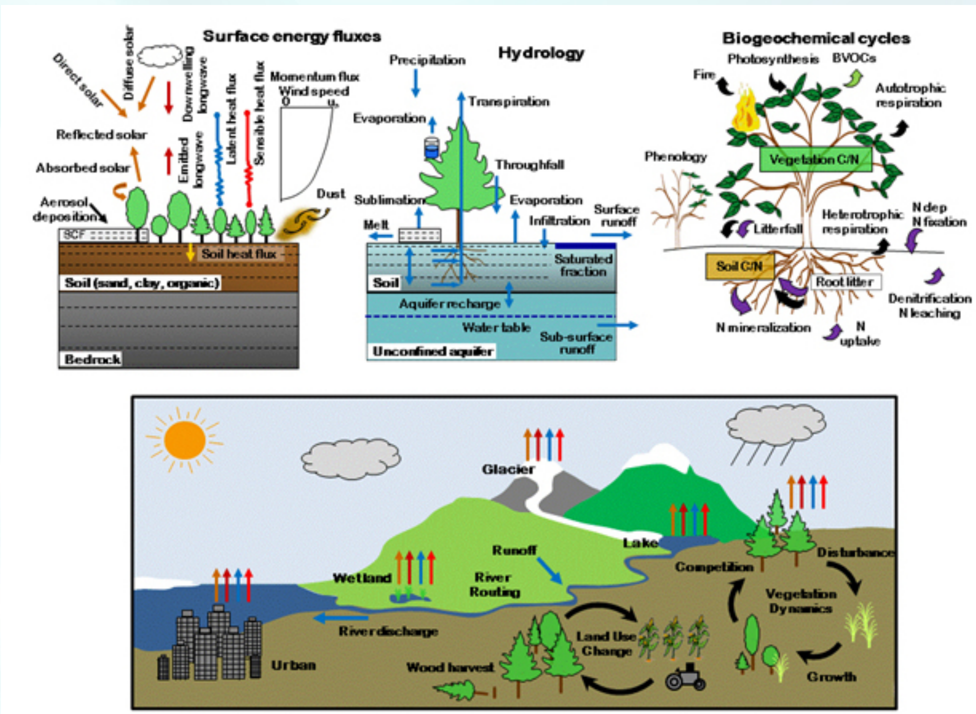
# Physics-informed Machine Learning for Uncertainty Quantification in E3SM Land Model

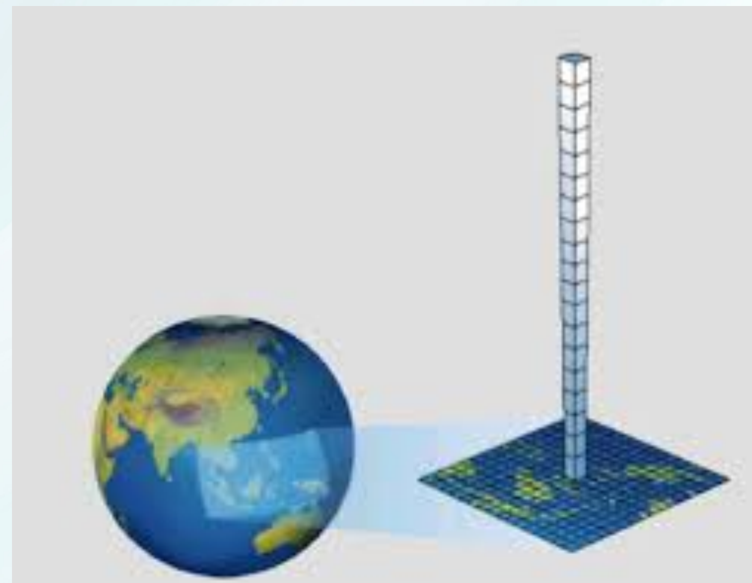
Khachik Sargsyan, Cosmin Safta, Vishagan Ratnaswamy (SNL-CA)
Daniel M. Ricciuto (ORNL)

