Using physics-based machine learning to estimate unobserved quantities:

A case study for landscape-scale soil and vegetation conductances to heat and water vapor

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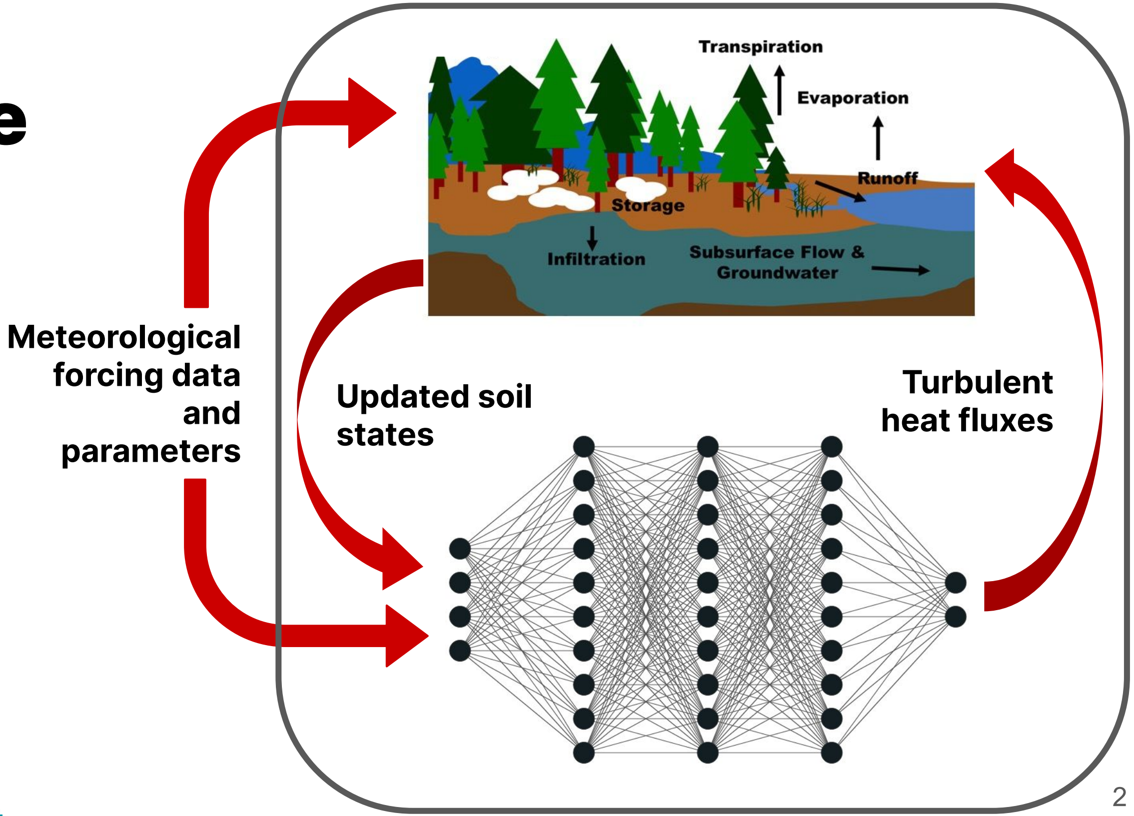
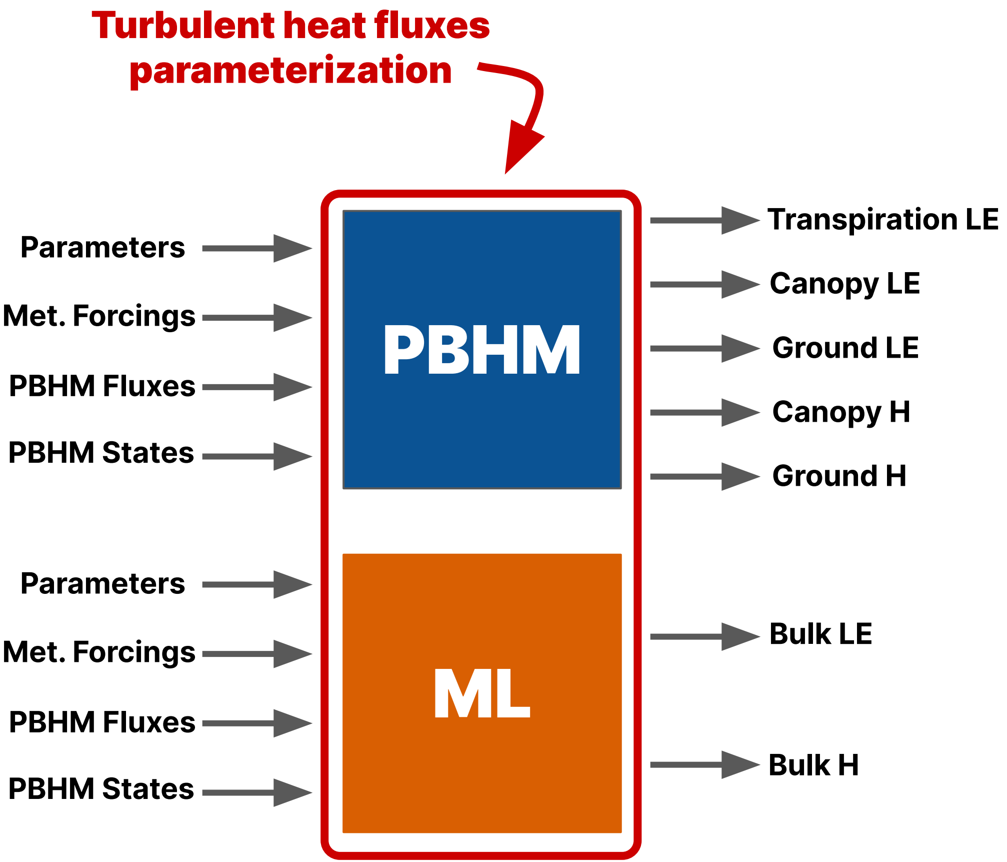
We previously showed that a coupled DL-PBHM approach can make better predictions of turbulent heat fluxes than a PBHM alone

Process based hydrologic model (PBHM)



Link to our previous work:
https://doi.org/10.1002/essoar.10505081.2

One of the major shortcomings is a mismatch between process fidelity and the observed data for training



