

Advancing X-ray Tomography using AI (TomoGAN)

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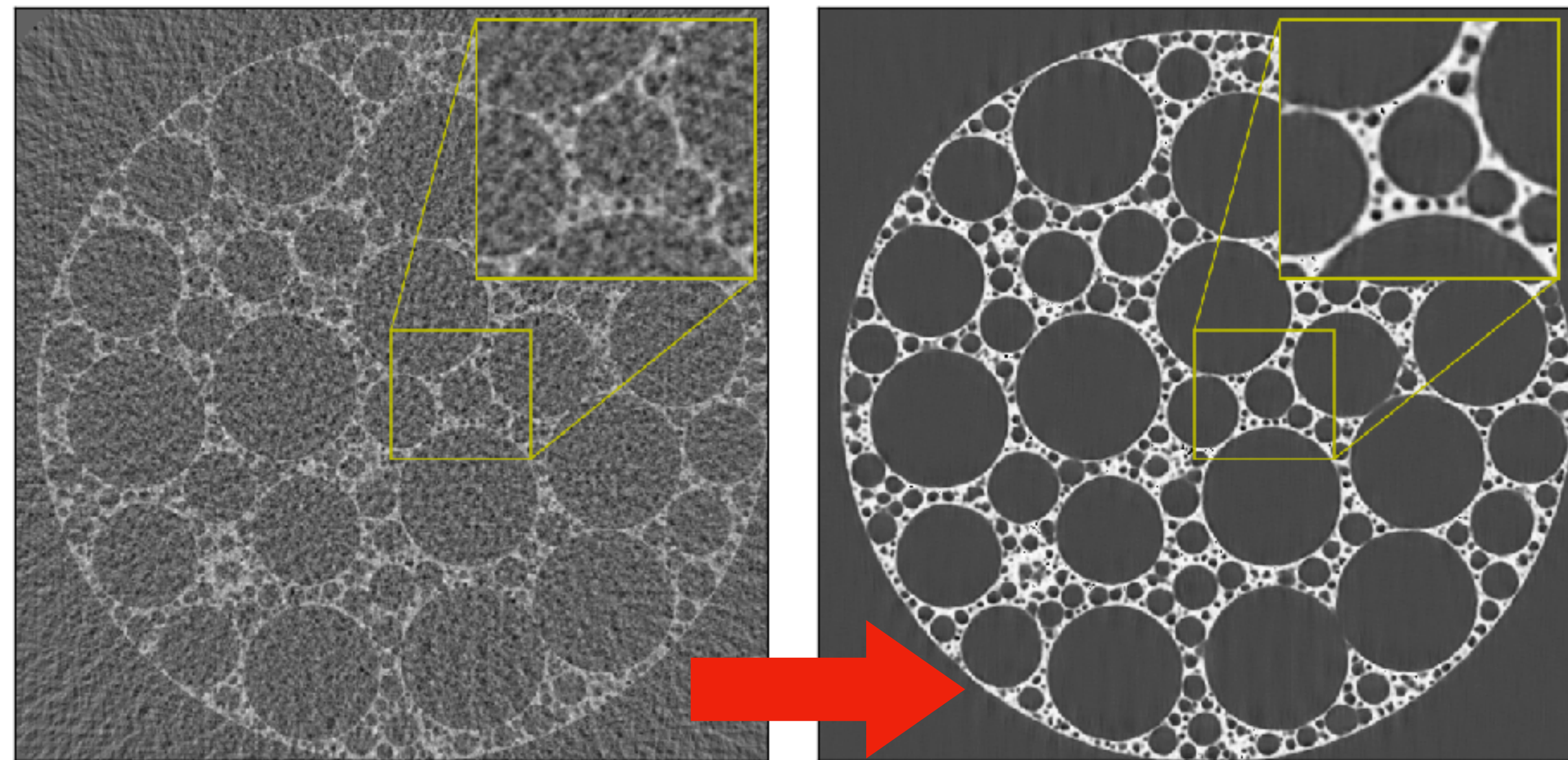
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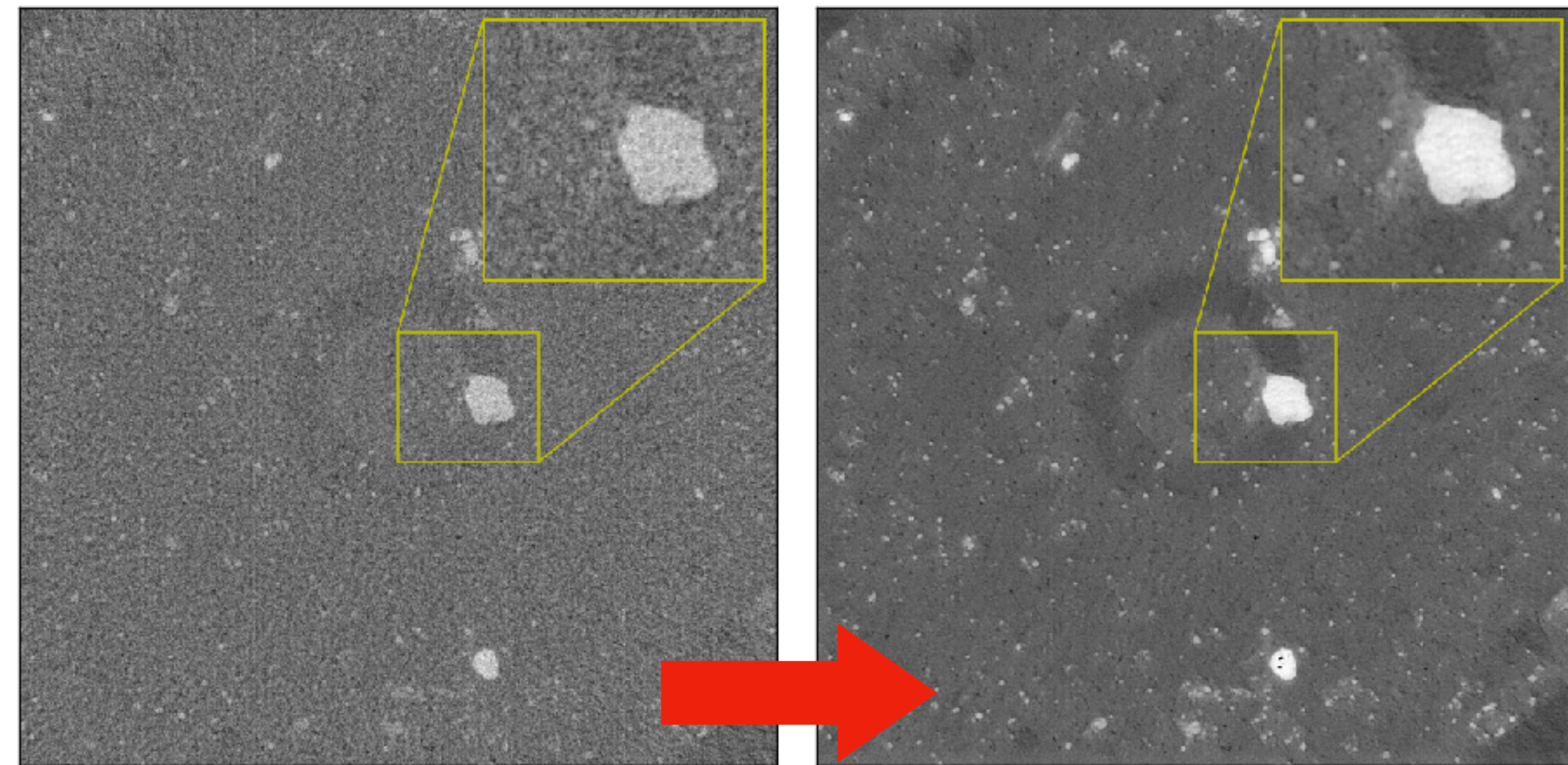
APS Internal AI/ML Workshop at Argonne National Laboratory

Motivation

- (1) lower X-ray dosage for sensitive sample like bio-sample;
- (2) faster experiment to capture dynamic features, like in fast chemical reaction processes;
- (3) smaller dataset and less computation for [near] realtime tomography imaging.



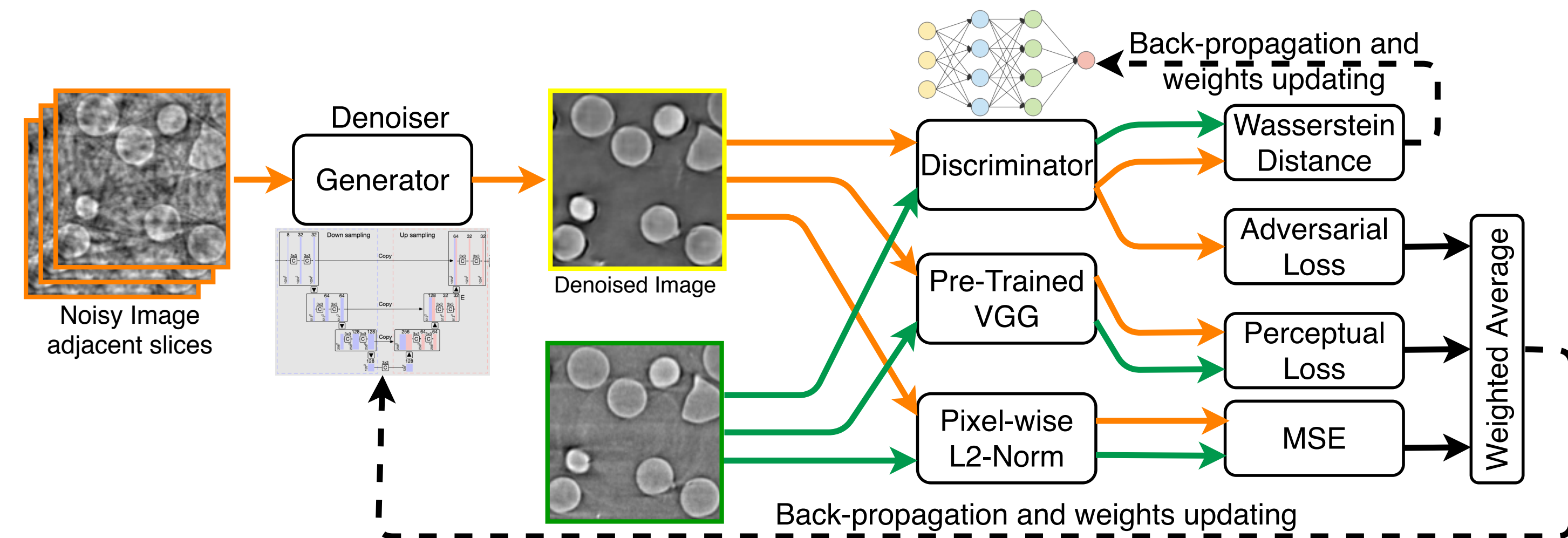
On the left, the results of conventional reconstruction, which are highly noisy. On the right, those same results after denoising with TomoGAN.



Model is trained with one shale sample imaged at APS and tested with **another** shale sample imaged at Swiss Light Source (SLS).

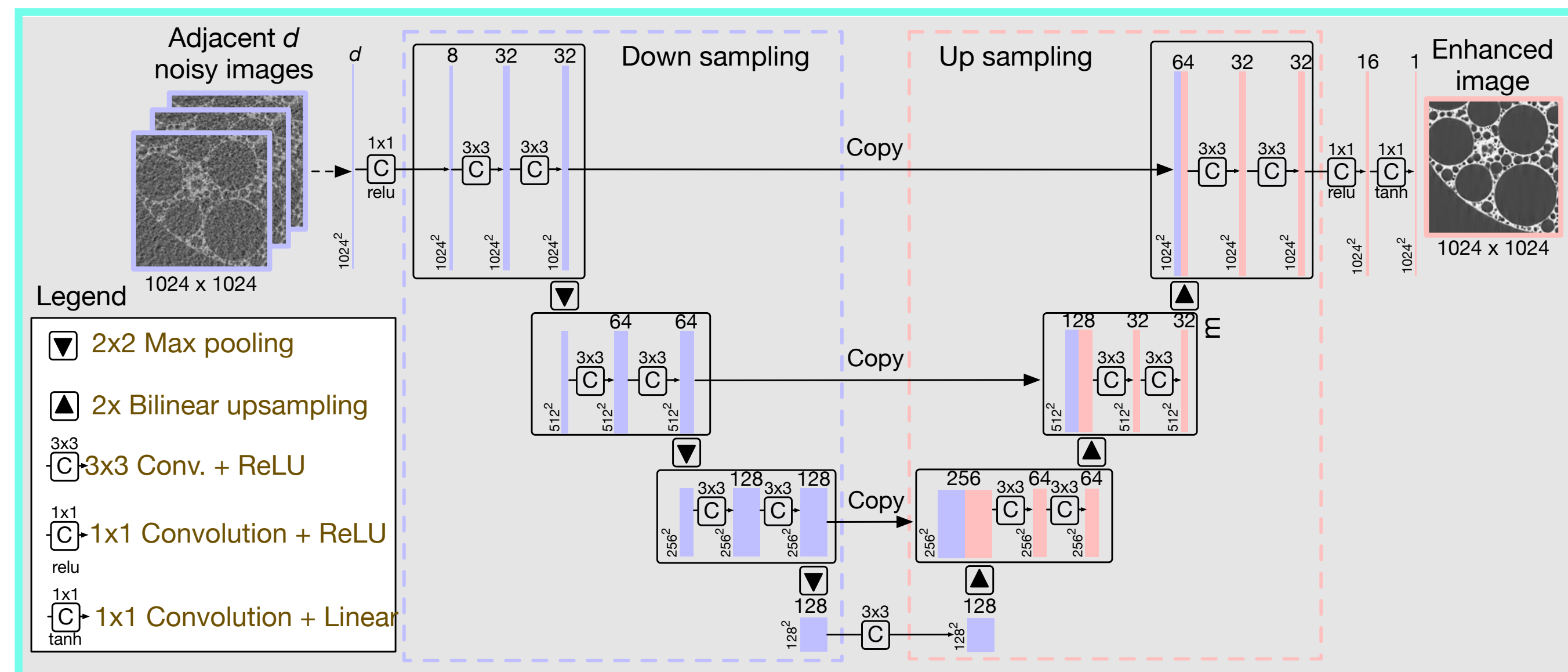
Method

A generative adversarial network (GAN) is a class of machine learning systems in which two neural networks, generator (G) and discriminator (D), contest with each other in a game (in the sense of game theory, often but not always in the form of a zero-sum game).



