

LocalDeblur: An automatic map sharpening by restoration of local resolution

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Cryo-EM maps benefit significantly of a “postprocessing” step, normally referred to as “sharpening”, that tends to increase signal at medium/high resolution. In this work we present a new method, LocalDeblur, in which our newly formulated local resolution approach [1] is used to restore the map. It works equally well, and beyond state of the art [2, 3, 4], for maps at medium and at quasi-atomic resolution.

INTRODUCTION

As a consequence of our work on local resolution [1], we achieve a local characterization of the map in terms of its locally variant monogenic signal. At this point it seemed natural to approach sharpening as a restoration considering this information. In this work we present our work on local deblurring, that applies equally well to quasi-atomic and to medium resolution maps, providing excellent results beyond state of the art [2,3,4]. Naturally, if structural models exist, a combination with methods such as locScale can be performed, further enhancing the results. We refer to our method as “LocalDeblur”.

METHOD

Let A be a linear operator that performs a local band-pass filter of a 3D map centered for each spatial location. The frequency at each location is given by a local resolution estimator (in our examples, we use Monores [1]). Let y be the 3D reconstructed volume and x the sharpened volume. We look the minimizer of the objective function:

$$\min \|y - Ax\|^2$$

The gradient descent iteration of this objective function is

$$x^{(k+1)} = x^{(k)} + \lambda A^T (y - Ax^{(k)})$$

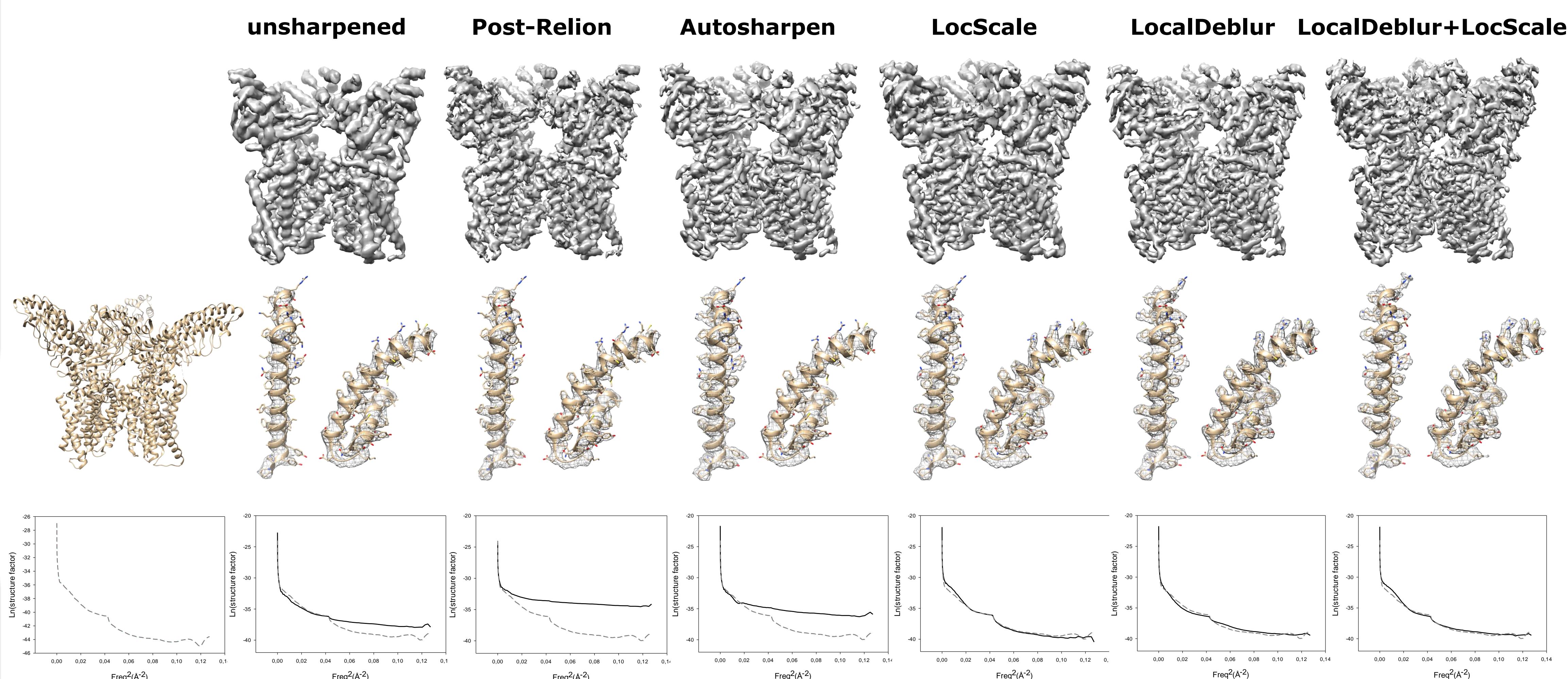
This iteration is known as the Richardson-Lucy algorithm in image restoration. We start with $x^{(0)} = y$.

