

Rich and Nonabelian Tomography: strain and magnetic fields

Bill Lionheart Naeem Desai Søren Schmidt Philip Withers

Tomography for Scientific Advancement, Bath 2016

Rich tomography

- ▶ Increasingly we need to image quantities with **more degrees of freedom** than a simple scalar
- ▶ Vector fields such as the magnetic field in a magnetic domain
- ▶ Tensor field such strain. To do this tomographically we need richer data than one scalar per line.
- ▶ We call such problems *Rich tomography*

New modalities

- ▶ In many cases the relevant transport equation involves matrix multiplication and this gives rise to **non-Abelian tomography** problems.
- ▶ In other cases what is measured is a projection of the vector or tensor field in the **transverse or longitudinal** directions.
- ▶ As new tomographic measurement modalities arise we need to understand what data is needed for a stable reconstruction and how to do that reconstruction numerically.

Transport/Beer Lambert

Transport equation, linear attenuation $-f$ photon flux u

$$\xi \cdot \nabla u(x, \xi) = \frac{\partial}{\partial s} u(x + s\xi, \xi) = f(x)u(x, \xi)$$

Data measured along a line (infinite but f only non-zero in some finite radius ball) input $u_- = u(x - \infty\xi, \xi)$ and output $u_+ = u(x + \infty\xi, \xi)$ results in solution to differential equation

$$\ln(u_+/u_-) = \int_{-\infty}^{\infty} f(x + s\xi) ds$$

Transverse and Longitudinal ray transform

For a scalar f the x-ray transform

$$Xf(x, \xi) = \int_{-\infty}^{\infty} f(x + s\xi) ds \quad (1)$$

For a tensor (matrix) f the longitudinal ray transform

$$If(x, \xi) = \int_{-\infty}^{\infty} \xi \cdot f(x + s\xi)\xi ds \quad (2)$$

...and transverse ray transform

$$Jf(x, \xi) = \int_{-\infty}^{\infty} \Pi_{\xi} f(x + s\xi)\Pi_{\xi} ds \quad (3)$$

Where $\Pi_{\xi} = I - \xi\xi^T$ is the projection matrix perpendicular to ξ

Inversion

- ▶ X can be inverted plane-by-plane (Radon transform inversion) [5]
- ▶ I cannot be inverted – it takes linear strains (symmetric derivatives of vector fields) to zero. $f_{ij} = \partial g_i / \partial x_j + \partial g_j / \partial x_i \implies If = 0$
- ▶ J can be inverted plane-by-plane easily with **six** rotation axes using Radon transform inversion [6]
- ▶ J can be inverted from data from three rotation axes by a more complicated method [4].

A tale of two strain tomographies

- ▶ Both x-rays and neutrons are *diffracted* by crystals, this is widely used for crystallography
- ▶ Metals are *polycrystalline*, that is they consist of small randomly oriented crystals.
- ▶ For polycrystalline materials the diffraction pattern is averaged over the group of rotations in three space.
- ▶ If the metal is subjected to linear elastic strain the crystals are deformed changing their diffraction pattern.
- ▶ Using a narrow collimated beam of x-rays or neutrons we might hope to get some kind of average strain along the beam.
- ▶ While this has not yet been done experimentally there has been some feasibility studies for two possible methods.

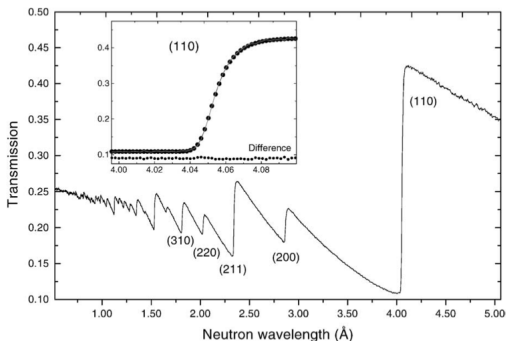
Bragg edge tomography

From Santiseban *et al*, 'Strain imaging by Bragg edge neutron transmission', Nuclear Instruments and Methods in Physics Research A, 481,765768,2002.

