

Rapid emulation of a physics-based hydrology simulator with knowledge guided deep learning models

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PRINCETON
UNIVERSITY



HydroGEN



Climate change is hitting the Colorado River 'incredibly fast and incredibly hard'

The warming climate is intensifying drought, contributing to fires and drying out the river's headwaters, sending consequences cascading downstream.

Ian James, Arizona Republic

Published 7:37 AM MST Jan. 1, 2021 | Updated 9:30 AM MST Jan. 8, 2021



The Water Wars that Defined the American West Are Heading East

Urban growth and surge in irrigation fuel fight between Georgia and Florida; soybeans or oysters?

Groundwater is critical to understanding and simulating changing watersheds

NAS

Global models underestimate large decadal declining and rising water storage trends relative to GRACE satellite data

Bridget R. Scanlon^{a,1}, Zizhan Zhang^b, Himanshu Save^c, Alexander Y. Sun^a, Hannes Müller Schmied^{d,e}, Ludovicus P. H. van Beek^f, David N. Wiese^g, Yoshihide Wada^{f,h}, Di Longⁱ, Robert C. Reedy^a, Laurent Longuevergne^j, Petra Döll^{d,e}, and



PNAS PLUS

LETTER

<https://doi.org/10.1073/pnas.18-04244>

Sensitivity of atmospheric CO₂ growth rate to observed changes in terrestrial water storage

Vincent Humphrey^{1*}, Jakob Zscheischler¹, Philippe Ciais², Lukas Gudasz³,

LETTER

[doi:10.1038/nature20780](https://doi.org/10.1038/nature20780)

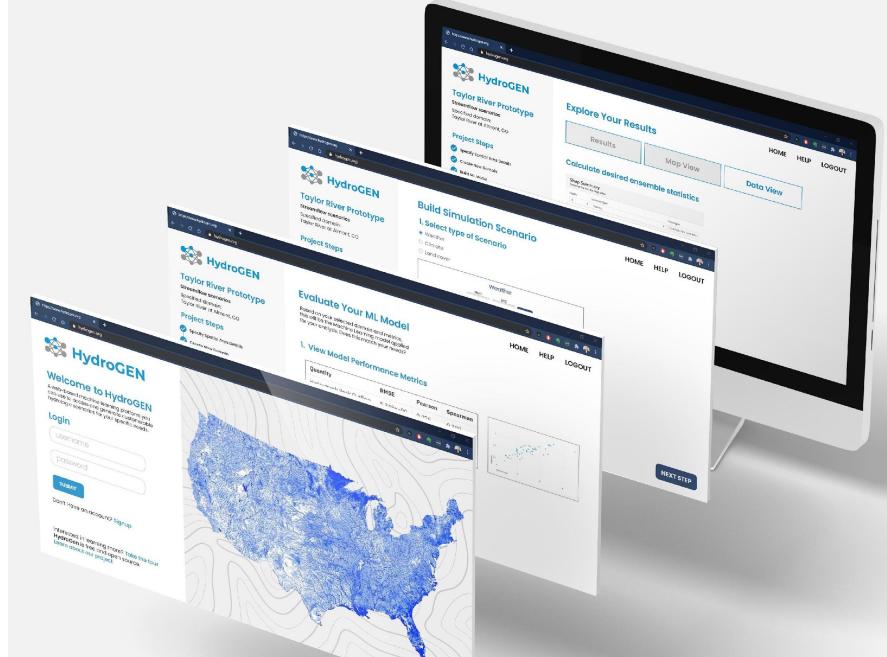
Compensatory water effects link yearly global land CO₂ sink changes to temperature

Martin Jungcl, Markus Reichstein^{1,2}, Christopher P. Schulze³, Chris Huntingford⁴, Stephen Sitch⁵, Anders Ahlström^{6,7}



HydroGEN

HydroGEN is a web-based platform that allows users to generate **seasonal forecasts** of watershed conditions **on demand**



We are a very interdisciplinary team across academia, industry, and government agencies



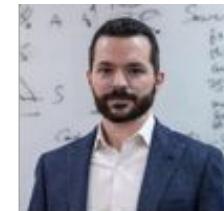
Hydrologists



Laura
Condon
Arizona



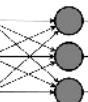
Reed Maxwell
Princeton



Peter Melchior
Princeton



Nirav Merchant
CyVERSE



ML Experts



Data Scientists



Elena
Leonarduzzi
Princeton



Hoang Tran
PNNL



Ben Horowitz
Princeton



Software Engineers

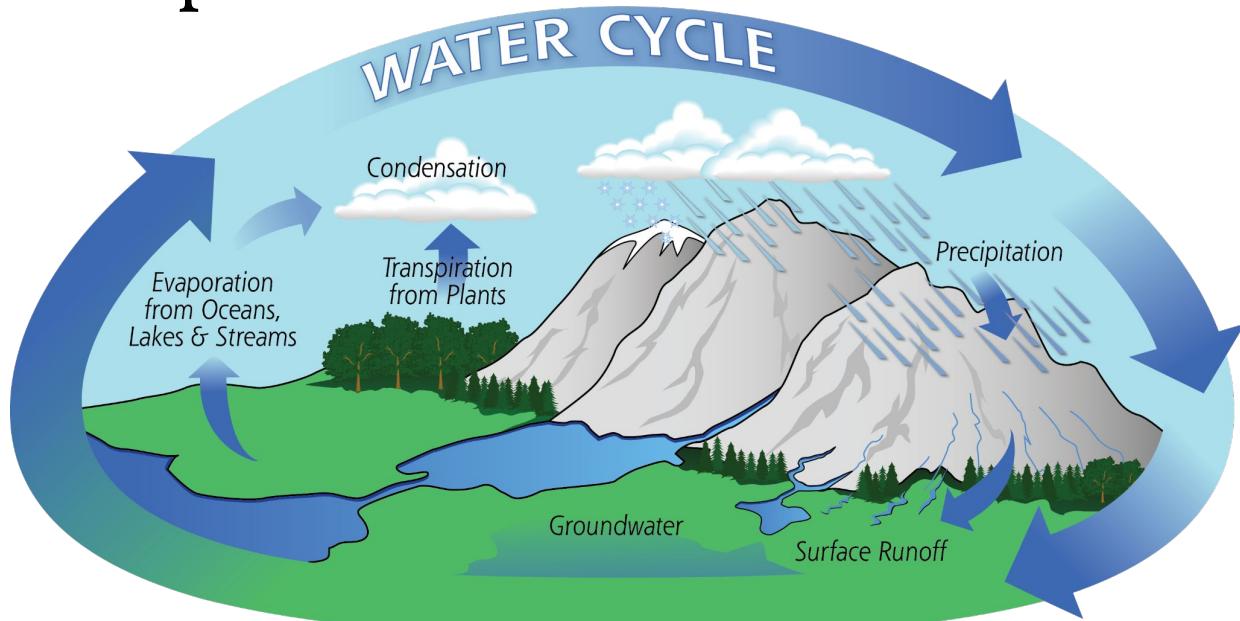


User Experience Specialists



Lindsay Bearup
Bureau of
Reclamation

Our goal is to jointly predict all major components of the terrestrial hydrologic cycle in a fully explicit spatiotemporal framework



This leads to an inherent tension:

Spatially-distributed and multi-process
implies process based models

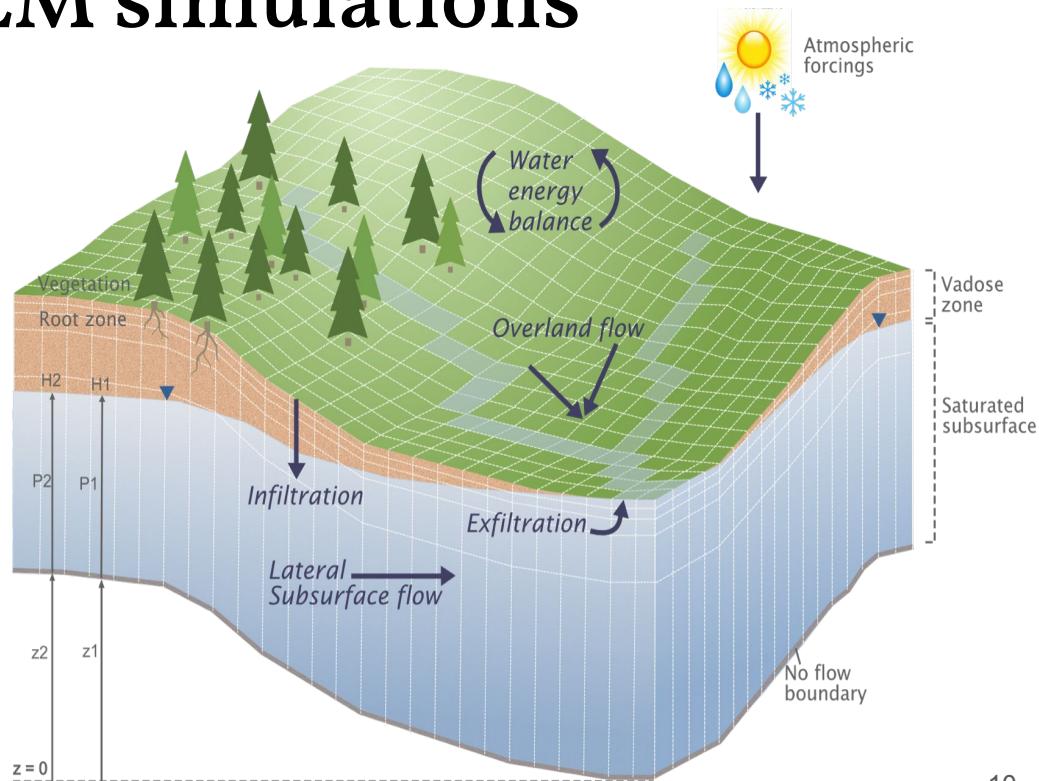
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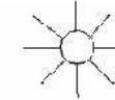
But speed, flexibility, and predictive skill
points toward data driven models