ESMD-E3SM PI Meeting
Oct 26-29, 2020

# Model of interest: E3SM Land Model (ELM)




## Single Column mode



# Ensemble-intensive studies require preconstructed surrogate models

**Surrogates are necessary for**

- Global sensitivity analysis
- Uncertainty propagation
- Model calibration/tuning
- Optimal experimental design

Design conditions (e.g. space/time)

Input parameters (uncertain)

$$f(x;\lambda) \approx f_s(x;\lambda)$$

Never analyze the ensemble directly: build a **surrogate** first
… otherwise called proxy, metamodel, emulator, response surface, <u>supervised ML</u>

Work with the model as a black-box (**non-intrusive**):
- create an ensemble of simulations with varying/perturbing $\lambda$ and *learn the relationship* $y = f(x;\lambda)$

# Temporal nature of the model requires special surrogate types

**Key Idea #1:**

Use Recurrent Neural Networks (RNN), such as Long Short Term Memory (LSTM) to capture temporal dependencies

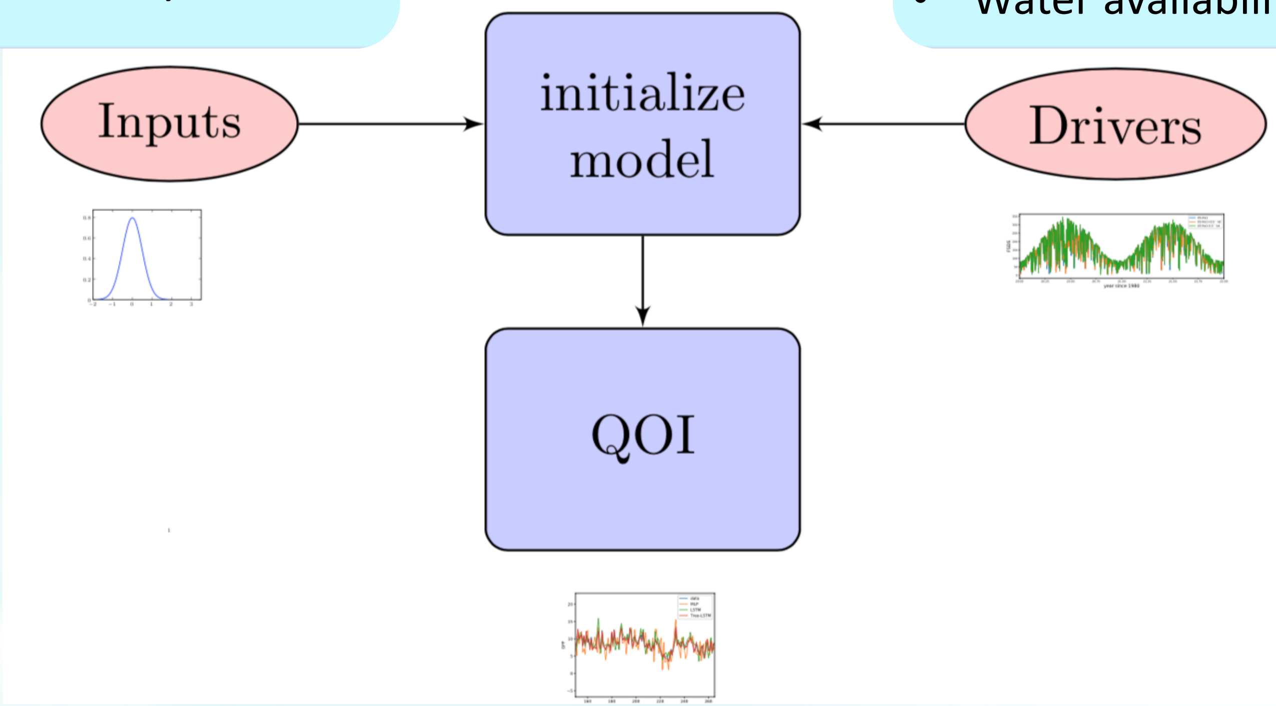
**Key Idea #2:**

Use physics-informed connections to build tree-based neural-network architecture for more efficient training and higher accuracy

