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

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https://github.com/mhpi

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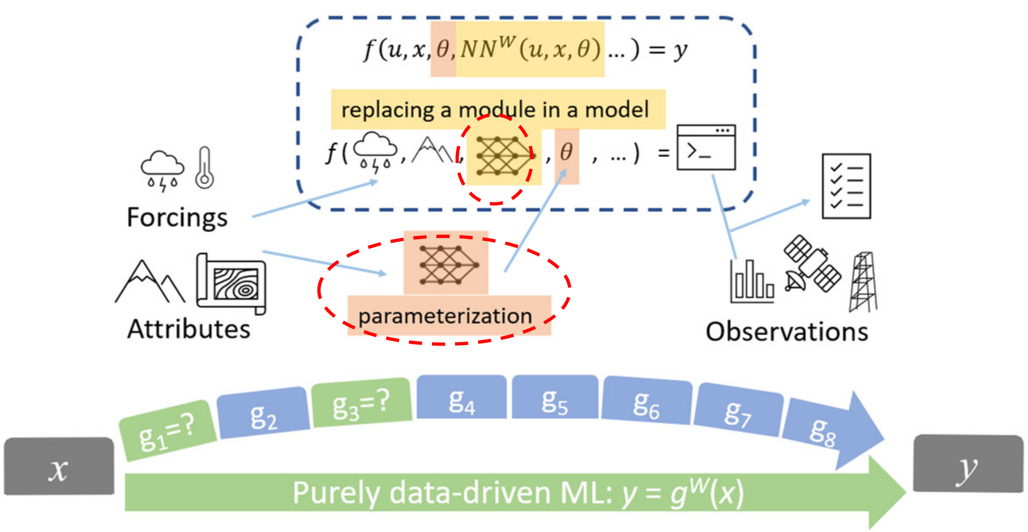
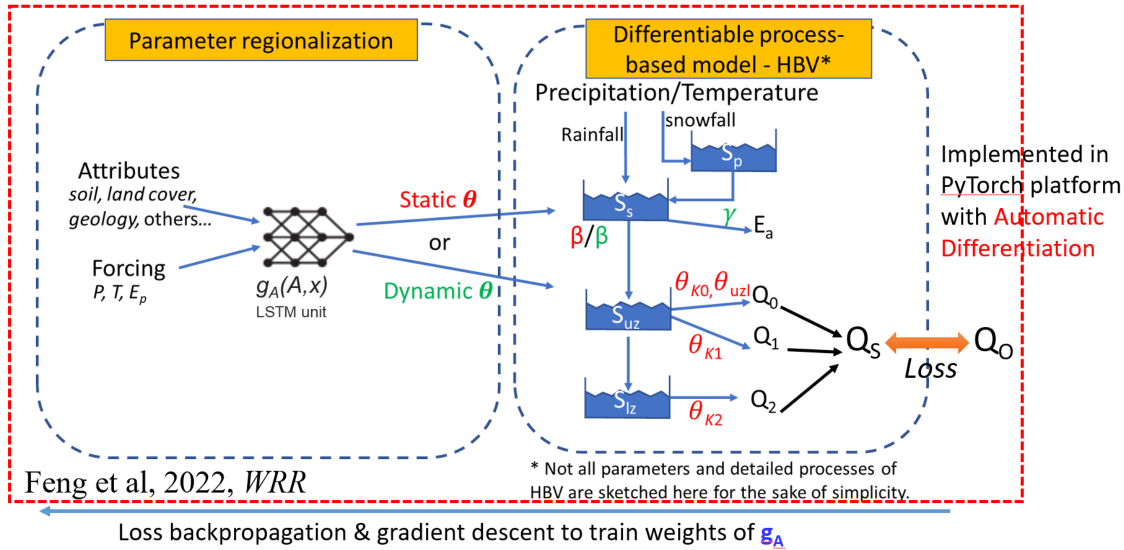
https://arxiv.org/abs/2301.04027

Differentiable Modeling in Geosciences



www.hydroml.org. HydroML Symposium Phase 2 in Berkeley. May 22-24 2023!

