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Beyond filtered backprojection: A reconstruction software package for ion beam microtomography data

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ABSTRACT

A new version of the TomoRebuild data reduction software package is presented, for the reconstruction of scanning transmission ion microscopy tomography (STIMT) and particle induced X-ray emission tomography (PIXET) images. First, we present a state of the art of the reconstruction codes available for ion beam microtomography. The algorithm proposed here brings several advantages. It is a portable, multi-platform code, designed in C++ with well-separated classes for easier use and evolution. Data reduction is separated in different steps and the intermediate results may be checked if necessary. Although no additional graphic library or numerical tool is required to run the program as a command line, a user friendly interface was designed in Java, as an ImageJ plugin. All experimental and reconstruction parameters may be entered either through this plugin or directly in text format files. A simple standard format is proposed for the input of experimental data. Optional graphic applications using the ROOT interface may be used separately to display and fit energy spectra. Regarding the reconstruction process, the filtered backprojection (FBP) algorithm, already present in the previous version of the code, was optimized so that it is about 10 times as fast. In addition, Maximum Likelihood Expectation Maximization (MLEM) and its accelerated version Ordered Subsets Expectation Maximization (OSEM) algorithms were implemented. A detailed user guide in English is available. A reconstruction example of experimental data from a biological sample is given. It shows the capability of the code to reduce noise in the sinograms and to deal with incomplete data, which puts a new perspective on tomography using low number of projections or limited angle.

1. Introduction

1.1. Reconstruction of STIMT and PIXET data: a brief overview

The idea to use a focused light ion beam, typically protons or alpha particles of a few MeV, to probe samples a few hundred micrometers in diameter, was initially implemented by Pontau et al. [1], Fischer and Mühlbauer [2] and Schofield and Lefevre [3]. Scanning transmission ion microscopy tomography (STIMT) gives access to 3D morphology, with a typical spatial resolution of a few micrometers, or even down to a few hundred nanometers in the most favorable cases [4]. More precisely, STIMT provides 3D maps of the mass density (in g/cm^3) within the analyzed volume. In addition to STIMT, particle induced X-ray emission tomography (PIXET) can be carried out to map elemental content. Multielement detection and trace element sensitivity, down to a few ppm, are recognized as the main advantages of the PIXE technique.

From an historical point of view, the processing of ion beam microtomography data has been inspired by the codes developed for medical imaging, starting with the so-called "Donner library" [5]. Very few research groups have been involved in this development. For this reason, we would like to cite very early works, as they can be still considered as valuable approaches. First STIMT reconstruction codes were proposed, based on filtered backprojection (FBP) [1,2,6], ART or entropy maximum [7]. In these first studies, the choice of experimental conditions was discussed: incident beam energy, number of events, number of projections, etc. Optimal ways to process data were also presented, taking into account methodological studies already performed for conventional (2D) STIM: mean or median filtering of the transmitted energy, calculation of stopping power, effect of the filters, etc. Over the years, the comparison of these approaches led the authors to prefer the FBP code to reconstruct STIMT data, for its simplicity, reliability and speed. Two main aspects justify this choice: (i) the STIMT projections, measured by transmission, usually have very little noise

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and (ii) the calculation of physical processes can usually be implemented following an analytical method. In this way, quantitative data can be obtained for thin samples [8].

The situation is more difficult for PIXET: the quantitative reconstruction of emission data requires an iterative algorithm, less sensitive to noise than FBP, and moreover able to take into account the attenuation of the emitted X-rays from their emission point to the detector. Pioneering studies were carried out by Schofield and Lefevre [3] and Antolak and Bench [9] using least squares methods derived from SPECT medical imaging (both from the Donner library). The second study improved the reconstruction process by combining the STIMT and PIXET reconstruction. In this way, local information about density is used to provide realistic attenuation factors, and reciprocally, local composition is used to calculate precise mass density. This more complete approach is required for the case of samples inhomogeneous in composition. A detailed study was carried out, where different sample compositions were compared, by increasing the levels or modifying the distribution of high Z elements in an organic matrix [9].

However, both approaches remained unsatisfactory in the sense that the X-ray detector was assumed point-like (zero solid angle). On the opposite, experimental conditions require that the detector should be as close as possible to the sample, in order to maximize counting statistics. The only code so far able to take into account the large solid angle required in real PIXET experiments was initially developed by Sakellariou et al. [10]. The DISRA program has remained the most complete code for the processing of STIMT/PIXET data, and has spread over the years in several research groups: Surrey [11], Leipzig [12], Bordeaux [13]. However, some restrictions inherent to the reconstruction method employed led some of them to explore other ways – although no complete solution has been reached so far. We would like here to summarize the main aspects of the reconstruction procedure in DISRA, to make clearer the origin of these limitations and how we could try to go beyond.

