Faster X-ray computed tomography in real-world dynamic applications

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Conclusions and outlook

This thesis took a journey along different components of fast tomographic pipelines. It discussed a customized set-up for fast imaging, deep learning in real-time pipelines, software for fast algorithms, and a self-supervised method for the removal of noise. These components were often connected: For example, the fast set-up yielded sparse-view data (Chapter 2), and consequently only the slower SIRT algorithm was able to achieve sufficient quality. Similarly, in the real-time learning pipeline of Chapter 3, the underlying numerical implementation of the tomographic algorithm proved crucial for on-the-fly training of the neural network.

In this section, we will take an overarching view on the results, reflect on the contributions of the papers, and provide directions for future research.

X-ray CT set-ups In Chapter 2, the authors investigated an ultra-sparse set-up for imaging the phenomena of fluidized beds. Fluidized beds behave similar to fluids, e.g., voids in fluidized beds can disperse and merge, similar to bubbles in a liquid. The authors first addressed several difficulties with the construction of the set-up, such as its calibration procedure to retrieve the positions and orientations of three sources and detectors, and the temporal synchronization of the three detectors. For bubbling fluidized beds, the set-up also required a tailored referencing procedure in order to extract the bubbles from radiographs with fluctuating backgrounds of particles.

In this research, their main contribution was to enable *time-resolved and fully-3D* reconstruction of gas-solids beds. Despite the ultra-sparse geometry, the high-resolution flat-panel detectors provided sufficient information that allowed inferring bubble characteristics, such as their shape, location and density in the volume. For example, phantom experiments were conducted to demonstrate that the new method enables reliable estimation of bubble diameters. Compared to existing set-ups, which, e.g., only image in a small horizontal slice, or are not time-resolved, this set-up has the unique ability to look at large-scale dynamic evolution of the beds.

To achieve the sparse-angle reconstruction, the authors leveraged SIRT (cf. Chapter 1). This algebraic technique enables the integration of prior information, which to some extent absorbed the difficulties of the sparse-view geometry and fast acquisition. We found two main factors to play a pivotal role in the reconstruction accuracy. The first was the usage of simple prior information, such as a masking region and box constraints, constraining the solution to the physically-attainable gas-solids ratios. The second was the amplitude of noise in the data. The most prominent source of noise was due to cross-scattering from the non-facing sources, and another was due to the granularity of particles in the data. Without mask or box constraints, or with high noise, SIRT cannot recover the smooth boundaries of bubbles. Instead, its solutions reflect the geometry of the set-up, and the bubbles become hexagonally-shaped in the horizontal plane. In real-world data, however, this effect was somewhat reduced, due to the smooth interfaces of bubbles: the SIRT solution only "hexagonalizes" uniform regions in the reconstruction.

One clear research direction is to study joined denoising-and-reconstruction technique in combination with the data retrieved from the set-up, as pursued in Chapter 5.2.2. Another straightforward way to further increase the accuracy of the reconstruction, is to extend the set-up with additional source-detector pairs. However, the existing set-up may also already be improved by changing its geometry, e.g., the sources and detectors could be aligned on a Cartesian coordinate system. A next direction for research would be to integrate (deep learned) priors about fluidized beds into the iterative method. Yet another would be to explore the temporal aspect of fluidized beds. Since bubbles are subject to morphological changes as they travel upwards, dynamic priors about the bubbles' positions or gas contents could be incorporated in the reconstruction process. However, bubbles in a bed borrow from, and release to, interstitial gas, and learning these complex dynamics may prove challenging, especially when the timesteps between reconstruction frames are large.

Real-time tomographic pipelines In Chapter 3, a neural network training strategy was introduced for real-time tomographic pipelines, such as are used within synchrotron beamlines. In these pipelines, off-the-shelf deep-learned algorithms (e.g. trained on pictures of photo cameras) do not generalize well due to the properties of experimental data. In this chapter, the authors pioneered a learning technique for on-the-fly reconstruction and training of neural networks, using a proof-of-concept implementation on intercepted radiographs of the RECAST3D pipeline software. They investigated different buffer sizes, fast and slow dynamics, and several variations of U-Net network architectures, on dissolving tablets from the FleX-ray laboratory with the Noise2Inverse denoising task.

In the research, it was found that pretrained CNNs (i.e., networks that are trained until convergence, on a hold-out part of the experimental data) cannot be expected to generalize well on out-of-distribution samples. While, for the FleX-ray experiments, such networks would generalize well for the next 12 seconds, the pretrained CNNs had diminishing performance under changing experimental conditions or diverging experimental dynamics. At the same time, networks that were trained for during the experiment could quickly anticipate changes in the data and deliver much better results on unseen data.

While the results of just-in-time learning are promising for synchrotron light sources, the idea is still in a conceptual stage. Even though customized software and patch-based training made the idea feasible, the main challenge remains the efficiency of training CNNs on-line. The experiments in the article used a region-of-interest FDK, a relatively simple training task, relatively slow experimental dynamics, and small network architectures. These properties proved realistic for the Noise2Inverse task, but for extending them to high-resolution, fully-3D reconstructions, fast dynamics, or complex learning tasks, the approach would require further research and would likely need much more computational resources (e.g., parallelization over a cluster of GPUs).

