Inversion of the spherical Radon transform by means of Gabor and Wavelet frames with applications in diffraction tomography

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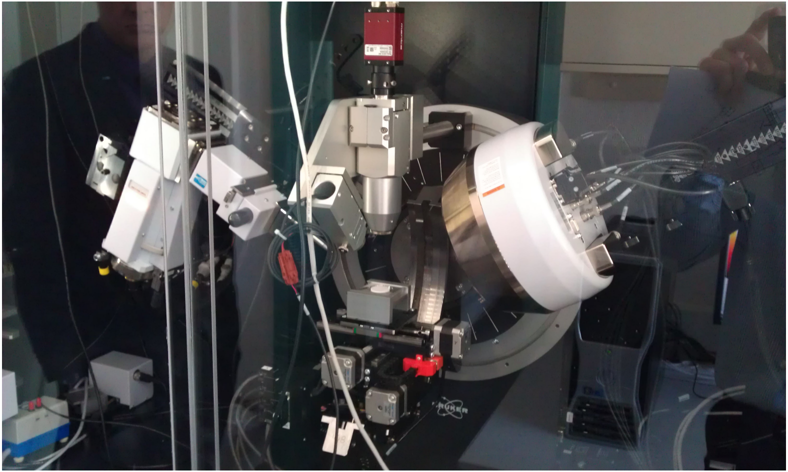
Diffraction tomography



Texture goniometry corresponds to evaluate a orientation density function (ODF) by means of X-ray diffraction *without* destroying it.

- Texture analysis with X-ray diffraction data $\hookrightarrow$ analysis of orientation distribution by volume;
- Polycrystalline specimen carries crystal grains with orientation within a given range $\mathcal{G}^*$ of all feasible orientations $\mathcal{G} \subset SO(3)$;
- Density of orientation function f: for given $g \in SO(3)$, we have $\frac{\Delta V_g}{V} \to f(g)dg$;
- Pole figure $P_x(y)$: a correspondence of a fixed crystal direction x with a test direction y, that is, $\frac{\Delta V_g}{V} \to P_x(y)dy$ for $g(x) = y$;

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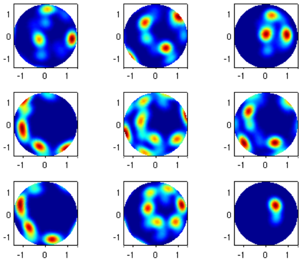
Pole figures example



These pole figures correspond to nine fixed crystal directions $x \in S^2$ and all test directions $y \in S^2_+$;

Polar density function $\mathcal{P}f : \mathbb{S}^2 \times \mathbb{S}^2 \to \mathbb{R}^+$, where $\mathcal{P}f(x, y)$ denotes the probability that a given crystal direction x or its symmetric $-x$ coincide with a specific direction y.

Therefore,

$$\mathcal{P}f(x, y) = \frac{1}{2} \left(\mathcal{R}f(-x, y) + \mathcal{R}f(x, y) \right),$$

where $\mathcal{R}f$ denotes the spherical X-ray transform

$$\mathcal{R}f(x, y) = \frac{1}{2\pi} \int_{\mathcal{G}_{xy}} f(g)dg, \quad and\ \mathcal{G}_{xy} = \{g \in SO(3) : g(x) = y\}.$$

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$$\mathcal{R}f(x, y) = \frac{1}{2\pi} \int_{\mathcal{G}_{xy}} f(g) dg, \quad \textit{and } \mathcal{G}_{xy} = \{ g \in SO(3) : g(x) = y \}.$$

Motivation: Spherical X-Ray transform

An integral transform $\mathcal{R} : L_2(Spin(3)) \mapsto L_2(S^2 \times S^2)$ such that

$$\begin{aligned}\mathcal{R}f(x,y) &= \frac{1}{2\pi}\int_{g\in Spin(3):y=g(x)} f(g)dg \\ &= 4\pi\int_{Spin(3)} f(g)\delta_y(g(x))dg \\ &= 4\pi\int_{C(x,y)} f(q)dq,\end{aligned}$$

where $C(x,y) = \{q \in S^3 \sim \mathbb{H} : qx\overline{q} = y\}$ is a great circle in $S^3 \sim \mathbb{H}$.

