

## **Development of a molecularly informed biogeochemical framework for reactive transport modeling of subsurface carbon inventories, transformations and fluxes**

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### **Project Abstract:**

To understand how soils moderate heterotrophic and autotrophic respiration of CO<sub>2</sub>, our project is using field and laboratory measurements of soil respiration, soil *p*CO<sub>2</sub> and soil organic carbon (SOC) content across the montane to sub-alpine ecosystems of the Rocky Mountain Biological Laboratory surrounding Gothic, CO watershed. Given the importance of exchanges across scales for improving modeling abilities, our project considers soil functional complexity in three conceptual dimensions: temporal variability, molecular diversity and spatial heterogeneity. Along the temporal axis of variability, we find that model structures that account for dormancy in response to pulsed wetting events, as well as plant phenology (*e.g.*, senescence) are critical for capturing the response of soil respiration to changes in the timing and magnitude of both snowmelt and the summer monsoonal precipitation. In terms of molecular diversity, we extended the SOC functional group abundance (SOC-fga) method that combines Fourier transform infrared spectroscopy (FT-IR) and bulk carbon X-ray absorption spectroscopy (XAS) to evaluate the density fractions within multiple meadow depth profiles. We find site-to-site variations in light and occluded fractions that contrast with the consistency in the heavy fraction between sites (polysaccharide and amide), indicating that regardless of carbon input, the residual products of SOC turnover have very similar structures, possibly due to sorption on mineral surfaces. In terms of spatial heterogeneity, we have combined airborne remote sensing with ground-truth SOC inventories to map the spatial heterogeneity in soil carbon. We find that depositional zones, including floodplains and fens, have an outsized control on carbon accumulation, but are difficult to predict based on topographic constraints alone. In these environments, we also find evidence for active methane cycling that shifts the functional complexity, pointing to a need for better characterization to understand how their temporal response and molecular diversity compares to the hillslope sites. Collectively, our results indicate that the spatially averaged fluxes may not equate to fluxes calculated for the averaged compartments, requiring consideration of not only the soil functional complexity but the upscaling methods used to represent it.