

Ming Du Ph.D.

Computational imaging and applied AI | Scientific software, machine learning, high-performance computing

Identity information intentionally omitted

Profile

- Computational scientist with 10+ years of experience across X-ray imaging, scientific machine learning, and semiconductor inspection.
- Develops algorithms and software for autonomous experiments, GPU-accelerated image reconstruction, distributed model training, and production C++ image analysis.
- Combines physics-based modeling, experimental validation, and software engineering to translate research methods into tools for scientific facilities and industrial inspection.

Experience

Computational Scientist

Oct 2025 – Present

Assistant Computational Scientist

Oct 2023 – Oct 2025

Argonne National Laboratory, Lemont, IL, USA

- Developed an agent harness for natural-language control and automation of scientific experiments, demonstrated at the Advanced Photon Source (APS) on feature search, X-ray optics focusing, and interactive data acquisition.
- Built an automated research harness that generates and evaluates scientific image-processing algorithms, with holdout testing to assess generalization; demonstrated on image registration, diffraction peak detection, and segmentation.
- Lead development of Pty-Chi, an open-source PyTorch library for GPU-accelerated ptychographic image reconstruction, with modular algorithms and multi-GPU support; adopted at multiple synchrotron facilities and universities.
- Developed Bayesian adaptive sampling for X-ray absorption near-edge structure (XANES) spectroscopy. Reported test cases used 15–20% of dense-scan measurement points, with normalized root-mean-square errors generally below 0.005; demonstrated the workflow in a live battery experiment at APS.
- Developed phase retrieval with neural-network priors. A deep image prior improved contrast and suppressed artifacts after removing 98% of measured diffraction patterns from a test-pattern dataset; a separate diffusion-based method reduced grid artifacts and multislice crosstalk while enforcing consistency with the physics model and measured data.
- Built distributed training workflows with MPI and PyTorch DistributedDataParallel (DDP), running jobs on more than 100 GPUs on Argonne's Polaris supercomputer. Trained ConvNeXt models on 30 million simulated and experimental samples to predict crystal symmetry and lattice parameters.
- Deploy on-premises infrastructure for collaborative model training, experiment tracking, and research software delivery.

Senior Algorithm Engineer

Mar 2023 – Sep 2023

Algorithm Engineer

Apr 2021 – Mar 2023

KLA Corporation, Ann Arbor, MI, USA

- Developed production C++ algorithms for image formation and defect detection in photomask inspection systems supporting sub-3-nm semiconductor processes.
- Led deep learning work for defect detection and artifact suppression, improving precision by 10%, reducing false positives by 60%, and cutting residual image artifacts by over 70%. Optimized model inference with OpenVINO.
- Mentored an intern on model-augmented deep learning to simulate inspection artifacts and accelerate algorithm validation.

Postdoctoral Scholar

Aug 2019 – Mar 2021

Argonne National Laboratory, Lemont, IL, USA

- Developed Adorym, an open-source framework using automatic differentiation with PyTorch and Autograd for large-scale 2D and 3D X-ray image reconstruction and joint refinement of experimental parameters.
- Developed a deep-image-prior method to reduce crosstalk between reconstructed sample layers in multislice ptychography.
- Contributed to distributed wave-propagation algorithms for high-performance computing.
- Led an ASCR Leadership Computing Challenge project on distributed wave propagation and large-scale 3D reconstruction beyond the depth-of-focus limit.

Ph.D. Researcher

Sep 2015 – Jun 2019

Northwestern University, Evanston, IL, USA

- Co-developed Tomosaic, a Python package for X-ray tomography of samples larger than the beam's field of view; demonstrated a 9.36-trillion-voxel reconstruction from 5.8 TB of measurements on an HPC cluster.
- Developed differentiable multislice imaging methods that account for wave propagation through thick samples,

enabling 3D reconstruction beyond the depth-of-focus limit.

