Literature review: GNN-Surrogate: A Hierarchical and Adaptive Graph Neural Network for Parameter Space Exploration of Unstructured-Mesh Ocean Simulations

Motivation

Problem

Explore the parameter space of ocean climate simulations.
Model for simulation of the global ocean system: MPAS-Ocean
Parameter space exploration is important for domain scientists to understand the influence of input parameters (e.g., wind stress) on the simulation output (e.g., temperature).

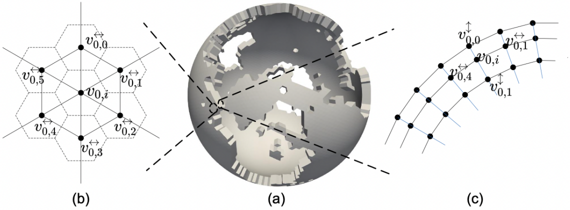


Fig. 1. (a) MPAS-Ocean's structure. (b) Horizontal Voronoi polygons. Dashed lines form Voronoi polygons. $v_{0,i}$, $v^{\leftrightarrow}_{0,0}$, $v^{\leftrightarrow}_{0,1}$, $v^{\leftrightarrow}_{0,2}$, $v^{\leftrightarrow}_{0,3}$, $v^{\leftrightarrow}_{0,4}$, $v^{\leftrightarrow}_{0,5}$ are Voronoi polygon cell centers. Solid lines link cell centers. (c) Cross section. $v^{\updownarrow}_{0,0}$, $v^{\updownarrow}_{0,1}$ are $v_{0,i}$'s vertical neighbors. Blue lines link vertical neighbors.

Motivation

- large problem size: 15-model-day ocean simulations; 60 horizontal layers; each layer 235,160 Voronoi cells; 1.00 GB space; 50 minutes to directly compute the simulation output on CPUs.
- EC60to30 [26] mesh, the grids' cell sizes vary from 30km to 60km. **unstructured-mesh simulations**

Existing parameter space exploration work

- Traditional parameter space exploration: first collect the simulation input and output pairs from ensemble runs, and perform parameter space exploration on the collected pairs.
- Surrogate models: 1. the image level, InSituNet (simulation output is only visualized with several predefined visual mappings)
  2. the data level, machine learning, gaussian process (only on regular grids.)

Graph Neural Networks surrogate

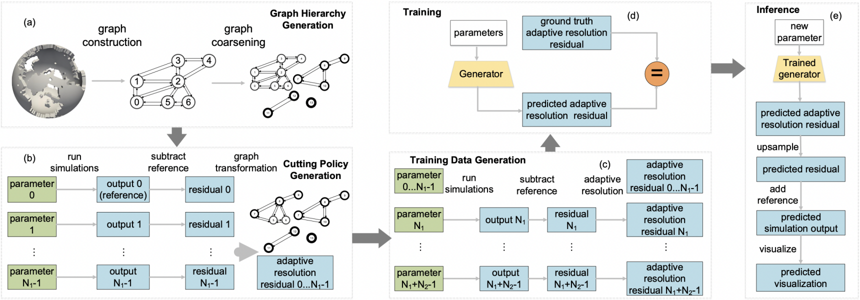
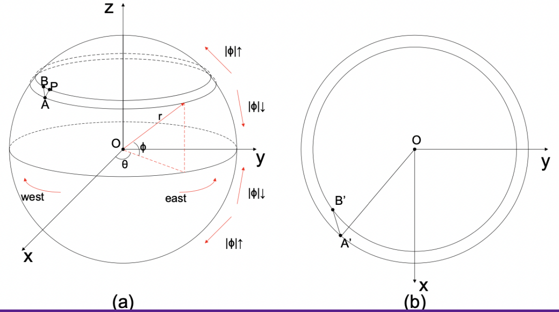


Fig. 2. Workflow of our approach. (a) Given the MPAS-Ocean mesh structure, a corresponding graph hierarchy is generated. (b) A few simulations are run for generating the graph hierarchy cutting policy. The cutting policy is used to guide representing the simulation output with adaptive resolutions. (c) Another batch of ensemble simulations is run for collecting the training data. (d) A deep surrogate model (i.e., GNN-Surrogate) is trained based on the generated training dataset. (e) In the inference stage, GNN-Surrogate is used to predict the simulation output. The predicted simulation output can be visualized later for parameter space exploration.

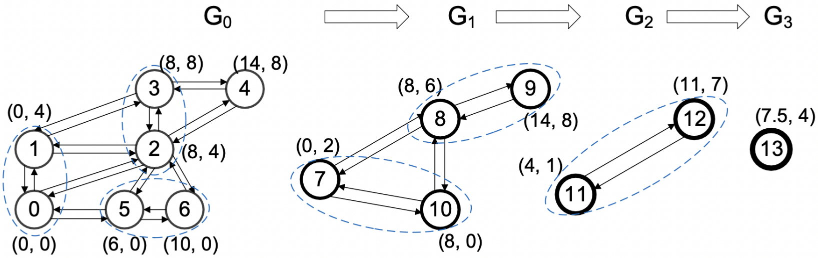
1. HIERARCHICAL GRAPHS FOR DATA WITH ADAPTIVE RESOLUTIONS

- $F(P_{sim}) = F_{ar\rightarrow s}(F_{p\rightarrow ar}(P_{sim}))$
- Use hierarchical graphs $(G0, G1, G2, ...)$ to represent outputs with adaptive resolutions.
- $G_0 = (V_0, E_0)$: built on the meshes with full resolution.
- node $v_{0,i}$ is defined as a variable of interest (cell-centered) such as temperature. Cartesian coordinate & spherical coordinate
- Edges are decomposed into horizontal edges and vertical edges. $E_0 = E_0^{\leftrightarrow} \cup E_0^{\updownarrow}$



Graph coarsening

The graph coarsening operation receives an input graph Gl and outputs the next level coarser graph G_{l+1} which has fewer nodes and edges but preserves the input graph's topological structures. Repeat until get a single node.

