Tencent AI Lab

GeoEnsemble for Open Catalyst Challenge 2022

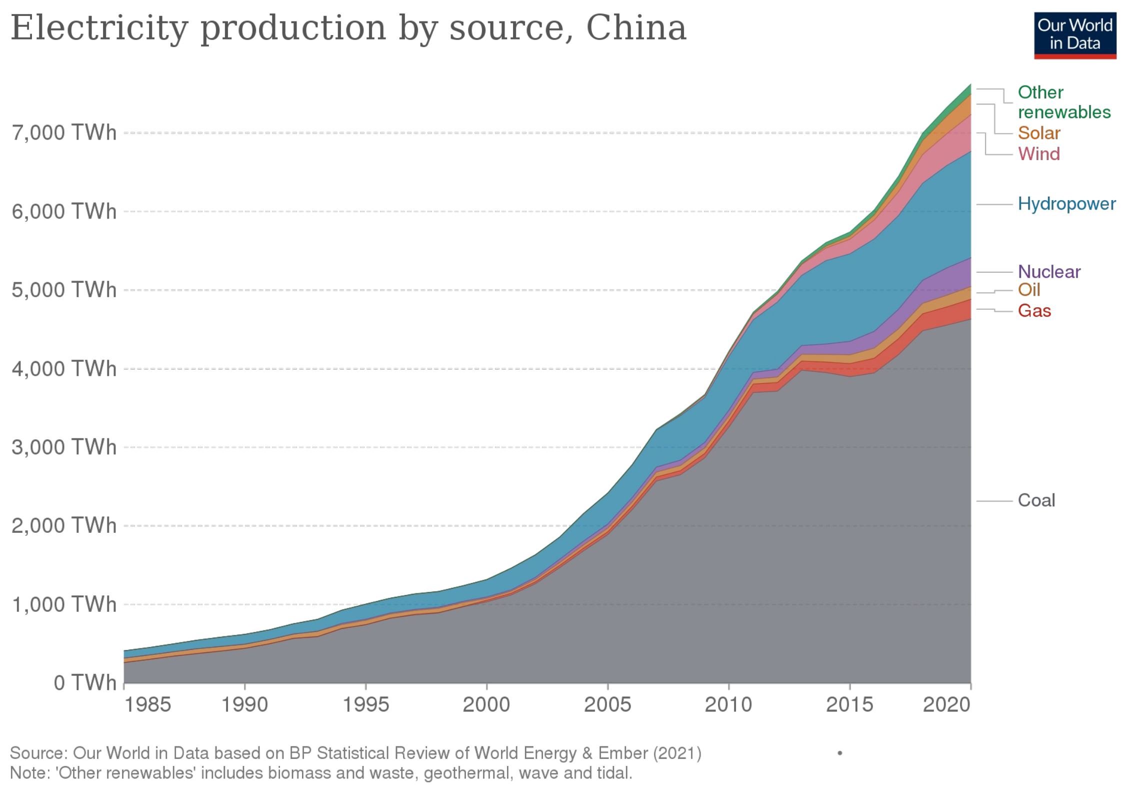
Jiaqi Han (intern) , Tian Bian (intern), Geyan Ye, Kaili Ma (intern), Yuduo Zhi, Kangfei Zhao, Tingyang Xu, Wenbing Huang, Yu Rong

Tencent AI Lab
Tsinghua University
Renmin University of China
The Chinese University of Hong Kong,

清華大學 Tsinghua University
香港中文大學 The Chinese University of Hong Kong
中国人民大學 RENMIN UNIVERSITY OF CHINA