In our model, the discriminator's job remains unchanged, but the generator is tasked not only with fooling (indistinguishable) the discriminator but also with being near the ground truth output in an L2 sense.

The discriminator works as a helper to train the generator that we need to denoise images.



Our Generator Architecture

Training

Discriminator Wasserstein GAN [1] + gradient penalty [2]

$$L(\theta_D) = \frac{1}{m} \sum_{i=1}^m \left[D(G(I_{LD}^i)) - D(I_{ND}^i) \right] + \lambda_D \frac{1}{m} \sum_{i=1}^m \left[\left(\left\| \nabla_{\bar{I}} D(\bar{I}^i) \right\|_2 - 1 \right)^2 \right],$$

Generator Weighted average of Adversarial loss, Perceptual loss, and Pixel-wise MSE

$$\ell^G = \lambda_g \ell_{adv} + \lambda_p \ell_{mse} + \lambda_v \ell_{vgg}$$

$$\ell_{adv}(\theta_G) = -\frac{1}{m} \sum_{i=1}^m D(G(I_{LD}^i))$$

$$\ell_{vgg} = \sum_{i=1}^{W_f} \sum_{j=1}^{H_f} \left(V_{\theta_{vgg}}(I^{ND})_{i,j} - V_{\theta_{vgg}}(G_{\theta_G}(I^{LD}))_{i,j} \right)^2$$

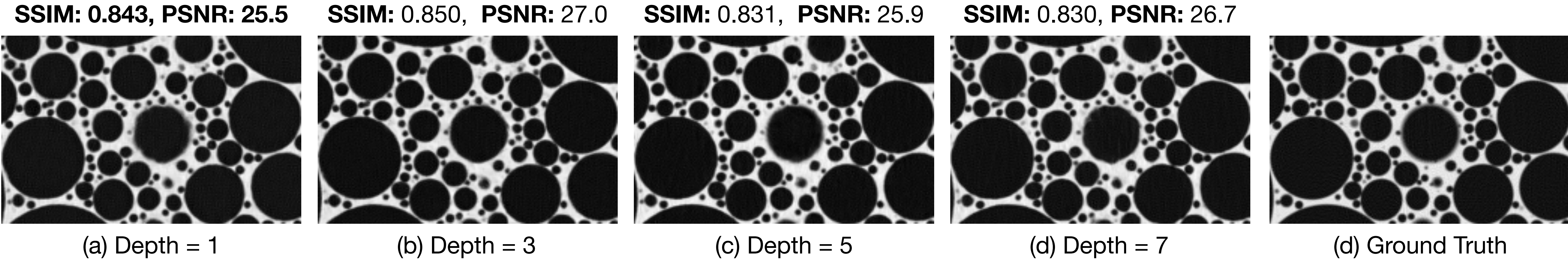
$$\ell_{mse} = \sum_{c=1}^W \sum_{r=1}^H \left(I_{c,r}^{ND} - G_{\theta_G}(I^{LD})_{c,r} \right)^2$$

[1] Wasserstein GAN. M. Arjovsky, S. Chintala, L. Bottou. arXiv:1701.07875

[2] Improved Training of Wasserstein GANs. I. Gulrajani, F. Ahmed, M. Arjovsky, V. Dumoulin, A. Courville. arXiv:1704.00028

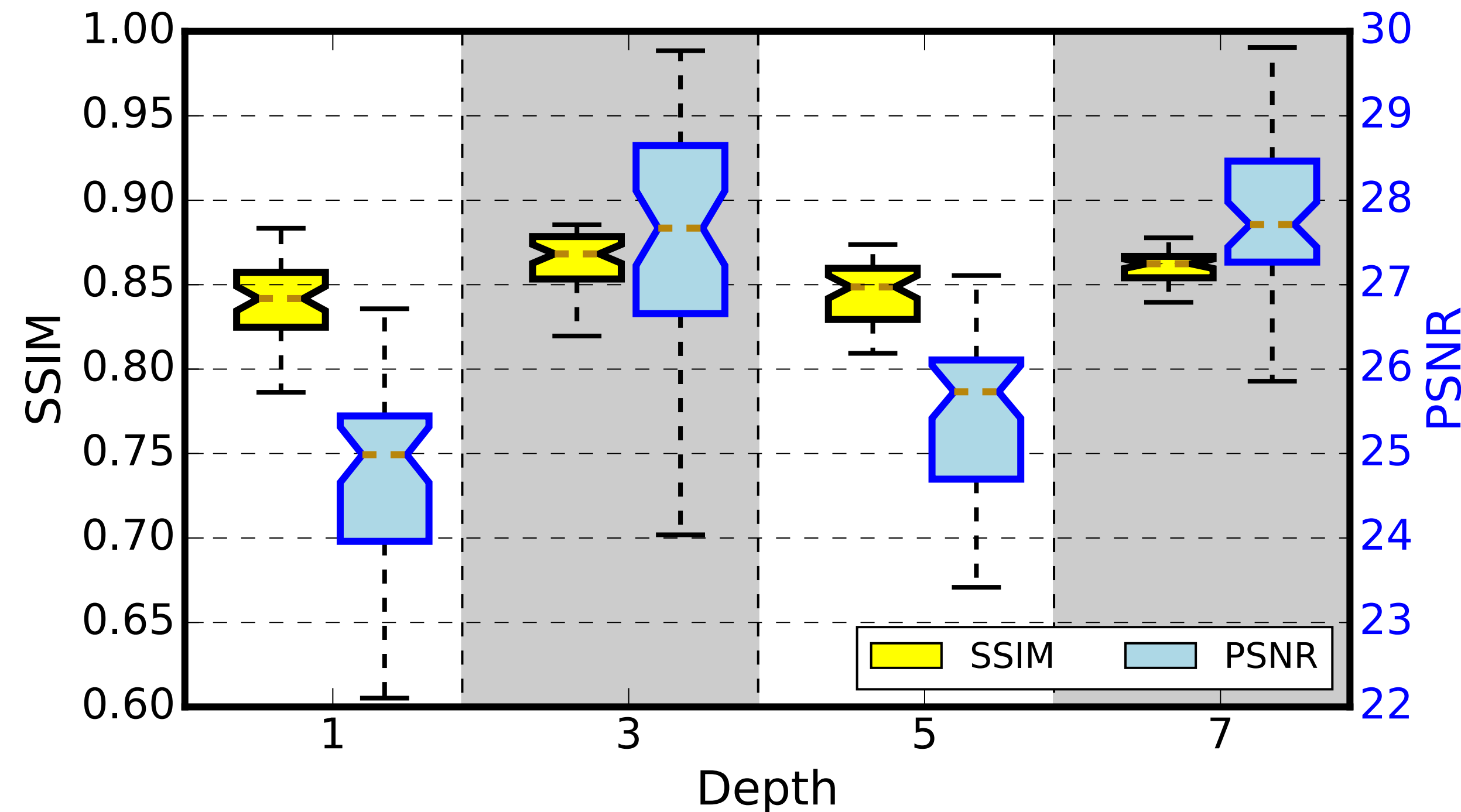
Results - Adjacent slices

Effectiveness of using adjacent slices in image enhancement



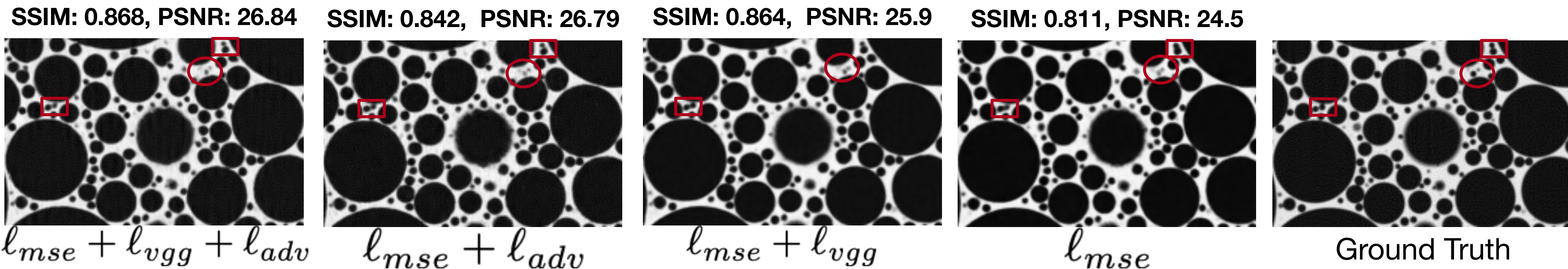
The input depth d has big influence on mode performance, and that $d=3$ gets the best quality, especially when the original feature edge is not sharp (e.g., the center circle).

We note that the best depth d depends on dataset characteristics such as feature resolution. $d=3$ may not be the best for other datasets where feature sizes change slowly across slices.



