The Tricomi approach to Chebfun Imaging in Electron Paramagnetic Resonance Tomography : Towards a Unifying Imaging Process for Cultural Heritage

Yann LE DU[1,2], Mariem EL AFRIT[1,2], Rafaël DEL PINO [3]

[1]PSL Research University, Chimie ParisTech-CNRS, Institut de Recherche Chimie Paris, UMR8247, 75005 Paris, France

[2]Centre de Recherche et de Restauration des Musées de France, C2RMF, Palais du Louvre - Porte des Lions, 14 Quai François Mitterand, 75001 Paris, France

[3]ENS 45 rue d'ulm 75005 Paris

yann.ledu@chimie-paristech.fr, mariem.el-afrit@chimie-paristech.fr, delpino@ens.fr

Résumé – Les besoins en imagerie pour l'étude des objets du patrimoine culturel nécessitent la manipulation d'un objet numérique unique qui combine les images obtenues à la fois à différentes échelles et à différentes longueurs d'onde, avec la possibilité de choisir une représentation à deux ou trois dimensions. Nous proposons un traitement unifié des données en imagerie fondé sur la technologie de Tchebychev telle qu'implémentée dans le logiciel libre Chebfun, et décrivons notre version de la backprojection filtrée adaptée au paradigme Chebfun, avec une application spécifique en Imagerie par Résonance Paramagnétique Électronique, une technique spectrométrique que nous avons récemment appliquée à l'études d'objets du patrimoine.

Abstract – Cultural heritage imaging has specific needs with regards to the analysis of images that require the manipulation of a single digital object that combines the images obtained both at different scales and at different wavelengths, with the further possibility of selecting two or three dimensional representations. We propose a unified imaging data processing approach based on the Chebyshev Technology powered open source Chebfun software, and describe our Chebfun-based filtered backprojection with an example application to Electron Paramagnetic Resonance Imaging, a spectrometric technique that we recently applied to the study of cultural heritage objects.

1 Image processing and cultural heritage

Together, the Institut de Recherche de Chimie Paris (IRCP[1]) and Centre de Recherche et de Restauration des Musées de France (C2RMF[2]) have set up a mixed research team, Physico Chimie des Matériaux Témoins de l'Histoire (PCMTH), in order to bring new solutions to the challenges facing the analysis, conservation and restoration of cultural heritage objects, and one of the team's ambitious research projects concerns digital images : how to best acquire, store, analyze and combine them. The C2RMF tools of the trade include optical and X-ray photography[3], and, thanks to the expertise in *Electron Paramagnetic Resonance* (EPR) brought by the team's IRCP component who pioneered the application of EPR imaging (EPR-I) to exobiology [5], has decided to use EPR-I in order to image specific chemical species which X-rays and other traditional techniques are unable to specifically target, like the different layers of carbon-related material found inside paintings.

However, this EPR-I information needs to be merged with the one gathered from other sources, be it X-rays or optical photography in order to provide a single object to which we may attach an interface for subsequent manipulations. This merging would be greatly simplified if we could unify the different pipelines that take raw data and transform them into images. At the moment, there are different pipelines (programs and associated algorithms) for each imaging technique, and even the data formats are different. This actually stands as a major global challenge : many domain specific techniques exist to solve particular problems in imaging, yet the final results obtained after applying each technique are difficult if not impossible to combine. The PCMTH team, in association with the C2RMF imaging team, is thus developing a generic approach which would allow a single pipeline to process all the different kinds of data, with a single unifying data structure and mathematical model founded on *Chebyshev technology* [3], as championed by the Oxford University Numerical Analysis Group through the development of *Chebfun* [4], an open-source software system for numerical computing with functions. The mathematical basis of Chebfun is piecewise polynomial interpolation and in this paper we describe the role Chebfun plays

[1]The IRCP is the research branch of *Chimie ParisTech*, covering many domains of chemistry.

[2]The C2RMF is an institution of the Ministry of Culture devoted to the analysis and conservation of the cultural heritage of the French Museums.

[3]A paper detailing those activities was submitted by *Boust et al.* to that same GRETSI conference.

in our unifying approach to image data processing[4], and more specifically how we managed to fit the key tomographic process of *backprojection* into the Chebfun paradigm. We show that this approach provides a promising imaging data processing unification without having to pay a performance cost : it is a zero-cost abstraction[5].

2 Chebfun for experimental data

The Chebfun approach allows a particular representation of any function based on Chebyshev polynomials, making the latter as easy to subsequently manipulate as polynomials [11]. Chebfun is both the name of the software and of the underlying mathematical object (*chebfun*, all in lowercase) that have a software implementation, and chebfuns can be described using a programming language terminology : a chebfun is an *object* with an *interface*. The mathematical concepts of integral, derivative, maxima and other similar ones become *methods* of the chebfun interface.