We developed an emulator based on coupled ParFlow-CLM simulations

- Unique national simulations that extend from the bedrock to the top of the treetops
- Solving physical equations for water and energy fluxes
- High resolution (1km)
- **Computationally expensive**

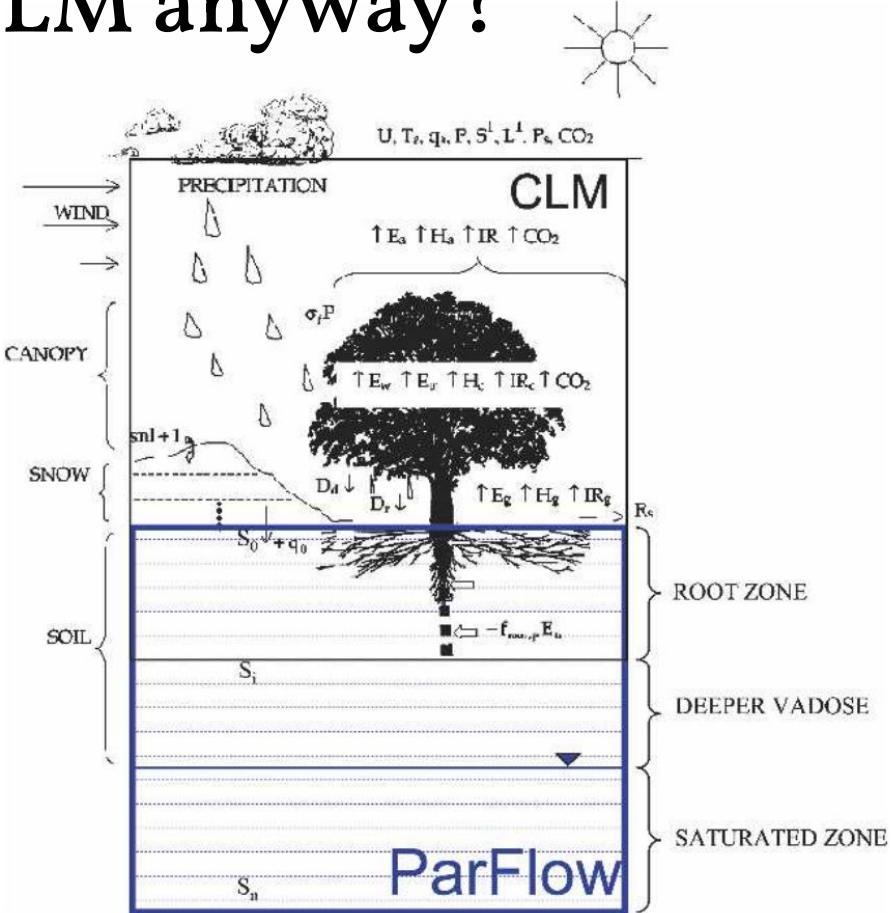


But what is ParFlow-CLM anyway?

