Variational Methods for Computational Microscopy

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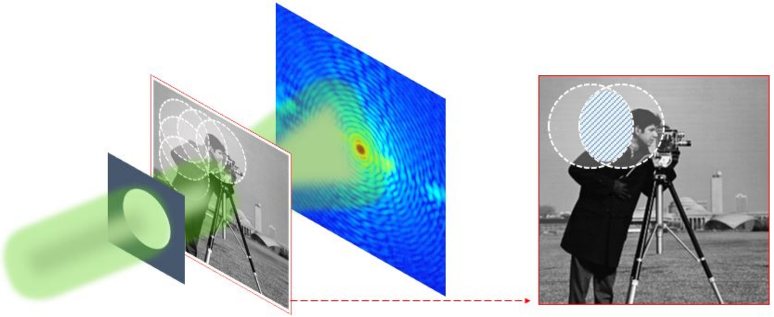
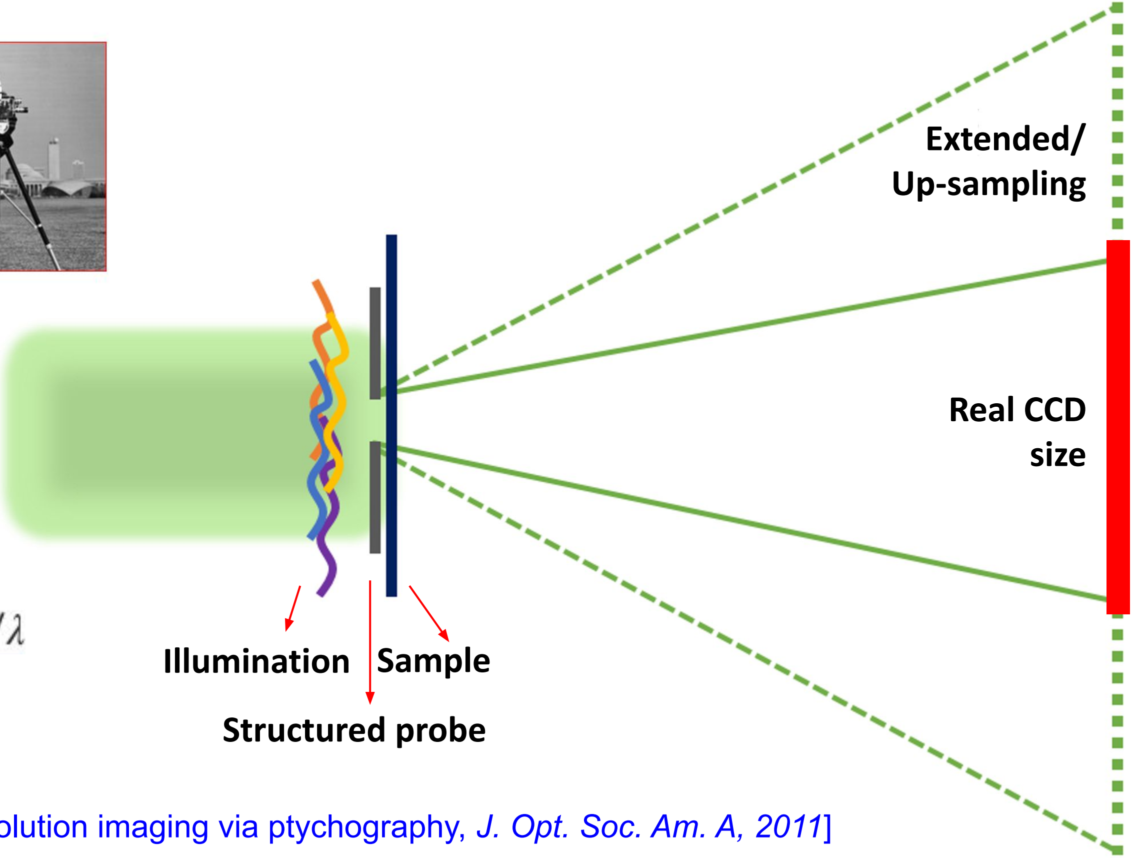
Content

