ETH zürich

Department of Mathematics
Computational Science Engineering

Semester Project Kick off meeting

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21-09

Outline

1. Introduction
2. Background
3. Methodology
4. Experiment
5. Future work

Outline

Finite Element Analysis

Strong Form : $\nabla \cdot \sigma(\varepsilon) + f = \rho \frac{\partial^2 u}{\partial t^2}$

Weak form : $\int_\Omega \sigma : \nabla v + b \cdot v \mathrm{d}\Omega - \int_{\partial\Omega} (\sigma \cdot n) \cdot v \mathrm{d}S = \rho \int_\Omega \frac{\partial^2 u}{\partial t^2} \cdot v \mathrm{d}\Omega$

Galerkin discretilization : $K_{ij} = \int_\Omega \sigma(\sum u_i \phi_i) : \nabla \psi_j + b \cdot \psi_j \mathrm{d}\Omega \quad \phi_i = N_i, \psi_j = N_j$

- σ stress, it's a function of strain $\sigma(\varepsilon)$
  Lame's approximation:
  $\sigma = \lambda \mathrm{Tr}(\varepsilon) I + 2\mu\varepsilon \quad \lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}, \mu = \frac{E}{1+2\nu}$
- ε strain, $\varepsilon = \nabla u$
- : double contraction, $\sigma : \nabla v = \nabla v^\top \cdot \sigma \cdot \nabla v \quad \sigma \in \mathbb{R}^{d \times d}, \nabla v \in \mathbb{R}^d$
- bilinear form : $a(u, v) = \int_\Omega \sigma(\varepsilon) : \nabla v + b \cdot v \mathrm{d}\Omega$ and linear form : $\ell(v) = \int_{\partial\Omega} (\sigma \cdot n) \cdot \mathrm{d}S$

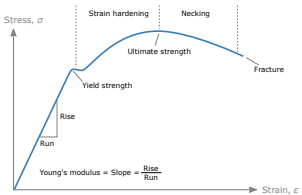


Figure: stress-strain relation

Linear Case

When **Dirichlet Boundary Condition** applied to mesh $\mathcal{M}$, $u_B, K, f \rightarrow u_I$

$$\begin{bmatrix} K_{II} & K_{IB} \\ K_{IB}^\top & K_{BB} \end{bmatrix} \begin{bmatrix} u_I \\ u_B \end{bmatrix} = \begin{bmatrix} f_I \\ f_B \end{bmatrix} \rightarrow K_{II} x_I = f_I - K_{IB} x_B$$

- $A_{\{II,BB,IB\}}$: Galerkin matrix for interior/boundary/interior-boundary connection
  - element matrix : $K_e = \int_\Omega B_e^\top D_e B_e \mathrm{d}\Omega$
  - B : Strain-Displacement Matrix, $\varepsilon = Bu = \frac{1}{2}(\nabla u + \nabla u^\top)$
    - Triangle Element : $B = \begin{bmatrix} \frac{\partial N_1}{\partial x} & 0 & \frac{\partial N_2}{\partial x} & 0 & \frac{\partial N_3}{\partial x} & 0 \\ 0 & \frac{\partial N_1}{\partial y} & 0 & \frac{\partial N_2}{\partial y} & 0 & \frac{\partial N_3}{\partial y} \\ \frac{\partial N_1}{\partial y} & \frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial y} & \frac{\partial N_2}{\partial x} & \frac{\partial N_3}{\partial y} & \frac{\partial N_3}{\partial x} \end{bmatrix} \quad \varepsilon = \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ 2\varepsilon_{xy} \end{bmatrix}$
  - D : Material's Constitutive (Elasticity) Matrix, $\sigma = D\varepsilon = DBu$
    - Triangle Element : $D = \frac{E}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & 0 \\ \nu & 1-\nu & 0 \\ 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix}$
- $u_{\{I,B\}}$: displacement for interior/boundary nodes
- $f_{\{I,B\}}$: applied force for interior/ boundary nodes