Example 3. differentiable, learnable models to learn functions



Evolve model structure

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

nature COMMUNICATIONS

ARTICLE

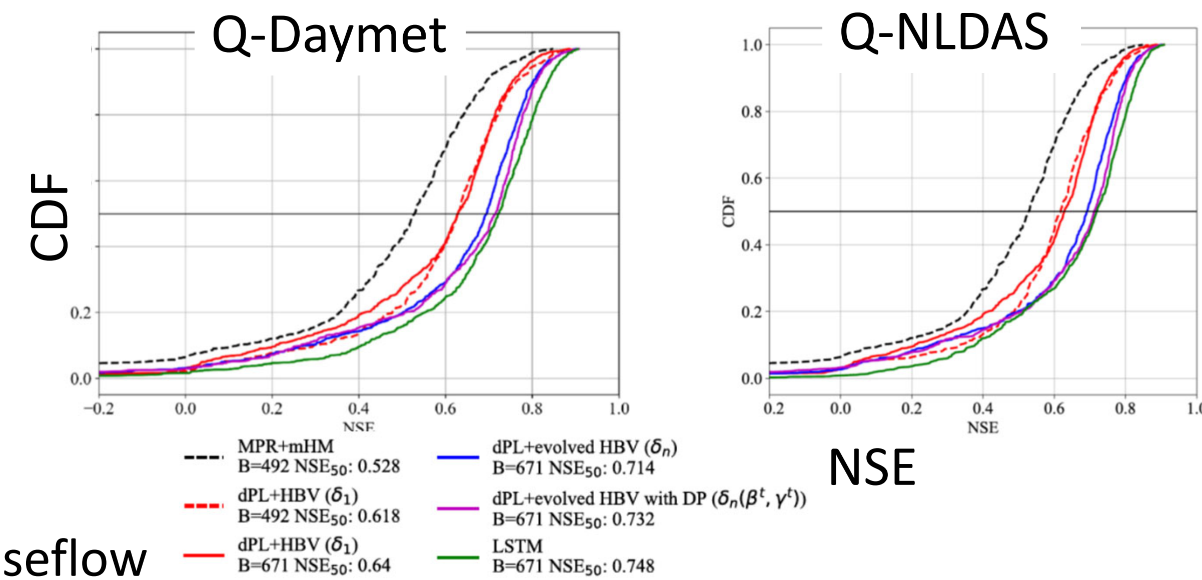
https://doi.org/10.1038/s41467-021-26107-z OPEN

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

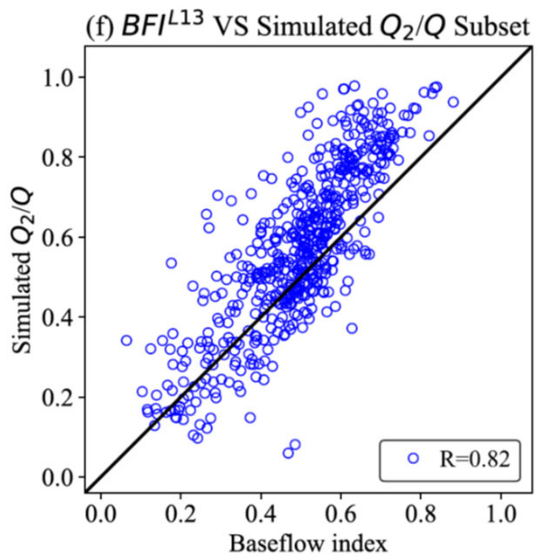
Wen-Ping Tsai[1], Dapeng Feng[1], Ming Pan[2,3], Hylke Beck[4], Kathryn Lawson[1,5], Yuan Yang[6,7], Jiangtao Liu[1] & Chaopeng Shen[1,5]

Approaching LSTM!
But....

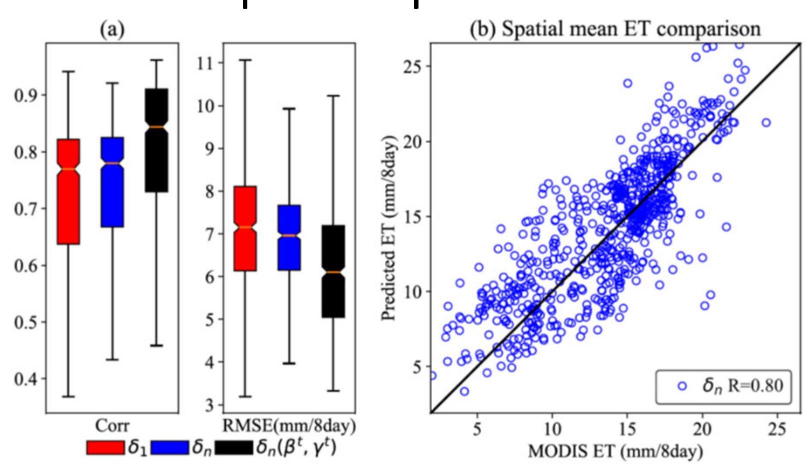
- Output untrained variables.
- Multivariate constraints.
- It extrapolates better.
- It can help us answer questions!

