Materials Characterization 139 (2018) 259–268

Contents lists available at ScienceDirect

Materials Characterization

journal homepage: www.elsevier.com/locate/matchar

Piecewise linear fitting in dynamic micro-CT

Marjolein Heyndrickx[a,*,1], Matthieu Boone[a], Thomas De Schryver[a], Tom Bultreys[b,2], Wannes Goethals[a], Glenn Verstraete[c], Valérie Vanhoorne[c], Luc Van Hoorebeke[a]

[a] UGCT/Radiation Physics, Dept. Physics and Astronomy, Ghent University, Proeftuinstraat 86, N12, Ghent 9000, Belgium
[b] UGCT/PProgRess, Dept. Geology and Soil Science, Ghent University, Krijgslaan 281 - Building S8, Ghent 9000, Belgium
[c] Laboratory of Pharmaceutical Technology, Ghent University, Ottergemsesteenweg 460, Ghent 9000, Belgium

ARTICLE INFO

Keywords:
X-ray micro-computed tomography
Analysis
Image processing
Reconstruction
Signal-to-noise ratio

ABSTRACT

Piecewise linear fitting, the technique proposed in this paper, performs data reduction on a large dynamic CT dataset and it already takes a step in the direction of the data analysis and characterization that needs to be performed afterwards. In addition, it drastically improves the signal-to-noise ratio. This is demonstrated on two complementary samples: a Bentheimer sandstone and a pharmaceutical tablet.

This technique is developed for dynamic high-resolution CT scanning or 4D-µCT, a tool to study dynamic processes in situ on the micro-scale. We propose to start from the low quality reconstruction and perform a piecewise linear fit in the time direction for each voxel. This effectively uses the nearby temporal information, regardless of the nature of the dynamic process, without introducing spatial correlation.

1. Introduction

In various scientific domains the ability to observe dynamic processes inside samples as they take place yields invaluable information. A dynamic process gives rise to an ongoing change in the structure of the sample: for example fluid filling up pores [1], crack formation under stress [2], the weathering of building stones [3] or limestones [4], self-healing materials upon fracturing [5] or structure changes due to temperature variations [6]. All these processes present us with the same problem: we should be able to observe the inside of the sample without disturbing the very process we want to study. As such, in the vast majority of the cases visible light is not a suitable probe as in most cases it has only a very limited penetration depth in the sample, and cutting the sample open is clearly destructive.

The use of X-ray computed tomography (i.e. CT scans) is in many cases a suitable solution. Observing the inside without cutting or destroying the sample is precisely what the technique is intended for [7]. Next to medical applications, there are also numerous other applications that make use of CT scans, such as airport security [8], geological research [9], historical artefacts [10], biology [11], and material science [12]. A CT scan, performed on an object, results in a complete virtual 3 dimensional representation of the object revealing both its internal and external features.

In brief, during a CT scan, a sample undergoes a rotation relative to an X-ray source-detector system while a (large) number of radiographic images (called projections) are taken at various rotation angles. The relative rotation can be the sample rotating around its own axis with stationary source and detector, or the source-detector system rotating around the stationary sample. The rotation can be complemented with a relative translation, e.g. in a helical trajectory [13]. These radiographic images are reconstructed to a 3D volume consisting of an array of voxels (3D pixels) using an appropriate reconstruction algorithm. The algorithm can be filtered back projection (FDK for cone-beam setups [14]), a technique that is less computationally intensive, or iterative algorithms [15], which has the advantage of being more easily extendible, for example by incorporating beam hardening corrections [16]. This algorithm yields the local X-ray linear attenuation coefficient for the material in each voxel. The attenuation coefficient can be visualised by a grey value. Afterwards, the 3D volume can be analysed, either by visual assessment or by complex automated analysis, or a mixture of both [17, 18].

The above describes the 3 dimensional case. In the case of dynamic CT scans, we add the fourth dimension, time, to obtain a "4D-µCT scan". The µ or micro- indicates a CT scanner with a resolution of at

* Corresponding author.
E-mail addresses: marjolein.heyndrickx@ugent.be (M. Heyndrickx), matthieu.boone@ugent.be (M. Boone), thomas.deschryver@xre.be (T. De Schryver), t.bultreys@imperial.ac.uk (T. Bultreys), wannes.goethals@ugent.be (W. Goethals), glenn.verstraete@ugent.be (G. Verstraete), valerie.vanhoorne@ugent.be (V. Vanhoorne), luc.vanhoorebeke@ugent.be (L. Van Hoorebeke).
[1] Present address: XRE nv, Bollebergen 2B bus 1, 9052 Ghent, Belgium.
[2] Present address: Imperial College London, Dept. of Earth Science and Engineering, SW7 2AZ London, United Kingdom.

https://doi.org/10.1016/j.matchar.2018.03.007
Received 5 January 2018; Received in revised form 2 March 2018; Accepted 7 March 2018
Available online 09 March 2018

least 100 μm, for certain very high-resolution systems even being as good as 1 μm or better. In a 3D + time scan, each scanned time step is reconstructed separately, resulting in a time-series of 3D volumes. In the case of a continuous 4D-μCT scan, where multiple rotations are performed continuously while taking projections, the series of projections is divided into separate rotations, each corresponding to a certain "time range". Each of these is reconstructed in a 3D way, also resulting in a time-series of 3D volumes. In a continuous scan, the defined time ranges can overlap and the time distance between two sequential time steps can be chosen freely. Each time range should preferably correspond to a fully sampled dataset [19], in order to avoid limited angle artefacts caused by a lack of angular information [20].