GNN view

Traditional Case:

$$Ku = f \Leftrightarrow u = \text{GNN}(A, f) \quad A_{ij} = K_{ij} > 0$$

considering **Dirichlet Boundary Condition**

$$K_{II}u_I = f_I - K_{IB}u_B \Leftrightarrow u_I = \text{GNN}(A_{II}, f_I - A_{IB}u_B)$$

Neumann Boundary Condition and Radiation Boundary can be coupled in the PDE form, which is simulated by the GNN

GNN is used as an inverse operator/sparse linear system solver

Traditional sparse linear system solver method: LUsparse, conjugated gradient .etc

Chanllege and Purpose

1. Theoretical proof of boundary condition GNN for FEM
2. End2end GNN framework applied to Dirichlet Boundary Condition
3. Better precision
4. Faster speed, larger scale (distributed, and even on disk)
5. Non-Lame's approximation

Outline

Graph Neural Network

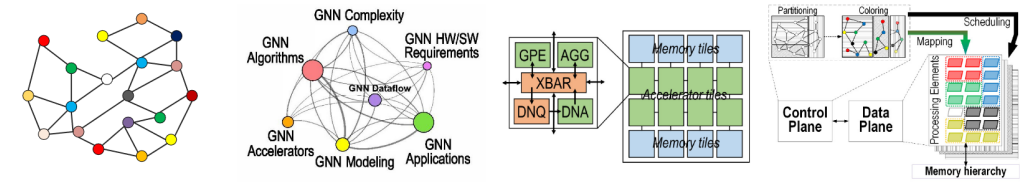


Figure: Graph Neural Network Survey: Algorithms, Application, Modeling, Accelerators [1]

Large Scale Graph Neural Network(1/4)

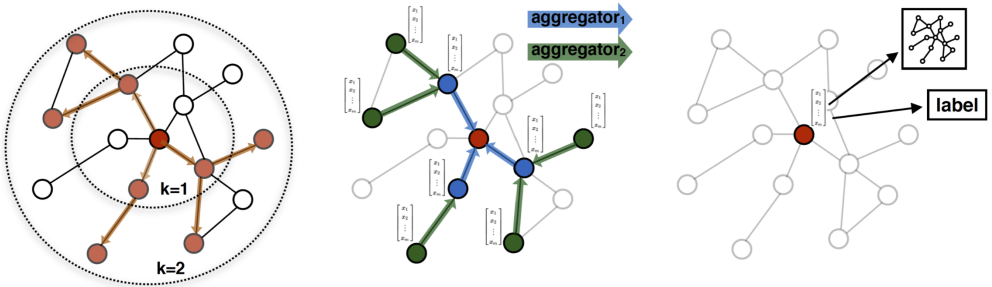


Figure: GraphSAGE:Sample K-hop neighbors to train as large graph [12]

Large Scale Graph Neural Network(2/4)

GraphSAINT: Sample random subgraph by weight to train as large graph [22]

- Aggregation : $\xi_v^{l+1} = \sum_{u \in \mathcal{N}(v)} \frac{\mathbf{A}_{u,v}}{\alpha_{u,v}} x_u^l \quad \alpha_{u,v} = \frac{p_{u,v}}{p_v}, p_{u,v} \propto \frac{1}{\text{deg}(u)} + \frac{1}{\text{deg}(v)}$
- Loss function : $\mathbb{E}[L] = \frac{1}{|\mathbb{G}|} \sum_{\mathcal{G}_s \in \mathbb{G}} \sum_{v \in \mathcal{V}_s} \frac{L_v}{\lambda_v} \quad \lambda_v = |\mathcal{V}| \cdot p_v$

