

Derek Anthony Mendez Jr. (dermen@lbl.gov)

Project scientist (<https://biosciences.lbl.gov/profiles/derek-mendez/>)

Lawrence Berkeley National Lab (Molecular Biophysics and Bioimaging Division)

Current role

Developing a pixel modeling approach to serial femtosecond crystallography data reduction. We use forward modeling of the measured spots combined with a gradient descent on GPUs in order to optimize the structure factors as free parameters. The work falls under the scope of the computational crystallography initiative (<http://cci.lbl.gov/>).

- Leadership class computing (NERSC, OLCF), with heavy focus on MPI, CUDA, and OpenMP acceleration.
- Computational crystallography toolbox (CCTBX) developer
- Exascale computing collaboration with SLAC
- X-ray free electron laser (XFEL) beamtime support

First author publications

- Observation of correlated X-ray scattering at atomic resolution , Philos. Trans. R. Soc. B, 369 (2013)
- Angular correlations of photons from solution diffraction at a free-electron laser encode molecular structure, IUCrJ, 3 (2016)
- Beyond integration: modeling every pixel to obtain better structure factors from stills, IUCrJ, 7 (2020)

Postdoctoral Research Associate (March 2017 - October 2018)

- Time-resolved solution scattering of rhodopsin in detergent micelles at X-ray free electron lasers
- Serial Laue crystallography at synchrotrons on small crystals of membrane proteins (DOI: 10.1107/S205225251900263X)

PhD in Applied Physics, Stanford University (June 2010 - March 2017)

- Research Advisor: Sebastian Doniach (sxdwc@slac.stanford.edu)
- Thesis topic: Fluctuation X-ray scattering (<https://searchworks.stanford.edu/view/11954441>)

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

Work skills

Python, C++, CUDA, MPI, OpenCL, OpenMP, HIP, git, Tkinter, shell scripting (BASH, CSH), R, MatLab, MySQL, Pandas, Latex, Markdown, Office

Key talks

- 23rd Congress and general assembly of the International Union of Crystallography (2014 Montreal), Correlated scattering: probing atomic structure of molecules and nanoparticles
- 16th International conference on small angle scattering (2015 Berlin), Observation of twinning in gold nano-particles using correlated x-ray scattering
- Invited speaker at Coherence (2018 Port Jefferson, New York), Correlated X-ray solution scattering in practice
- Honorary speaker, Stanford Physics graduation commencement (2017)
- American Crystallographic Association (2019 Covington, Kentucky), Application of anomalous techniques in macromolecular crystallography

Fellowships

- NIGMS: Maximizing access to research careers; T34 (2008 - 2010, <https://www.nigms.nih.gov/Training/MARC/Pages/USTARAwards.aspx>)

- Stanford NIH Biotech. training program (2011 - 2014, <https://btp.stanford.edu/>)

Previous Work experience

- Contract data manager, Institute for Pacific Island Forestry (IPIF) in Hilo HI (April 2015 - Sept 2015)
- Cardinal Scholars private tutor (2014/2015)
- Teaching assistant (June 2007-May 2008)
- Supplementary Instructor UT San Antonio (Aug. 2006 - May 2008)

Websites

- **Pubs:** <https://scholar.google.com/citations?user=7hIRrWEAAAAJ&hl=en&authuser=1>
- **Code:** <http://stackoverflow.com/users/2077270/dermen>

Extracurricular

folk singing, guitar playing