Part I: Super-resolution Ptychography

Super-resolution Ptychography





Math

✔ **sub-pixel step size + up-sampling**

✔ **Regularization**

Physics

Cut-off frequency: $(\mathrm{NA}_{\mathrm{illum}} + \mathrm{NA}_{\mathrm{obj}})/\lambda$

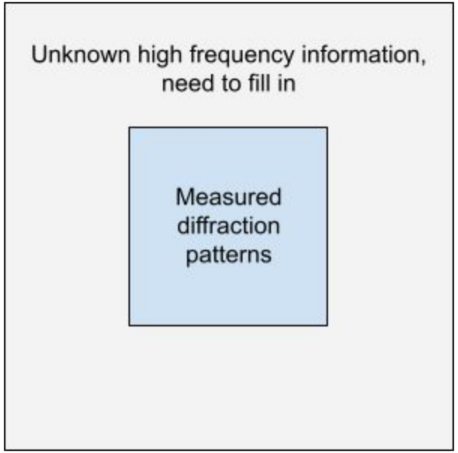
✔ **Structured probe / illumination**

- Bi-/tri- modes illumination
- Probe before/on the sample (4f)

[A. Maiden, Superresolution imaging via ptychography, *J. Opt. Soc. Am. A, 2011*]

Super-resolution Ptychography requirement

Determining the high frequency information of ptychography images encounters difficulty: Under-constrained system



With high overlap scanning, we can obtain high frequency information of ptychography images

To obtain super-resolution Ptychography, we need:

1. A structured probe: to obtain high frequency information
2. A regularizer for Ptychography algorithm.
3. Smaller and sub-pixel scanning step-size

Super-resolution Ptychography optimization

Original Ptychography minimization problem:

$$\min_{P,O} \; \frac{1}{2}\sum_n \| |\mathcal{F}(PO_{\Omega_n})| - \sqrt{I_n} \|^2$$

The optimization problem needs a regularizer.

$$\min_{P,O} \; \frac{1}{2}\sum_n \| |\mathcal{F}(PO_{\Omega_n})| - \sqrt{I_n} \|^2 + \gamma TV(O_{\Omega_n})$$

Total variation helps to stabilize the Ptychography reconstruction and remove noise.