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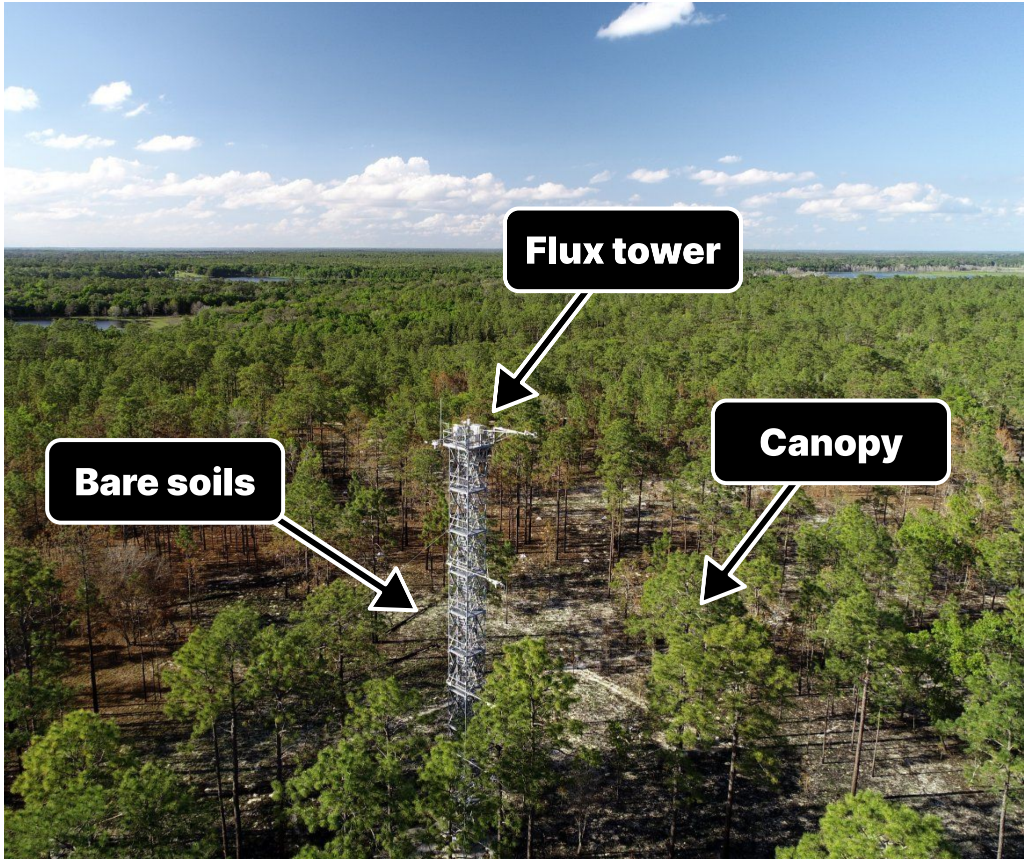
A reminder: The land surface is heterogeneous!

Flux towers measure bulk fluxes

But we want to model the various components

Without fancy techniques supervised machine learning can only learn bulk fluxes from observations then

This presentation is about one of these “fancy techniques”



So, we've got tradeoffs

	Process based model	Machine learned model
Superior performance	✗	✓
Process fidelity	✓	✗


Why don't we have both?

So, we've got tradeoffs

	Process based model	Machine learned model
Superior performance	✗	✓
Process fidelity	✓	✓

Why don't "physics" based models perform well?

These bulk transfer equations are very common in hydrologic and land surface modeling:

- Andreadis et al., 2009
- Bonan, 1991
- Inclan and Forkel, 1995
- Sellers et al., 1986
- Mahat et al., 2013
- Clark et al., 2015
- ...

$$\left.\begin{aligned} Q_h^{veg} &= -\rho_{air} c_p C_h^{veg} \left(T^{veg} - T^{cas} \right) \\ Q_h^{sfc} &= -\rho_{air} c_p C_h^{sfc} \left(T^{sfc} - T^{cas} \right) \end{aligned}\right\} \text{Sensible heat fluxes}$$

$$\left.\begin{aligned} Q_{evap}^{veg} &= -\frac{L_{vap} \rho_{air} \varepsilon}{P_{air}} C_{evap}^{veg} \left[e_{sat} \left(T^{veg} \right) - e^{cas} \right] \\ Q_{trans}^{veg} &= -\frac{L_{vap} \rho_{air} \varepsilon}{P_{air}} C_{trans}^{veg} \left[e_{sat} \left(T^{veg} \right) - e^{cas} \right] \\ Q_l^{sfc} &= -\frac{L_{vap} \rho_{air} \varepsilon}{P_{air}} C_w^{sfc} \left[\phi_{hum}^{sfc} e_{sat} \left(T^{sfc} \right) - e^{cas} \right] \end{aligned}\right\} \text{Latent heat fluxes}$$

Why don't "physics" based models perform well?

These consist of three main parts

1. Constants & parameters
2. Temperature or moisture gradients
3. Conductance terms

$$Q_h^{veg} = -\rho_{air} c_p C_h^{veg} \left(T^{veg} - T^{cas}\right)$$

$$Q_h^{sfc} = -\rho_{air} c_p C_h^{sfc} \left(T^{sfc} - T^{cas}\right)$$

Sensible heat fluxes

$$Q_{evap}^{veg} = -\frac{L_{vap}\rho_{air}\varepsilon}{P_{air}} C_{evap}^{veg} \left[e_{sat}\left(T^{veg}\right) - e^{cas}\right]$$

$$Q_{trans}^{veg} = -\frac{L_{vap}\rho_{air}\varepsilon}{P_{air}} C_{trans}^{veg} \left[e_{sat}\left(T^{veg}\right) - e^{cas}\right]$$

$$Q_l^{sfc} = -\frac{L_{vap}\rho_{air}\varepsilon}{P_{air}} C_w^{sfc} \left[\phi_{hum}^{sfc} e_{sat}\left(T^{sfc}\right) - e^{cas}\right]$$

Latent heat fluxes

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$$\theta \bullet C \bullet \Delta$$

Why don't "physics" based models perform well?

These consist of three main parts

1. **Constants & parameters**
2. **Temperature or moisture gradients**
3. Conductance terms

I'm going to argue these are either:

1. Pretty well known
2. Parts of other processes

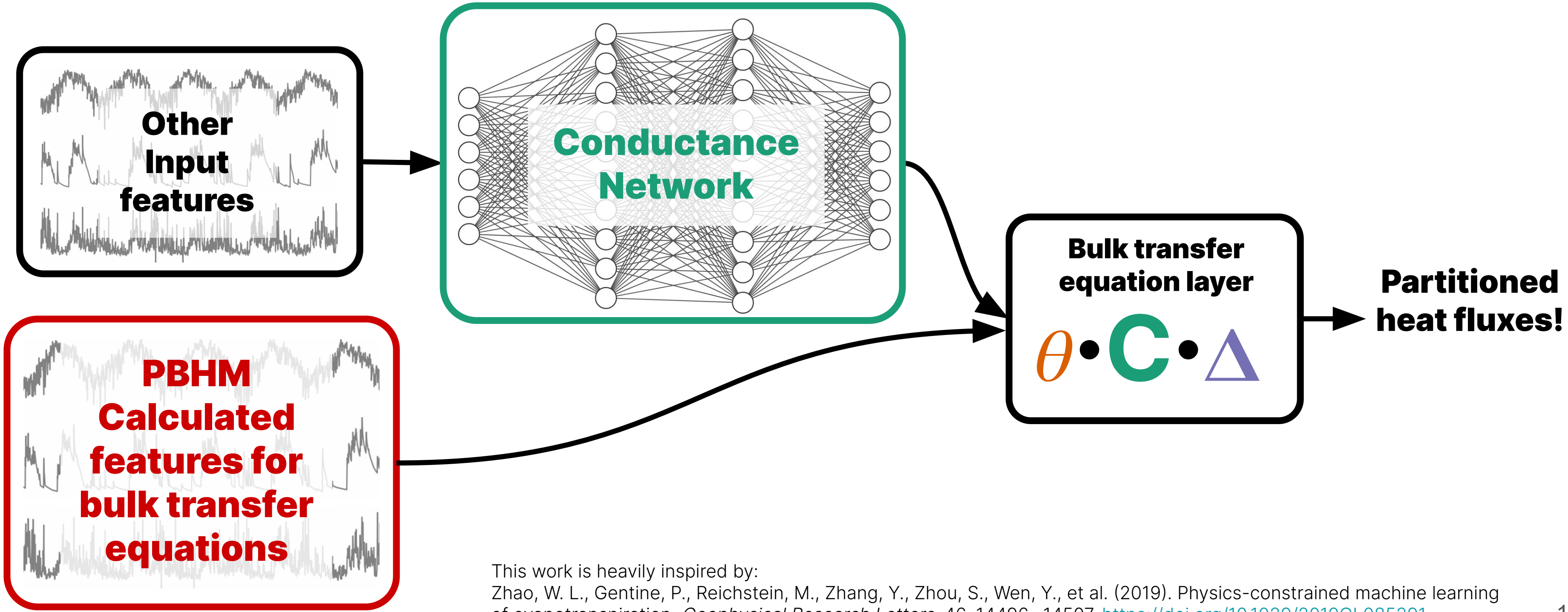
Why don't "physics" based models perform well?