The transmission spectrum of thermal neutrons through a polycrystalline sample displays sudden, well-defined increases in intensity as a function of neutron wavelength (Fig. 1). These Bragg edges occur because for a given $\{h,l,k\}$ reflection, the Bragg angle increases as the wavelength increases until 2θ is equal to 180° . At wavelengths greater than this critical value, no scattering by this particular $\{h,l,k\}$ lattice spacing can occur, and there is a sharp increase in the transmitted intensity.

766

J.R. Santisteban et al. / Nuclear Instruments and Methods in Physics Research A 481 (2002) 765–768

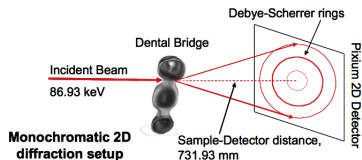


Bragg edge tomography

- ▶ A later paper Abbey *et al*, Feasibility study of neutron strain tomography, Procedia Engineering 1 (2009) 185188, states that “ Analysis of the shape, position and relative magnitude of these Bragg edges can yield two-dimensional information about the component of the average elastic strain within the sample that is collinear with the incident beam.”
- ▶ Although the mathematical details are sketchy they use a curve fitting technique to find the magnitude of the average strain projected in the direction of the beam. Their test object has rotational symmetry making the measurement and reconstruction simpler.
- ▶ Using this approach we believe what they have estimated is the *Longitudinal ray transform* $I\epsilon$ of the strain.
- ▶ As linear strain is the symmetric derivative of the deformation vector this technique measures just.... the change in thickness!

A different approach

A different approach is suggested by Korsunsky *et al* in Strain tomography of polycrystalline zirconia dental prostheses by synchrotron x-ray diffraction, *Acta Materialia*, 59, 2501–2513, 2011. They notice that the diffraction pattern for a narrow beam of monochromatic x-rays through a polycrystalline material on a distant screen forms concentric circular Debye-Scherrer rings.



Korsunsky *et al* Fig 3

If the material in the beam was subjected to a uniform linear elastic strain the rings would become concentric ellipses, and the matrix defining each ellipse is proportional to the *strain tensor projected in the direction normal to the beam*. They presume without proof that for a non-uniform strain fitting an ellipse to the diffraction pattern results in an average of this transverse strain.

What can you get from one projection?

- ▶ In general 'Rich Tomography' is still line integrals of a parameterized function of the unknowns. We might hope to get the *distribution of values* on the line, i.e. the **histogram** without knowing what order they are in.
- ▶ Let us consider a line parallel to the x_3 axis each value of the transverse strain ϵ_{ij} , $1 \leq i, j \leq 2$ results in a contribution to the intensity on the screen equally distributed on the ellipse

$$\epsilon_{11}q_1^2 + 2\epsilon_{12}q_1q_2 + \epsilon_{22}q_2^2 = 1$$

in normalized screen coordinates $q = (q_1, q_2)$.

- ▶ let $\phi(\epsilon)$ be the density of strain values on along the line. The intensity at q is then

$$\mathcal{I}(q) = \int_{\epsilon: \epsilon_{11}q_1^2 + 2\epsilon_{12}q_1q_2 + \epsilon_{22}q_2^2 = 1} \phi(\epsilon) d\epsilon_{11} d\epsilon_{12} d\epsilon_{22}$$

- ▶ This is an integral over a *two parameter* family of planes in *three dimensional* ϵ space. A restricted Radon plane transform.
- ▶ No unique solution ϕ with out *a priori information*.

Diffraction Strain Tomography works

We can reduce the data from each ray (which also makes it practically manageable) and then reconstruct as a tensor ray transform.

- ▶ A careful analysis shows that by taking appropriate moments of the diffraction pattern we recover the transverse ray transform of the strain.
- ▶ Specifically let $\mathcal{I}(q)$ be the intensity of the light in the diffraction pattern where $q \in \mathbb{R}^2$ is a vector in the coordinates of the screen, the moment

$$\int r \mathcal{I}(r^{-1/2} q) dr = q \cdot J\epsilon(x, \xi) \cdot q$$

for any unit vector q normal to the ray ξ where ϵ is the infinitesimal strain (and x a point on the ray).

