



MEGA AI
FOUNDATION
MODELS FOR
SCIENCE & SECURITY
@PNNL



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Mega AI, an internal investment at Pacific Northwest National Laboratory, aims to develop next-generation artificial intelligence (AI) capabilities unique to the Department of Energy's national laboratory system. These capabilities will be used to address research gaps in large-scale, multimodal representation learning; multitask inferences; and the need for increased generalizability, rapid adaptivity, and usability of AI technologies. In this newsletter, we highlight recent developments in the research community on next-generation AI technologies focusing on massive-scale model development, deployment and evaluation, data and code availability, model interactions, and new features and capabilities that are relevant to Mega AI's goals and science and security applications.



NEW MODELS AND CAPABILITIES

- **January 3 | Code:** The Illustrated Retrieval Transformer. [HERE](#)
- **January 13 | Blog:** *Scaling Vision with Sparse Mixture of Experts*. [READ MORE](#)
Publication: [READ MORE](#), **Blog:** [READ MORE](#), and **Code:** [HERE](#)
- **January 14 | Blog:** *Learning to Route by Task for Efficient Inference*. [READ MORE](#)
- **January 19 | Publication:** *CM3: A Causal Masked Multimodal Model of the Internet*. [READ MORE](#)
- **January 19 | Blog:** *DeepSpeed: Advancing MoE inference and training to power next-generation AI scale*. [READ MORE](#)
- **January 21 | Publication:** *GreaseLM: Graph REASoning Enhanced Language Models for Question Answering*. [READ MORE](#)

- **February 4 | Publication:** *Using DeepSpeed and Megatron to Train Megatron-Turing NLG 530B, A Large-Scale Generative Language Model.* [READ MORE](#)
- **February 7 | Publication:** *Improving Language Models by Retrieving from Trillions of Tokens.* [READ MORE](#), **Blog:** [READ MORE](#)
- **March 2 | Publication:** *A ConvNet for the 2020s.* [READ MORE](#), **Code:** [HERE](#)
- **Publication |** *Beyond Distillation: Task-level Mixture-of-Experts for Efficient Inference.* [READ MORE](#)
- **Publication |** *FastMoE: A Fast Mixture-of-Expert Training System.* [READ MORE](#)
- **Publication |** *UC2: Universal Cross-lingual Cross-modal Vision-and-Language Pre-training.* [READ MORE](#)
- **Publication |** *SMILES Transformer: Pre-trained Molecular Fingerprint for Low Data Drug Discovery Publication.* [READ MORE](#)
- **Publication |** *SMILES-BERT: Large Scale Unsupervised Pre-Training for Molecular Property Prediction.* [READ MORE](#)
- **Publication |** *ChemBERTa: Large-Scale Self-Supervised Pretraining for Molecular Property Prediction.* [READ MORE](#)
- **Blog |** *WebGPT: Improving the factual accuracy of language models through web browsing.* [READ MORE](#)



NEW CODE FOR REPRODUCIBILITY

- **January 21 | GeekWire:** *Ai2 releases demo of question-answering model it claims outperforms GPT-3.* [READ MORE](#)
- **GitHub | Code:** Official codebase for running the small, filtered-data GLIDE model from GLIDE: Towards Photorealistic Image Generation and Editing with Text-Guided Diffusion Models. [READ MORE](#)
- **Website |** First QA demo from Ai2 for large-scale LMs. [READ MORE](#)



NEW DATASETS FOR TRAINING AND EVALUATION

- **Website |** *DUE Benchmark – a Document Understanding Benchmark.* [READ MORE](#)
GitHub: [READ MORE](#), **Publication:** [READ MORE](#)



HIGHLIGHTED TECHNICAL RESOURCES

- **January 31 | Blog:** *OpenAI's InstructGPT Leverages RL From Human Feedback to Better Align Language Models With User Intent.* [READ MORE](#)
- **Github |** Reading List for Topics in Multimodal Machine Learning maintained by CMU. [READ MORE](#)
- **Video Playlist |** [Multimodal playlist](#) by [AI Coffee Break](#)
- **Publication |** *Graph Neural Networks for Natural Language Processing: A Survey.* [READ MORE](#)
- **Website |** *Open Catalyst Project: Using AI to model and discover new catalysts to address the energy challenges posed by climate change.* [READ MORE](#)
- **Publication |** *Multimodal Research in Vision and Language: A Review of Current and Emerging Trends.* [READ MORE](#)