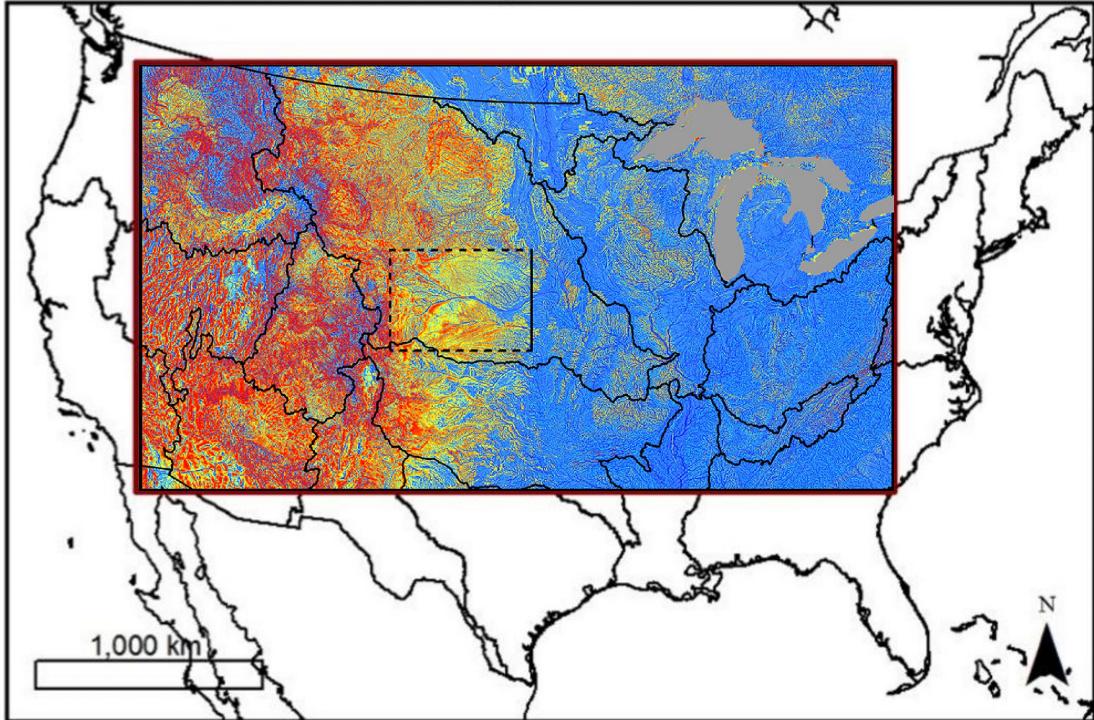


CLM is a model of
the land surface

ParFlow is a model
of the subsurface

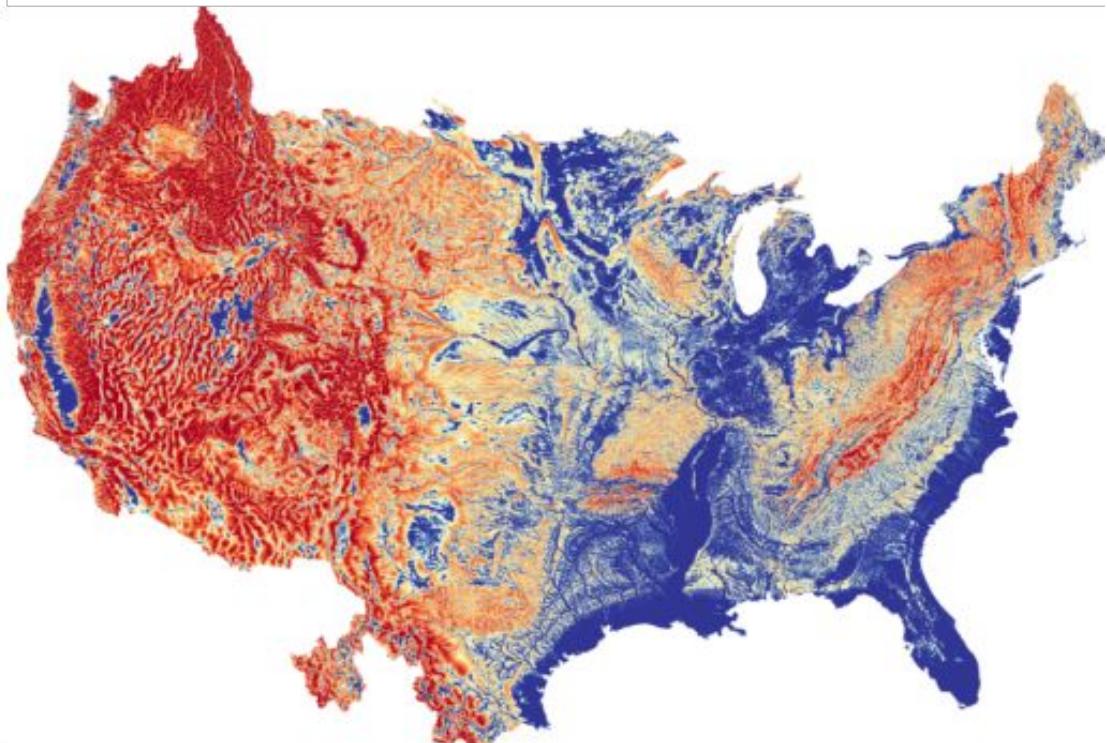


Our current
model domain
covers the
majority of the
Continental
United States

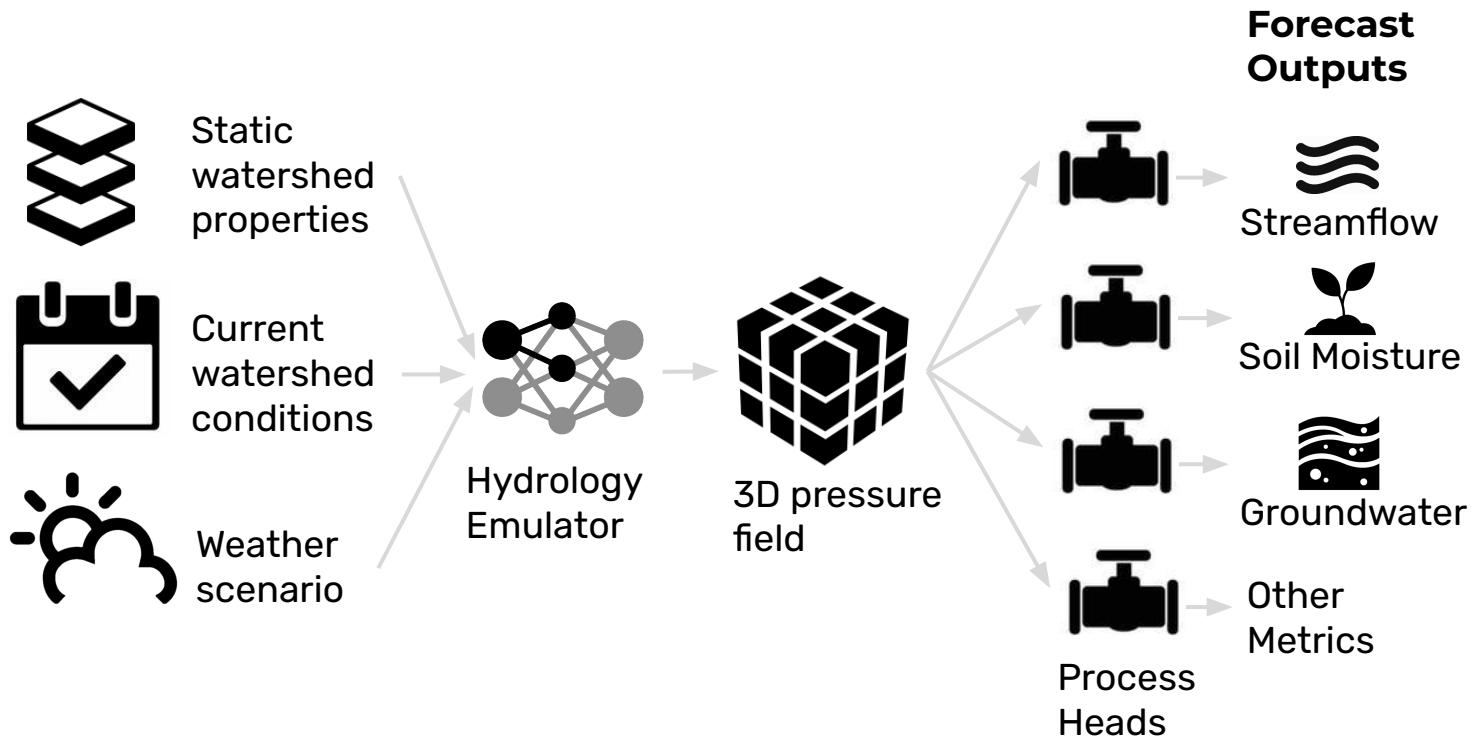


Maxwell, R. M., Condon, L. E., & Kollet, S. J. (2015). A high-resolution simulation of groundwater and surface water over most of the continental US with the integrated hydrologic model ParFlow v3. *Geoscientific Model Development*, 8(3), 923–937.
<https://doi.org/10.5194/gmd-8-923-2015>

We will be expanding
to the full contiguous
US soon!



Our machine learning approach for forecast generation

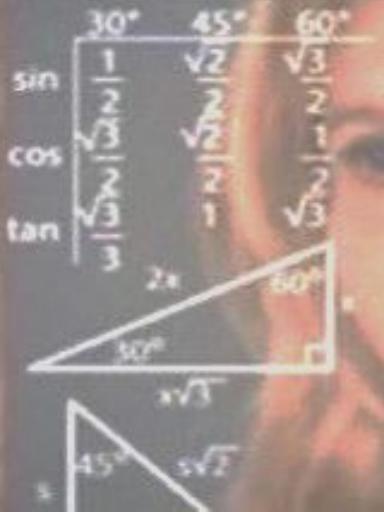
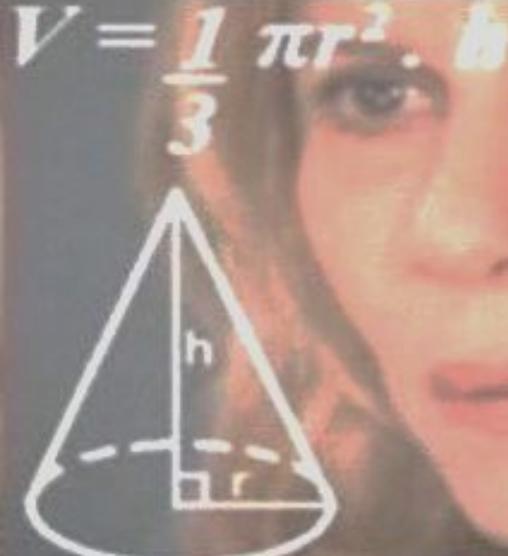


$$y = ax^2 + bx + c$$

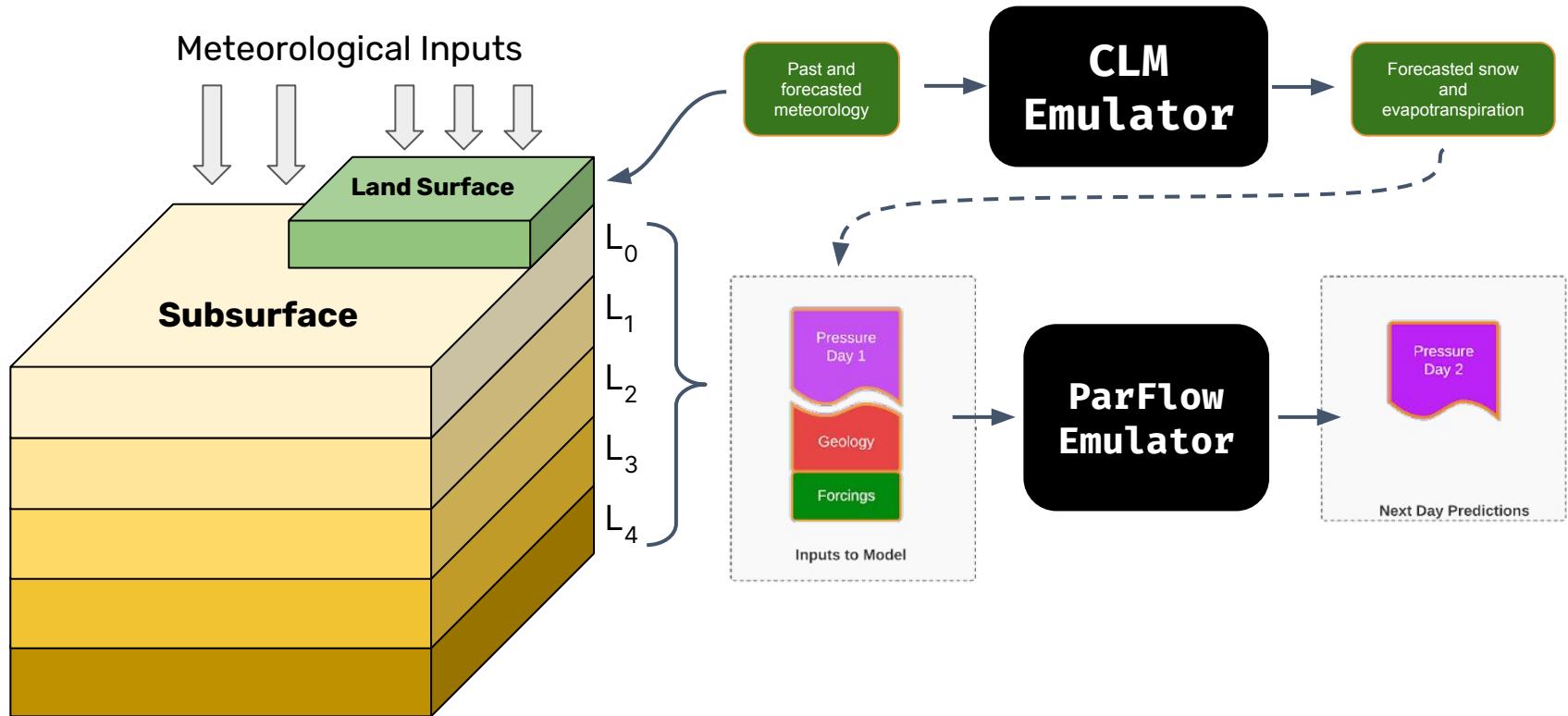
$$(x_1, x_2) = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$\Delta = \sqrt{b^2 - 4ac}$$

Methods



The emulator approach



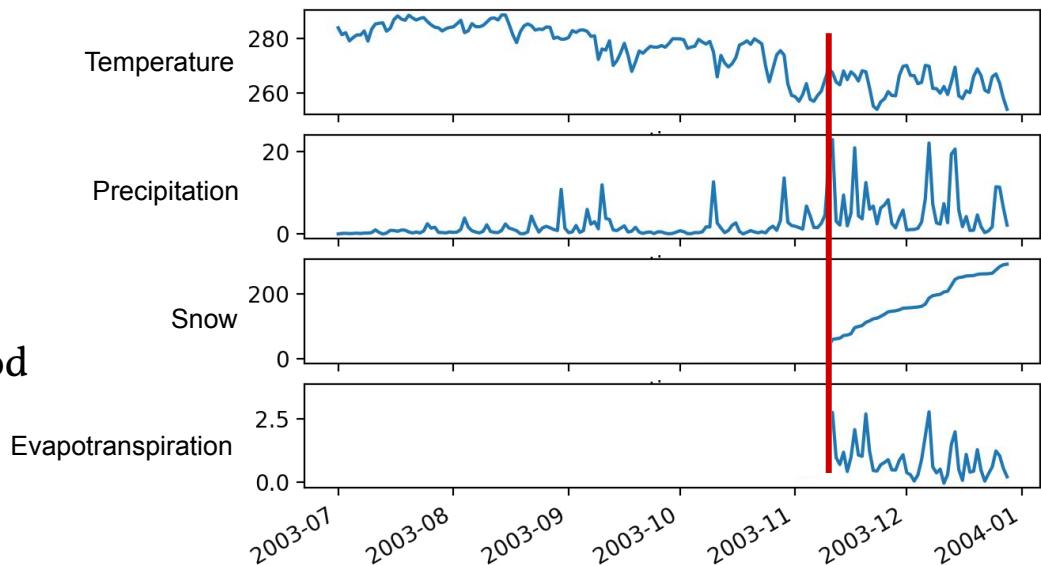
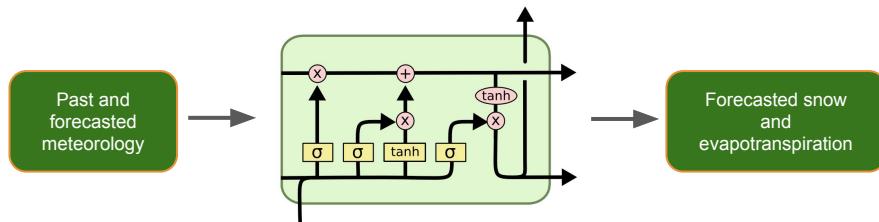
The land surface component is an LSTM