Properties

- $\mathcal{R}f$ satisfies the ultra-hyperbolic equation $(\Delta_x - \Delta_y)\mathcal{R}f = 0$
- Regularity: $\mathcal{R} : L_2(Spin(3)) \mapsto H^{1/2}(S^2 \times S^2) \cap \ker(\Delta_x - \Delta_y)$ and $||f||_{H^{1/2}(S^2\times S^2)} := ||(-2\Delta_{S^2\times S^2} + 1)^{1/4} f||_{L_2(S^2\times S^2)}$
- $\mathcal{R}$ is an isometry: $||\mathcal{R}f||_{H^{1/2}(S^2\times S^2)} = 16\pi^2||f||_{L_2(Spin(3))}$
- Inversion formula: $f(g) = \frac{1}{4\pi}\int_{S^2}(-2\Delta_{S^2\times S^2} + 1)^{1/2}\mathcal{R}f(x, gx)dx$
- For more details see also works of V. Palamodov, S. Helgason, and others

Motivation: Statement of Main problem

- Given the map $R : L_2(Spin(3)) \mapsto L_2(S^2 \times S^2)$ and data $y = Rf$ how retrieve f ?
- Questions:
  - how to expand f ? Spherical frame expansion
  - how to compute/approximate R^{-1}? Iterative Approach
  - how to treat noisy data $y_\delta, |y - y_\delta| \leq \delta$? Regularization

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What is a frame?

Frame definition

We call a system $\{\psi_i\}_{i\in I}$ a frame for X if for all $f \in X$ there exists constants $A, B > 0$ such that

$$\frac{1}{A}||f||^2 \leq \sum_{i\in I} | < f, \psi_i > |^2 \leq \frac{1}{B}||f||^2$$

Dual frame

Given a frame $\{\psi_i\}_{i\in I}$ there exists a dual frame $\{\psi_i^*\}_{i\in I}$ such that for all $f \in X$ one has

$$f = \sum_{i\in I} < f, \psi_i^* > \psi_i.$$

How we can work with frames?

- $\{\psi_i : x_i \in X_i\}$ has a dual frame, i.e.

$$f = \sum < f, \tilde{\psi}_i > \psi_i$$

- In practical terms:
  Given $(< f, \psi_i >)$ how to calculate $(< f, \tilde{\psi}_i >)$?
- Frame operator $F : f \mapsto (< f, \psi_i >) = (c_i)$
- Adjoint operator $F^* : (c_i) \mapsto \sum \psi_i c_i$
- Given system $F^* c = f$

Gabor frames - Concept in $\mathbb{R}^n$

- signal $f \in L_2(\mathbb{R}^n)$
- windowed Fourier transform:

$$V_\psi f(\omega, b) = \int_{\mathbb{R}^n} f(x)\psi(x-b)e^{i<\omega,x>}dx$$

- group-based interpretation:

$\pi : G = \mathbb{R}^n \times \mathbb{R}^n \mapsto \mathcal{U}(L_2(\mathbb{R}^\ltimes))$ via $\pi(\omega, b)\psi(x) = e^{i<\omega,x>}\psi(x-b)$

$$V_\psi f(\omega, b) = \int_{\mathbb{R}^n} f(x)\pi(\omega, b)\psi(x)dx$$

Gabor frames - Concept in S^3

- signal $f \in L_2(S^3)$
- proper windowed Fourier transform:

  translations and modulations on the sphere
  $G := E(4) = Spin(4) \ltimes \mathbb{R}^4$
- Representation of G in $L_2(S^3)$:

$$\pi(s,p)f(q) = f(\bar{s}qs)e^{i\langle p,q\rangle}$$

- windowed Fourier transform:

$$V_\psi f(s,p) = \int_{S^3} f(q)\psi(\bar{s}qs)e^{i\langle p,q\rangle}\,dS_q$$

Gabor frames - Concept in S^3

- Problem: representation is not square-integrable, i.e.

$$\|V_\psi f\|_{L_2(G)} \text{ is not finite}$$

- group is too “large”
- therefore choose some closed subgroup H and consider $X = G/H$ with G-invariant measure $d\mu(x)$
- example: $H = \{(0,0,0,p_4) \in G, p_4 \in \mathbb{R}\}$
- consider instead for $(s,p) \in X$,

$$V_\psi f(s,p) =< f, \pi(\sigma(s,p)^{-1})\psi >$$

- Admissibility condition:

$$\int_X |\langle f, \pi(\sigma(s,p)^{-1})\psi\rangle|^2 d\mu(x) = \langle A_\sigma^\psi f, f\rangle \quad \forall f \in L_2(S^3)$$

