Laura Hellwege*, Carla Gensana Claus, Moritz Schaar, Thorsten M. Buzug and Maik Stille

Generation of realistic multi-energetic cone-beam CT datasets based on medical software phantoms

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Abstract: Multi-energy reconstructions have become an important research field in computed tomography in recent years. Since modern reconstruction and postprocessing techniques often employ deep learning strategies, there is a high need for large, diverse and adaptable multi-energy datasets. Therefore, this work proposes a straightforward pipeline for the generation of multi-energy cone-beam CT projection data based on the established XCAT software phantom with arbitrary desired X-ray spectra. We evaluate the effort and time required for dataset generation and utilize the generated data for model-based iterative reconstruction exemplarily. This approach provides an understanding of the current pipeline's bottlenecks while demonstrating its suitability in producing high-quality projection datasets and reconstructions. Thus, we contribute to open knowledge on generation of large multi-energetic CT datasets for deep learning purposes.

Keywords: Multi-energy CT, simulation, deep learning, data generation

1 Introduction

Modern multi-energy CT allows for more precise tissue characterization and material identification than conventional CT. Due to significant technological advancements in the form of photon-counting detectors, this research field is of even greater interest today. Considering that modern reconstruction and postprocessing techniques aim to employ deep learning strategies [1], there is a high need for large amounts of multi-energy data that is adaptable to application specifications. To our knowledge, there exist no medical open-access datasets that include complete multi-energy cone-beam CT projection data. Even if such data was provided, some multi-energy techniques also require exact knowledge of the X-ray spectra and detector response of the underlying CT system. In general, this information is not provided.

The XCAT software phantom [2] uses a specific set of parameters to define a virtual patient with realistic shapes of all body parts and organs. Each part is defined by non-uniform rational B-Splines (NURBS). These splines can be visualized as a curved 2D surface that forms a closed 3D shape. NURBS surfaces are uniquely defined by so-called control points, which are stored for each body part of the virtual patient. Additionally, every body part has a material identifier that represents its attenuation properties.

Simulation of physical processes like X-ray transmission can be achieved with a variety of software products. In this work, the X-ray projections are computed with aRTist [3], a software that accepts arbitrary X-ray spectra and detector response definitions and applies ray-casting to obtain realistic projection values. aRTist supports virtual scene generation from 3D object models of STL (Standard Tessellation Language) or PLY (Polygon) format.

2 Methods

This work focuses on three tasks: First, the cone-beam CT (CBCT) data generation from medical software phantoms itself. Second, usage of the generated data with a physics-informed material decomposition to exemplarily evaluate accuracy of the image's expected Hounsfield unit (HU) values. Third, the consideration of time requirements for large dataset generation. The proposed pipeline relies on different software products that support GPU parallelization. The computation time is dependent on the computational resources available. In this work a workstation with AMD Ryzen 9 9900x processor, 64 GB RAM, and NVIDIA GeForce RTX 3080 Ti GPU with 16 GB VRAM is employed.

2.1 Data generation pipeline

We propose a semi-automatic pipeline for multi-energy data generation of virtual patients. It is visualized in **Figure 1** and consists of four main steps:

***Corresponding author: Laura Hellwege**[1,2], e -mail: l.hellwege@uni-luebeck.de, **Carla Gensana Claus[2], Moritz Schaar[2], Thorsten M. Buzug[1,2] and Maik Stille[2]**
[1]Institute of Medical Engineering, University of Lübeck, Ratzeburger Allee 160, Lübeck, Germany
[2] Fraunhofer Research Institution for Individualized and Cell-Based Medical Engineering IMTE, Lübeck, Germany