Simulation results

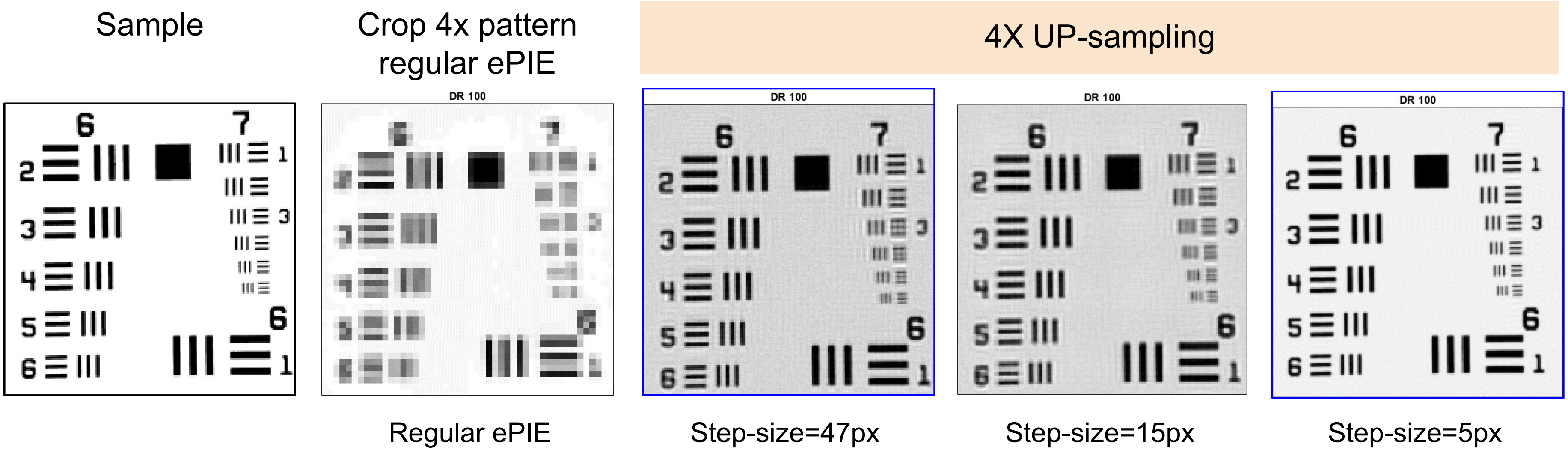
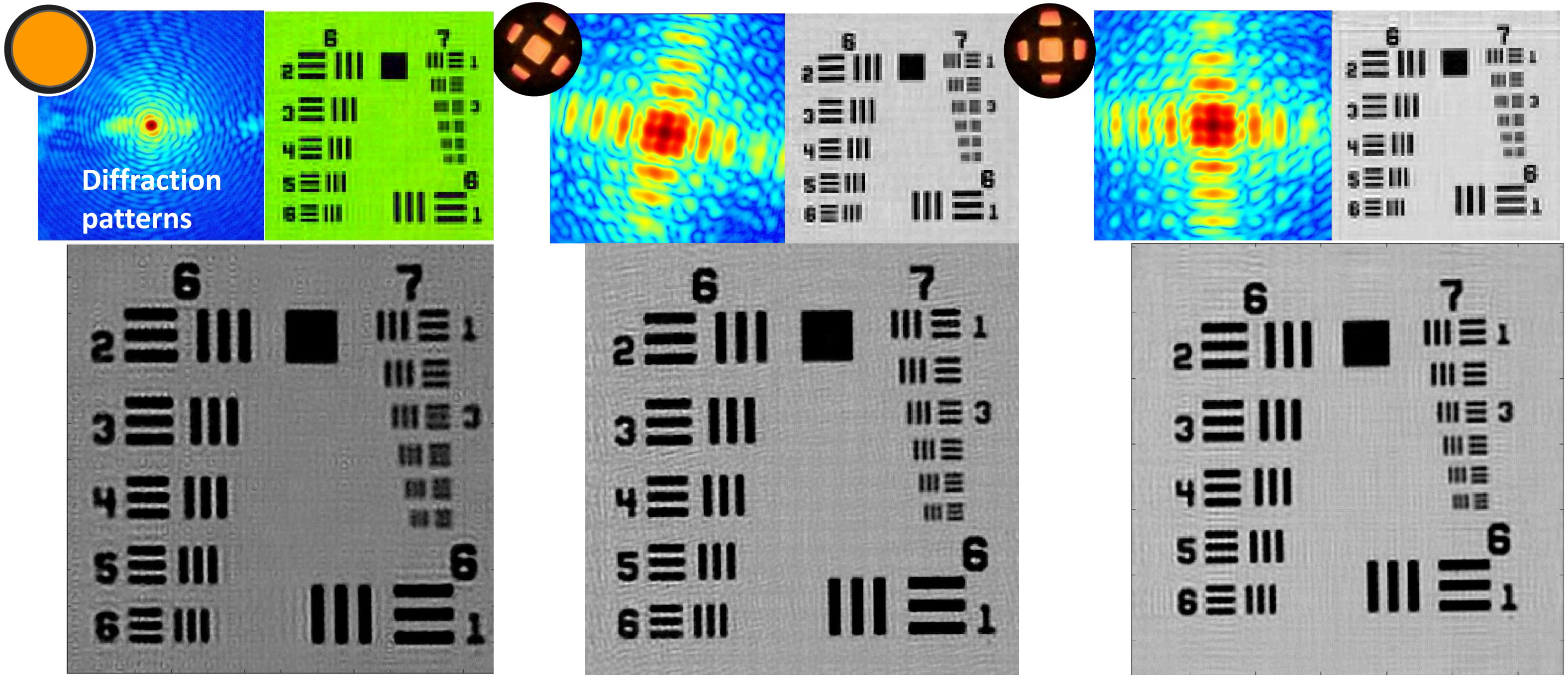


Figure: simulation and reconstruction of USAF using regular Ptychography ePIE, and super-resolution technique. **High overlap** and **sub-pixel scanning step size** help to improve the resolution