- Conducted tomography and ptychography experiments and helped commission the AuTomo and Ripple automated data-processing workflow at APS beamline 32-ID.
- Developed models to estimate image contrast and radiation dose for X-ray imaging of thick, hydrated specimens.

Research Intern

Jan 2014 – Jun 2014

Singapore Institute of Manufacturing Technology, Singapore

- Investigated how voltage and electrolyte temperature affect pore size during anodic aluminum oxide fabrication.
- Built an unsupervised analysis tool to extract trends from experimental data.

Education

Ph.D., Materials Science and Engineering

2015 – 2019

Northwestern University, Evanston, IL, USA

Advisor: Prof. Chris Jacobsen. Thesis: *To the Breadth, and to the Depth: Scalable 3D Imaging of Extended Objects with High Resolution Using X-ray Microscopy.*

B.Eng., Materials Science and Engineering

2011 – 2015

National University of Singapore, Singapore

Graduated with first-class honours and a minor in Physics.

Certifications and Training

2023	AWS Certified Machine Learning – Specialty, Amazon Web Services Training and Certification.
2022	Deep Learning for Computer Vision (EECS 598-008, grade A), University of Michigan, Ann Arbor.
2022	Bayesian Statistics specialization, Coursera.
2020	Statistical Thinking in Python and Unsupervised Learning in Python, DataCamp.

Teaching

Teaching Assistant, Northwestern University

- MSE 395-4: Computational Thermodynamics and Kinetics (Winter 2018).
- MSE 401: Chemical and Statistical Thermodynamics of Materials (Fall 2018).
- MSE 361: Crystallography and Diffraction (Winter 2018).

Publications

- [1] B. L. Boyce et al. *Materials Behavior as Mechanism Ensembles: A Probabilistic Framework for Emergent Behaviors*. 2026. arXiv: [2607.27163 \[cond-mat.mtrl-sci\]](#).
- [2] X. Yin, **M. Du**, M. H. Prince, and M. J. Cherukara. *Artifact-centered claim-aware observability for autonomous scientific agents*. 2026. arXiv: [2608.18312 \[cs.CL\]](#).
- [3] J. McCourt, S. Seifert, Z. Cheng, **M. Du**, B. Zhang, M. R. Jones, M. Cherukara, B. Lee, and J. Deng. “Pty-co-SAXSNN: CNN-based deconvolution for simultaneous X-ray ptychography and SAXS nanostructure characterization”. In: *MRS Communications* (2026). DOI: [10.1557/s43579-026-01027-5](#).
- [4] **M. Du**, X. Yin, Y. Luo, D. Beniwal, S. Tang, H. Sharma, and M. J. Cherukara. *CVEvolve: Autonomous Algorithm Discovery for Unstructured Scientific Data Processing*. 2026. arXiv: [2605.11359 \[cs.AI\]](#). URL: <https://arxiv.org/abs/2605.11359>.
- [5] **M. Du**, Y. Luo, S. Banerjee, M. Wojcik, J. Popovic, and M. J. Cherukara. “Experiment automation agents: automating materials characterization with vision language model agents”. In: *npj Computational Materials* (July 31, 2026). DOI: [10.1038/s41524-026-02213-8](#). URL: <https://www.nature.com/articles/s41524-026-02213-8>.
- [6] N. Andrejevic*, **M. Du***, H. Sharma, J. P. Horwath, A. Luo, X. Yin, M. Prince, B. H. Toby, and M. J. Cherukara. *AlphaDiffract: Automated Crystallographic Analysis of Powder X-ray Diffraction Data*. 2026. arXiv: [2603.23367 \[cond-mat.mtrl-sci\]](#).
- [7] **M. Du**, V. Rose, J. Deng, D. Singh, S. Chen, and M. Cherukara. “Fidelity-preserving enhancement of ptychography with foundational text-to-image models”. In: *Optica* 13.1 (2026), pp. 45–56. DOI: [10.1364/OPTICA.579456](#).
- [8] **M. Du**, M. Wolfman, C. Sun, S. D. Kelly, and M. J. Cherukara. “Demonstration of an AI-driven workflow for dynamic x-ray spectroscopy”. In: *npj Computational Materials* 11.1, 320 (2025). DOI: [10.1038/s41524-025-01771-7](#).
- [9] **M. Du** et al. *Pty-Chi: A PyTorch-based modern ptychographic data analysis package*. 2025. arXiv: [2510.20929 \[physics.optics\]](#). URL: <https://arxiv.org/abs/2510.20929>.