Pretty simple architecture, just a couple LSTM layers with about 256 nodes

Inputs (lookback 180 days) are:

- Max temp
- Min temp
- Precipitation
- Shortwave radiation
- Topographic index

Outputs are SWE and ET for last 60 (configurable) days of the input period



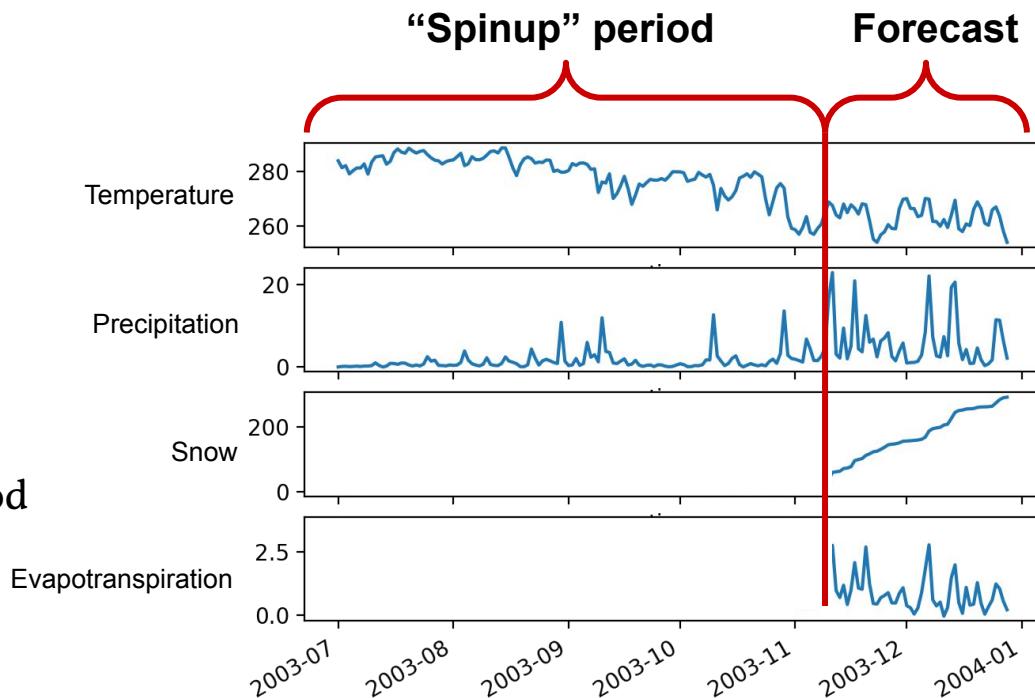
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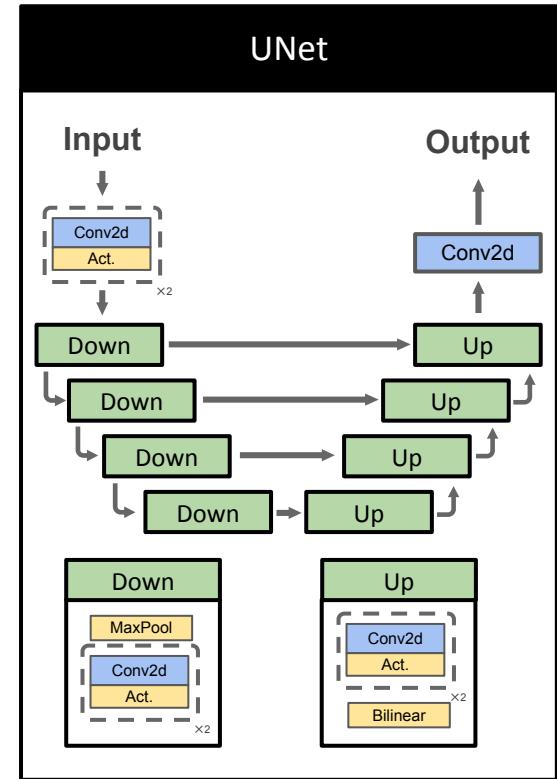
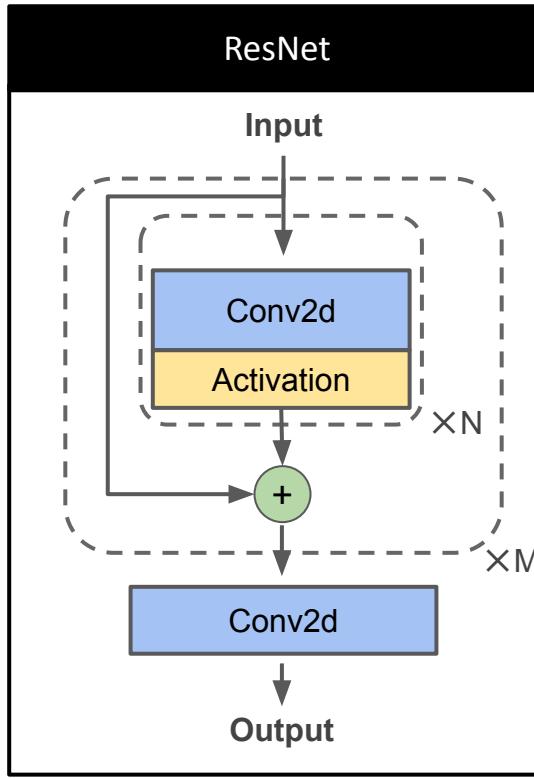
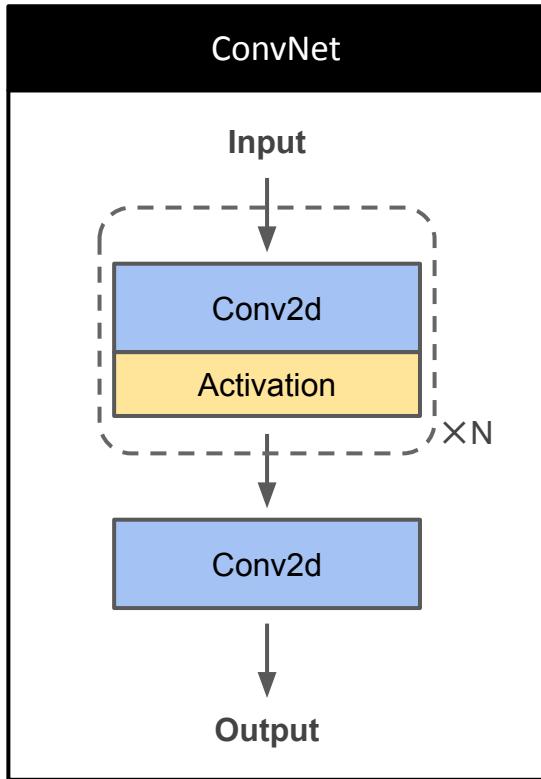
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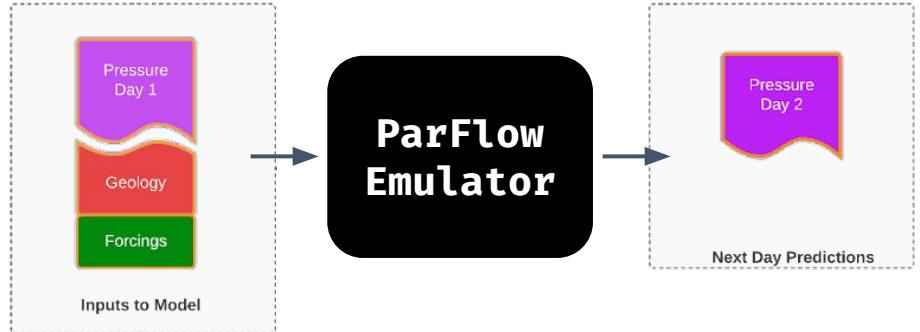
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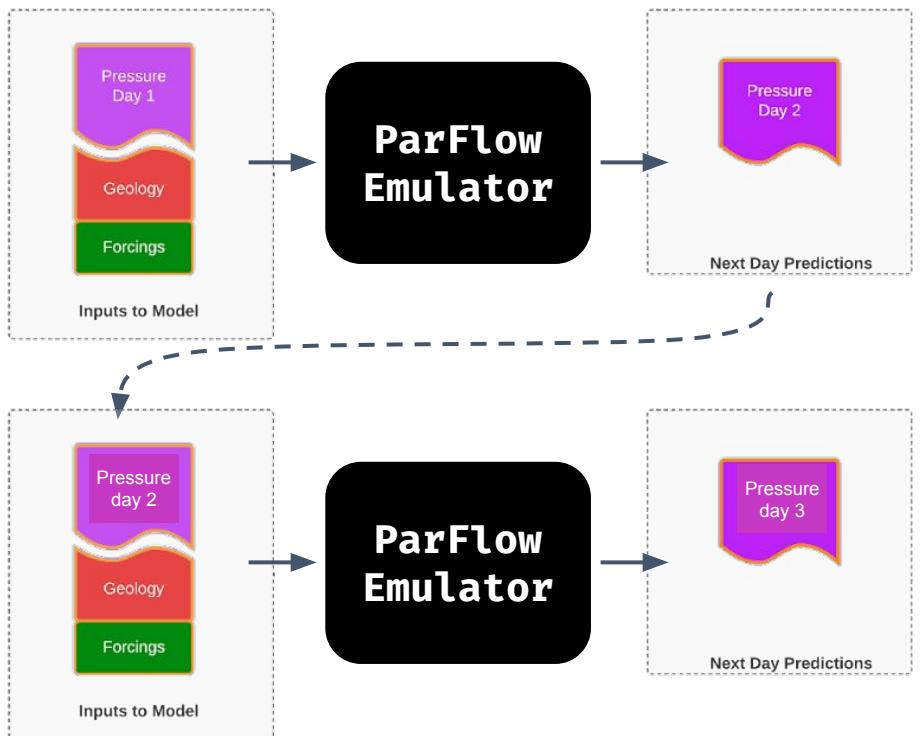
We have multiple architectures for the ParFlow emulator piece



