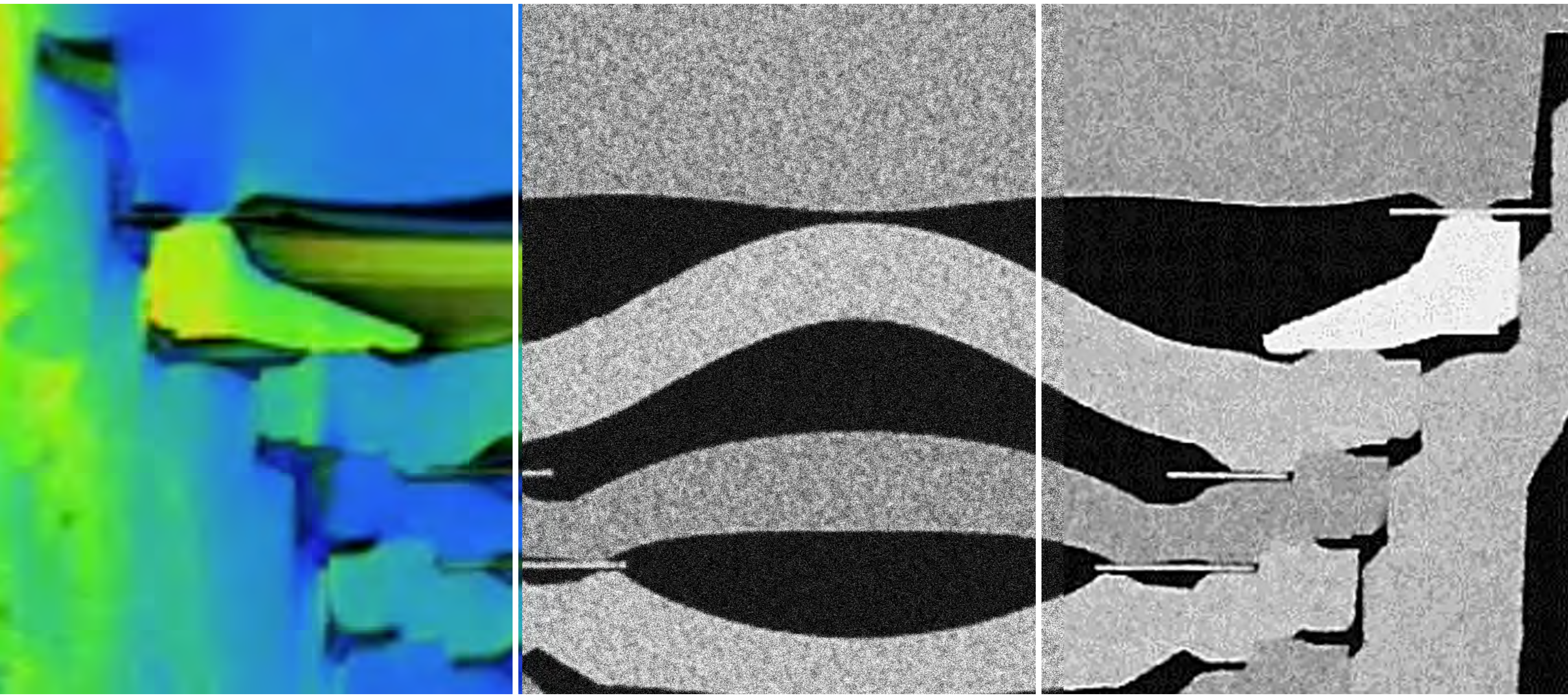
Technical Note

Advanced Reconstruction Technologies

ZEISS Xradia 3D X-ray Microscopes



Seeing beyond

Authors: Matthew Andrew, Ph.D.
Ravikumar Sanapala, M.S.
ZEISS Research Microscopy Solutions
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Leading academic and industrial researchers in the world rely on 3D X-ray microscopy as an effective non-destructive imaging technique to produce remarkable scientific insights. To obtain useful 3D volumetric data from X-ray microscopy, 2D projections first need to be interpreted and combined using tomographic image reconstruction algorithms. Such reconstruction technologies typically have certain requirements, assumptions, advantages and drawbacks which make them specifically well suited towards particular applications. Many different techniques are available, which enables incremental performance to be extracted from datasets but may not be universally applicable across all sample classes, applications or usage modes. The ZEISS Advanced Reconstruction Toolbox from ZEISS is aimed at making these techniques available to scientists, engineers and technicians, improving performance of 3D X-ray microscopes in their specific application and use cases. The performance improvements that can be achieved with the advanced reconstruction toolbox can be in terms of throughput, image quality, field of view, and ease-of-use. This toolbox acts as a platform to launch the next series of ground-breaking improving.