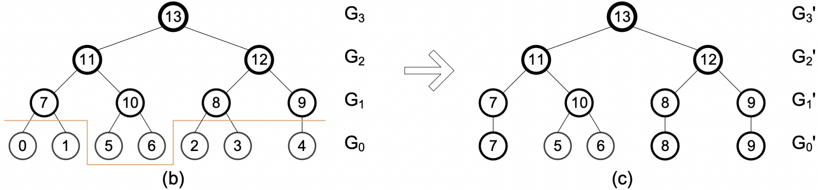


(a)

1. HIERARCHICAL GRAPHS FOR DATA WITH ADAPTIVE RESOLUTIONS

Graph hierarchical tree cutting.

For each simulation output residual, cut where computation and memory are reduced to support training GNN-Surrogate given limited computing resources. Node $v_{l,j}$ is cut after the integration only if its parent has the approximating ability for all the residuals.



2. ARCHITECTURE AND OPERATIONS

Perform linear transformation for the input feature map by dense matrix-vector multiplication; the weighted sum by sparse matrix-vector multiplication; matrix multiplication operations in parallel by PyTorch Sparse library.

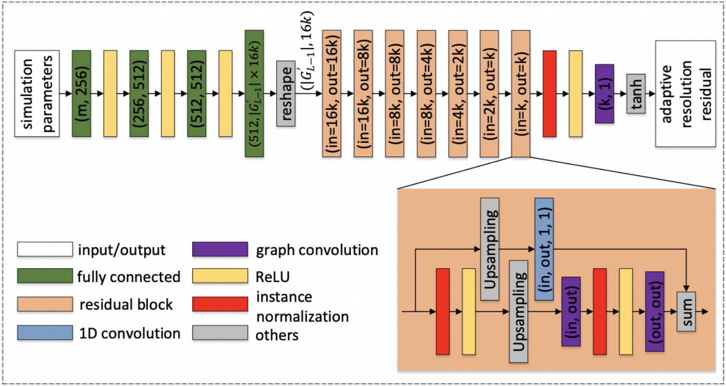
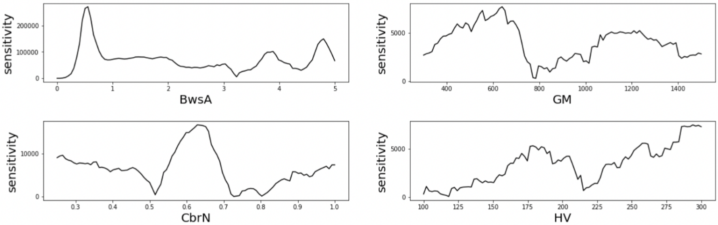


Fig. 7. Upsampling-convolution generator architecture of GNN-Surrogate.

Sensitivity Analysis

We aggregate the predicted field (e.g., L1 norm of the data values) to obtain a scalar value and compute the **derivative** of that scalar value with respect to one selected parameter.



$BwsA > CrbN > GM > HV$

EXPERIMENTS

Study the impact of four parameters (BwsA, CrbN, GM, HV) on output.

- 100 parameter settings from the parameter space, 70 training (N1=16), 30 testing; 15-model-day ocean simulations, grids with EC60to30 resolution (repres. temperature).
- Each mesh structure 60 horizontal layers, each layer 235,160 Voronoi cells; One generated ensemble member takes 1.00 GB space with a temperature field of size 107.65 MB within it.
- training and testing: on one NVIDIA Volta V100 GPU 16GB. training time to 36 hours
- a single forward pass through the trained GNN-Surrogate: ¡2s; direct simulation on cluster CPUs: 50 mins.
- Metrics: Data-level metrics (PSNR, MD); Geometry-level metrics (ITL); Image-level metrics (Structural similarity index measure (SSIM) and earth mover's distance (EMD) between color histograms); both global and specific regions of interest (ROI)

EXPERIMENTS

TABLE I

Quantitative comparison of the output predicted with GNN-Surrogate, radial basis function (RBF) interpolation, and inverse distance weighting (IDW) interpolation.

	GNN-Surrogate	IDW Interp	RBF Interp
PSNR (global, dB)	**50.7, 2.52**	47.7, 5.72	32.43, 8.91
MD (global)	0.1965, 0.0415	0.1721, 0.0562	**0.1397, 0.0398**
PSNR (ROI, dB)	**39.5, 3.06**	33.6, 6.03	27.43, 7.27
MD (ROI)	0.1774, **0.0332**	0.1673, 0.0672	**0.1573**, 0.0605
params (GB)	**2.18**	7.18	10.27

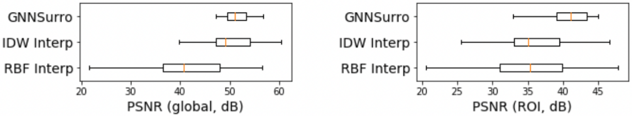


Fig. 8. The box plot showing the PSNR deviation on global and ROI temperature maps from 30 different testing ensemble members.