MS42-O5

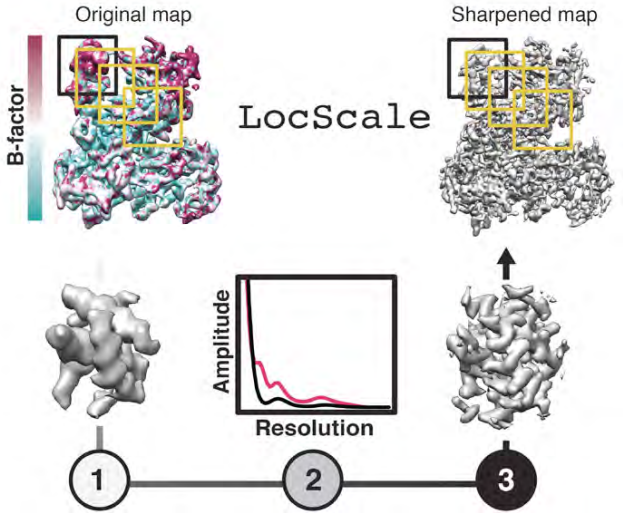
Reference-based restoration of local contrast for cryo-EM density interpretation

Arjen Jakobi[1]

1. Department of Bionanoscience, Kavli Institute of Nanoscience, Delft University of Technology, Delft, Netherlands (Holland, Europe)

email: a.jakobi@tudelft.nl

Improvements in detector technology and image processing algorithms have rendered single-particle cryo-EM capable of routinely delivering structures of macromolecular assemblies at near-atomic resolution, permitting building and refining of atomic models. Yet, the interpretation of cryo-EM density maps with atomic models often remains challenging due to specific properties such as inherent contrast loss and spatial variation in map resolution. Variations in map resolution, if combined with global contrast restoration procedures, may result in density maps with locally inappropriate sharpening levels that are prone to hamper or even misguide misguide atomic model building. We have recently suggested a reference-based sharpening procedure to restore local structural features in cryo-EM density maps more faithfully [1]. We here present this procedure and explore the conditions for which local sharpening provides benefits over global contrast restoration procedures. Based on a systematic analysis of local vs. global sharpening procedures using publicly available datasets from the EMDB we identify boundary conditions for which local reference-based contrast restoration can be effective tool for map sharpening. We will illustrate pitfalls in atomic model building resulting from map sharpening artifacts and we outline practical issues affecting optimal sharpening results. The presented procedures should help overcome common difficulties in map interpretation using high-resolution cryo-EM density maps.



References:

[1] Jakobi et al, eLife 6: e27131 (2017)

Keywords: cryo-EM, map sharpening, model building

MS43 Topological analysis of structures: algorithms and software

Chairs: Prof. Patrick McArdle, Prof. Vladislav Blatov

MS43-O1

Distinguishing metal-organic frameworks

Senja Barthel[1], Eugeny V. Alexandrov[2], Davide M. Proserpio[3], Berend Smit[1]

1. Laboratory of Molecular Simulation, EPFL Valais Wallis, Sion, Switzerland
2. Samara Center for Theoretical Material Science, Samara University and Samara State Technical University, Samara, Russia
3. Dipartimento di Chimica, Università degli Studi di Milano, Milano, Italy

email: senja.barthel@epfl.ch

We consider two metal−organic frameworks as identical if they share the same bond network respecting the atom types. An algorithm is presented that decides whether two metal−organic frameworks are the same. It is based on distinguishing structures by comparing a set of descriptors that is obtained from the bond network. We demonstrate our algorithm by analyzing the CoRe MOF database of DFT optimized structures with DDEC partial atomic charges using the program package ToposPro.

References:

doi: 10.1021/acs.cgd.7b01663

Keywords: metal-organic frameworks, topological analysis