Structure of probe

probe



Super-resolution ePIE:
d=100um, step=15um
lamda=0.543um

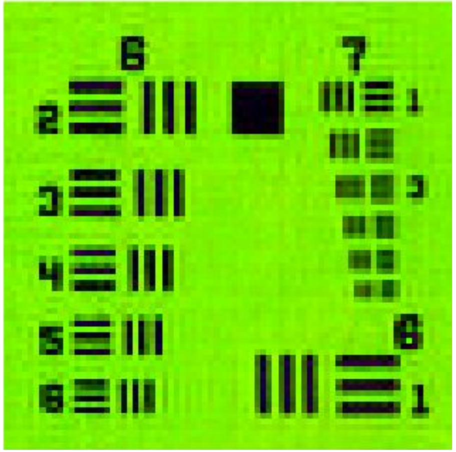
Super-resolution ePIE with
structured probe
step=15um z=1.72e5um
pixel size=3.88um

step=10um z=1.72e5um
pixel size=4um

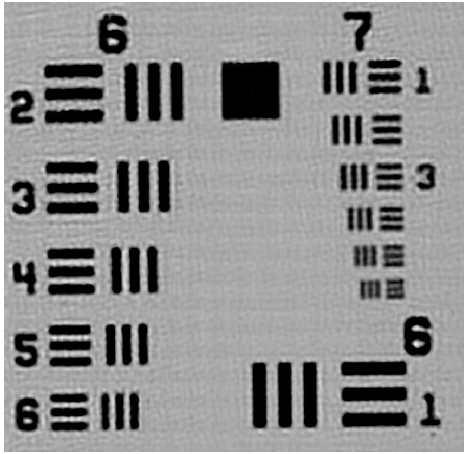
Image reconstruction is independent of the probe rotation

Super-resolution Ptychography with TV regularization

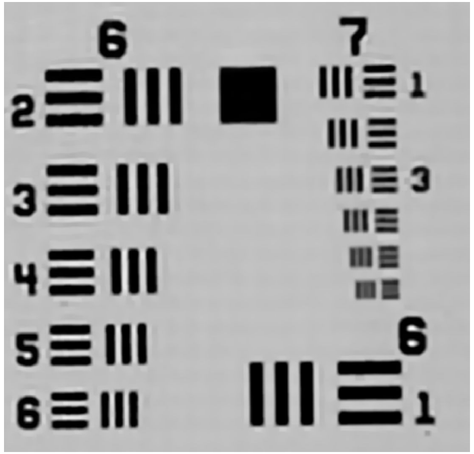
Before up-sampling
+ circle probe



up-sampling
+ structured probe



up-sampling
+ structured probe
+ regularization



Remark:

1. The reconstruction is unstable without regularizer.
2. There is a tradeoff between denoising and high frequency information

Ongoing Research

1. Need better structured probes.
2. Experiment with biological samples.
3. Continue improving algorithms.

Part II: Vector Tomography

Part II: Vector Tomography

Goal: 3D magnetic texture, spin-engineered magnetic materials

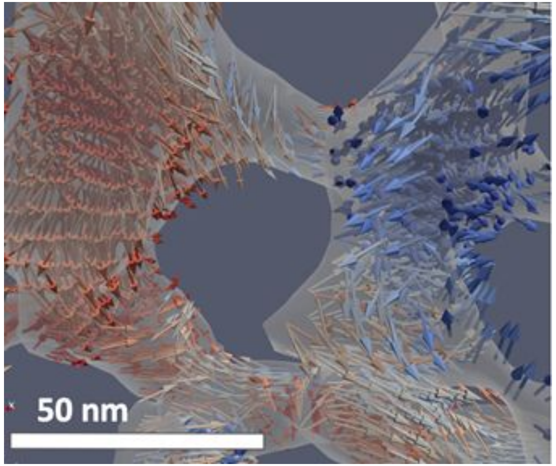


Figure: Imaging the 3D spin textures in a magnetic metalattice sample using vector ptycho-tomography. The 3D magnetization field is overlaid on the reconstruction of the Ni (gray) and silica (voids) metalattice.

Question:

- How to design experiment? How many tilt series are required?
- Algorithm?