These consist of three main parts

1. Constants & parameters
2. Temperature or moisture gradients
3. Conductance terms

And likewise, this is where the model uncertainty really is...

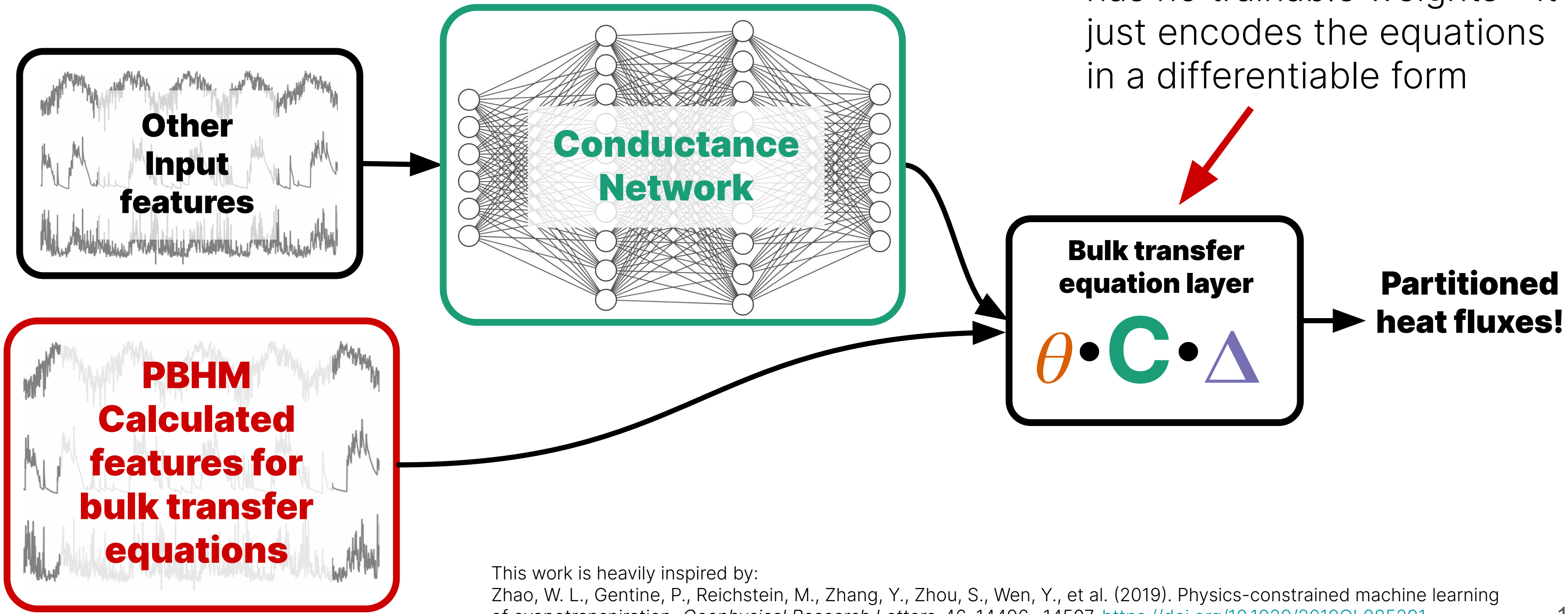
The hybrid neural network architecture



This work is heavily inspired by:
Zhao, W. L., Gentine, P., Reichstein, M., Zhang, Y., Zhou, S., Wen, Y., et al. (2019). Physics-constrained machine learning of evapotranspiration. *Geophysical Research Letters*, 46, 14496– 14507. https://doi.org/10.1029/2019GL085291

The hybrid neural network architecture

Technical note: This "layer" has no trainable weights - it just encodes the equations in a differentiable form



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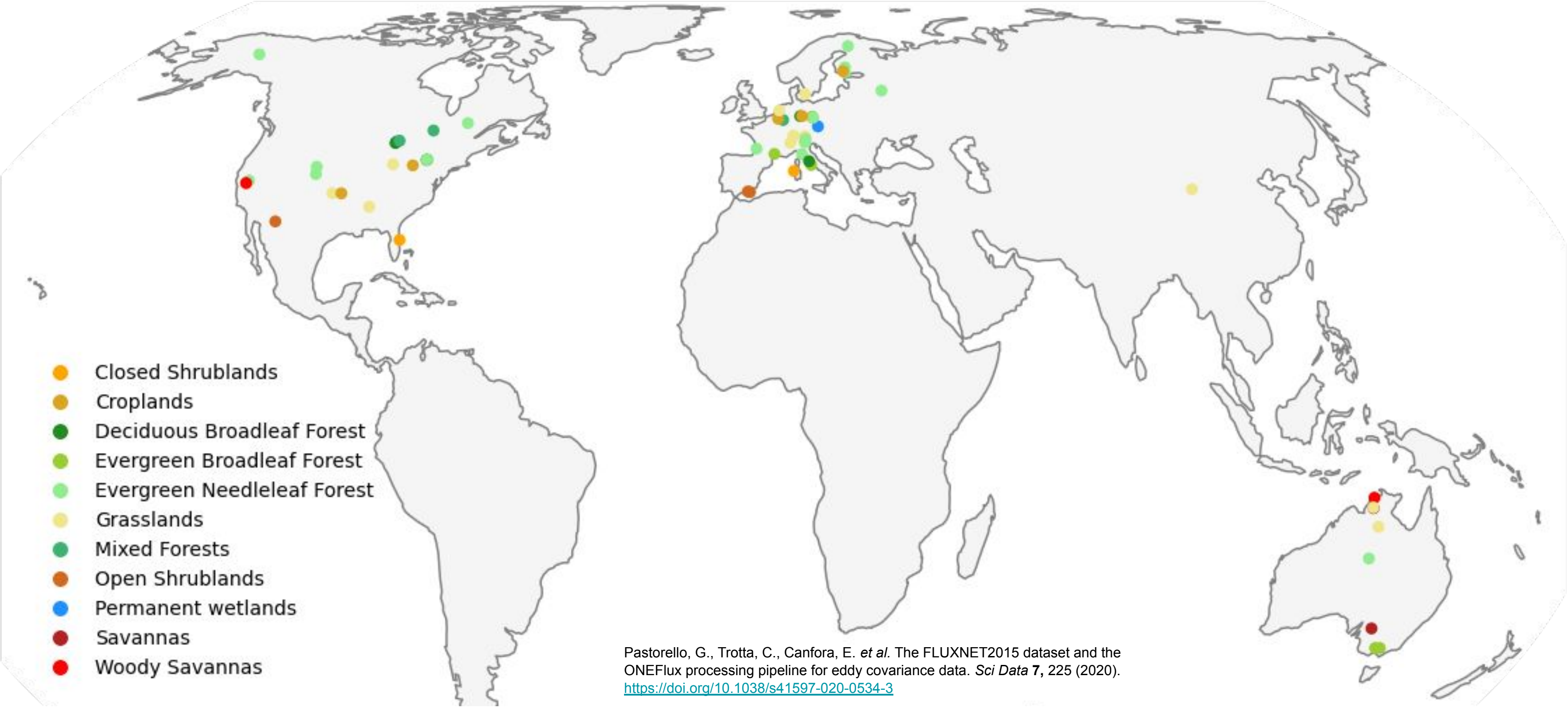
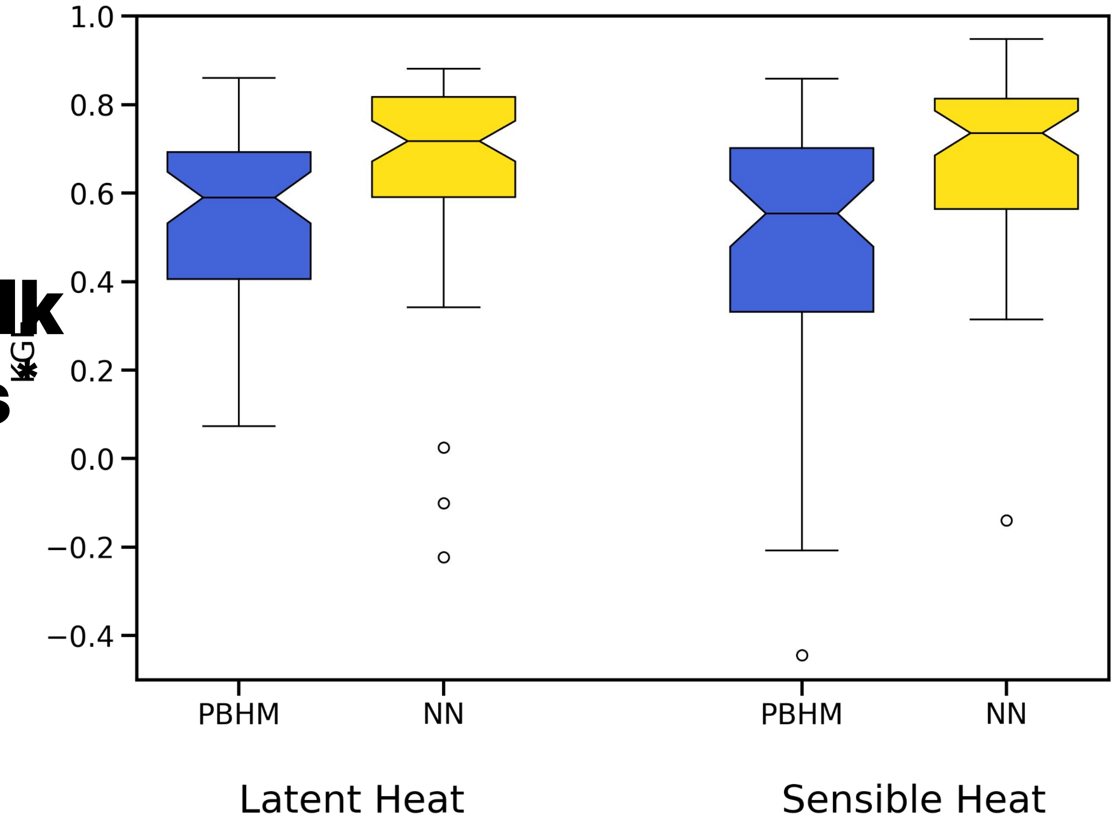
We gathered data from 60 FluxNet sites, totalling over 500 site-years of half-hourly data