Spherical Gabor transform

Lemma (admissibility and isometry)

Assume that the window $\psi \in L_1(S^3) \cap L_2(S^3)$ is such that $\mathrm{supp}(\psi) \subseteq S^3_+$

$$0 \neq C_\psi = 64\pi^5 \int_0^{2\pi} \int_0^{\pi} \int_0^{\pi/2} \frac{|\psi(q(\theta,\alpha,\phi))|^2}{\cos\phi} \, d\phi \, d\alpha \, d\theta < \infty. \tag{1}$$

Then the map

$$f \in L^2(S^3) \mapsto \frac{1}{\sqrt{C_\psi}} V_\psi f \in L^2(Spin(4) \times \mathbb{R}^3)$$

is an isometry, i.e.

$$\int_{Spin(4)\times\mathbb{R}^3} |V_\psi f(s,p)|^2 \, d\mu(s) \, dp = C_\psi \int_{S^3} |f(q)|^2 dS_q.$$

Spherical Gabor transform

Corollary (reconstruction)

Any $f \in L^2(S^3)$ can be reconstructed by

$$f(q) = \frac{1}{C_\psi} \int_{\mathrm{Spin}(4)} \int_{\mathbb{R}^3} V_\psi f(s,p) e^{-i\langle \bar{s}ps, q\rangle} \psi(sq\bar{s})\, dp\, d\mu(s).$$

No discrete expansion formula

Possible choice of window function:

$$\psi(q) = \cos^\eta(\alpha \arccos(q_0))\chi_{[\frac{\pi}{6},\frac{\pi}{2}]}(q_0)$$

Dual window is given approximately by finite linear combination of "shifted" windows.

Spherical Gabor transform

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Continuous Wavelet transform - Concept in $\mathbb{R}$

- Wavelet:

$$\psi_{a,b}(x) = \pi(a,b)\psi(x) = \frac{1}{\sqrt{a}}\psi\left(\frac{x-b}{a}\right),$$

  with $(a,b) \in \mathbb{R} \setminus \{0\} \times \mathbb{R}$

- $$\pi(a_1,b_1)\pi(a_2,b_2)\psi = \pi(a,b)\psi$$

  with $(a,b) = (a_1 a_2, a_1 b_2 + b_1)$

- Wavelet transform

$$V_\psi f(a,b) = \int_{\mathbb{R}} \pi(a,b)\psi(x)f(x)dx$$

Extensions to the sphere

- Many constructions based on approximate identities
- Diffusive wavelets using the heat kernel by S. Ebert (PhD thesis 2011)
- Using the Iwasawa decomposition of $SO(n+1,1)$ by Antoine, Vandergheynst 1998
- Using the Cartan decomposition of $Spin(n+1,1)$ by M. Ferreira 2005

Conformal group of the ball

- Lorentz group Spin$(1, n)$ - conformal group of the ball.
- Cartan decomposition Spin$(1, n)$=Spin$(n)\times$Spin$(1, 1)\times$Spin(n).
- For $n \geq 3$ representations are not square-integrable $\Rightarrow$ need to factorize
- Spin$(n)\times$Spin$(1, 1)$ $\Rightarrow$ Wavelet analysis
- Spin$(1, 1)\times$Spin(n) $\Rightarrow$ function theory in the unit ball
- Spin$(1, 1)\times$Spin(n) - “group of Möbius transformations” does NOT form a group $\Rightarrow$ representation theory for gyrogroups - M. Ferreira 2007

Gyrogroup

Definition

A groupoid $(G, \oplus)$ is a gyrogroup if its binary operation satisfies the following axioms:

1. There is at least one element 0 satisfying $0 \oplus a = a$, for all $a \in G$;
2. For each $a \in G$ there is an element $\ominus a \in G$ such that $\ominus a \oplus a = 0$;
3. For any $a, b, c \in G$ there exists a unique element $\mathrm{gyr}[a, b]c \in G$ such that the binary operation satisfies the left gyroassociative law $a \oplus (b \oplus c) = (a \oplus b) \oplus \mathrm{gyr}[a, b]c$;
4. The map $\mathrm{gyr}[a, b] : G \to G$ given by $c \to \mathrm{gyr} c$ is an automorphism of the groupoid $(G, \oplus)$, that is $\mathrm{gyr}[a, b] \in \mathrm{Aut}(G, \oplus)$;
5. The gyroautomorphism $\mathrm{gyr}[a, b]$ possesses the left loop property

$$\mathrm{gyr}[a, b] = \mathrm{gyr}[a \oplus b, b]$$

Spherical Wavelet Transform

Consider the Möbius transformations:

$$\varphi_a(x) = (a - x)(1 - \bar{a}x)^{-1}, |a| < 1$$

.