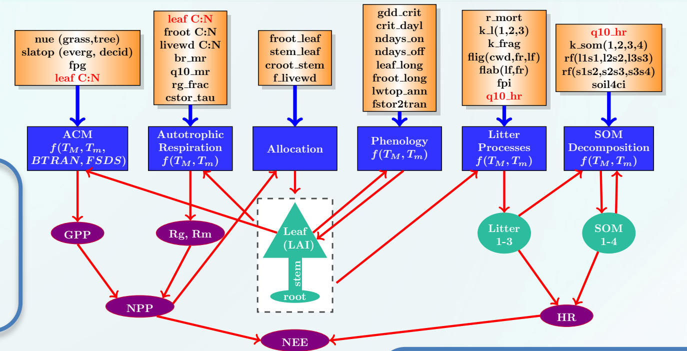
# I/O structure of single column ELM

- 10-100 input parameters
- Usually uncertain

- Day of year
- Min/Max Temp
- Solar radiation
- Water availability

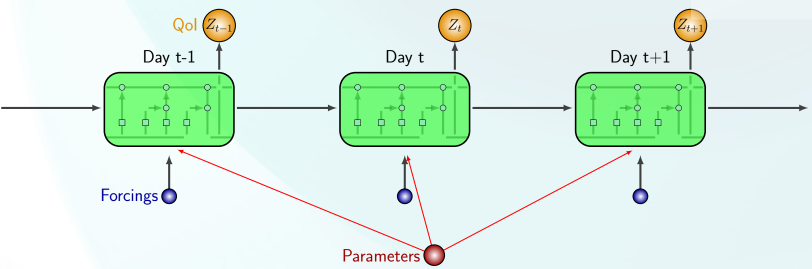


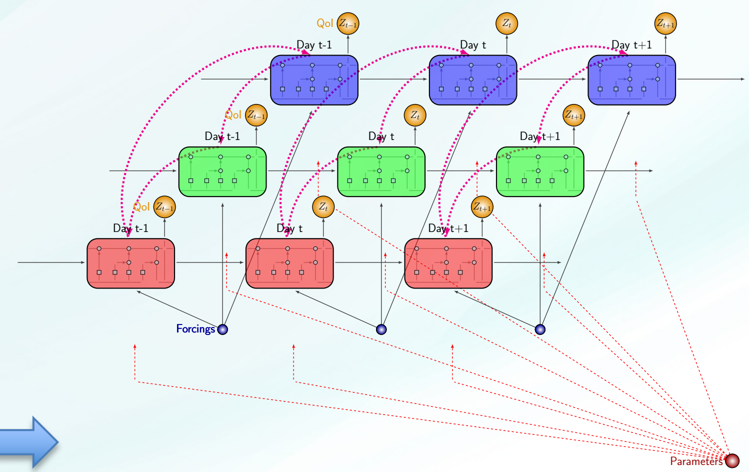
# LSTM architecture handcrafted according to known physical connections




Vanilla LSTM:
One network per QoI

Physics-informed LSTM:
accounts for QoI connections




- Long short term memory (LSTM), a variant of Recurrent Neural Network (RNN)
- Much better than conventional polynomial regression or multilayer NN
- But the winner is ….
  physics-informed architecture