Pastorello, G., Trotta, C., Canfora, E. *et al.* The FLUXNET2015 dataset and the ONEFlux processing pipeline for eddy covariance data. *Sci Data* **7,** 225 (2020). https://doi.org/10.1038/s41597-020-0534-3

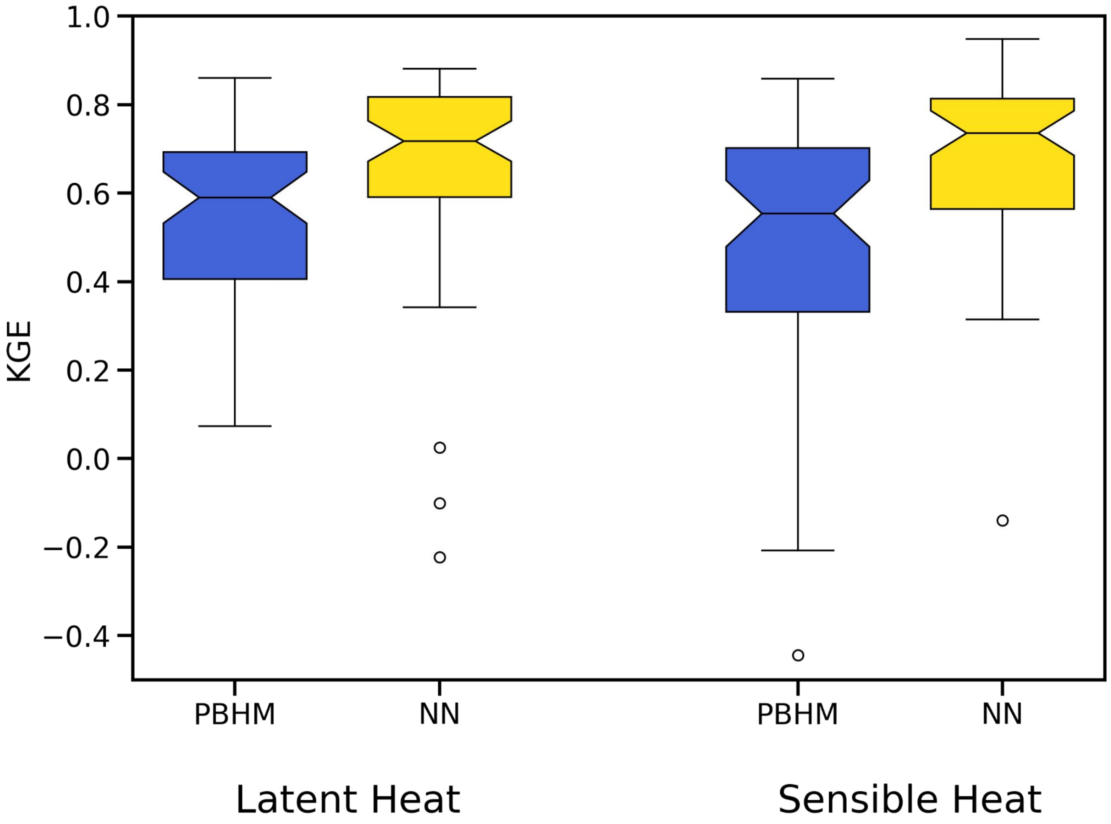
We're still able to outperform a calibrated PBHM using the same bulk transfer equations*



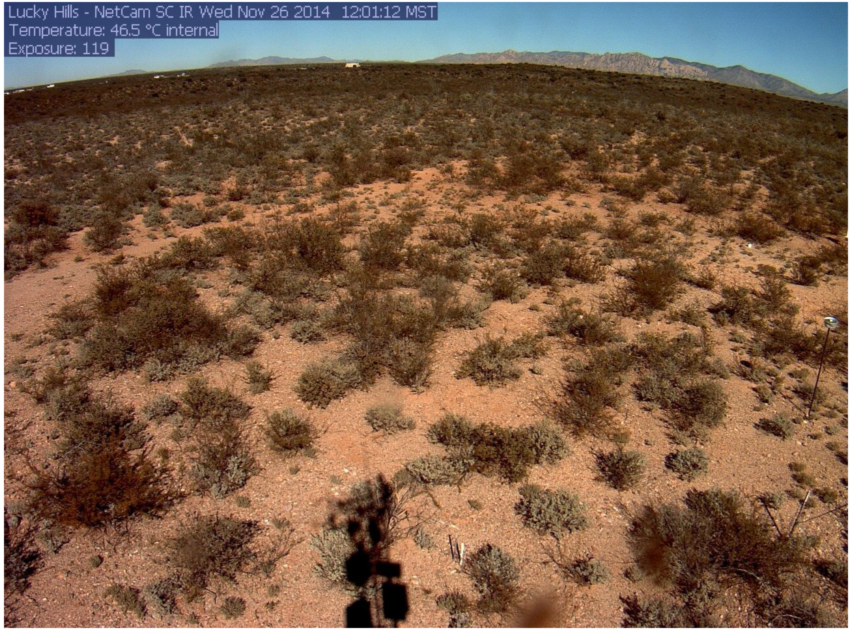
**other pure ML based approaches outperform this but that's asking a different question*

