

**Derek Anthony Mendez Jr.** (dermen@slac.stanford.edu).  
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**Staff scientist** Stanford Synchrotron Radiation Lightsource, Structural and Molecular Biology Group (Nov. 2021-present).

- **Director** of computational resources (XMed).
  - Oversee development and implementation of in-silico methods for the X-ray Accelerated Medicines Development Consortium, the result of a new 3 year, multi-institutional grant running through 2026. Areas of focus
    - AI classification and analysis of crystallization outcomes
    - Molecular dynamics for drug design
    - Virtual ligand screening, linking and merging
    - High throughput job offloading to NERSC Perlmutter using the superfacility API
  - Supervise classes and internships for STEM undergraduates working on grant-related projects (including a partnership with UT San Antonio)
- **Algorithms development** for beamline software. Notable contributions include:
  - A generalized CUDA-port of the EMC algorithm (Expand, expectation Maximize, Compress) for solving protein structures from sparse crystallographic data.
  - A novel physics-informed crystallography artificial intelligence software suite (called Resonet) for training deep neural networks to process diffraction data and monitor user experiments.
- **Teaching and mentoring** undergraduates in STEM fields.
  - UCSB Data Science Capstone sponsor (Winter and Spring 2023, Winter 2024).
  - DOE funded Community College Internship mentor (Summer 2023, 2024).
  - DOE Brave internship mentor (Summer 2024)
- **Affiliate** at Lawrence Berkeley National Lab, Molecular Biophysics and Bioimaging Division (Nov 2021 - present).
  - Developing the GPU-based diffraction modeling program *diffBragg* for use at synchrotrons and leadership class compute facilities (Perlmutter, Frontier).
- Supervised by Aina Cohen (acohen@slac.stanford.edu)

## Work skills

- **Computer programming**
  - Proficient in: C++, CUDA, Git, Matplotlib, MPI, Numpy, Pandas, Python, Scipy, Scipy.optimize
  - Moderate experience with: BASH, Boost.Python, Latex, Markdown, MatLab, MySQL, Office, OpenCL, OpenMP, Pyopencl, PyTorch, R, Sklearn, TCSH, Tkinter
- **High performance computing**
  - Multi process/Multi GPU programming using MPI, CUDA, and Kokkos
  - SLURM
- **Scientific writing, data visualization and graphics, tutorials**
  - Peer-reviewed publications and grant proposals
  - Online tutorials and manuals, e.g., (<https://prickly-pythons.github.io/pythoncode/prickliesspeedops.html>)
  - Advanced Matplotlib for publication graphics
- **Physics-based simulations**
  - Full forward model simulations of X-ray scattering experiments (solution scattering and crystallography) based on kinematic diffraction theory.
- **Numerical optimization**
  - Proficient with L-BFGS, LevMar, Sparse LevMar, and Machine Learning methods to fit complicated functions to observed data.
  - Building frameworks for fitting large systems, sometimes fitting millions of parameters to terabytes of data.
  - Training deep neural networks on supercomputers.
- **X-ray crystallography** (rotation and serial)
  - Proficient data processing using DIALS, CCTBX, and CrystFEL, as well as customized code for unique experiments.
  - Data collection at synchrotron and XFEL facilities (including SSRL, APS, ALS, PAL, EuXFEL, LCLS, SACLA), sample delivery using jets, mix-and-inject setups, and traditional collection using e.g., BluICE.
- **X-ray solution scattering at XFELs**
  - Probing water soluble and detergent systems at LCLS and SACLA, with emphasis on exploring the dynamics of bovine rhodopsin.
  - Data processing for small and wide-angle X-ray scattering experiments, as well as generalized SAXS/WAXS, otherwise known as Fluctuation X-ray scattering. First-principles simulations of conventional and fluctuation solution scattering experiments for comparison with data.
- **X-ray time-resolved studies**
  - Mix and inject setups for probing long time delays (milliseconds to seconds)
  - Femtosecond and picosecond timing for laser driven reactions at both CXI (LCLS) and SACLA. Time-tool analysis for sorting data with 100 femtosecond timing accuracy. Smart database development for storing and quickly sorting intensity profiles and doing dimensionality reduction for cluster analysis (e.g. K-means).

