Physics-Informed Deep Learning for Multiscale Water Cycle Prediction

Authors

Brenda Ng, ng30@llnl.gov, Lawrence Livermore National Laboratory, ***Machine Learning***

Vidya Samadi, samadi@clemson.edu, Clemson University, ***Hydroinformatics***

Cheng Wang, wangcheng@anl.gov, Argonne National Laboratory, ***Integrated watershed modeling***

Jie Bao, jie.bao@pnnl.gov, Pacific Northwest National Laboratory, ***Surface/subsurface flow modeling***

Focal Area(s)

This paper falls under Focal Area #2: *Predictive modeling through the use of AI techniques and AI-derived model components; the use of AI and other tools to design a prediction system comprising of a hierarchy of models (e.g., AI-driven model/component/parameterization selection)*.

Science Challenge

The goal of this white paper is to advocate the use of physics-informed deep learning techniques to improve the Earth system predictability by implementing a multiscale predictive system for the integrated water cycle, including the relevant processes contributed by atmospheric, terrestrial (above and below ground), oceanic, and human system components.

Rationale

Human actions, driven by agriculture, transportation, domestic and industrial needs, have long been altering the water cycle. In addition to direct alterations (e.g., dams and canals), human-induced climate change is resulting in a catastrophic redistribution of precipitation patterns, resulting in a domino effect of perturbations to surface water flow and energy balance, which in turn exacerbates the situation of droughts, floods and other extreme-weather events.

To raise awareness and inform policies, we need a decision support system that can be used to evaluate the impact of different mitigation strategies. This decision support system will require an integrated and intelligent Earth system predictive framework that couples the geophysical models (e.g., E3SM[1] and CCSM[2]) and transport models (e.g., PFLOTRAN) with deep learning algorithms to extract non-physical insights from multi-source data (e.g., drone/satellite imagery over arid zones, soil surveys, water use

[1] E3SM contains 3 geophysical models: (1) atmosphere, (2) land and energy, and (3) ocean, sea ice, land ice.
[2] CCSM contains 5 geophysical models: (1) atmosphere, (2) sea-ice, (3) land, (4) ocean, and (5) land-ice.

DOI: https://doi.org/10.2172/1769760
DOE BER, AI4ESP 2021 #AI4ESP1100 (https://www.ai4esp.org)

data, etc.). To implement such an integrated prediction system, the following computational challenges must be addressed:

- ***How to efficiently couple the computationally expensive numerical (PDE-based) models that operate at different spatial-temporal scales***: Currently, the geophysical models are generally run in tandem and a "coupler" manages the up- or down-sample required to resolve the resolutions to coordinate information between the models. (E.g., within the E3SMv1, atmosphere and land are modelled by 110 km grid cells, ocean and sea ice by 30-60 km variable grid cells, and river transport by 55 km grid cells.) These couplers require much time and domain expertise to develop. A more scalable (potentially semi-automated) approach to coupling the models is necessary to support the development of a multiscale prediction system.
- ***How to bridge knowledge gaps by leveraging multi-source data***: [Sun et al., 2020] integrated satellite observations and human water use data to understand water storage in North China. [Dadsetan et al., 2020] applied deep-learning-based computer vision methods to high-resolution aerial imagery to identify nutrient deficiency stress in US-based corn and soybean fields. These successful studies reveal that much insights can be gleaned from imagery data. Available big data can be leveraged by the suitable machine learning algorithms (e.g., deep learning) to bridge gaps in knowledge that are not covered by the geophysical or transport models.

Narrative

We propose a hybridization of physics-based models and data-driven prediction to create a physics-inspired deep learning[3] framework. In our proposed framework, neural networks (NNs) will be used to (1) emulate computationally intensive Earth numerical models, as well as (2) extract patterns to bridge knowledge gaps that are not spanned by the numerical models. A hierarchical mesh graph network will be applied to learn the resolution-agnostic dynamics between the components of geophysical models. ***The proposed framework will deliver a machine learning capability to enable an integrated predictive framework that can harness the power of complex physical phenomena, data intelligence, and neural networks, for multiscale water cycle prediction.***

Depending on the way scientific principles inform the design or training of the NNs, physics-based DL is categorized into five classes [Willard et al., 2020]: (1) physics-guided loss function with which the NN is trained; (2) physics-guided initialization of NN parameters prior to training; (3) physics-guided design of NN architecture; (4) residual modeling in which a NN models the discrepancy between the physics-based model and the data; and (5) hybrid physics-DL models that embed the physics-based model directly into an NN, or vice versa. For our proposed framework, we will be focusing on the R&D of class-3 and class-5 methods, e.g., graph neural networks [Scarselli et al., 2008], mesh graph networks

[3] Deep learning (DL) is synonymous with deep neural networks, which are neural networks with many layers between the input and output layers.