[A. Rana, Direct observation of 3D topological spin textures and their interactions using soft x-ray vector ptychography, *2021*]

Vector Tomography algorithm

3D magnetic components $\overrightarrow{\boldsymbol{m}} = (m_x, m_y, m_z)$ and the scalar part O are coupled via a linear integral constraint

$$\int_{L_\theta} \langle \overrightarrow{\boldsymbol{m}}(x,y,z), \boldsymbol{R}_{\boldsymbol{\theta}}^{\dagger} \overrightarrow{\boldsymbol{e}_{\boldsymbol{z}}} \rangle + O(x,y,z)\, dz = P_{\boldsymbol{\theta}}(x,y)$$

- Use left and right polarization to eliminate the dependency of the scalar part O.
- Rewrite the equation in algebraic way.

Vector Tomography minimization problem:

$$\min_{\overrightarrow{\boldsymbol{m}}} \ \varepsilon(\overrightarrow{\boldsymbol{m}}) = \frac{1}{2} \sum_{\boldsymbol{\theta}} \left\| \alpha_{\boldsymbol{\theta}} \, \Pi_{\boldsymbol{\theta}}(m_x) + \beta_{\boldsymbol{\theta}} \, \Pi_{\boldsymbol{\theta}}(m_y) + \gamma_{\boldsymbol{\theta}} \, \Pi_{\boldsymbol{\theta}}(m_z) - b_{\boldsymbol{\theta}}^{+} \right\|^2$$

Vector Tomography algorithm

$$\min_{\vec{\boldsymbol{m}}} \; \varepsilon(\overrightarrow{\boldsymbol{m}}) = \frac{1}{2} \sum_{\boldsymbol{\theta}} \left\| \alpha_{\boldsymbol{\theta}} \, \Pi_{\boldsymbol{\theta}}(m_x) + \beta_{\boldsymbol{\theta}} \, \Pi_{\boldsymbol{\theta}}(m_y) + \gamma_{\boldsymbol{\theta}} \, \Pi_{\boldsymbol{\theta}}(m_z) - b_{\boldsymbol{\theta}} \right\|^2$$

Method: gradient descent

$$\frac{\partial \varepsilon}{\partial m_x} = \sum_{\boldsymbol{\theta}} \alpha_{\boldsymbol{\theta}} \, \Pi_{\boldsymbol{\theta}}^T \left(\alpha_{\boldsymbol{\theta}} \, \Pi_{\boldsymbol{\theta}}(m_x) + \beta_{\boldsymbol{\theta}} \, \Pi_{\boldsymbol{\theta}}(m_y) + \gamma_{\boldsymbol{\theta}} \, \Pi_{\boldsymbol{\theta}}(m_z) - b_{\boldsymbol{\theta}} \right)$$

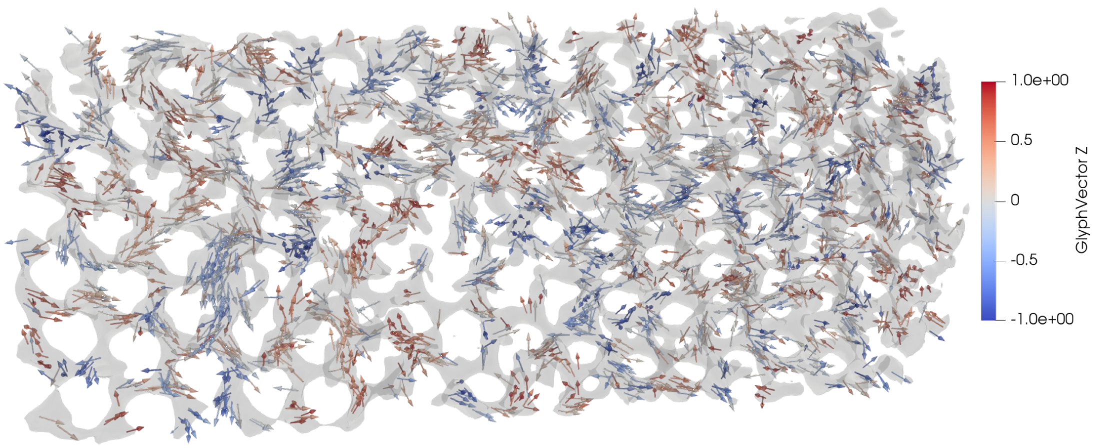
We use Fourier slice theorem to show that the reconstruction requires three tilt series: one original set, one in-plane rotation set, and one side rotation set.