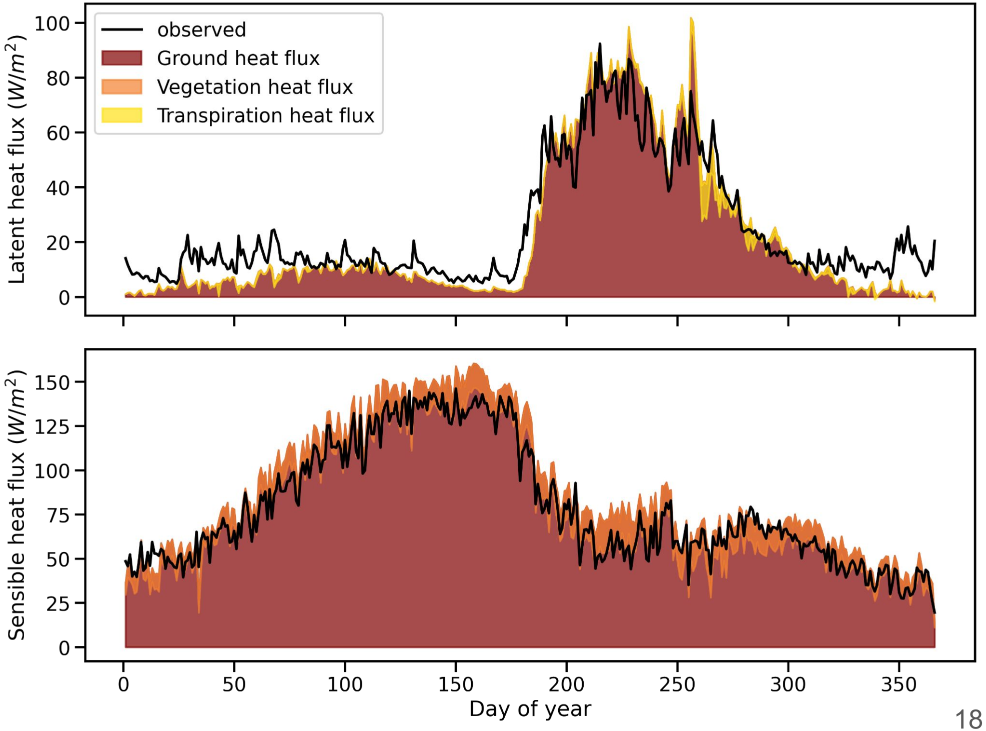
Perhaps a rough upper bound on the performance of the “physics” based equations?

more work remains to be done to ensure that these performance results are optimal (notably fixing outliers)