To train the ParFlow emulator we unroll in time

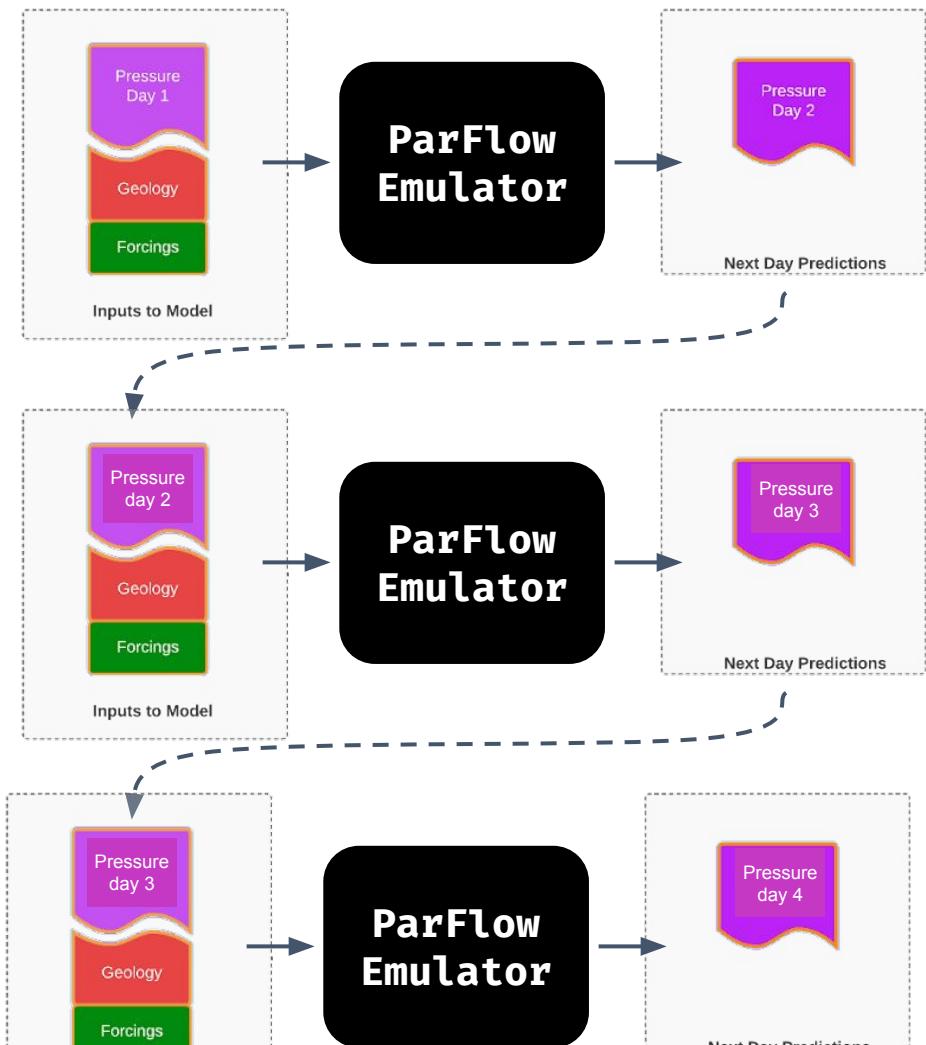


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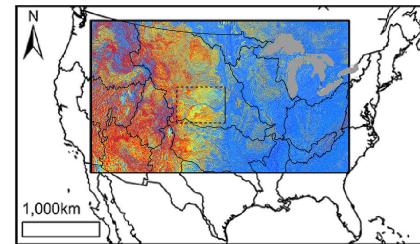
To train the ParFlow emulator we unroll in time

During training we increase the rollout, usually to ~30 days



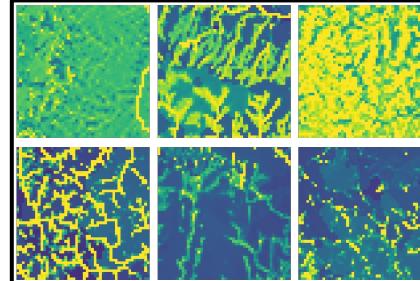
The training data is sampled patch-wise from the full domain

Raw data from Parflow-CLM



- 1 Read full data catalogue
- 2 Sample from geographies
- 3 Extract & prepare features

Machine learning ready data

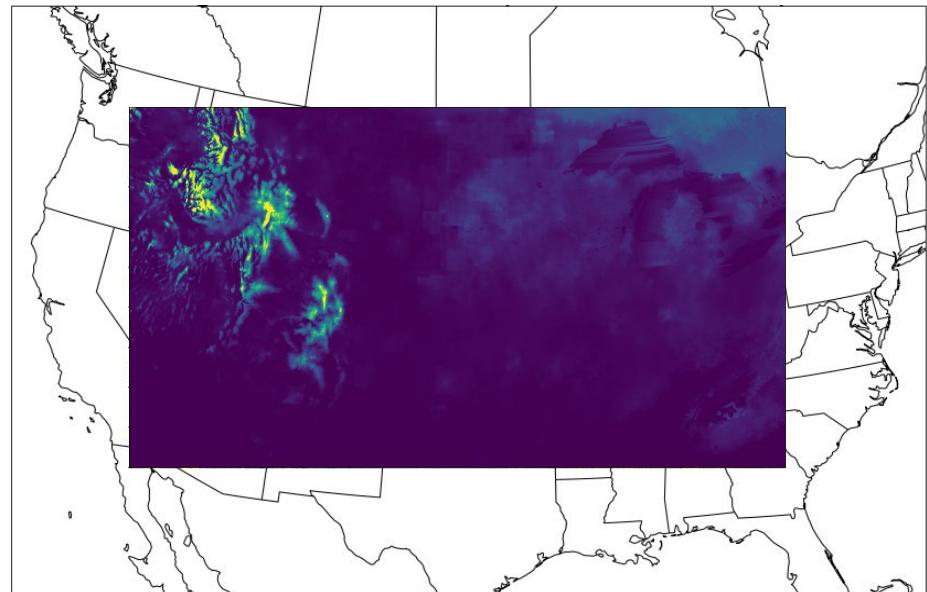


**Some
brief results**

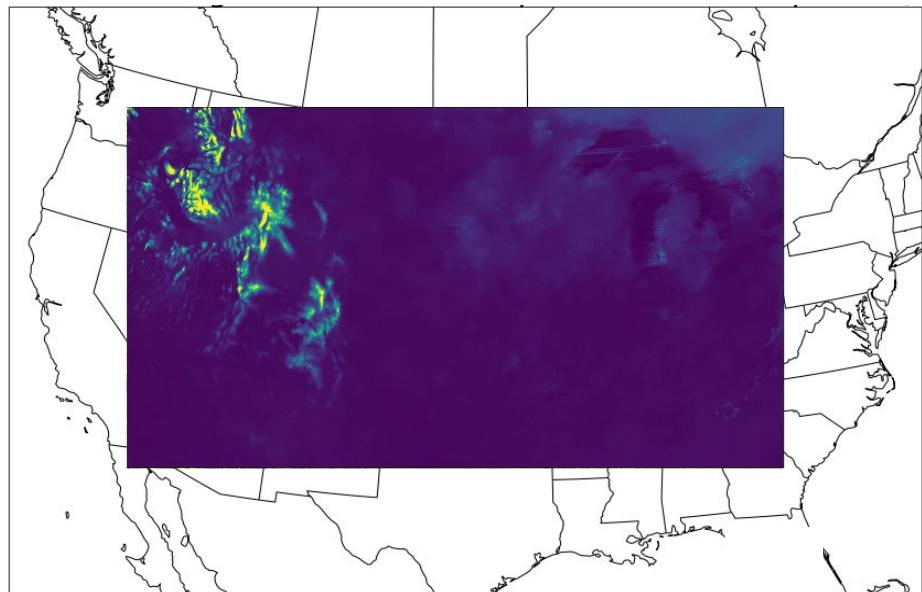


We're able to match snow patterns generally

Parflow-CLM



Emulator

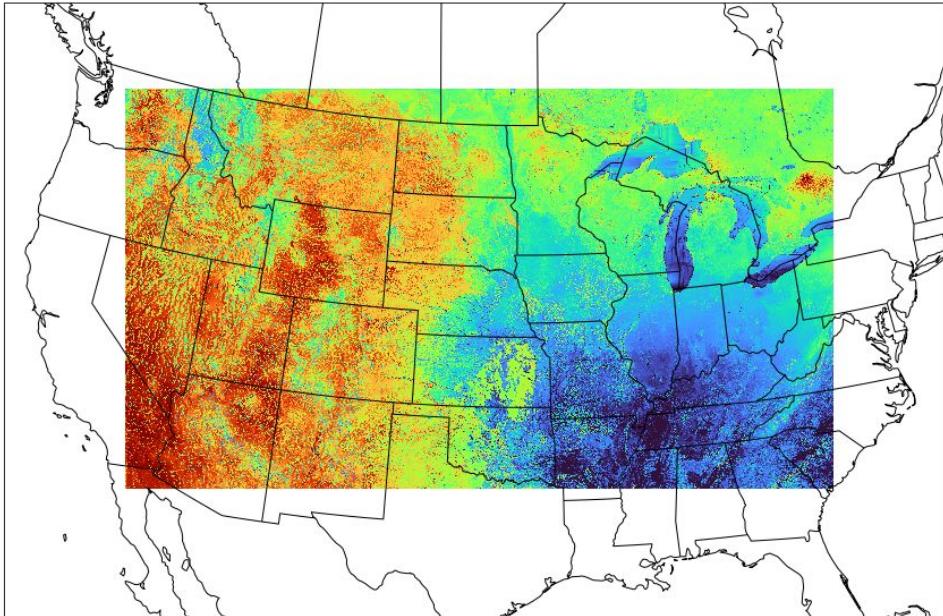


SWE [mm]