Remark:

1. Side rotation is infeasible.
2. However, support constraint can help (3D magnetic field only appears in the vacancy of magnetic materials).

[M. Pham, Real space iterative reconstruction engine for Tomography, *arxiv, 2021*]

Vector Tomography: Constraint Support



1. Support constraint helps the reconstruction.
2. Magnetic field only appears in the vacancy of the materials (the space between atoms)

Figure: Reconstructed magnetization vector field of a Nickel infiltrated meta-lattice.

Remark: Simulation & experimental data shows the method works fine without side rotation when support constraint is enforced.

Scalar Tomography: Constraint Support

Q: How to compute the support?
A: Obtain Scalar reconstruction, then use hard thresholding,
or better, we use l1 minimization

$$\min_O \; \varepsilon(O) = \frac{1}{2} \sum_{\boldsymbol{\theta}} \left\| \Pi_\theta(O) - b_{\boldsymbol{\theta}} \right\|^2 + \gamma \|O\|_1$$

Augmented Lagrangian: exploit dual variable.

$$\mathcal{L}(O, Y, \lambda) = \frac{1}{2} \sum_{\boldsymbol{\theta}} \left\| \Pi_\theta(O) - b_{\boldsymbol{\theta}} \right\|^2 + \gamma \|Y\|_1 + \frac{t}{2} \|O - Y + \frac{\lambda}{t}\|^2$$

where Y and λ and auxiliary and dual variables

Scalar Tomography: l1 minimization

Augmented Lagrangian:

$$\mathcal{L}(O,Y,\lambda) = \frac{1}{2}\sum_{\boldsymbol{\theta}} \left\|\Pi_\theta(O) - b_{\boldsymbol{\theta}}\right\|^2 + \gamma\|Y\|_1 + \frac{t}{2}\|O - Y + \frac{\lambda}{t}\|^2$$

Algorithm: linearized ADMM.

$$O^{k+1} = Y^k - \frac{\lambda^k}{t} - \frac{1}{t}\sum_\theta \Pi^T(\Pi_\theta O^k - b_\theta)$$

$$Y^{k+1} = Shrink(O^{k+1} + \frac{\lambda^k}{t}, \frac{\gamma}{t})$$

$$\lambda^{k+1} = \lambda^k + t(O^{k+1} - Y^{k+1})$$

where Shrink operator is soft thresholding.

Why linearized ADMM: inverse is expensive

Scalar Tomography: l1 minimization

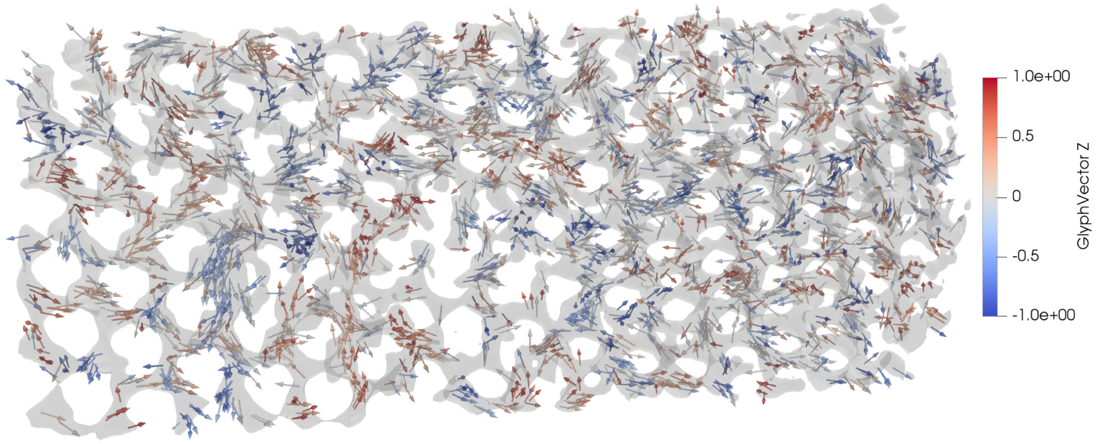


Figure: Reconstructed magnetization vector field of a Nickel infiltrated meta-lattice with l1-mimization to find the support

