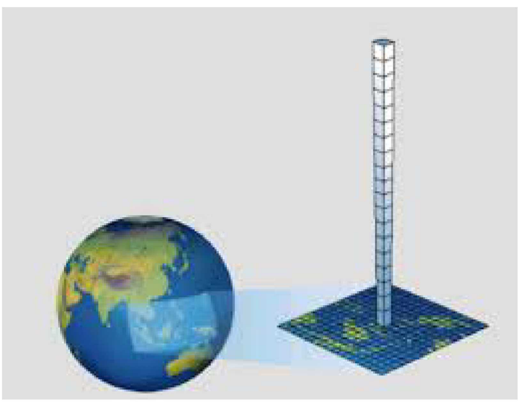
SAND2019-15074C

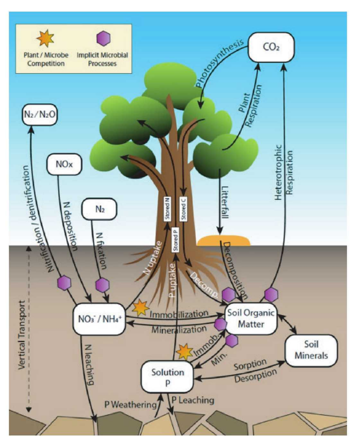
Physics Informed Neural Network Surrogate for E3SM Land Model

Vishagan Ratnaswamy[1], Cosmin Safta[1], Khachik Sargsyan[1], and Daniel Ricciuto[2]

Sandia National Laboratories[1], Livermore CA
Oak Ridge National Laboratory[2], Oak Ridge TN

Surrogate Construction for Land Model





Major challenges

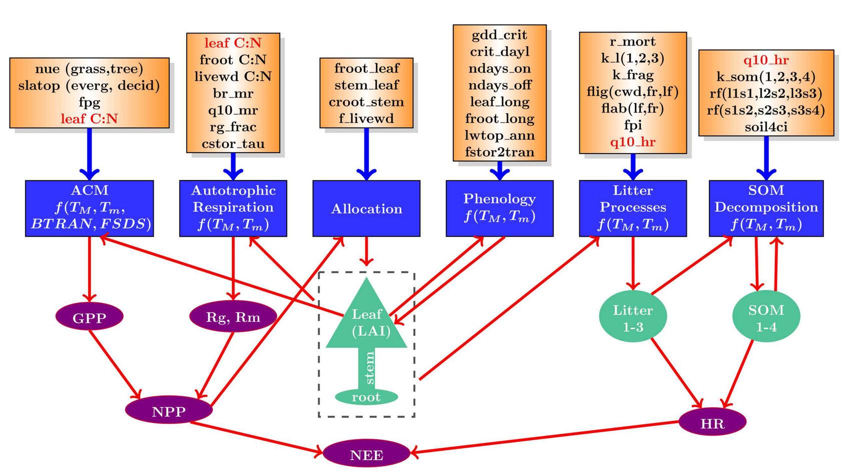
- High-dimensionality: complex climate models typically include a large number of input parameters
- Expense: a single simulation takes hours/core
- Uncertainty quantification studies, such as calibration or sensitivity analysis are infeasible
- Need to pre-built surrogates to replace the model

Key ideas

- *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

Hierarchical Structure of E3SM Land Model

- Land Model is driven by given daily **Forcings** (Precipitation, Min/Max Temp, Radiation) and ~ 50 **Input Parameters** (not known precisely)
- Connections between input parameter, forcings and output QoIs are known *a priori* - we want to use this knowledge for a better NN architecture!