In the field of experimental science, we do not collect functions, but rather function samples. We need to transform data points into a chebfun, giving us access to the same interface as the one Chebfun originally provides for functions ; any data-related query thus becomes a call to a chebfun method, from simple ones like finding the maximum or the integrated signal, to more complex ones like "what image is produced with this data", and "how close is this image to that one". The key idea remains the same : transform data into a chebfun, and then use the available methods or add new ones to that same object's interface.

Within the existing Chebfun implementation as available in the eponymous Matlab toolbox, we can transform arbitrary data into a chebfun object ; we use the very practical `FUNQUI` function which takes a series of data points supposed to vary with a single underlying variable [6], which builds an appropriate Chebfun object. Hence in the rest of the paper we shall consider that the data is appropriately represented by a chebfun.

Now, it would be easy to apply the traditional data processing algorithms to sampled chebfuns, but that would defeat the whole purpose of the Chebfun approach and make it a waste of time. Instead, because data is a chebfun, we may now consider algorithms from their operator aspect and thus interpret any subsequent operation on the data as the application of an operator to a chebfun. This means that in order not to switch back to sampled data, we need to find ways of mapping any subsequent transform to a composition of more or less simple operations on the chebfun itself. For example, if we wanted to find the derivative of the "Chebfunized" data, we could always resort to sampling the chebfun and compute the discretized derivative, but that is exactly what we would like to avoid : we should instead compute the derivative of the underlying chebfun mathematical object. The default interface provided by the toolbox already exposes many such operations, and our goal is to enrich that interface with methods useful for tomography, and imaging in general.

[4]We can find more details on our website HPU4science [2]

[5]We import that concept from the field of computer languages, especially from the abstractions provided by the C++ STL and implemented using Stepanov's generic programming approach [10].

3 EPR Imaging

EPR spectrometry monitors the absorption of oncoming microwaves by a sample as we vary an applied magnetic field ; the combination of the microwave frequency with the magnetic field intensity at which absorption is maximized constitutes the signature of a particular chemical species, thus revealing its presence in the sample. Figure 2 shows a typical real EPR spectrum with a reasonably clear resonance magnetic field value, and unavoidable noise. *EPR imaging* (EPR-I) is an extension of EPR spectrometry, similar in principle to Magnetic Resonance Imaging [9] : a magnetic field gradient is added to the global magnetic field and maps the different positions of atoms responsive to EPR spectrometry to different magnetic field resonance values on a spectrum ; if a chemical species has a zero gradient resonance spectrum s, then, given a magnetic gradient G and global magnetic field B, the linear density of the species is mapped to a spectrum according to

$$r(B) = \int_{\text{sample}} c(x) \cdot s(B + G \cdot x)\, dx \qquad (1)$$

where the integral has the form of a convolution, and is applied on the sample in the direction of the magnetic field gradient. The linear density c is itself related to the volume density ρ by a surface integral : $c(x)$ is the integral of ρ on the plane orthogonal to the direction of the magnetic field gradient at the position x on that direction ; the problem is to find ρ given only the EPR spectra, i.e. r and s.

Different solutions exist and our own which is summarized in figure 1. In order to simplify the problem, we shall consider the sample to be a 2D flat surface, thus transforming the surface integral relating ρ to c into a line integral (along the direction AB in figure 4), leading to the Radon transform $\mathcal{R}$ representation of c as being $c = \mathcal{R}\rho$ which allows us to rewrite equation 1 more abstractly as $r = s \star \mathcal{R}\rho$; Given that simplification, figure 4 describes the EPR imaging process.

The problem is now to find ρ, a flat surface density which thus depends on the variables (x, y), given the experimental spectra r and s. It is a typical inverse problem, involving the well-known Fredholm integral equation of the first kind which the convolution equation 1 is an example of, together with the Radon transform, thus requiring two inversions : the first is a deconvolution, and the second the *filtered backprojection* operator that involves the naive backprojection $\mathcal{B}$. As for the convolutional part, this blurring of the density is traditionally dealt with using Fourier transforms directly on r, but it turns out that the deconvolution can be performed on the final image thanks to the linearity property of the backprojection operator with respect to convolution :

$$\mathcal{B}\left(s \star \mathcal{R}\rho\right)(x,y) = \left(\mathcal{B}s \star \rho\right)(x,y) \tag{2}$$

This property allows us to postpone the deconvolution and apply it only on the blurred reconstructed image, instead of the blurred linear density. But in this paper, we shall even further simplify the problem and suppose that the EPR spectra are a direct mapping of the linear density, a simplification fully justified by the property expressed in equation 2, and we shall just inverse the simplified equation $r = \mathcal{R}\rho$ but with the requirement that the inversion fits into the Chebfun paradigm : we would like to find an inverse transform that maps to simple operations on the chebfun itself, without having to mediate those transformations through sampling. In our general methodology we thus focus on three specefic nodes of the more general approach depicted in figure 1.