Require: Training graph $G(V, E, X)$; Labels Y; Sampler SAMPLE
Ensure: GCN model with trained weights
1: **Pre-processing:** Setup SAMPLE parameters; Compute normalization coefficients α, λ.
2: **for** each minibatch **do**
3: $Gs(Vs, Es) \leftarrow$ Sampled sub-graph of G according to SAMPLE
4: GCN construction on Gs.
5: $\{y_v | v \in Vs\} \leftarrow$ Forward propagation of $\{x_v | v \in Vs\}$, normalized by α
6: Backward propagation from λ-normalized loss $L(y_v, y_v)$. Update weights.
7: **end for**

Large Scale Graph Neural Network(3/4)

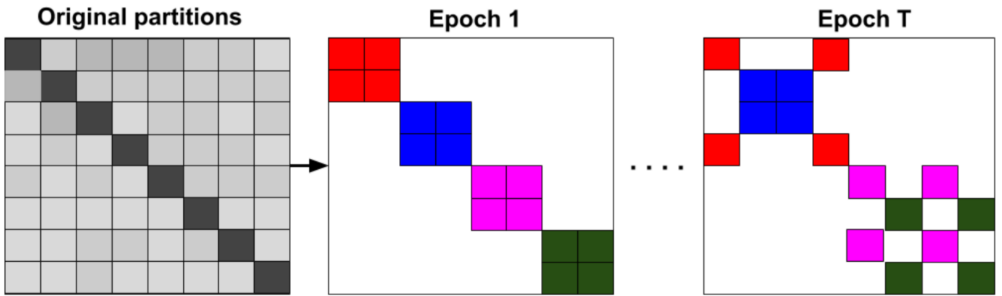


Figure: ClusterGCN:Partition Graph Manually rather than sample [12], commonly by METIS [14]

Large Scale Graph Neural Network(4/4)

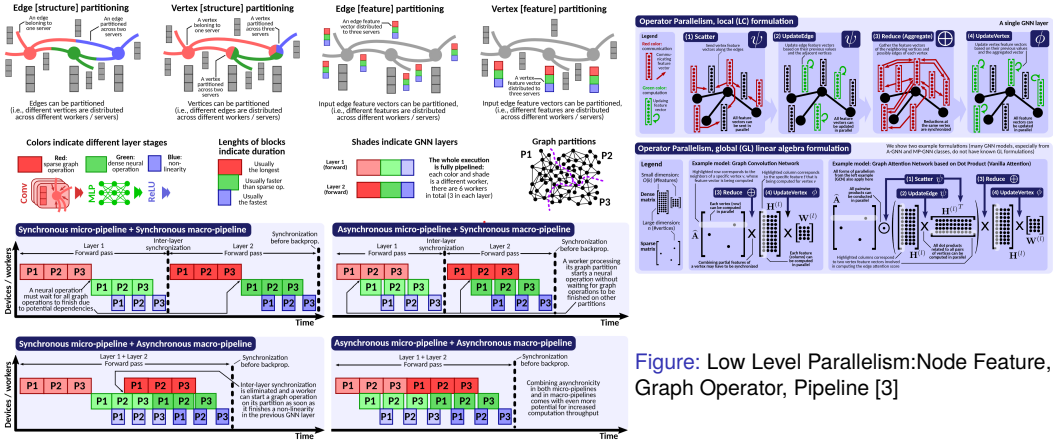


Figure: Low Level Parallelism:Node Feature, Graph Operator, Pipeline [3]

GNN for FEM(1/2)

- No Neighbor Explosion
- No super node

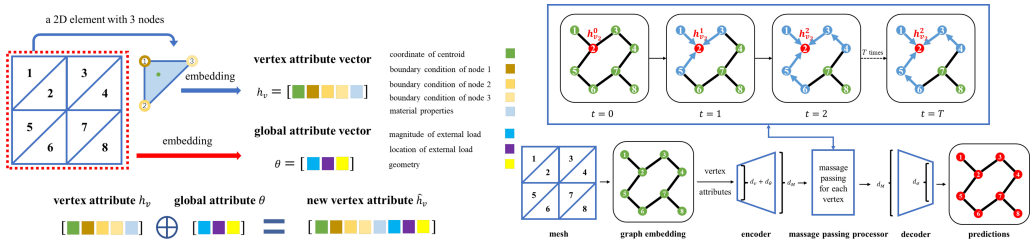


Figure: Encoder-Decoder structure [13]