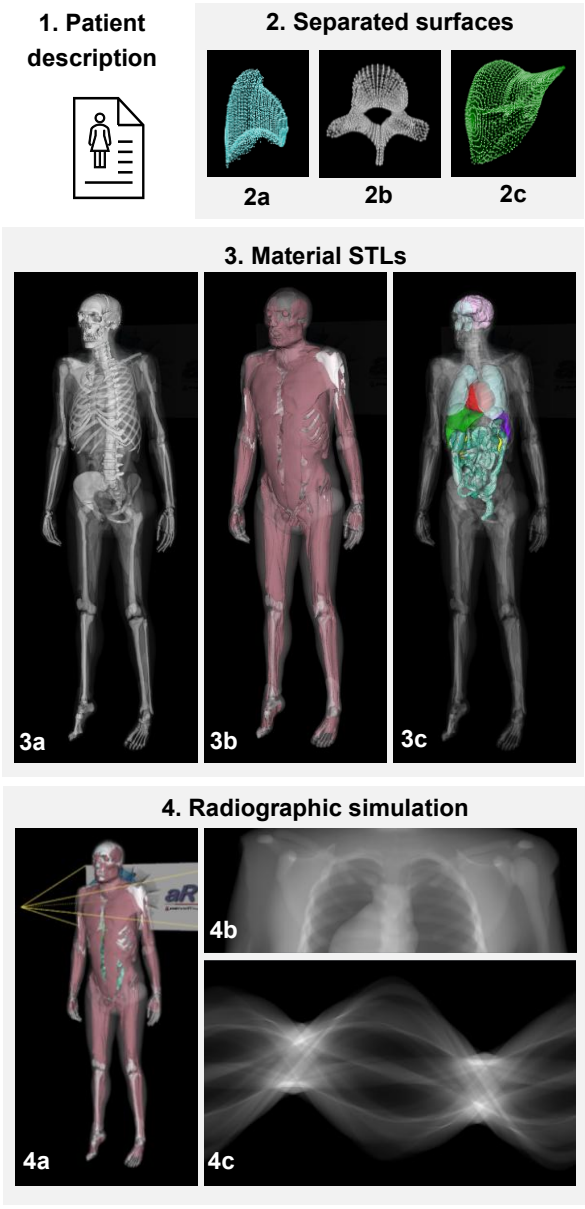

Figure 1: Visualization of proposed pipeline. First, the patient is described in form of a parameter file. The second step generates separated surfaces in form of NURBS control points from XCAT phantom (**2a** right lung, **2b** vertebra, **2c** liver). In the third step, the software solution achieves conjoined material STLs (**3a** bone materials, **3b** muscle, **3c** different organ materials). Lastly, a complete CT scan is performed in aRTist simulation (**4a** simulated patient with source and detector placement, **4b** single projection image, **4c** sinogram of single detector row).

Patient description

Each virtual patient is described by a parameter file consisting of randomized the parameters for XCAT phantom generation. The patients are chosen to be female or male with a probability of 50% each. All other parameters contain information on the patients' body part dimensions and follow a uniform distribution within a specified parameter interval.
Headline 3rd level

Generation of body part surfaces

For each virtual patient, XCAT Phantom is employed to extract the NURBS control points and the material identifier for each body part surface. As suggested in [4], these surfaces should be converted to STL for simulation time optimization.

Conversion to material selective STLs

For further processing we conjoin body part surfaces of the same material identifier to reduce the number of loading and material selecting steps. This is achieved by loading the NURBS surfaces into a parametric modelling software. We employ Rhino3D® since it supports programming via customized Python scripts. The data for each material identifier are selected and the respective NURBS information is converted into surfaces of triangular facets. The converted triangulation is stored as an STL file.

Radiographic simulation

For accurate simulation with aRTist, some crucial properties must be defined:
The material selective STLs are imported into aRTist, where they appear as separate layers. The attenuation coefficients for each layer and for all relevant X-ray energies can be extracted from the XCAT Phantom software. This information is reformatted and loaded into aRTist's material database. It is important to load the STLs in the correct order since aRTist overwrites material information of overlapping regions, e.g. for the spine and the spinal cord. For each STL material layer a material from the material database must be selected.
For multi-energy simulation at least two different X-ray spectra must be utilized – one in each simulation process. In this work, we focus on a dual-energy approach, resulting in two spectra. Both are simulated as a tungsten source spectrum. For the low energy spectrum, the source operates on 90 kVp with a spectral filter of 3.5 mm aluminium. The high-energy spectrum is produced with 150 kVp with a spectral filter of 2.0 mm copper. An energy-integrating detector of 2862 × 954 pixels with 0.15 mm detector pixel spacing and aRTist default detector response is simulated. The detector response function can be extracted for later use in the reconstruction. A fixed maximum detector exposure is chosen, such that no over- or under-exposure occurs while scanning. Furthermore, we employ aRTist's multisampling option with 10 samples per projection value. A standard circular trajectory around the patient's chest with 720 projections in 0.5° angular steps is selected. The source-isocenter distance (SID) and source-detector distance (SDD) are chosen such that the full torso can

be imaged from all angles (SID 500 mm; SDD 1000 mm). The background intensity is estimated in a region of interest and used for normalization on all projection images. To reduce noise, the projection images are rebinned to 954×318 pixels (with spacing 0.45 mm). The projections are stored as a 3D sinogram in NIfTI format.

