PennState

Differentiable and physics-informed modeling to unify machine learning and physical models and advance Geosciences

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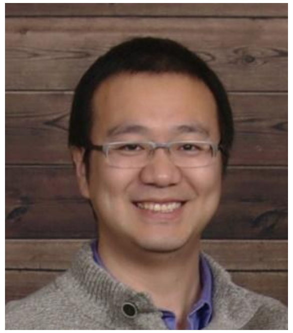


https://github.com/mhpi
Hydroml.org

@ChaopengShen

Hydroml.org
HydroML Symposium, May 22-26, 2023, Berkeley, CA

Overview

- ***What*** is the fundamental strengths of ML models compared to process-based models?
- ***What*** is *differentiable modeling in geosciences*?
- ***Examples*** of *differentiable modeling in geosciences*?

nature reviews earth & environment https://doi.org/10.1038/s43017-023-00450-9

Perspective

Check for updates

Differentiable modelling to unify machine learning and physical models for geosciences

A list of authors and their affiliations appears at the end of the paper

Water Resources Research

RESEARCH ARTICLE
10.1029/2019WR026793

Special Section:
Big Data & Machine Learning in Water Sciences: Recent Progress and Their Use in Advancing Science

Enhancing Streamflow Forecast and Extracting Insights Using Long-Short Term Memory Networks With Data Integration at Continental Scales

Dapeng Feng[1], Kuai Fang[1,2], and Chaopeng Shen[1]

[1]Civil and Environmental Engineering, Pennsylvania State University, State College, PA, USA, [2]Now at: Earth System Science, Stanford University, Stanford, CA, USA

Streamflow long-term projection or short-term forecast

Geophysical Research Letters

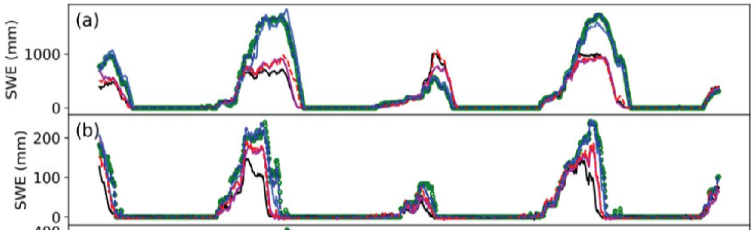
Research Letter | Full Access

A multiscale deep learning model for soil moisture integrating satellite and in-situ data

Jiangtao Liu, Farshid Rahmani, Kathryn Lawson, Chaopeng Shen

First published: 14 March 2022 | https://doi.org/10.1029/2021GL096847

Multiscale soil moisture



Song, et al., 2023, ***Snow Water Equivalent*** (under review)

Geophysical Research Letters

Research Letter | Full Access

Mitigating Prediction Error of Deep Learning Streamflow Models in Large Data-Sparse Regions With Ensemble Modeling and Soft Data

Dapeng Feng, Kathryn Lawson, Chaopeng Shen

First published: 30 June 2021 | https://doi.org/10.1029/2021GL092999 | Citations: 1

Data-sparse region

Hydrological Processes

RESEARCH ARTICLE | Full Access

Deep learning approaches for improving prediction of daily stream temperature in data-scarce, unmonitored, and dammed basins

Farshid Rahmani, Chaopeng Shen, Samantha Oliver, Kathryn Lawson, Alison Appling

Rahmani et al., 2021b, ***water temperature***

Water Resources Research

Technical Reports: Methods | Full Access

Transferring Hydrologic Data Across Continents – Leveraging Data-Rich Regions to Improve Hydrologic Prediction in Data-Sparse Regions

Kai Ma, Dapeng Feng, Kathryn Lawson, Wen-Ping Tsai, Chuan Liang, Xiaorong Huang, Ashutosh Sharma, Chaopeng Shen

Ma et al., 2021, ***Transfer Learning***

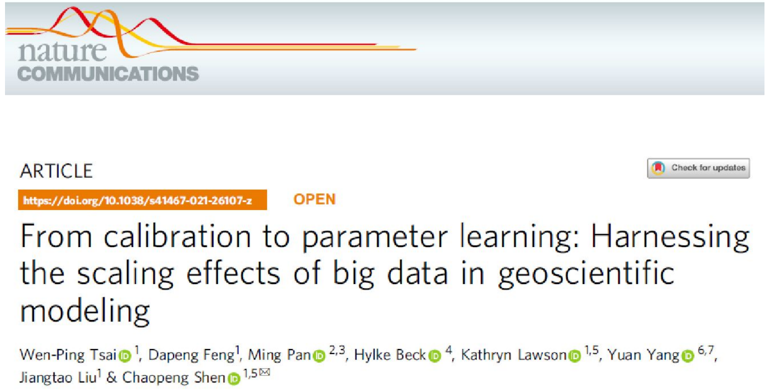
The first phase of hydrologic DL

- Success:
  1. DL models very often outperform existing models in accuracy: traditional models **were flawed**.
  2. With some adaptations, DL can offer **an ecosystem of services**.
  3. There is synergy of **big data**.
- Lessons:
  1. DL models are still **difficult to interpret** or extracting scientific insights from.
  2. Surrogate model □ how to improve above the raw model?
  3. May not learn causal relationships.
  4. DL models are limited by the issues of their training data:
  Only output observed data; limited data quality; nonstationarity

Similarity & Differences between deep learning (DL) and process-based models (PBM)?

