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Bayesian Library for the Analysis of Neutron Diffraction Data[1]
WILLIAM RATCLIFF, NIST - National Institute of Standards Technology , JOSEPH LESNIEWSKI, Georgetown University, DYLAN QUINTANA, Carnegie Mellon University — During this talk, I will introduce the Bayesian Library for the Analysis of Neutron Diffraction Data. In this library we use of the DREAM [1] algorithm to effectively sample parameter space. This offers several advantages over traditional least squares fitting approaches. It gives us more robust estimates of the fitting parameters, their errors, and their correlations. It also is more stable than least squares methods and provides more confidence in finding a global minimum. I will discuss the algorithm and its application to several materials. I will show applications to both structural and magnetic diffraction patterns. I will present examples of fitting both powder and single crystal data. [1] Jasper A. Vrugt, Cajo J. F. ter Braak, Martyn P. Clark, James M. Hyman, and Bruce A. Robinson, WATER RESOURCES RESEARCH, VOL. 44, W00B09 (2008)

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