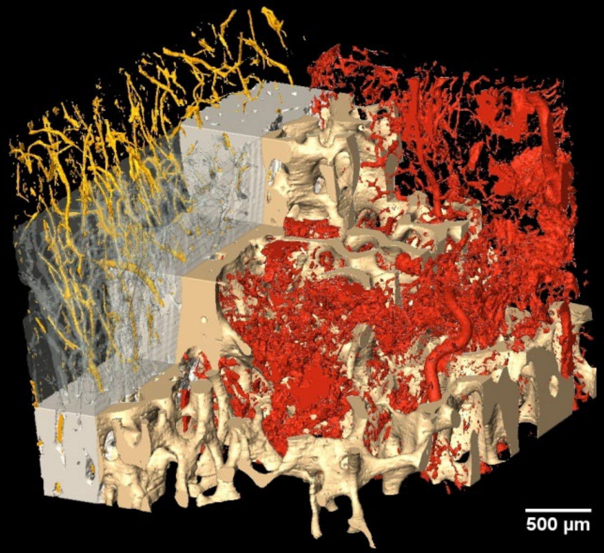
Deep learning for phase retrieval in propagation-based X-ray phase contrast imaging

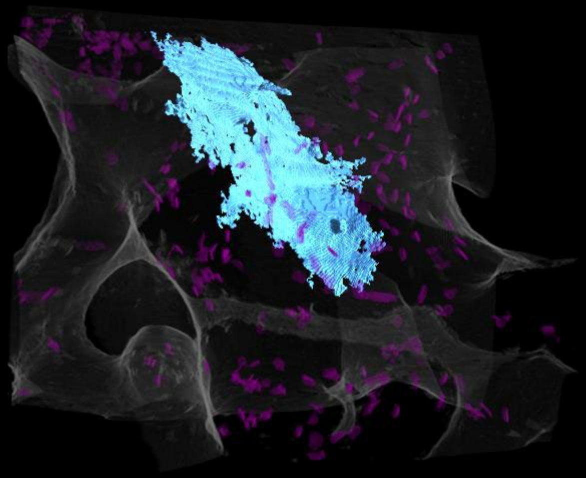
Kannara Mom, Bruno Sixou, Max Langer

Université Grenoble Alpes, CNRS, UMR 5525, VetAgro Sup, Grenoble INP, TIMC, 38000 Grenoble, France

max.langer@univ-grenoble-alpes.fr

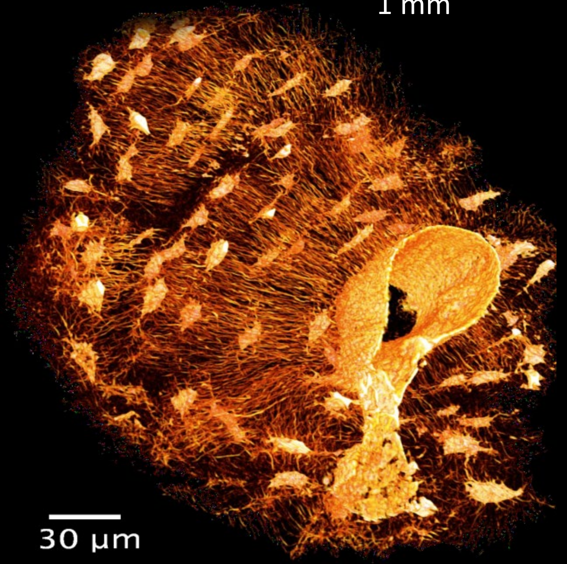
Quantitative X-ray tomography through the scales