- encoder-decoder structure
- element as node (FVM)

GNN for FEM(2/2)

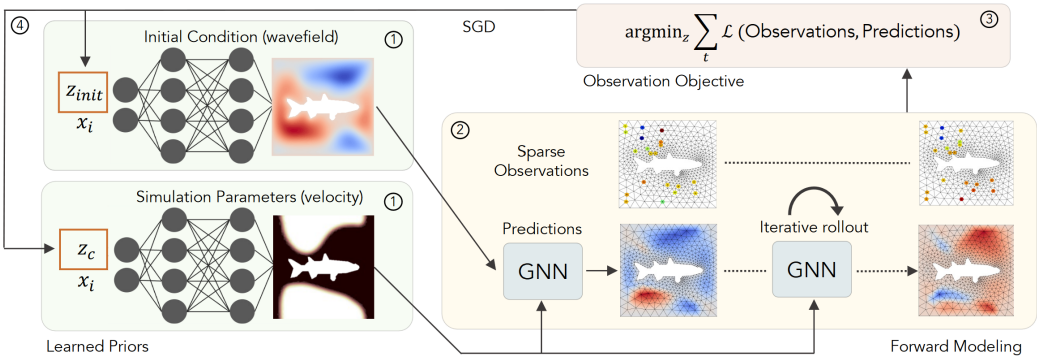


Figure: Inverse Problem [16]

- focus on inverse time sequencing problem
- data driven

GNN for FEM DBC(1/2)

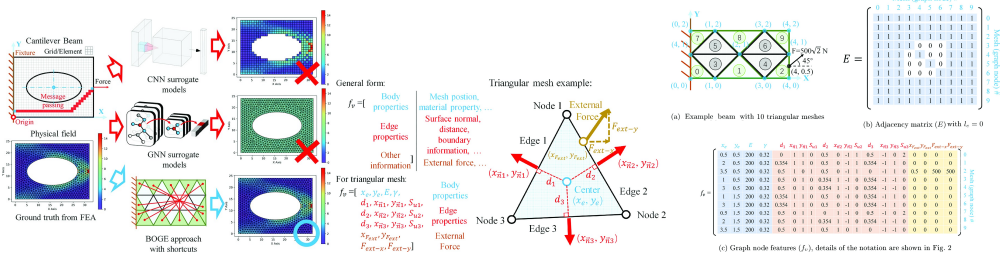


Figure: Fully Connected Solution: each $(v_i, v_j) \in \hat{\mathcal{E}} \quad \forall v_i \in \mathcal{M}_I \quad \forall v_j \in \mathcal{M}_B$, interior nodes and boundary nodes fully connected, element as node in graph [9]

GNN for FEM DBC(2/2)

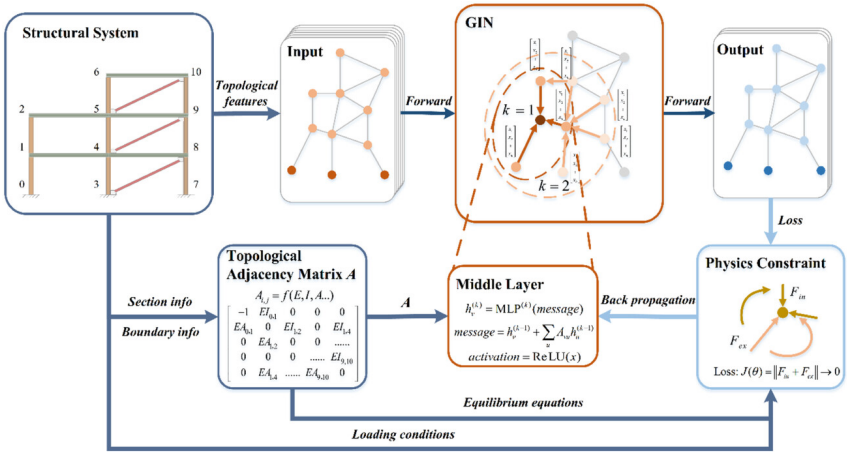


Figure: Physics Informed: $\|f_I + f_B\| = 0$, node as node in graph [20]