Results - Loss

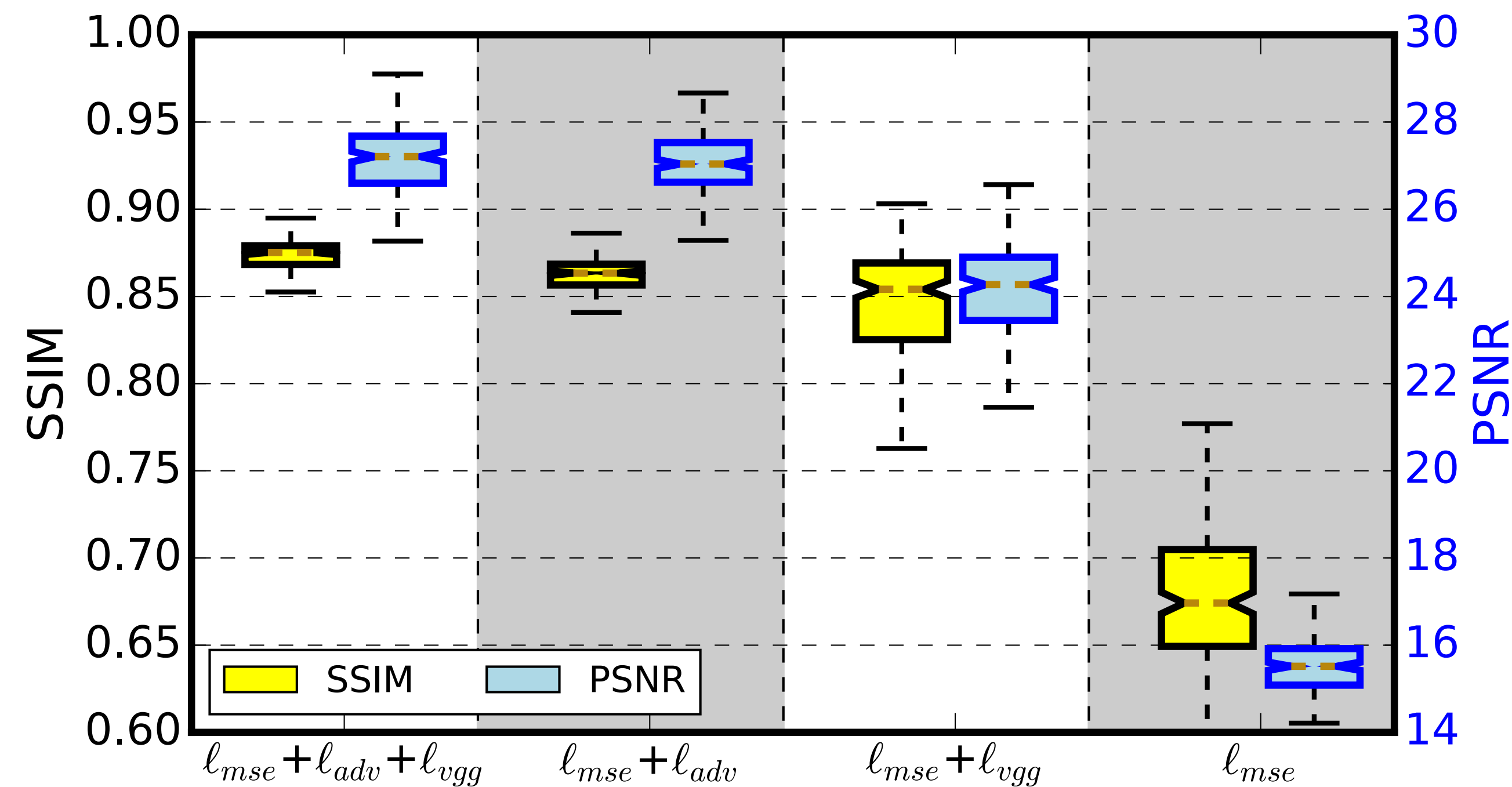
Importance of the various loss terms



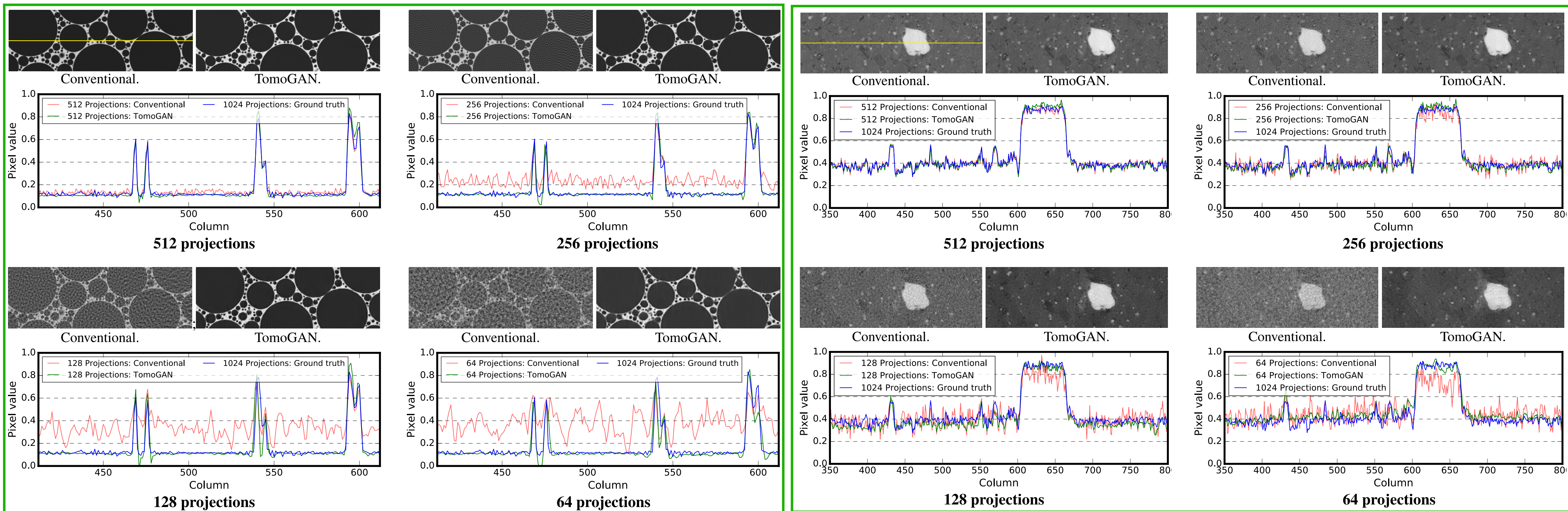
MSE is necessary to enforce correctness of low-frequency structures but MSE alone is not enough.

The adversarial and perceptual loss terms each provide considerable improvements when used in isolation.

The two together are only slightly better than adversarial loss alone.

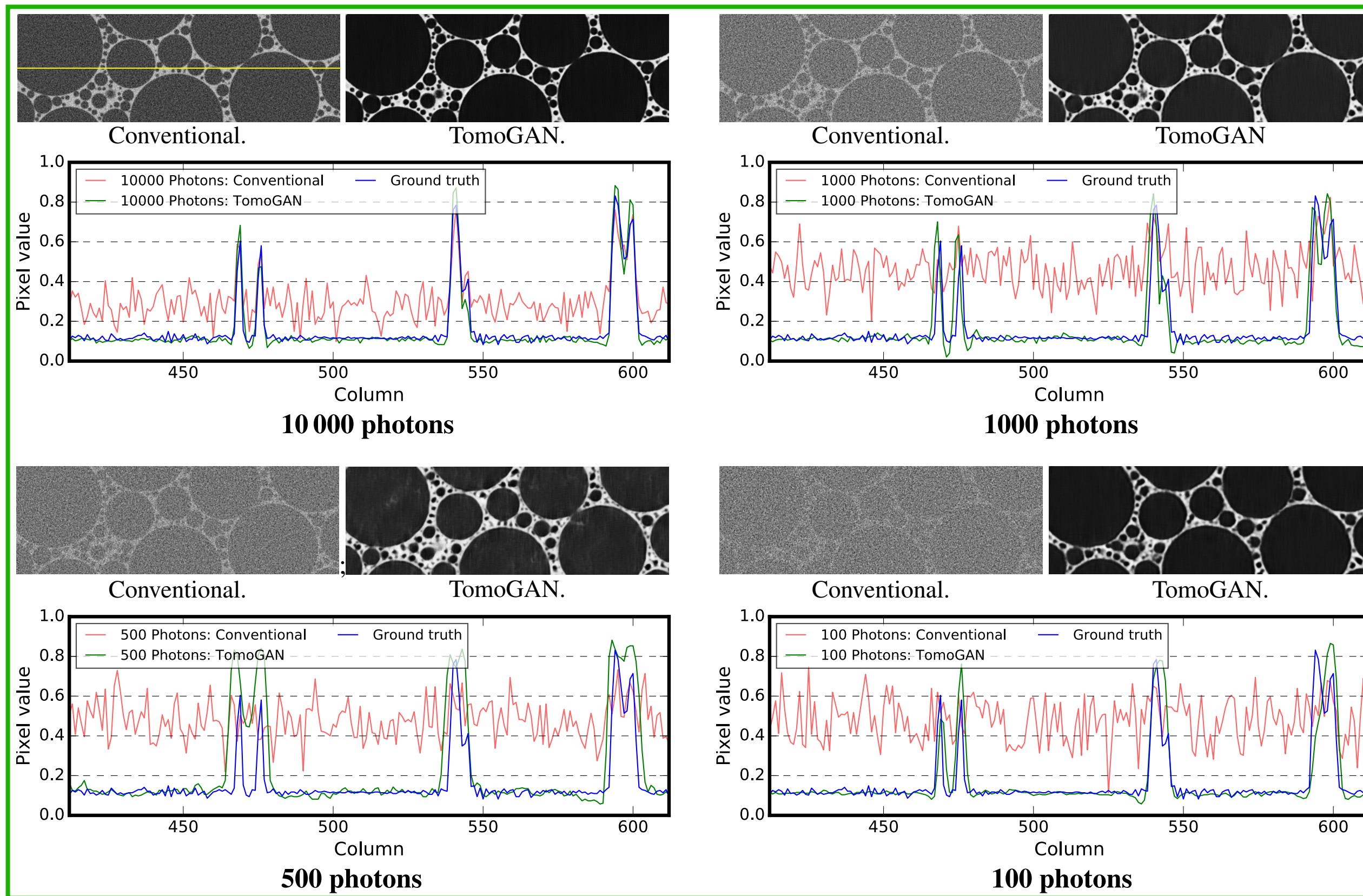


Results - Sparse views

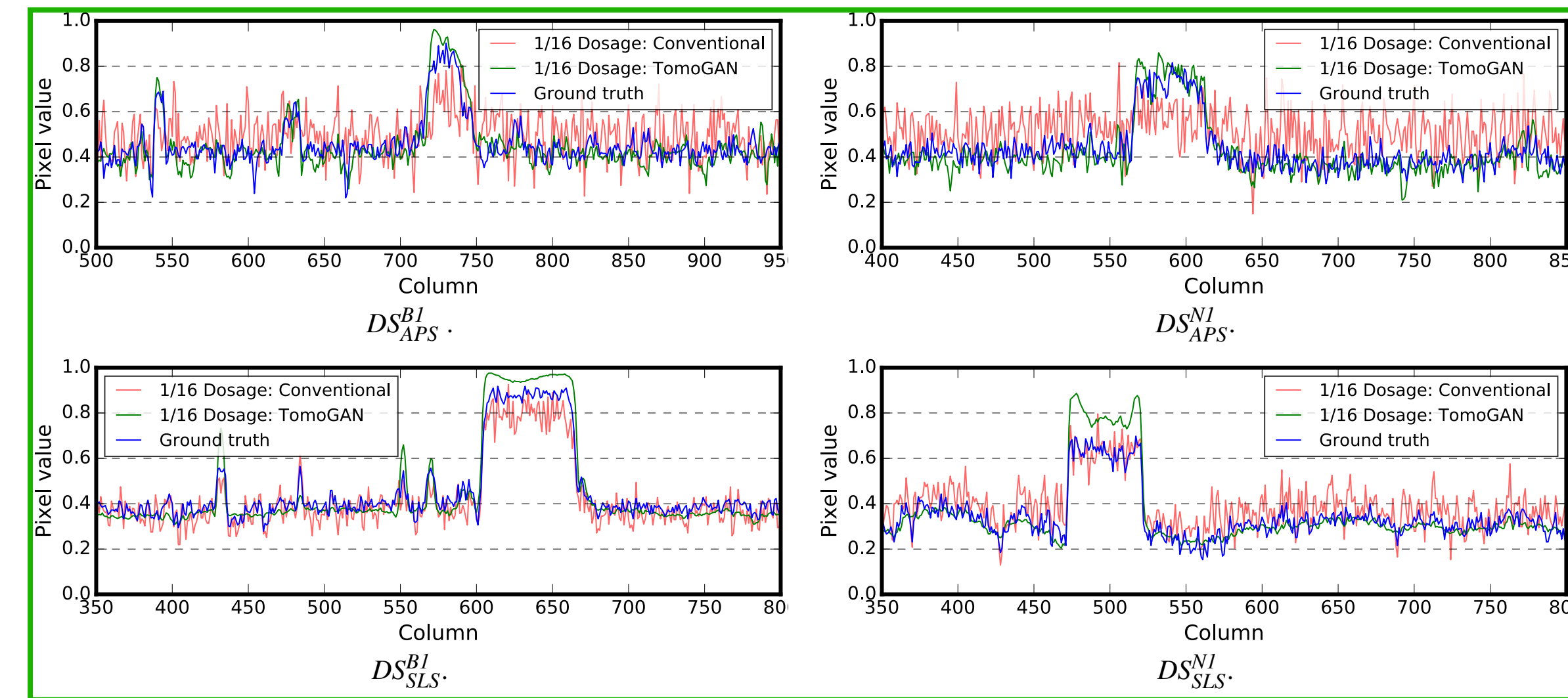


Conventional vs. TomoGAN-enhanced reconstructions of simulated (left) data and shale (right), subsampled to (512, 256, 128, 64) projections. In each group of three elements, the two images show conventional and TomoGAN reconstructions, while the plot shows conventional, TomoGAN, and ground truth values for the 200 pixels on the horizontal line in the top left image.

Results - Short exposure time



Pixel values of an arbitrarily chosen feature in each of the four experimental datasets, with projections generated by using 1/16 of the normal exposure time. Feature shapes are different for each dataset.



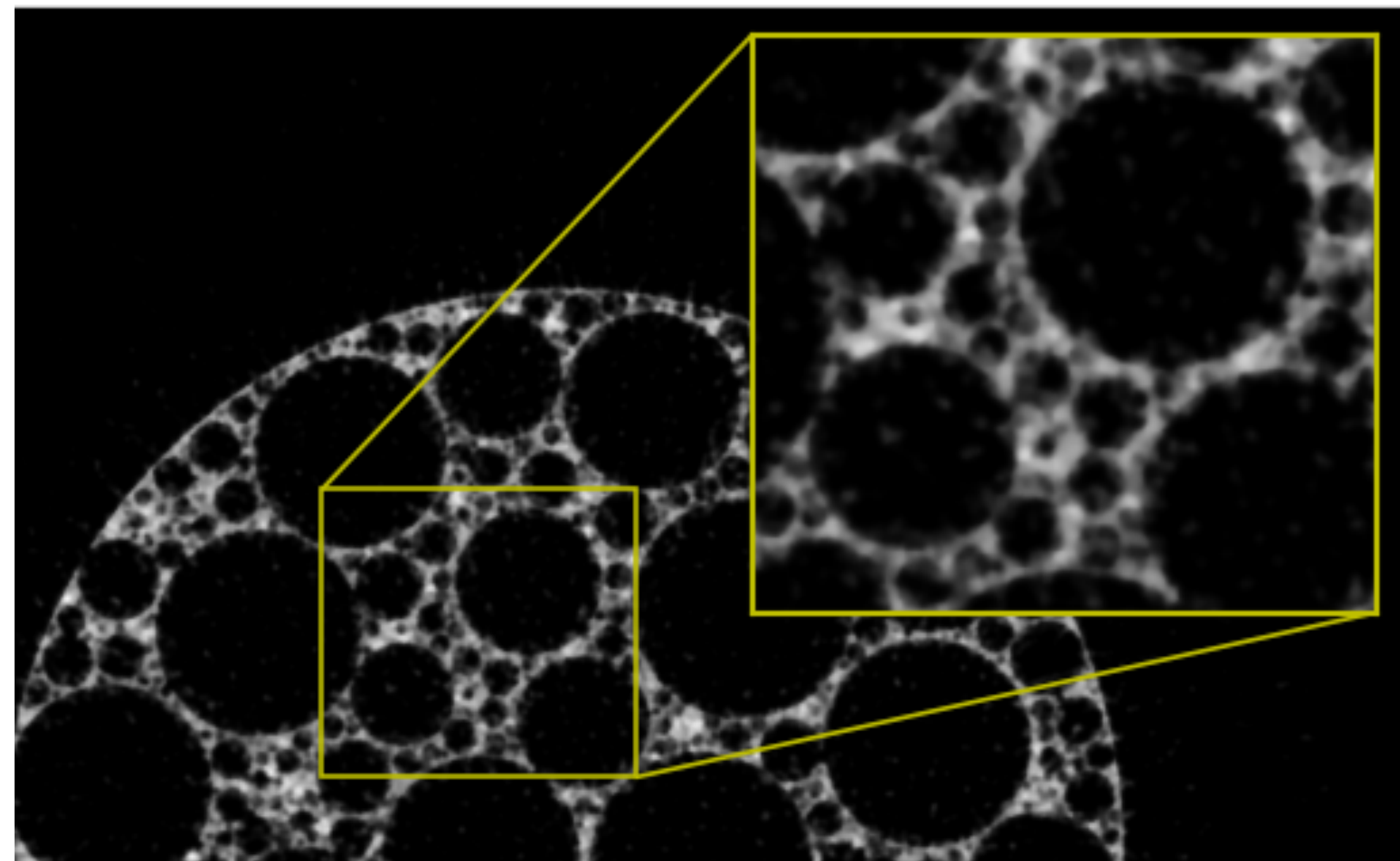
Conventional vs. TomoGAN-enhanced reconstructions of simulated data with intensity limited to 10000, 1000, 500, 100 photons per pixel.

