Abstract Submitted
for the 4CS19 Meeting of
The American Physical Society

Parallel Density and Root-Mean-Square Analyses in MDAnalysis
NIKOLAUS AWTREY, SHUJIE FAN, OLIVER BECKSTEIN, Arizona State University Department of Physics — MDAnalysis is a widely used Python library for the analysis of particle-based simulations in the biomolecular and materials science communities. Parallel MDAnalysis, known as PMDA, is being developed to make use of modern multicore computers as well as high performance supercomputing resources. PMDA uses functions from MDAnalysis along with Dask to seamlessly construct parallel versions of the analyses in MDAnalysis. We added two new analysis tools to PMDA: DensityAnalysis and RMSF. DensityAnalysis gives users the ability to find concentrations of molecules around proteins and other biophysical systems. RMSF calculates the positional root mean square fluctuations of proteins as a measure of their flexibility. We developed a new parallel algorithm for RMSF based on partial means and sums of squares [1]. The results are consistent with the serial version in MDAnalysis and have been verified using the NumPy standard deviation functions on arbitrary data sets. Benchmark results are shown corresponding to typical use.

[1] T. F. Chan, G. H. Golub, and R. J. LeVeque. In COMPSTAT 1982, Ed. by H. Caussinus, P. Ettinger, and R. Tomassone. (1982), doi: 10.1007/978-3-642-51461-6$_3$.

Nikolaus Awtrey
Arizona State University Department of Physics

Date submitted: 13 Sep 2019 Electronic form version 1.4