Isaac (Xin) Ju

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Skills

Programming Languages: Python, Modern C++, MATLAB, Fortran, bash

Software Engineering Tools: Pytorch, PyG, TensorFlow, ParMETIS, NetworkX, Git, CMake, GoogleTest, Linux

High-Performance Computing: OpenMP, MPI, CUDA, PETSc

Numerical Modeling & Analysis: Virtual Element Method, Finite Element Method, Computational Fluid Dynamics, Multiphysics Modeling

Education

Stanford University — Stanford, CA

PhD Candidate *in Energy Resources Engineering, GPA: 3.7* — *Sept. 2021 – Present*

- **Minor**: Computer Science
- **Concentrations**: High-Performance Physics-Based Modeling & Deep-Learning-Based Simulation
- **Selected Coursework**: Machine Learning with Graphs, Machine Learning, Deep Learning, Linear Algebra with Application to Engineering Computations, Numerical Analysis, Finite Element Analysis

Research & Work Experience

TotalEnergies E&P USA, Inc — Stanford, CA

Machine Learning Research Intern — *Jun. 2022 – Sept. 2022*

- Developed a deep-learning-based surrogate model for subsurface flow simulations with unstructured mesh using graph neural networks (GNNs).
- Designed recurrent GNNs that combine graph-based long-short-term-memory (LSTM) model with MeshGraphNet (MGN) to allow for stable temporal predictions of interested dynamical variables.
- The developed surrogate model provides solutions to the situation where capturing subsurface structure with unstructured mesh is necessary for quantifying uncertainties related to flow simulations (MGN-LSTM).

Stanford University — Stanford, CA

Research Assistant — *Jul. 2021 to present*

- Designed a graph neural network using Encoder-Processor-Decoder architecture to model physical dynamics in reservoir simulations with unstructured meshes.
- Enhanced computational geometry features in (GEOS) open-source HPC simulation framework.
- Implemented Virtual Element Method (VEM) for mechanical simulation with arbitary polyhedral mesh.
- Developed innovative algorithms combining the Lagrange Multiplier Method and VEM to address contact problems on polyhedral meshes.

Lawrence Livermore National Laboratory — Livermore, CA

Academic Graduate Appointee — *Jul. 2019 to Jun. 2021*

- Collaborated in an agile team to implemenet physics modules to GEOS, an open-source exascale HPC platform optimized for GPUs (www.geosx.org).
- Enhanced GEOS with capabilities to model thermo-hydro-mechanical (THM) processes in fluid-driven fracturing.

- Introduced an efficient coupling scheme integrating the THM model with a fracture mechanics module.
- Incorporated PETSc's parallel linear solvers into GEOS for robust handling of linear systems from multiphase flow simulations in fracture-matrix systems.
- Utilized GEOS modules to produce synthetic data aiding machine learning in history-matching workflows for Geological Carbon Sequestration.

Project

CS224W Group Project: Learning Mesh-Based Flow Simulations on Graph Networks
Stanford University, CS224W: Machine Learning with Graphs *Blog*

- Collaboratively designed and developed a graph-based simulator as part of the CS224W course project.
- Utilized MeshGraphNet (MGN) to learn and simulate mesh-based flow dynamics.
- Authored a comprehensive Medium blog post detailing the project's objectives, methodology, results, and insights.
- Demonstrated the potential of graph networks in accurately capturing the intricacies of mesh-based flow simulations.

Publication

- X. Ju, F. P. Hamon, G. Wen, R. Kanfar, M. Araya-Polo, and H. A. Tchelepi, *Learning co_2 plume migration in faulted reservoirs with graph neural networks*, arXiv preprint arXiv:2306.09648, (2023)(link).
- M. Tang, X. Ju, and L. J. Durlofsky, *Deep-learning-based coupled flow-geomechanics surrogate model for co_2 sequestration*, International Journal of Greenhouse Gas Control, 118 (2022), p. 103692(link).
- H. Tang, P. Fu, C. S. Sherman, J. Zhang, X. Ju, F. Hamon, N. A. Azzolina, M. Burton-Kelly, and J. P. Morris, *A deep learning-accelerated data assimilation and forecasting workflow for commercial-scale geologic carbon storage*, International Journal of Greenhouse Gas Control, 112 (2021), p. 103488(link).
- X. Ju, P. Fu, R. R. Settegast, and J. P. Morris, *A coupled thermo-hydro-mechanical model for simulating leakoff-dominated hydraulic fracturing with application to geologic carbon storage*, International Journal of Greenhouse Gas Control, 109 (2021), p. 103379(link).
- X. Ju, F. Liu, P. Fu, M. D. White, R. R. Settgast, and J. P. Morris, *Gas production from hot water circulation through hydraulic fractures in methane hydrate-bearing sediments: Thc-coupled simulation of production mechanisms*, Energy & Fuels, 34 (2020), pp. 4448–4465(link).

Academic Service

- **Journal Reviewer**: Reviewed articles for esteemed journals such as Geoenergy Science and Engineering, SPE Journal, Geomechanics for Energy and the Environment, and Petroleum Science Bulletin.
- **Organizer of Stanford Reading Group for Machine Learning in Simulation**: Led and coordinated the Stanford Reading Group focused on the intersection of Machine Learning and Simulation. Facilitated discussions on cutting-edge ML research, fostering collaboration among 50 participants from more than 20 institutes.
- **Teaching Assistant**: Collaborated with Dr. Franklin M. Orr to curate and deliver content for ERE251, a graduate course on Carbon Capture & Sequestration (CCS), with an enrollment of 33 students. Presented on CCSNet.ai, an innovative machine learning tool for real-time CO_2 plume migration prediction.