Energy Scarcity and Climate Change

- **Energy Scarcity and Climate Change**

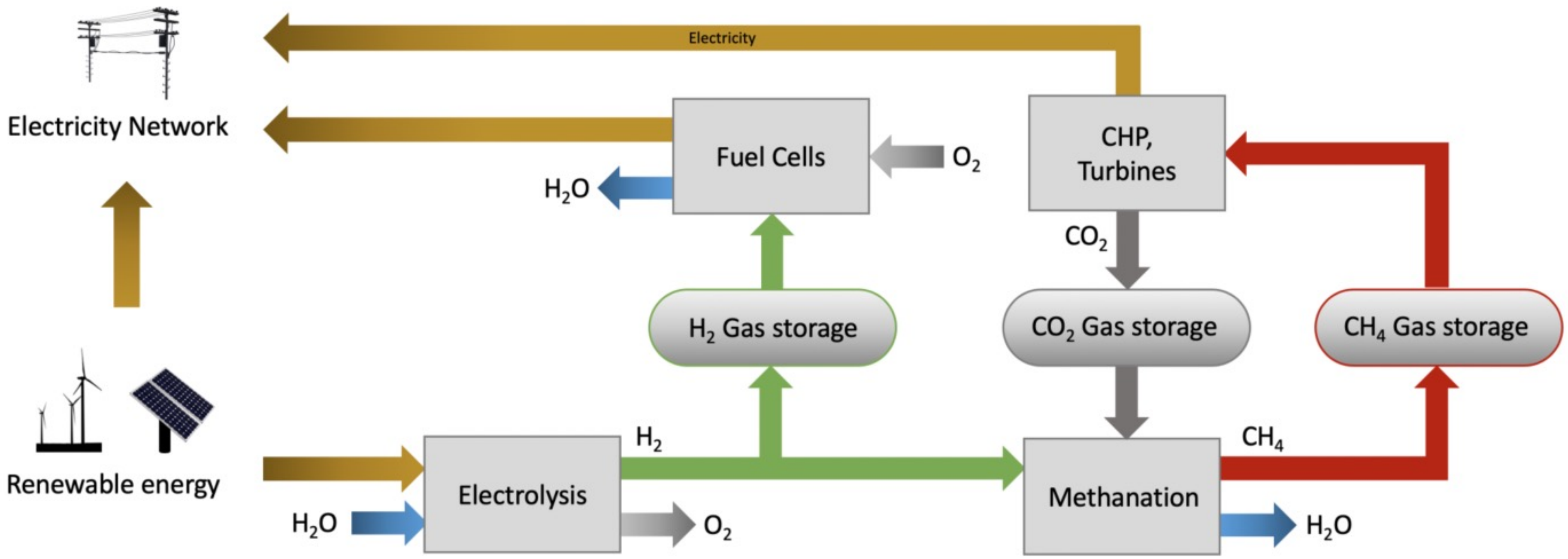


Wind farm in Xinjiang, China

[1] https://en.wikipedia.org/wiki/Electricity_sector_in_China

Energy Scarcity and Climate Change

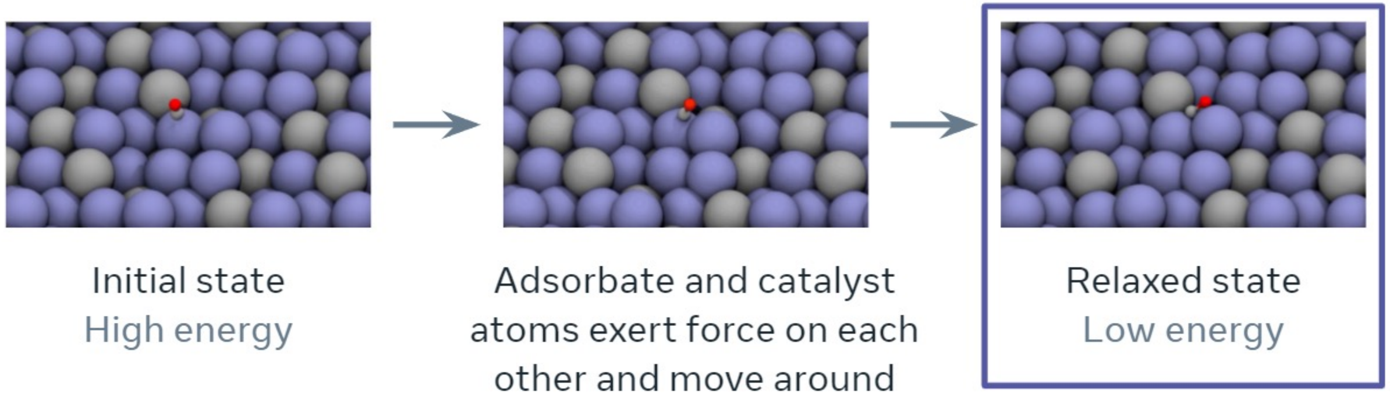
- **Discovery of catalyst for Efficient Energy Storage**