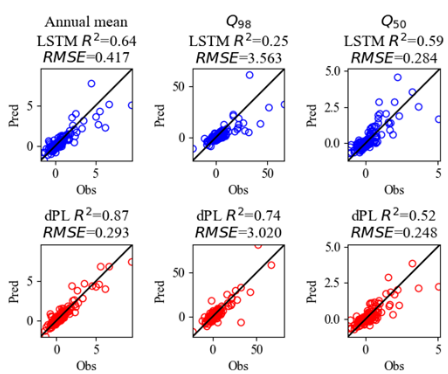


Baseflow



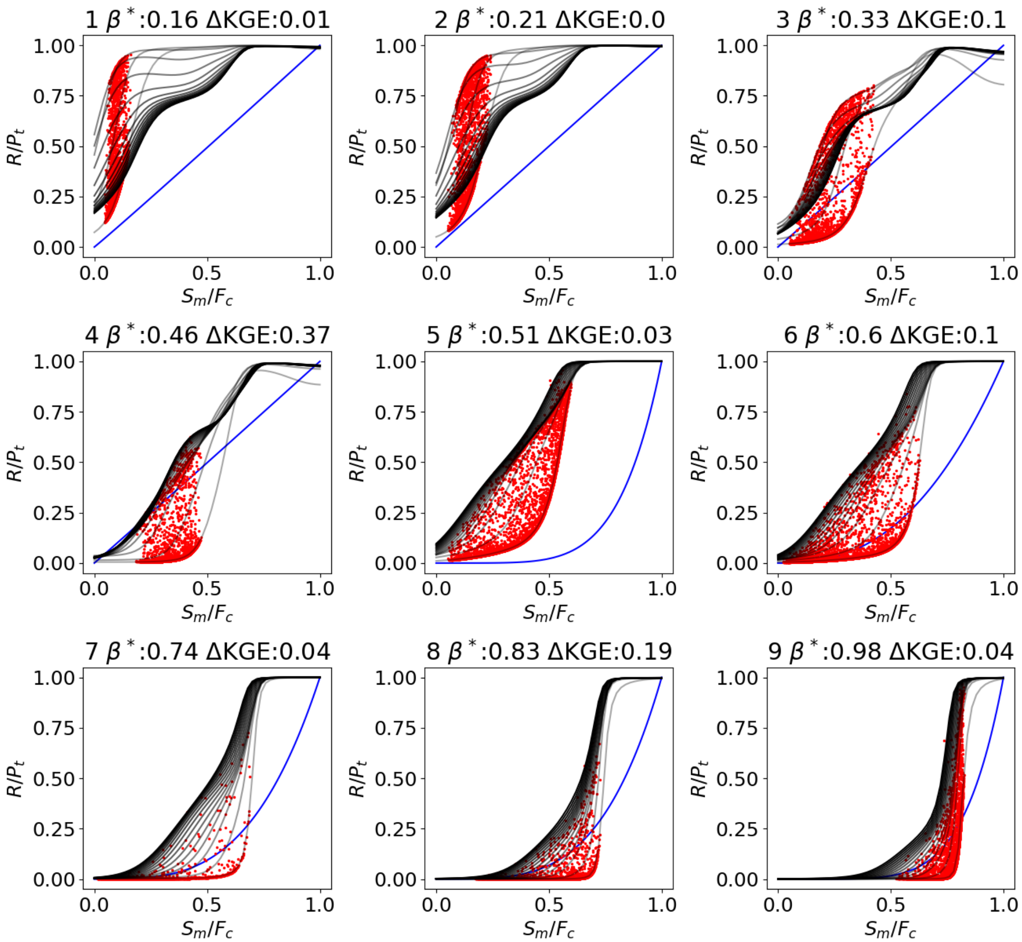
Evapotranspiration





https://hess.copernicus.org/preprints/hess-2022-245/

What the ANN learned functions look like?



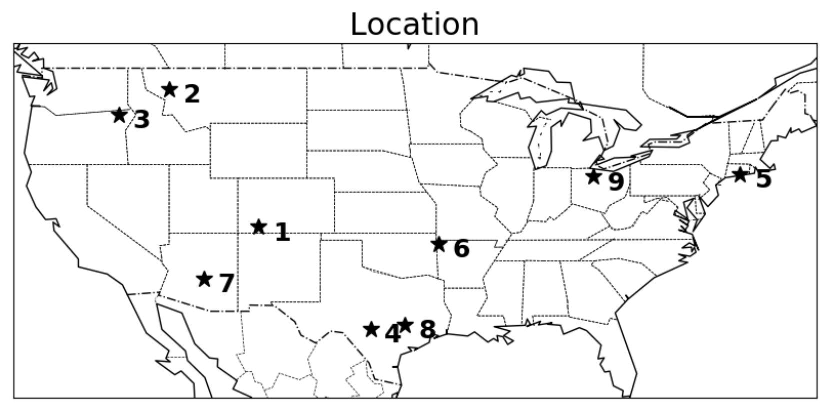
$$R/P_t = (S_m/F_c)^{\beta}$$

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

Blue line: original power law relation

Red dots: ANN simulations

Black lines: continuous plotting of ANN functions



Thank you!