Graph Pooling(1/4)

Method	**Select**	**(Feature) Reduce**	(Edge) Connect
DiffPool [21]	$\mathbf{S} = \text{GNN}_1(\mathbf{A}, \mathbf{X})$	$\mathbf{X}' = \mathbf{S}^\top \cdot \text{GNN}_2(\mathbf{A}, \mathbf{X})$	$\mathbf{A}' = \mathbf{S}^\top \mathbf{A} \mathbf{S}$
MinCut [4]	$\mathbf{S} = \text{MLP}(\mathbf{X})$	$\mathbf{X}' = \mathbf{S}^\top \mathbf{X}$	$\mathbf{A}' = \mathbf{S}^\top \mathbf{A} \mathbf{S}$
NMF [2]	Factorize : $\mathbf{A} = \mathbf{W}\mathbf{H} \rightarrow \mathbf{S} = \mathbf{H}^\top$	$\mathbf{X}' = \mathbf{S}^\top \mathbf{X}$	$\mathbf{A}' = \mathbf{S}^\top \mathbf{A} \mathbf{S}$
LaPool [19]	$\begin{cases} \mathbf{V} = \lvert\mathbf{L}\mathbf{X}\rvert_d \\ \mathbf{i} = \{i \lvert \forall j \in \mathcal{N}(i) : \mathbf{V}_i > \mathbf{V}_j\} \\ \mathbf{S} = \text{SparseMax}\left(\beta \frac{\mathbf{X}\mathbf{X}_\mathbf{i}^\top}{\lVert\mathbf{X}\rVert \lVert\mathbf{X}_\mathbf{i}\rVert}\right) \end{cases}$	$\mathbf{X}' = \mathbf{S}^\top \mathbf{X}$	$\mathbf{A}' = \mathbf{S}^\top \mathbf{A} \mathbf{S}$
Graclus [7]	$S_k = \left\{ \mathbf{x}_i, \mathbf{x}_j \middle\vert \underset{j}{\text{argmax}} \left(\frac{\mathbf{A}_{ij}}{\mathbf{D}_{ii}} + \frac{\mathbf{A}_{ij}}{\mathbf{D}_{jj}} \right) \right\}$	$\mathbf{X}' = \mathbf{S}^\top \mathbf{X}$	METIS [14]
NDP [5]	$\mathbf{i} = \{i \lvert u_{max,i} > 0\}$	$\mathbf{X}' = \mathbf{X}_\mathbf{i}$	Kron [8]
Top-K	$y = \frac{\mathbf{X}\mathbf{p}}{\lVert\mathbf{p}\rVert}; \mathbf{i} = \text{top}_K(y)$	$\mathbf{X}' = (\mathbf{X} \odot \sigma(y))_\mathbf{i}$	$\mathbf{A}' = \mathbf{A}_{\mathbf{i},\mathbf{i}}$
SAGPool [15]	$y = \text{GNN}(\mathbf{A}, \mathbf{X}); \mathbf{i} = \text{top}_K(y)$	$\mathbf{X}' = (\mathbf{X} \odot \sigma(y))_\mathbf{i}$	$\mathbf{A}' = \mathbf{A}_{i,i}$

Table: Incomplete Summary of Graph Pooling [18, 11]

Graph Pooling(2/4)