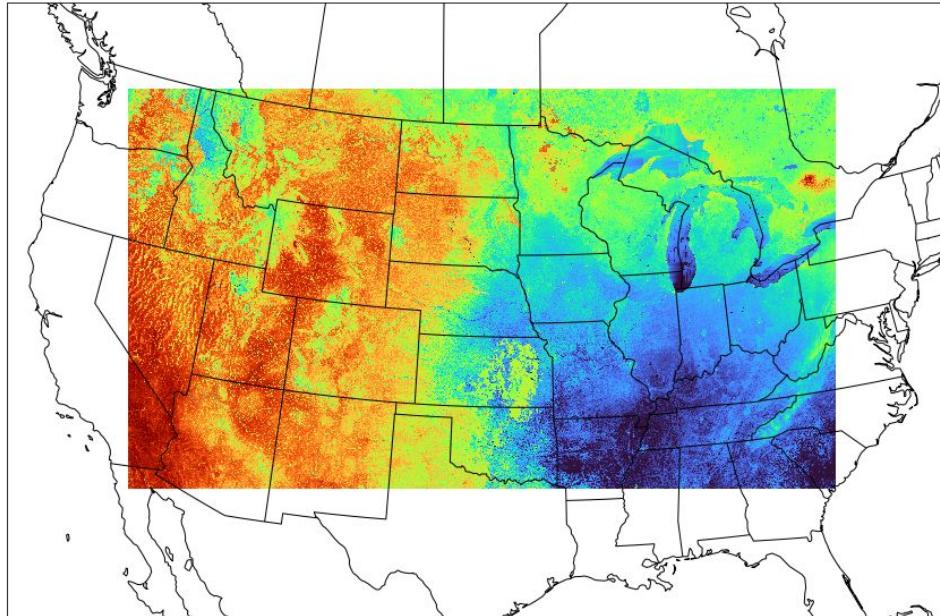


Same for ET, largely

Mean ET from ParFlow-CLM

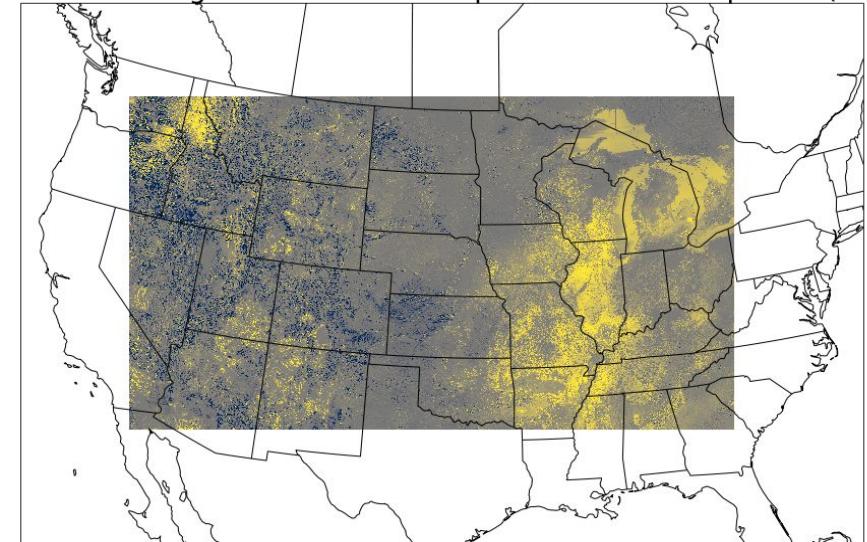


Mean ET from emulator

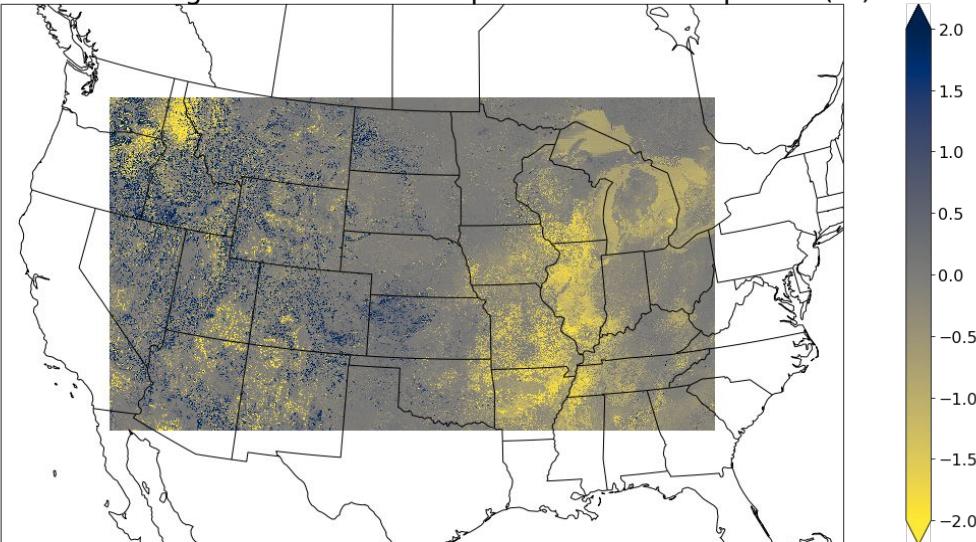


Emulator shows promising performance across the Continental US (CONUS)

Parflow change in water table depth over forecast period (m)

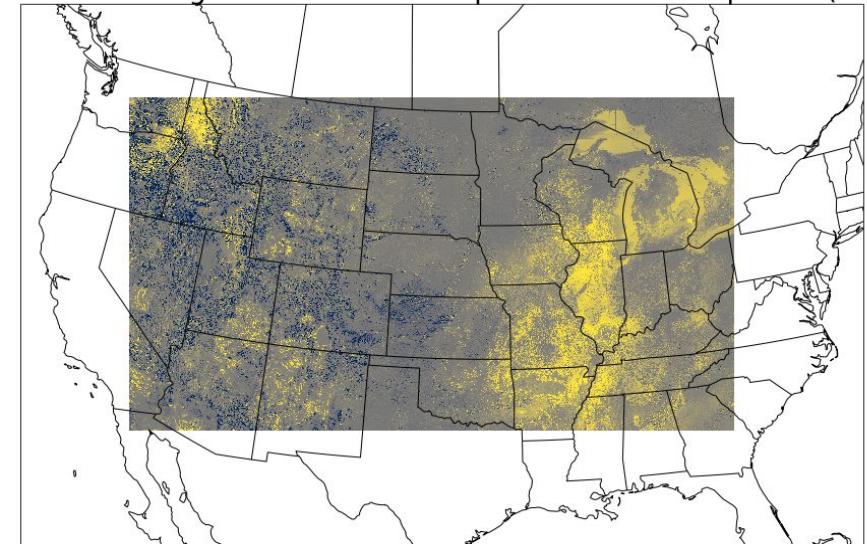


Emulated change in water table depth over forecast period (m)

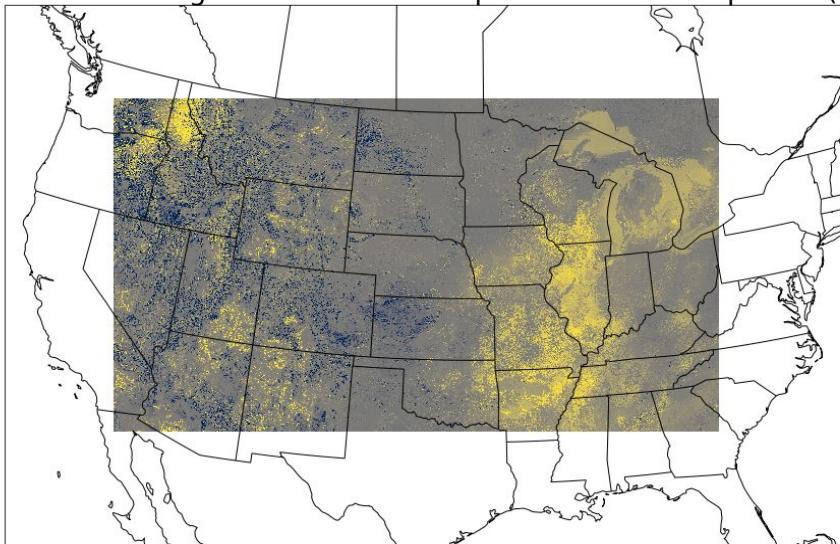


We get good performance in the subsurface generally too

Parflow change in water table depth over forecast period (m)



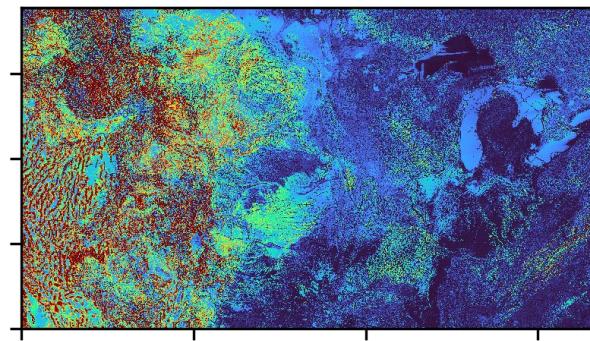
Emulated change in water table depth over forecast period (m)



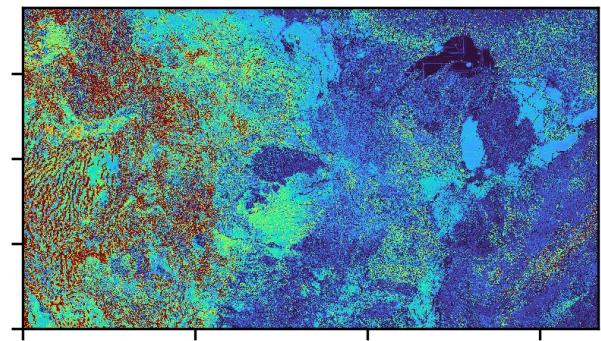
- 90 day forecast takes ~10 minutes on 1 GPU
- >50x speedup vs Parflow on 1,000 cores
- Saturation, water table depth and streamflow calculated by process heads off the simulated pressure field