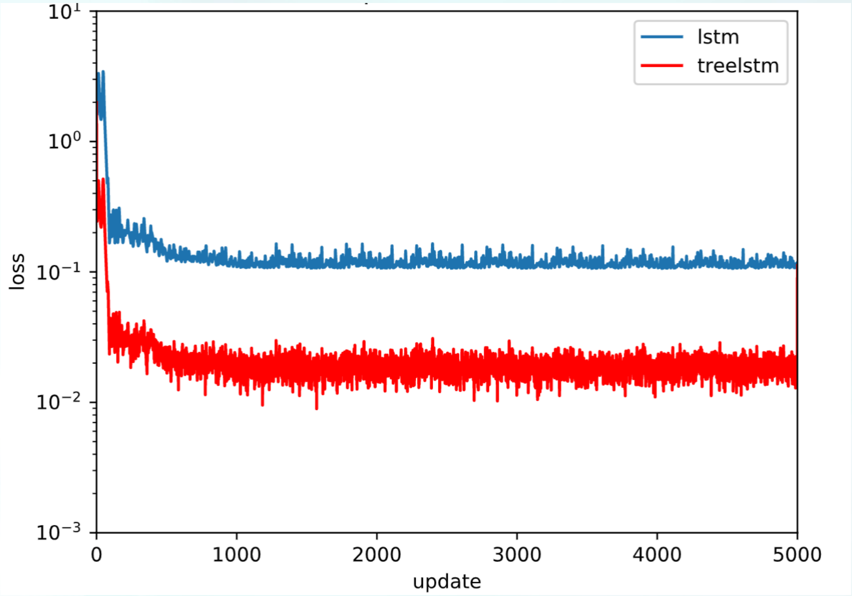
# Model and training details

- Initial work on sELM, simplified py version for UQ analysis
- Represents land biogeochemistry (carbon cycle processes)
- 47 parameters (subset of ELM) – prior distributions from literature
- Can run point to global-scale simulations

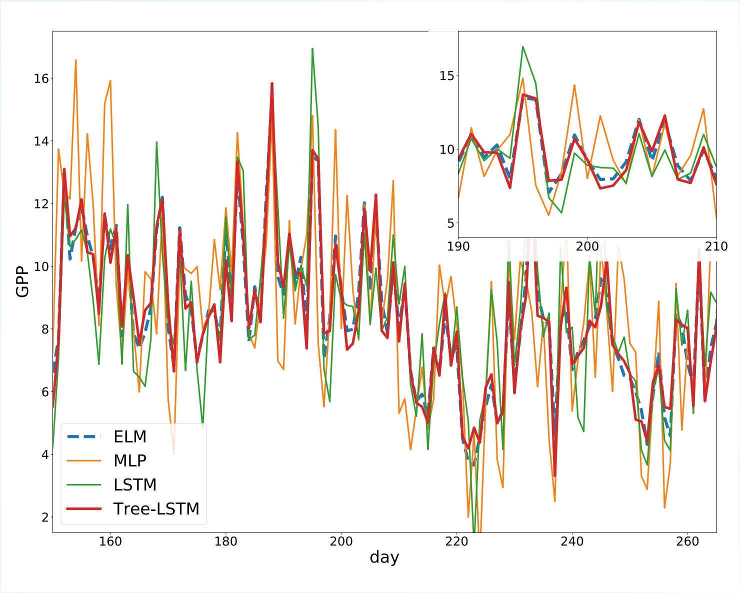
- Trained on simulations at various FLUXNET sites
- Dropout Regularization
- 500 training samples, 500 validation samples
- Three hidden layers, each 150 units

