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FEM: Feature Enhanced Map

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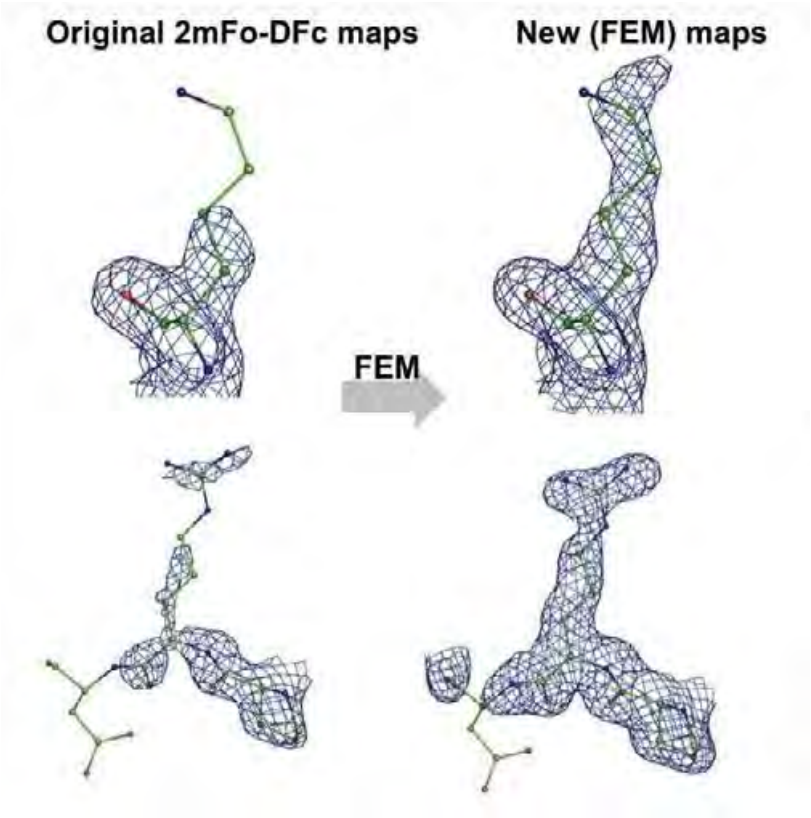
A method is proposed that modifies 2Fo-Fc σA-weighted map such that the resulting map has significantly reduced amount of noise and model bias, and at the same time the weak signal is enhanced so it is visible as good as the strong signal. We call the new map Feature Enhanced Map (FEM). An atomic model is a result of interpretation of the electron density map. There are at least three fundamentally different sources of map imperfections that affect quality of this interpretation. 1) Errors. Fourier map artifacts due to finite resolution and completeness of data, errors in experimental data and crystal model parameters result in noise peaks in map that oftentimes appear very much similar to the true atomic structure and in turn may be erroneously interpreted as such. Also, the noise may obscure or corrupt the signal making its meaningful interpretation difficult or even impossible. 2) Signal strength. Not all the signal presented in the map has the same strength: a strong signal arising from a heavy atom derivative may obscure weak signal arising from a partially occupied very mobile ligand or residue side chain alternative conformation or hydrogen atoms. It is common that such weak signals are near or below the noise level. 3) Model bias. Crystallographic maps are calculated using model phases alone or a combination of model and experimental phases. Once placed, correctly or not, atoms feed back revealing themselves in the map. Therefore erroneously placed atoms may be positively confirmed against the map resulting in an incorrect structure. All three sources of map imperfections are always present together. They make interpretation of crystallographic maps never unambiguous, trivial, or unique at typical macromolecular resolutions. The new method aims to overcome these problems and is available in Phenix software. More information: http://www.phenix-online.org/presentations/fem_SEP2013.pdf



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