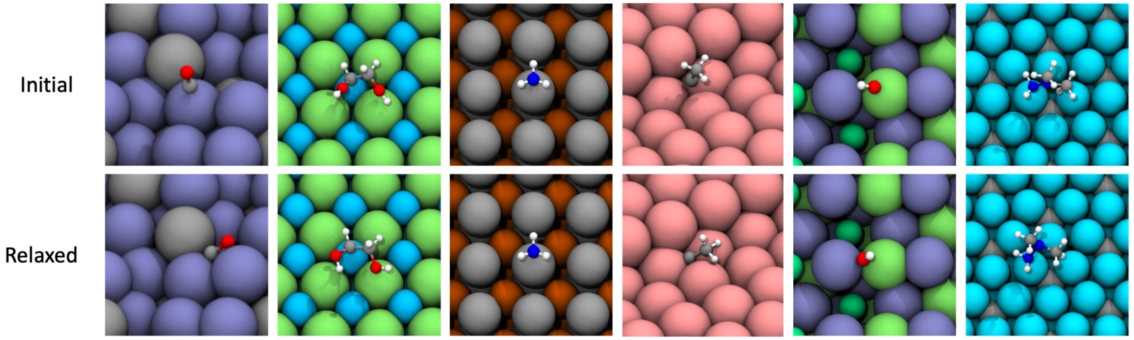
[2] Zitnick C L, Chanussot L, Das A, et al. An introduction to electrocatalyst design using machine learning for renewable energy storage[J]. arXiv preprint arXiv:2010.09435, 2020.

Energy Scarcity and Climate Change

- **Discovery of catalyst for Efficient Energy Storage**



Can be used to determine reaction rate



[3] https://github.com/Open-Catalyst-Project/ocp/blob/main/tutorials/OCP_Tutorial.ipynb.
[4] Zitnick C L, Chanussot L, Das A, et al. An introduction to electrocatalyst design using machine learning for renewable energy storage[J]. arXiv preprint arXiv:2010.09435, 2020.

Challenges

How to model the complex mechanisms of the dynamics of particles ?

How to incorporate the S2EF and IS2RE data.

GMN-OC: Adaptation of GMN on OC data

- Basic layers:

Universal multi-channel O(3)-equivariant function[1]:

$$\varphi(\vec{Z}, h) = \vec{Z}\sigma(\vec{Z}^\top \vec{Z}, h), \quad \text{(O(3)-equivariant case)}$$

$$\psi(\vec{Z}, h) = \gamma(\vec{Z}^\top \vec{Z}, h). \quad \text{(O(3)-invariant case)}$$

GMN Layer:

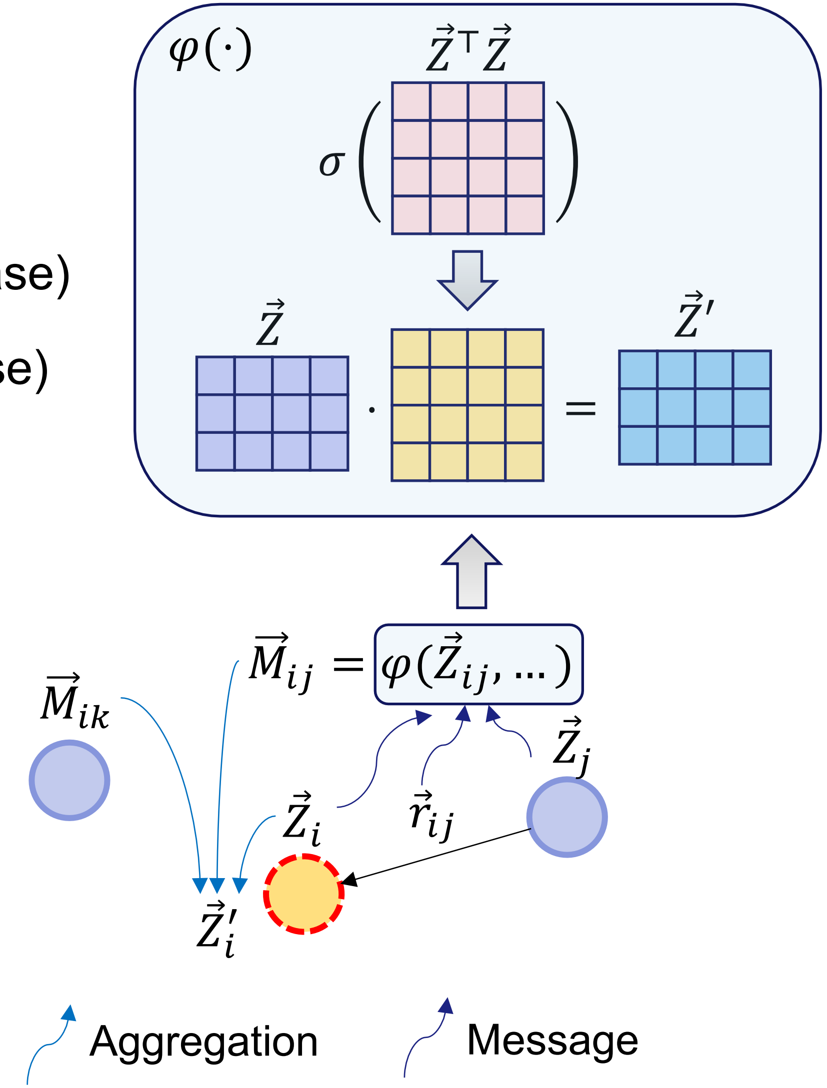
$$\vec{Z}_{ij} = [\vec{Z}_i - \vec{Z}_j, \vec{r}_{ij}],$$

