Stanford



Derek Mendez

Staff Scientist - Biomedicine, Stanford Synchrotron Radiation Lightsource

NIH Biosketch available Online Curriculum Vitae available Online

Bio

CURRENT ROLE AT STANFORD

Computational staff scientist at the Stanford Synchrotron Radiation Lightsource (SSRL), in the Macromolecular Crystallography group (Structural and Molecular Biology division).

Main activities revolve around a 3 year BRaVE-funded project to build a new X-ray resource for the acceleration of medicines development (XMeD). Active in-silico areas of research are in the characterization of crystallization outcomes, virtual and experimental screening of ligands, in-silico methods for lead molecule optimization, and extremely sensitive absorption profile characterization using machine learning techniques. A major computational goal is to determine the most valuable tools (and develop new ones) for future XMeD users.

Beyond XMeD, we are focusing on using GPUs and machine learning models to accelerate processing and characterization of user diffraction data that is collected at SSRL beamlines 12-1, 12-2, 14-1, and 9-2. In addition, we are aiming to make available to users new methods that process X-ray diffraction data at the pixel-level in order to extract more information to better resolve structural changes in proteins arising from e.g., binding events and light/chemical driven dynamics.

We are also partnering with NERSC to build a framework for our beamline users to offload computationally intensive jobs to the Perlmutter GPU cluster.

EDUCATION AND CERTIFICATIONS

- BS, University of Texas at San Antonio , Physics, Math (2010)
- PhD, Stanford University , Applied Physics (2017)

PERSONAL INTERESTS

Diffraction AI: https://smb.slac.stanford.edu/~resonet/

EasyBragg diffraction simulators for Python: https://smb.slac.stanford.edu/~dermen/easybragg/

The last question: https://users.ece.cmu.edu/~gamvrosi/thelastq.html

LINKS

- The last question: https://users.ece.cmu.edu/~gamvrosi/thelastq.html
- AI for diffraction (Resonet): https://smb.slac.stanford.edu/~resonet/
- Simulate diffraction with easyBragg: https://smb.slac.stanford.edu/~dermen/easybragg/

Publications

PUBLICATIONS

- **Deep residual networks for crystallography trained on synthetic data.** *Acta crystallographica. Section D, Structural biology*
  Mendez, D., Holton, J. M., Lyubimov, A. Y., Hollatz, S., Mathews, I. I., Cichosz, A., Martirosyan, V., Zeng, T., Stofer, R., Liu, R., Song, J., McPhillips, S., Soltis, et al
  2024

- **Beyond integration: modeling every pixel to obtain better structure factors from stills.** *IUCrJ*
  Mendez, D., Bolotovsky, R., Bhowmick, A., Brewster, A. S., Kern, J., Yano, J., Holton, J. M., Sauter, N. K.
  2020; 7 (Pt 6): 1151–67

- **Angular correlations of photons from solution diffraction at a free-electron laser encode molecular structure** *IUCRJ*
  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, et al
  2016; 3: 420-429

- **Observation of correlated X-ray scattering at atomic resolution.** *Philosophical transactions of the Royal Society of London. Series B, Biological sciences*
  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, et al
  2014; 369 (1647)

- **Real-time XFEL data analysis at SLAC and NERSC: A trial run of nascent exascale experimental data analysis** *CONCURRENCY AND COMPUTATION-PRACTICE & EXPERIENCE*
  Blaschke, J. P., Brewster, A. S., Paley, D. W., Mendez, D., Bhowmick, A., Sauter, N. K., Kroger, W., Shankar, M., Enders, B., Bard, D.
  2024; 36 (12)

- **Accelerating x-ray tracing for exascale systems using Kokkos** *CONCURRENCY AND COMPUTATION-PRACTICE & EXPERIENCE*
  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.
  2024; 36 (5)

- **Interpreting macromolecular diffraction through simulation.** *Methods in enzymology*
  Young, I. D., Mendez, D., Poon, B. K., Blaschke, J. P., Wittwer, F., Wall, M. E., Sauter, N. K.
  2023; 688: 195-222

- **Chemical crystallography by serial femtosecond X-ray diffraction.** *Nature*
  Schriber, E. A., Paley, D. W., Bolotovsky, R., Rosenberg, D. J., Sierra, R. G., Aquila, A., Mendez, D., Poitevin, F., Blaschke, J. P., Bhowmick, A., Kelly, R. P., Hunter, M., Hayes, et al
  1800; 601 (7893): 360-365

- **Untangling the sequence of events during the S2 S3 transition in photosystem II and implications for the water oxidation mechanism.** *Proceedings of the National Academy of Sciences of the United States of America*
  Ibrahim, M., Fransson, T., Chatterjee, R., Cheah, M. H., Hussein, R., Lassalle, L., Sutherlin, K. D., Young, I. D., Fuller, F. D., Gul, S., Kim, I., Simon, P. S., de Lichtenberg, et al
  2020

- **SAD phasing of XFEL data depends critically on the error model.** *Acta crystallographica. Section D, Structural biology*
  Brewster, A. S., Bhowmick, A., Bolotovsky, R., Mendez, D., Zwart, P. H., Sauter, N. K.
  2019; 75 (Pt 11): 959-968

- **High-viscosity injector-based pink-beam serial crystallography of microcrystals at a synchrotron radiation source.** *IUCrJ*
  Martin-Garcia, J. M., Zhu, L., Mendez, D., Lee, M. Y., Chun, E., Li, C., Hu, H., Subramanian, G., Kissick, D., Ogata, C., Henning, R., Ishchenko, A., Dobson, et al
  2019; 6 (Pt 3): 412-425

- **Processing simultaneously collected MAD data from two closely spaced (90 eV) wavelengths measured at an X-ray free-electron laser**
  Mendez, D., Weis, W., Brunger, A., Wakatsuki, S., Sauter, N.
  INT UNION CRYSTALLOGRAPHY.2019: A244