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HIGH RESOLUTION ORIENTATION DISTRIBUTION FUNCTION

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Abstract. A new method for reconstructing a High Resolution Orientation Distribution Function (HRODF) from X-ray diffraction data is presented. It is shown that the method is capable of accommodating very localized features, e.g. sharp peaks from recrystallized grains on a background of a texture component from the deformed material. The underlying mathematical formalism supports all crystallographic space groups and reduces the problem to solving a (large) set of linear equations. An implementation on multi-core CPUs and Graphical Processing Units (GPUs) is discussed along with an example on simulated data.

Introduction

Reconstruction of the Orientation Distribution Function (ODF) from diffraction data is a well established discipline, see e.g. [1,2,3]. Here, we present a new method that facilitates reconstruction of High Resolution ODF (HRODF) from synchrotron diffraction data. The aim of the method is to optimize the use of the information content from far field detectors to explore the substructure of the individual diffraction features. The method relies on a new parameterization of the orientation space [4], which extends the properties of the Rodrigues-Frank space [5] to include the full orientation space and thus supporting all space groups.

Mathematical Framework

In the following the mathematical framework for HRODF is outlined and it is shown that properties of the Rodrigues-Frank (RF) space can be extended to include the full orientation space and thus supporting all space groups.
The crystallographic orientation given by the unit quaternion $Q = (q_1, q_2, q_3, q_4) = (q_1, \mathbf{q})$, i.e. $\sqrt{q_1^2 + q_2^2 + q_3^2 + q_4^2} = 1$, can be parameterized by the rotation axis $\mathbf{n} = (\mathbf{n_1}, \mathbf{n_2}, \mathbf{n_3})$ (unit 3-vector) and a rotation angle, ω, around the rotation axis,

$$Q = (\cos\frac{\omega}{2}, n_1 \sin\frac{\omega}{2}, n_2 \sin\frac{\omega}{2}, n_3 \sin\frac{\omega}{2}). \quad (1)$$

The *gnomonic* projection maps the quaternion into the RF space,

$$Q \to \frac{\mathbf{q}}{q_1} = \tan\frac{\omega}{2}\mathbf{n} \equiv \mathbf{r}. \quad (2)$$

For two diffraction vectors in reciprocal space, **h** and **g**, the set of orientations that maps **h** onto **g**, *the geodesic*, is represented as a straight line in RF space. For high symmetry space groups the RF space is finite, but infinite when $\omega \to \pi$ needed for the low symmetry space groups. The space is not Euclidian and the density of orientations drops off as $1/\left(\pi(1+|\mathbf{r}|^2)\right)^2$.

The singularity in Eq.(2) can be avoided if we apply a generalized gnonomic map $\mathcal{G}$,

$$\mathcal{G} : Q \to \frac{1}{q^{max}} Q, \quad q^{max} = \max\{|q_1|, |q_2|, |q_3|, |q_4|\}. \tag{3}$$

As a result there are 8 three dimensional domains, or bounding cubes (four possibilities of the origin of q^{max} in addition to the sign of q^{max}), called *frustums*. The frustums are labelled F_k with $\pm k \in \{1, 2, 3, 4\}$ and $k = 1$ if $q_1 = q^{max}$ or $k = -1$ if $q_1 = -q^{max}$, and so on. Each frustum constitutes a cube with side length of 2 and $F_{\pm k} = \{(x_1, x_2, x_3, x_4) \,|\, x_k = \pm 1, -1 \leq x_i \leq 1, i \neq k\}$. The generalization of Eq.(2) then reads,