$$h_{ij} = [h_i, h_j, G(||\vec{r}_{ij}||)],$$

$$\vec{M}_{ij} = \varphi(\vec{Z}_{ij}, h_{ij}),$$

$$\vec{Z}_i' = \vec{Z}_i + \sum_{j \in \mathcal{N}(i)} \vec{M}_{ij}.$$

$G(\cdot)$: Guassian basis function



[1] Wenbing Huang*, Jiaqi Han*, Yu Rong, Tingyang Xu, Fuchun Sun, Junzhou Huang. Equivariant Graph Mechanics Networks with Constraints. ICLR 2022.

GMN-OC: Towards larger capacity of GMN

- 1. Stacking multiple layers:

- 2. Global shared representation:

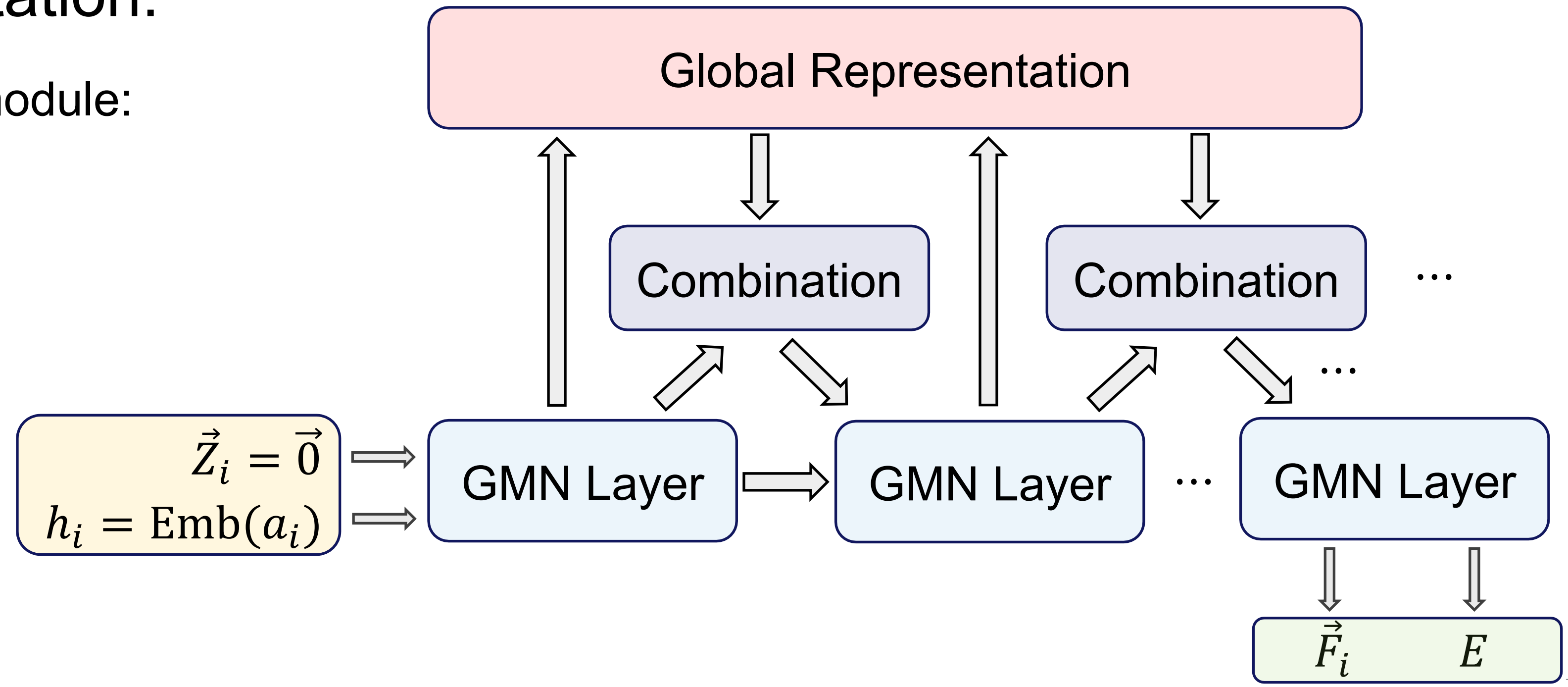
Global shared representation module:

$$\vec{V}_i = \varphi_g(\vec{Z}_i, h_i).$$

Combination layer:

$$W_{ij} = \psi(\vec{Z}_{ij}, h_{ij}),$$

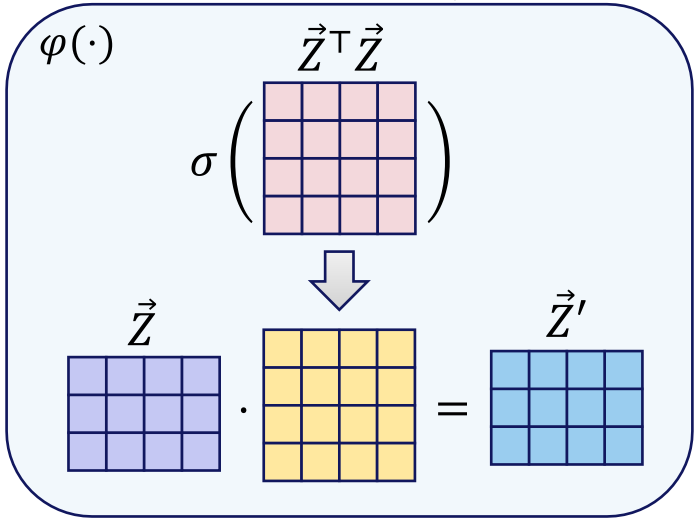
$$\vec{Z}_i' = \vec{V}_i \sum_{j \in \mathcal{N}(i)} W_{ij}\ .$$



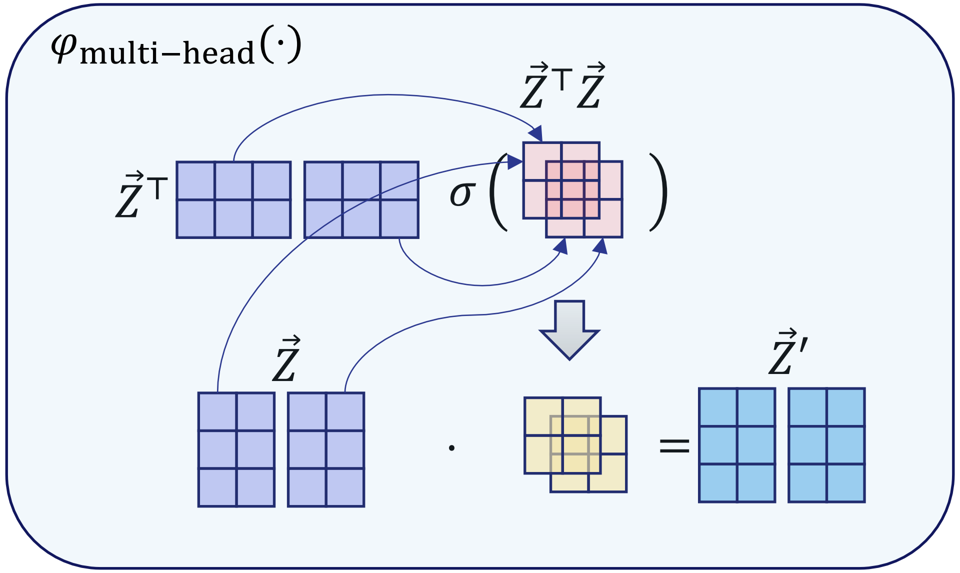
GMN-OC: Towards larger capacity of GMN

- 3. Multi-head GMN Layer:

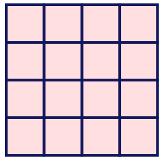
Plain GMN Layer



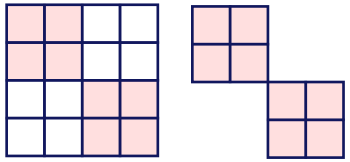
Multi-head GMN Layer



Parameter Complexity



$O(H^2)$



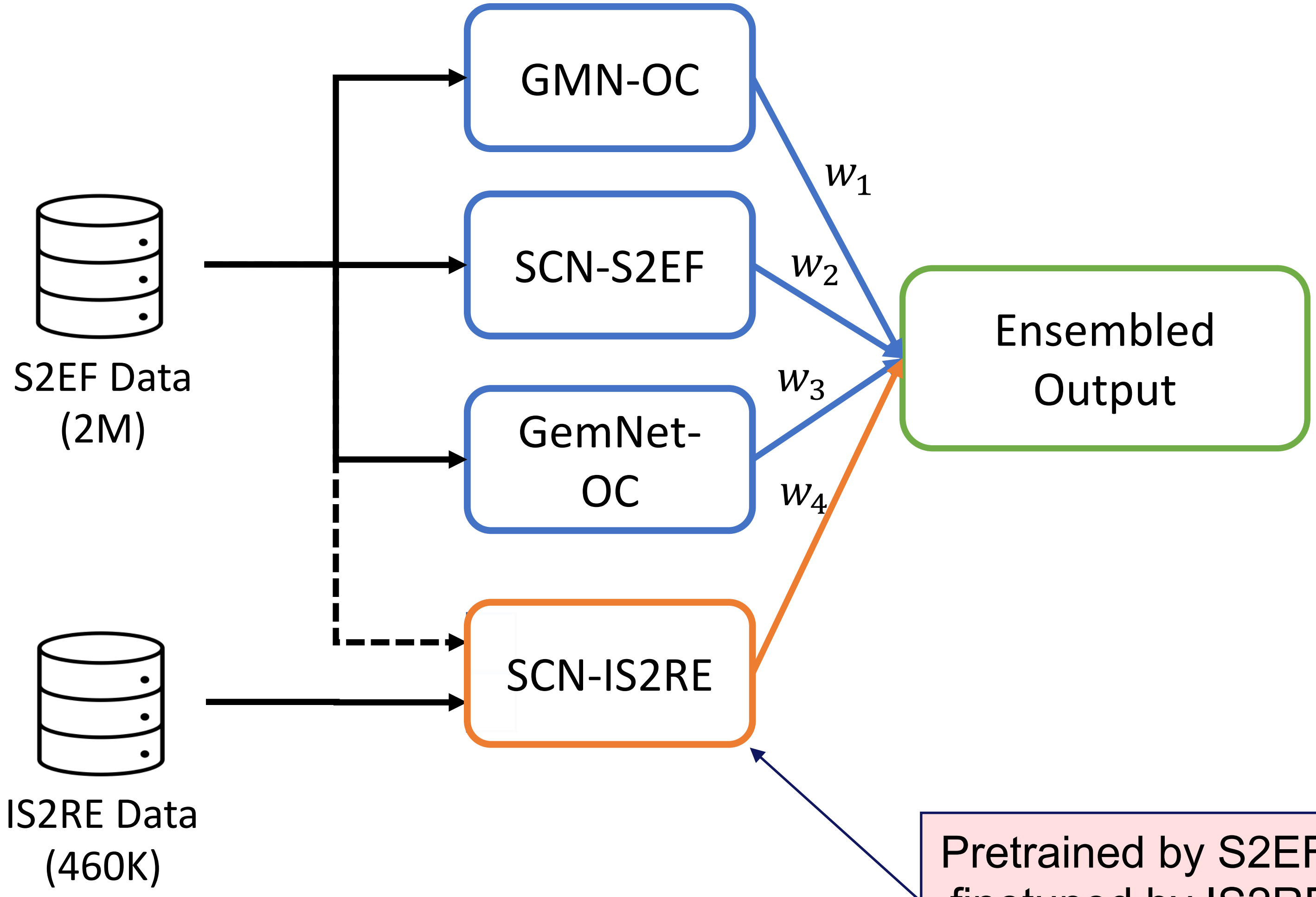
$O(H^2/\text{n\_head})$

H is the number of vector channels.

n_head is the number of heads.