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Hydroml.org
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

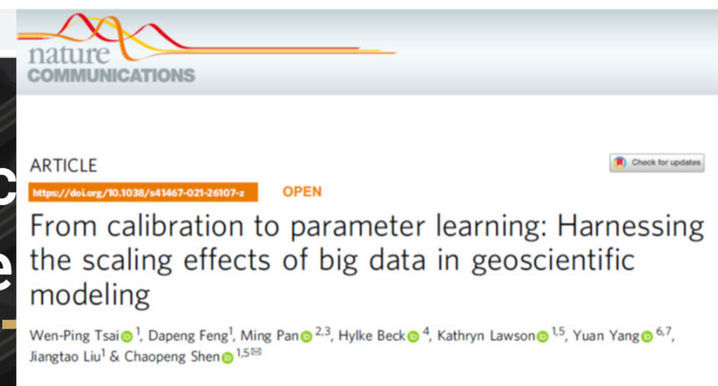
REVIEW ARTICLE
10.1029/2018WR022643

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]

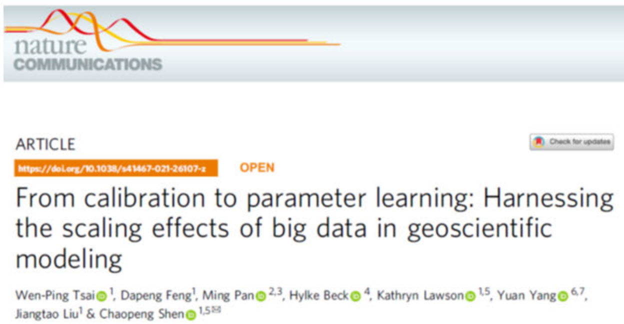
[1]Civil and Environmental Engineering, Pennsylvania State University, University Park, PA, USA


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

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]

Differentiable parameter learning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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

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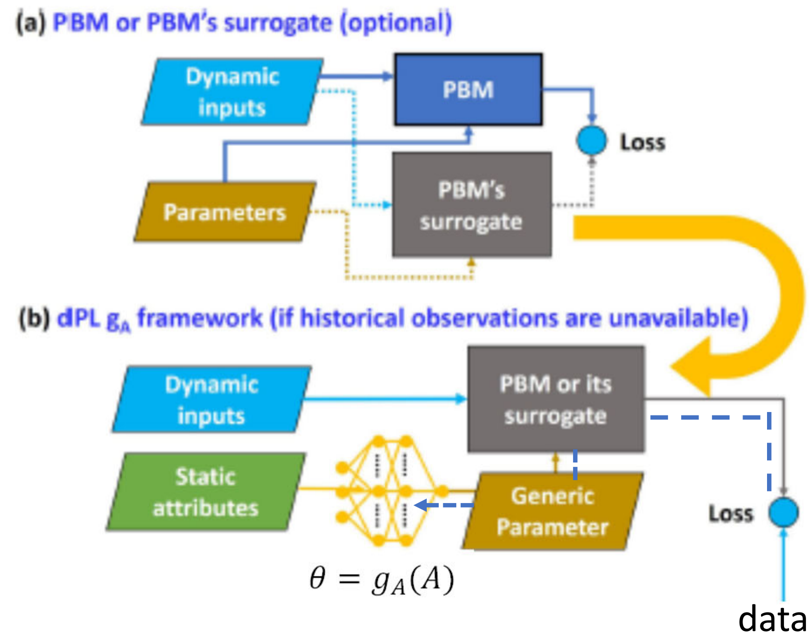
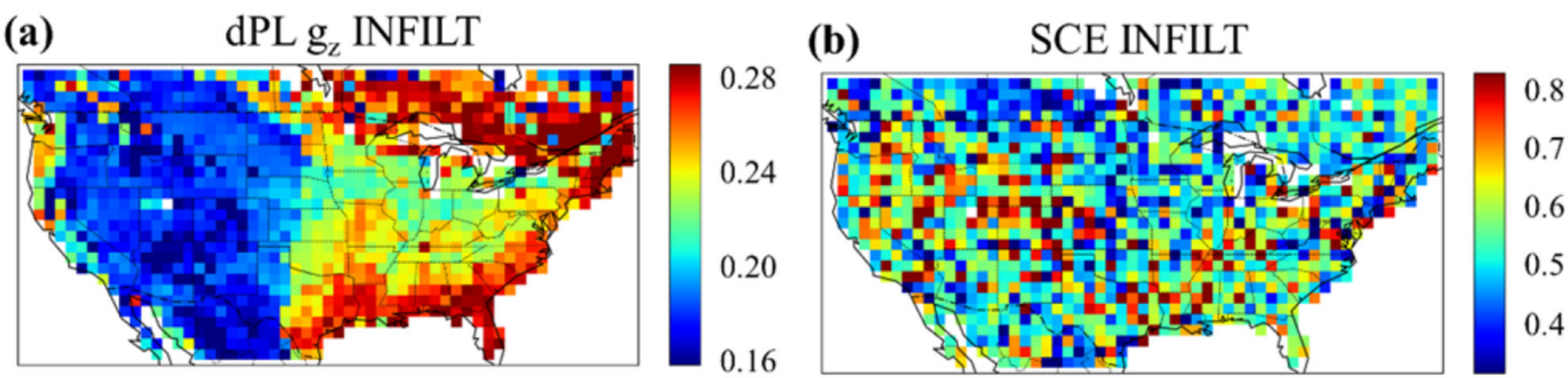




Point #1. Data scaling relationships (network effect?)