One of the principal challenges when applying X-ray microscopy to solve industrial problems is a compromise one needs to make between imaging throughput and image quality. High resolution 3D X-ray microtomography acquisition times can be on the order of several hours, which can lead to challenging return-on-investment (ROI) calculations when weighing the relative advantage of high accuracy 3D analysis with cheaper, less capable analytical techniques. To tackle this issue, optimization of each step in the production of the actionable information required by these industrial users is required. For 3D X-ray microtomography, these steps typically consist of sample mounting, scan setup, 2D-projection image acquisition, 2D to 3D image reconstruction, image post-processing and segmentation, and final analysis. In repetitive workflows (where many similar samples are run sequentially and image processing and analysis workflows are well understood), the slowest step is image acquisition and subsequent reconstruction. Even in academic environments where ROI is less of a concern, *in situ* analyses can require very high absolute temporal resolutions when performing 4D (time-resolved) scanning. Beyond this require-ment, the analysis of subtle chemical or compositional differences, which may only exhibit very slight greyscale or textural contrasts, requires extremely low noise levels to accurately segment and classify. This means that even when acquisition time is less of a concern, image quality may require the use of advanced reconstruction technologies.

In this technology note, we will review a range of different reconstruction technologies, specifically analytical, iterative and deep learning-based reconstructions that are launched as part of the ZEISS Advanced Reconstruction Toolbox. These technologies are targeted to enhance throughput and image quality of ZEISS Xradia 3D X-ray microscopes. In analytical reconstruction (of which by far the most common type is "filtered back projection" for cone-beam based systems, typically known as Feldkamp-Davis-Kress algorithm or FDK [1]), the entire volume is reconstructed in a single step. While this has advantages in terms of computational simplicity, it is prone to the impacts of both artifacts and noise, requiring either a large number of 2D projections and/or long exposure times, both of which result in reduced imaging throughput.

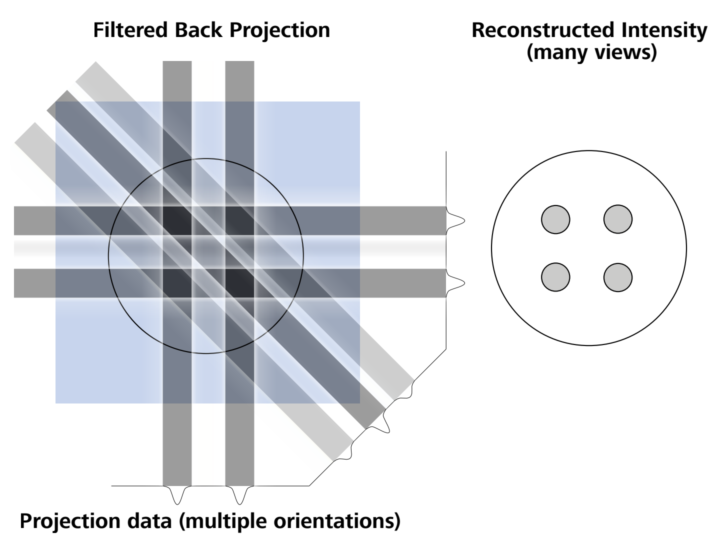


Figure 1 *Filtered back projection. Projection data is filtered using a frequency domain filter, reducing image blurring.*

On the cover Smartphone camera module images from ZEISS Xradia Versa 3D X-ray microscope. (1) Capture from 3D image. (2) 2D projection, standard reconstruction. (3) 2D projection with ZEISS OptiRecon reconstruction, acquired in ¼ the time with superior image quality.

During iterative reconstruction, a volume is progressively created over multiple iterations, and a model set of projections from this volume is compared with the real set of projections, minimizing the difference between the two, and thereby minimizing the impact of artifacts and noise in the final reconstruction. Deep learning-based reconstruction is a new technology where trained neural networks are introduced between the projections and the final reconstructed volume. This has the effect of drastically denoising the data, as well as reducing any reconstruction associated artifacts.