- ▶ From the polarization identity we can now find $J\epsilon(x, \xi)$

We hope to test this at the Diamond Light Source

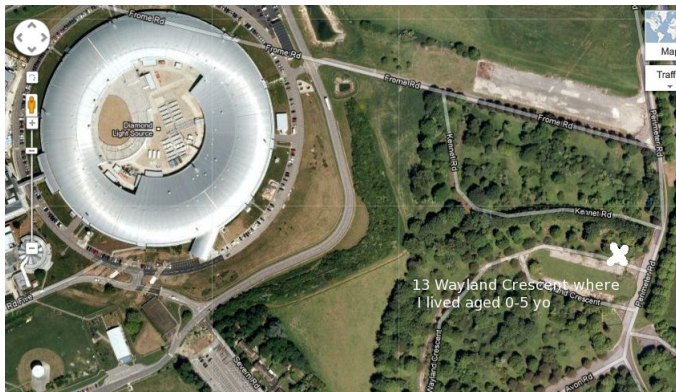


Photo: Google Earth

This synchrotron at Harwell provides a monochromatic collimated x-ray source. Manchester has its own beam and lab at Harwell as part of Manchester X-ray Imaging Facility.

Inverting the transverse ray transform

Consider a fixed unit vector η then for all ξ normal to η

$$\eta \cdot JF(x, \xi)\eta = \int \eta \cdot \Pi_\xi \cdot F(x + s\xi)\Pi_\xi\eta ds = X(\eta \cdot F\eta)(x, \xi)$$

So we can invert to get $\eta \cdot F\eta$ as a Radon transform in each plane. This means we need to rotate the sample half a turn about six axes η and measure the η moment the diffraction pattern for each ray. Of course this is very time consuming and better to get more data for each ray, Desai and Lionheart[4] show how to do it with three rotations for a general tensor... but for a **strain only two orthogonal rotation axes** are sufficient.

Neutron spin tomography

In Neutron spin tomography [1, 7, 8, 3] slow neutrons are fired with a known spin direction through a material that has a spatially varying magnetic field and measure the spin state when it emerges.

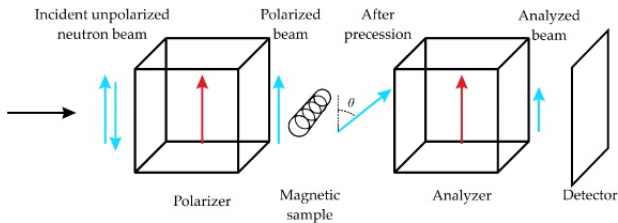


Figure : A schematic diagram of the experimental setup used for polarized neutron imaging on the cold neutron radiography and tomography station (CONRAD) at the Helmholtz Centre Berlin, from Dawson et al [1]

For simplicity take the initial spin states to be each unit basis vector then assemble the resulting spin states along a ray as a 3×3 matrix u . The transport law is

$$\xi \cdot \nabla u(x, \xi) = M(B(x))u$$

where $B(x)$ is the magnetic field and $M(B)$ is proportional to skew symmetric matrix of the linear map $v \mapsto v \times B$, the vector product. Eskin's theorem[2] then gives us $M(B(x))$ for B smooth and from this we can deduce B uniquely, as there is phase wrapping ambiguity. Note that neutron spin tomography can be done a plane at a time so the planar result is enough. But **not constructive** and requires C^∞ **smoothness**.

Linearization I

Let D be the unit disk centred on the origin in \mathbb{R}^2 . Suppose the line $x + s\xi$ intersects D first at $s = s_-(x, \xi)$ and leaves for $s = s_+(x, \xi)$ and let B be continuous. We want to compute the linearization of $S(M(B))(x, \xi) = u(x + \infty\xi, \xi) = u(x + s_-\xi, \xi)$ with respect to B . For $B = 0$ we have $u = I$ so for some B let $u = I + v$ then v satisfies