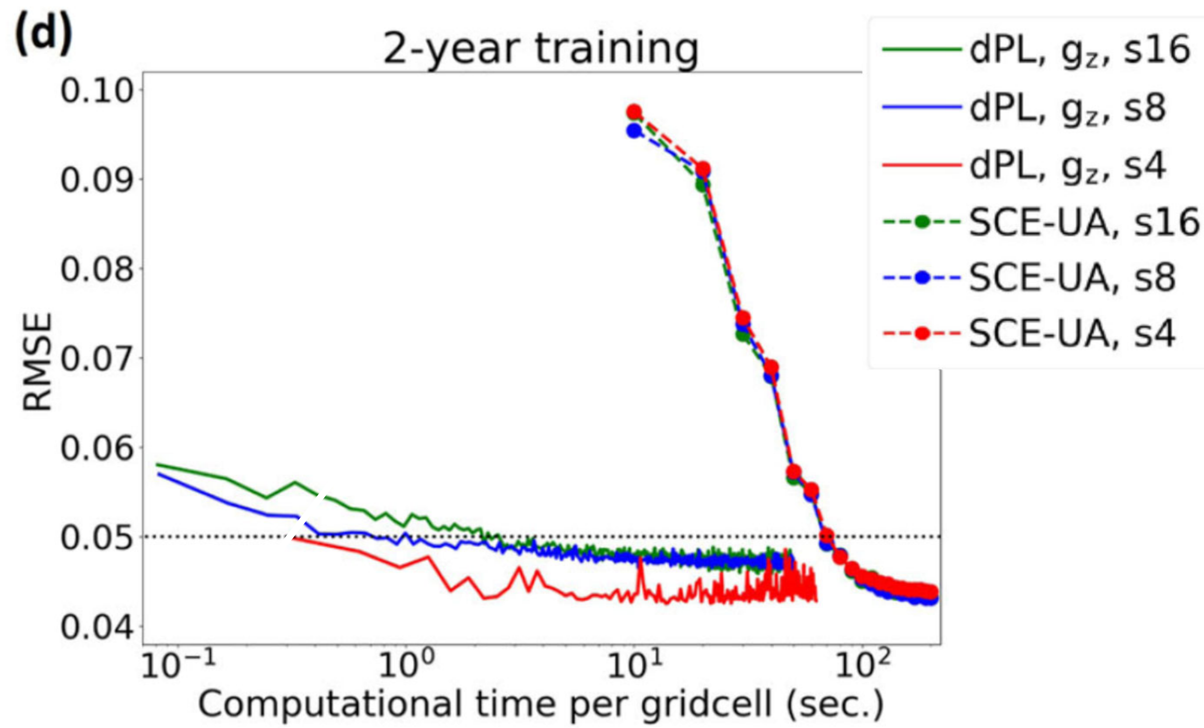
1. dPL = SCEUA for lowest RMSE

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!

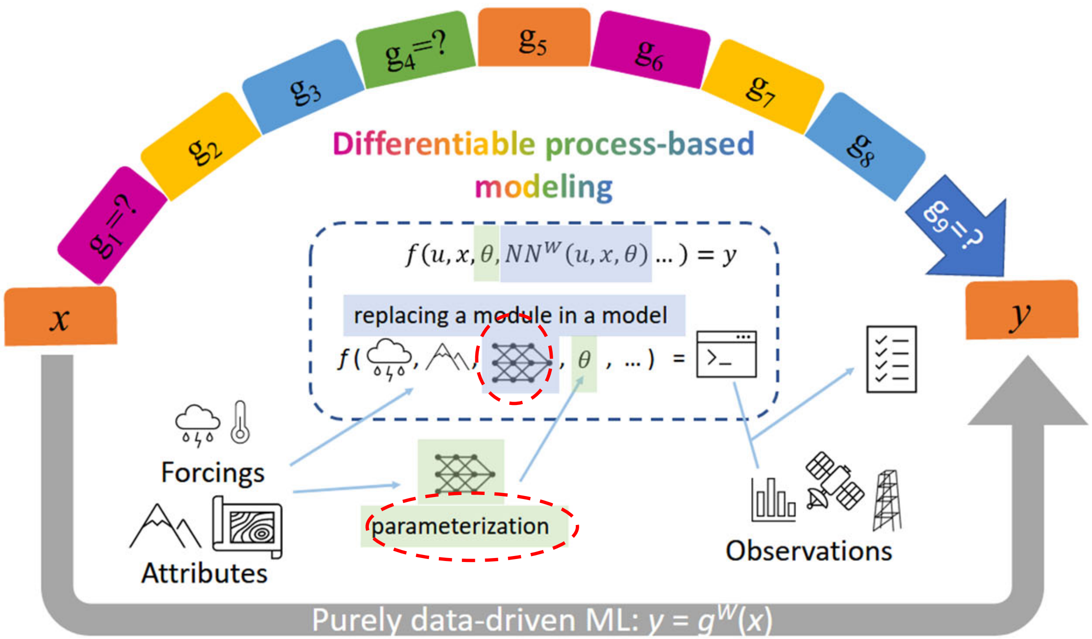
Relies on differentiable programming!



