Automatic calculation of Local Resolution with MonoRes: A new approach, its assessment and new applications.

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Resolution has always being a key topic in cryoEM [1]. The ability to calculate local (per pixel) resolution, first accessible with Blocres [2] and then with the very successful ResMap [3] approach, has had an important impact in the field. Building on the successful use of local resolution estimations, we introduce MonoRes, a new approach that provides fully automatic and fast estimations, rendering a locally-filtered (per pixel) map that can be used as input to any modelling or docking approach. Naturally, an assessment of MonoRes as compared to previous methods is also presented. Finally, we note that an extension of MonoRes towards Tomography is currently under analysis.

The roots of MonoRes algorithm are the named monogenic signals [] which represent mathematical generalization to several dimensions of the well-known 1D analytic signals. These kind of signal allow to decompose instantaneously (locally) a function into an envelope and phase terms. Thus the algorithm use a sweep of frequencies, starting the filtering process of the input density map at a given frequency and calculated the monogenic signal at each frequency. Hence, the so-called monogenic amplitude (local energy or envelope) is computed. The values of local resolution are obtained by comparison of the monogenic amplitude to the distribution of noise energy at that frequency, allowing to determine if at that resolution and that location monogenic amplitude is significantly higher than noise. Noise estimation can be performed either using two volumes calculated from two halves of the data or, instead, taking into account those voxels within a user defined mask.

The method has been tested with many experimental volumes, in particular, the chosen data set to illustrate the capabilities of the new algorithm, was the RNA polymerase I at 3.4 Å (EMDB entry 3593) [5]. The results agree with the FSC, casting the median value of the resolution histogram close to the FSC.

MonoRes and ResMap are available within the Scipion image processing framework [4], as well as freely served over the Web as part of Scipion Web Tools (http://scipion.cnb.csic.es/m/services/), accessible both from Madrid and the EMDB (under “Validation”)

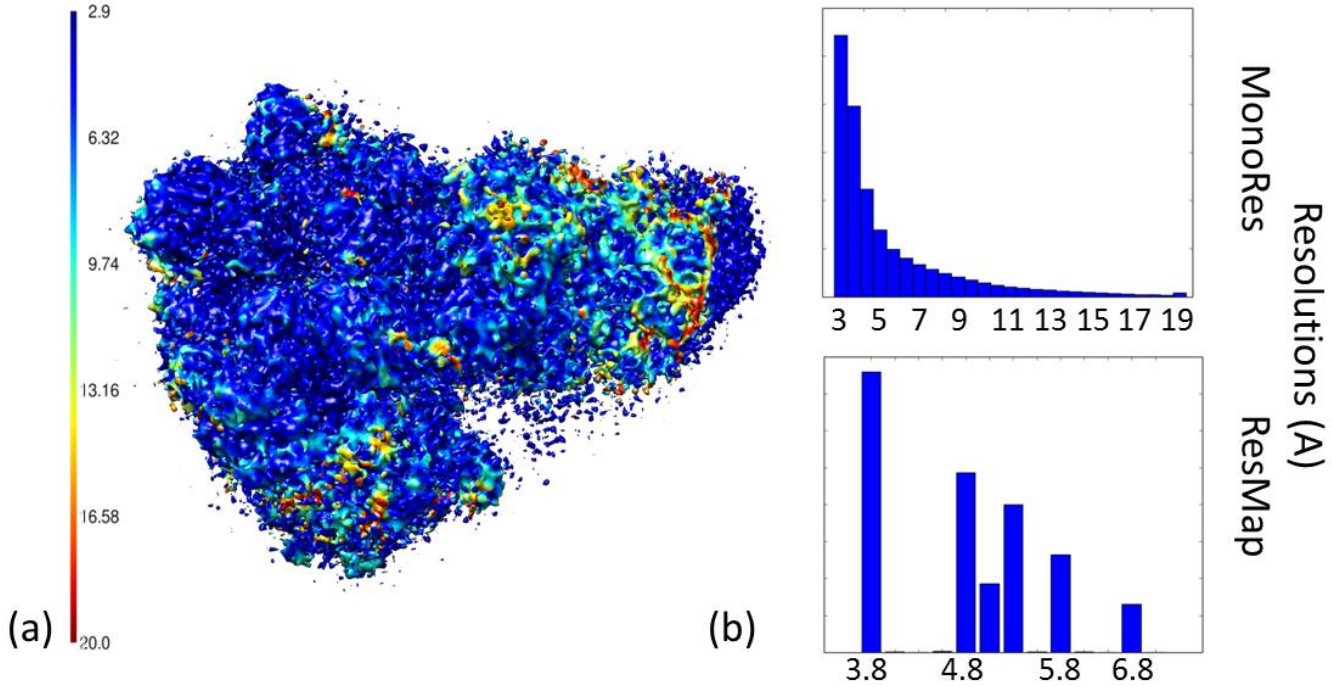

Figure 1. (a) Resolution map cast by Monores for the EMDB 3592 (FSC 2.8 Å at 0.143) . (b) The resolution histograms obtained with MonoRes and ResMap.

References:

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The authors would like to acknowledge economical support from: The Comunidad de Madrid through grant CAM(S2010/BMD-2305), the Spanish Ministry of Economy and Competitiveness through Grants AIC-A-2011-0638, and 335 BIO2013-44647-R, and the Fundación General CSIC (Programa ComFuturo).