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Quantitative X-ray imaging at Lawrence Livermore National Laboratory (LLNL)

Massimiliano Ferrucci[1], K. Aditya Mohan[2], Brian Giera[1]

[1] *Materials Engineering Division, Lawrence Livermore National Laboratory*
[2] *Computational Engineering Division, Lawrence Livermore National Laboratory*

ferrucci2@llnl.gov

Abstract
X-ray imaging, in particular X-ray computed tomography (CT), is commonly used for non-destructive inspection of additively manufactured (AM) parts [1-5]. X-ray imaging is increasingly used for in-situ inspection of the AM process [6-16]. We provide an overview of quantitative X-ray CT imaging at Lawrence Livermore National Laboratory (LLNL), including how we can reconstruct into physical units using Livermore Tomography Tools (LTT) software suite, the challenges of using X-ray CT for the development of AM digital twins, and a brief discussion on efforts to standardize the use of CT to perform dimensional measurements.

X-ray computed tomography, non-destructive measurement, digital twins, additive manufacturing, standardization

1. Introduction

At Lawrence Livermore National Laboratory (LLNL), we use the term ‘quantitative X-ray imaging’ to denote the representation of X-ray computed tomography (CT) data in terms of values that can be directly related to a physical quantity. Various efforts at the lab fall under the scope of quantitative imaging and are discussed in the following sections:

2. Reconstructing into physically relevant values
3. CT in support of AM digital twins
4. Standardization of CT for dimensional measurements

2. Reconstructing into physically relevant values

X-ray imaging exploits principles of X-ray attenuation to produce a visual representation of the imaged samples. X-ray attenuation is dependent on material properties of the imaged sample, namely electron density and effective atomic number, and on the energy of the X-ray photons.

If data is acquired using monochromatic X-rays, attenuation is reduced to a function of electron density, which is proportional to bulk density, and material composition. If the material composition of the imaged sample(s) is known, then changes in the X-ray image values can be related to changes in bulk density. Gaining access to a monochromatic X-ray source, such as a synchrotron facility, requires lengthy procedures that are not suitable for high-throughput inspections. Cabinet X-ray systems can more readily accommodate high throughput inspections, though X-rays produced in cabinet systems are typically polychromatic. In this case, decoupling material composition from bulk density becomes more difficult, particularly in the case of multi-material parts, due to the energy dependence of X-ray attenuation. Energy-resolving detectors are a promising solution but are currently limited in the maximum photon flux of reliable operation. Traditional dual-energy approaches do not fully account for the spectral dependence of X-ray interactions and will therefore provide different results given different acquisition settings and across imaging systems.

Nevertheless, with a little extra effort on the part of the users, polychromatic data can be reconstructed into physically relevant values. The mathematical algorithms for these capabilities are provided in the Livermore Tomography Tools (LTT) [17] software package developed at LLNL (figure 1).

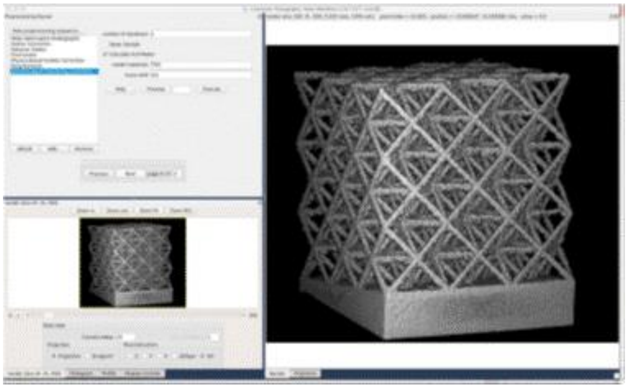

Figure 1. LTT’s graphical user interface, showing the reconstruction of a Titanium alloy truss [17].

LLNL employs more than a dozen CT systems, both home-built and commercial, to non-destructively image parts of various materials and sizes. Our CT systems therefore span a broad range of geometries, detector and source technologies, and maximum operating energies [18]. LTT was originally developed to reconstruct data acquired on our home-built systems. Data acquired on commercial systems was typically reconstructed on vendor-provided software.

