

**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
- American Crystallographic Association (2019 Covington, Kentucky), Application of anomalous techniques in macromolecular crystallography

## **Fellowships**

- Minority access to research careers (MARC) fellowship (2008 - 2010)
- NIH Biotech. training grant fellowship (2011 - 2014)

## 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