At the same time, there exist many opportunities to further improve the concept. An interesting, more theoretical inclined direction, is that of on-line learning. In the proof-of-concept, a simple capacity queue was used to decide which selection of historic radiographs was used as training samples. The size of the queue was hand-picked. However, a more intelligent selection has large potential to improve generalization. For example: under rapidly changing dynamics, the training procedure should focus only on the most recently reconstructed samples. And, with slower dynamics, also older radiographs should be included to prevent catastrophic forgetting. A further research direction that could prove helpful for training tasks that are more complex than denoising, is to combine the just-in-time strategy with transfer learning. For example, one could train a neural network partially off-line, and then continuously fine-tune it during the experiment.

Software for tomographic projectors In Chapter 4, the authors introduced ASTRA KernelKit, a Python software package that enables easy customization of tomographic projectors. Within the software, “projectors” not only refer the computational operations of the X-ray transform, but also include, e.g., memory management on the CPU and GPU, as well as preparatory calculations for the projection and volume geometries. The software was initially developed for Chapter 3 to facilitate the generation of reconstruction patches while the neural network training is ongoing, and then was then continued in its own project.

To motivate the new software package, the paper authors had first investigated several existing packages for Computed Tomography. Many, if not all, of those packages assumed a “user philosophy”, that is, they were built for users to launch efficient pre-implemented CT algorithms. The latent CUDA kernels of these packages were similar in terms of efficiency, since they all followed best-practices for single three-dimensional reconstruction volumes. Unfortunately, the philosophy is problematic for researchers that need to experiment with custom algorithms, for example for neural networks or high-dimensional problems. KernelKit therefore instead takes a “researcher philosophy”: Both Python and CUDA operations are easily accessible, allowing researchers to extend or modify the core routines to fit their needs. In the results, the software was demonstrated for tomographic pipelines. The examples were: CUDA graphs for neural networks, slice-based reconstruction with RECAST3D (Chapter 3), and kernel tuning for the fluidized-bed set-up (Chapter 2).

There are two main research directions for this project. One is the project itself, and the other is the utilization of KernelKit in other research projects. Within the project itself, there are several possibilities for extensions. Currently, KernelKit only implements the standard ASTRA kernels. However, it could benefit from recent developments for CT, such as the distance-driven projectors. Another technical direction is to support more devices, for example, AMD ROCm architectures, or NVIDIA Hopper or Grace architectures. The possible of run-time compilation also allow software features that accommodate to different reconstruction problems: For example, KernelKit could automatically compile a kernel that skips all computations inside a masked area of the volume.

The second research direction is in projects that have become possible or easier with KernelKit. One particular interesting direction is kernel tuning. Currently, KernelKit compiles a standard kernel when the user does not specify parameters, such as the number of X, Y, and Z CUDA threads that determine how the workload is divided. Oftentimes, tomographic algorithms can take several minutes or longer to compute, with the projectors taking the majority of the computation time. Probing the parameter space before of the start of the algorithm can take as little as a few seconds, and can increase the efficiency of the algorithm or lower its power consumption.

Self-supervised denoising of radiographs Lastly, in Chapter 5, the paper authors sought a solution for self-supervised blind-spot denoising of radiographs. As explained in Chapter 1 and 5, blind-spot denoisers work for noisy images without paired ground truths, but unlike zero-shot denoisers, e.g., the Deep Image Prior, can still take information from large data sets of single noisy images.

The motivation for this research originated from the set-up of Chapter 2, which provided a data set comprising many noisy radiographs of bubbles. At that time, no self-supervised learning techniques existed that could take advantage of this noisy data. They required, for example, paired noisy radiographs, radiographs from nearby angles, repeated patches within a radiograph (similar to BM3D), or downsampling, to make sure that multiple independent noisy samples could be extracted from the data. In the research, the authors investigated why the most promising class of self-supervised denoisers, the blind-spot denoisers, did not work for the radiographs from X-ray detectors, and found the cause to be due to correlated photon fluctuations inside scintillator detectors. Since correlations were isotropic for real-world Caesium-Iodine scintillator detectors, they could be described by a uniform convolution. From here, a simple sampling-decorrelation workflow was derived, and the method tested successfully for the bubble radiographs and the SIRT reconstruction outlined in Chapter 2.

In this research, there are again two promising continuations. The first is a further improvement of the denoising workflow, i.e., as outlined in the conclusions at the end of Chapter 5: It can be tested for different different set-ups and detectors (e.g. monolithic detectors, different scintillator crystals), and it may be possible to suppress the side-effects of additive Gaussian noise. A possible improvement could be to extend the model to nonuniform deconvolution as to further reduce model mismatch (e.g. for heterogeneous pixel technology, or Swank noise).

An open question is if and how the denoising framework can be further integrated with with self-supervised tomographic reconstruction. In our work, it was considered as a preprocessing technique before sparse-view reconstruction. Preprocessing can be more memory-efficient compared to, e.g., iterative learned techniques, such as the learned primal-dual. On the other hand, for situations where the learned 3D reconstruction would be possible (small volumes, or 2D parallel beam), an opportunity could be to integrate blind-spot denoising in the reconstruction. This would have the advantage that neural network filters work on reconstructed data (where the image features are local), while the loss is taken on the radiographs (where the noise is local).

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