$$\mathcal{G} : Q = q_1 + q_2\mathbf{i} + q_3\mathbf{j} + q_4\mathbf{k} \to \frac{Q}{q^{\max}} = \begin{cases} \left(\frac{q_2}{(1-q_1^2)^{1/2}}, \frac{q_3}{(1-q_1^2)^{1/2}}, \frac{q_4}{(1-q_1^2)^{1/2}}\right) \tan\frac{\omega_1}{2}, & \text{if } |q_1| = q^{\max} \\ \mathbf{i}\left(-\frac{q_1}{(1-q_2^2)^{1/2}}, \frac{q_4}{(1-q_2^2)^{1/2}}, -\frac{q_3}{(1-q_2^2)^{1/2}}\right) \tan\frac{\omega_2}{2}, & \text{if } |q_2| = q^{\max} \\ \mathbf{j}\left(-\frac{q_4}{(1-q_3^2)^{1/2}}, -\frac{q_1}{(1-q_3^2)^{1/2}}, \frac{q_2}{(1-q_3^2)^{1/2}}\right) \tan\frac{\omega_3}{2}, & \text{if } |q_3| = q^{\max} \\ \mathbf{k}\left(\frac{q_3}{(1-q_4^2)^{1/2}}, -\frac{q_2}{(1-q_4^2)^{1/2}}, -\frac{q_1}{(1-q_4^2)^{1/2}}\right) \tan\frac{\omega_4}{2}, & \text{if } |q_4| = q^{\max} \end{cases}, \tag{4}$$

where $\tan\frac{\omega_k}{2} = \frac{\sqrt{1-q_k^2}}{q_k}$. The inverse map from Frustum to quaternion space is simply

$$\mathcal{G}^{-1} : X \to \frac{X}{||X||}. \tag{5}$$

Each Frustum preserves the properties of the RF space locally. In quaternion space the geodesic is a great circle on the 3-sphere and can be parametrized with a orthogonal quaternion pair, Q_1 and Q_2,

$$C_{(Q_1,Q_2)}(u) = Q_1 \cos u + Q_2 \sin u, \quad u \in [0 : 2\pi) \tag{6}$$

with

$$Q_1 = \left(\cos\frac{\nu}{2}, \frac{\mathbf{g}\times\mathbf{h}}{|\mathbf{g}\times\mathbf{h}|}\sin\frac{\nu}{2}\right), \quad Q_2 = \left(0, \frac{\mathbf{g}+\mathbf{h}}{|\mathbf{g}+\mathbf{h}|}\right), \quad \cos\nu = \frac{\mathbf{g}\cdot\mathbf{h}}{|\mathbf{g}||\mathbf{h}|}. \tag{7}$$

The ODF reconstruction can then be formulated as an inverse problem,

$$\int_{C_{(Q_1,Q_2)}} f(s)ds = \int_0^{\pi} f(Q_1\cos t + Q_2 \sin t)dt = I_{(\mathbf{g},\mathbf{h})}, \tag{8}$$