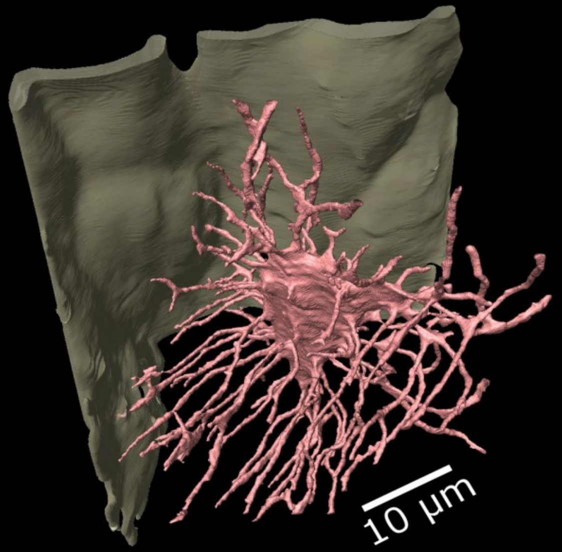


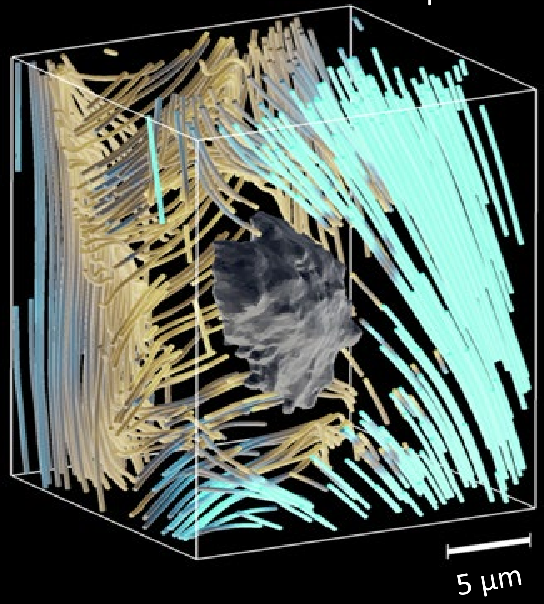


1 mm

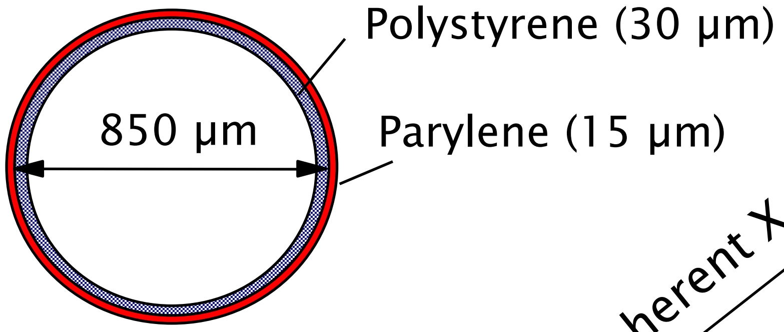
50 µm

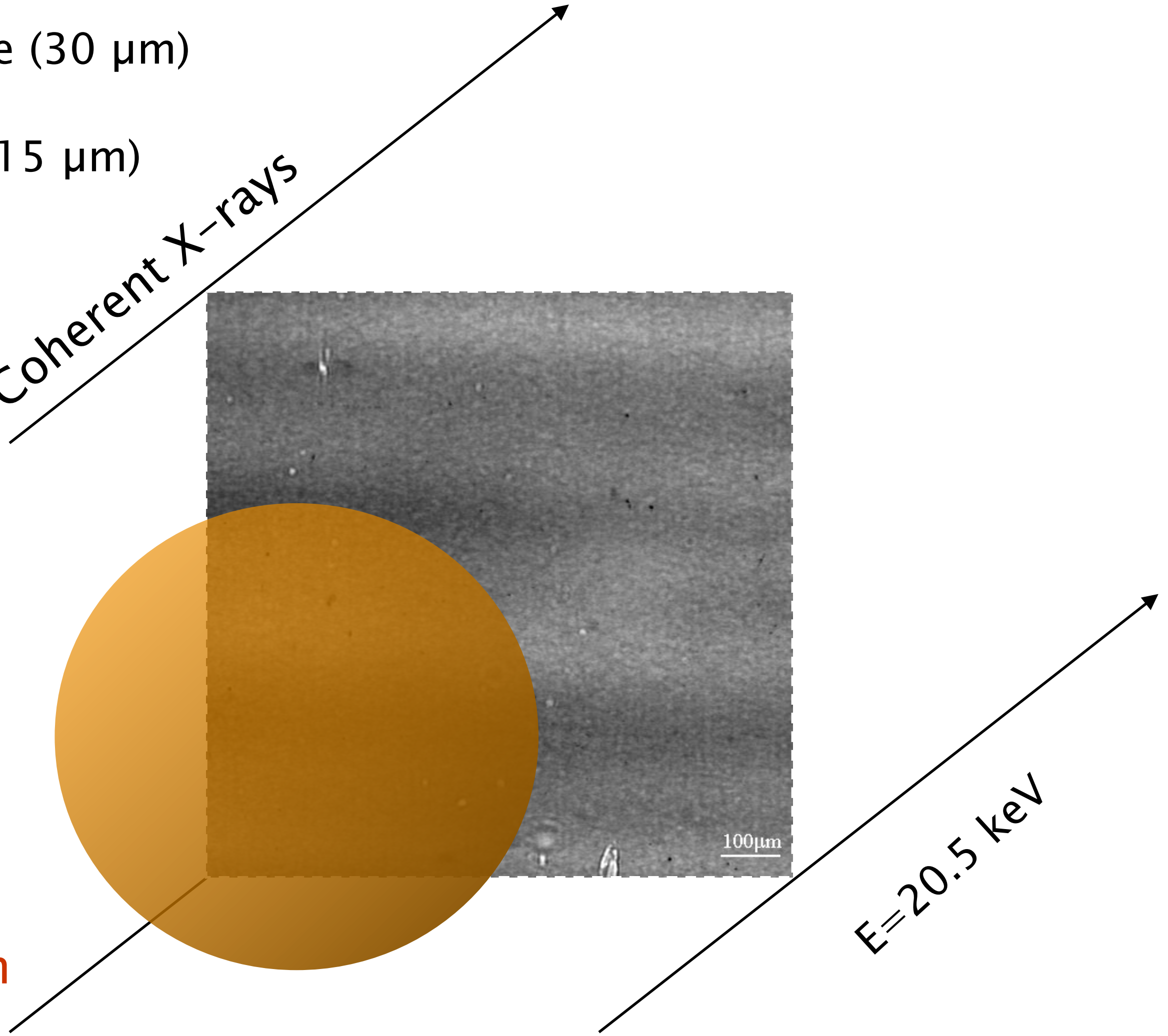






In-line X-ray phase contrast imaging



