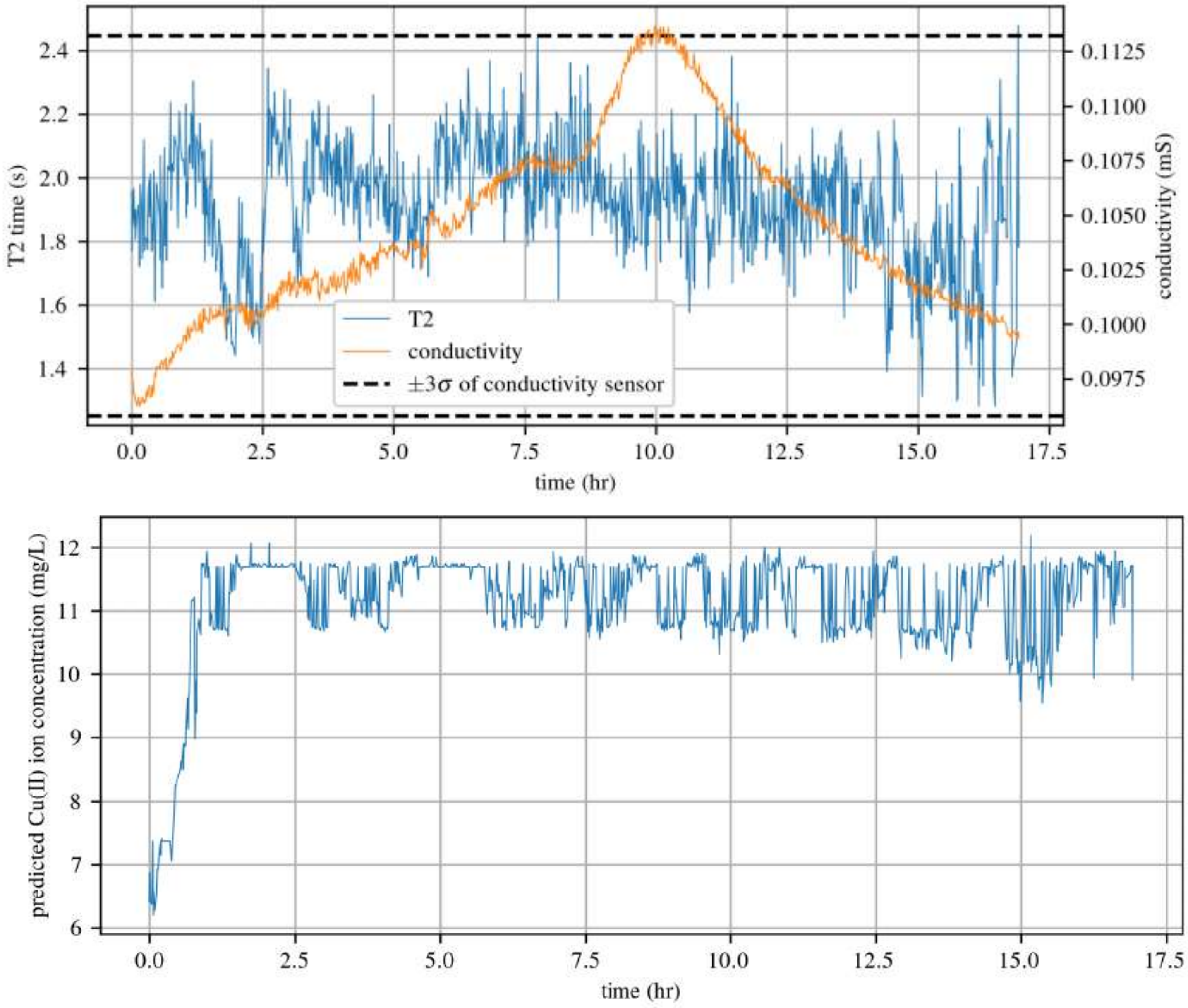
- Partial dependence plot: indicates low T2 and high conductivity cause high Cu(II) concentration and high T2 and low conductivity cause low Cu(II) concentration
- Importance plot: shows that T2 and conductivity are by far the most important
- Together, they indicate the model is thinking correctly





Rocky Branch Creek Data

- T2 and conductivity data collected in-situ over 17 hours
- T2 and conductivity (within 3σ) stay the same
- Model predictions agreeing with the consistency of data collection



Conclusion

- NMR can be used to quantify magnetic particle concentration related to ash contaminated water due to wildfires
- A remote-deployable system has been designed, built, and tested with ML functionality to quantify magnetic content based on T2, water quality data, and time series parameters
- The system will be further developed to be able to distinguish and quantify different contaminants

Acknowledgement

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Thank You for Your Time

GitHub Repository

https://github.com/ARTS-Laboratory/Paper-2025-Continuous-Water-Quality-Monitoring-using-Field-Deployable-NMR

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