Model architectures
have different
performance
characteristics, but
generally all capture
broad patterns

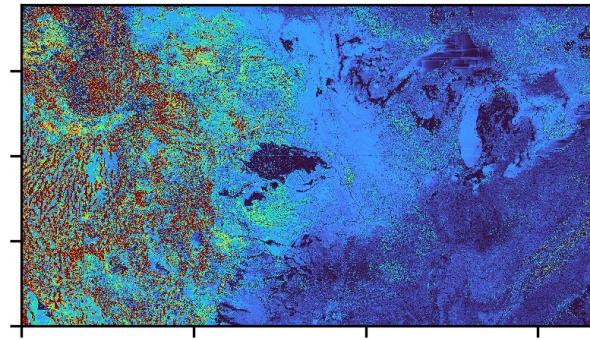
ParFlow



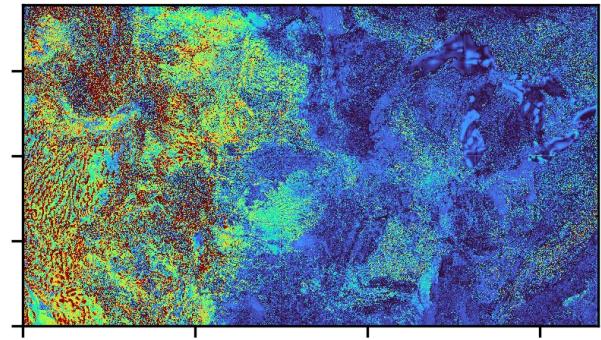
ConvNet



ResNet

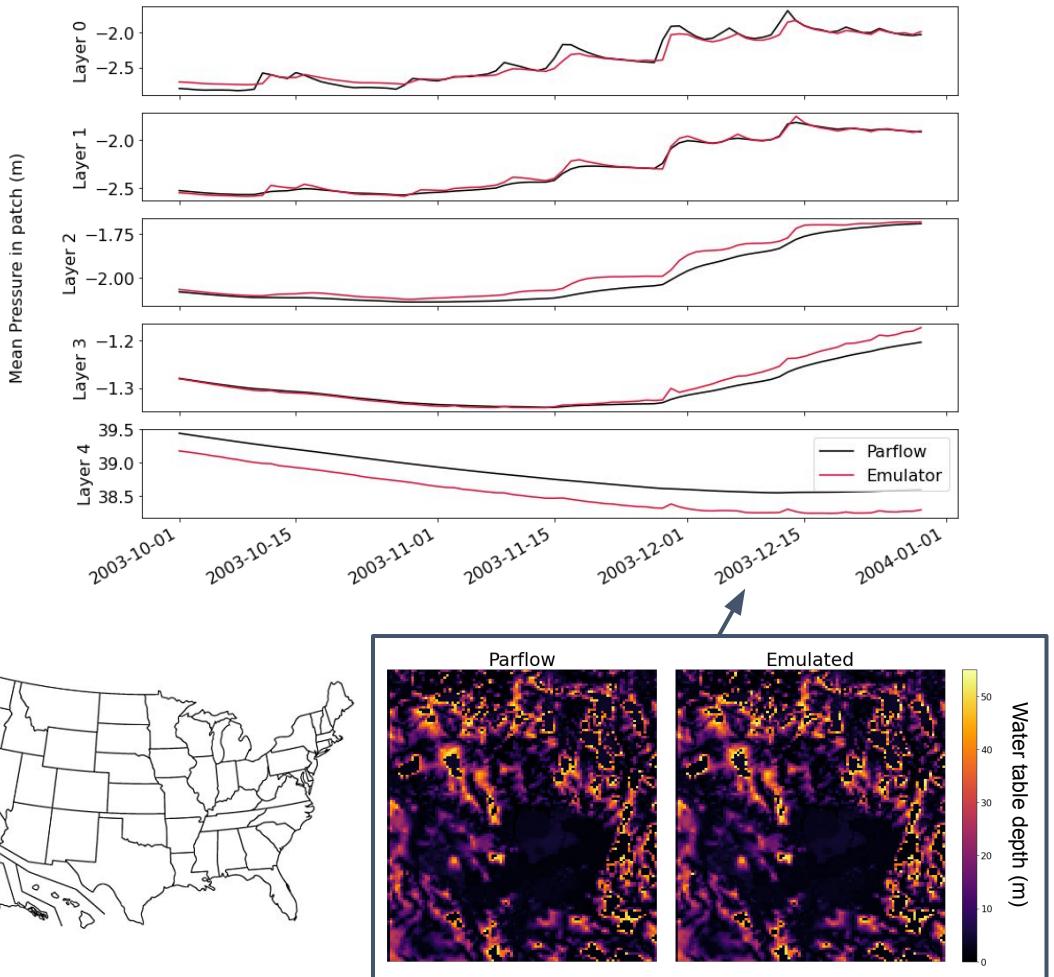


UNet



90 day rollouts match dynamics well too

- Here we show 90 timeseries for all 5 layers of the pressure
- Showing for a location in eastern Oregon state marked by red star on map
- Again, patterns are captured well, but bottom layer has a constant bias
- Zooming in we see spatial patterns of water table depth are very well captured



The messy bits



We are actually
deploying these
models in a webapp

 **HydroGEN**

Overview **Repositories** 30 Projects Packages Teams 5 People 30

Type ▾ Language ▾ Sort ▾

hydrodata Private
Python 0 ⚡ 0 ⚫ 0 ⚪ 0 Updated 5 hours ago

hydrogen-service Private
Python 1 ⚡ 0 ⚫ 0 ⚪ 0 Updated 2 days ago

hydrogen-frontend Private
Hydrogen Frontend web application
JavaScript 0 ⚡ 0 ⚫ 0 ⚪ 0 Updated 2 days ago

HydroGEN-NationalData Private
Python 1 ⚡ 0 ⚫ 0 ⚪ 0 Updated 2 days ago

hydrogen-hydroml Private
Python 0 ⚡ 0 ⚫ 5 ⚪ 0 Updated 3 days ago

We are actually
deploying these
models in a webapp

It turns out MLOps
is not an easy task

The screenshot shows a GitHub-like interface for the 'HydroGEN' organization. The top navigation bar includes links for Overview, Repositories (30), Projects, Packages, Teams (5), People (30), and search/filter options for Type, Language, and Sort.

Below the navigation, there is a search bar with placeholder text 'Find a repository...' and filter buttons for Type, Language, and Sort.

The main content area displays five repository cards:

- hydrodata** (Private)
Python 0 stars 0 forks 0 updated 5 hours ago
- hydrogen-service** (Private)
Python 1 star 0 forks 0 updated 2 days ago
- hydrogen-frontend** (Private)
Hydrogen Frontend web application
JavaScript 0 stars 0 forks 0 updated 2 days ago
- HydroGEN-NationalData** (Private)
Python 1 star 0 forks 0 updated 2 days ago
- hydrogen-hydroml** (Private)
Python 0 stars 5 forks 0 updated 3 days ago