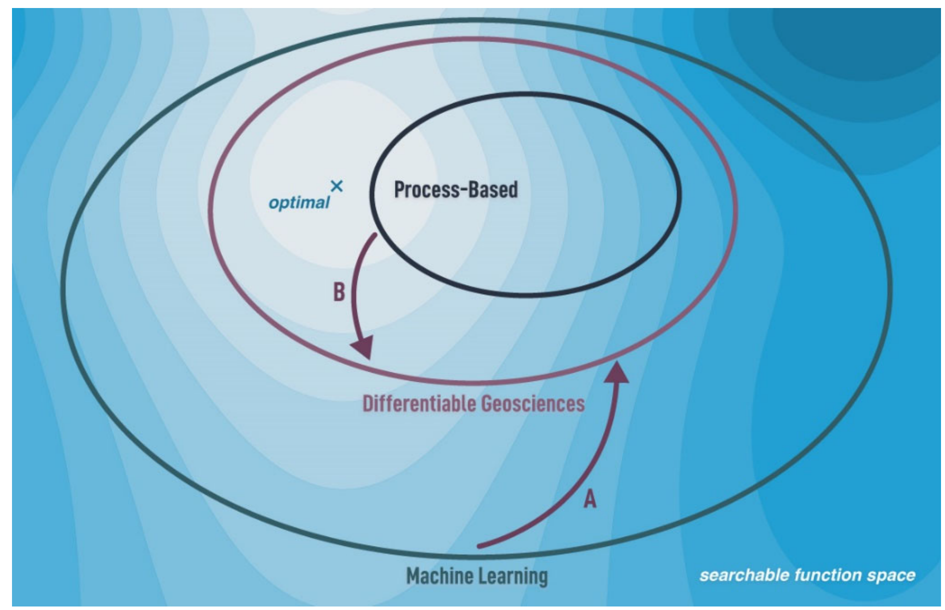
Tsai et al. 2021, Nature Communications

What is Differentiable Geoscientific Modeling (DG)?