Purely data-driven NNs	Purely process-based models
Similarities	

Differentiable parameter learning


nature COMMUNICATIONS

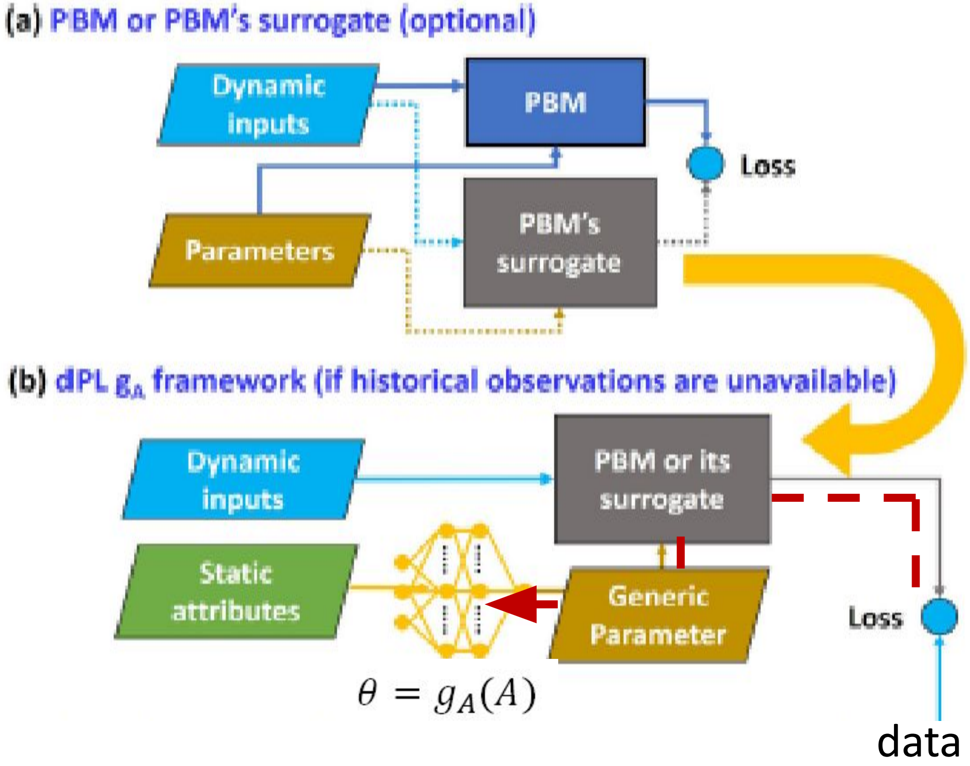
ARTICLE

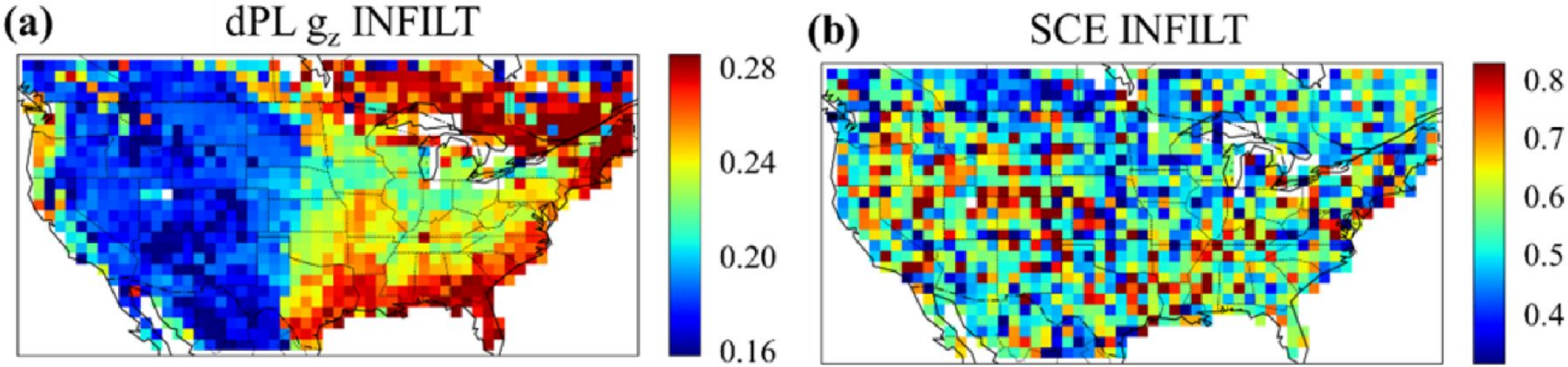
Check for updates

https://doi.org/10.1038/s41467-021-26107-z OPEN

From calibration to parameter learning: Harnessing the scaling effects of big data in geoscientific modeling

Wen-Ping Tsai[1], Dapeng Feng[1], Ming Pan[2,3], Hylke Beck[4], Kathryn Lawson[1,5], Yuan Yang[6,7], Jiangtao Liu[1] & Chaopeng Shen[1,5]

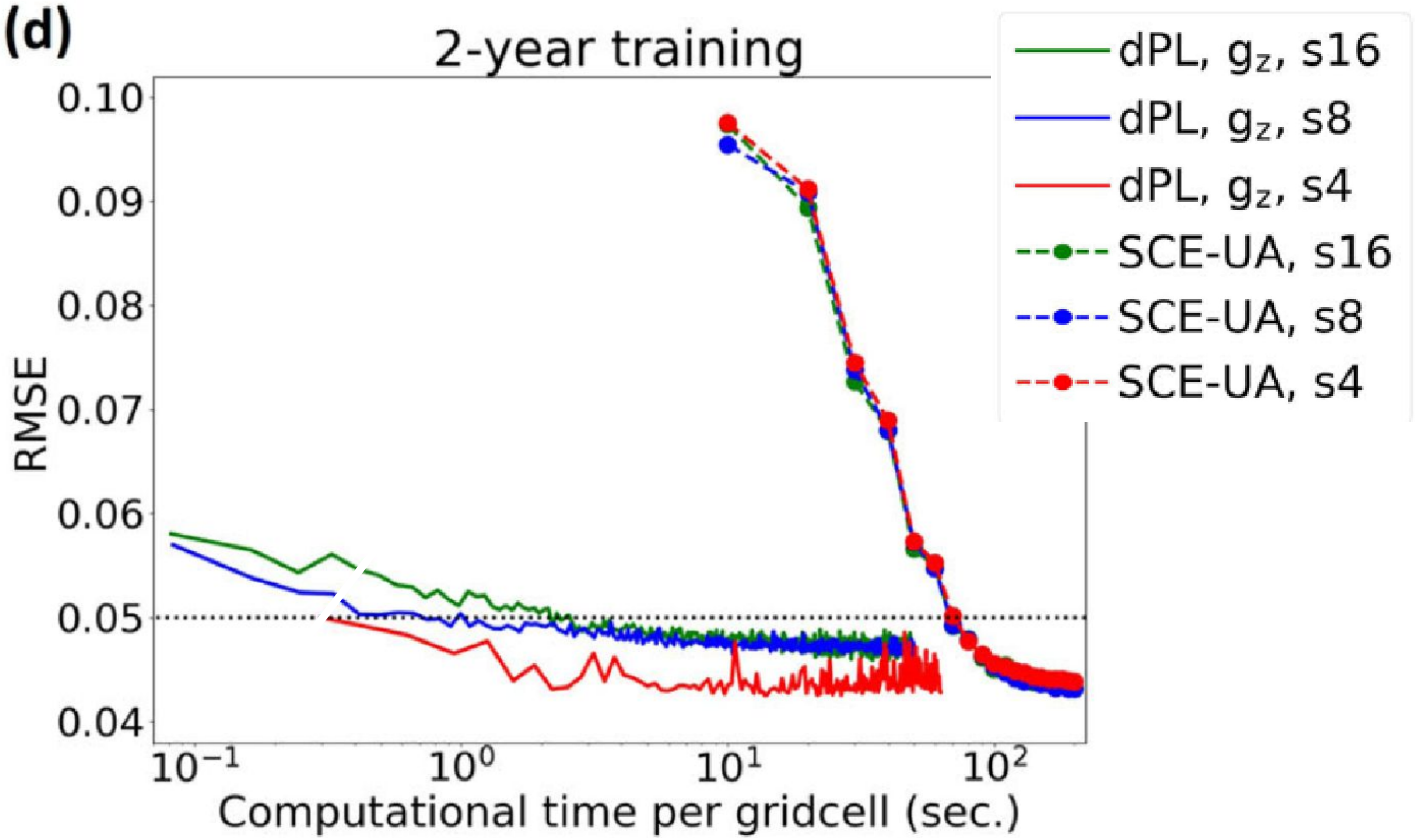




Point #1. Data scaling relationships (network effect?)

1. dPL = SCEUA for lowest RMSE
2. dPL scales better with more data
3. Orders of magnitude more efficient
4. (not shown) better results for **untrained** variables and better **spatial generalization** than traditional approach!

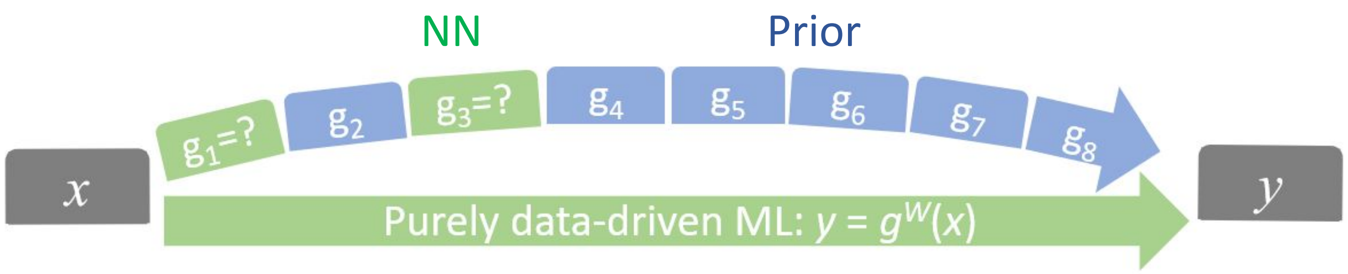
Relies on differentiable programming!