- [10] **M. Du**, T. Zhou, J. Deng, D. Ching, S. Henke, and M. Cherukara. “Predicting ptychography probe positions using single-shot phase retrieval neural network”. In: *Optics Express* 32 (2024), pp. 36757–36780. DOI: [10.1364/OE.524317](https://doi.org/10.1364/OE.524317).
- [11] X. Liu et al. “Origin and regulation of oxygen redox instability in high-voltage battery cathodes”. In: *Nature Energy* 7 (2022), pp. 808–817. DOI: [10.1038/s41560-022-01036-3](https://doi.org/10.1038/s41560-022-01036-3).
- [12] **M. Du**, X. Huang, and C. Jacobsen. “Using a modified double deep image prior for crosstalk mitigation in multislice ptychography”. In: *Journal of Synchrotron Radiation* 28 (2021), pp. 1137–1145. DOI: [10.1107/S1600577521003507](https://doi.org/10.1107/S1600577521003507).
- [13] **M. Du**, S. Kandel, J. Deng, X. Huang, A. Demortiere, T. T. Nguyen, R. Tucoulou, V. de Andrade, Q. Jin, and C. Jacobsen. “Adorym: a multi-platform generic X-ray image reconstruction framework based on automatic differentiation”. In: *Optics Express* 29 (2021), pp. 10000–10035. DOI: [10.1364/OE.418296](https://doi.org/10.1364/OE.418296).
- [14] **M. Du**, Z. W. Di, D. Gürsoy, R. P. Xian, Y. Kozorovitskiy, and C. Jacobsen. “Upscaling X-ray nanoimaging to macroscopic specimens”. In: *Journal of Applied Crystallography* 54 (2021), pp. 386–401. DOI: [10.1107/S1600576721000194](https://doi.org/10.1107/S1600576721000194).
- [15] P. Huang, **M. Du**, M. Hammer, A. Miceli, and C. Jacobsen. “Fast digital lossy compression for X-ray ptychographic data”. In: *Journal of Synchrotron Radiation* 28 (2021), pp. 292–300.
- [16] S. Ali, **M. Du**, M. F. Adams, B. Smith, and C. Jacobsen. “Comparison of distributed memory algorithms for X-ray wave propagation in inhomogeneous media”. In: *Optics Express* 28 (2020), pp. 29590–29618. DOI: [10.1364/OE.400240](https://doi.org/10.1364/OE.400240).
- [17] **M. Du**, D. Gürsoy, and C. Jacobsen. “Near, far, wherever you are: simulations on the dose efficiency of holographic and ptychographic coherent imaging”. In: *Journal of Applied Crystallography* 53 (2020), pp. 748–759. DOI: [10.1107/S1600576720005816](https://doi.org/10.1107/S1600576720005816).
- [18] **M. Du**, Y. S. G. Nashed, S. Kandel, D. Gürsoy, and C. Jacobsen. “Three dimensions, two microscopes, one code: Automatic differentiation for x-ray nanotomography beyond the depth of focus limit”. In: *Science Advances* 6 (2020), eaay3700. DOI: [10.1126/sciadv.aay3700](https://doi.org/10.1126/sciadv.aay3700).
- [19] J. Prasad, A. Balwani, E. Johnson, J. Miano, V. Sampathkumar, V. De Andrade, K. Fezzaa, **M. Du**, et al. “A three-dimensional thalamocortical dataset for characterizing brain heterogeneity”. In: *Scientific Data* 7 (2020), p. 358. DOI: [10.1038/s41597-020-00692-y](https://doi.org/10.1038/s41597-020-00692-y).