NEW REPORTS AND STUDIES

- **January 20 | Publication:** *LaMDA: Language Models for Dialog Applications.* [READ MORE](#)
- **February 7 | Publication** *data2vec: A General Framework for Self-supervised Learning in Speech, Vision, and Language.* [READ MORE](#)
- **Poster |** *True Few-Shot Learning with Language Models.* [READ MORE](#)
- **Poster |** *Multimodal Few-Shot Learning with Frozen Language Models.* [READ MORE](#)
- **Poster |** *MERLOT: Multimodal Neural Script Knowledge Models.* [READ MORE](#)
- **Poster |** *Mind the Gap: Assessing Temporal Generalization in Neural Language Models.* [READ MORE](#)
- **Publication |** *Sparse is Enough in Scaling Transformers.* [READ MORE](#)
- **Publication |** *GraphFormers: GNN-nested Transformers for Representation Learning on Textual Graph.* [READ MORE](#)
- **Poster |** *Rethinking Graph Transformers with Spectral Attention.* [READ MORE](#)
- **Poster |** *Robust Counterfactual Explanations on Graph Neural Networks.* [READ MORE](#)
- **Poster |** *SaIKG: Learning from Knowledge Graph Explanations for Commonsense Reasoning.* [READ MORE](#)
- **Poster |** *Mind the Gap: Assessing Temporal Generalization in Neural Language Models.* [READ MORE](#)
- **Publication |** *FLEX: Unifying Evaluation for Few-Shot NLP.* [READ MORE](#)
Leaderboard: [READ MORE](#), **Code:** [READ MORE](#)
- **Website |** *Multimodal Few-Shot Learning with Frozen Language Models.* [READ MORE](#)
- **Publication |** *VATT: Transformers for Multimodal Self-Supervised Learning from Raw Video, Audio, and Text.* [READ MORE](#)

- **Publication** | [GemNet](#): Universal Directional Graph Neural Networks for Molecules. [READ MORE](#)
- **Publication** | Flow Network based Generative Models for Non-Iterative Diverse Candidate Generation. (GNN + Reward) [READ MORE](#)
- **Publication** | A 3D Generative Model for Structure-Based Drug Design. [READ MORE](#), **Code**: (Autoregressive), [READ MORE](#)
- **Publication** | Large-Scale Representation Learning on Graphs via Bootstrapping. [READ MORE](#)
- **Publication** | Learning in High Dimension Always Amounts to Extrapolation. [READ MORE](#)
- **Publication** | Math-word embedding in math search and semantic extraction. [READ MORE](#)
- **Article** | Advancing mathematics by guiding human intuition with AI. [READ MORE](#)
- **Publication** | Memorizing Transformers. [READ MORE](#)



EVENTS

- **January 11** | **Video**: Machine Learning Street Talk episode on interpolation and extrapolation. [WATCH](#)
- **Recording** | From VQA to VLN: Recent Advances in Vision-and-Language Research workshop on CVPR2021. [WATCH](#)
- **Recording** | Pay Attention to What You Need: Do Structural Priors Still Matter in the Age of Billion Parameter Models? (NeurIPS 2021 Panel) [WATCH](#)
- **Recording** | The Consequences of Massive Scaling in Machine Learning. (NeurIPS 2021 Panel) [WATCH](#)
- **Recording** | Self-Supervised Learning: Self-Prediction and Contrastive Learning. (NeurIPS 2021 Panel) [WATCH](#)
- **Github** | **Code**: Graph Neural Networks for Natural Language Processing. [HERE](#), **Slides**: [READ MORE](#)



COMMUNITY DISCUSSION

- **January 3** | 2021's Top Stories About AI. [READ MORE](#)
- **January 11** | **Blog**: Google Research: Themes from 2021 and Beyond. [READ MORE](#)
- **January 14** | **Article**: Google AI Introduces V-MoE: A New Architecture for Computer Vision Based On A Sparse Mixture Of Experts. [READ MORE](#)
- **January 19** | **Article**: Are Universal Self-Supervised Learning Algorithms Within Reach? [READ MORE](#)

- **January 24 | Blog:** *Meta AI's OMNIVORE: A Modality-Agnostic Single Vision Model With Cross-Modal Generalization.* [READ MORE](#)
 - **January 24 | Blog:** *Meta Works with NVIDIA to Build Massive AI Research Supercomputer.* [READ MORE](#)
 - **January 27 | Article:** *MIT News: Demystifying machine-learning systems | MIT News | Massachusetts Institute of Technology.* [READ MORE](#)
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