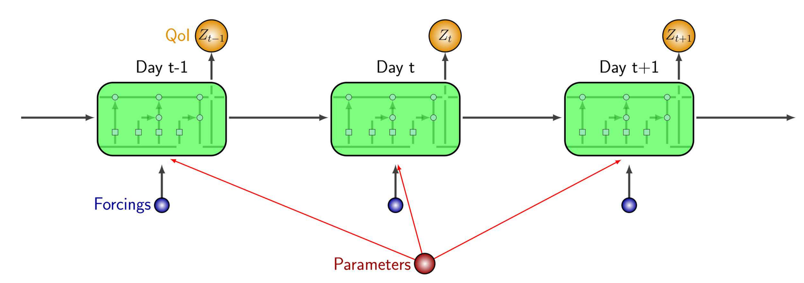


Connectivity of parameters/forcings/outputs

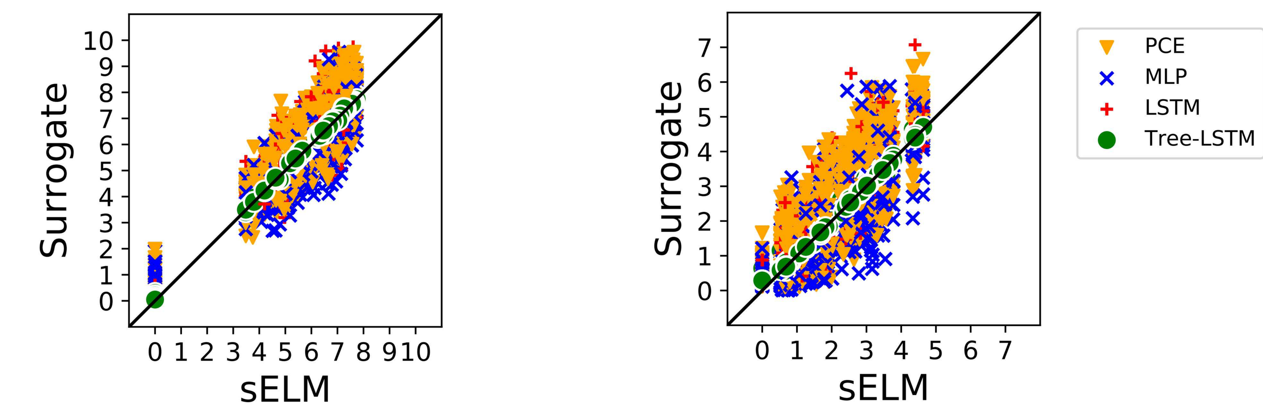
Physics Informed Machine Learning Methodology

Main features

- Land model $Z(x,t;\lambda)$, where x are forcings, t is time, and λ are parameters
- Vanilla LSTM captures time dynamics well
- We developed multiple-QoI network architecture with special connections between QoIs, forcings and parameters, based on code inspection
- Physics-informed Tree LSTM captures known relationships between QoIs and leads to more efficient training
- Flexibility to train on daily or monthly QoIs
- Physics-informed LSTM drastically improves surrogate accuracy