[Pfaff et al., 2021], neural ODEs [Chen et al., 2018], universal differential equations [Raukauckas et al., 2020] and implicit layers [Zhang et al., 2020], as the DL components in the proposed framework.

The technical approach is outlined as follows:

- A relevant set of geophysical (numerical) models from open-source efforts would be identified. These models would be partitioned into an *analytic* set (i.e., models which would be called by the framework) and an *approximate* set (i.e., models which would be replaced by fast surrogates).
- Within the approximate set, surrogate models would have to be developed to replace the computationally expensive models. Depending on the degree of “first-principles preservation”, the specific form of the surrogate might range from a NN (purely data- driven) to a universal differential equation (preserving some first principles but using NNs to learn missing terms in the governing equations). A universal differential equation is a neural ODE that incorporates physics structure. A neural ODE is the continuous limit of a residual NN, and can naturally handle irregularly-sampled data.
- To couple the models within the analytic and approximate sets, we would apply a “backbone” mesh graph network (MGN) to learn the *inter-model* interactions from available open-source data from NOAA, NASA, USGS, etc. The mesh graph network (MGN) is a cutting-edge deep learning model that uses adaptive meshes and graph neural networks (GNNs) to efficiently learn and produce mesh-based simulations at variable resolutions. Like a GNN, an MGN represents a complex system as a graph that encapsulates the state of the system and uses message-passing to update the graph to reflect changes in the system. An MGN learns resolution-independent dynamics, which makes it the ideal “coupler” between the geophysical models, since up- and down-sample would no longer be required to sync up the geophysical models of different resolutions.

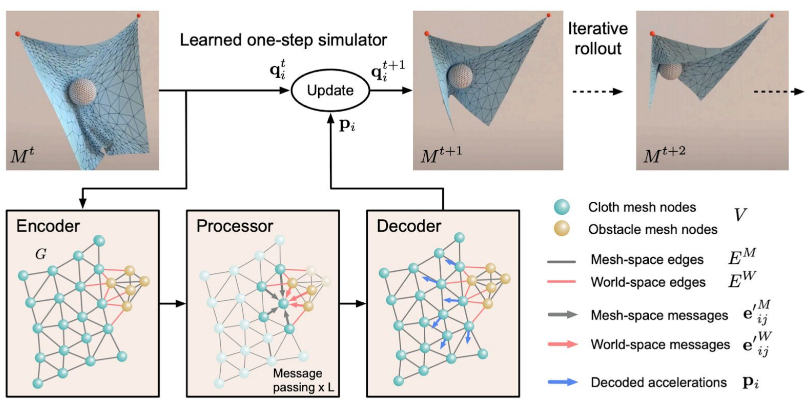

Figure 1. Schematic of MeshGraphNets (MGN) [Pfaff et al., 2021]

The code developed under this proposed effort will be open-source to encourage collaborative development by the hydrology, climate and the machine learning communities. This work will follow FAIR principles applied to software: We will host the code on Github to ensure findability and accessibility. For interoperability, our documentation will include a list of dependencies (e.g., external geophysical libraries) with instructions for their installation. For reusability, we would release the weights (i.e., trained parameters) to our DL components so others may reproduce our results.

Physics-Informed Deep Learning for Multiscale Water Cycle Prediction

Suggested Partners/Experts

- **Dr. Chris Rackaukas**, contact@chrisrackauckas.com, MIT, ***Scientific Machine Learning***
- **Dr. David Gochis**, gochis@ucar.edu, National Center for Atmospheric Research, ***Hydrometeorology***
- **Dr. Chaopeng Shen**, cshen@engr.psu.edu, Penn State Univ, ***Hydrologist & Machine Learning***
- **Dr. Alex Tartakovsky**, amt1998@illinois.edu, UIUC, ***Flow and Transport Modeling & Machine Learning***
- **Dr. Glenn Hammond**, glenn.hammond@pnnl.gov, PNNL, ***Lead Developer for PFLOTRAN***
- **Dr. Amy McGovern**, amcgovern@ou.edu, Univ of Oklahoma, ***Director of AI2ES***
- **Dr. Christa Peters-Lidard**, christa.d.peters-lidard@nasa.gov, NASA, ***Deputy Director for Hydrosphere, Biosphere, and Geophysics in the Earth Sciences Division***