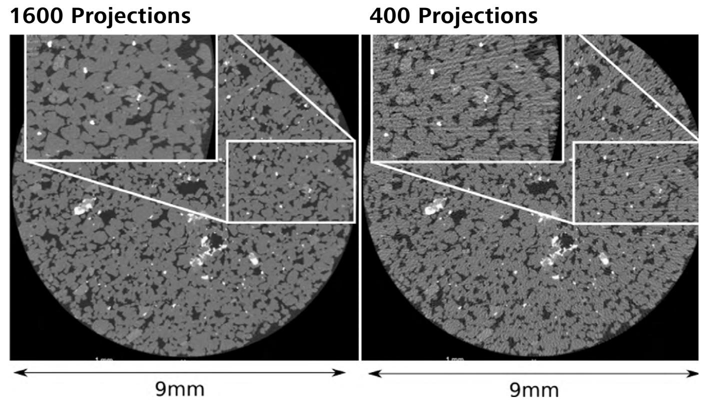


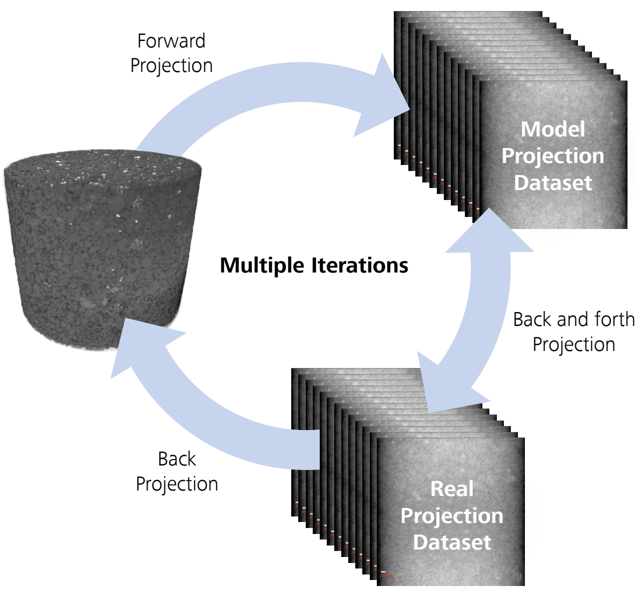
Figure 2 *3D reconstructed volume (using FDK algorithm) of sandstone sample using 1600 projections, showing few artifacts, and 400 projections, showing much greater impact of sampling artifacts and noise. The darkest phase in this image represents the pore space of the rock and the light phase represents the grains in the rock.*

Filtered Back Projection (a.k.a Feldkamp-Davis-Kress reconstruction, or FDK)

In order to reconstruct a 3D volume from a series of sequentially acquired 2D X-ray projections, traditionally FDK filtered back is used in cone beam CT geometric reconstruction. In this technique, projections are weighted and filtered before being distributed across image volume along all their projection directions (Figure 1). If many projections, ideally thousands, are used, an accurate representation of the 3D volume of the sample is achieved.

This technique works well with many views, however, relies on the assumption that the total projection dataset contains sufficient projections spaced at small angular intervals (the data is "well sampled") and does not contain significant noise.

These assumptions are frequently broken in the interest of improving throughput by reducing total tomography acquisition time (e.g., for increasing temporal resolution in *in situ* experiments or, during industrial applications, to reduce the effective cost per sample), leading to errors in the reconstructed image (Figure 2). This, in turn, leads to errors in segmentation and any resulting analysis from the data.



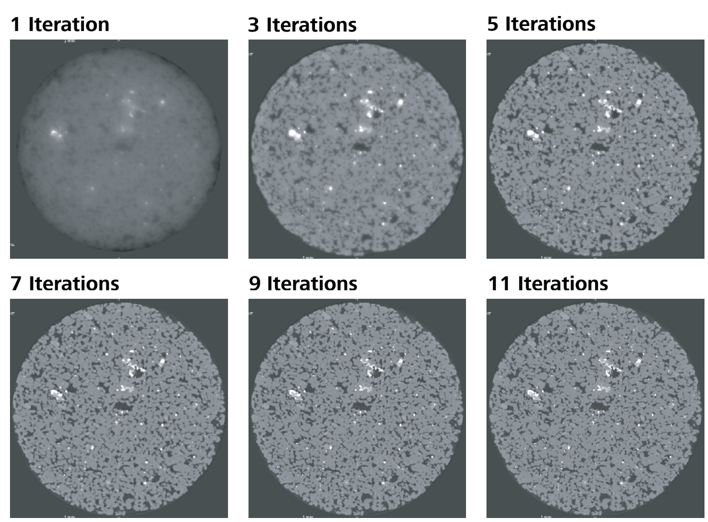


Figure 3 *Statistical Iterative Reconstruction. The model dataset is continually compared with the real projection dataset, and the difference between them back projected, gradually creating a 3D model that closely resembles the real 3D sample geometry*

Iterative Reconstruction

While filtered back projection is the most commonly used reconstruction technique, statistical iterative reconstruction (SIR) is a new technology allowing for many of the limitations encountered using filtered back projection to be overcome [2]. In this technology, a 3D model of the sample is gradually built up over the course of many iterations. At each iteration this 3D model is forward-projected, creating an estimated set of projections, which is compared to the original (real) dataset. The difference between the real projection dataset and the estimated projection dataset is then back-projected and added to the volume, reducing the difference between the 3D model and the sample. When the 3D model is subsequently forward-projected the difference between the real projection dataset and the estimated (forward-projected) dataset is reduced (Figure 3). When some stopping criterion is met (e.g., a certain difference between the real and the estimated projection datasets, or a fixed total number of iterations), the final reconstructed volume is reported.