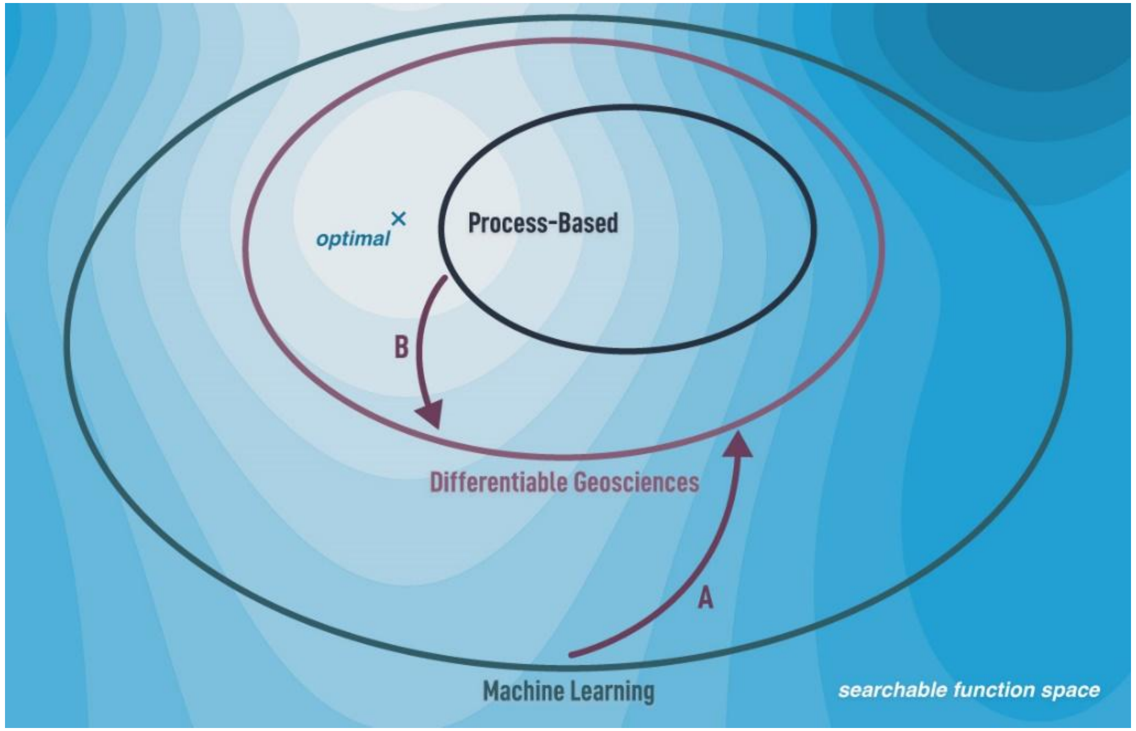
Tsai et al. 2021, Nature Communications

What is Differentiable Modeling (DM) in Geosciences?

Why is it difficult to understand ML
Why can we understand and learn DM better?



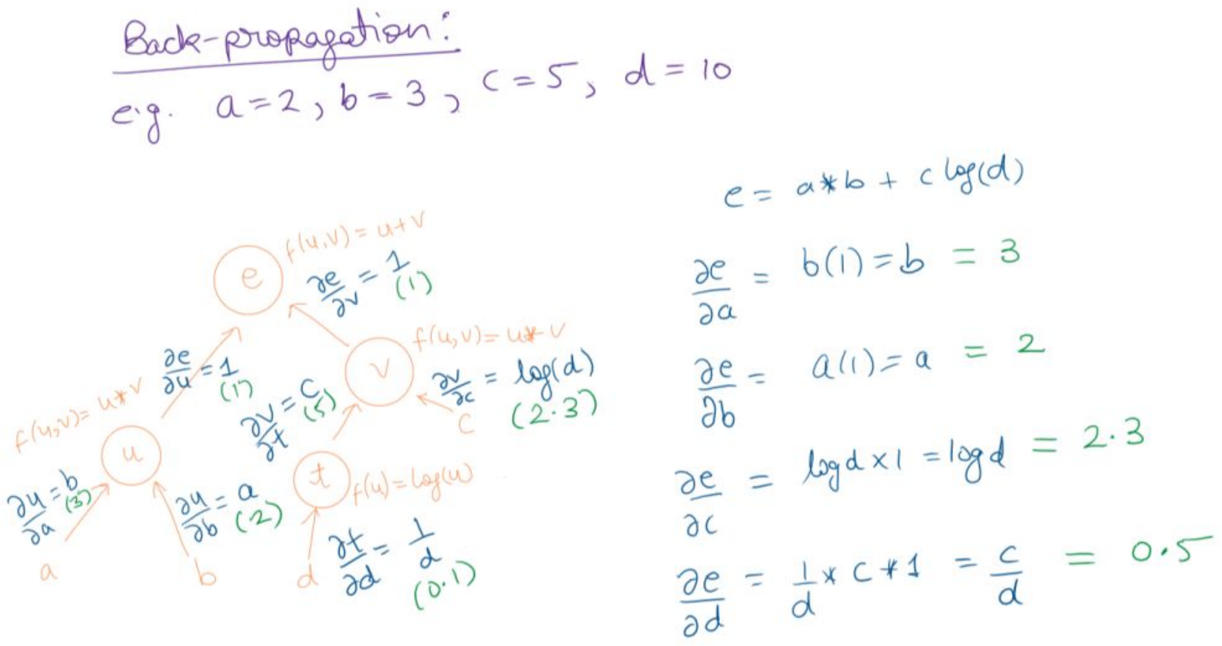
2 perspectives



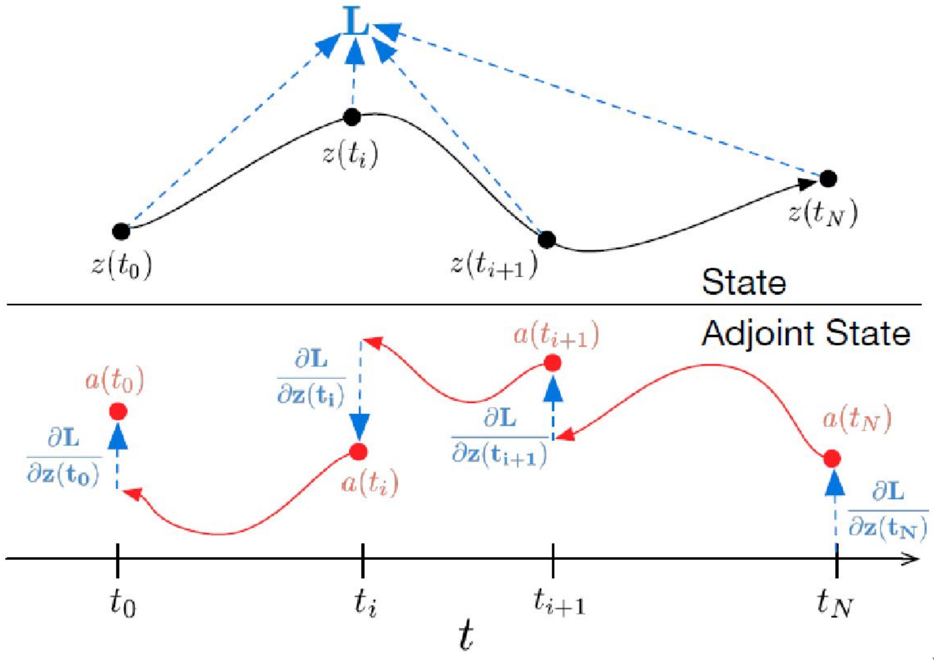
What does “Differentiable” mean?

- The ability to rapidly compute gradients $\frac{dL}{d\theta}$
- Enabling training by gradient descent

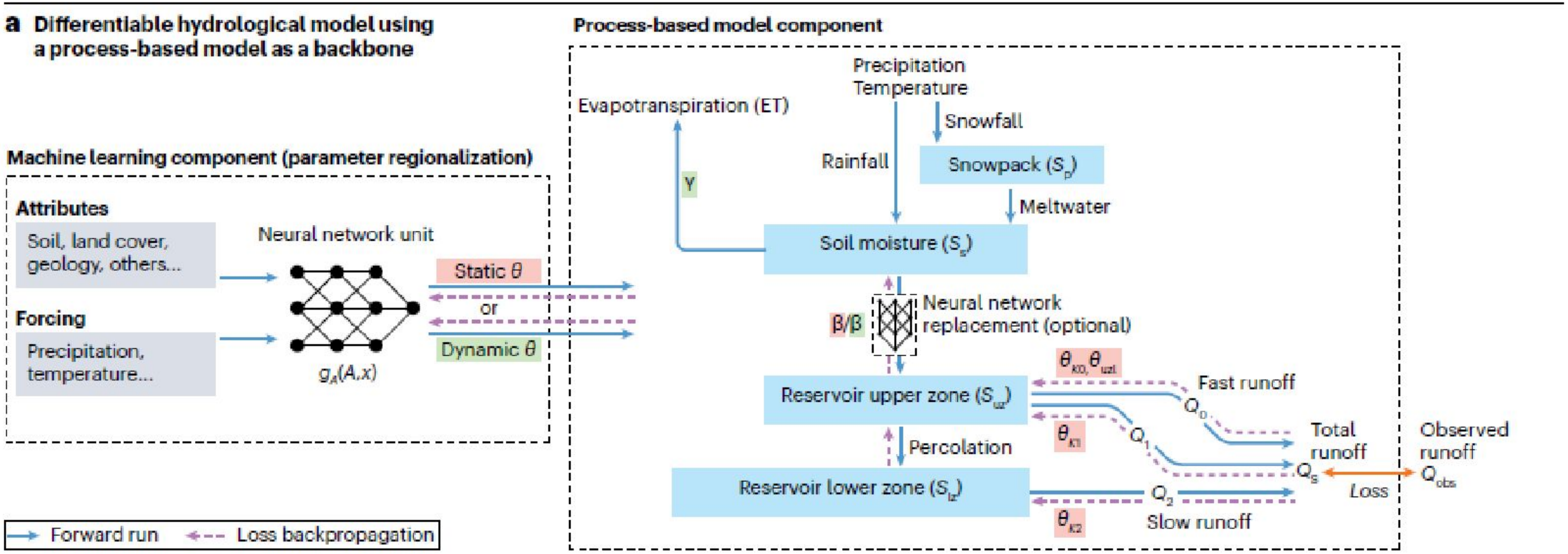
Automatic differentiation



Adjoint State method



Example 2. differentiable, learnable models to learn functions



Water Resources Research

Research Article Full Access

Differentiable, learnable, regionalized process-based models with multiphysical outputs can approach state-of-the-art hydrologic prediction accuracy