# Physics-informed LSTM neural network accurately resolves time evolution

Loss function of vanilla LSTM and physics-informed LSTM




Comparison of sELM and NNs

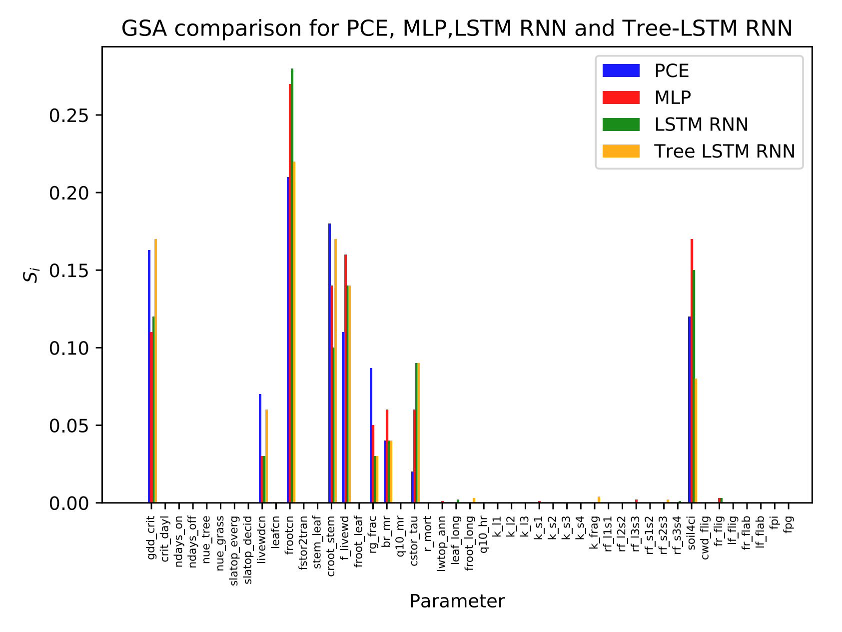


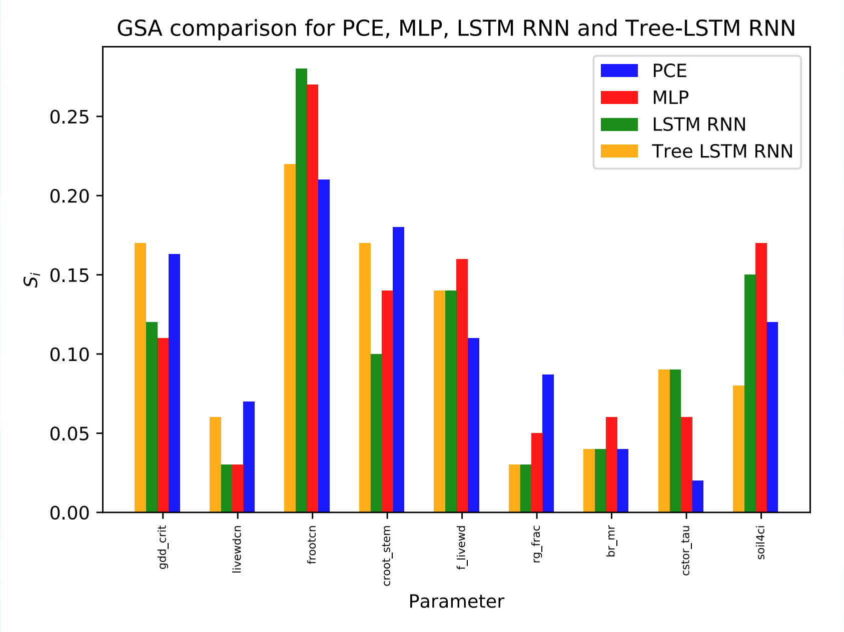

LSTM NNs approximates the sELM behaviour
with respect to perturbations in 47 parameters, with a fraction of the cost

# Global Sensitivity Analysis (GSA) enables parameter selection

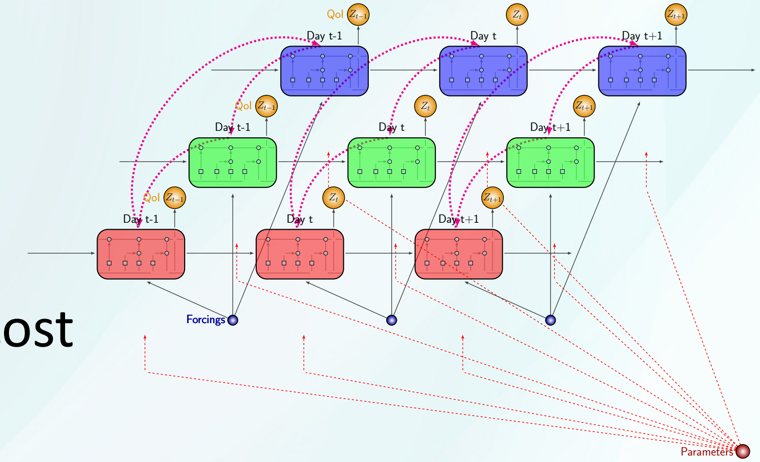
… otherwise called Sobol indices, variance-based decomposition

Attribute fractions of output variance to input parameters

# Summary




- Physics-informed NN architecture helps build a time-resolved accurate surrogate

- The cost of surrogate evaluation is a fraction of the land model evaluation cost

- Surrogate is employed for uncertainty propagation and global sensitivity analysis

- Surrogate will be employed for parameter calibration/tuning

- Marry temporal surrogate with a spatially resolved surrogate