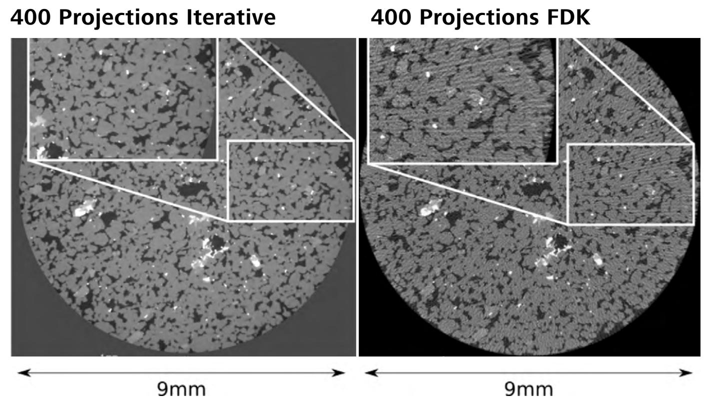


Figure 4 *Iterative reconstruction (left) vs. FDK reconstruction at reduced number of projections (400). The use of iterative reconstruction techniques greatly reduces the impact of noise and sampling artifacts on the resulting reconstructed data, while maintaining image sharpness.*

As the data is not ramp filtered, the resulting image is less susceptible to the sampling artifacts of traditional filtered back projection algorithms. Also, as any change to the reconstructed volume is consistently and continually checked against the real projection dataset, powerful denoising algorithms (called "regularization") and noise weighting models can be introduced to reduce the impact of noise in the final reconstruction with an edge toward preserving performance significantly better than FDK (Figure 4).

Three of the major challenges of iterative reconstruction are computational cost, parameter selection and sample specificity. As iterative reconstruction consists of multiple pairs of forward and backward projections, substantial computational resources are required than for traditional filtered back projection. ZEISS OptiRecon solves this challenge relying on a highly efficient multi-GPU based implementation and dedicated high performance workstation. This implementation can reconstruct a one-billion-voxel 3D image in less than 5 minutes.

The second major challenge faced by iterative reconstruction is parameter optimization, particularly for the edge-preserving denoising regularization algorithm, which can have many variables to optimize. This typically requires substantial expertise of the operator to achieve useful results. To solve this challenge, ZEISS OptiRecon has implemented a user friendly two-parameter optimization interface whereby the edge preservation parameter is determined by an initial unconstrained reconstruction of a small characteristic portion of the sample. The smoothing parameter is then determined for a sequence of displayed values, ensuring neither over-smoothing nor under-smoothing of the final reconstructed dataset.

The third major challenge is sample specificity due to the assumptions made during reconstruction. As shown below, ZEISS OptiRecon demonstrated superior results compared to FDK for typical samples in oil and gas applications that can be described as "sparse," meaning the features are relatively large compared to the voxel size. ZEISS OptiRecon, launched as part of the ZEISS Advanced Reconstruction Toolbox, expands this superior iterative reconstruction capability to a broader set of sample classes.

Results & Examples

In order to quantitatively compare the performance of differing reconstruction techniques, we evaluate (1) signal-to-noise ratios (SNR) to measure the impact of noise, and (2) edge sharpness profiling, where we assume an analytical profile for a particular phase interface with a specified characteristic length scale, to measure the impact of reconstruction method on image sharpness. SNR is calculated by measuring the mean (signal) and standard deviation (noise) of the gray scale values in two regions of interest representing the two phases of grain and pore.

SNR is then given by the difference of the mean values divided by the average of the standard deviations. Edge sharpness is determined by fitting a logistics function to a gray scale line profile across the edge, and the edge sharpness in voxels is given by the width (in voxels, smaller means sharper) of the transition of the fitted line (inverse of the parameter k of the logistics function). When using these metrics on the dataset shown in Figure 4, iterative reconstruction techniques give a reconstructed SNR value approximately three times higher than when using FDK (with values of 15.4 vs. 5.55 for iterative reconstruction and FDK respectively). This was achieved while decreasing the characteristic edge length (representing edge width or image sharpness) by approximately a factor of 1/3 (Table 1). It can also be shown (not presented here) that applying edge-preserving noise reduction filters to FDK reconstructions with few projections does not achieve the same level of image quality improvements and artifact reduction as the iterative algorithm does.