$$\frac{dv}{ds} - M(B)v = M(B)$$

Now define \mathcal{M} by

$$\mathcal{M}(w)(s) = \int_{s_-}^s M(B(x(s')))w(s') ds'$$

and notice this is bounded, and also is a bounded linear operator in B . We have

$$(I - \mathcal{M})(v)(s) = \mathcal{M}(s)$$

Linearization II

and hence for $\sup |B|$ small enough the operator series

$$v(s) = \left(\sum_{k=1}^{\infty} (\mathcal{M})^k I \right) (s)$$

converges and we see the Fréchet at 0 of $S(M(B))$ wrt B is \mathcal{M} . .
Specifically for ξ in some plane we can solve the linear approximation for small B simply by solving the two dimensional ray transform

$$e_1 \cdot S(M(B))(x, \xi) e_2 = X(B_3)(x, \xi)$$

and cyclic permutations. This can be done using any two-dimensional Radon inversion method, and this is the approach taken by the experimentalists, eg [3].

Numerical examples

- ▶ A magnetic field example is calculated analytically
- ▶ The reconstruction is on a 90×90 pixel grid.
- ▶ Data consists of 117 rays of neutrons parallel beam at 1 degree increments.
- ▶ The forward problem is solved by intersecting rays with pixels (using our ray tracing code `jacobs_rays`), and assuming B is pw analytic on pixels the ODE is solved analytically on each pixel.
- ▶ The inverse Radon transform is calculated using a Ram-Lak filter computed using FFT, and the backprojection operator is *matched*, that is it implements the transpose of the forward projector
- ▶ Noise was added to simulated data using a Gaussian pseudo random number generator.
- ▶ These results are for small B and one iteration. Preliminary indications are that when the spin rotates more than a few degrees several iterations are needed.

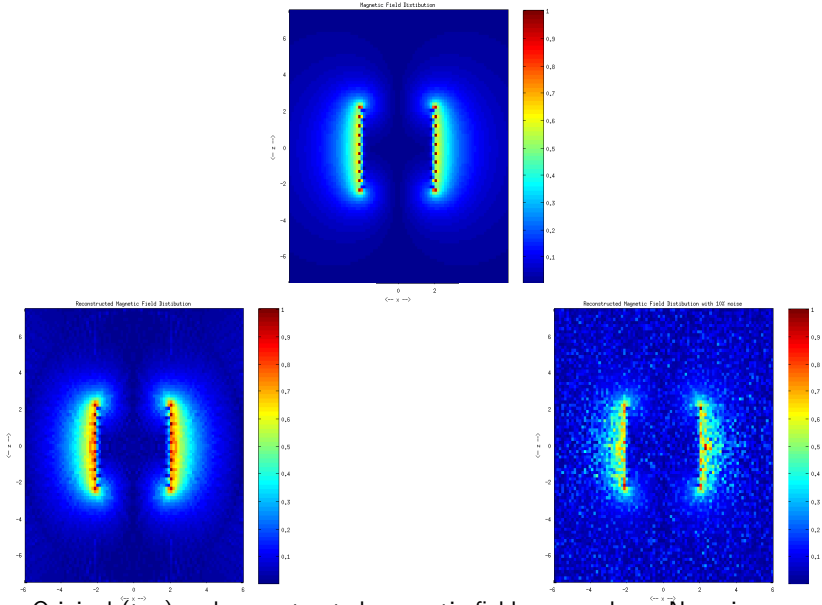


Figure : Original (top) and reconstructed magnetic field – x_1x_3 plane. No noise left and 10% noise right