RESULTS

We have used two cryo-EM maps to illustrate our approach. The first one corresponds to TRPV1 and the second to RIBOSOME. In the two cases the lay out of the Figures is similar. We present from left to right the unsharpened map (in both cases obtained by Relion), and then the sharpened versions corresponding to Relion postprocessing [2] (Post-Relion), Phenix sharpening [3] (Autosharpen), LocScale [4], LocalDeblur and LocalDeblur+LocScale. Zoom-out of significant areas are presented in all cases [(TRPV1: residues 419-465 and 568-642) (RIBOSOME: residues 283-378 and 149-283)]. On the bottom of the two Figures, we show a B-factor plot.

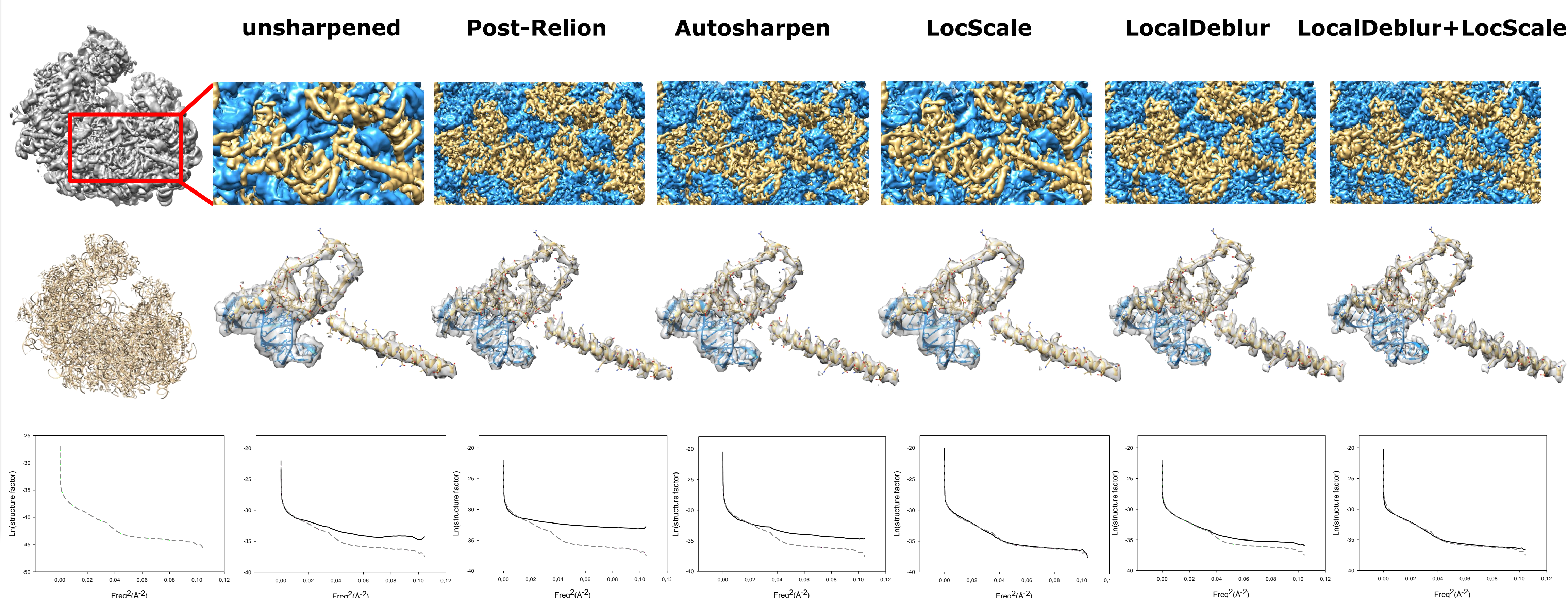
TRPV1

Structure of the capsaicin receptor



RIBOSOME

Structure of the *Plasmodium falciparum* 80S ribosome



CONCLUSION

LocalDeblur, is showing a very significant increase in the interpretability of cryo-EM maps at the same time that restores very well structure factors. The method is applicable to a broad range of maps, at medium or high resolution.

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