However, we are increasingly using LTT to also reconstruct data acquired on commercial systems to ensure consistency and therefore comparability of tomographic data across all CT systems and acquisition parameters. To this end, LTT attempts to reconstruct into values that can be related to physical quantities, such as linear attenuation coefficient (LAC, in cm^{-1}) from a single acquisition (section 2.1), or, in the case of dual-energy acquisitions, into electron density ρ_e (in electron-moles·cm^{-3}) and effective atomic number Z_e (section 2.2). These physics-based algorithms require knowledge of the system's spectral response (section 2.3). The presence of scattered X-rays in the projection data is detrimental to the performance of these algorithms; while LTT can approximately model X-ray scatter and subtract it from the projections (section 2.4), attempts should be made to suppress scatter during the acquisition.

2.1. Reconstructing into linear attenuation coefficients (LACs)

Acquiring a single set of polychromatic projections, users can reconstruct into linear attenuation coefficients (mm^{-1}) from a single polychromatic acquisition (figure 2). The iterative beam hardening correction (iBHC) algorithm in LTT can be used to convert the polychromatic projections to synthesized monochromatic projections. To do this, iBHC requires the elemental composition of the sample material(s) and an estimate of the X-ray spectrum. Users can optionally specify the reference energy E_R at which the monochromatic projections will be synthesized. If a reference energy is not specified, LTT will use the mean spectral response. Applying filtered back-projection (FBP) to the monochromatic projections will provide an LAC reconstruction C_{E_R} at the reference energy.

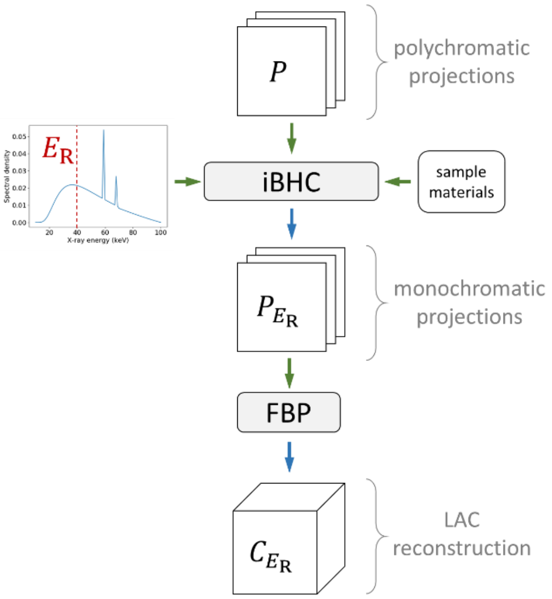

Figure 2. Diagram illustrating how LTT can be used to reconstruct projections acquired at a single polychromatic spectrum into LACs.

2.2. Reconstructing into ρ_e and Z_e

Acquiring X-ray projections at two distinct spectra (i.e., dual-energy acquisition), users can reconstruct into electron density ρ_e and effective atomic number Z_e (figure 3) [19]. Dual energy decomposition (DED) converts polychromatic projections acquired under known low-energy (L) and high-energy (H) spectra to synthesized monochromatic basis (SMB) projections at two energies: E_L and E_H. To do this, DED requires estimates of the X-ray spectra for each acquisition. The user can optionally specify these two energies; otherwise, LTT will use the mean spectral responses. Performing filtered back-projection (FBP) on each SMB projection dataset provides linear attenuation coefficient (LAC) reconstructions C_{E_L} and C_{E_H}. For each voxel in the pair of LAC reconstructions, ρ_e and Z_e are determined by solving a system of two equations.