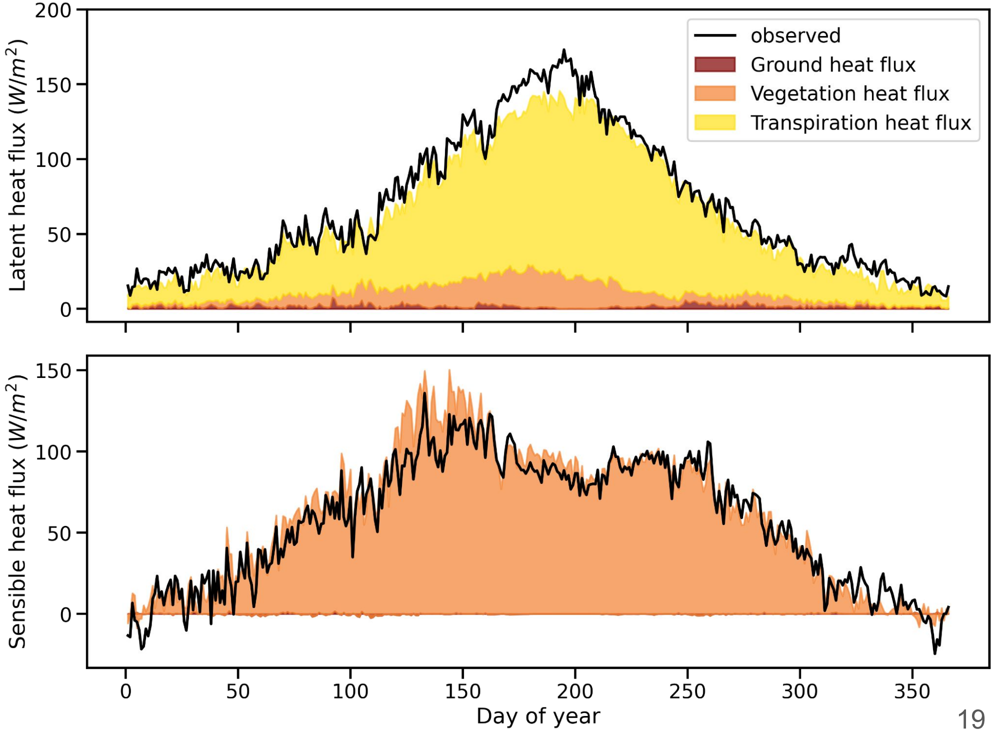


Walnut Gulch near Tombstone, AZ (US-Whs) shows ground component is largest

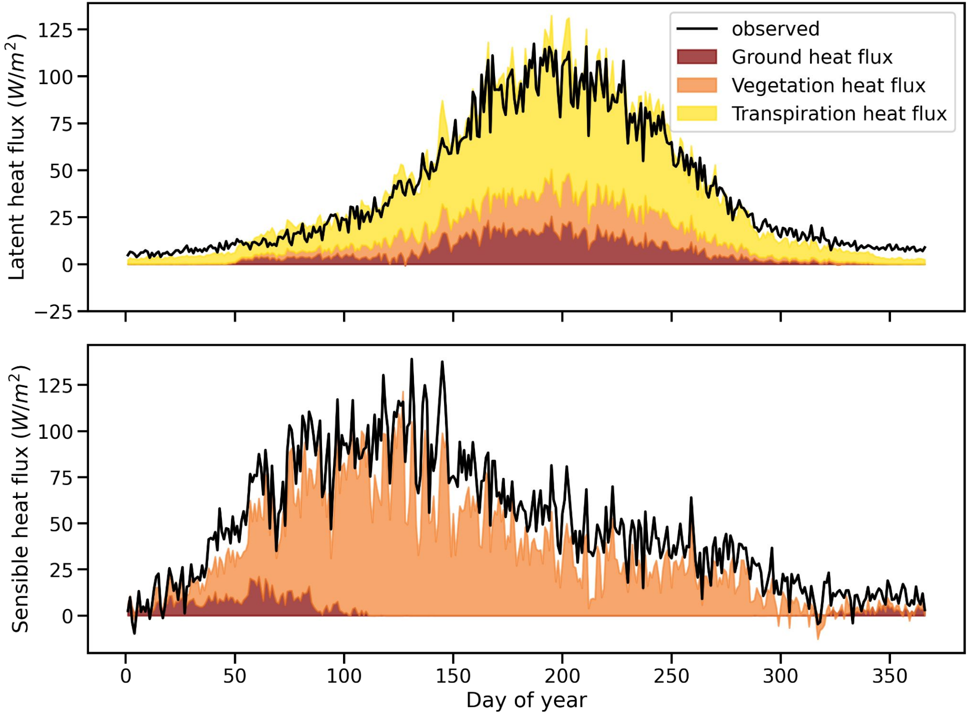




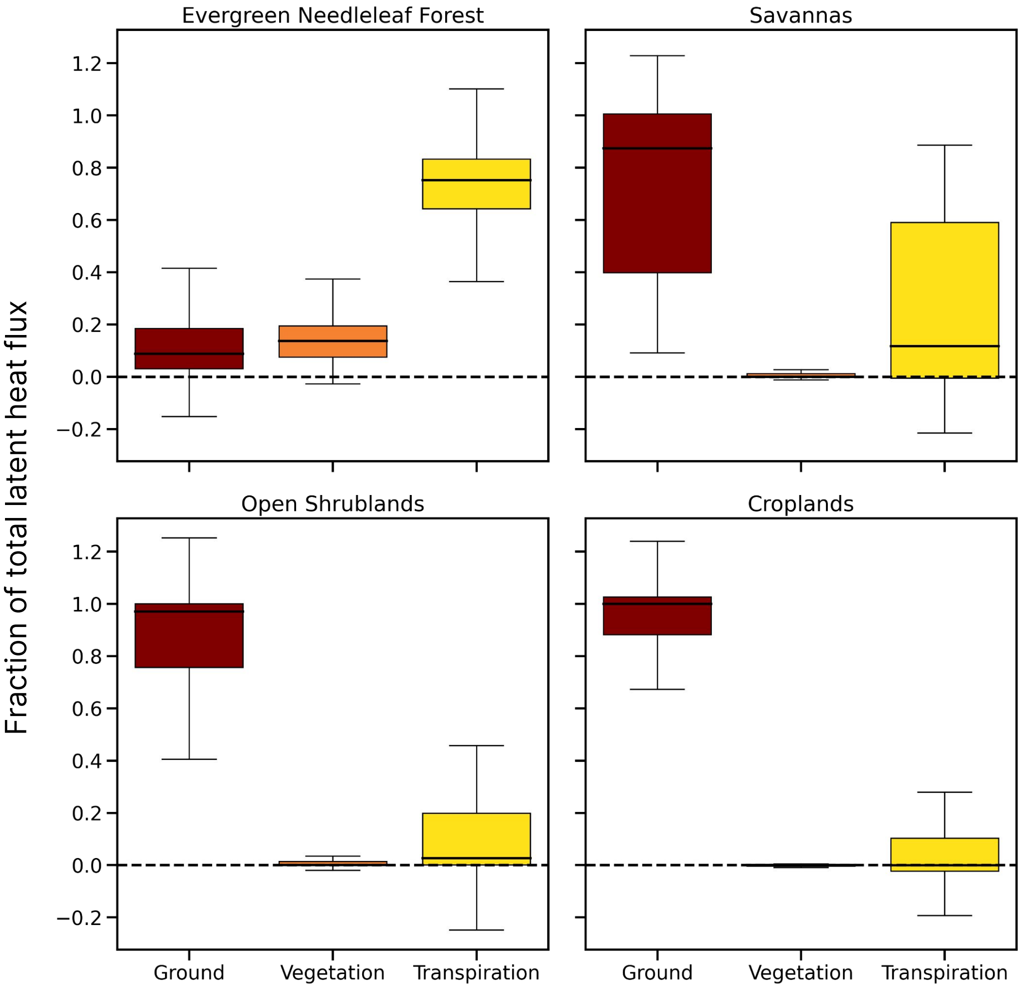
Blodgett Forest near Sacramento, CA (US-Blo) shows vegetation components are largest