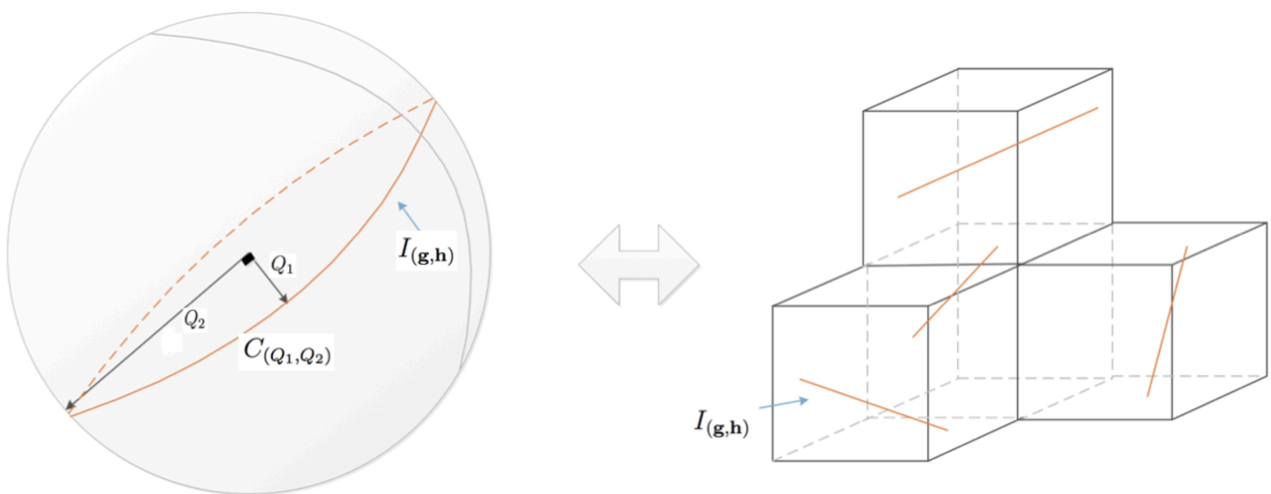

Fig. 1: The geodesic on the 3-sphere corresponds to piecewise straight lines through the frustums.

i.e. the integral over the geodesic $C(Q_1, Q_2)$ is given by the measured intensity $I_{(\mathbf{g},\mathbf{h})}$. Here **h** is a theoretical diffraction vector that maps onto the measured diffraction vector **g**. Since the ODF is an even function it is only necessary to integrate over half of the great circle. Consequently, the full orientation space can be represented by $F_1, ..., F_4$, i.e. $\cup_{k=1}^4 F_k$. The gnomonic projection of $C_{(Q_1,Q_2)}(u)$, $u \in [0, \pi)$ traverses between two to four frustums and within each frustum the projection is a straight line, as illustrated in Fig. 1. There exists an analytical solution for finding the entry and exit points of the geodesic within each of the visited frustums. We refer the reader to [4] for a detailed description. By subdividing each frustum into N^3 voxels, each voxel having a side length of $2/N$, the ODF reconstruction reduces to solving a (large) set of linear equations. More specifically, for each measurement the set of visited voxels can be derived by performing ray tracing through the voxel mesh connecting the frustum entry and exit points. The integral equation (8) reduces to

$$\sum_j a_{ij} x_j = I^i_{\mathbf{g},\mathbf{h}} \tag{9}$$

for the ith measurement. Here, x_j is the ODF density in the jth voxel, a_{ij} is the weight (path length through the jth voxel normalized by π). As the geodesic is a 1D intersection with a 3D object the set of linear equations is very sparse. In fact, at most $12N - 8$ weights out of $4N^3$ are nonzero.
For $N = 1000$ an average resolution of the HRODF below 0.2 degrees can be obtained for the lowest symmetry space group. As the RF space is not Euclidian the resolution varies across the frustums when using uniformed voxel size. By rescaling the voxels sizes according to the local geometric properties in the RF space a more homogeneous overall resolution can be obtained.

Implementation

Even though the sparsity of the linear problem is high a straightforward reconstruction of the HRODF puts very high demand on memory storage. E.g. for $N = 1000$ the memory consumption of the $\{a_{ij}\}$ matrix alone would require 44 TB, far beyond the capability of conventional computers. Instead, by making on-the-fly calculations of the $\{a_{ij}\}$ matrix the same problem can be handled by less than 128 GB of memory, which is within reach of the largest conventional computers today. An HRODF reconstruction Toolbox has been developed [6] with these considerations in mind. Along with the diffraction data the user specifies the unit cell and space group of the material. Inside the toolbox several reconstruction procedures are available, using various linear solvers and ray tracers. These can be adapted to the specific needs of the reconstruction task at hand. The toolbox utilizes multiple CPU cores for reconstruction.If Graphical Processing Units (GPUs) from NVIDIA are available in the computer, then solving can be accelerated by distributing part of the workload to the GPUs. This is due to the highly parallel architecture of the GPUs, especially beneficiary for ray tracing, but also some linear solvers.