Computational superiority

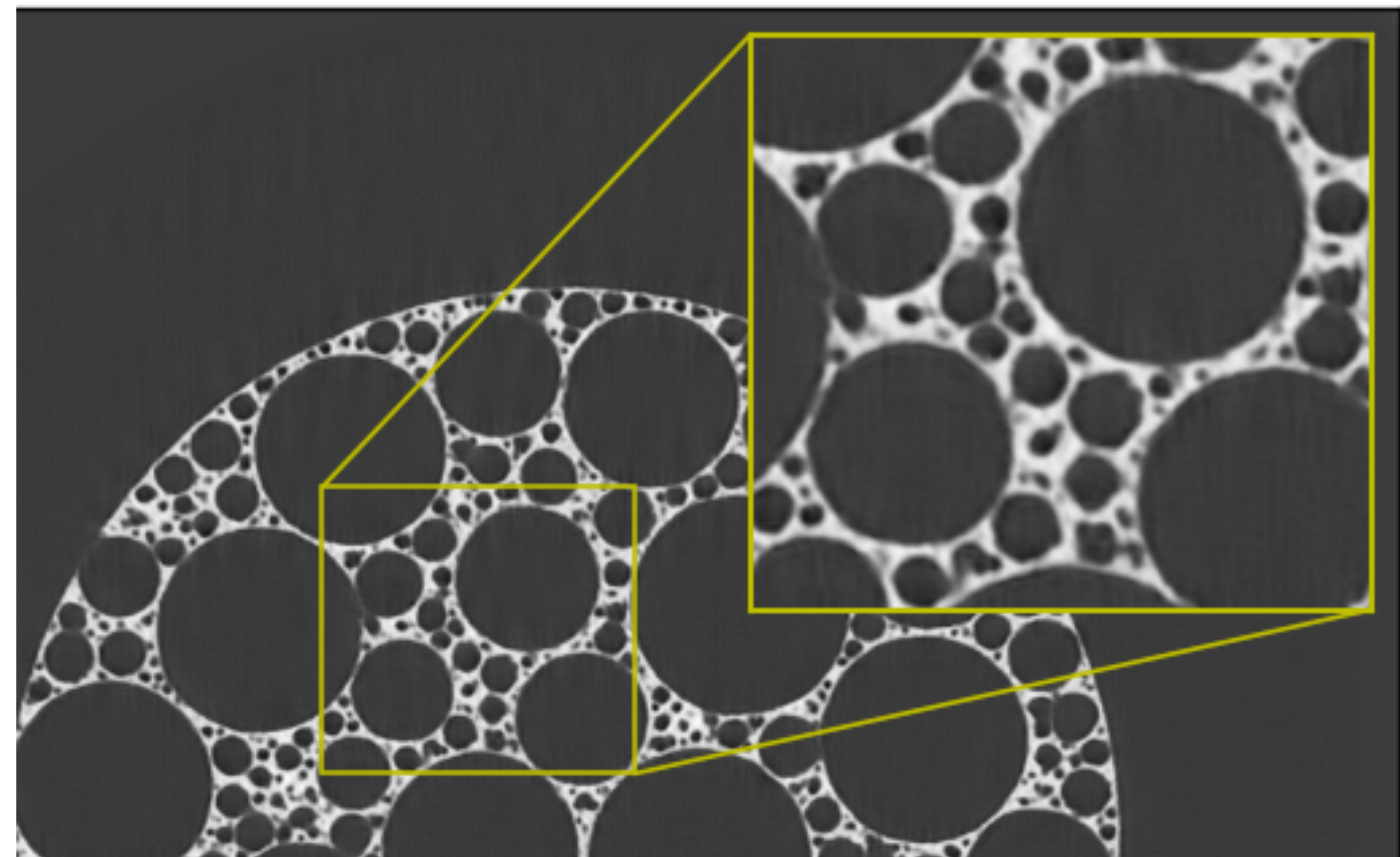
The filtered back projection (FBP) algorithm takes 40 ms to reconstruct one image (using TomoPy) and TomoGAN takes 30 ms to enhance the reconstruction, totals **70 ms** per image.

In contrast, the SIRT based solution (using TomoPy) takes **550 ms** (400 iterations), i.e., 8x faster. Times are measured using one Tesla V100 graphic card.

Moreover, iterative reconstruction does not provide better image quality than does our method.



SIRT + total variation postprocess.

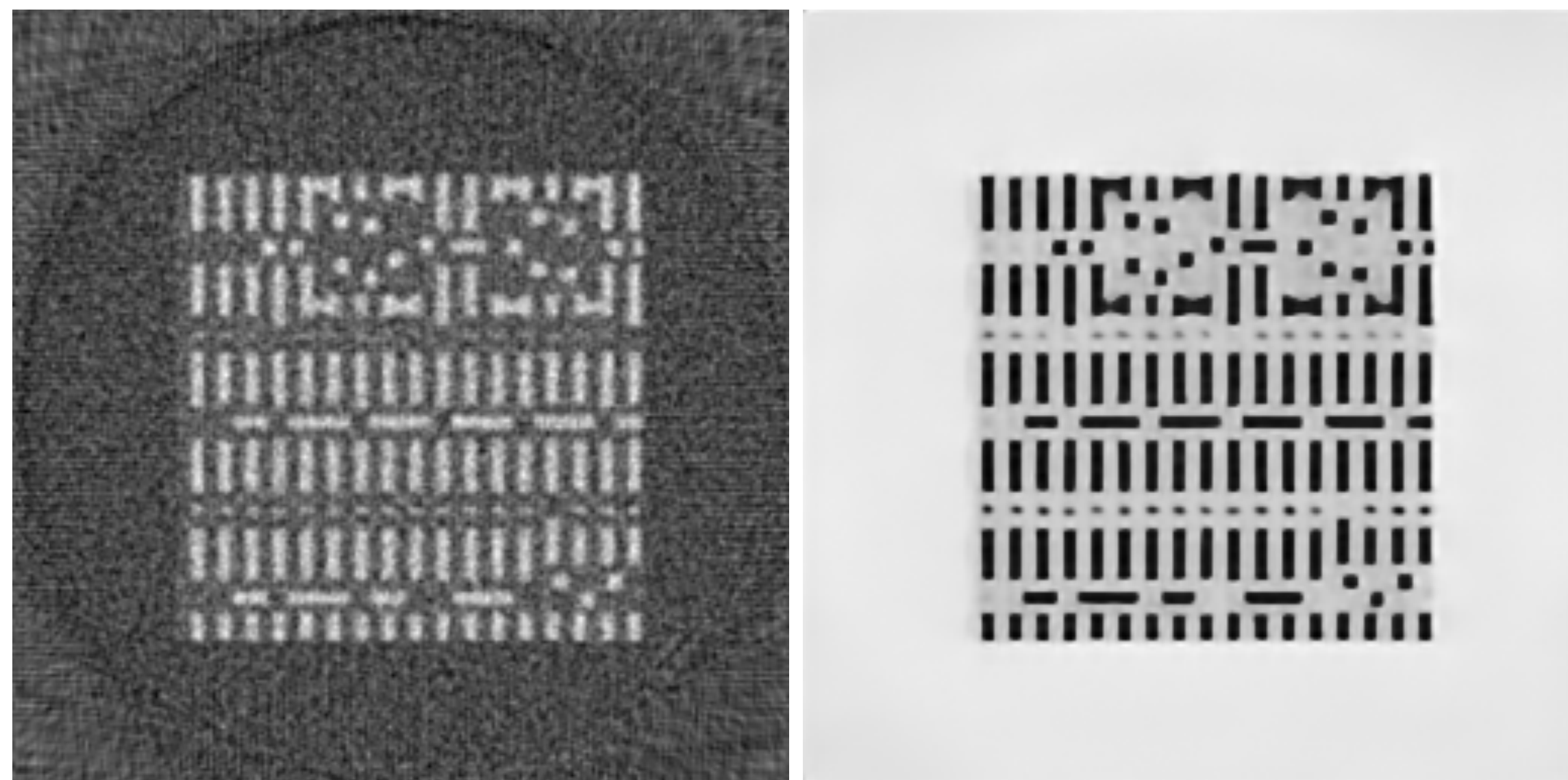


Filtered back projection + TomoGAN post-process.

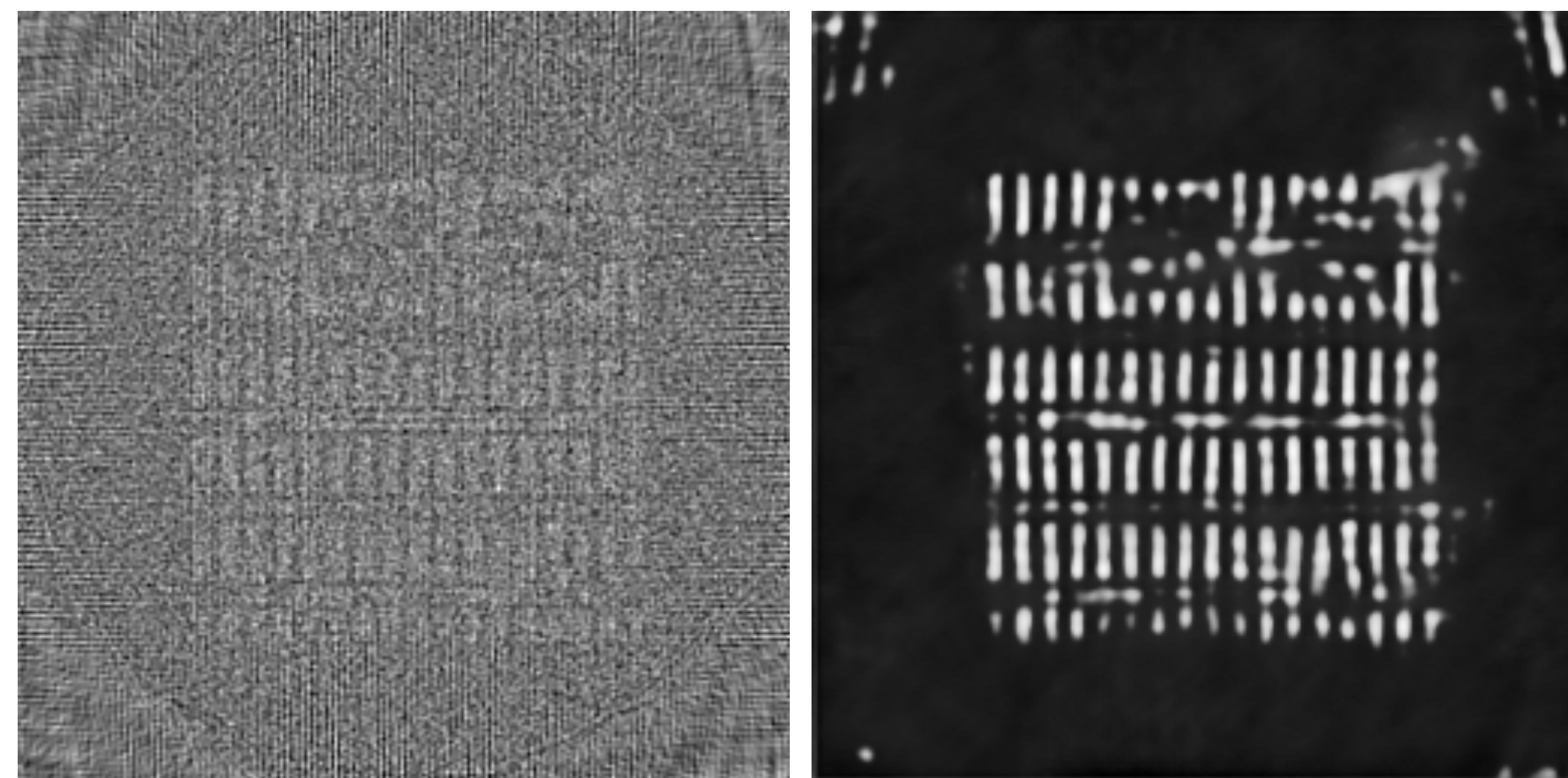
TomoGAN - Extend use case - ADMM

It has been applied to the joint ptycho-tomography problem for reconstructing the complex refractive index of a 3D object.

