From: Colin Nave
To: CCP4BB@JISCMAIL.AC.UK
Subject: Re: [ccp4bb] Fwd: [ccp4bb] FW: [ccp4bb] Resolution and distance accuracies
Date: Thursday, January 06, 2011 6:14:27 AM

I too think the phrase super-resolution is rather misleading, in particular the analogy with light microscopy methods. Super-resolution in these latter cases is achieved via different physical phenomena (think excitations not waves).

Would one claim super-resolution when refining the relative positions of the carbon atoms in benzene given the constraints of 6 fold symmetry and a carbon carbon distance of 1.39 angstroms?

What would Moliere think?

However, to quote from the DEN paper
"Our approach is a major advance over conventional modeling of low resolution X-ray diffraction data by fitting rigid bodies since it accounts for deformations of the models while at the same time using a minimal set of variables (the single-bond torsion angles)"

Overall this seems a reasonable claim.
Colin

From: CCP4 bulletin board [mailto:CCP4BB@JISCMAIL.AC.UK] **On Behalf Of** Charles W. Carter, Jr
Sent: 06 January 2011 09:52
To: CCP4BB@JISCMAIL.AC.UK
Subject: [ccp4bb] Fwd: [ccp4bb] FW: [ccp4bb] Resolution and distance accuracies

Begin forwarded message:

From: "Charles W. Carter, Jr" <carter@med.unc.edu>
Date: January 6, 2011 10:51:20 AM GMT+01:00
To: Gerard Bricogne <gb10@GLOBALPHASING.COM>
Subject: Re: [ccp4bb] FW: [ccp4bb] Resolution and distance accuracies

I echo Gérard's thought.

Pascal Retailleau did a relevant experiment published in Acta D:

Retailleau, et al., (2001) High-resolution experimental phases for tryptophanyl-tRNA synthetase
(TrpRS) complexed with tryptophanyl-5'AMP, Acta Cryst, D57, 1595–1608

He determined three independent sets of experimental phases for two different 1.7 Å selenomethionine structures (SAD) plus a 1.6 Å native (MIRAS) and refined the structures independently. The rmsd between the

two SeMet structures was 0.25 Å, whereas that between the two SAD structures and the native structure was 0.39 Å, sufficient to demonstrate significant differences between the SeMet and native proteins. This experimental variance is a quite considerable indication of the magnitude of coordinate errors.

Thus, as Gérard, who also was an author on that work together with Bob Sweet, points out, we're delighted to discover we have been achieving super-resolution to use Axel's neologism!

Charlie

On Jan 6, 2011, at 10:13 AM, Gerard Bricogne wrote:

Dear Axel,

On Sun, Dec 26, 2010 at 01:15:44PM -0800, Axel Brunger wrote:

We defined "super-resolution" in our DEN paper as
achieving coordinate accuracy better than the resolution
limit d_min of the diffraction data. We proposed this
definition in analogy to its use wide-spread use in optical microscopy:
"super-resolution" methods such as STORM, PALM, and STED achieve
accuracy of positions of fluorescent labels significantly better than the
diffraction limit (in some cases, sub-nanometer accuracy -
Pertsinidis, Zhang, Chu, Nature 466, 647-651, 2010).

In that case, all crystallographers doing stereochemically restrained refinement will now have become aware, to their great delight, that they have been unknowingly achieving "super-resolution" all the time, from the grand old days of Bob Diamond's real-space refinement program - just like Monsieur Jourdain found out that he had been speaking in prose all his life without realising it.

I guess that "super-resolution" is a sexier keyword in the mind of editors of Nature that "restrained crystallographic refinement" :-)) !

With best wishes for the New Year,

Gerard.

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We found DEN to be useful to move some atoms into correct
positions in cases where electron density maps are difficult or
impossible to interpret at low resolution. By default, DEN is

active during the first torsion angle molecular dynamics stages, but then turned off during the last two stages. In addition, the DEN network is deformable. Thus, DEN is very different from "secondary structure" restraints or point restraints to reference models which are "on" all the time. Rather, DEN steers or guides the torsion angle conformational search process during refinement.

Cheers,
Axel

On Dec 24, 2010, at 2:14 PM, Bernhard Rupp (Hofkristallrat a.D.) wrote:

> > I find the "super-resolution" claims in this paper a bit of a conjuring
> trick.
>
> I think it is understood that information cannot come from nothing. You
> cannot cheat in basic physics. Interestingly, I had the same discussion with
> bioinformatics colleagues a short time ago. The problem is the same and
> seems of a semantic nature. They are using prior information of some sort
> (undisclosed) to successfully improve maps and they suggested to call this
> 'resolution increase'. I had the same objection and said that in
> crystallography resolution is a relatively hard term defined by the degree
> to which experimental observations are available, and as crystallographers
> we won't like that claim at all.
>
> On the other side it is uncontested that as long as the model fits
> (crossvalidation-) data better when prior information is used, something
> useful has been achieved - again with all the caveats of weights and