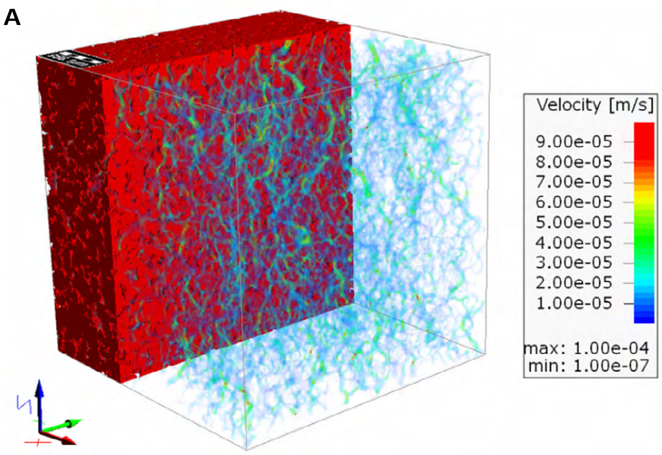
One of the primary areas of application for this technology is that of digital rock physics whereby the pore space of rock cores from petroleum reservoirs are imaged using X-ray microscopy and segmented. This segmentation is then used as the input to a pore scale computational model, the results of which are used to inform and populate the reservoir models that make predictions about petroleum production and reservoir performance. One of the biggest challenges associated with this workflow, however, is cost and, by extension, acquisition time. The use of iterative reconstruction will let researchers and service companies reduce acquisition time and thus the "cost per sample" of this workflow.

To characterize the impact of reconstruction on resulting petrophysical properties, permeability and mercury intrusion capillary pressure was simulated through the pore network of the sample shown in Figure 4, reconstructed using both FDK (with 1,600 projections) and iterative reconstruction (with 400 projections). These reconstructions were then segmented using Otsu automated selection [3] and

	Iterative Reconstruction (ZEISS OptiRecon)	FDK Reconstruction
Signal to Noise Ratio	15.4	5.6
Edge sharpness (voxels)	0.31	0.45

Table 1 *Quantitative comparison of signal-to-noise and edge sharpness for iterative reconstruction vs. FDK reconstruction. Edge sharpness is measured in voxels, so a smaller number denotes a sharper edge.*

A



B

	X	Y	Z
FDK	4.0	3.4	3.7
Iterative	4.4	3.8	4.0

C

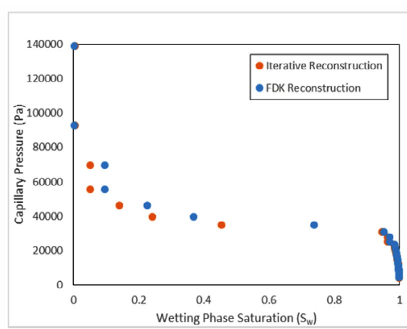


Figure 5 *Simulations through the same volume reconstructed using filtered back projection using 1,600 projections and iterative reconstruction using 400 projections. (A) Velocity field, shown through the FDK reconstructed image. (B) Permeability tensor components (in Darcy units) (C) Simulated capillary pressure curve.*

hydraulic parameters were simulated using GeoDict (Math2Market GmbH), showing very little difference between simulations from the filtered back projection reconstruction and the iterative reconstruction (Figure 5).

Iterative reconstruction also has great potential application in the performance of dynamic, time-resolved *in situ* experiments, as it could greatly increase their temporal resolution, reducing typical acquisition times from several hours down to tens of minutes. In the field of flow and transport porous media, this could allow for processes of chemical reaction (occurring over several hours) to be examined with a much greater precision than previously possible.

Finally, iterative reconstruction may open up an exciting new area of application for X-ray microscopy: liberation analysis within the comminution process in the mining industry. During comminution, the process of reducing a mineral ore into its constituent mineral grains for subsequent extraction, the "liberation" of a particle, is the proportion of that particle made of the mineral of interest (rather than other minerals, forming the rest of the "gangue" mineralogy of the rock). This analysis is traditionally done in 2D using SEM-based automated mineralogy. X-ray microscopy, however, has the potential of both greatly speeding up and removing the stereological biases inherent in 2D analysis if it can be delivered at high image quality with a fast (and economical) acquisition time. When examining such mineralogy feed samples, a great improvement in image quality can be seen when comparing traditional filtered back projection and iterative reconstruction techniques (Figure 6).