2.2 Multi-energy reconstruction

To evaluate the usefulness and accuracy of the created dual-energy sinograms, we perform model-based iterative reconstruction (MBIR) to decompose into two basis materials [5]. This method utilizes a physics model to calculate polychromatic projections. Let $\mu_j^b(E_k)$ be the attenuation of material $b \in \{1, \dots, B\}$ in voxel $x_j^b, j \in \{1, \dots, N\}$, where N is the total number of voxels, for energy $E_k \in \{10, 11, \dots, 150\}$ keV. Then the projection value at detector element i is given by

$$p_i^S = \sum_{E_k} S(E_k) \exp\left(- \sum_{b=1}^{B} \mu_j^b(E_k) \sum_{j=1}^{N} a_{ij} x_j^b \right), \quad (1)$$

with a_{ij} indicating the system matrix entry for voxel j in ray i. In the effective spectrum S, the information on the X-ray spectrum and the detector response is combined. We employ two basis materials ($B = 2$). MBIR computes the material images x_j^b by executing two steps: First, calculating the current sinogram value and comparing it to the expected sinogram value. Second, calculating a gradient from the sinogram difference that adapts the image for the next iteration. We apply MBIR with an almost-zero initialization image (value 10^{-6} in all voxels) and with pseudo-Huber regularization. The algorithm converges if a predefined tolerance between the estimated sinogram from equation (1) and the expected sinogram values is reached. As basis materials, calcium (300 mg/ml) and polymethyl-methacrylate (short: PMMA, a soft tissue equivalent material) is chosen. Virtual monoenergetic images (VMIs) can visualize a CT image as if measured with a monoenergetic X-ray source. They can be calculated from the material decomposed images $x_j^{\{b=1\}}, x_j^{\{b=2\}}$ (with μ_j^b as defined for eq. (1)) as

$$\mathrm{VMI}_j(E) = \mu_j^1(E) \cdot x_j^1 + \mu_j^2(E) \cdot x_j^2.$$

The energy E can be chosen arbitrarily since the attenuation values for each individual basis material are known from physics databases (e.g. NIST [6]).

3 Results

Figure 2 shows the exemplary generated projection datasets of a virtual patient for both X-ray spectra employed. Since the underlying geometry, spectra and detector properties are known, the desired model-based reconstruction technique is

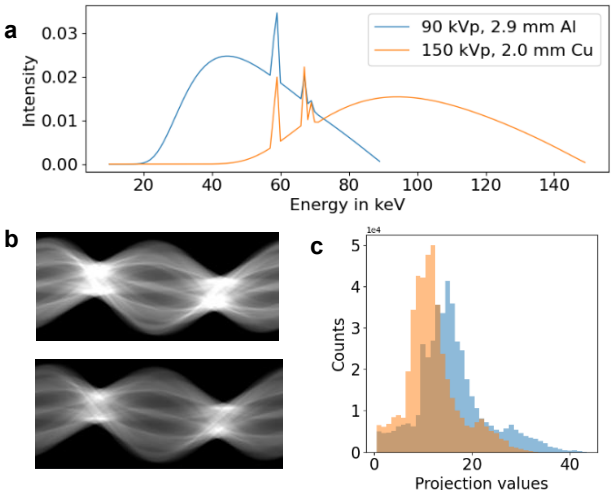

Figure 2: Results of multi-energy simulation. **a** X-ray spectra, **b** low and high energy projection data for the center detector row over a full rotation, and **c** distribution of projection values.

applicable to the generated data. Gradient-based MBIR achieves realistic results as shown in **Figure 3**. The image slice in Figure 3a is taken as our baseline. The material decomposition results in Figure 3b and 3c show expected behaviour as only bone structures are visible in the calcium image and seem virtually removed in the PMMA image. The created VMI exhibits accuracy in terms of HU values for different material ROIs as shown in **Table 1**. An important aspect of creating big virtual datasets is the required generation time. **Table 2** provides benchmark timings for each step of the proposed pipeline. It is apparent that the X-ray simulation itself, even if executed with parallelization via GPU, takes up the biggest percentage of pipeline execution time (ca. 89.5%).