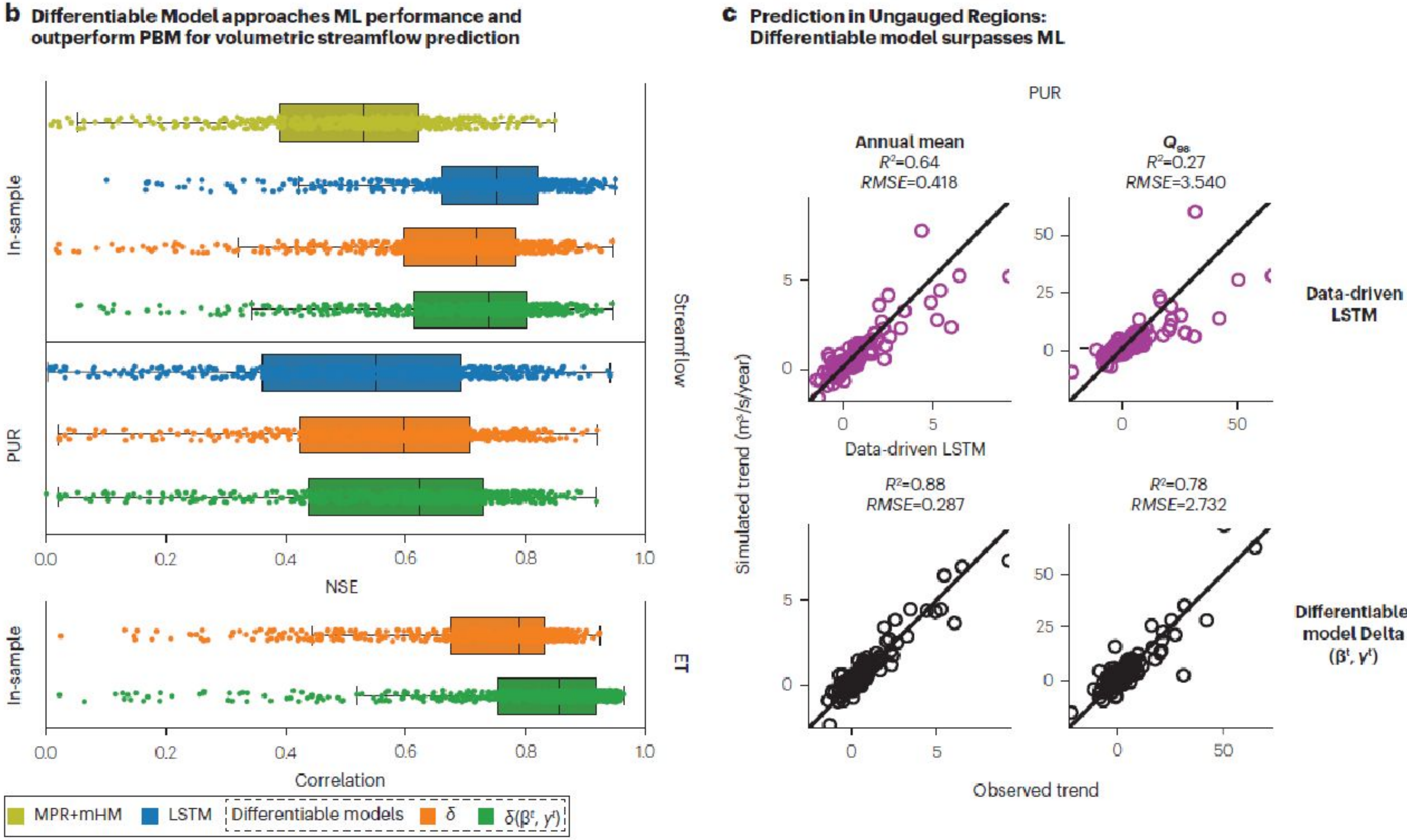
Dapeng Feng, Jiangtao Liu, Kathryn Lawson, Chaopeng Shen

First published: 19 September 2022 | https://doi.org/10.1029/2022WR032404

Evolve model structure

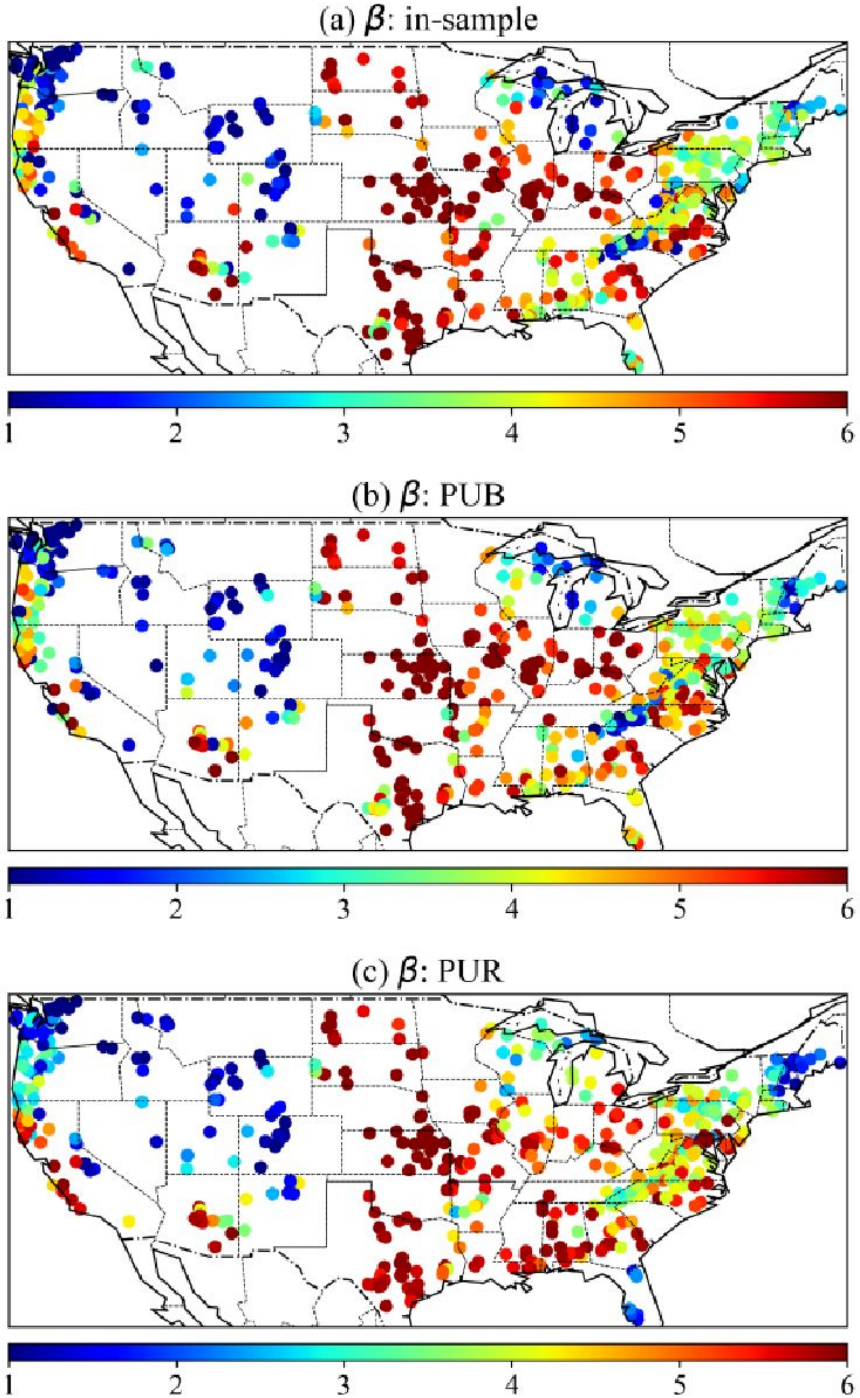
Approaching deep networks! And….