Representation:

$$\pi_1(s, a_\phi)\psi(x) = \left(\frac{1 - |a_\phi|^2}{|1 - a_\phi \bar{s}xs|^2}\right)^{\frac{n-1}{2}} \psi(\varphi_{-a_\phi}(\bar{s}xs))$$

$V_\psi : L_2(S^{n-1}) \to L_2(G)$

$$\begin{aligned} V_\psi f(s, a_\phi) &= < \pi_1(s, a_\phi)\psi, f > \\ &= \int_{S^{n-1}} \overline{\left(\frac{1 - |a_\phi|^2}{|1 - a_\phi \bar{s}xs|^2}\right)^{\frac{n-1}{2}} \psi(\varphi_{-a_\phi}(\bar{s}xs))} f(x)\, dS(x) \end{aligned}$$

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Spherical Wavelet transform

Lemma (admissibility)

Assume that the Fourier coefficients of $\psi \in L_2(S^3)$ satisfy

$$\frac{1}{N(n,l)} \sum_{M=1}^{N(n,l)} \int_{-1}^{1} |\hat{\psi}_{\sigma(te_n)}|^2 d\mu(te_n) < \infty \tag{2}$$

uniformly in l then the map

$$f \in L^2(S^3) \mapsto W_\psi f \in L^2(Spin(4) \times Spin(1,1))$$

is an invertible operator, i.e.

$$\int_{Spin(4)\times Spin(1,1)} |W_\psi f(s,p)|^2 \, d\mu(s) \, dp = \int_{S^3} \overline{(A_\sigma^\psi f)(q)} f(q) dS_q.$$

Spherical Wavelet transform

Corollary (reconstruction)

Any $f \in L^2(S^3)$ can be reconstructed by

$$f(q) = \int_{-1}^{1} \int_{\mathrm{Spin}(4)} W_\psi f(s, \sigma(te_n)) \left[R_s (A_\sigma^\psi)^{-1} D_{\sigma(te_n)} \psi \right] (q) d\mu(s) d\mu(te_n).$$

No discrete expansion formula

Admissible wavelets using Cayley transform:

$$g : H_4 \to S^3, g(x) = (x + e_4)(1 + e_4 x)^{-1}$$

Spherical Wavelet transform

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Frames via coorbit space theory

Correspondence principle

Let π be a square integrable representation of the Euclidean group $Spin(4) \ltimes \mathbb{R}^4$ mod (H, σ) with an admissible pair (ψ, σ). Then V_ψ is a bijection of $L_2(S^3)$ onto the RKHS $\mathcal{M}_2$
$\mathcal{M}_2 = \{F \in L_2(X) : \langle R(g, \cdot), F\rangle = F(g)\}$ where

$$R(g, l) := \langle \psi, \pi(\sigma(h)\sigma(l)^{-1})\psi\rangle = V_\psi(\pi(\sigma(l)^{-1})\psi)(h)$$

Two classic assumptions:

1. $R(g, l)$ is absolutely integrable over the group
2. Representation is irreducible
3. Coorbit space $Co(Y) = \{T \in S' | V_\psi T \in Y\}$

Gabor Frames via coorbit space theory

- Choose $\mathcal{U}$-dense and relatively separated family $\{x_i\}_{i\in I} \subset X$
- Define the oscillation kernel

$$\mathrm{osc}_{\mathcal{U}}(l,h) := \sup_{u\in\mathcal{U}} \left|\langle \psi, \pi(\sigma(l)\sigma(h)^{-1})\psi - \pi(u^{-1}\sigma(l)\sigma(h)^{-1})\psi\rangle_{L_2(S^3)}\right|$$