DeepRecon

An extremely exciting new area of imaging technologies is the integration of deep learning-based techniques into the image reconstruction workflow. The last ten years have seen a transformation in a wide array of advanced statistical inference techniques broadly grouped together under the umbrella of "machine learning." While these technologies have transformed sectors as wide as medical diagnostics to stock market analysis, their practical application to X-ray microscopy is still in its early stages. During visual examination, the brain of a trained scientist,

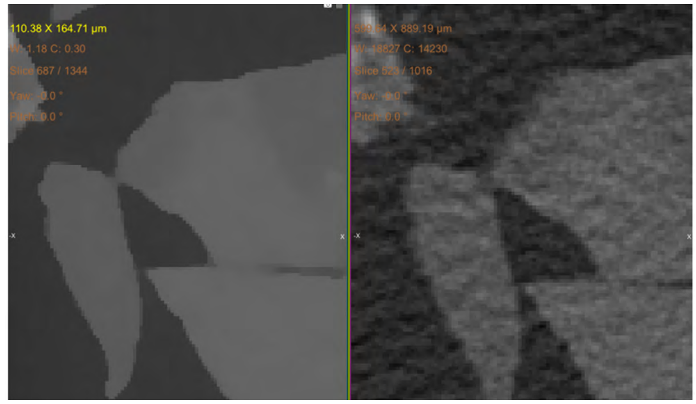


Figure 6 *Iterative (left) and FDK (right) reconstruction of a mining sample from 400 projections.*

engineer, or analyst act to integrate features across multiple scales, removing noise and artifacts to extract features and objects of interest. This has traditionally been extremely challenging to capture in a computational form as it involves much more than local greyscale, integrating local and non-local greyscale, gradient and textural features.

Most of machine learning applications to date have been focused on post-processing for image segmentation, feature classification, or object recognition [4, 5]. It has not been integrated deeply inside an instrumental workflow, especially in one as complex as 3D X-ray microscopy. The dual "projection-to-image volume" nature of X-ray microscopy presents specific challenges to machine learning workflows, as the training of networks requires highly consistent spatially registered datasets with consistent scaling and noise profiles. The line-integral projection process from X-ray source to detector incorporates a range of inherent non-linearities that make the creation of well-matched datasets for network training extremely challenging. This challenge is exacerbated by the range of standard image corrections frequently applied to X-ray data (such as center shift offset or beam hardening corrections), which can further effect scaling or data matching between pairs.

ZEISS DeepRecon is an integrated package of software that allows for this process of image improvement, interpretation, and retrieval to be performed using a trained neural network, allowing for high quality reconstructed data to be achieved despite rapid acquisitions using a small number of projections or short exposures (Figure 7).

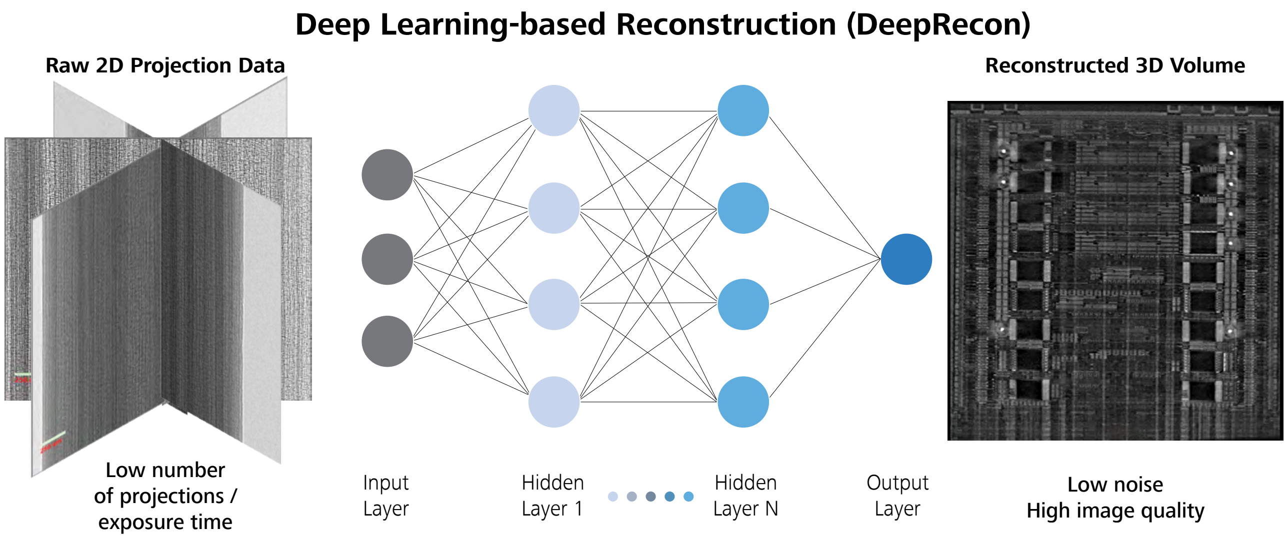


Figure 7 *By integrating a pre-trained neural network between detected raw projection data and reconstructed data, high quality reconstructions can be achieved with low numbers of projections, or short exposures.*

These techniques allow for extreme throughput improvements, potentially up to 10X improvement over standard filtered back projection techniques (Figure 8). These techniques are particularly useful for applications and industries where repetitive, similar samples are frequently imaged with 3D X-ray microscopes. This is because a single model can be used across most of the samples imaged, rather than requiring frequent time-expensive model retraining.