MLFlow has been key for tracking and preparing models for deployment

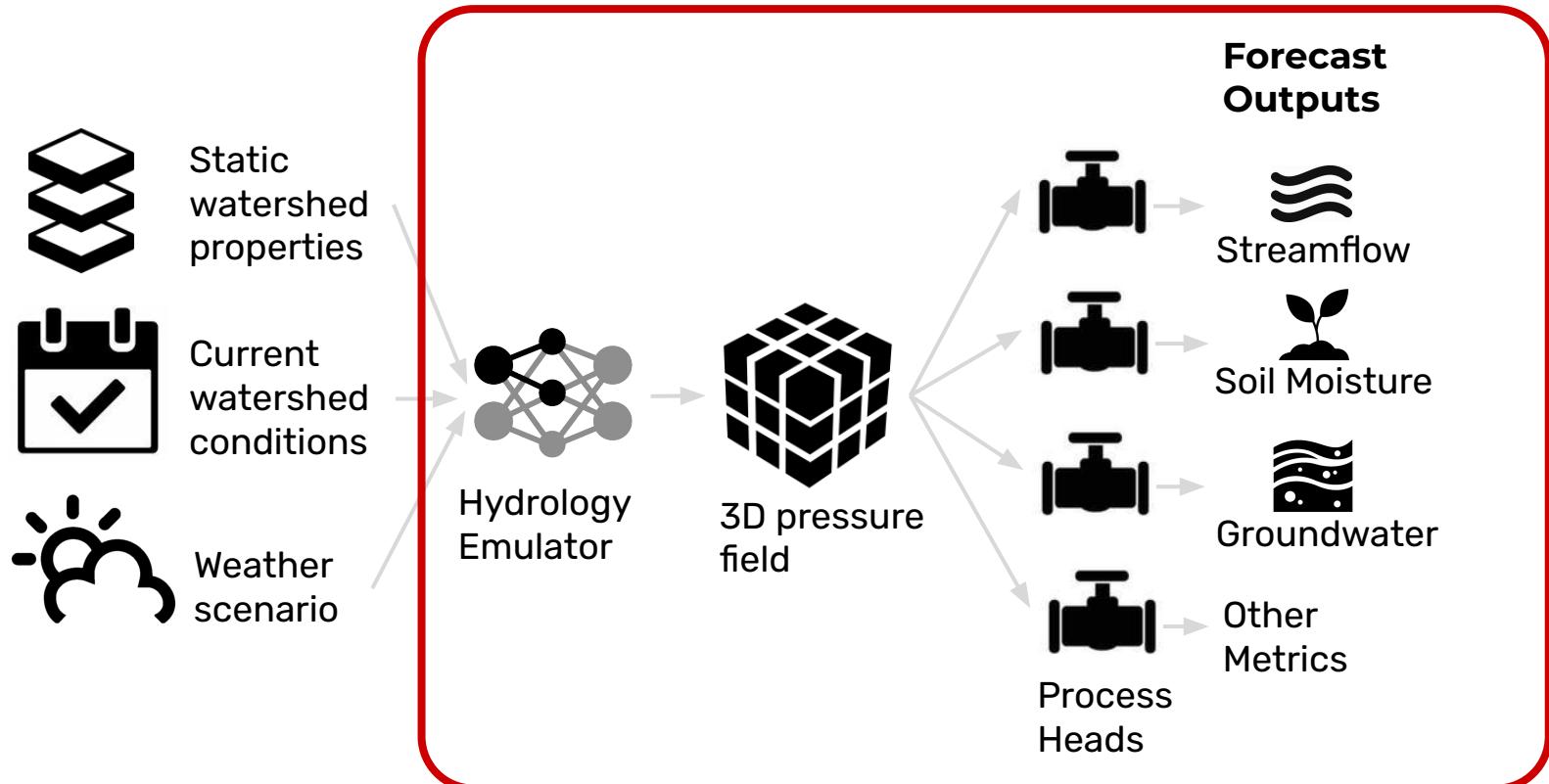


MLFlow has been key for tracking and preparing models for deployment

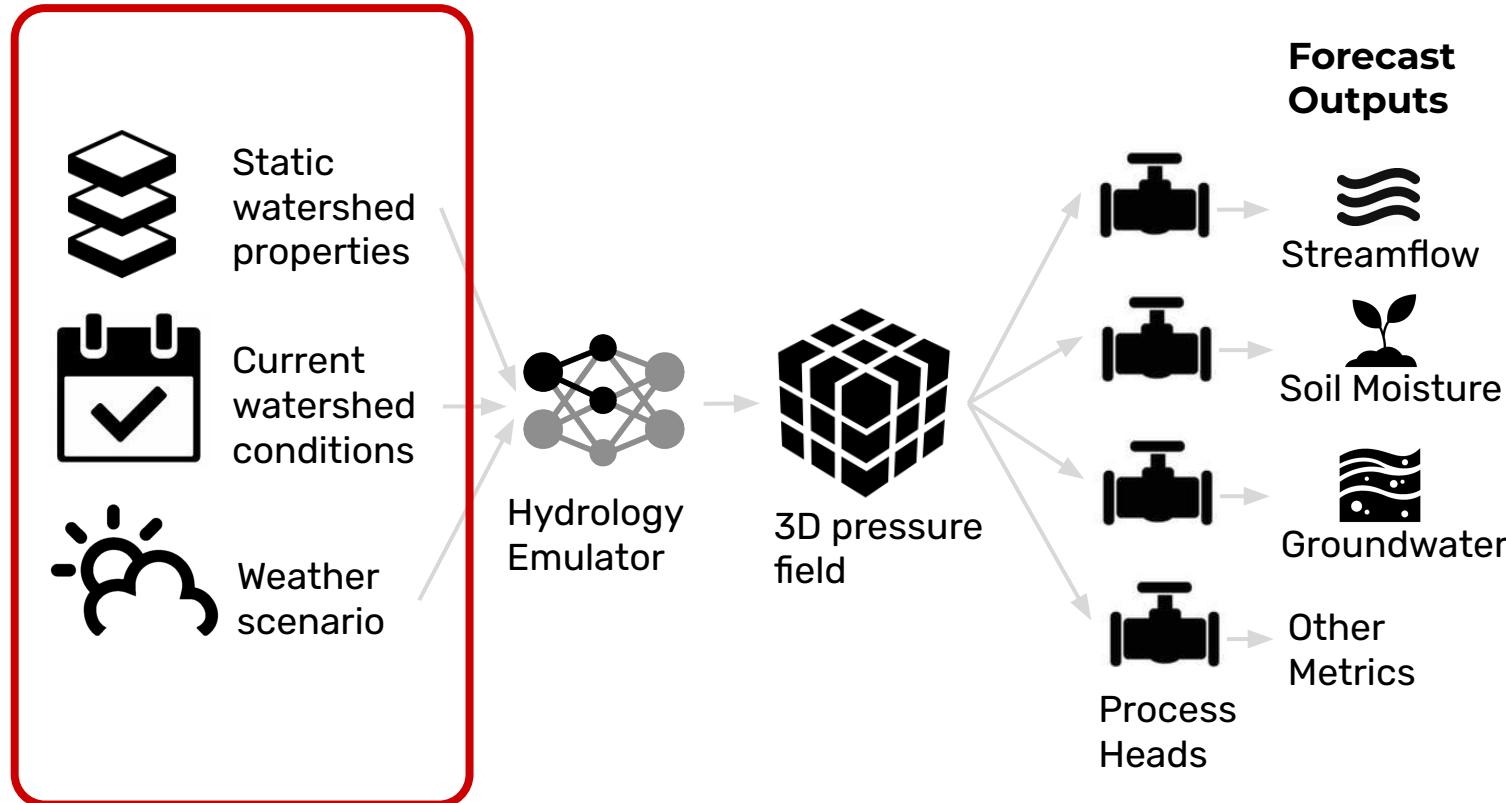
But still at the end of the day, we end up with some shims for the “model zoo”

```
INS (base) (base) model_zoo >>> tree
.
├── convnet_configurable_091922
│   ├── conus1.scalers
│   ├── convnet_train_configurable_7day_1M.pt
│   ├── multilstm_sept8.pt
│   ├── subsurface_config.json
│   └── surface_config.json
└── emulator1
    ├── lstm_swe_et_2layer_120_lookback_2022-06-02_0.pt
    ├── mvp_conus1.scalers
    ├── new_data_stacked_unet_2022-05-29_1.pt
    ├── subsurface_config.json
    └── surface_config.json
└── los_sunus_060122
    ├── lstm_swe_et_2layer_120_lookback_2022-06-02_0.pt
    ├── mvp_conus1.scalers
    ├── new_data_stacked_unet_2022-05-29_1.pt
    ├── subsurface_config.json
    └── surface_config.json
```

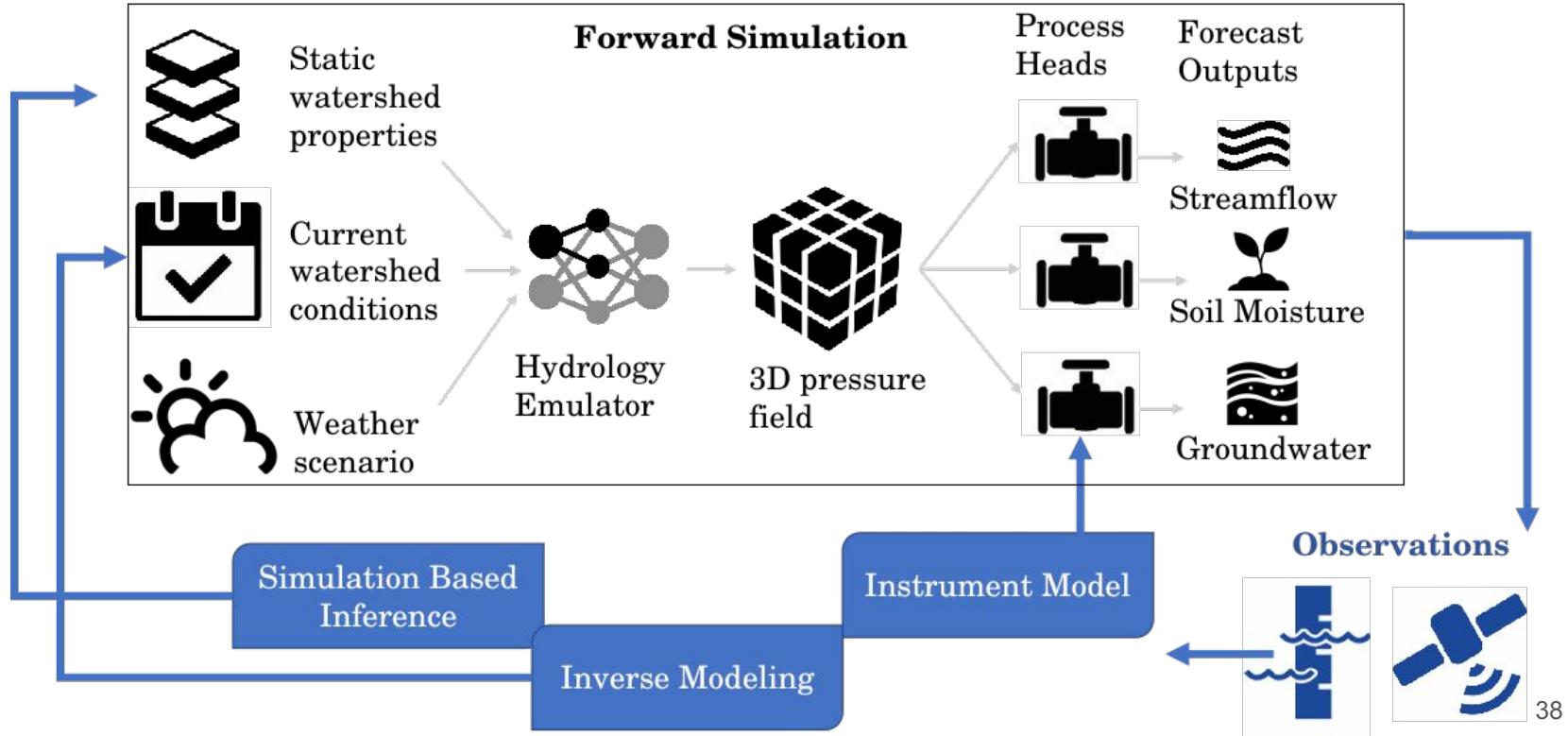
And that's not even the full system



Each of these pieces need to be automated too!



To do this we are bringing in a diverse sets of observations



Still tons of work to do...

- Continue to improve emulator by training on more data, using data augmentation, more training steps, etc
- Perform more comprehensive selection of input data for surface module
- Train directly on derived processes such as water table depth and streamflow
- SBI and inverse modeling to get initial state and parameter values to be more predictive of observations

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- SBI and inverse modeling to get initial state and parameter values to be more predictive of observations

Thanks for listening!
Questions?

Email: andrbenn@email.arizona.edu

Twitter: @arbennett_

Time permitting, a demo!

<https://hydro-dev.princeton.edu/>