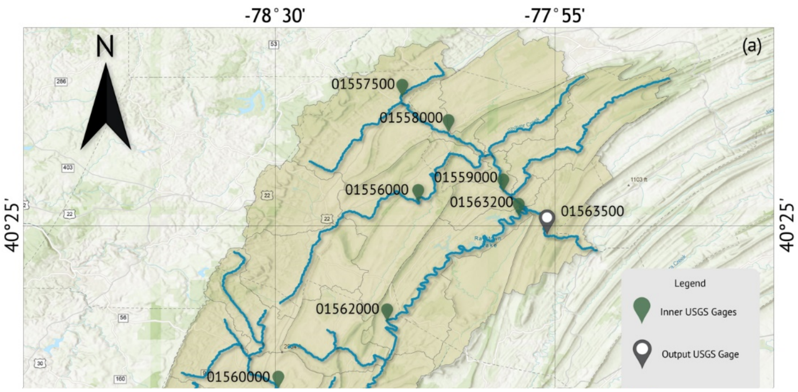
Inserting “?” anywhere

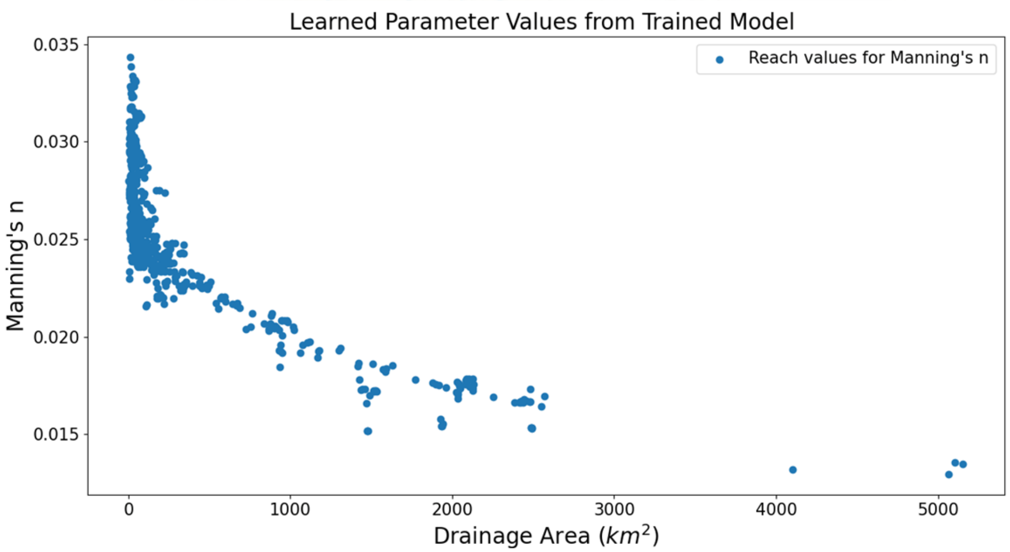


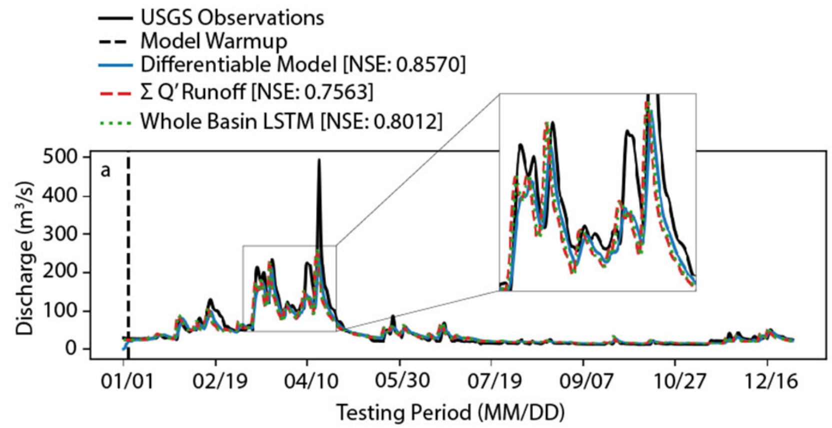
2 perspectives

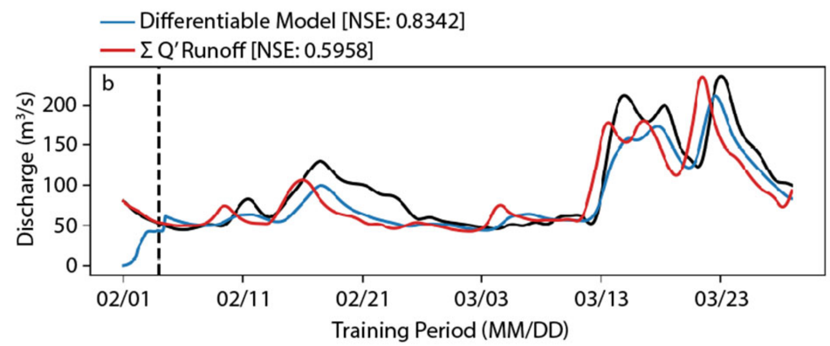


Example 2. River graph







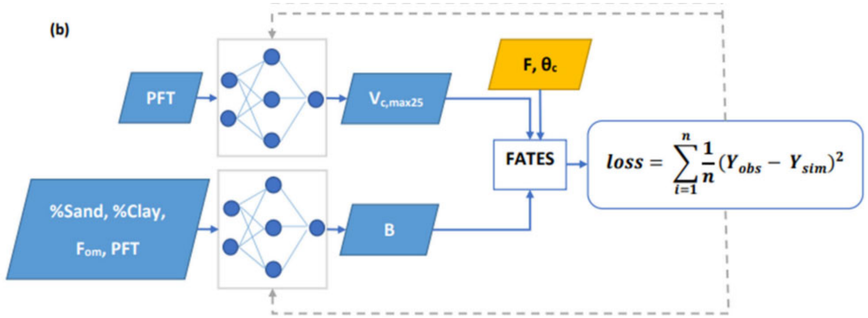


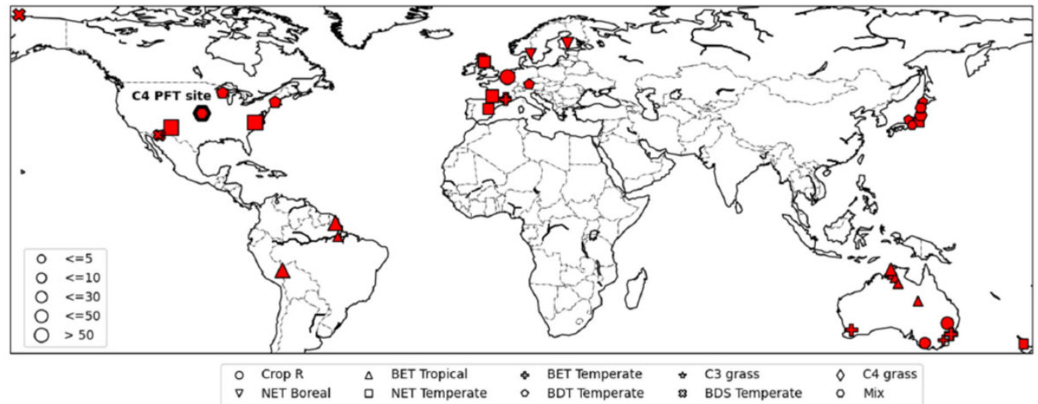
Learn physics on the river graph

https://doi.org/10.1002/essoar.10512512.1

Example 3. Ecosystem modeling (photosynthesis)