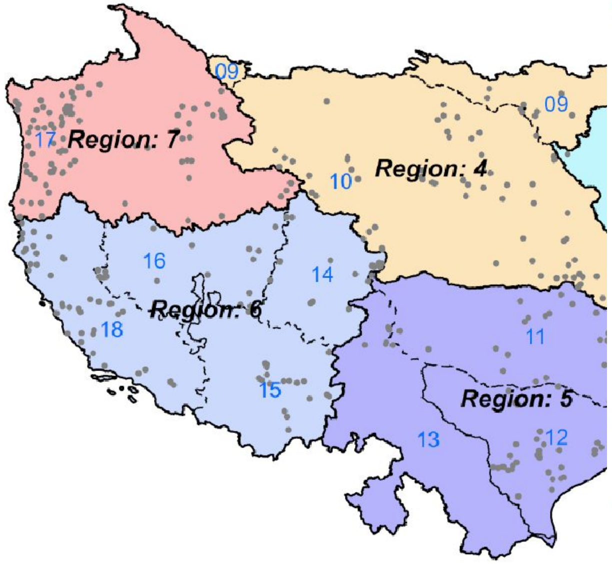
- Output untrained variables.
- Multivariate constraints.
- It extrapolates better.
- It can help us answer questions!

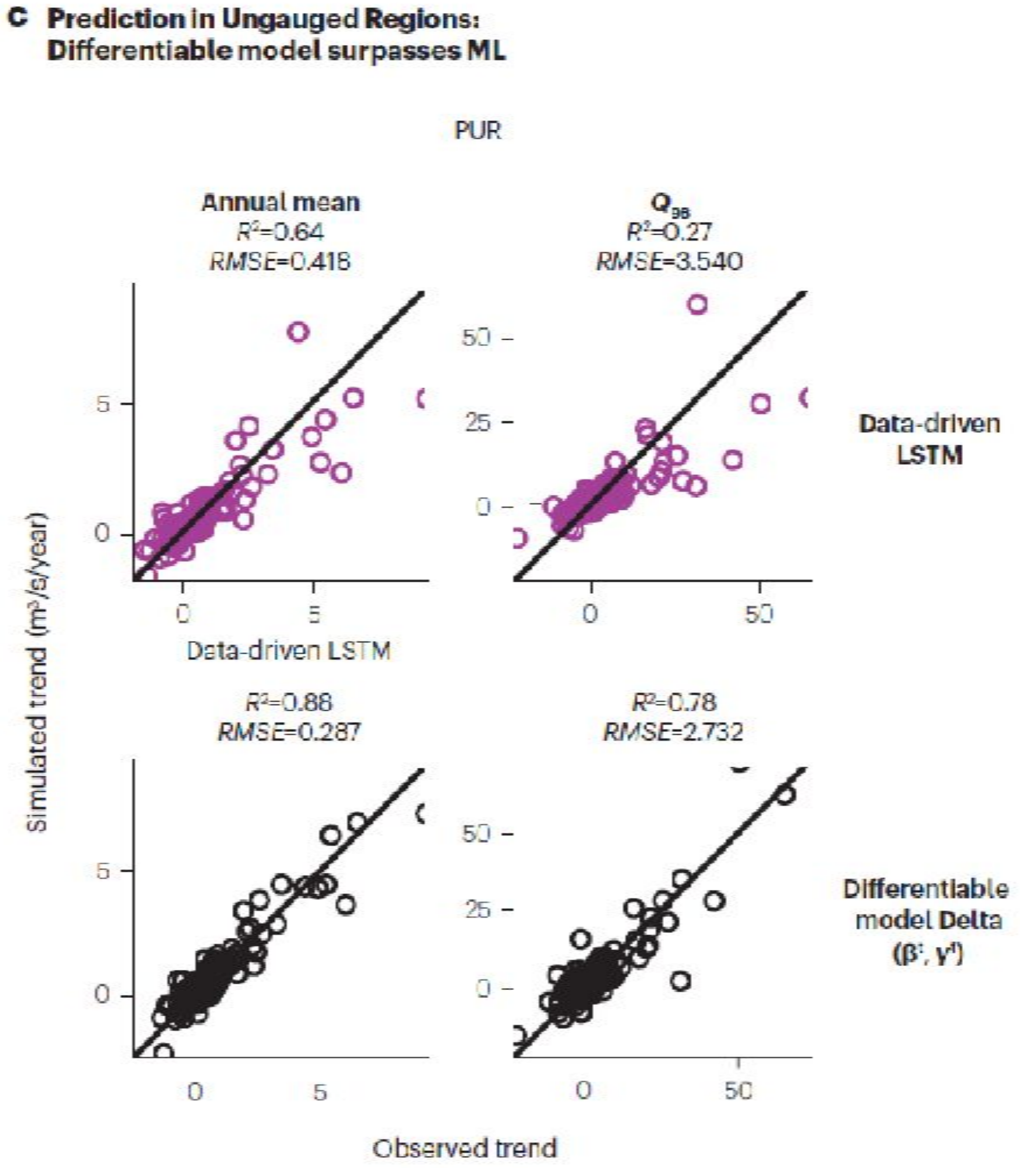


Caveat: not using the ensemble
-- first iteration. Priors do matter.

Great for extrapolation!