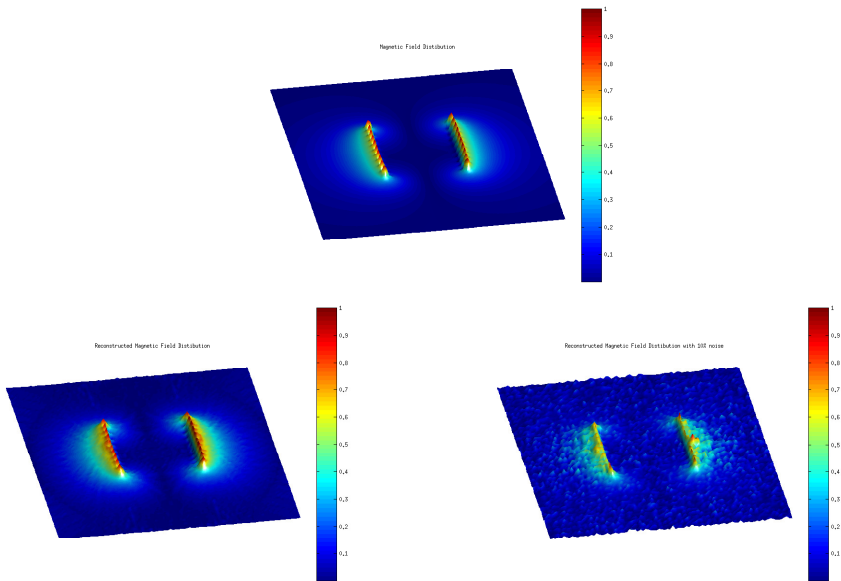


Figure : Original (top) and reconstructed magnetic field – x_1x_3 plane. No noise left and 10% noise right(surface plots).

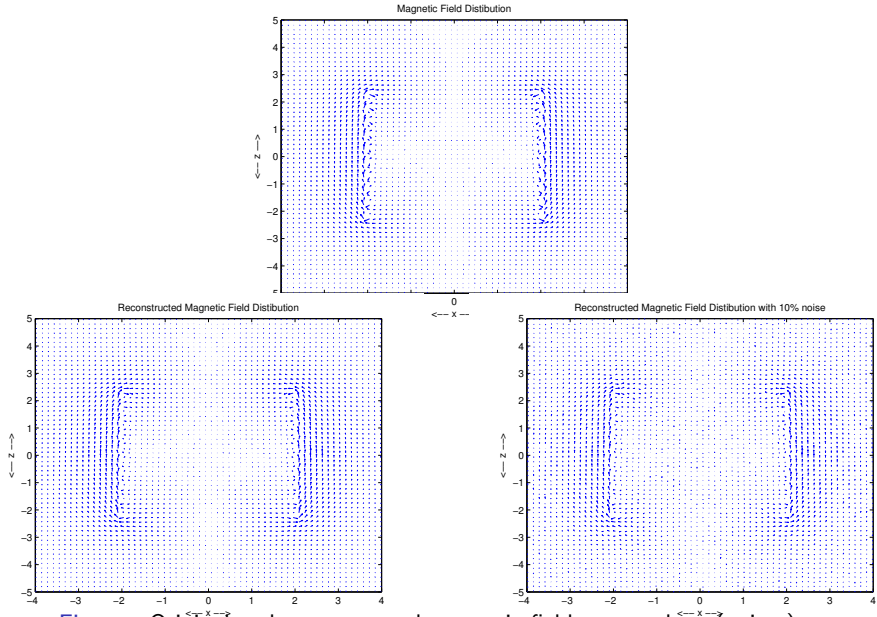


Figure : Original and reconstructed magnetic field – x_1x_3 plane (quiver).

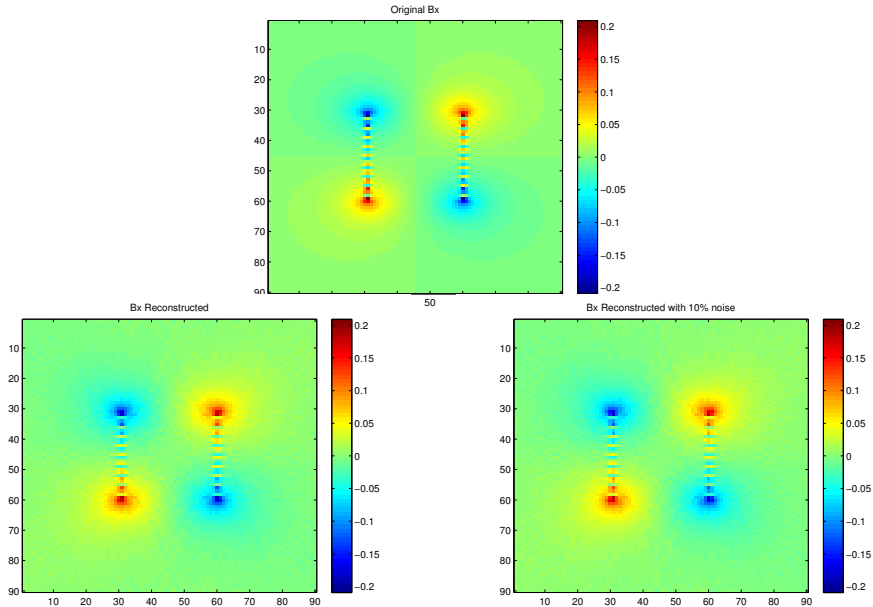


Figure : Original and reconstructed B_1 component - x_1x_3 plane.