Mixed forest near Vielsalm, Belgium shows a larger mixture between components

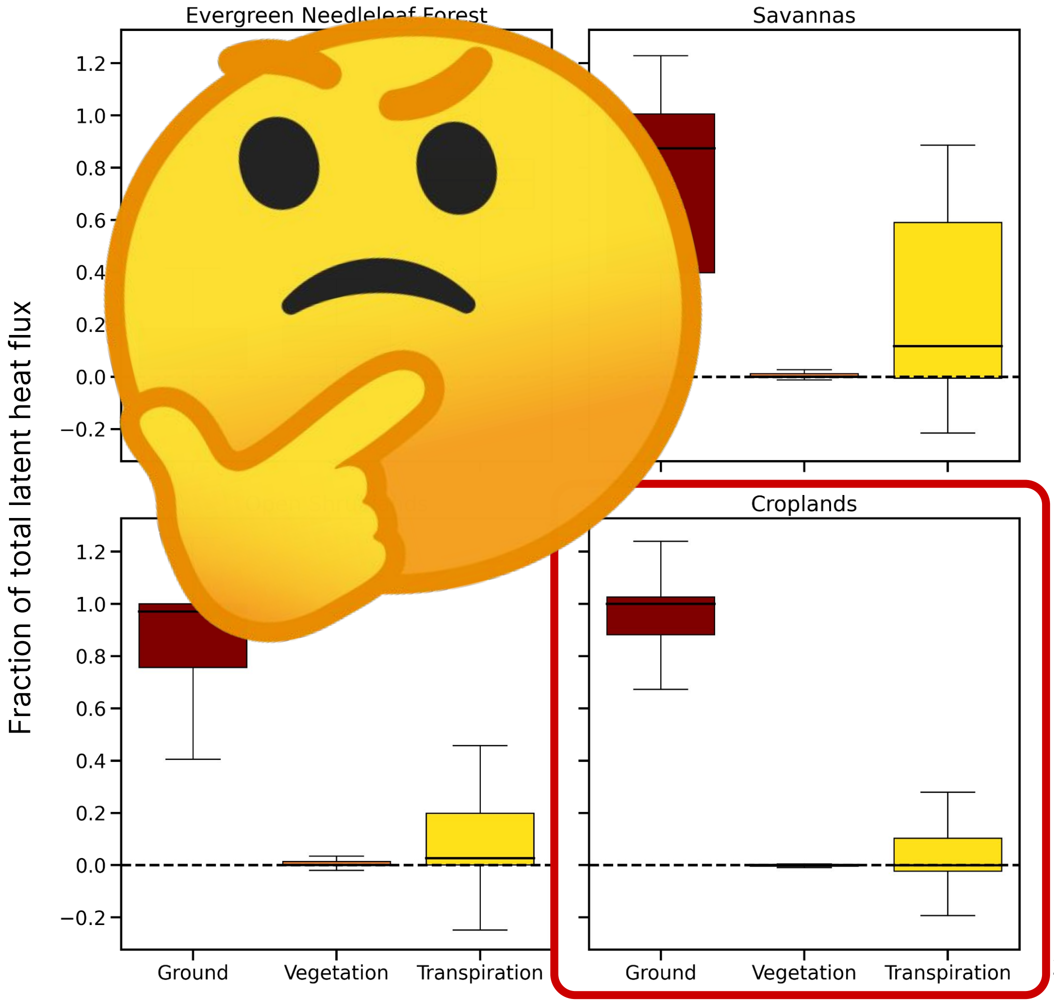


The overall partitioning matches physical intuition to a first order



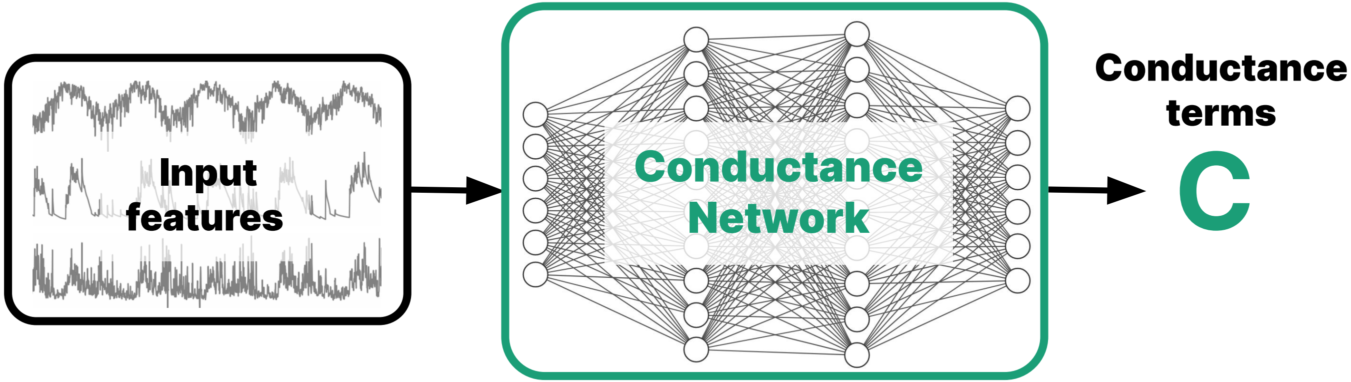
Note: values can be <0 and >1 because condensation exists

The overall partitioning matches physical intuition to a first order, mostly

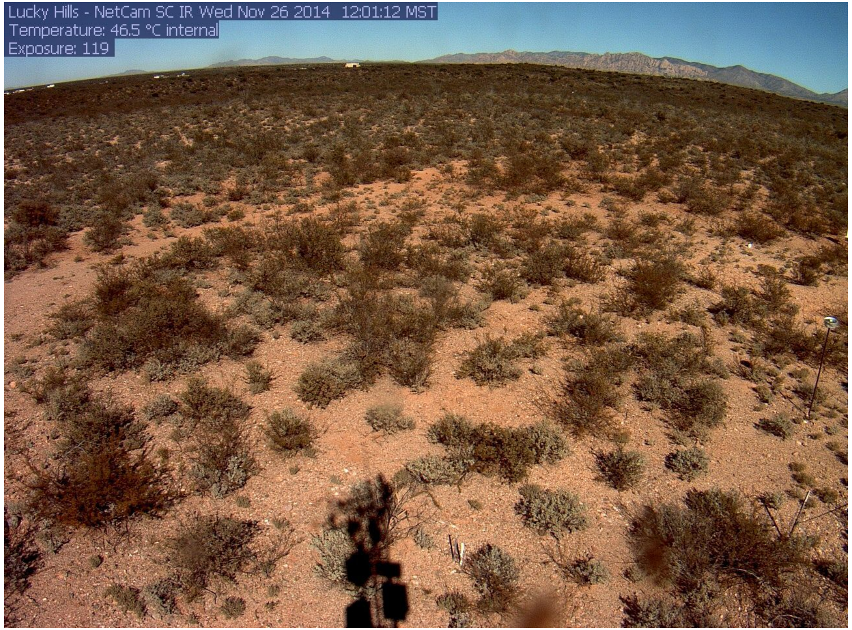


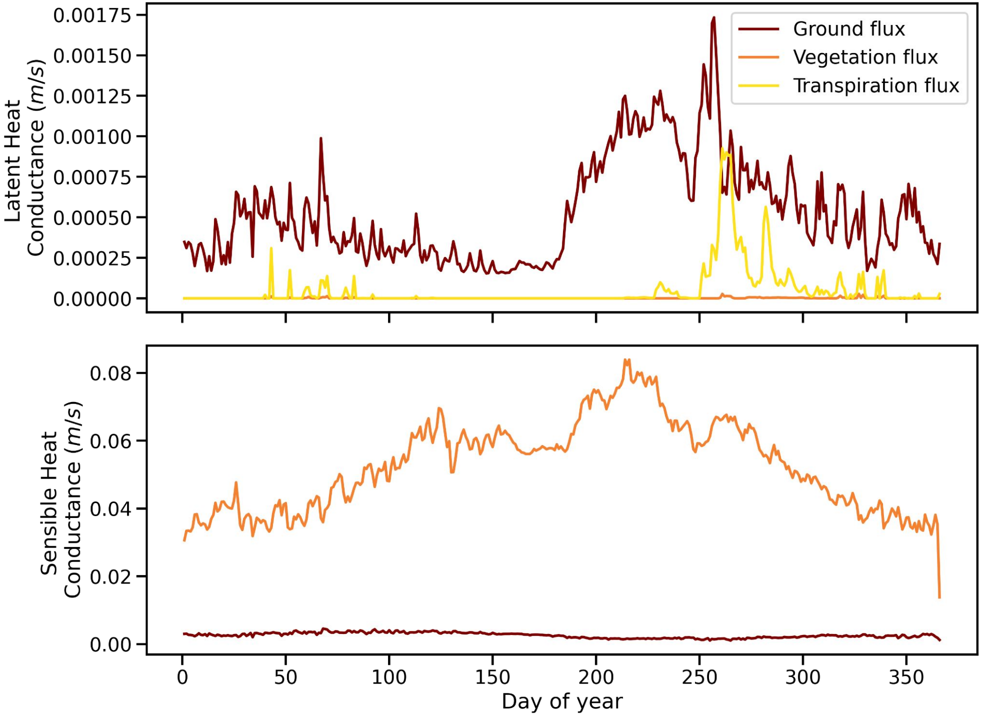
Note: values can be <0 and >1 because condensation exists

We can also truncate the network to analyze the conductances!

