On the Appearance of Crystals during Diffusion MRI

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INTRODUCTION: In this work, we demonstrate a remarkable phenomenon in diffusion MRI. When pure dihydrogen monoxide (maintained at room temperature) is sampled with a carefully-calibrated sampling scheme comprising six sampling vectors (arranged according to a model of electrostatic repulsion), peaks in the orientational density function are distributed with incredible regularity. Despite the absence of apparent structure outside the scanner, our analysis shows that a combination of high B0-field (3000 mT!!!!), and rapidly changing magnetic field gradients, leads to alignment of the eigenvectors of the tensor produce a regular crystalline dodecahedral arrangement.

METHODS: A spherical phantom, filled with non-doped dihydrogen monoxide, was fully visually inspected, placed in the centre of the magnet, and allowed to stabilize for 24 hours prior to the start of the experiment. Diffusion-weighted data were collected using sampling schemes comprising 6, 8, 10 and 12 unique directions (distributed according to an electrostatic repulsion algorithm). 2.4 mm isotropic resolution, and a b-value of approximately 600 s/mm^2 (optimized to provide precise estimates of the diffusivity). The diffusion tensor was estimated within each voxel according to a weighted linear least squares routine – for each of the different acquisitions and the principal eigenvector computed in each voxel. For each sampling scheme, the orientation of the principle eigenvector was plotted for every voxel on the unit sphere. Due to an unfortunate incident during the preparation of this abstract, the actual data were lost – but with careful Monte Carlo simulations, we were able to simulate the results from dihydrogen monoxide to the extent that, as far as we recall, resemble those obtained from the phantom.

RESULTS: With a low number of gradient sampling vectors (n = 6), we found a regular pattern of orientation of the principal eigenvector. Figure 1 shows the distribution of these eigenvectors alongside the orientation of the sampling vectors. The regularity was so remarkable that, using a simulated annealing algorithm, we were able to fit a dodecahedron to the points – therefore revealing a true crystalline structure. As the number of unique orientations was increased, the regularity of this crystalline structure weakened and disappeared. (see Figure 1). At the completion of scanning, the phantom was removed from the magnet and inspected – and the substrate inside again appeared amorphous.

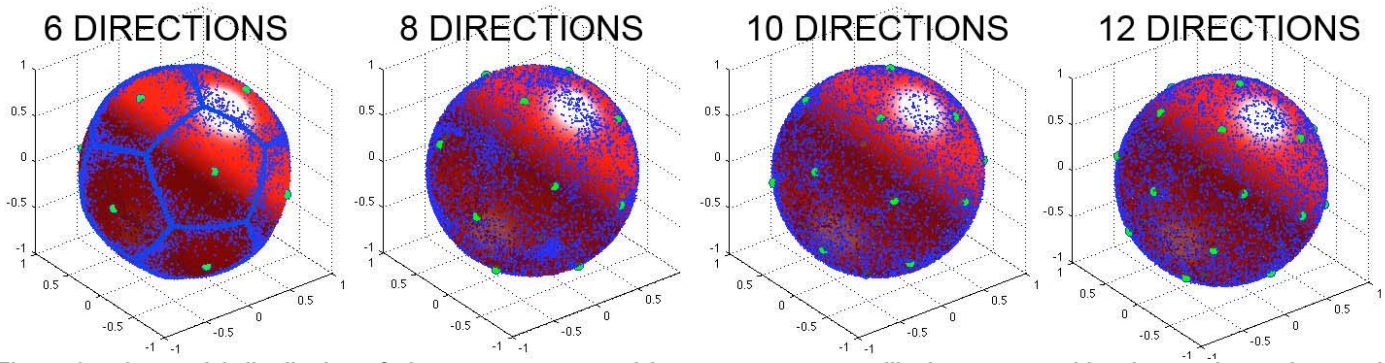

Figure 1 – the spatial distribution of eigenvectors measured in room temperature dihydrogen monoxide when an increasing number of gradient sampling vectors is used. Green dots = sampling vectors, blue dots = eigenvectors For the 6-direction ('perfectly' symmetric) sampling scheme, the eigenvectors are sufficiently uniform that they can be fitted with a dodecahedron – using simulated annealing

DISCUSSION: Several important observations can be made:

1. The crystalline structure only appeared at the start of the experiment – when six directions were used.
2. The vertices of the crystal are not aligned with the sampling vectors. In fact, almost no eigenvectors are aligned with the sampling vectors.
3. Crucially, we find that increasing the number of encoding vectors serves to dissolve this transient structure.

Thus, we have discovered a new mechanism for generating a crystalline form of dihydrogen monoxide, using only a superconducting magnet and time-varying magnetic field gradients. The exact mechanism underpinning our crystallisation process has yet to be established. We have considered many important factors. Notably, the six-direction sampling scheme is the only one where the electrostatic (Coulombic) forces are truly balanced. Perhaps this symmetry invokes further symmetry in the substrate. As more directions are added, the electrostatic forces involved (and perhaps associated heat dissipation) serve to break down the symmetry seen at $N = 6$. We have considered conducting more experiments in this domain to learn more. However, a colleague (I.C. Orl) has recently pointed out (*personal communication)* that:

1. Dihydrogen monoxide may be crystallised more cheaply and efficiently using domestic refrigeration devices
2. The appearance of the crystalline structure is purely an artefact of the Rician noise distribution

He went on to say that in each voxel the principal eigenvector points along the axis of *highest* diffusivity. If the SNR is such that the Rician noise floor is encountered, then the diffusivity along the sampling vector will be *under*estimated and therefore the lowest– (something to do with squashing peanuts). Thus the eigenvectors will point 'anywhere but along the sampling vectors'. As the number of sampling vectors becomes higher, this becomes harder – and thus – the distribution becomes more uniform. To refute his assertions, we conducted further simulations – but this time with Gaussian noise – but he was right! The crystalline structure did indeed disappear. Thus, our colleague was right on his point 2 – so we now resort to his point 1 – and each time we wish for some crystalline dihydrogen monoxide in our beverages, we go to the fridge. Lesson learnt.

CONCLUSION: A small number of sampling vectors in an isotropic medium leads to a very non-uniform distribution of eigenvectors if plotted across all voxels. One *might* have anticipated a uniform distribution of eigenvectors. However, the Rician noise-distribution in complex data means that there is an intrinsic bias *away* from the sampling vectors leading to a non-uniform distribution that is, at first, non-intuitive. Checking for the uniformity of the eigenvectors in an isotropic medium – as a method of quality assurance on gradient calibration (i.e. agreement between gradient axes) – would require a larger number of sampling vectors.