(b)

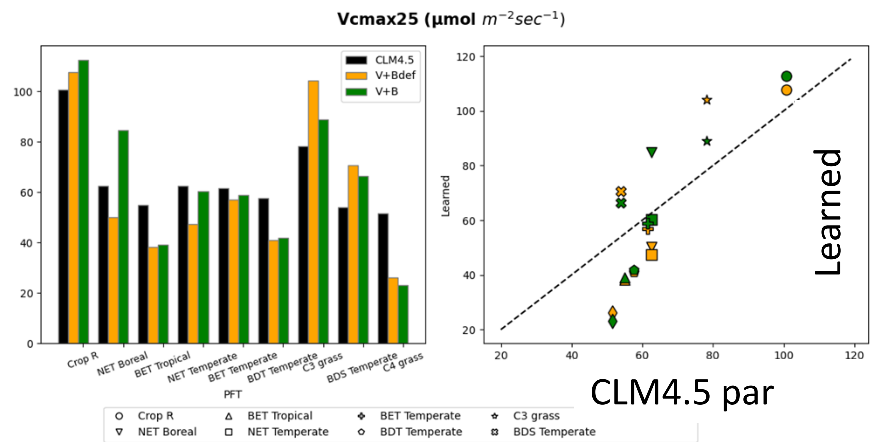




(a) Temporal holdout test for the following system

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*



Ecosystem modeling – DoE SC0021979

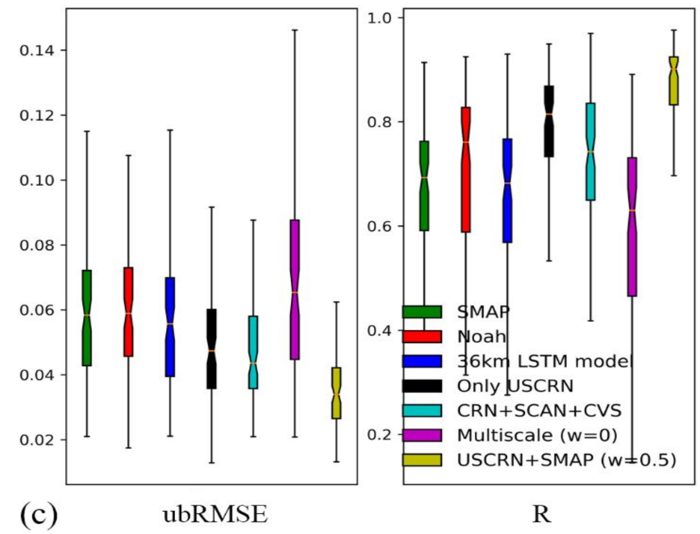
https://bg.copernicus.org/preprints/bg-2022-211/bg-2022-211.pdf

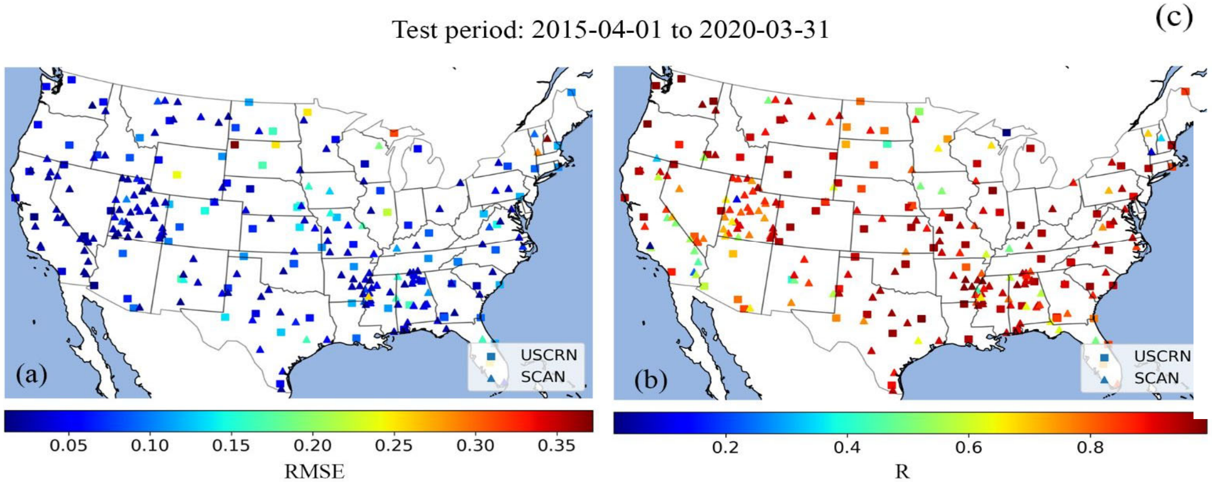
Example 4. Multiscale soil moisture – learning from two teachers

High-res sim - - - - - In-situ data

Coarsen ↓

Low-res sim - - - - - Satellite data





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