- There is a ptychography process to reconstruct projections needed for tomography. but it is very time consuming to image the sample (month).
- Less datapoint results in noisier ptychography reconstruction and worse tomography images.
- TomoGAN here was used to enhance tomography images with less data points need to collect, i.e., faster experiment.

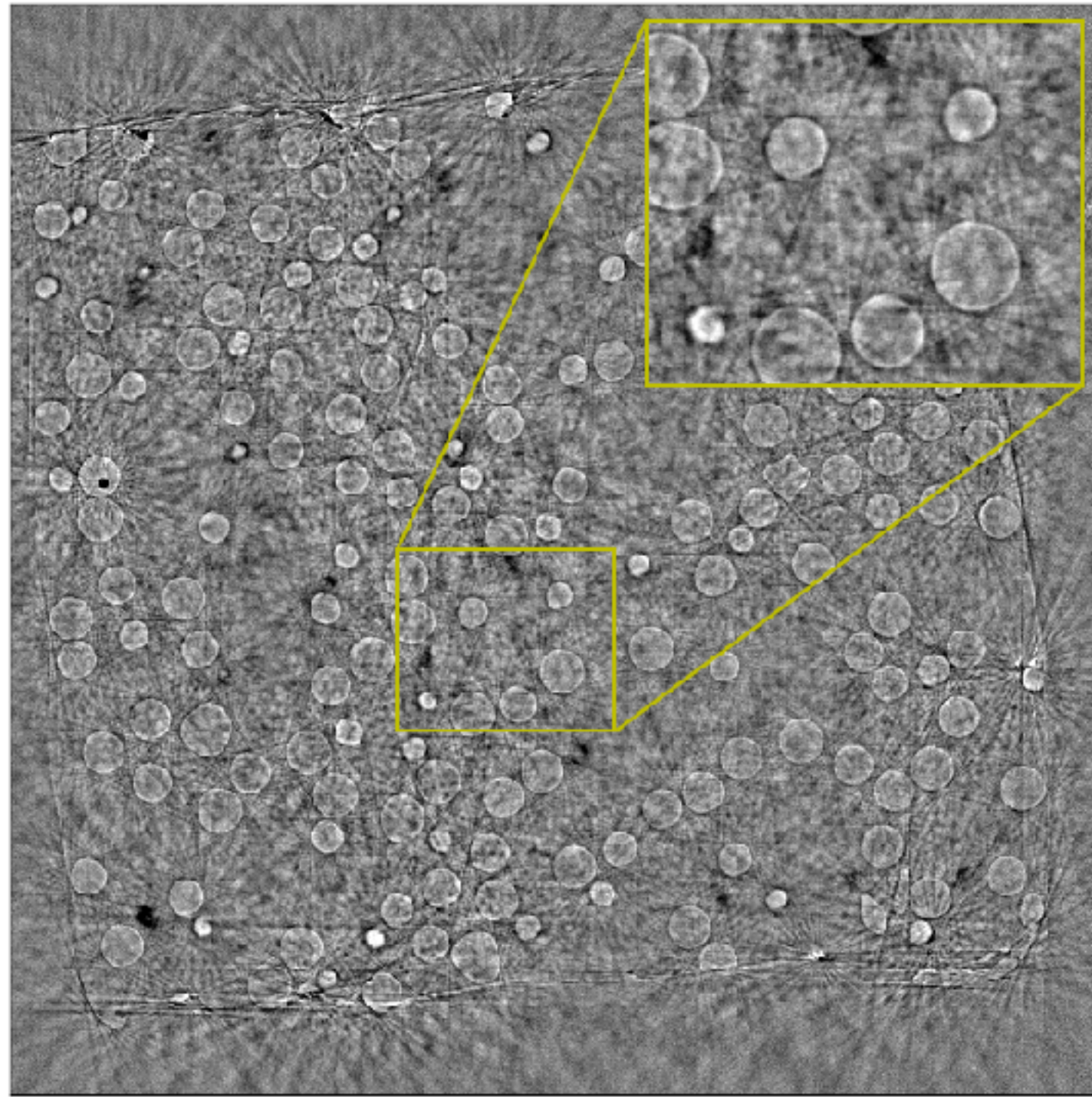


Delta, 0.003

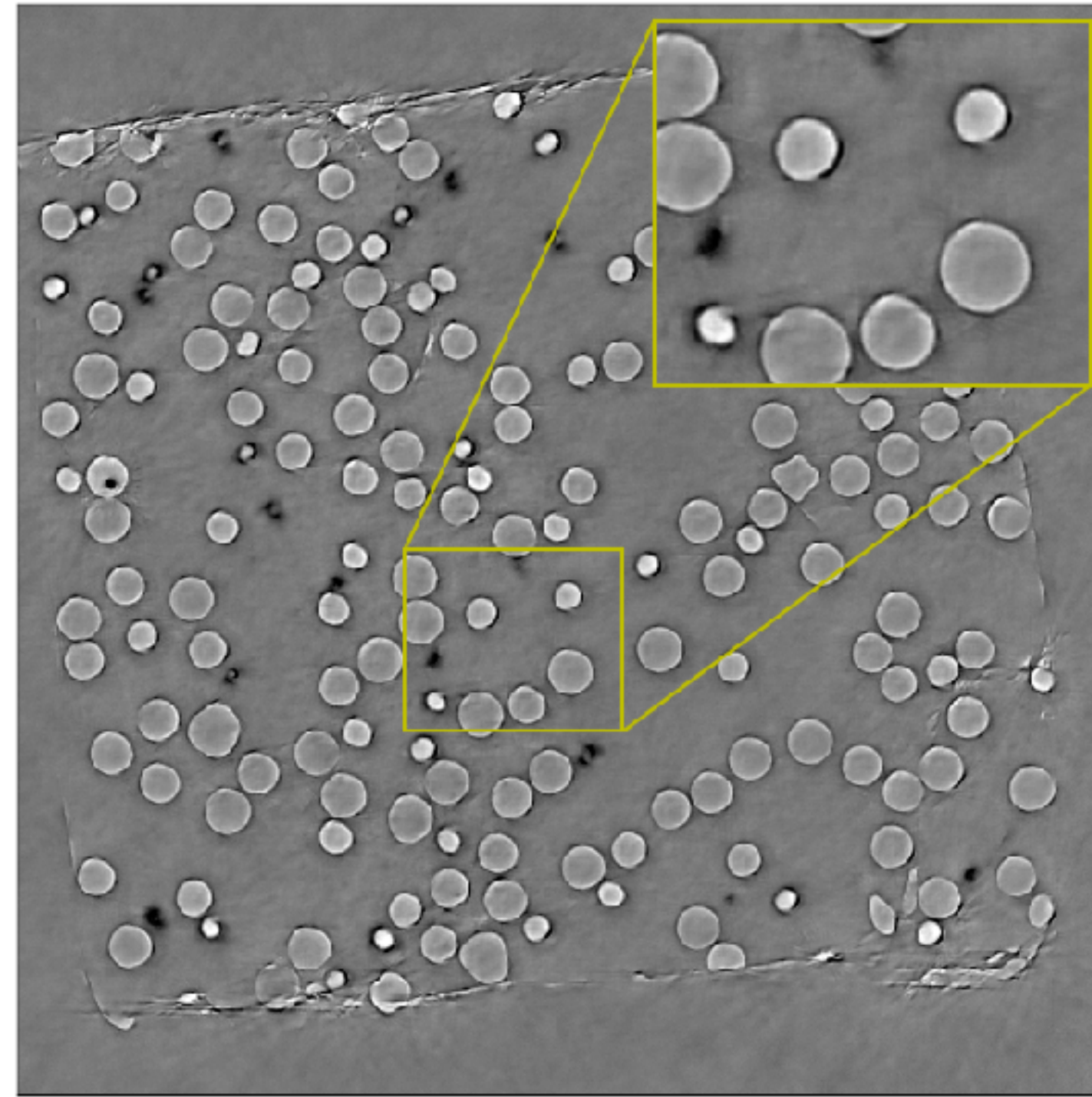


Beta, 0.03

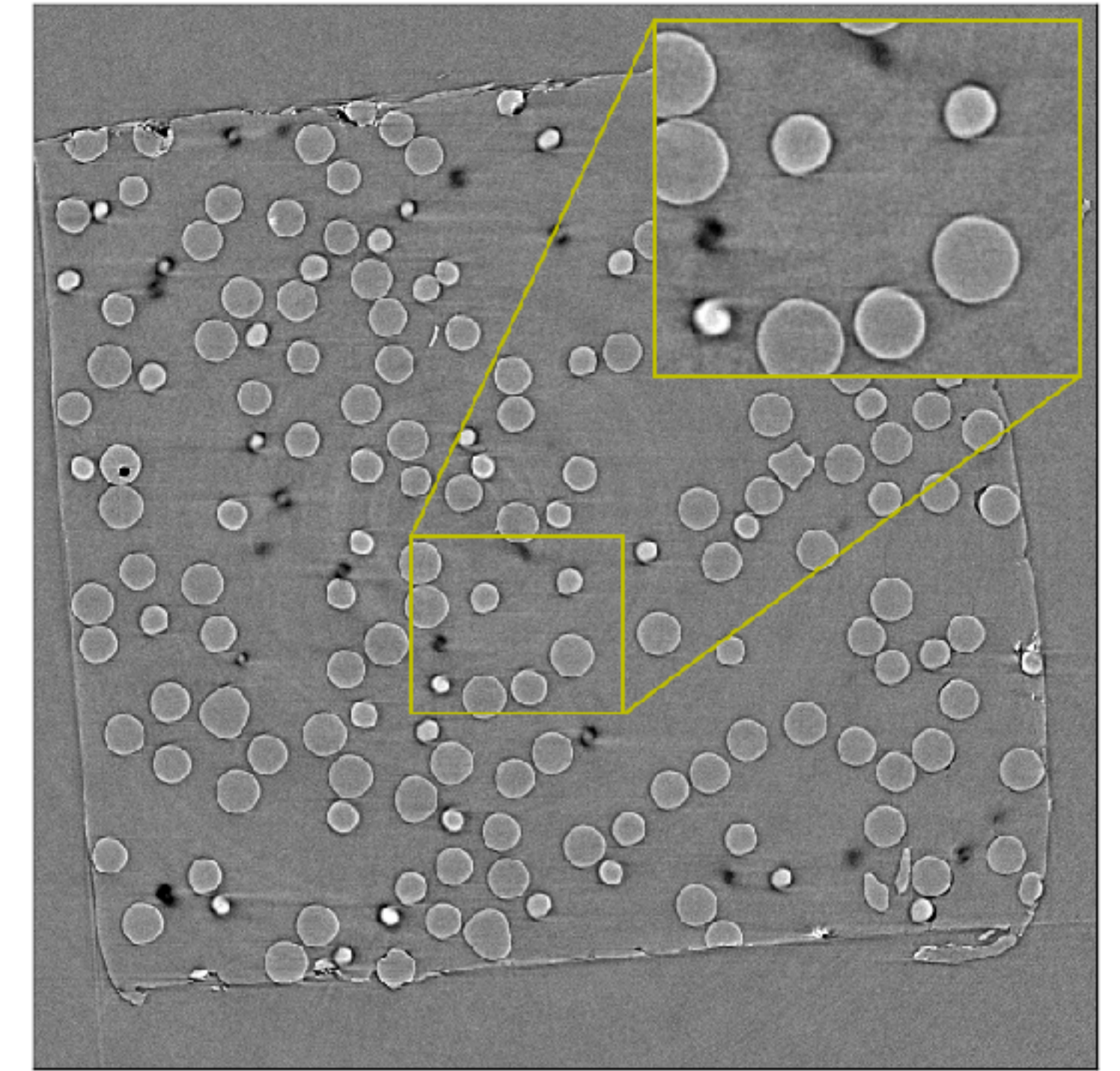
TomoGAN - Extend use case - Streaming tomography



with data up to 462s (480 projections), before enhancement;



with the same data, after enhancement;

