

Chen Zhang

GitHub: github.com/KedoKudo | LinkedIn: [linkedin.com/in/chen-z-5a081725](https://www.linkedin.com/in/chen-z-5a081725)

Summary

Computational scientist with expertise in neutron science, machine learning, and graph neural networks. Experienced in developing advanced algorithms for neutron imaging, AI-driven data analysis, and interdisciplinary collaborations. Skilled in Python, C++, and FORTRAN, with a focus on high-performance computing, scientific software development, and materials characterization techniques.

Professional Experience

Oak Ridge National Laboratory (ORNL)

August 2020 – Present

R&D Associate Staff

- Lead development of BM3DORNL, an open-source library for ring artifact removal in neutron tomography, enhancing data quality at the Multimodal Advanced Radiography Station (MARS) at the High Flux Isotope Reactor (HFIR) and the Versatile Neutron Imaging Instrument (VENUS) at the Spallation Neutron Source (SNS)
- Developed Fusion Graph Neural Network (FuGNN) for dynamic graph problems, advancing neutron reflectometry and power-grid stability analysis
- Created DocSAGE, a local large language model (LLM) and retrieval augmented generation (RAG) system for AI-driven research in neutron science
- Established Python packaging standards adopted by the Neutron Data Project (NDP) and Los Alamos National Laboratory (LANL)
- Provided critical support during VENUS@SNS commissioning
- Led Laboratory Directed Research & Development (LDRD) and SEED proposals to expand AI applications in neutron science

Colorado School of Mines & Advanced Photon Source

September 2019 – August 2020

Post-Doctoral Fellow

- Developed semi-automated data processing pipeline for the high throughput high energy diffraction microscopy (HT-HEDM) instrument at Advanced Photon Source
- Created x-proc, a collection of meta-packages to streamline post-processing of tomography, far-field HEDM (ff-HEDM), and near-field HEDM (nf-HEDM) data
- Participated in the deployment of the new HT-HEDM at 6-ID-D at Advanced Photon Source
- Conducted synchronization analysis of duo-detector configuration for the ff-HEDM experiment with HT-HEDM instrument
- Led the development of a modern Python-based experiment control system for the HT-HEDM instrument

Carnegie Mellon University & Advanced Photon Source

September 2018 – August 2019

Postdoctoral Research Associate

- Developed tomoproc, a Python meta-package for automated tomography reconstruction
- Participated in the development of HEXOMAP, a GPU-based microstructure reconstruction library for processing nf-HEDM data
- Conducted tomographic characterization of solid oxide fuel cells using high-energy transmission X-ray microscopy

Michigan State University
Graduate Research Assistant

August 2010 – August 2018

- Studied plastic deformation history of Ti-5Al-2.5Sn using crystal plasticity modeling, electron backscatter diffraction (EBSD), and differential aperture X-ray microscopy (DAXM)
- Maintained and developed constitutive models for the open-source material analysis toolkit: Düsseldorf Advanced Material Simulation Kit (DAMASK)
- Developed Python package CYXTAL for materials informatics, including residual lattice stress-strain extraction and dislocation content mapping
- Developed new algorithms for spatially resolved dislocation density information analysis and 3D dislocation network reconstruction

Michigan State University
Teaching Assistant

August 2010 – April 2017

- Taught undergraduate students to implement various algorithms using MATLAB and Excel
- Instructed standard experimental techniques for materials characterization

Oak Ridge National Laboratory
Visiting Scholar

February 2013

- Developed computational toolkit for analyzing and visualizing subsurface dislocation content using micro-Laue diffraction data

Max-Planck-Institut für Eisenforschung GmbH
R&D Intern

June 2012

- Developed 3D microstructure reconstruction algorithm for crystal plasticity simulation using computer vision and data mining

Education

Michigan State University
Ph.D. in Materials Science and Engineering

August 2010 – August 2018

GPA: 3.8/4.0

Shanghai Jiao Tong University

2006 – 2010

B.S. in Materials Science and Engineering, Minor in Management GPA: 3.7/4.0

Technical Skills

Programming:	Python, C++, FORTRAN, R, MATLAB, LaTeX, SQL
Tools & Frameworks:	MPI, Cython, Git, GNU Make, Machine Learning, Graph Neural Networks
Experimental Techniques:	X-ray diffraction, Electron Backscatter Diffraction (EBSD), Finite Element Analysis (FEA), Differential Aperture X-ray Microscopy (DAXM)