- [20] R. Vescovi*, **M. Du***, V. de Andrade, W. Scullin, D. Gürsoy, and C. Jacobsen. “Tomosaic: efficient acquisition and reconstruction of teravoxel tomography data using limited-size synchrotron X-ray beams”. In: *Journal of Synchrotron Radiation* 25 (2018), pp. 1478–1489. DOI: [10.1107/S1600577518010093](https://doi.org/10.1107/S1600577518010093).
- [21] **M. Du**, R. Vescovi, K. Fezzaa, C. Jacobsen, and D. Gürsoy. “X-ray tomography of extended objects: a comparison of data acquisition approaches”. In: *Journal of the Optical Society of America A* 35 (2018), p. 1871.
- [22] M. A. Gilles, Y. S. G. Nashed, **M. Du**, C. Jacobsen, and S. M. Wild. “3D x-ray imaging of continuous objects beyond the depth of focus limit”. In: *Optica* 5 (2018), pp. 1078–1086.
- [23] A. Shahbazi et al. “Flexible learning-free segmentation and reconstruction of neural volumes”. In: *Scientific Reports* 8 (2018), p. 1448.
- [24] R. Chard, R. Vescovi, **M. Du**, H. Li, K. Chard, S. Tuecke, N. Kasthuri, and I. Foster. “Autonomous infrastructure for science”. In: *Proceedings of AI-Science’18*. 2018, pp. 1–7.
- [25] **M. Du**, R. Vescovi, R. Chard, N. Kasthuri, C. Jacobsen, E. Dyer, and D. Gürsoy. “An automated pipeline for the collection, transfer, and processing of large-scale tomography data”. In: *Biophotonics Congress: Biomedical Optics Congress*. Paper BF4C.2. 2018.
- [26] M. Tondravi, W. Scullin, **M. Du**, R. Vescovi, V. D. Andrade, C. Jacobsen, K. P. Kording, D. Gürsoy, and E. Dyer. “A pipeline for distributed segmentation of teravoxel tomography datasets”. In: *Microscopy and Microanalysis* 24 (2018), pp. 166–167.
- [27] **M. Du** and C. Jacobsen. “Relative merits and limiting factors for X-ray and electron microscopy of thick, hydrated organic materials”. In: *Ultramicroscopy* 184 (2018), pp. 293–309.
- [28] C. J. Jacobsen, V. D. Andrade, J. Deng, **M. Du**, D. Gürsoy, Y. S. Nashed, and T. Peterka. “Digital holography and three-dimensional imaging”. In: *Digital Holography and Three-Dimensional Imaging*. Paper W2A.12. 2016.
- [29] **M. Du**, X. Yin, C. Tang, T. J. Huang, and H. Gong. “Takovite-derived 2-D Ni/Al double hydroxide monolayer and graphene hybrid electrodes for electrochemical energy storage applications with high volumetric capacitance”. In: *Electrochimica Acta* 190 (2016), pp. 521–530.
- [30] X. Yin, T. J. Huang, C. Tang, **M. Du**, L. Sun, Z. Shen, and H. Gong. “Significantly different mechanical properties and interfacial structures of Cu₂ZnSn(S,Se)₄ films prepared from metallic and sulfur-contained precursors”. In: *Solar Energy Materials and Solar Cells* 134 (2015), pp. 389–394.
- [31] **M. Du**, X. Yin, and H. Gong. “Effects of triethanolamine on the morphology and phase of chemically deposited tin sulfide”. In: *Materials Letters* 152 (2015), pp. 40–44.