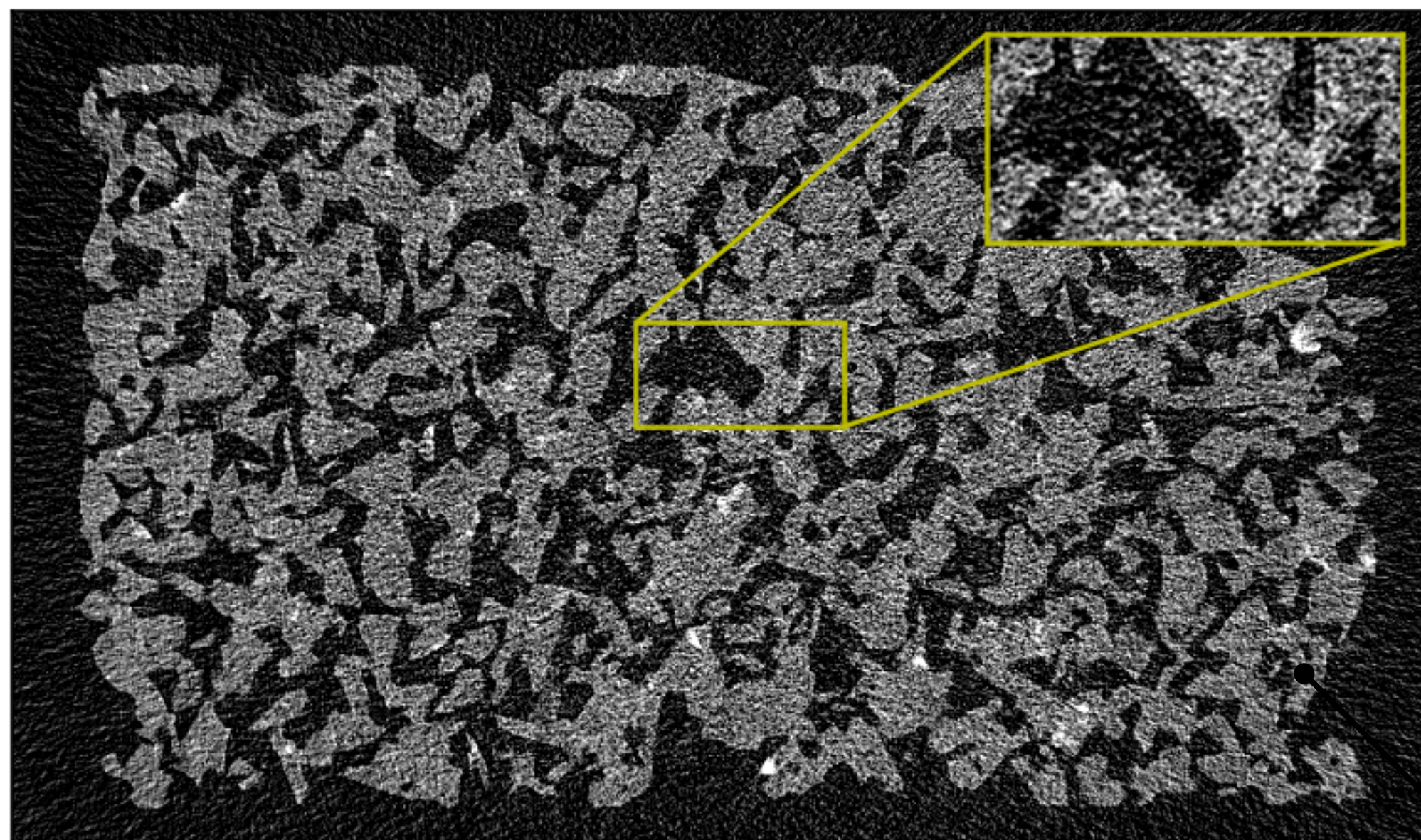


with data up to 1433s (1504 projections), before enhancement.

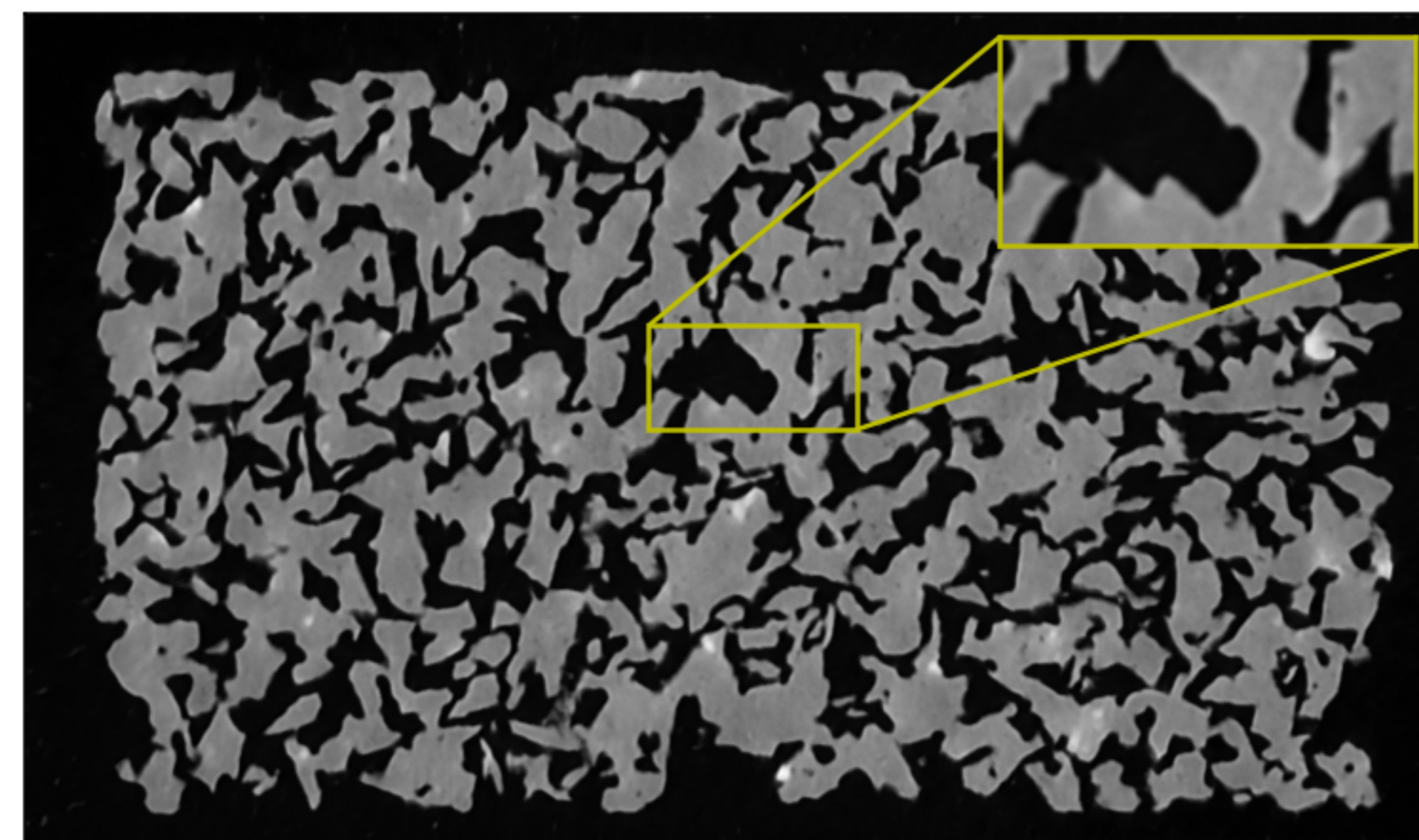
Three times faster turnaround time for domain scientists. A.K.A., three times increased throughput for the light source and computing facility.

Important as enablers of experiment steering, where quick turnaround is required.

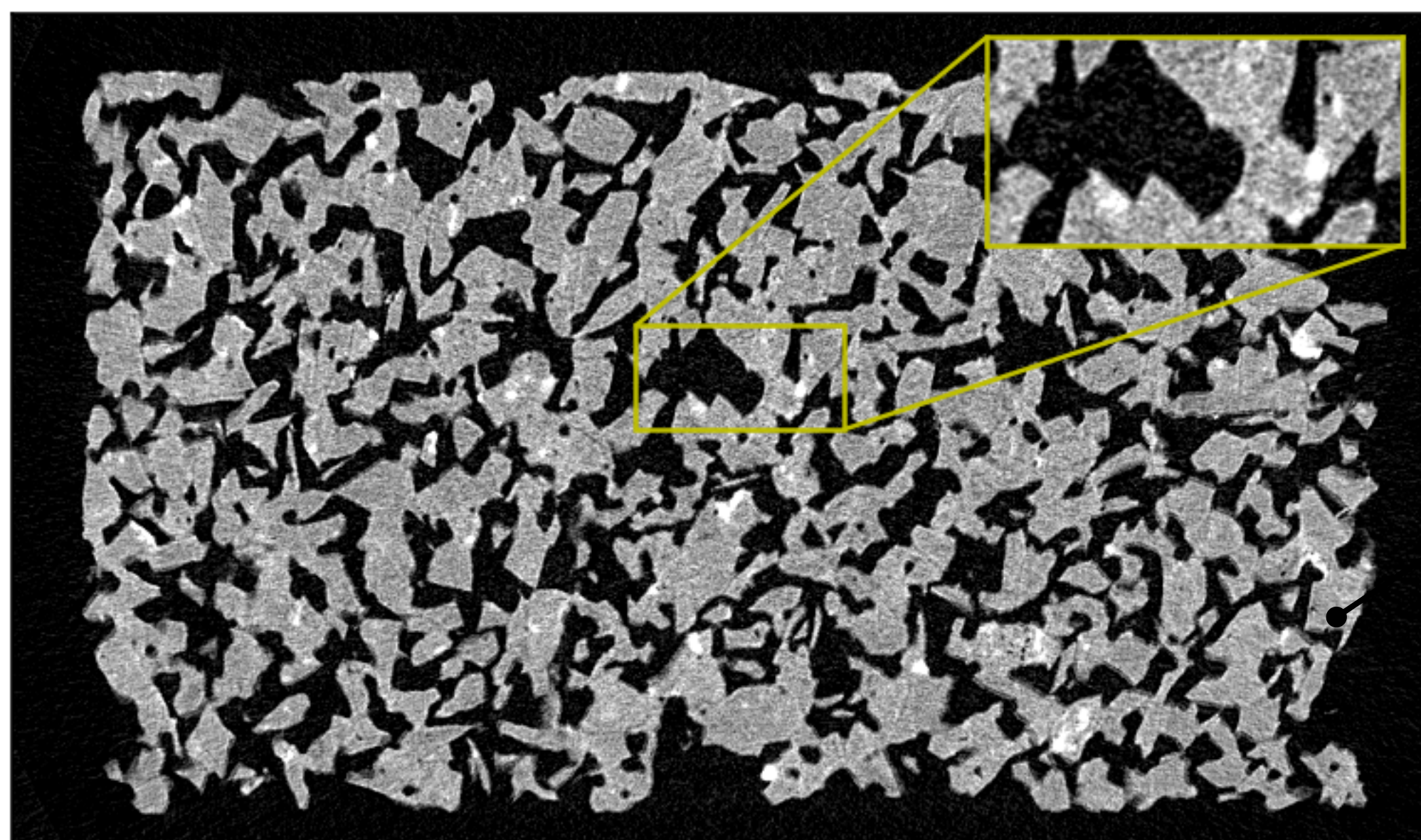
TomoGAN - Extend use case - 3M with alignment issue



180°, large step size, no frame avg. (45 minutes)



TomoGAN enhanced (**Model Output**)

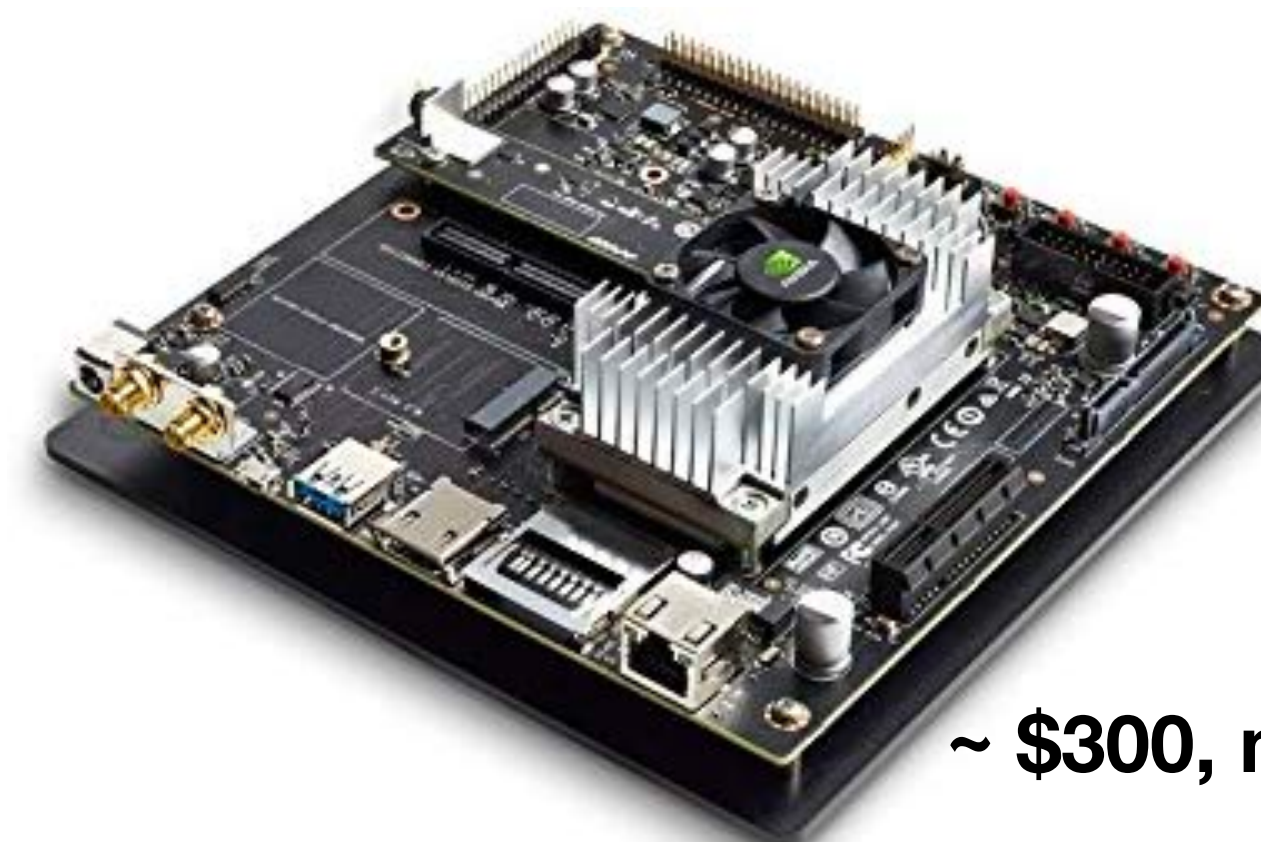
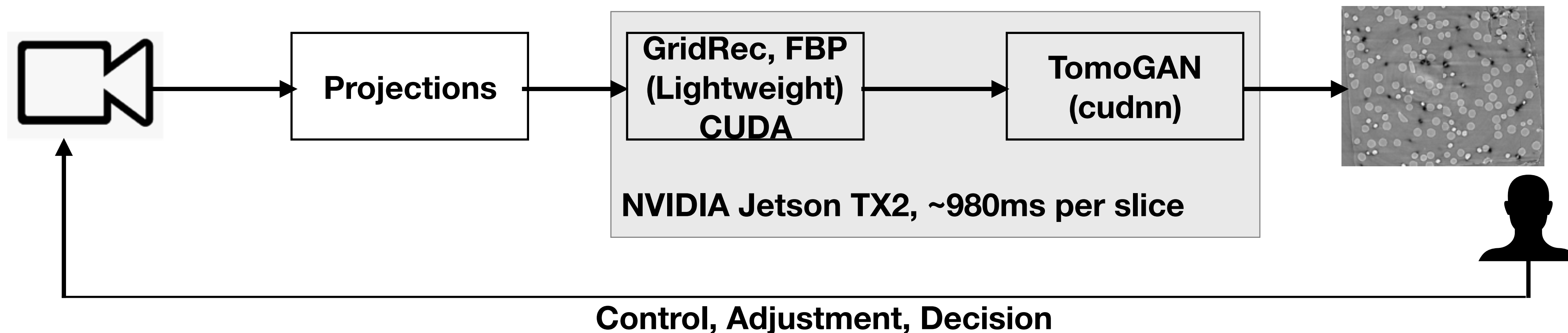