There is a lower limit on the time required per full rotation of the scanner. This limit can be caused by the speed of the rotation stage or by the combination of the required (and available) X-ray flux per radiograph and the angular spacing, both contributing to the resolution and signal to noise ratio of the scan. To optimize the temporal resolution, the time for one full rotation needs to be minimized under these limitations. Indeed, during the full rotation time, the dynamic process may already introduce changes in the sample. The reconstruction algorithm assumes the scanned sample did not change during the scan or in this case, during the used time range (i.e. it was a "static sample"). This assumption may be violated due to the dynamical processes. The result is the appearance of movement artefacts.

As such, to stay as close as possible to the assumption of a static sample, the rotation should happen much faster than the time scale of the dynamic process taking place in the sample. A typical 3D micro-CT scan in the lab takes minutes to hours. Yet, we are often interested in processes with temporal resolutions of some seconds to sub-seconds. A 4D micro-CT scan therefore rotates much faster than for a static scan, currently a few seconds (12 and up) on our system at UGCT, the EMCT micro-CT scanner [21].

However, decreasing the acquisition time introduces another problem: because the data acquired for one 3D reconstruction is taken during the shortest possible time period, the projections contain less detected photons, hence more image noise. This results in low quality 3D reconstructions and, since these are the building blocks of the 4D result, a low quality 4D reconstruction. In addition, while there were projections taken a short time apart, each containing information on a specific time point, the time range of the 3D reconstructions will usually consist of multiple projections, providing a worse temporal resolution.

When prior knowledge is available, techniques to exploit all available information become available. The prior knowledge of which regions of the sample will be static and which will be dynamic gives the option of using a method such as presented by Myers et al. [22] or region based 4D tomographic reconstruction [23]. If the sample consists of a few different compositions with known grey values, it is possible to use discrete reconstruction techniques such as DART [24]. The latter technique requires less projections for one reconstruction, thus improving the temporal resolution in a dynamic experiment. If the physics of the dynamic process poses certain constraints to the reconstructed grey values, this can be used in a Bayesian approach: the MAP-EM framework (maximum a posteriori - expectation-maximisation) [25], where different physical effects or other a priori information can be included. A more limiting case is the MAP algorithm presented in [26].

The technique developed in this paper, piecewise linear fitting, addresses the noise and dynamic changes in a 4D CT scan by using the time as a connecting dimension. The starting point will be the low quality, low temporal resolution 4D reconstruction described above. The piecewise linear fitting approach will be applied after the volume reconstruction to increase the signal-to-noise ratio and also already provides information that can be readily used in the analysis of the 4D dataset. In short, a piecewise linear function will be fitted to the time evolution of the grey value of each voxel.

An analogue can be drawn with local regression [27] with a polynomial of the order of 1. In a technique called LOESS, a line is fitted for each data point, including its direct neighbours. The result is a smoothing of the data. This means noise will be reduced, just as with piecewise linear fitting. On the other hand, the smoothing applies over the discontinuities in the time dimension as well, which is an unwanted effect. At the same time, the result would not be a simple set of parameters that can be used for further analysis.

Similar observations can be made about other 1D smoothing algorithms or noise filters applied to the temporal dimension, such as smoothing splines [28] or Savitzky-Golay filters [29]. These will have similar noise repression behaviour, but lack the sharp breakpoints and the final parameters that can be a starting point for analysis. The breakpoints are sharp edges in the time dimension, such as when a material moves into a voxel.

Fitting a function to the reconstructed data has been done in literature when there is more information available on the functional behaviour of the time evolution. For example, in [30], a 3-piece piecewise constant function is fitted to the time evolution of fluid flow through rock, with the first and third piece being the same. This yields excellent results, but it can only be used for samples that follow this particular time evolution. In [31] and [32] the fitted function is a linear combination of gamma variates. The application consists of dynamic brain scans, which are performed precisely to determine information that is contained in the parameters of this function, such as peak height and mean transit time. Again, this particular function can only be used for this particular application. It also requires some segmentation beforehand, since the curves are fitted to regions of interest (arteries) where the contrast agent appears.

Dynamic PET or SPECT scan users have been fitting time dependency models to their reconstructed data for some time already, as can be read in [33–35]. Some replace the reconstructed voxel values by the fitted values, as is the case in this paper, while others use some sort of average between the two. They use a compartment model for the intake and outflow of substances in (parts of) the human body. This is therefore a combination of spatial and temporal fitting. In addition, they combine the fitting and reconstruction steps. This means they go directly from projections to the fitted parameters. Since the compartment model is specific to the substance and human body, this is not applicable to applications other than the one for which it is developed. It is also harder to combine with other reconstruction improvement techniques.

If the data corresponds to a specific, known function, in many cases it is best to use these techniques (or a similar one with that known function), as shown in literature. However, in absence of such prior information, a piecewise linear function is a good choice. Its advantages are 1) its simplicity, 2) the broad possible applications, 3) the fact that no prior knowledge is needed and 4) that it can be used as a starting point for further analysis of the sample.

Compared to other 4D noise reduction techniques, such as anisotropic hybrid diffusion with continuous switch [36], piecewise linear fitting is remarkably simpler, yet it can capture temporal discontinuities. Anisotropic hybrid diffusion with continuous switch is actually a combination of two noise filters and has quite some parameters to tune, although the authors provide an estimated good value for a number of them. Some samples need this more complex approach, but for many, a simple one is adequate.

Section 2 explains how the developed method works, how it is implemented (Section 2.2) and why specifically we chose a piecewise linear function as opposed to any other function (Section 2.1). Then, we provide a description of two samples that were used to test piecewise linear fitting: a Bentheimer sandstone and a pharmaceutical tablet (Section 2.3). Section 3 shows the results of this method on the two chosen samples, demonstrating its ability to reduce noise while maintaining resolution. The conclusions are presented in Section 4.