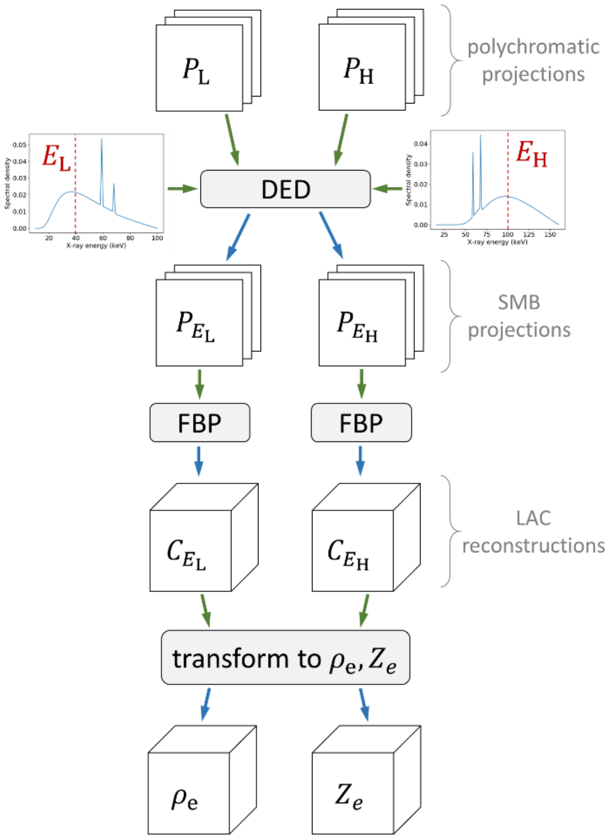

Figure 3. Diagram illustrating how LTT reconstructs projections acquired at two distinct polychromatic spectra into ρ_e and Z_e.

2.3. System spectral response

The system's spectral response is the product of the X-ray source spectrum (considering any materials in the path except the sample) and the detector's spectral response. An initial estimate of the system's spectral response can be determined using LTT's physics-based modelling, which requires information about the system construction and acquisition parameters (see table 1 for a list). Information that is proprietary to the system manufacturer might be obtainable through a non-disclosure agreement (NDA), for example. The user can also load their own spectral response if this is available. The initial estimate can subsequently be refined by applying a least-squares minimization (within LTT) of measured and modelled transmission data of a reference phantom of known geometry and material. Projections of high-purity cylindrical phantoms, e.g., wires, acquired under equivalent spectra can be used in this spectrum refinement step.

Table 1 Parameters needed to model X-ray system's spectral response.

Category	Parameters	
Source[1]	- target elemental composition - take-off angle	- anode normal - voltage
Filtration[2]	- elemental composition - density	- thickness
Scintillator	- elemental composition - density	- thickness
Acquisition	- source voltage - source current	

[1] *Currently, only reflection sources are supported, though transmission targets are envisioned in future releases.* [2] *Filtration comprises any object in the path of the X-rays prior to scintillation, though not including the sample(s) and any sample mounting components. Objects in this category include, e.g., source aperture window, beam filters, and protective materials at the scintillator.*

2.4. Scatter correction

The presence of X-ray scatter in the projections due to the sample can either be suppressed prior to reaching the detector, e.g., using an anti-scatter grid, or can be determined experimentally or from numerical modelling and subsequently subtracted from the projections. LTT's physics-based modelling allows the user to model scatter given an accurate estimate of the source spectrum and material information about the sample.

3. CT in support of AM digital twins

Performing ex-situ inspection, e.g., with X-ray CT, on each additively manufactured part is cost prohibitive. At LLNL, we are developing digital twins of the AM process that, when fed with in-situ diagnostics, will enable virtual inspection of the parts as they are being built. The hope is that virtual inspection can remove the need for ex-situ inspection of each manufactured part, translating to significant cost savings. The reliability of the virtual inspection relies on the accuracy of the in-situ diagnostics and on the correctness of the digital twin's physics-based models. X-ray CT measurements are used as ground truth to benchmark the virtual inspection results and to adapt the digital twin as necessary. However, acquiring low uncertainty X-ray CT measurements is not a trivial task. Imaging artifacts, e.g., cone-beam, beam hardening, scatter, degrade image quality and must be minimized or altogether avoided. To perform dimensional measurements, a surface must be determined from the CT image. Correct surface determination relies on a correct gray value threshold, which can be determined from the CT measurement of a separate calibrated phantom of similar composition, size, and acquisition parameters to the test part. The gray value threshold that minimizes the error between CT measurements and calibrated values is then used to determine the surface on the CT image of the test part. This task of calibrating a reference phantom is not straightforward when the test part is made from a soft material, such as siloxane. Traditional tactile measurement techniques will provide erroneous surface representations due to elastic deformation upon contact. In the talk, we address these considerations and present approaches to overcome them.

4. Standardization of CT for dimensional measurements

Researchers from LLNL are leading the development of a new standard on controlling CT dimensional measurement performance by using representative quality indicators (RQIs) within the American Society for Testing and Materials (ASTM) Committee E07 on non-destructive testing. The standard will serve as a guide for using a calibrated surrogate that is radiologically similar to the test part(s) to ensure accurate and repeatable CT dimensional measurements of the test part(s). Working group WK84977 is looking for members representing industrials users of CT systems. Interested parties should contact the corresponding author for more information.

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