We can significantly increase the number of channels for multi-head GMN layer.

The Overall Model: GeoEnsemble



Model	Type	# of Params
GMN-OC	Relaxation	81M
SCN-S2EF	Relaxation	124M
GemNet-OC	Relaxation	38M
SCN-IS2RE	Direct	168M

Pretrained by S2EF, then finetuned by IS2RE with delta-position loss.

Training & Inference Details

Model	Type	Dataset	# of Params	GPUs	Training GPU Hours	Inference GPU Hours
GMN-OC	Relaxation	S2EF-2M	81M	V100	3200 Hours	128 Hours
GemNet-OC	Relaxation	S2EF-2M	38M	V100	1060 Hours	144 Hours
SCN-S2EF	Relaxation	S2EF-2M	124M	A100	3072 Hours	105.6 Hours
SCN-IS2RE	Direct	Pretrain: S2EF-2M Finetune: IS2RE-460K	168M	A100	4096 Hours 896 Hours	4.2 Hours

Public Leaderboard

TEAM	METHOD	EWT (%)	ENERGY MAE (EV)	SUBMITTED
FAIR +CMU	SCN (relaxation)	14.25	0.3221	2022/5/19
TTRC	GeoEnsemble (Relax, S2EF-2M data)	10.11	0.3428	2022/11/1
TUM + FAIR	GemNet-OC-Large-force relaxations + GemNet-OC-Large-energy	14.97	0.3477	2022/7/14
FAIR + NERSC	GemNet-XL	11.13	0.3712	2021/9/27
TUM + FAIR	GemNet-T-EFwT-Relaxation-All	9.86	0.3997	2021/8/23
TTRC	GMN-OC, Relaxation, S2EF-2M data	8.2	0.4212	2022/10/15
FAIR + CMU	spinconv-force-centric-relaxation-all	7.9	0.4343	2021/6/3
FAIR + NERSC	GemNet-XL (Finetuned)	5.6	0.4623	2021/10/5
Atomic Architects MIT	Equiformer (IS2RE training data only with IS2RS and Noisy Nodes. Direct.)	5.66	0.466	2022/5/20
Machine Learning	3d-Graphormer (Direct, IS2RE data only)	6.1	0.4722	2021/10/6
Deep Mind	GNS + Noisy Nodes (IS2RE Only)	6.5	0.4728	2022/2/15

The data is collected on 2022-11-08.

The Lessons

Things tried but do not work yet	Things worked but haven't been applied to the solution
• Sophisticated design of components in Transformer. • Prediction with gas energy. • Elastic network loss. • Different relaxation strategy.	• Finetuning with Fake IS2RE data from S2EF dataset. • Recycle module in model design.

Future Directions

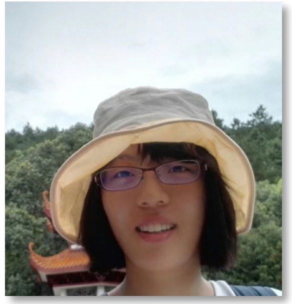
- More inspirations from the real physical process.
- More exploitations of the existing data.
- Training process optimization.

Teams

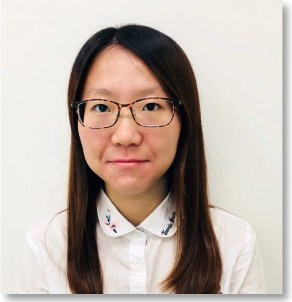

Jiaqi Han

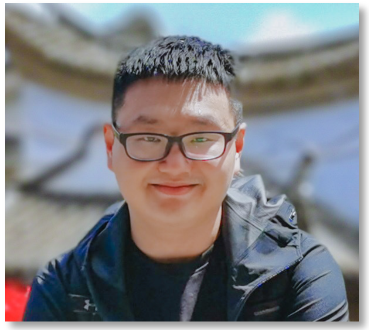

Tian Bian


Geyan Ye

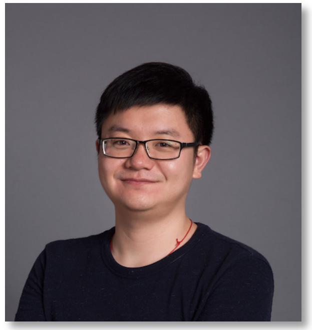

Kaili Ma


Yuduo Zhi


Kangfei Zhao


Tingyang Xu


Wenbing Huang


Yu Rong

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