- Estimate

$$\begin{aligned} \leq \quad & \sup_{u\in\mathcal{U}} \left| \int_{S^3_+} e^{i\langle q, p - s_1\overline{s_2} r s_2 \overline{s_1}\rangle} \left(\psi(s_2\overline{s_1} q s_1 \overline{s_2}) - \psi(s_2\overline{s_1} s_u q \overline{s_u} s_1 \overline{s_2})\right) \overline{\psi}(q)\, dS_q \right| \\ & + \sup_{u\in\mathcal{U}} \left| \int_{S^3_+} e^{i\langle q, p - s_1\overline{s_2} r s_2 \overline{s_1}\rangle} \left(1 - e^{i\langle q, s_1\overline{s_2} p_u s_2 \overline{s_1}\rangle}\right) \psi(s_2\overline{s_1} s_u q \overline{s_u} s_1 \overline{s_2}) \overline{\psi}(q)\, dS_q \right| \end{aligned}$$

Gabor Frames

Theorem (frames)

Assume

$$\int_X \mathrm{osc}_{\mathcal{U}}(l,h)\,d\mu(l) < \frac{\eta}{C_\psi} \quad \textit{and} \quad \int_X \mathrm{osc}_{\mathcal{U}}(l,h)\,d\mu(h) < \frac{\eta}{C_\psi} \tag{3}$$

with $\eta < 1$. Then the set $\{\psi_i := \pi(\sigma(x_i))\psi : i \in I\}$ is a frame for $L_2(S^3)$. This means that

1. $f \in L_2(S^3) \Leftrightarrow \{\langle f, \psi_i \rangle\}_{i \in I} \in \ell_2$,
2. there exists constants $0 < A \leq B < \infty$ such that
$$A\|f\|_{L_2(S^3)} \leq \|\{\langle f, \psi_i \rangle\}_{i \in I}\|_{\ell_2} \leq B\|f\|_{L_2(S^3)} ,$$
3. there exists a bounded, linear synthesis operator $S : \ell_2 \to L_2(S^3)$ such that $S(\{\langle f, \psi_i \rangle\}_{i \in I}) = f$.

Difference with case of spherical wavelets

$$R(t,s,t',s') = \int_{\mathbb{S}^3} \left[\left(\frac{1-\alpha^2}{|1-\alpha e_n \bar{s}' s x \bar{s} s'|^2} \right)^{\frac{n-1}{2}} \psi(\varphi_{-\alpha e_n}(\bar{s}' s x \bar{s} s')) \overline{\psi(x)} \right] dS_x$$

- L_1-integrability is difficult to achieve
- Way out: Use $T = \cap_{p>1} L_p$ as target space (S. Dahlke, et al., JFAA, 2016)
- $T = \cap_{p>1} L_p$ is still closed under convolution!

Frames via coorbit space theory

- Choose $\mathcal{U}$-dense and relatively separated family $\{x_i\}_{i\in I} \subset X$
- Define the oscillation kernel

$$\mathrm{osc}_{\mathcal{U}}(l,h) := \sup_{u\in\mathcal{U}} |\langle\psi, \pi(\sigma(l)\sigma(h)^{-1})\psi - \pi(u^{-1}\sigma(l)\sigma(h)^{-1})\psi\rangle_{L_2(S^3)}|^p$$

- Estimate the decay of the Fourier coefficients of the oscillation kernel

Wavelet Frames

Theorem (frames)

Assume

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Construction of wavelet frame

- Dilation discretization via a hyperbolic lattice for $te_3, t \in [-1, 1]$
- Lattice for Spin(4) via a subdivision scheme (G. Nawratil, H. Pottmann, 2007) $\rightarrow$ quasi-uniform distribution
- Consider the function

$$h(x) = \begin{cases} \cos(2\pi f(2x)) & \frac{1}{8} \leq |x| \leq \frac{1}{4} \\ \sin(2\pi f(x)) & \frac{1}{4} \leq |x| \leq \frac{1}{2} \\ 0 & \end{cases}$$

with $f_\epsilon(x) = \frac{\lambda(\epsilon(\frac{1}{2}-x))}{4\left(\lambda(\epsilon(x-\frac{1}{4})+\lambda(\epsilon(\frac{1}{2}-x)))\right)}$, $\lambda(x) = e^{-|x|^2}$.