Selected Publications

1. C. Zhang, V. A. Niemann, P. Benedek, T. F. Jaramillo, and M. Doucet, "Extracting thin film structures of energy materials using transformers," JACS Au, 2024. (Under revision)
2. B. Liu, C. Zhang, J. Dong, P. Balaprakash, Y. Liu, and B. Eiffert, "Enhancing Power Distribution System Resilience with Fusion-GNN: A Dynamic Graph Representation Learning Approach," Proc. IECON 2024 - 50th Annual Conference of the IEEE Industrial Electronics Society, 2024. (Accepted)

3. F. Funama, S. Chong, M. Loyd, K. J. Gofron, Y. Zhang, S. J. Kuhn, C. Zhang, M. R. Fitzsimmons, A. Khaplanov, B. Vacaliuc, L. Crow, F. Li, "Scintillator-based Timepix3 detector for neutron spin-echo techniques using intensity modulation," *Rev. Sci. Instrum.* 95(3): 033304, 2024.
4. J. C. Bilheux, et al. (including C. Zhang), "Neutron imaging software tools at the Oak Ridge National Laboratory," *Journal of Physics: Conference Series*, vol. 2605, no. 1, pp. 012014, Sep. 2023.
5. W. T. Heller, et al. (including C. Zhang), "drtsans: The data reduction toolkit for small-angle neutron scattering at Oak Ridge National Laboratory," *SoftwareX*, Volume 19, 2022.
6. C. Zhang, S. Balachandran, P. Eisenlohr, M.A. Crimp, C. Boehlert, R. Xu, T.R. Bieler, "Comparison of dislocation content measured with transmission electron microscopy and micro-Laue diffraction based streak analysis," *Scripta Materialia*, 2018.
7. C. Zhang, H. Li, P. Eisenlohr, W. Liu, C.J. Boehlert, M.A. Crimp, T.R. Bieler, "Effect of realistic 3D microstructure in crystal plasticity finite element analysis of polycrystalline Ti-5Al-2.5Sn," *International Journal of Plasticity*, 2015.
8. T.R. Bieler, P. Eisenlohr, C. Zhang, H. Phukan, M.A. Crimp, "Grain boundaries and interfaces in slip transfer," *Current Opinion in Solid State and Materials Science*, 2014.
9. M. Diehl, P. Eisenlohr, C. Zhang, J. Nastola, P. Shanthraj, F. Roters, "A Flexible and Efficient Output File Format for Grain-Scale Multiphysics Simulations," *Integrating Materials and Manufacturing Innovation*, 2017.
10. C. Zhang, B. Lv, Y. Wang, "Study of sand mold strength in cast magnesium alloy production," *Foundry Engineering*, 2009.

Notable Projects

- BM3DORN: Open-source BM3D algorithm with Numba and CuPy acceleration for ring artifact removal in tomography
- FuGNN: Generic graph neural networks library for temporal dynamic graph representation learning
- DocSAGE: Application for Retrieval Augmented Generation (RAG) with local large language models (LLMs)
- NTRACE: Transformer-based material parameters estimator for neutron reflectometry
- iMars3D: Core neutron reduction for MARS@HFIR and VENUS@SNS
- NeuNorm: Open-source neutron imaging data normalization
- iBeatles: Application for Bragg Edge imaging at VENUS@SNS
- Shiver: Desktop application for examining Time of Flight (ToF) inelastic neutron data
- CYXTAL: Python package for materials informatics, including residual lattice stress-strain extraction and dislocation content mapping
- HEXOMAP: GPU-based microstructure reconstruction library for processing nf-HEDM data

Professional Activities

- Invited reviewer for journals including *Materials Science and Engineering A (MSEA)* and *Journal of Open Source Software (JOSS)*
- Active contributor to open-source projects in scientific computing and neutron science
- Organizer of AI seminars and tutorials at ORNL
- Member of the US Research Software Engineer Association (US-RSE) award committee
- Contributor to the organization of Oak Ridge Software Data Expo 2024 (OSDX2024)