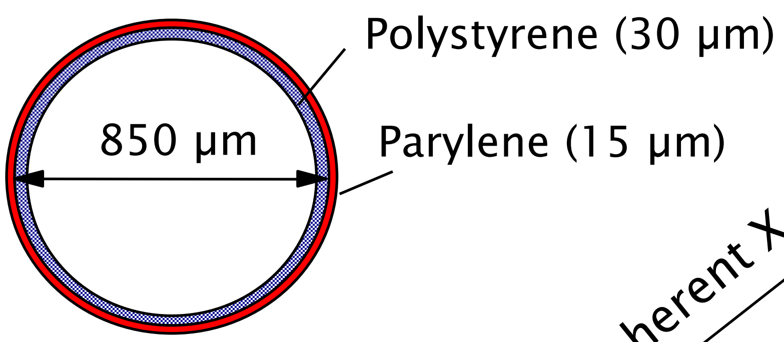


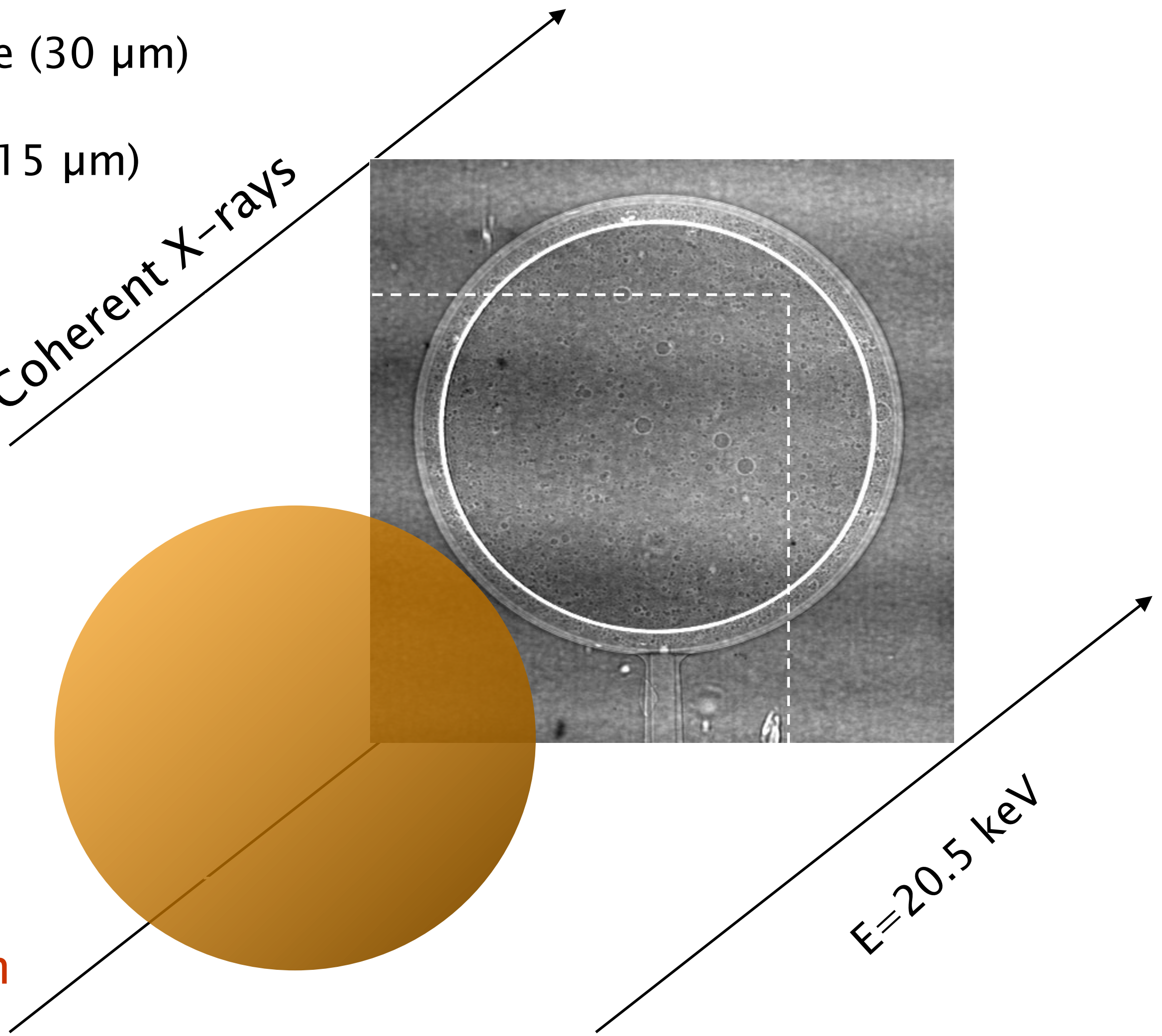
Attenuation at zero distance

Phase contrast downstream

Phase contrast up to three orders of magnitude more sensitive than absorption contrast in hard X–ray region