Inversion of X-ray transform

- R is an integral transfrom $\rightarrow$ Rf belongs to smoothness space
- only noisy data y^δ available: $Rf + \epsilon = y^\delta \in L_2(S^3 \times S^3)$ with $|y - y^\delta| \leq \delta$
- Assume f has a sparse expansion within $\{\psi_i\}_{i \in I}$

$$f(p) = Fc(p) = \sum_{i \in J \subset I, |J| \text{small}} c_i \psi_i(p)$$

Inversion of X-ray transform

- Optimization problem:

$$\min_{c \in B_R} ||y^\delta - R(Fc)||^2$$

with $B_K = \{c \in l_2(I) : ||c||_{l_1(I) \leq K}\}$

- Minimization through projected steepest descent with step length control

$$c_i^{n+1} = P_K \left(c_i^n + \frac{\beta_n}{r} (F^* R^* (y - R(Fc_i^n))) \right)$$

Given	operator R, some initial guess c^0, and K (sparsity constraint ℓ_1-ball B_K)
Initialization	$\lVert RF^* \rVert^2 \leq r$, set $q = 0.9$ (as an example)
Iteration	**for** $n = 0, 1, 2, \ldots$ **1.** $\beta^n = C \cdot \sqrt{\frac{D(x^0)}{D(x^n)}}$, $C \geq 1$ (greedy guess) **2.** $c^{n+1} = P_K\left(c^n + \frac{\beta^n}{r} FR^*(y - R(F^*(c^n)))\right)$; **3.** verify (B2): $\beta^n \lVert R(F^* c^{n+1}) - R(F^* c^n) \rVert^2 \leq r \lVert c^{n+1} - c^n \rVert^2$ **if** (B2) is satisfied increase n and go to **1.** **otherwise** set $\beta^n = q \cdot \beta^n$ and go to **2.** **end**

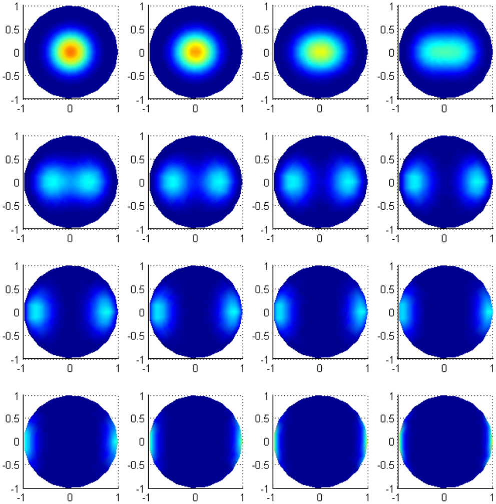
Numerical Simulation with Gabor frames

- Simple analyzing atom

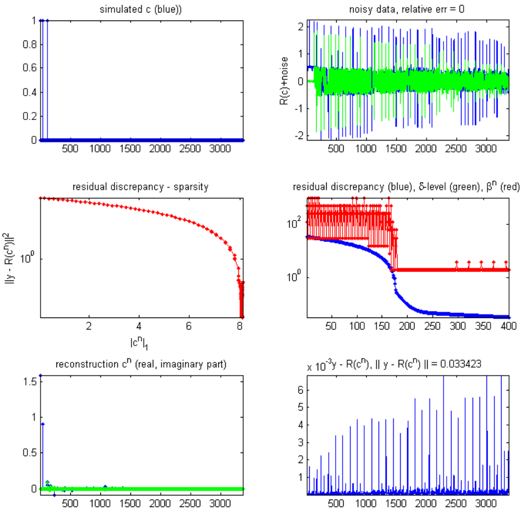
$$\psi(q) = \cos^6(2.6 \arccos(q_0)), \quad \frac{\sqrt{3}}{2} \leq q_0 \leq 1,$$

- Frame grid: frequency $\mathbb{Z}_3$, rotation 120 vertices of the 600-cell
- 17 of the 32 space groups are subgroups of the 600-cell
- (synthetic) example of an ODF with orthorhombic crystal symmetry and triclinic symmetry for the specimen
- 3 cases: no noise, 5% noise, 10% noise