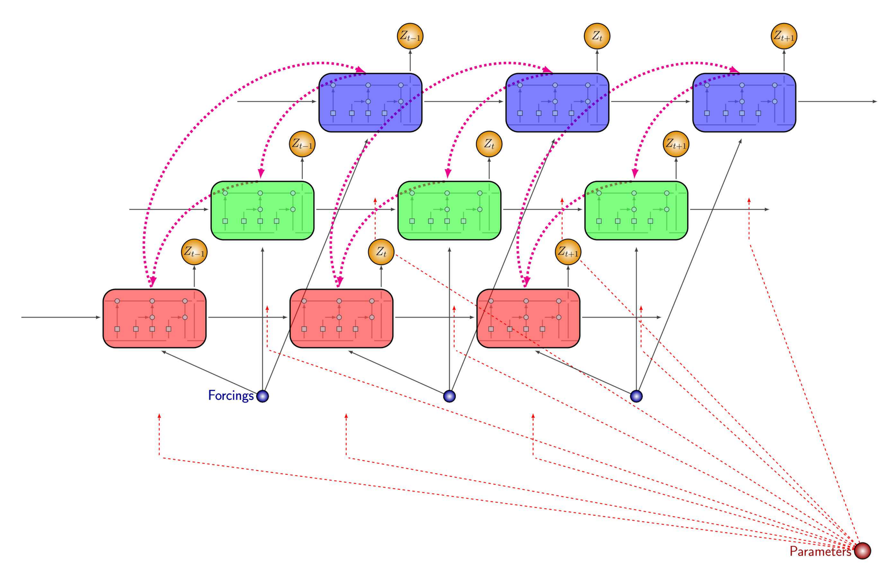


Vanilla LSTM network

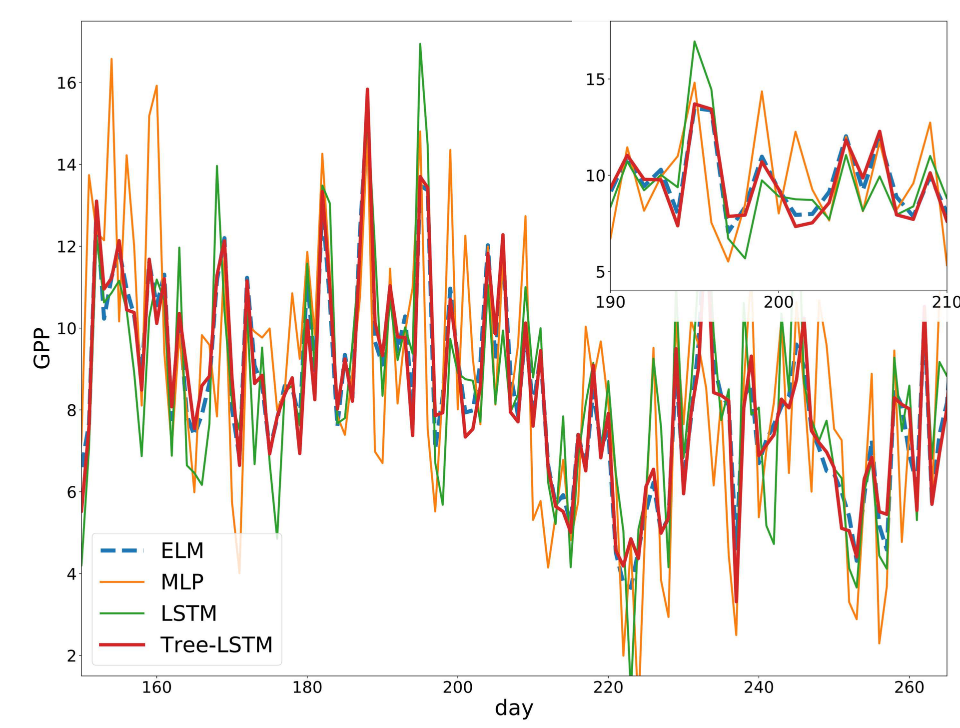


Training details

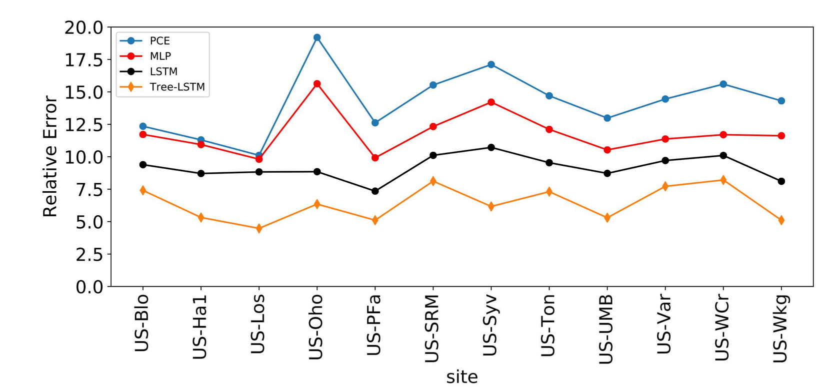
- Trained on simulations at 12 FLUXNET Sites
- Dropout Regularization
- 500 training samples, 500 validation samples
- Hyperparameter optimization on learning rate, number of neurons (~ 150), hidden layers (2 or 3)



Tree-LSTM network builds in custom connections between QoIs, forcings and parameters