In-line X-ray phase contrast imaging





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Phase contrast downstream

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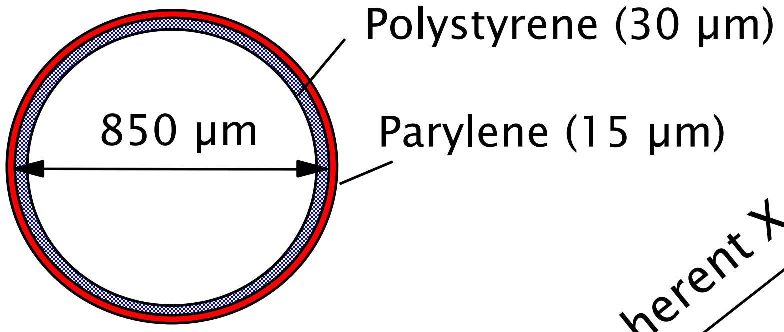
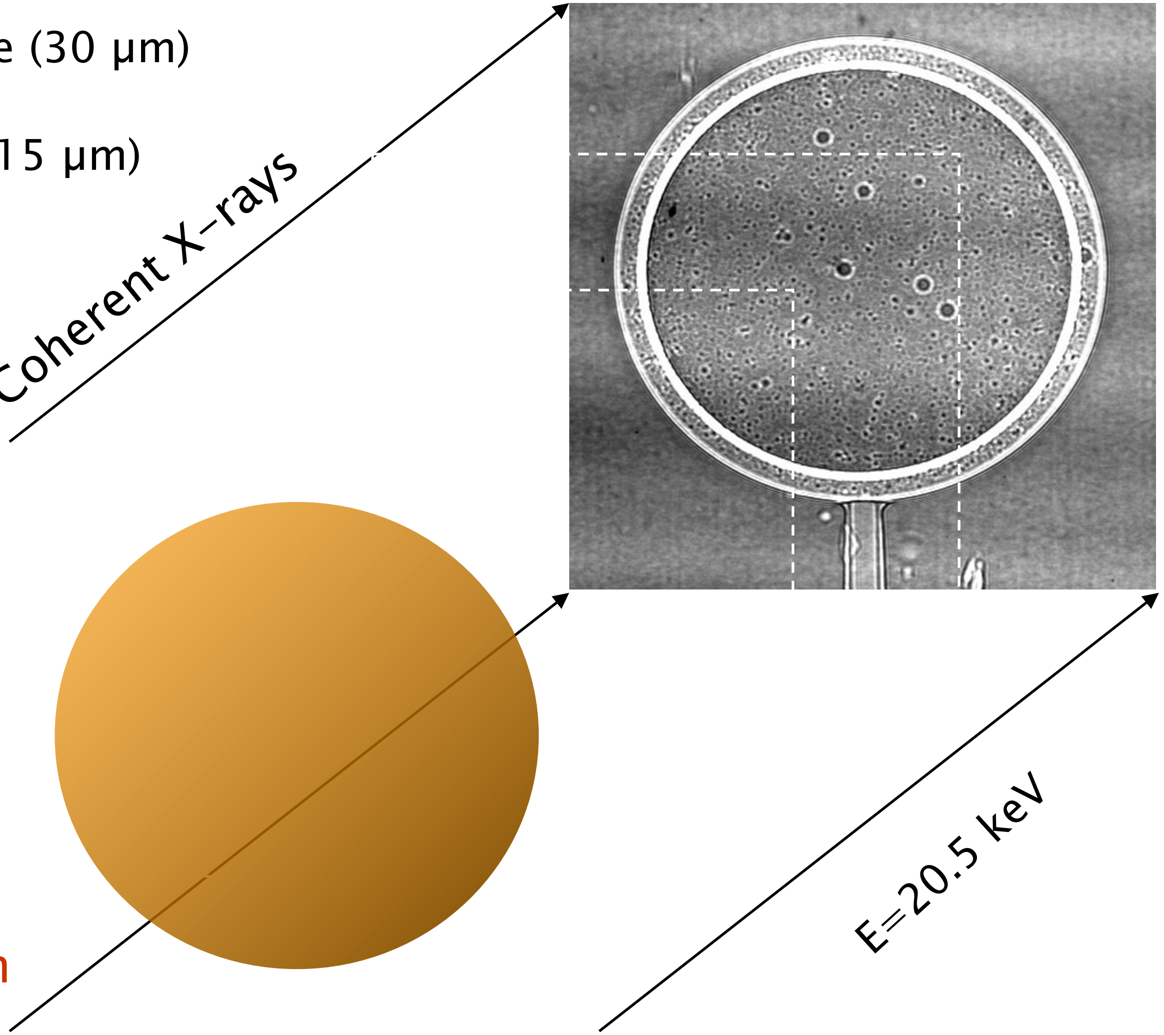
In-line X-ray phase contrast imaging



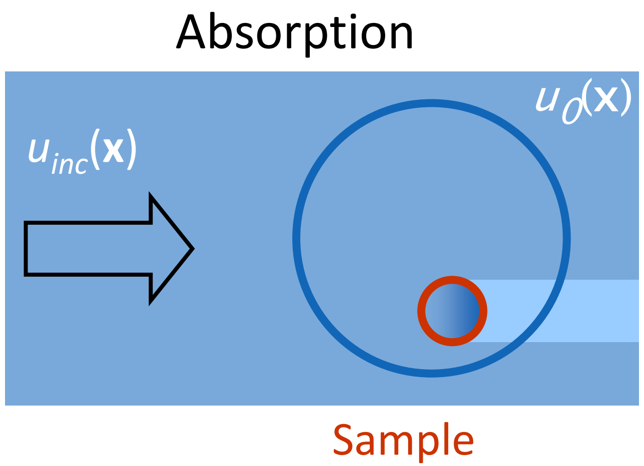


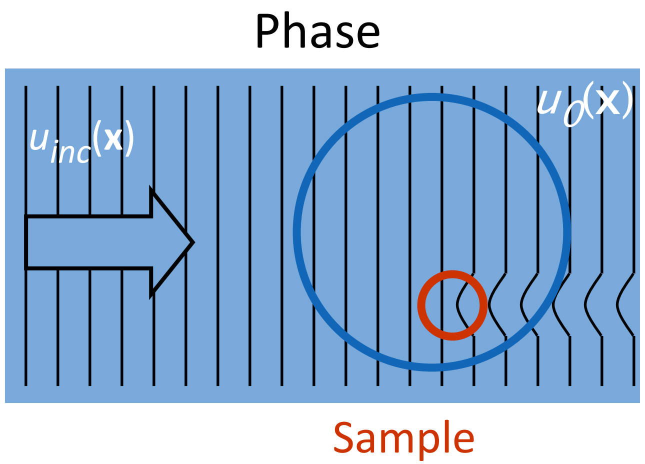
Attenuation at zero distance

Phase contrast downstream

Phase contrast up to three orders of magnitude more sensitive than absorption contrast in hard X-ray region