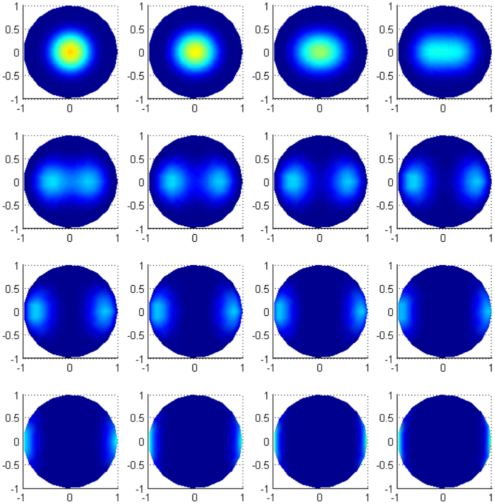
Original configuration



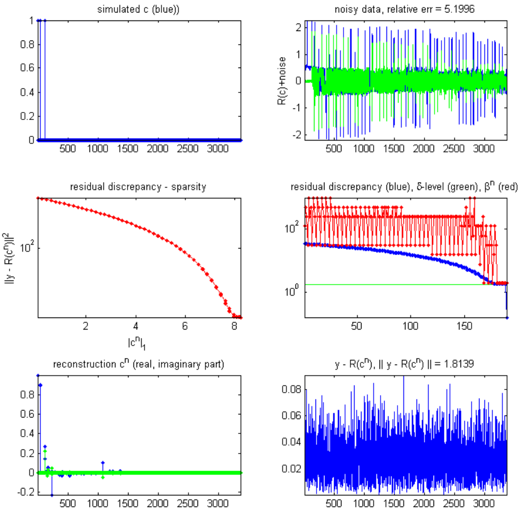
Reconstruction without noise



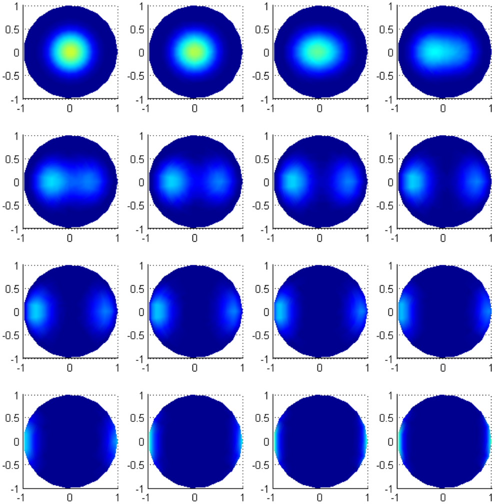
Reconstruction without noise



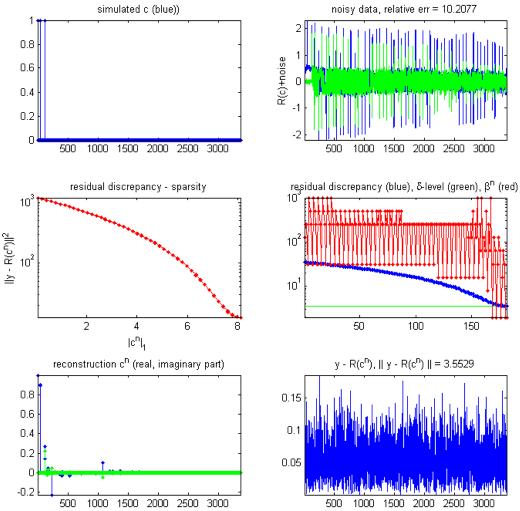
Reconstruction with 5% error



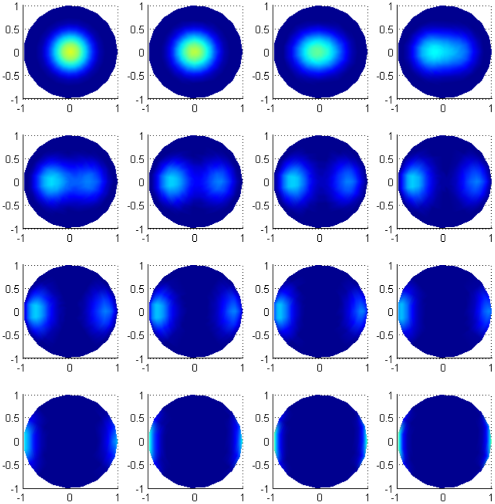
Reconstruction with 5% error



Reconstruction with 10% error



Reconstruction with 10% error



The end!

Thank you for your attention.

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FCT Fundação para a Ciência e a Tecnologia

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