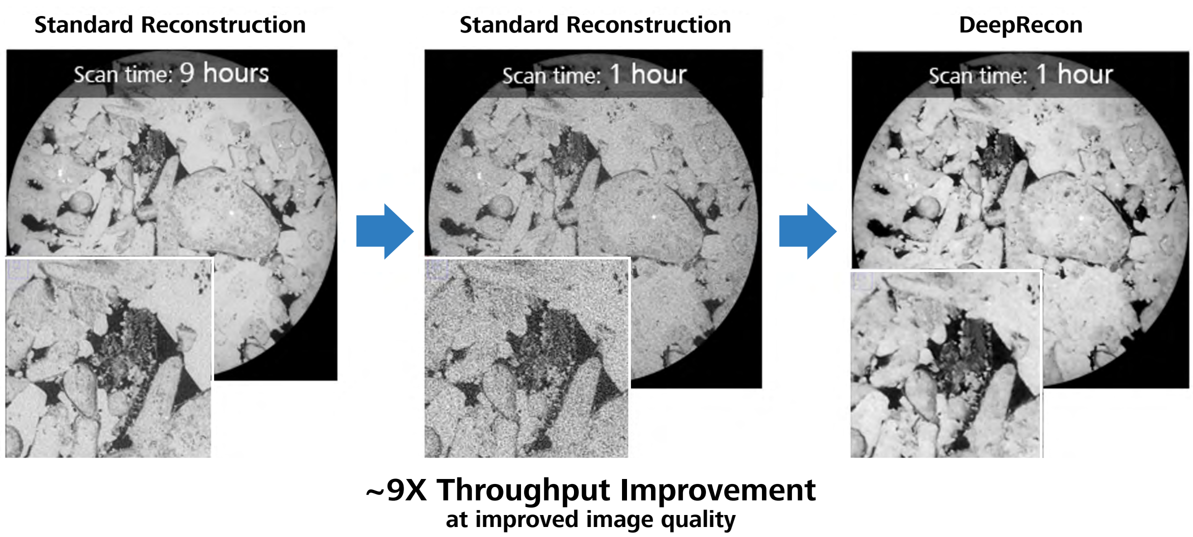


Figure 8 *Extreme throughput improvements can be achieved using DeepRecon. In this example of a porous rock sample, an effective ~9X improvement in throughput even further enhancing image quality is observed. The images were obtained with ZEISS Xradia 620 Versa.*

Conclusions & Future Views

Reconstruction technologies are critical to 3D X-ray microscopy, and novel reconstruction methods have the potential of greatly enhancing the product performance of ZEISS 3D X-ray microscopes. The advanced reconstruction toolbox from ZEISS will pave a path for continuous innovations in reconstruction technologies that can significantly enhance the performance of ZEISS 3D X-ray microscopes thereby helping scientists, researchers and lab technicians to enrich their scientific explorations. The first version of ZEISS Advanced Reconstruction Toolbox consists of two reconstruction technologies, ZEISS OptiRecon and ZEISS DeepRecon, both of which are targeted to significantly improve the image quality or throughput of ZEISS 3D X-ray microscopes, providing the researcher with ultimate flexibility.

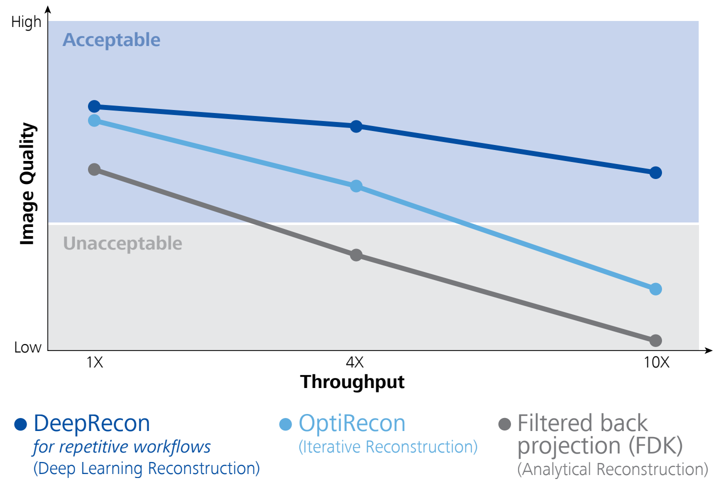


Figure 9 *Schematic representation of performance improvement with advanced reconstruction technologies (DeepRecon and OptiRecon) compared to standard reconstruction (FDK)*