Wave-Object Interaction





- Object described by 3D complex refractive index $n(x, y, z) = 1 - \delta(x, y, z) + i\beta(x, y, z)$

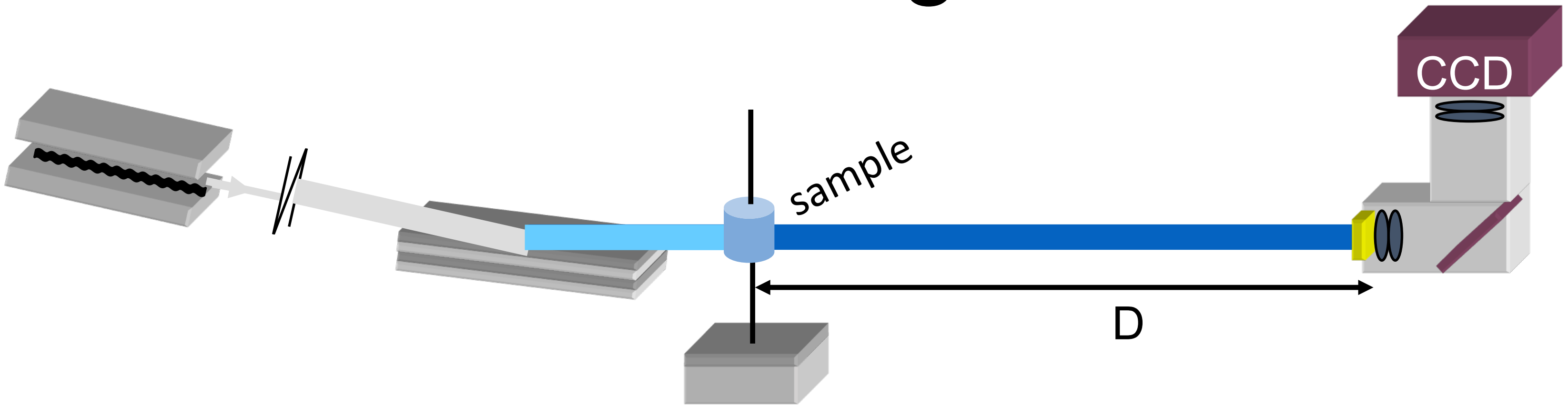
- Wave-object interaction described by a transmittance function: $u_0(\mathbf{x}) = T(\mathbf{x})u_{inc}(\mathbf{x})$, $\mathbf{x} = (x, y)$
- Induces amplitude (absorption) and phase modulation: $T(\mathbf{x}) = A(\mathbf{x})e^{i\varphi(\boldsymbol{x})}$

- Both amplitude and phase modulation are given by projections through $n(x, y, z)$

Amplitude $A(\mathbf{x}) = e^{-\frac{2\pi}{\lambda}\int \beta(x,y,z)\mathrm{d}z} = \mathrm{e}^{-\frac{1}{2}\int \mu(x,y,z)\mathrm{d}z}$

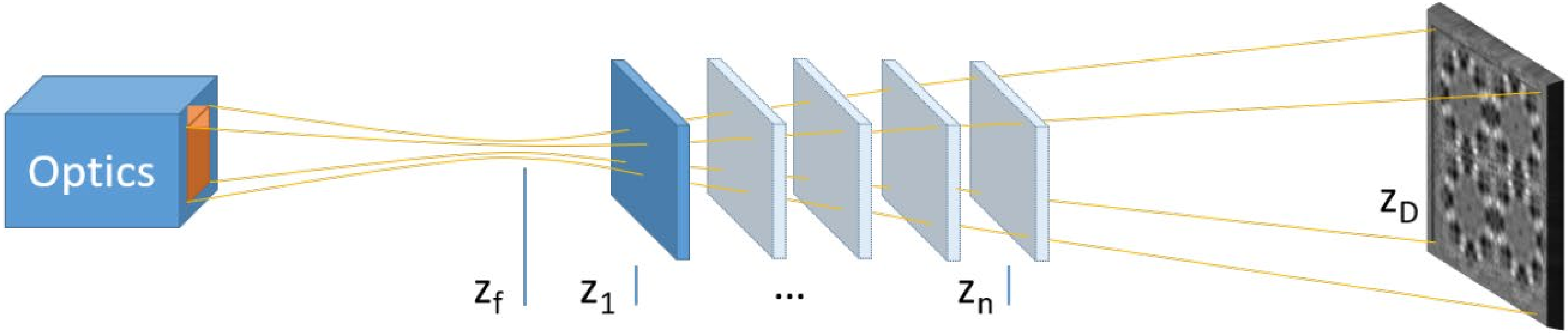
Phase $\varphi(\mathbf{x}) = \varphi_o - \frac{2\pi}{\lambda}\int \delta(x, y, z)\mathrm{d}z$