Best attempt (4 hours)

- ❑ (X,y) pair comes from two experiments;
- ❑ Impossible to perfectly aligned, like rotated a bit;
- ❑ Not a big problem for scientists but a big problem to ℓ_{mse}
- ❑ Tune the weight of ℓ_{mse} , ℓ_{vgg} and ℓ_{adv} works.

TomoGAN - Tomography at Edge

- Both Tomography and DL are computation intensive but both GPU typically helps a lot;
- A GPU friendly tomography for a rough (noisy) results plus DL based enhancement;
- Fusion of analytical (human knowledge) and deep learning (data driven).



~ \$300, maximum 15 watts

Make it usable

Hack and Play

open source implementation, better to have a GPU for training

```
Git clone git@github.com:ramsesproject/TomoGAN.git

python ./train.py -ld noise-img.hdf5 -nd clean-img.hdf5

python ./infer.py -ld ld-prod.hdf5
```

X as a Service

DLHub

Data and Learning Hub for Science



B. Blaiszik. arXiv:1811.11213

```
from dlhub_sdk.client import DLHubClient
dlhub = DLHubClient()

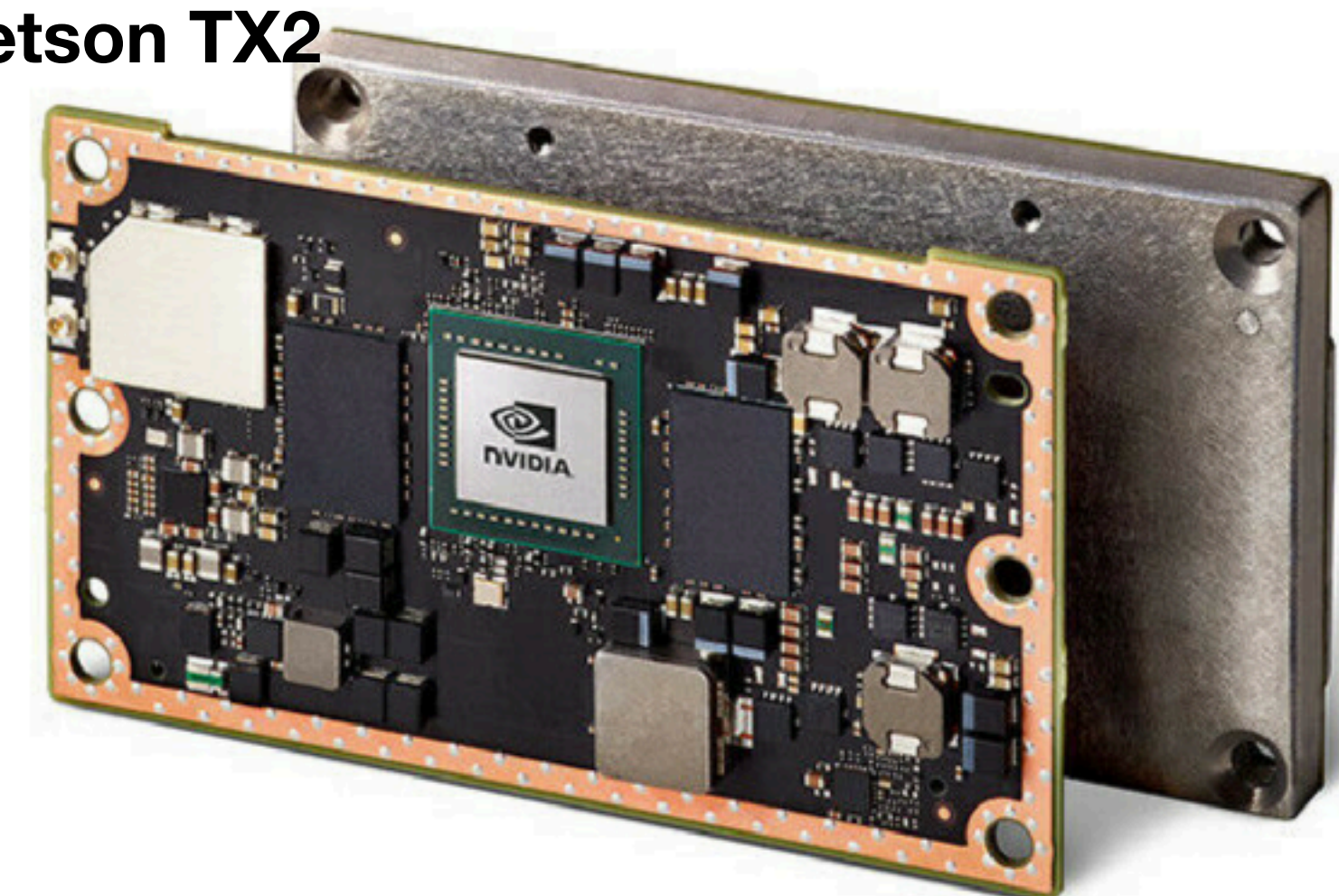
model = dlhub.get_id_by_name("tomoGAN")
data = h5py.File("tomo_ld.hdf5", "r")["ld_img"]
pred = dl.run(model, data)
```

Plug and Play Abeykoon et al.

Edge TPU

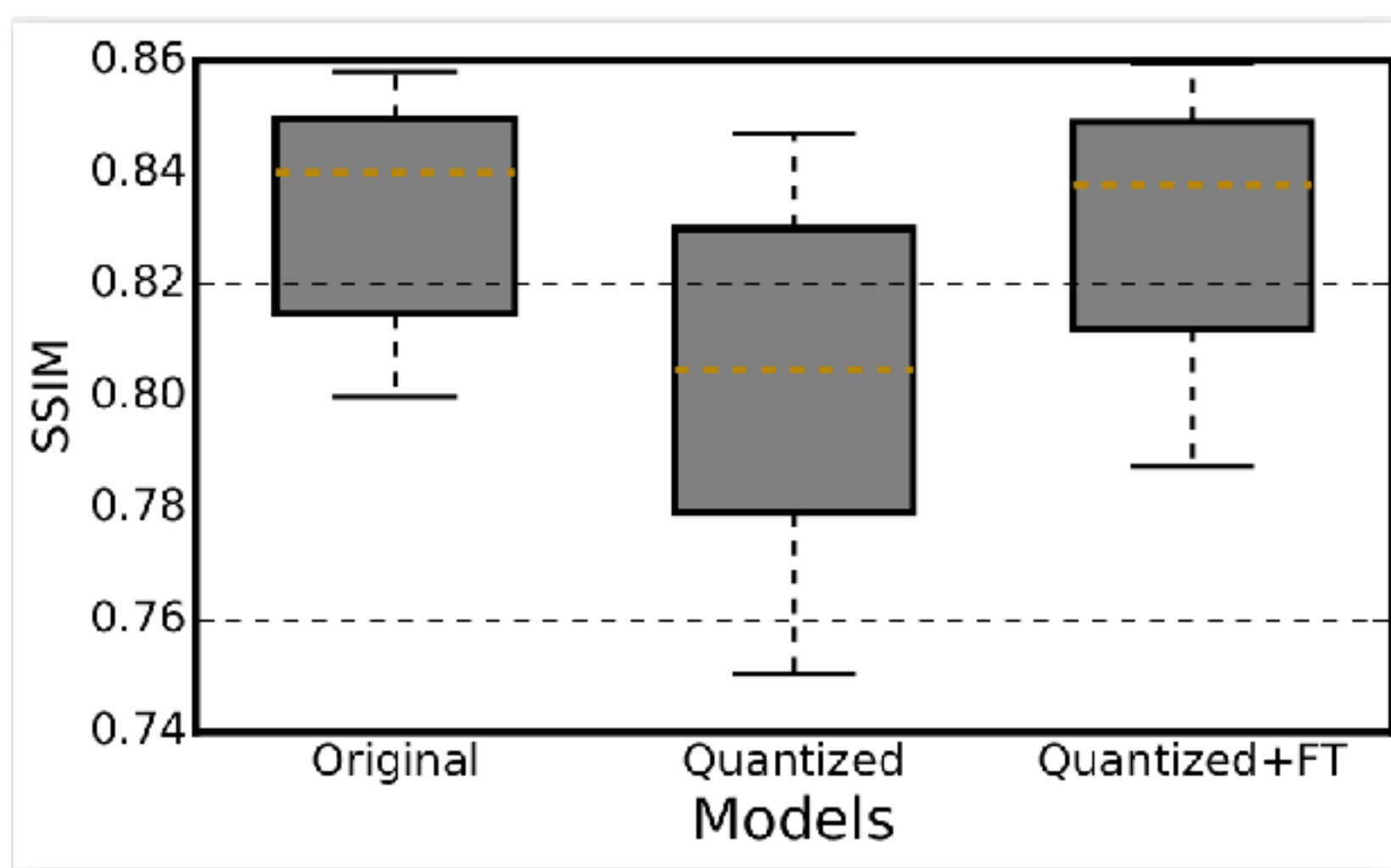
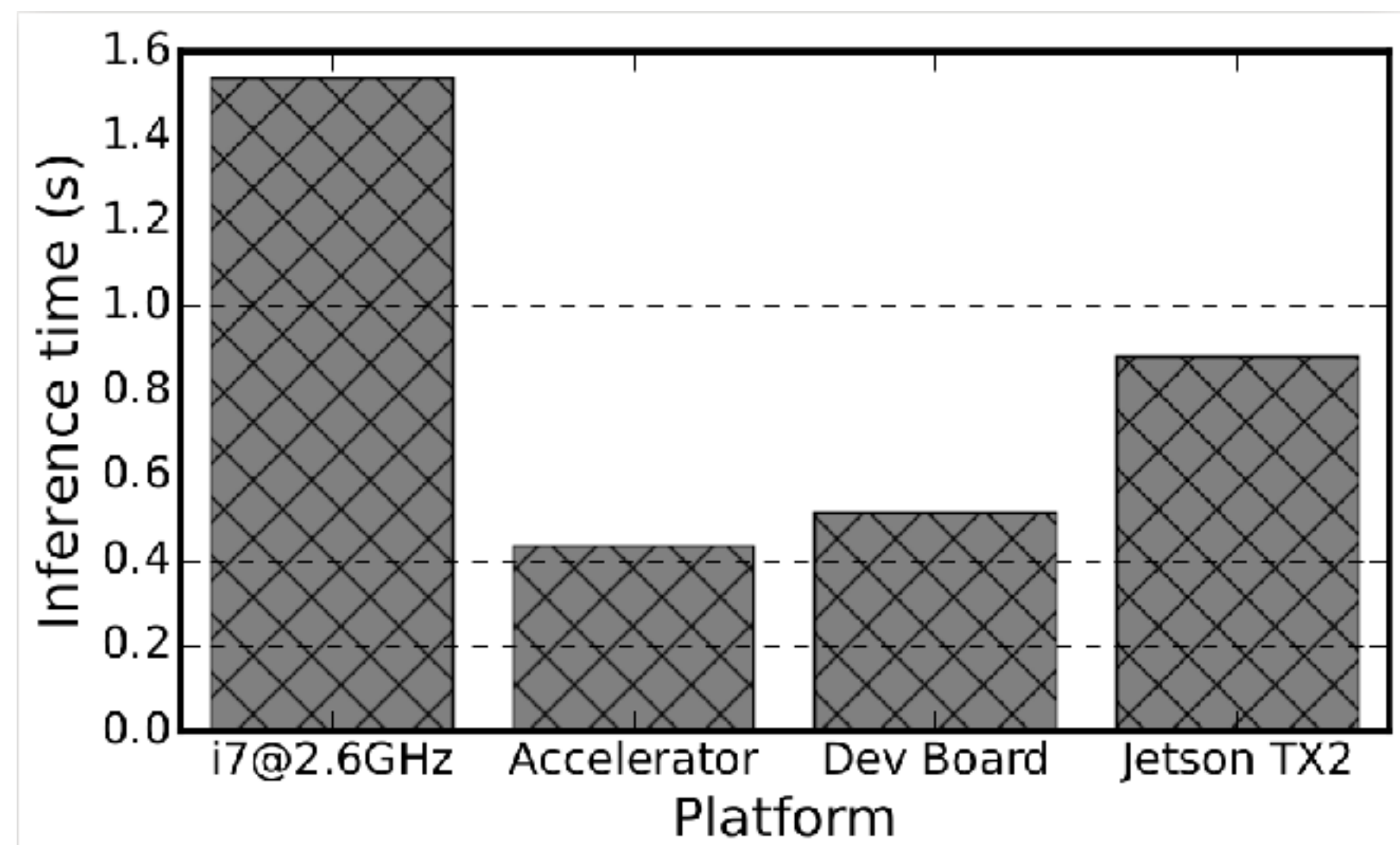
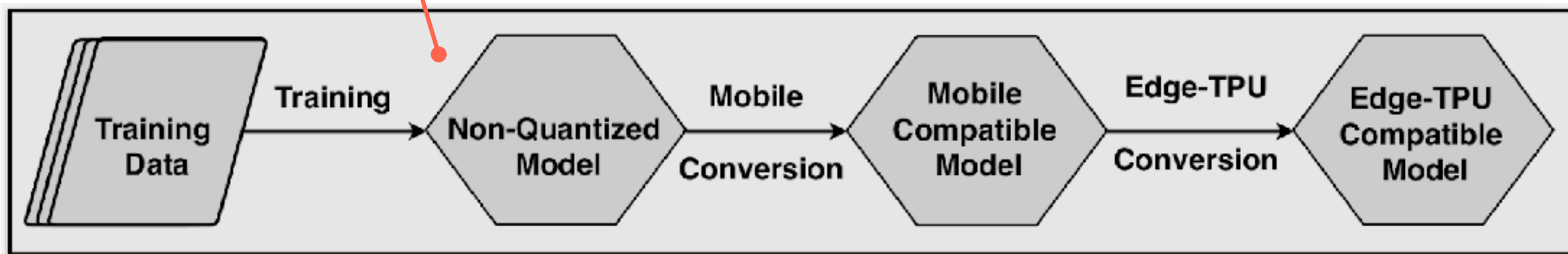
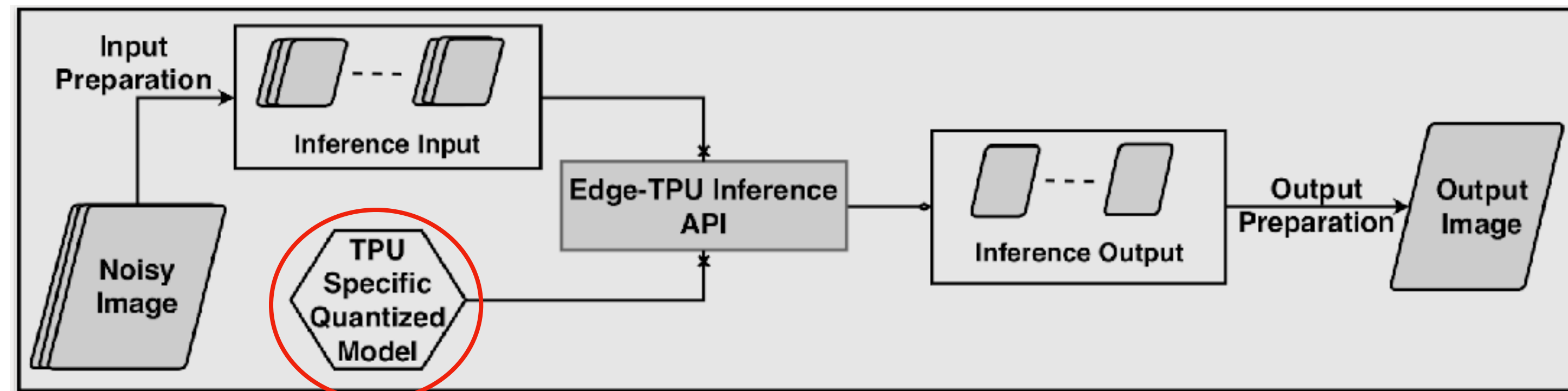