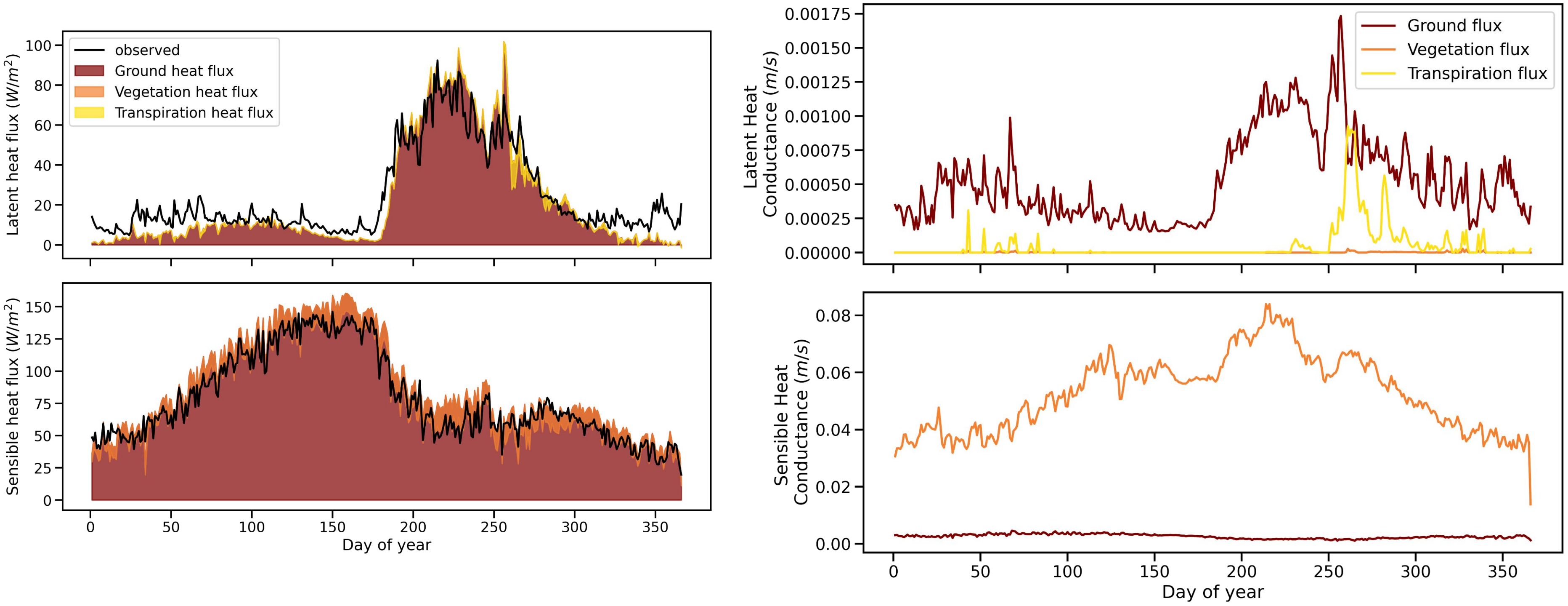


Conductances at Walnut Gulch

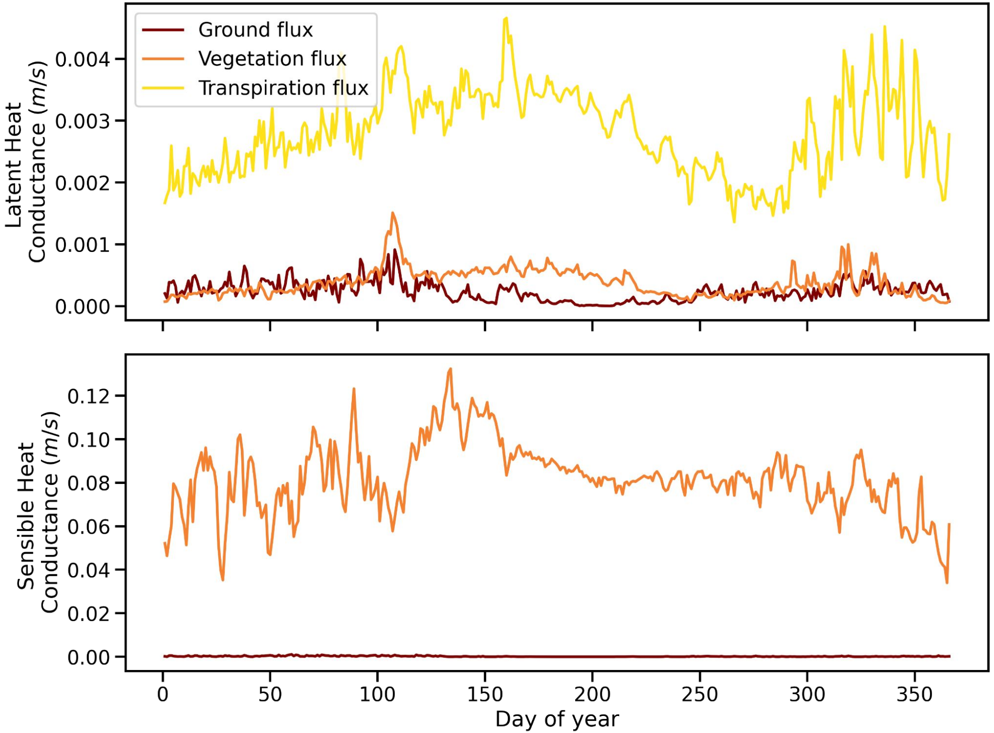




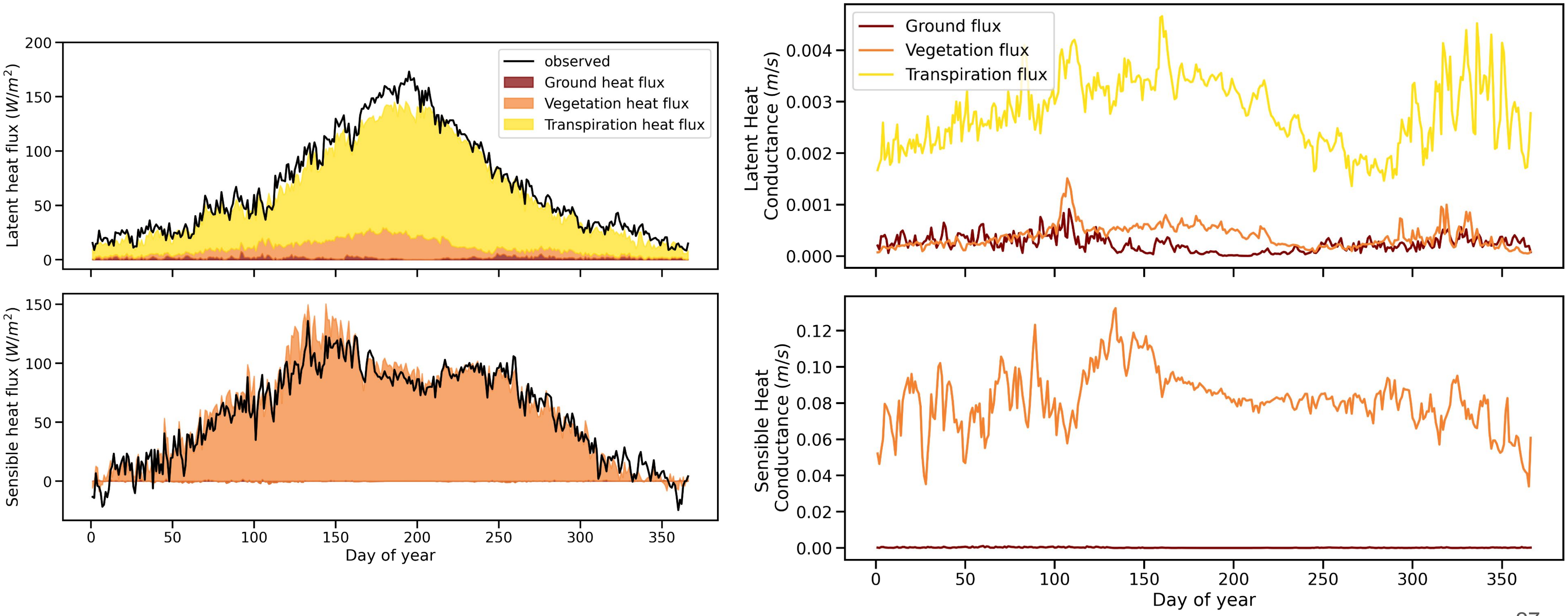
Conductances are not 1-1 with heat fluxes



Conductances at Blodgett Forest



Conductances are not 1-1 with heat fluxes *still*



Wrapup, future work, and some conceptual takeaways

We've quantified that a large amount of predictive performance is due to conductance terms

Need methods/data to better constrain the partitioning, particularly at sites with human interventions, like croplands

Coupling to the PBHM is still incomplete, but needed to analyze the effects on the full water cycle

My big takeaway: Process-based vs data-driven modeling should be a spectrum rather than a binary choice