Direct Problem – Image Formation

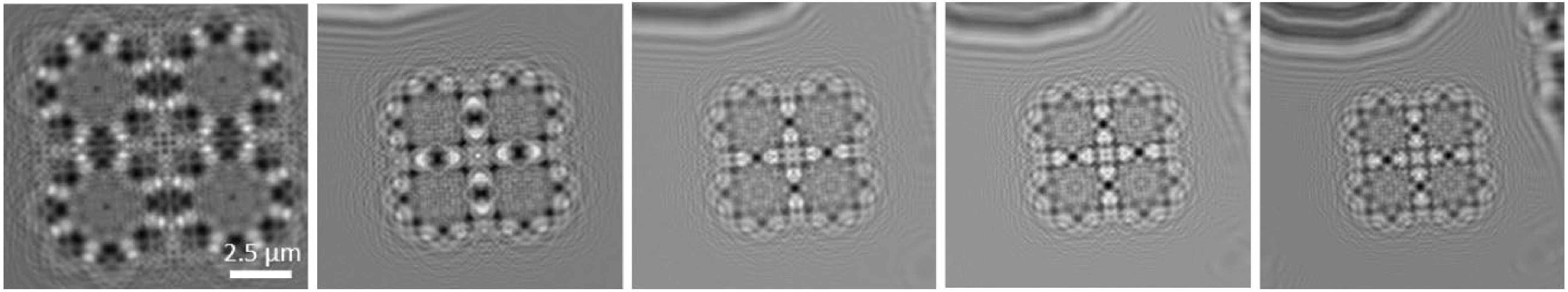


- Propagation over finite D is described by Fresnel diffraction
- Propagation is a linear system w.r.t. the wave (Fresnel transform)
  - Convolution of wave $u_D(\mathbf{x}) = (P_D * u_0)(\mathbf{x})$ with propagator $P_D(\mathbf{x}) = \frac{-i}{\lambda D} \exp\left(\frac{i\pi}{\lambda D}|\mathbf{x}|^2\right)$
  - Fourier domain: Multiplication with propagator $\tilde{P}_D(\mathbf{f}) = \exp(-i\pi\lambda D|\mathbf{f}|^2)$
- Non-linear w.r.t intensity: squared modulus of wave: $I_D(\mathbf{x}) = |u_0(\mathbf{x})|^2$
- Fourier transform of intensity: $\tilde{I}_D(\mathbf{x}) = \iint T\left(\mathbf{x} - \frac{\lambda D\mathbf{f}}{2}\right) T^*\left(\mathbf{x} + \frac{\lambda D\mathbf{f}}{2}\right) \exp(-i2\pi\mathbf{x}\cdot\mathbf{f})\, d\mathbf{x}$

High resolution phase contrast imaging



- With X-ray focusing optics : allows **high resolution** imaging.



Absorption & Phase retrieval : Estimating $\boldsymbol{B}$ & $\boldsymbol{\varphi}$ from recorded intensity

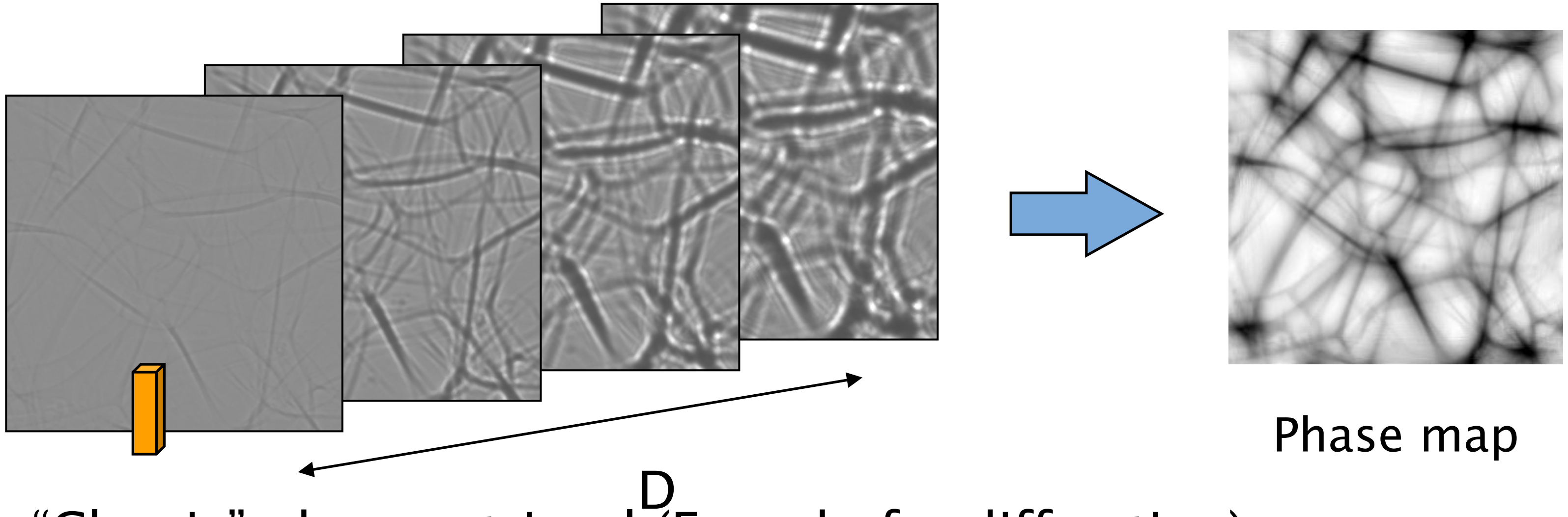
Phase Retrieval

- Quantitative, non-linear relationship between phase shift and contrast

$$I_D(\mathbf{x}) = \left|\mathrm{Fr}_{D,\lambda}[\mathrm{T}_{A,\varphi}(\mathbf{x})]\right|^2$$