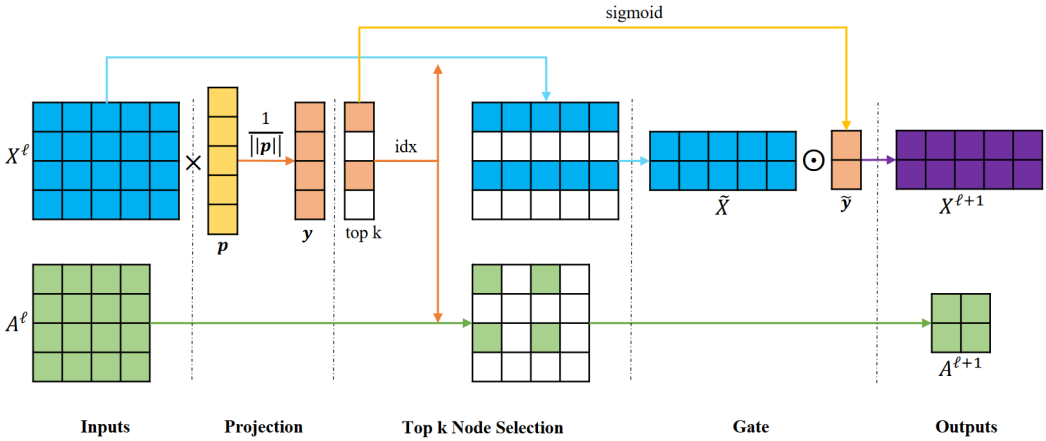
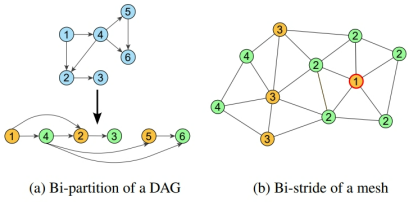


Figure: Naive Pooling [10]

Graph Pooling(3/4)



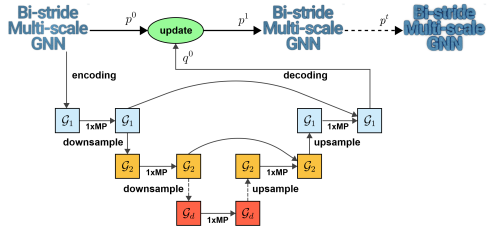
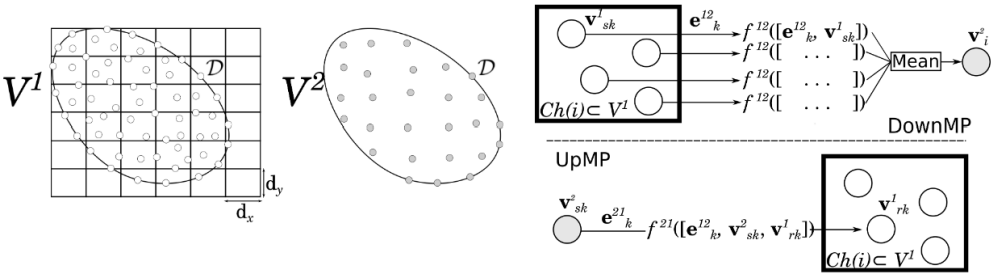


Figure: 2-Strided Pooling [6]

Graph Pooling(4/4)



(a) Building V^2 from V^1 (b) DownMP and UpMP layers

Figure: Rasterization Pooling [17]

- Also U-Net structure
- Looks like Particle To Cell method (widely used in N-body problem simulation)

Outline

Methodology

- GNN Introduction
- How FEM different boundary condition be tackled
- How our method work(Sampled Graph U Net)

Outline

Experiment

- Strain-Stress precision and baseline comparison
- Case study on airfoil example
- Parameter Sensitivity
- Speed/Memory Comparation(and compare with FEM)
- Topology Optimization? $z = \underset{z}{\text{argmin}} \sum_{e=1}^{N} (z_e)^p u_e^\top A_e u_e \quad z_e > 0$

Outline

Future work

- FEM for Structure Engineering Benchmark / Leaderboard?
- FEM for torch

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The current project description is available at walkerchi.github.io/ETHz-SP/kickoff

D MATH

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