4 The Chebfun backprojection

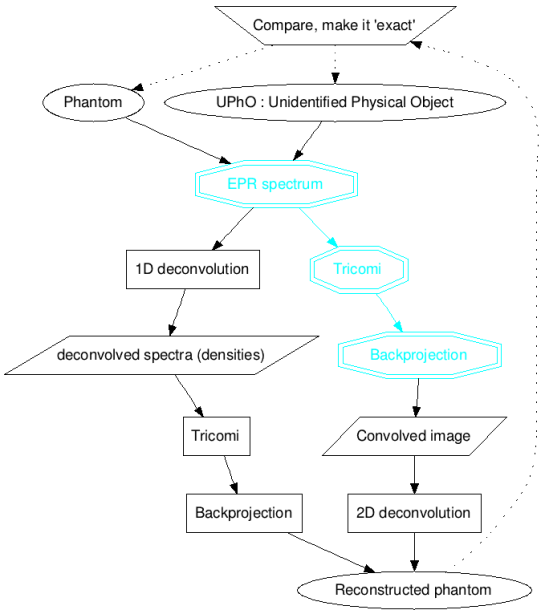


Figure 1 – Our approach to tomography uses two mathematically equivalent yet implementation-wise different paths : in this paper, we describe the three nodes which are highlighted in blue and with double-line contours. The key steps are the transformation of spectra into chebfuns, and the formulation of the inverse problem solution using the Tricomi transform. The third node, the backprojection itself, is not described in this paper yet used for the reconstructions.

In order to inverse the Radon transform, the common practice is to *filter* the naive backprojection $\mathcal{B}$ and we may retrieve the density ρ by using the well known *Fourier form* of the filtered backprojection [8] which has an equivalent form that uses the *Hilbert transform* [8]. Thanks to the commutativity of the latter with the derivative, we can write

$$\rho\left(x,y\right) = -\frac{1}{2}\mathcal{B}\left[\frac{\partial\mathcal{H}\left(\mathcal{R}\rho\right)(t,\theta)}{\partial t}(t,\theta)\right](x,y) \tag{3}$$

If we now recall that the $\mathcal{R}\rho$ are the EPR spectra, we can consider each of those to be a chebfun (as we previously discussed in section 2) which we shall call P_θ, by defining

$$Q_\theta\left(t\right) = P_\theta\left(t\right)\cdot\sqrt{1-t^2} \tag{4}$$

we obtain that in equation 3,

$$\mathcal{H}\left(\mathcal{R}\rho\right)(t,\theta) = \mathcal{H}\left(P_\theta\right)(t) = \mathcal{H}\left(\frac{Q_\theta\left(t\right)}{\sqrt{1-t^2}}\right)(t) \tag{5}$$

We can now express Q_θ as a combination of the Chebyshev polynomials of the first kind T_n with coefficients C_n, so that from equation 5 we obtain

$$\mathcal{H}\left(P_\theta\left(t\right)\right)(t,\theta) = \sum_n\left(C_n\left(\theta\right)\cdot\mathcal{H}\left(\frac{T_n\left(t\right)}{\sqrt{1-t^2}}\right)(t)\right) \tag{6}$$

Because we study physical objects which have a finite extension and under the hypothesis that the corresponding chebfun will also have a finite support, our Hilbert transform becomes a *Tricomi transform* [12] $\mathcal{T}$. This, together with the very useful property of the Tricomi transform

$$\mathcal{T}\left(\frac{T_n\left(t\right)}{\sqrt{1-t^2}}\right)(t) = -\frac{1}{n}\frac{\partial T_n\left(t\right)}{\partial t} \tag{7}$$

allows us to rewrite [7] equation 6 as

$$\mathcal{H}\left(P_\theta\left(t\right)\right)(t,\theta) = -\sum_n\left(\frac{C_n\left(\theta\right)}{n}\cdot\frac{\partial T_n\left(t\right)}{\partial t}\right) \tag{8}$$

and finally equation 3 becomes

$$\rho\left(x,y\right) = \frac{1}{2}\mathcal{B}\left[\frac{\partial^2}{\partial t^2}\left(\sum_n\left(\frac{C_n\left(\theta\right)}{n}\cdot T_n\left(t\right)\right)\right)\right](x,y) \tag{9}$$

This last expression reveals the simple relationship between the spectrum chebfun, obtained directly from the raw (sampled) spectrum, and the reconstructed image, which can easily be expressed as an algorithm amenable to a Chebfun compatible implementation :

1. Prefactor the raw spectra $r(t)$ by $1/\sqrt{1-t^2}$;
2. transform each prefactored spectrum into a chebfun with the `FUNQUI` function ;
3. apply the square brackets part of equation 9 ;
4. apply the naive backprojection $\mathcal{B}$ that constitutes the remaining part of equation 9.