- Phase retrieval: inverse problem of calculating phase shift from phase contrast images at different distances

$$\varphi(\mathbf{x}) = \underset{\varphi}{\operatorname{argmin}} \left\| \left|\mathrm{Fr}_{D,\lambda}[\mathrm{T}_{A,\varphi}(\mathbf{x})]\right|^2 - I_D(\mathbf{x}) \right\|^2$$



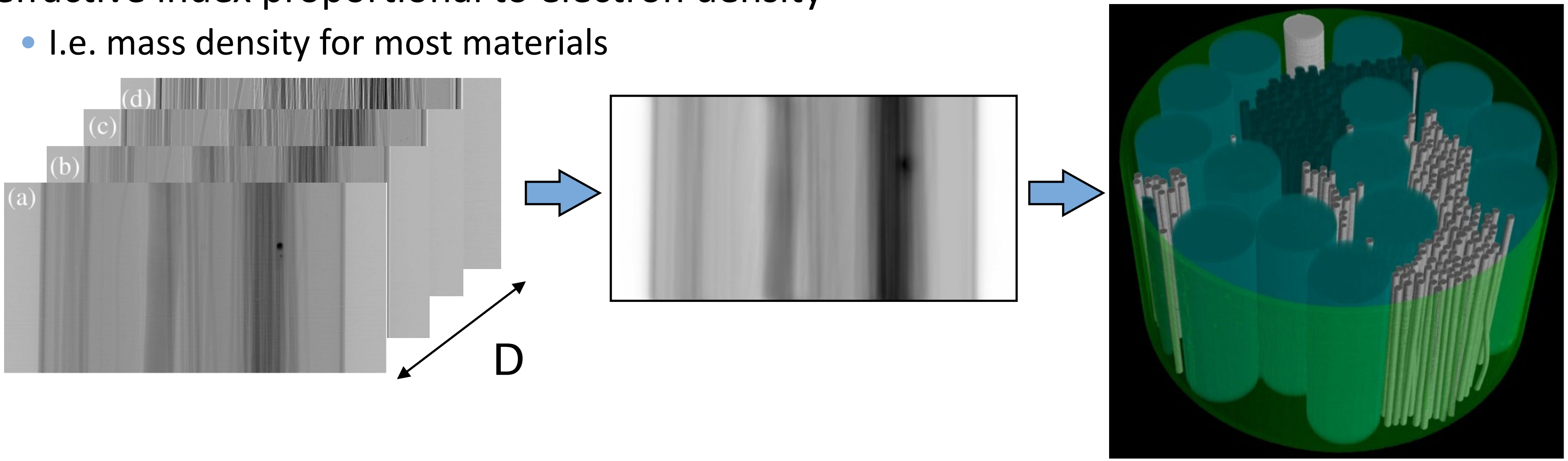
Phase map

- Cf. “Classic” phase retrieval (Fraunhofer diffraction)

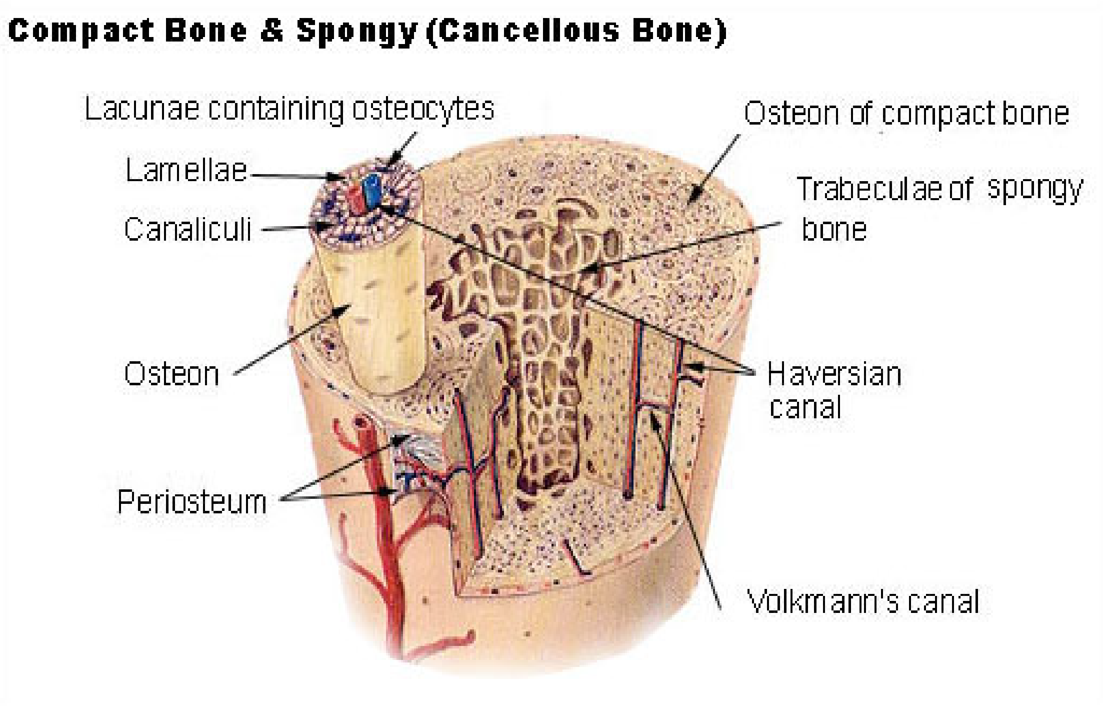
$$I_D(\mathbf{x}) \propto \left|\widetilde{\mathrm{T}}_{A,\varphi}(\mathbf{f})\right|^2 \quad \left|\widetilde{\mathrm{T}}_{A,\varphi}(\mathbf{f})\right|\exp[i\psi(\mathbf{f})] = \int \mathrm{T}_{A,\varphi}(\mathbf{x}) \exp(-i2\pi\mathbf{f}\cdot\mathbf{x})\, d\mathbf{x}$$