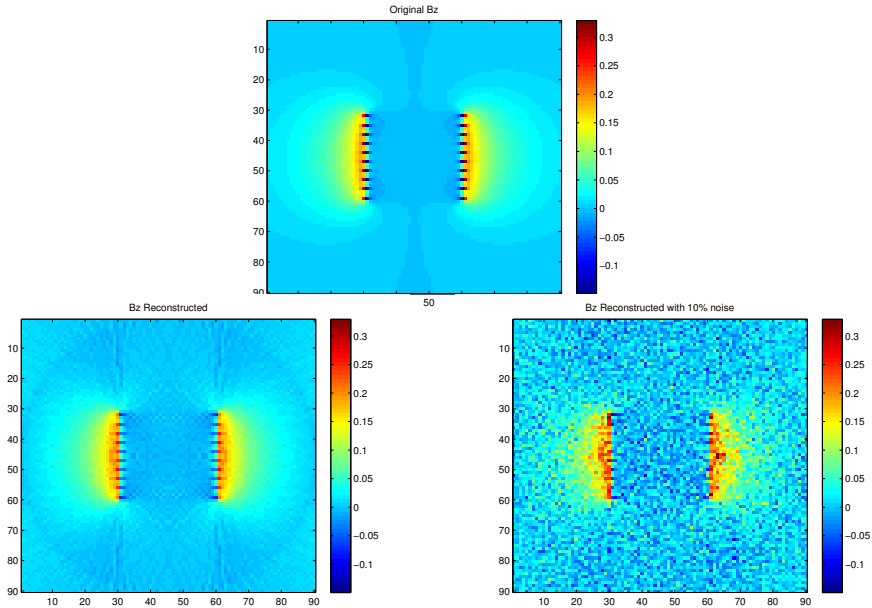


Figure : Original and reconstructed B_3 component - x_1x_3 plane.

References I

- [1] Martin Dawson, Ingo Manke, Nikolay Kardjilov, Andre Hilger, Markus Strobl, and John Banhart.
Imaging with polarized neutrons.
New Journal of Physics, 11(4):043013, 2009.
DOI 10.1088/1367-2630/11/4/043013.
- [2] Gregory Eskin.
On non-abelian radon transform.
Russ. J. Math. Phys., 11(4):391–408, 2004.
ArXIV math/0403447.
- [3] Nikolay Kardjilov, Ingo Manke, Markus Strobl, Andre Hilger, Wolfgang Treimer, Michael Meissner, Thomas Krist, and John Banhart.
Three-dimensional imaging of magnetic fields with polarized neutrons.
Nat Phys, 4:339–403, 10 2008.
DOI 10.1038/nphys912.
- [4] W R B Lionheart and N Desai.
Explicit reconstruction algorithm for the transverse ray transform with three axes.
Inverse Problems, 2016.
- [5] F. Natterer.
The Mathematics of Computerized Tomography.
Classics in Applied Mathematics. Society for Industrial and Applied Mathematics, 2001.
- [6] V.A. Sharafutdinov.
Integral Geometry of Tensor Fields.
Inverse and ill-posed problems series. VSP, 1994.
Also online.
- [7] Wolfgang Treimer.
Radiography and tomography with polarized neutrons.
Journal of Magnetism and Magnetic Materials, 350(0):188 – 198, 2014.
DOI 10.1016/j.jmmm.2013.09.032.
- [8] Treimera W, Ebrahimib O, and Karakasa N.
Imaging of quantum mechanical effects in superconductors by means of polarized neutron radiography.
Physics Procedia, 43(0):243 – 253, 2013.
DOI 10.1016/j.phpro.2013.03.028.