Example

In the following we will demonstrate, by means of simulated data, the capability of capturing both smooth and distinct features in the microstructure. The simulated ODF is given by a smooth component superimposed by local sharp features. The density of the smooth component reads $\rho(W) = 0.05w_0^2 + 0.02w_1^2 + 0.03w_2^2 + 0.06w_3^2$, where $W = (w_1, w_2, w_3, w_4)$ is a unit quaternion. In each frustum the sharp features are given by four ball-shaped entities with different densities: 0.02, 0.01, 0.015 and 0.005, respectively. The grid size of the simulated ODF is $N = 257$. A 2D cross section of the simulated ODF is shown in Fig. 3(A). The simulated data set is given by 10 million randomly chosen geodesics (i.e. orthogonal quaternion pairs $(Q_1, Q_2)_i$) passing though the simulated ODF. The integral along the individual geodesic provides the intensity $I^i_{\mathbf{g},\mathbf{h}}$. In real data this is related to the intensity from the diffraction vector **g**. The set of 10 million linear equations is then solved using the HRODF toolbox. In

Fig. 3(B) the resulting ODF after 2 hours of reconstruction with $N = 257$ is shown. Clearly additional iterations are needed in order to approach the correct solution. The reconstruction time can be improved by refining the grid size during the reconstruction, called the hierarchical method. Initially a solution is obtained on a coarse grid with $N = 17$. Next the solution is divided on a finer grid size $N = 33$ and a refined solution is reconstructed. The procedure continues with grid sizes of 65, 129 and 257. In Fig. 3(C) is hierarchical solution after 2 hours of reconstruction is shown. The residual of the hierarchical method is two orders of magnitude lower than the fixed grid size reconstruction.

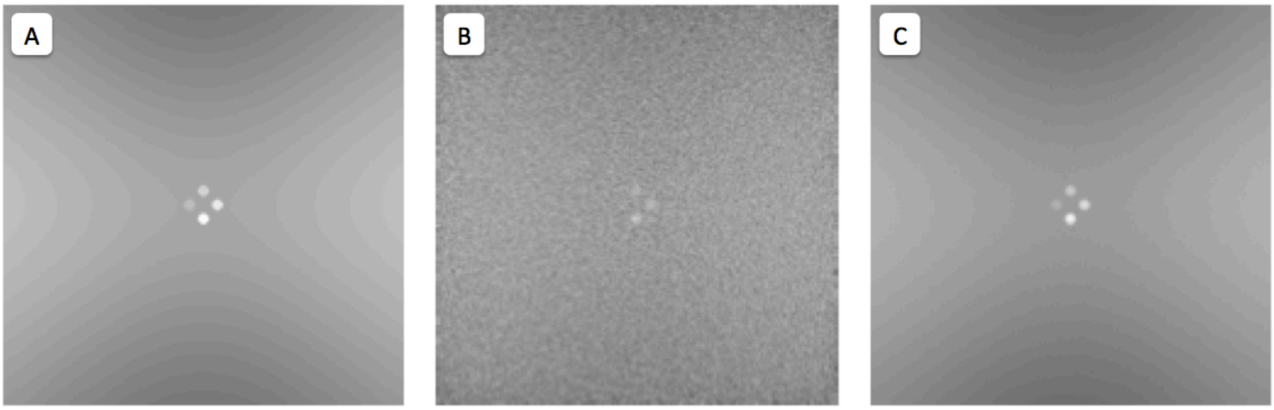

Fig. 2: Example of HRODF reconstruction on simulated data. A 2D cross section through frustum F_1, with grid size $N = 257$, is shown: In A the simulated ODF, in B the ODF reconstruction with constant grid size, and in C the hierarchical ODF reconstruction.

Summary

A novel procedure for reconstructing High Resolution Orientation Distribution Functions for all space groups from diffraction data has been developed. The implementation handles very large problems and facilitates a resolution of 0.2 degrees for the lowest symmetry space groups.

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