* Co-first authors with equal contributions.

Conference Presentations and Talks

- [1] “Adaptive sampling of XANES spectroscopy using Bayesian optimization with engineered acquisition function,” Denver X-ray Conference, Rockville, USA (2025).
- [2] “Ptychographic Scan Position Prediction Using Single-Shot Phase Retrieval Neural Networks,” Denver X-ray Conference, Westminster, USA (2024).
- [3] “Applications of automatic differentiation in image reconstruction and experimental parameter refinement for 3D microscopy,” 23rd Euro AD Workshop, virtual (2020).
- [4] “Three dimensions, two microscopes, one code: Automatic differentiation for x-ray nanotomography beyond the depth of focus limit,” ALCF Simulation, Data, and Learning Workshop, Lemont, USA (2019).
- [5] “A multifunctional tool for X-ray ptychographic and holographic 3D imaging beyond the depth-of-focus limit,” Gordon Research Seminar on X-ray Science, Easton, USA (2019).
- [6] “Using automatic differentiation for coherent diffraction imaging and reconstructing beyond depth of focus” (co-presented with S. Kandel), Ptycho Developer Meeting, Berkeley, USA (2019).
- [7] “3D object reconstruction beyond the depth-of-focus limit using automatic differentiation,” Coherence 2018, Port Jefferson, USA (2018).
- [8] “An automated pipeline for the collection, transfer, and processing of large-scale tomography data,” Biomedical Optics Congress, Hollywood, USA (2018).

Media Coverage

- [1] Beth Burmahl, “A new kind of microscope: Agentic AI turns simple language into self-guided experimentation,” *Argonne National Laboratory* (October 5, 2026). URL: anl.gov
- [2] Joseph E. Harmon, “Artificial intelligence makes X-ray spectroscopy five times faster, smarter and less prone to human error,” *Argonne Press Release* (2026). URL: <https://tinyurl.com/5ya82wmb>
- [3] Andre Salles, “Filling in the blanks: How supercomputing can aid high-resolution X-ray imaging,” *ALCF News Center* (2020). URL: <https://tinyurl.com/56pty3yc>
- [4] Argonne Leadership Computing Facility, “ALCF supercomputers power scientific breakthroughs in 2020,” *ALCF News Center* (2020). URL: <https://tinyurl.com/2vnvr2m5>
- [5] Sally Johnson, “Extreme 3-D,” *DEIXIS Magazine* (2021). URL: <https://tinyurl.com/5eacp988>

Awards

2025	Impact Argonne Award for extraordinary impact from rapid demonstration of integrated circuit imaging results.
2020	Named one of Optica’s most active reviewers of 2019.
2015	Materials Research Society (Singapore) Medal.

Research Leadership and Professional Service

2024	Lead principal investigator, Laboratory Directed Research and Development (LDRD) Swift project on AI-enabled scientific workflows.
2024	Co-principal investigator, LDRD Seed project on advanced computational imaging.
2020–2021	Principal investigator, ASCR Leadership Computing Challenge project “Distributed large wavefield propagation and 3D reconstruction beyond the depth of focus limit.”
2020	Selected participant, Argonne Training Program on Extreme-Scale Computing.
2020	Co-organizer, “Advances in Phase Retrieval Methods for High-resolution X-ray Imaging” workshop at the APS/CNM User Meeting.
2018–Present	Reviewer for <i>Optics Express</i> , <i>Applied Optics</i> , <i>Optics Letters</i> , <i>Biomedical Optics Express</i> , and <i>IU-CrJ</i> ; reviewer record: ResearcherID V-4905-2019.
2018–Present	Member, Optica (formerly The Optical Society of America).

Languages

English	Fluent
Chinese	Native
Japanese	Beginner
German	Beginner

Extracurricular Activities

2018–2019	Member, Northwestern University Society of Physics Students.
2017	Volunteer, Baxter Symposium at Northwestern University.
2013–2015	Co-chair, Movement for the Intellectually Disabled of Singapore (Fernvale branch).
2014	Chair, Movement for the Intellectually Disabled of Singapore (Fernvale branch) summer camp.