EGU23-15968, updated on 14 Apr 2024
https://doi.org/10.5194/egusphere-egu23-15968
EGU General Assembly 2023

Differentiable modeling to unify machine learning and physical models and advance Geosciences

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Process-Based Modeling (PBM) and Machine Learning (ML) are often perceived as distinct paradigms in the geosciences. Here we present differentiable geoscientific modeling as a powerful pathway toward dissolving the perceived barrier between them and ushering in a paradigm shift. For decades, PBM offered benefits in interpretability and physical consistency but struggled to efficiently leverage large datasets. ML methods, especially deep networks, presented strong predictive skills yet lacked the ability to answer specific scientific questions. While various methods have been proposed for ML-physics integration, an important underlying theme — differentiable modeling — is not sufficiently recognized. Here we outline the concepts, applicability, and significance of differentiable geoscientific modeling (DG). “Differentiable” refers to accurately and efficiently calculating gradients with respect to model variables, critically enabling the learning of high-dimensional unknown relationships. DG refers to a range of methods connecting varying amounts of prior knowledge to neural networks and training them together, capturing a different scope than physics-guided machine learning and emphasizing first principles. In this talk we provide examples of DG in global hydrology, ecosystem modeling, water quality simulations, etc. Preliminary evidence suggests DG offers better interpretability and causality than ML, improved generalizability and extrapolation capability, and strong potential for knowledge discovery, while

approaching the performance of purely data-driven ML. DG models require less training data while scaling favorably in performance and efficiency with increasing amounts of data. With DG, geoscientists may be better able to frame and investigate questions, test hypotheses, and discover unrecognized linkages.