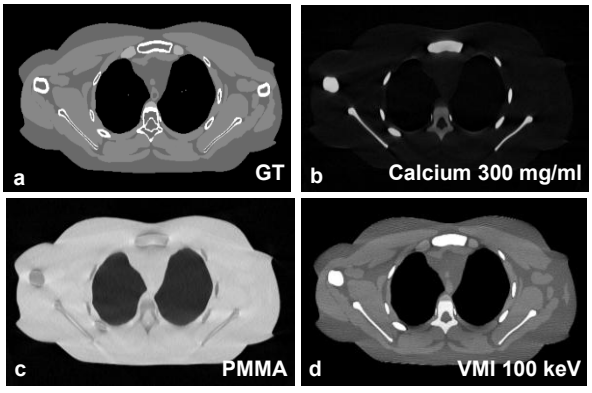

Figure 3: Qualitative results of multi-energy reconstruction. **a** Ground-truth phantom 100keV [Level: 0 HU, Window: 400 HU]. **b, c** Material decomposition results with basis materials calcium (300 mg/ml) and PMMA, [L: 0.5, W: 1.0]. **d** Example VMI at 100 keV calculated from decomposition results, [L: 0 HU, W: 400 HU]. All images are reconstructed using a pixel spacing of 0.75 mm. ROIs for HU evaluation are marked in red.

Additionally, it is noticeable that loading the data into Rhino3D and aRTist from disk memory takes up a significant amount of time (ca. 8.1%). It should be noted that the steps were performed by manual execution. This means that some amount of time is to be expected in between steps, depending on manual workforce availability.

Table 1: HU values for calculated VMI in ROIs (see Fig. 3)

Material	Tissue	Muscle	Lung	Spine
Ground truth	-25.7	14.2	-710.6	196.8
Mean in ROI ± std	-53.5 ± 50.3	-14.2 ± 63.4	-760.9 ± 55.8	173.7 ± 80.1

Table 2: Benchmark times with standard deviation for ten repetitions of each pipeline step and extrapolated time for 1000 virtual patients. For single patient: NURBS: ca. 1.1 m control points (40 MB), STL: ca. 19.7 m triangles (1 GB)

Step	Mean time (± std) for single virtual patient	Estimation for 1000 patients
1. Parameter generation	43.9 (± 11.7) ms	negligible
2. NURBS generation	2:02 (± 0:02) min	1 d 10 h
3. Rhino3D		
· Loading NURBS	4:03 (± 0:20) min	2 d 19 h
· STL generation	2:25 (± 0:03) min	1 d 16 h
4. aRTist		
· Loading STLs	7:01 (± 0:07) min	4 d 22 h
· Dual-energy X- ray simulation	121:48 (± 1:38) min	12 wks 14 h
Total	137:18 (± 2:11) min	12 wks 11 d

4 Discussion and Outlook

The suggested pipeline for simulated CBCT data generation is straightforward. We have shown that the simulated projections obtain realistic HU values in the VMIs when applying an exemplary multi-energetic reconstruction technique. In this work, dual-energy data for an energy-integrating detector was simulated. The simulation could be expanded for even more energy spectra or photon-counting. However, the simulation for each spectrum or photon-counting energy bin (Step 4, aRTist) must be executed additionally. Parallelization on multiple GPUs should be considered in this case. Furthermore, disk and memory space must be reviewed since they grow linearly with the number of spectral datasets. Preparation and simulation time as well as the amount of data could be reduced by utilizing only specific parts of the virtual patients and reducing detector size or detector resolution. These parameters should be chosen according to application need. As of now, the data generation is only semi-automatic: Some of the steps must be performed manually with periods of waiting time in between interactions. This makes the current pipeline somewhat inefficient. In the future, we hope to circumvent these problems by customized software solutions in Python for STL generation from NURBS (e.g. via NURBS-Python [7]) and process from working memory directly. This will reduce the time needed to load the different data formats from disk memory and improve automation. In conclusion, the proposed simulation pipeline is an important step towards large, adaptable and diverse medical datasets that are essential for training in deep learning tasks for medical multi-energy imaging.

Author Statement

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