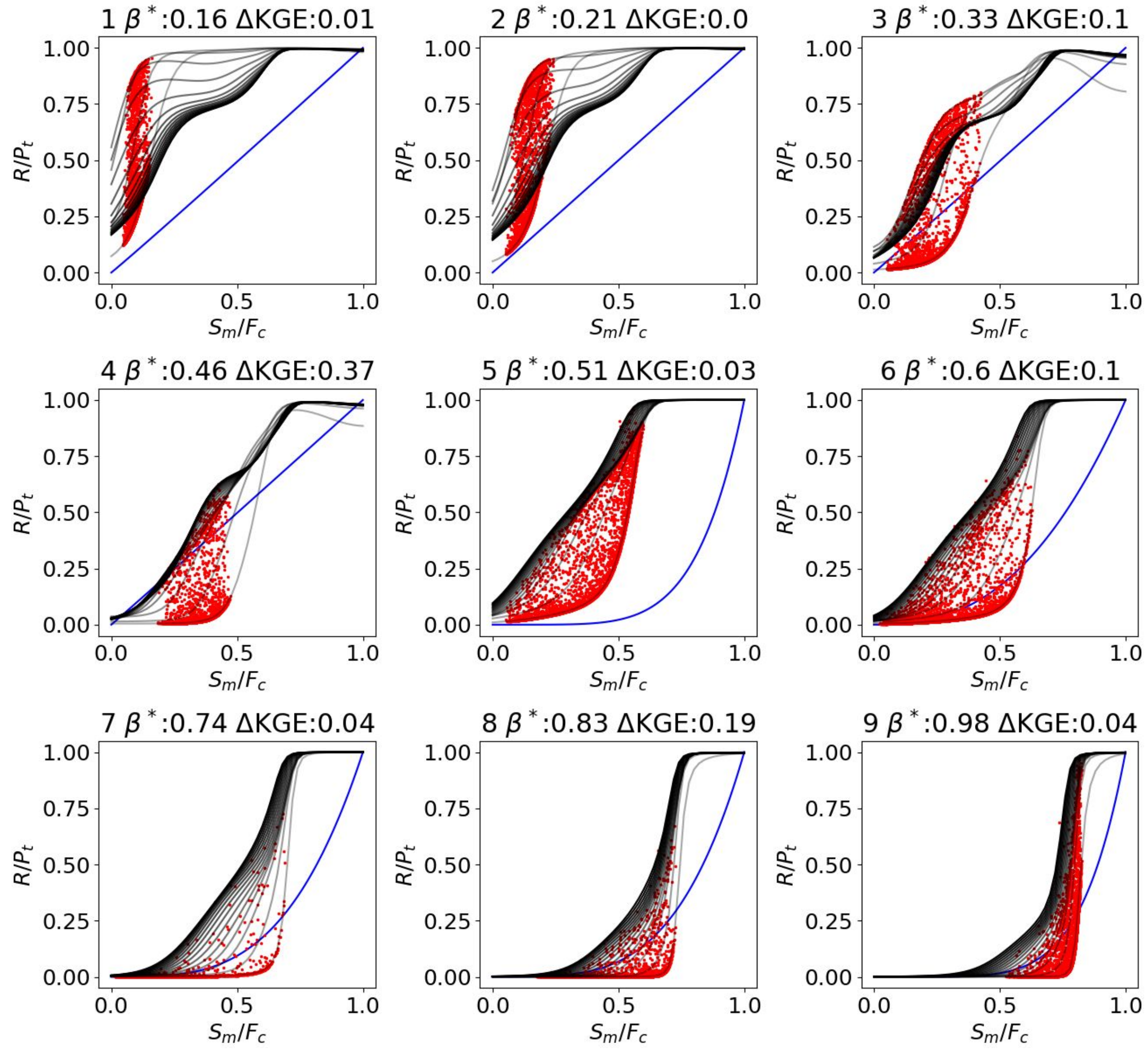






Feng 2022b HESSD
https://hess.copernicus.org/preprints/hess-2022-245/

What the ANN learned functions look like?

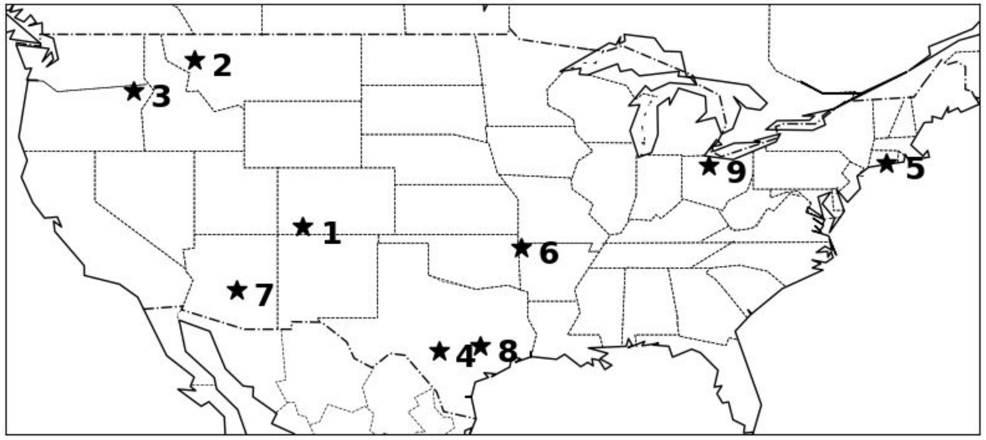


$$R/P_t = (S_m/F_c)^{\beta}$$

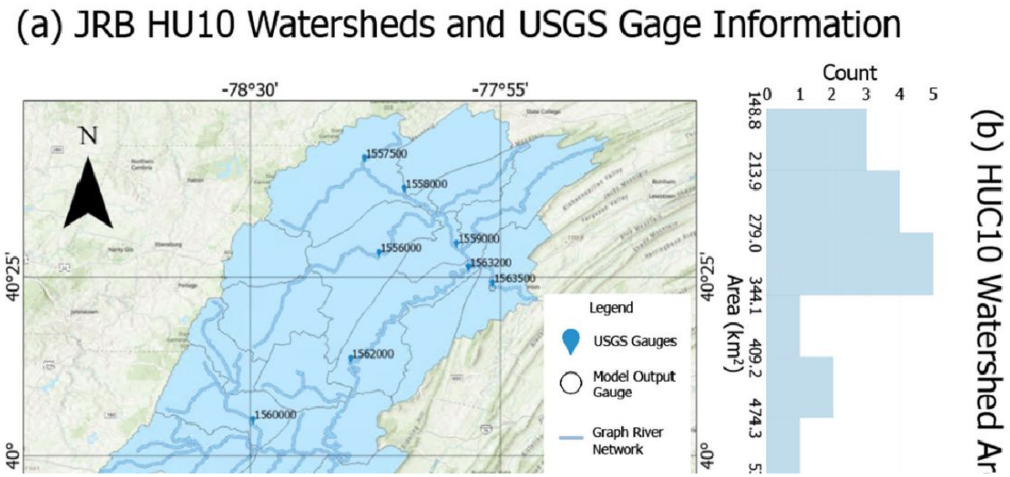
$$\boxed{R/P_t = ANN(\beta^*, F_c, S_m, S_m/F_c, P_t)}$$

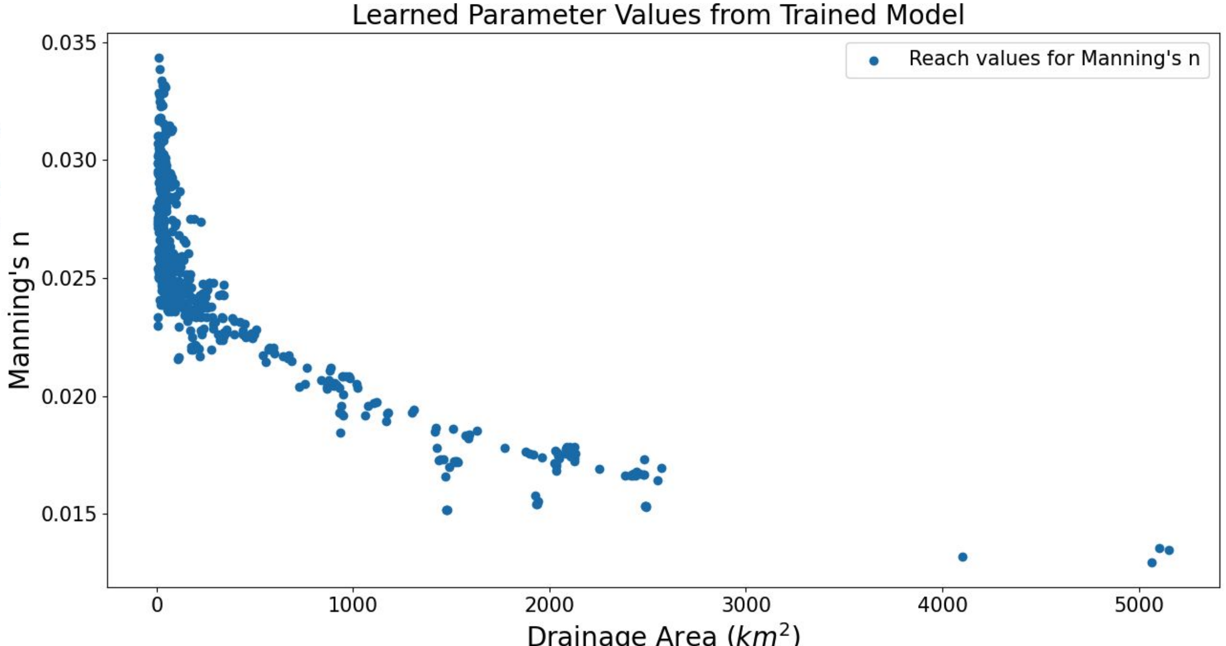
Blue line: original power law relation
Red dots: ANN simulations
Black lines: continuous plotting of ANN functions

