Representing low-resolution electron density maps from solution scattering data

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Many computational algorithms devoted to the interpretation and modeling of small angle scattering (SAS) data have been developed over the last several decades. In addition to the commonly used ASCII text files containing fits to data, real space transforms, modeling parameters, etc., modeling algorithms often generate coordinate files containing 3D coordinates of atomic or coarse-grained models to describe the object. Due to their versatility and community acceptance, coordinate files have become popular for representing models from a variety of different algorithms including bead modeling, rigid body modeling, ensemble modeling, flexible fitting, molecular dynamics, etc. and have found wide spread adoption in the SAS community. As novel algorithms are developed, new representations of particles are often required that may not be compatible with conventional coordinate models. Here I will describe the program DENSS[1] which generates low-resolution 3D density maps from 1D solution scattering data using a novel *ab initio* reconstruction algorithm. The primary output of DENSS is an MRC file, commonly used in the electron microscopy community (and similar to the CCP4 format used in crystallography), which represents objects on a 3D grid of voxels where each voxel has a value corresponding to the density at that location. DENSS offers advantages over conventional algorithms that are implicit to its use of density to represent particles. Accurate and unbiased interpretation of a density map requires understanding how visualization programs graphically represent the 3D grid of values and how the low-resolution nature of the reconstruction affects this visualization. This includes tasks such as selecting appropriate contour thresholds and how to accurately and unbiasedly display such low-resolution density maps in publication figures and archives. Community engagement in this area will help to generate a set of standards for accurately publishing low-resolution density maps to avoid overinterpretation, as has previously been done for validation of conventional SAS models[2].

[1] Grant, T.D. (2018). *Nature Methods.* **15,** 191–193.

[2] Trewhella, J., *et. al.* (2017). *Acta Cryst. D. Struct. Bio.* **79(9)**, 710-728.

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