Part III: Blind Deconvolution with CNN

Deconvolution with Deep learning

Convolutional neural networks acts as a high pass filter in denoising/deblurring.

$$\min_\theta \frac{1}{2} \sum_n \|x_n + f_\theta(x_n) - y_n\|^2$$

where $\{(x_n, y_n)\}_{n=1}^N$ are pairs of corrupted & clean images (training data)

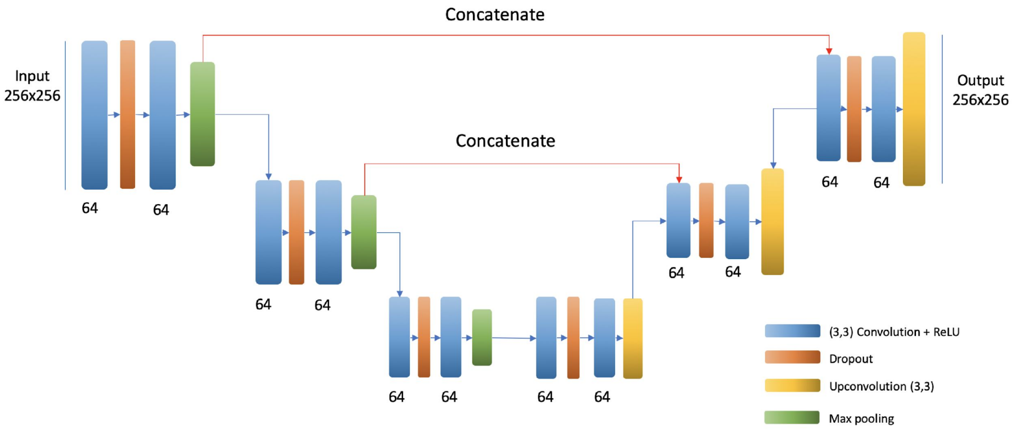


Figure 4: U-Net: a convolutional neural network that combines Encoder-Decoder with skip connection. U-Net uses down-sampling, up-sampling to extract high frequency of images.

Deconvolution with Deep learning

Enforce the commutative property of convolution: $K * D = D * K$

Send derivative in i and j directions to the neural networks:

$$\min_\theta \frac{1}{2} \sum_n \|x_n + f_\theta(x_n) - y_n\|^2 + \|D_i x_n + f_\theta(D_i x_n) - D_i y_n\|^2 + \|D_j x_n + f_\theta(D_j x_n) - D_j y_n\|^2$$

Advantage:

- A natural way to increase the training data size.
- Learn the high frequency information better
- Reduce bias
- Can help in the case of scarce data

Results

Figure: Deblurring with U-net and commutative property enforcement. PNSR improves 0.5-3.

Part IV: GPU high performance Computing

High performance computing:

1. CUDA/C++ implementation with highly parallel computing.
2. Ptychography.
3. Tomography: RESIRE2 algorithm which can work with extended objects and partially blocked projections.
4. on single or multi-GPU
5. Matlab friendly

Thank you

Reference

[1] Yuan, Y., Kim, D.S., Zhou, J. et al. Three-dimensional atomic packing in amorphous solids with liquid-like structure. Nat. Mater. 21, 95–102 (2022).

[2] Yang, Y., Zhou, J., Zhu, F. et al. Determining the three-dimensional atomic structure of an amorphous solid. Nature 592, 60–64 (2021)

[3] M. Pham, Y. Yang, A. Rana, J. Miao, and S. Osher. "RESIRE: real space iterative reconstruction engine for Tomography." arXiv preprint arXiv:2004.10445 (2021)

[4] M. Pham, “Core-CNN: Commutative reinforcement of convolutional neural network. An application to blind deconvolution.” Preprint

[5] M. Pham, “RESIRE-v: Real Space Iterative Reconstruction Engine for Vector Tomography.” Preprint

Collaborators: Xingyuan Lu, Arjun Rana, Mike Hung Lo, Yao Yang, Dennis Kim, Zhi Zhou