ZEISS OptiRecon is based on iterative reconstruction, which is a powerful technology with the potential of being transformative for X-ray microscopy workflows. It allows for high quality data to be acquired in a much-reduced period of time. This, in turn, allows for industrial workflows to be applied much more economically, at a reduced time per sample, and for academic analyses, particularly time resolved *in situ* analyses, to be performed at much greater temporal resolution. Iterative technologies, particularly their application to the big datasets produced by high resolution 3D X-ray microscopy, are in their infancy and have a great potential for future development. Here, we have demonstrated that OptiRecon can provide equivalent image quality while using only 1/4 of the number of projections, and therefore 1/4 of data acquisition time, e.g., for typical applications in oil and gas, resulting in 4X throughput improvement of the 3D X-ray microscope. Alternatively, OptiRecon can also be used to significantly enhance image quality at similar throughput as that of FDK reconstruction.

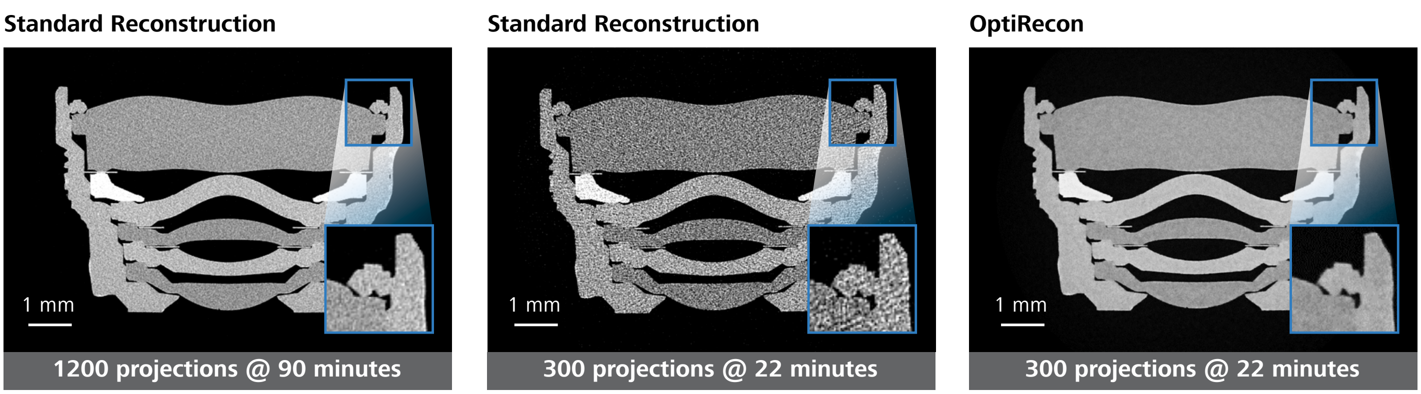


Figure 9 *Smartphone camera module images from ZEISS Xradia Versa 3D X-ray microscope. ZEISS OptiRecon reconstruction demonstrates 4X throughput improvement with excellent image quality.*

ZEISS DeepRecon is a novel reconstruction technology that is based on deep learning and is targeted to improve throughput or image quality of ZEISS 3D X-ray microscopes for repetitive workflow applications. DeepRecon can provide up to 10X throughput improvement at similar or better image quality compared to standard FDK reconstruction. This technology uniquely harvests the hidden dependencies in big data available from ZEISS X-ray microscopes and provides significant artificial intelligence-driven throughput or image quality improvement. The network models can be created per sample class and can be tailored to precisely fit customer applications.

The algorithms discussed here could be further extended to include multiscale analyses (reducing the noise level of high-resolution interior scanning) or innovative new noise reduction algorithms with the potential of removing noise while neither degrading edges nor removing small features. They could even be extended to include full spectral inversion, where rays are modelled as a range of energies, opening the door to both greater chemical sensitivity and the removal of the impact of the beam hardening artifacts associated with highly attenuating materials. Such improvements will extend the applicability of these reconstruction technologies to further extend the performance of ZEISS 3D X-ray microscopes.

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Carl Zeiss Microscopy GmbH
07745 Jena, Germany
microscopy@zeiss.com
www.zeiss.com/xray