1.2. The Discrete Image Space Reconstruction Algorithm (DISRA)

The DISRA code was derived from a method initially developed for Positron Emission Tomography (PET). It is based on successive projections/backprojections of simulated data. To summarize, the starting tomogram (simulated 3D object) at zero order is guessed from the direct FBP of experimental projections (i.e. energy loss for STIMT, number of events for PIXET). This initial tomogram is then weighted, using an a priori global scaling factor. This factor is applied so that the content of every voxel of the initial tomogram can be of the same order of magnitude as the real physical parameter to be reconstructed (i.e. a mass density for STIMT, or a mass fraction for PIXET). Additional corrections (normalization, zeroing, etc.) are also brought, that we will not discuss here.

From this first "numerically guessed" tomogram, the iterations start: the physical processes of X-ray emission and attenuation are simulated, taking into account the detection solid angle specified by the user. A local correction factor is applied at every step, by comparing, voxel by voxel, the FBP of simulated data to the FBP of experimental projections, taken as a "reference reconstruction". To avoid noise amplification inherent to FBP, the originality of DISRA is that every voxel value is limited by a bandwidth $\Delta D_{(i)}$ at the ith iteration. This limitation is performed in a smart way, as the bandwidth is reduced at each iteration, since the voxel values are getting closer to convergence. More precisely, it follows the formula:

$$\Delta D_{(i)} = d \times 2^{-(2+i)}$$

In this formula, d is an arbitrary numerical factor different for STIMT and PIXET data. The convergence is reached when the simulated data are found to be close enough to the experimental ones.

1.3. Current limitations and prospects

DISRA has been proven to generate accurate mass density and mass fractions results, both on simulated "phantom" objects and on experimental data [14], at least for inorganic samples presenting a good density contrast and high X-ray yields. However, for less contrasted objects, such as biological samples, limitations of DISRA may appear. From an experimental point of view, the duration of PIXET data acquisition may be of a few hours per slice, depending on the number of pixels, number of projections and element concentration. To give an example, for isolated cells or for small organisms such as the nematode presented here, it typically takes about 1–2 h beam time to map the mineral content (typical concentration about a few per thousand in dry mass). To give a comparison, a full 3D (128 slices) STIMT experiment may take about the same time. In these conditions, both experiment duration and sample damage would be prohibitive to perform 3D PIXET. Instead, it appears advisable to probe isolated PIXET slices, in regions of interest selected from 3D STIMT reconstruction. A modification of the DISRA code was introduced to handle this configuration [13].

A second difficulty in DISRA is the arbitrary numerical factor used for discretization. The default values imposed in the code can turn out to be inappropriate in certain conditions, such as for low mass fractions. In these conditions the iterations are prohibitively slowed down and the source code has to be modified "manually", according to the considered sample [15].

We could see a last obstacle to the application of DISRA for biological studies, which is inherent to the FBP process used for reconstruction. From an experimental point of view, the sample is mounted as freestanding, attaching to the top of the rotation axis. To prepare the sample this way can turn out to be a rather difficult task for fragile biological samples, such as isolated cells. A more convenient option would be to probe cells deposited on a 2D substrate, using limited angle tomography, as it is done for electron tomography for instance [16]. However, because of the FBP algorithm implemented at each iteration, this possibility cannot be handled by DISRA at this stage.

An innovative approach was proposed by Andrea et al. [17] for limited angle tomography of single cells, over an angular range of 120°. In this study, the missing STIMT projections, over the 60° angle range not covered by the beam, were interpolated using a back and forth numerical guess of the complete sinogram, based on a FBP method. Noise amplification in the image outside the sample was eliminated by image processing. Qualitative PIXET reconstruction was performed the same way. Satisfactory images were obtained. However, because FBP is intrinsically an analytical method, we believe that other algorithms should be considered as more promising options for limited angle tomography.

For all these reasons, we would like here to propose an alternative to FBP for the reconstruction of low-contrast objects such as biological samples. To tackle the full problem of the reconstruction of PIXET data as precisely as DISRA is able to do it (when all conditions are fulfilled for the convergence to be reached) will definitely take a long effort. We propose here a new development of the TomoRebuild data reduction software package [18], able to perform quantitative STIMT and qualitative PIXET reconstruction. To broaden the reconstruction possibilities, in addition to FBP, two iterative reconstruction methods are proposed, able to tackle the problems of noise amplification – even for a small number of projections – and limited range tomography. This development was made keeping as a main goals ease of use and portability, whatever the operating system and experimental conditions. Below, we present an example of experimental data reduction for a biological sample. However, the software package is more general and could be implemented for any type of sample.