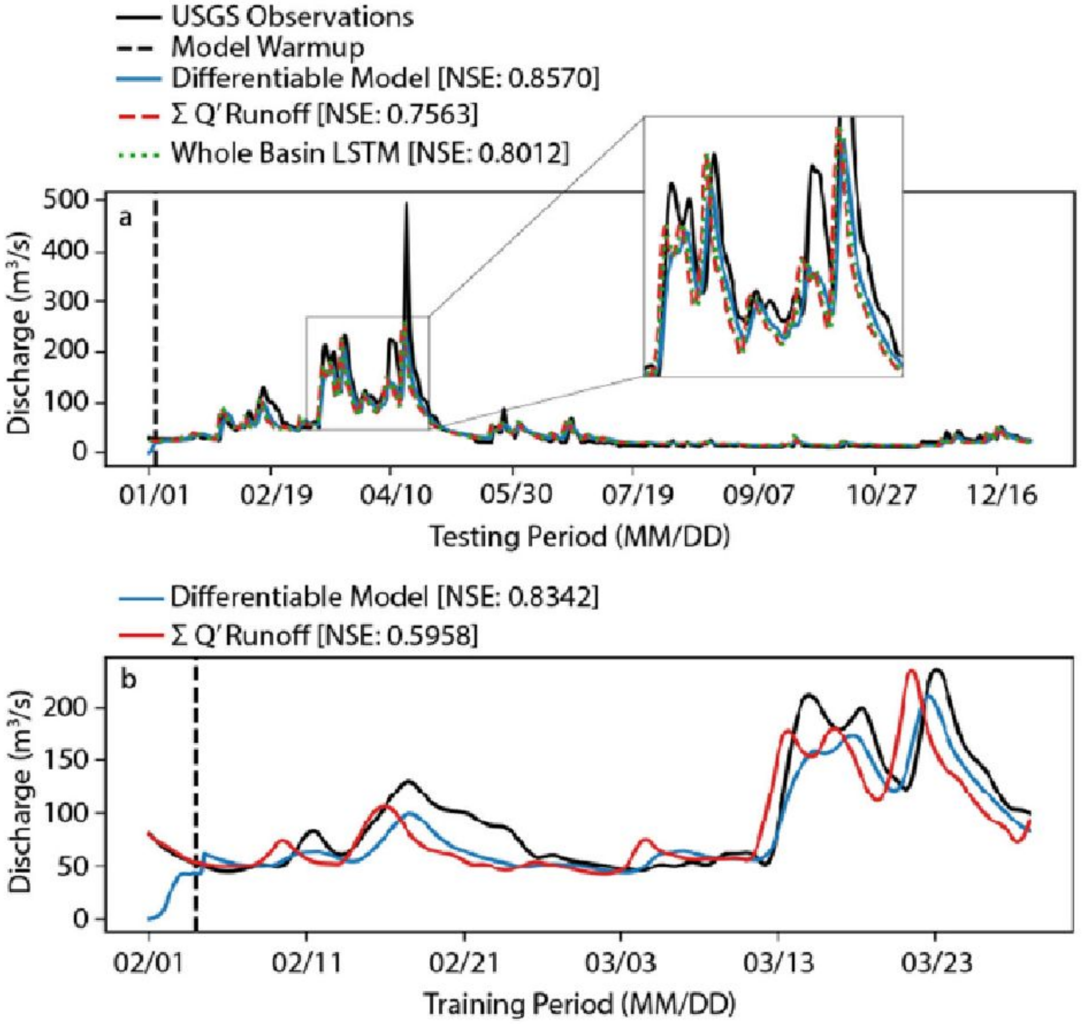
Location



Example 3. River graph



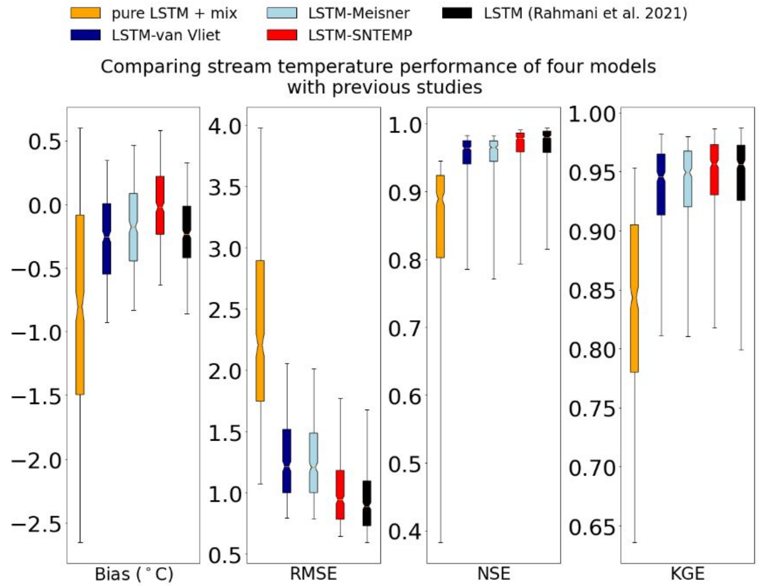




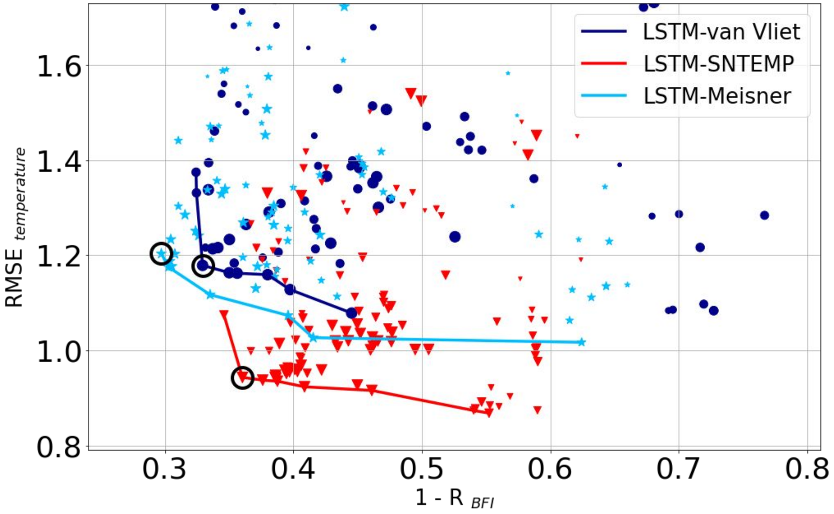
Learn physics on the river graph

https://doi.org/10.1002/essoar.10512512.1 Bindas (revision)

Example 4. *Water temperature modeling*



Prior assumptions matter!

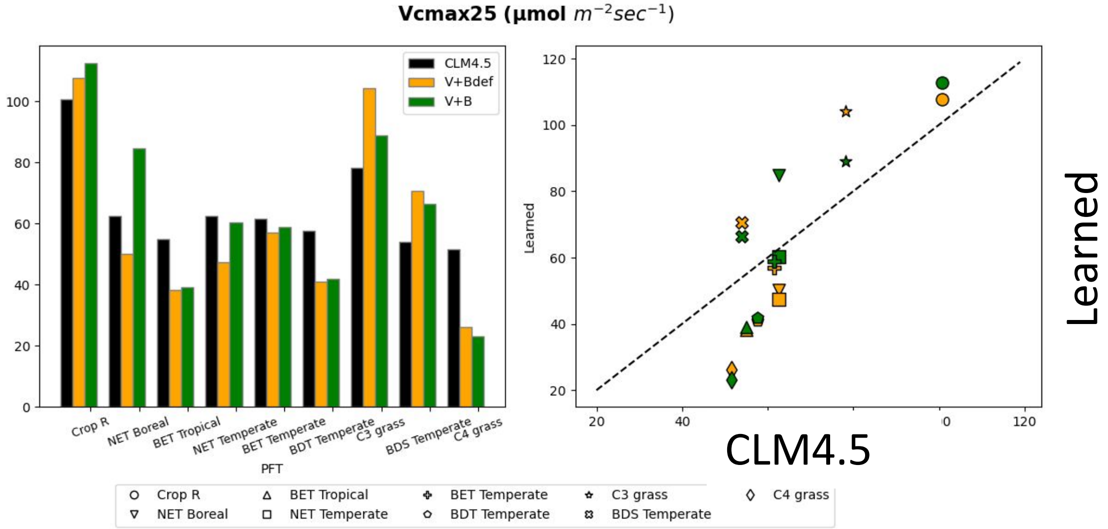


Example 5. *Ecosystem modeling*

(a) Temporal holdout test for the following system

Runs	Corr		RMSE (μmol m^{-2} s^{-1})		Bias (μmol m^{-2} s^{-1})		NSE	
	Train	Test	Train	Test	Train	Test	Train	Test
V_{def}+B_{def}	0.565		6.780		1.476		0.041	
V_{def}+B_{def} **	0.592		5.488		1.034		0.318	
V_{def}+B	0.678	0.547	5.887	6.730	1.353	1.754	0.321	-0.084
V+B_{def}	0.769	0.593	4.595	5.677	-0.129	-1.368	0.587	0.229
V+B	0.800	0.748	4.299	4.421	0.037	0.347	0.638	0.532
V+B **	0.774	0.768	4.269	4.198	0.056	0.092	0.597	0.581