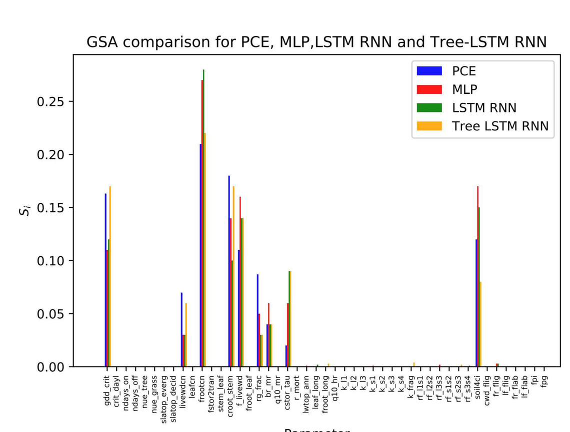
Daily series comparison



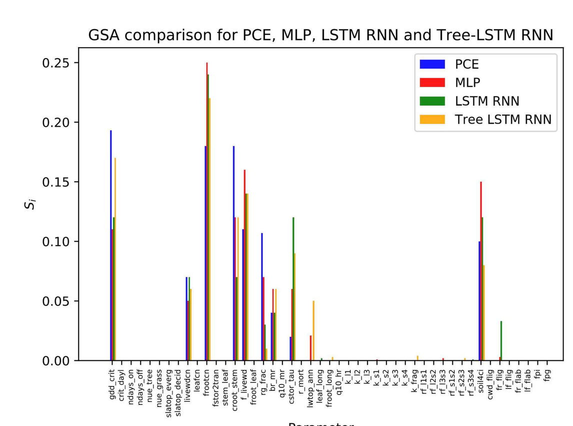
Relative errors for FLUXNET site surrogates

Global Sensitivity Analysis (GSA)

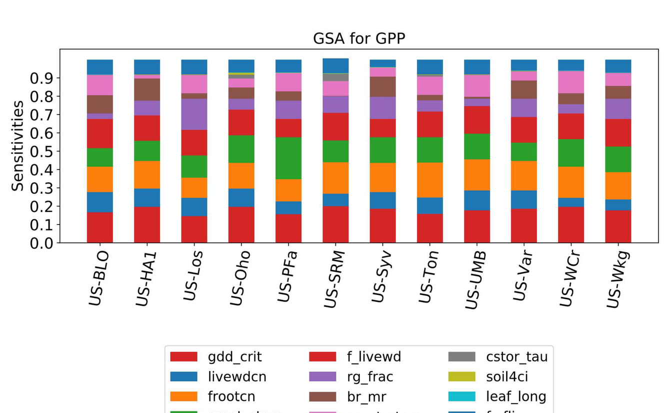
- Monte-Carlo based variance decomposition or Sobol sensitivity computation using NN surrogate, using 3000 samples
- More conventional polynomial chaos surrogate is less accurate but provides sensitivities for free
- Sensitivities are consistent across sites
- Dimensionality reduction: 8 parameters out of 47 with nearly all variance contribution
- Regional surrogates and single-site surrogates produce qualitatively similar sensitivities
- In agreement with the hierarchical nature of the ELM model



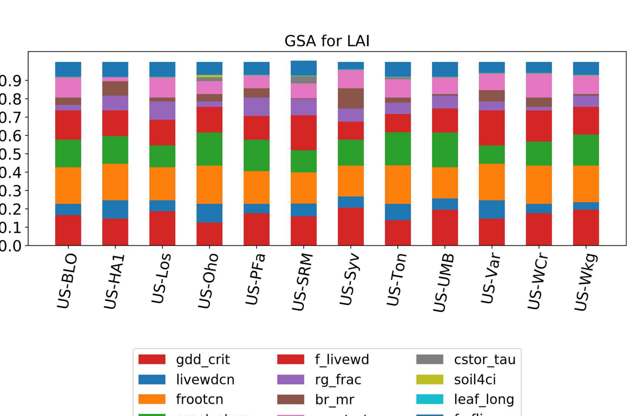
GSA for GPP
US-Harvard single site surrogate



GSA for LAI
US-Harvard regional surrogate



GSA for GPP for all 12 sites



GSA for LAI for all 12 sites

Summary

- Resolving temporal dynamics with LSTM
- Neural network architecture, informed by physics, provides much more accurate surrogates
- Physics-based architecture outperforms conventional LSTM, multilayer perceptron and polynomial chaos
- GSA consistent with prior findings

Current and future work

- Extend to regional surrogate construction
- Use tree-LSTM surrogates for model parameter calibration and design optimization

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research and Office of Biological and Environmental Research, Scientific Discovery through Advanced Computing (SciDAC) program. This research used resources of the National Energy Research Scientific Computing Center (NERSC), a U.S. Department of Energy Office of Science User Facility operated under Contract No. DE-AC02-05CH11231.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. Oak Ridge National Laboratory is managed by UT-BATTELLE for DOE under contract DE-AC05-00OR22725.