## Previous work experience

- **Project scientist**, Lawrence Berkeley National Lab, Molecular Biophysics and Integrated Bioimaging Dept. (Nov. 2018- Nov. 2021).
  - Leadership class computing (NERSC, OLCF), with focus on MPI, CUDA, and OpenMP acceleration of data modeling.
  - Computational Crystallography Toolbox (CCTBX) and DIALS developer.
  - Exascale computing collaboration with Stanford Linear Accelerator Center (SLAC).
  - Developed the program diffBragg for iteratively fitting a forward diffraction model to whole diffraction images.
  - X-ray free electron laser (XFEL) beamtime support.
  - Boss: Nick Sauter, nksauter@lbl.gov
- **Postdoctoral research associate**, Arizona State University, Physics Dept. (March 2017 - October 2018).
  - Time-resolved solution scattering of rhodopsin in detergent micelles at X-ray free electron lasers (collab with Michael Brown U. of Arizona).
  - Serial Laue crystallography at synchrotrons on small crystals of membrane proteins.
  - Boss: Rick Kirian, rkirian@asu.edu
- **Graduate Research Assistant**, Stanford University Applied Physics (Jan 2011 - March 2017)
  - Further developed the field of fluctuation X-ray scattering (first proposed in 1977). Conducted novel experiments demonstrating that spatial intensity correlations from solutions of nanoparticles can reveal hidden structural details that are undetectable using conventional wide-angle X-ray scattering. The technique was demonstrated at both a synchrotron (SSRL, beamline 12-1) and an XFEL (SACLA).
- **Database manager**, Institute for pacific island forestry (IPIF) in Hilo HI (Contract job from April 2015–Sept 2015).
  - Created a quality and control GUI for the standardization of tree census data collected on GIS tablets in the field.
  - Merged 5 years of tree census data from 4 Hawaiian sites to compute growth and biodiversity statistics of native Hawaiian plantlife.
  - Boss: Becky Ostertag, ostertag@hawaii.edu
- **Cardinal scholars private tutor** (2014-2015)
- **Teaching assistant**, UTSA physics dept. (June 2007–May 2008)
- **Supplementary instructor (SI)** for Physics and Economics UTSA (Aug. 2006 – May 2008)
- **Target** retail employee (cash register and food avenue) (2006-2007)
- **Six Flags Fiesta Texas** food vendor (Jay Vending) (March 2004 - Oct 2006)

## Education

- **PhD in applied physics, Stanford University** (June 2010 – March 2017)
  - Research advisor: Sebastian Doniach (sxdwc@slac.stanford.edu)
  - Thesis topic: correlated (fluctuation) X-ray scattering (<https://searchworks.stanford.edu/view/11954441>)
  - Stanford NIH biotech. training fellowship (2011 - 2014, <https://btp.stanford.edu/>)
- **BS physics, University of Texas at San Antonio** (Aug 2005 – May 2010)
  - GPA: 3.99; summa cum laude; minor in mathematics
  - Honors thesis: Steered molecular dynamics to probe membrane protein interactions (2010); advised by Robert Renthal
  - NIGMS Maximizing access to research careers T34 fellowship (2008 - 2010, <https://www.nigms.nih.gov/Training/MARC/Pages/USTARawards.aspx>)

## Key talks

- **American Crystallographic Association** (2024 Denver, CO), Towards processing diffraction data with deep residual networks.
- **7th Ringberg Workshop on Structural Biology (with XFELs)** (2024 Germany) Deep residual networks for crystallography trained on synthetic data.
- **American Crystallographic Association** (2023 Baltimore, MD), CRAIT: physics informed neural networks for guiding crystallography experiments.
- **CCP4 study weekend** (2023 University of Nottingham), Exascale computing for SFX data processing.
- **Diffraction Methods Gordon Research Conference** (2022 Lewiston, ME), Beyond integration with diffBragg: new methods for stills data processing.
- **American Crystallographic Association** (2019 Covington, KY), Application of anomalous techniques in macromolecular crystallography.
- **Coherence** (2018 Port Jekerson, New York), Correlated X-ray solution scattering in practice.
- **Stanford Applied Physics Dept. graduation commencement** (2017 Stanford, CA) Traversing the river of doubt.
- **16th International conference on small angle scattering** (2015 Berlin). Observation of twinning in gold nano-particles using correlated x-ray scattering.
- **23rd Congress and general assembly of the International Union of Crystallography** (2014 Montreal), Correlated scattering: probing atomic structure of molecules and nanoparticles.