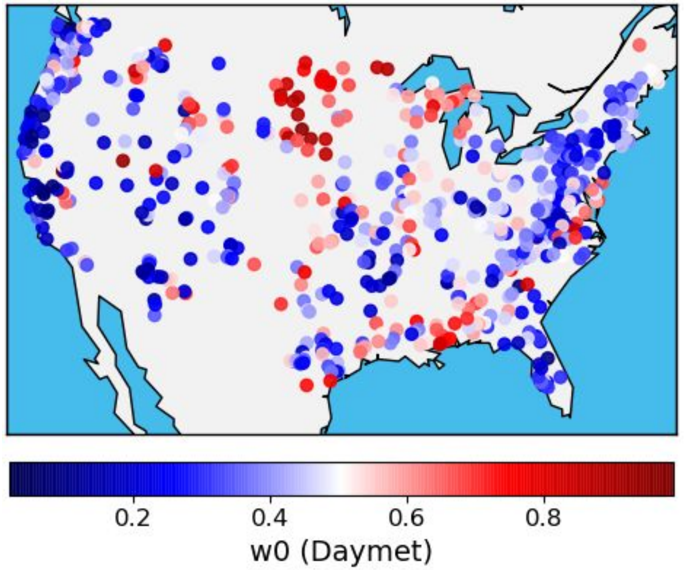
*** refers to using C3_only plants in dataset*

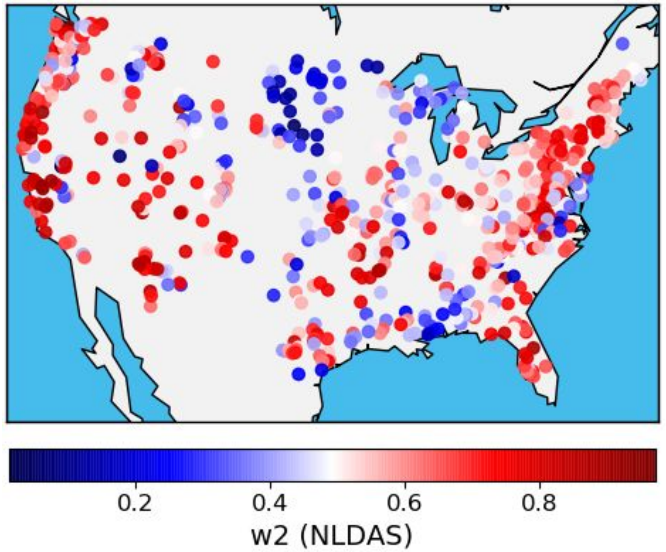


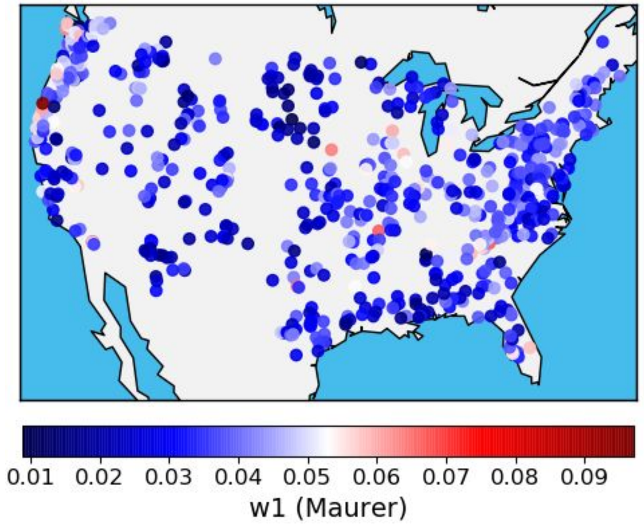
https://bg.copernicus.org/preprints/bg-2022-211/bg-2022-211.pdf

Example 5. Ongoing effort – using streamflow to learn precipitation bias

NLDAS (0.56) > Daymet (0.41) > Maurer (0.03)

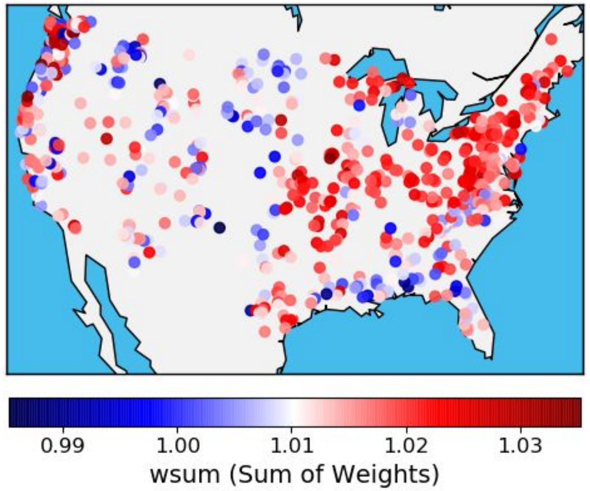






Simulation	Forcings	Median NSE	Median KGE	Low flow RMSE (mm/day)	ET correlation with MODS
LSTM	Daymet	0.747	0.720	0.249	-
Differentiable HBV with bias correction	Daymet	0.745	0.748	0.122	**0.82**
Multiforcing with bias correction	Daymet, Maurer, NLDAS	**0.770**	**0.780**	**0.082**	0.81

Low bias



Thank you!

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https://github.com/mhpi

http://water.engr.psu.edu/shen/hydroDL.html

CUAHSI cyberseminar series on BDML

WRR special issue on BDML

AGU Editor's review

Hydrol. Earth Syst. Sci., 22, 5639–5656, 2018
https://doi.org/10.5194/hess-22-5639-2018

Hydrology and Earth System Sciences

HESS Opinions: Incubating deep-learning-powered hydrologic science advances as a community

Chaopeng Shen[1], Eric Laloy[2], Amin Elshorbagy[3], Adrian Albert[4], Jerad Bales[5], Fi-John Chang[6], Sangram Ganguly[7], Kuo-Lin Hsu[8], Daniel Kifer[9], Zheng Fang[10], Kuai Fang[1], Dongfeng Li[10], Xiaodong Li[11], and Wen-Ping Tsai[1]

Water Resources Research

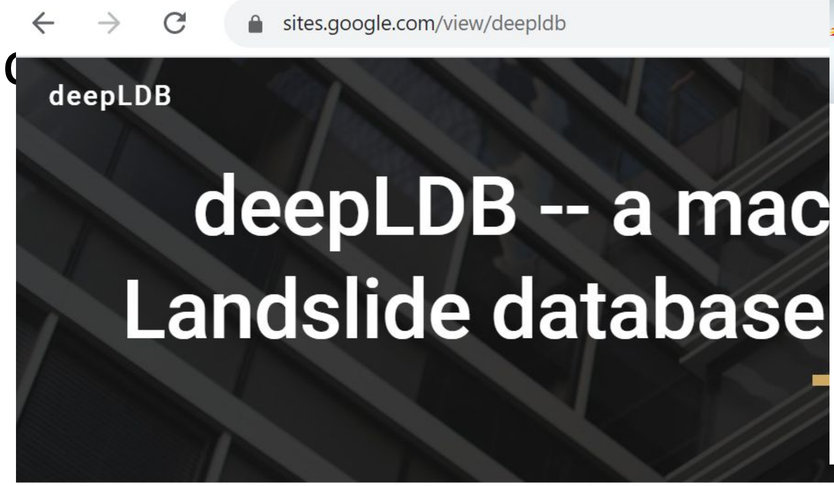
REVIEW ARTICLE
10.1029/2018WR022643

Special Section:
Big Data & Machine Learning in Water Sciences: Recent Progress and Their Use in Advancing Science

A Transdisciplinary Review of Deep Learning Research and Its Relevance for Water Resources Scientists

Chaopeng Shen[1]

[1]Civil and Environmental Engineering, Pennsylvania State University, University Park, PA, USA



nature COMMUNICATIONS

ARTICLE
https://doi.org/10.1038/s41467-021-26107-z OPEN
Check for updates

From calibration to parameter learning: Harnessing the scaling effects of big data in geoscientific modeling

Wen-Ping Tsai[1], Dapeng Feng[1], Ming Pan[2,3], Hylke Beck[4], Kathryn Lawson[1,5], Yuan Yang[6,7], Jiangtao Liu[1] & Chaopeng Shen[1,5]