Jetson TX2

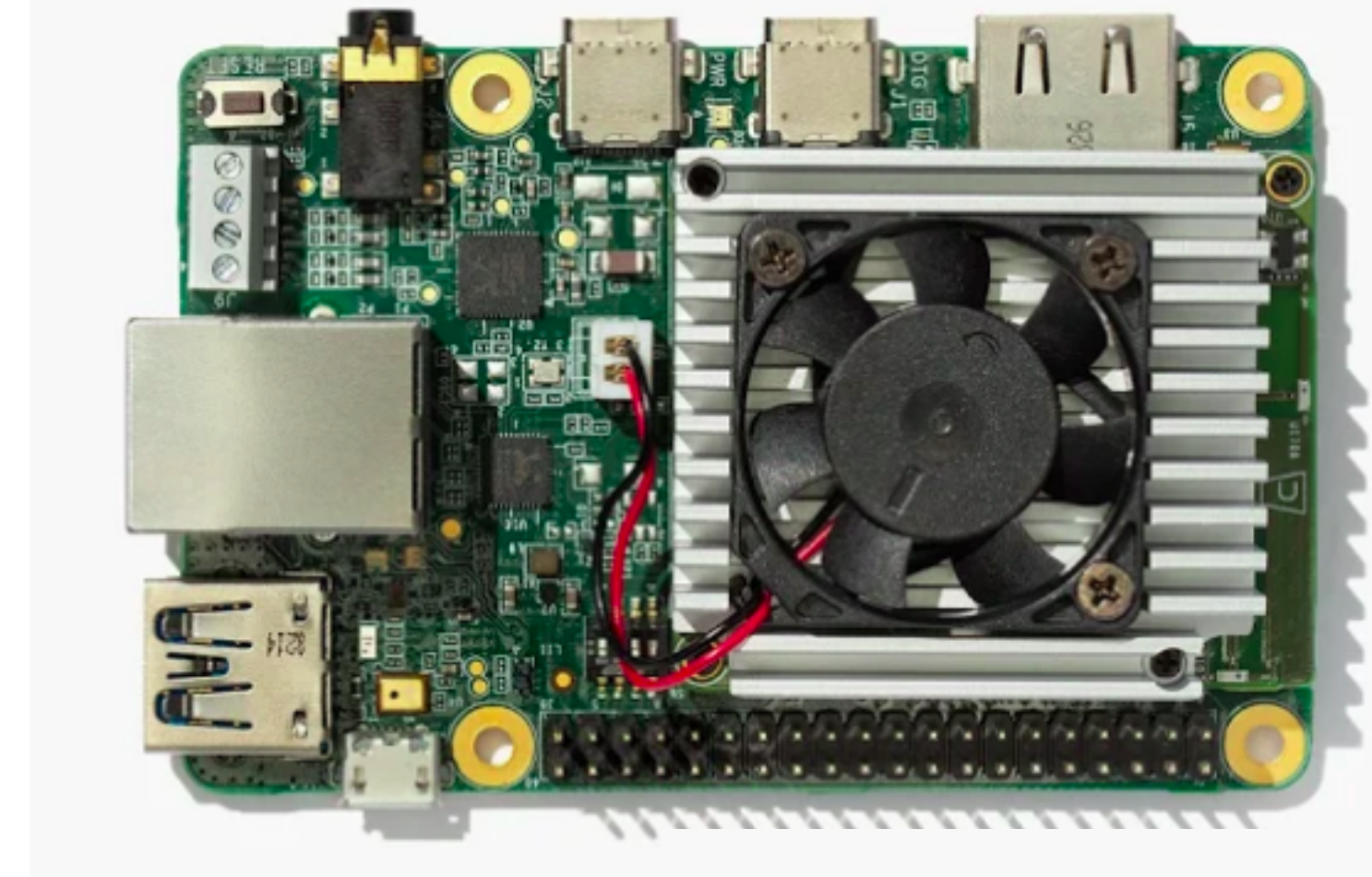


~700ms to denoise a 1k x 1k image

Make it usable - Continue Details



TPU Dev Board



TPU Accelerator

Self-driving Accelerator Operation

Powered by:

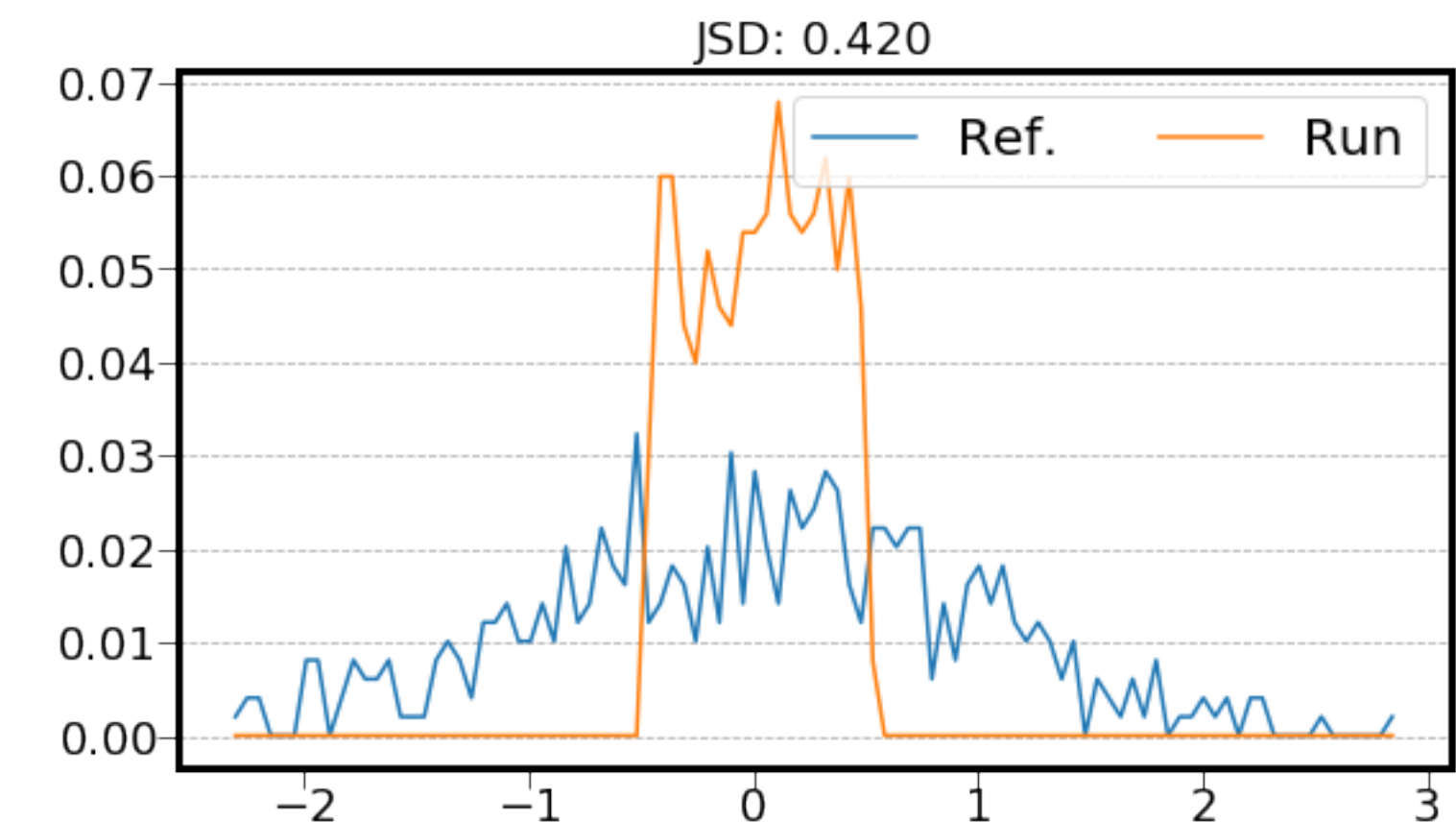
- 1,320 power supply controls the electron beam which provides X-ray radiation
- 20 years of monitoring every ~60s include: capacitor temperature, current, magnitude temperature, DAC, IGBT and voltage
- Currently dozens of failure annually
- It will be valuable for APS-U in its early stage or even testing stage.

Can we:

- Detect anomaly and raise alarms?
- Predict power supply failure before the weekly maintenance?
- Learn from expert, (adapt configuration) fix (some) potential power supply issue?

Plan and progress:

- Auto-encoder for anomaly detection, to understand if recorded data can (fully) characterize power supply status
- Conventional way for anomaly detection, statistical distance between known normal and realtime monitoring. Jensen-Shannon Divergence (JSD) works fine using 12 hours monitoring.
- Machine learning prediction for weekly maintenance intensive care.
- Learning from expert for auto-tuning



Thanks!

Open source at: <https://github.com/ramsesproject/TomoGAN>

python: Tensorflow.Keras based;

C++ : DNNL(MKL-DNN) based, good for CPU based e.g., KNL;

C++, CUDA: cuDNN and cuda based, good for NVIDIA GPU;