Step 4 of our algorithmic implementation above requires the computation of the naive backprojection. Here also we took advantage of the Chebfun approach, but describing that would lead us beyond the limits of the present paper.

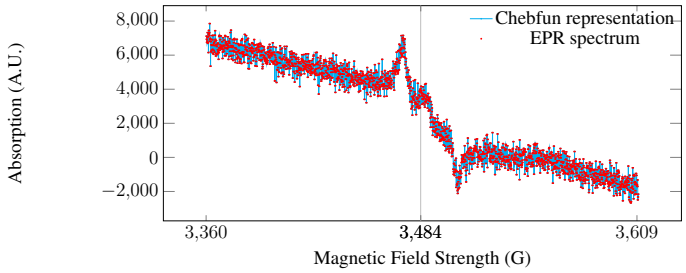
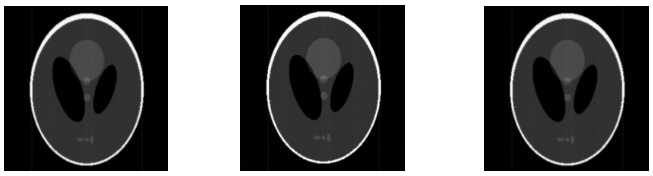


Figure 2 – An EPR spectrum with its Chebfun representation. The absorption (arbitrary units) is measured as the magnetic field is varied (abscissa, in Gauss) and the microwave frequency of the oncoming radiation kept constant (around 9.5GHz for X band EPR); EPR traditionally measures the derivative of that signal, explaining the bumps and troughs. The maximum absorption is here around 3500 G.

Figure 3 shows that our reconstruction is at least as good as the standard procedure using the vanilla Matlab imaging toolbox solution that uses the `IRADON` function. Figure 5 shows the application of our approach to experimental data : it does not yet include any noise filtering, yet it already improves on the traditional Fourier-based approach which black-box implementation is provided by the Bruker XEPR software suite that comes with the EPR imaging spectrometer [1].



(a) Original Shepp-Logan phantom.

(b) Standard Fourier reconstruction.

(c) Our Chebfun reconstruction, cf. figure 1.

Figure 3 – We tested our approach on the Shepp-Logan phantom (left). The other two figures show the phantom reconstruction using only the information provided by the Radon transform of the phantom sampled on the angles, cf. figure 4. We can see that our approach is at least as good as the standard one.

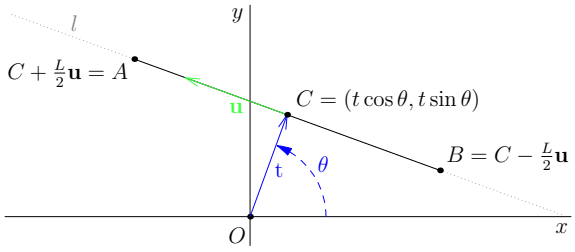
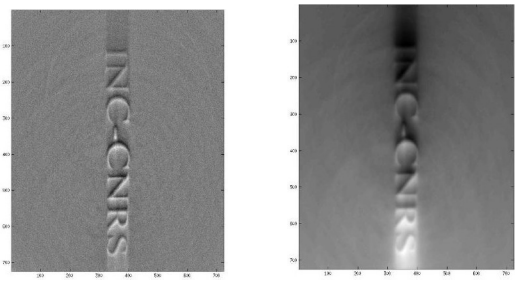


Figure 4 – Radon transform geometry : OC is the direction of the imaging magnetic gradient (every spectrum is given by the choice of θ and on a given spectrum every data point has an abscissa t and an ordinate giving the integrated density along the direction AB) ; l is the position along the Radon integration path, and L is the sample size.



(a) Our Chebfun/Tricomi reconstruction, cf. figure 1.

(b) Standard Fourier-based reconstruction.

Figure 5 – "I(nstitut) N(ational) de C(himie) - CNRS" was laser printed (heated toner is very responsive to EPR) on a piece of paper (1cm by 5cm), hidden in an EPR tube filled with sand (EPR neutral) positioned in a Bruker EPR imaging spectrometer. The reconstructions do not (yet) include noise filtering.

References

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