## Select publications

- **Mendez, D.**, Holton, J. M., Lyubimov, A. Y., Hollatz, S., Mathews, I. I., Cichosz, A., Martirosyan, V., Zeng, T., Stofor, R., Liu, R., Song, J., McPhillips, S., Soltis, M., & Cohen, A. E. (2024). "Deep residual networks for crystallography trained on synthetic data." Acta Crystallographica Section D Structural Biology, 80(1), 26–43. <https://doi.org/10.1107/S2059798323010586>
- Wittwer, F., Sauter, N. K., **Mendez, D.**, Poon, B. K., Brewster, A. S., Holton, J. M., Wall, M. E., Hart, W. E., Bard, D. J., & Blaschke, J. P. (2023). "Accelerating x-ray tracing for exascale systems using Kokkos. Concurrency and Computation: Practice and Experience", CPE 7944. <https://doi.org/10.1002/cpe.7944>
- Schriber, E. A., Paley, D. W., Bolotovskiy, R., Rosenberg, D. J., Sierra, R. G., Aquila, A., **Mendez, D.**, Poitevin, F., Blaschke, J. P., Bhowmick, A., Kelly, R. P., Hunter, M., Hayes, B., Popple, D. C., Yeung, M., Pareja-Rivera, C., Lisova, S., Tono, K., Sugahara, M., ... Hohman, J. N. (2022). "Chemical crystallography by serial femtosecond X-ray diffraction." Nature 2022 601:7893, 601(7893), 360–365. <https://doi.org/10.1038/s41586-021-04218-3>
- Blaschke, J. P., Brewster, A. S., Paley, D. W., **Mendez, D.**, Bhowmick, A., Sauter, N. K., Kröger, W., Shankar, M., Enders, B., & Bard, D. (2021). "Real-Time XFEL Data Analysis at SLAC and NERSC: a Trial Run of Nascent Exascale Experimental Data Analysis." <http://arxiv.org/abs/2106.11469> (accepted by CPE)
- **Mendez, D.**, Bolotovskiy, R., Bhowmick, A., Brewster, A. S., Kern, J., Yano, J., Holton, J. M., & Sauter, N. K. (2020). "Beyond integration: Modeling every pixel to obtain better structure factors from stills." IUCrJ, 7(6), 1151–1167. <https://doi.org/10.1107/S2052252520013007/ZF5012SUP1.PDF>
- Martin-Garcia et al J. M., Zhu, L., **Mendez, D.**, Lee, M.-Y., Chun, E., Li, C., Hu, H., Subramanian, G., Kissick, D., Ogata, C., & others. (2019). "High-viscosity injector-based pink-beam serial crystallography of microcrystals at a synchrotron radiation source." IUCrJ, 6(3).
- **Mendez, D.**, Watkins, H., Qiao, S., Raines, K. S., Lane, T. J., Schenk, G., Nelson, G., Subramanian, G., Tono, K., Joti, Y., Yabashi, M., Ratner, D., & Doniach, S. (2016). "Angular correlations of photons from solution diffraction at a free-electron laser encode molecular structure." IUCrJ, 3(6), 420–429. <https://doi.org/10.1107/S20522525160113956>
- **Mendez, D.**, Lane, T. J., Sung, J., Sellberg, J., Levard, C., Watkins, H., Cohen, A. E., Soltis, M., Sutton, S., Spudich, J., Pande, V., Ratner, D., & Doniach, S. (2014). "Observation of correlated X-ray scattering at atomic resolution." Philosophical Transactions of the Royal Society B: Biological Sciences, 369(1647). <https://doi.org/10.1098/rstb.2013.0315>