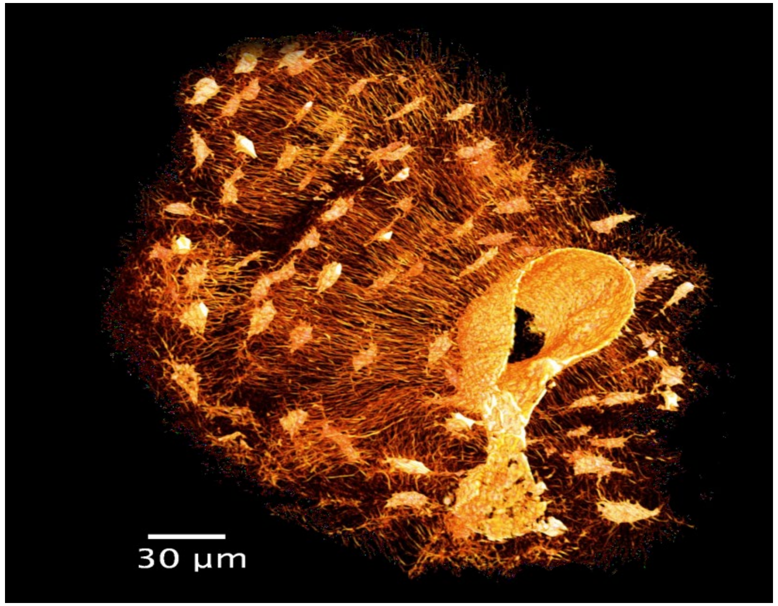
Phase Tomography

- Phase shift is projection through refractive index
- Refractive index can be reconstructed by tomography
- Phase tomography is usually divided into a two-step process
  - Phase retrieval (2D)
  - Repeated for each projection angle, tomography (3D)
- Refractive index proportional to electron density
  - I.e. mass density for most materials

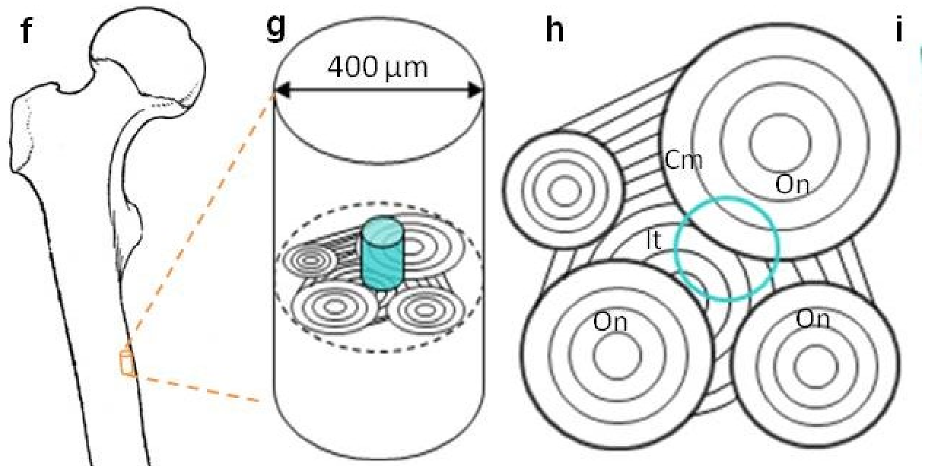


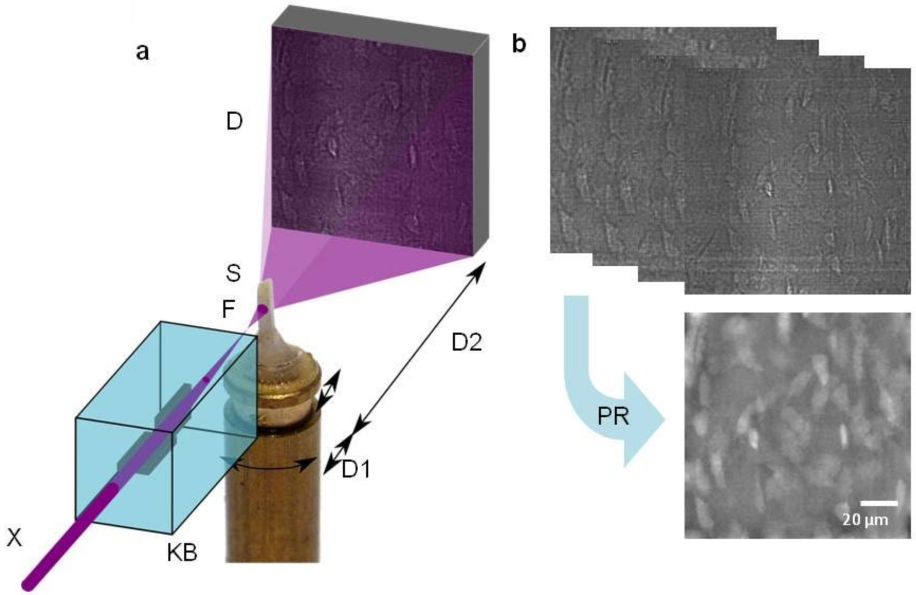
Phase nanotomography of bone



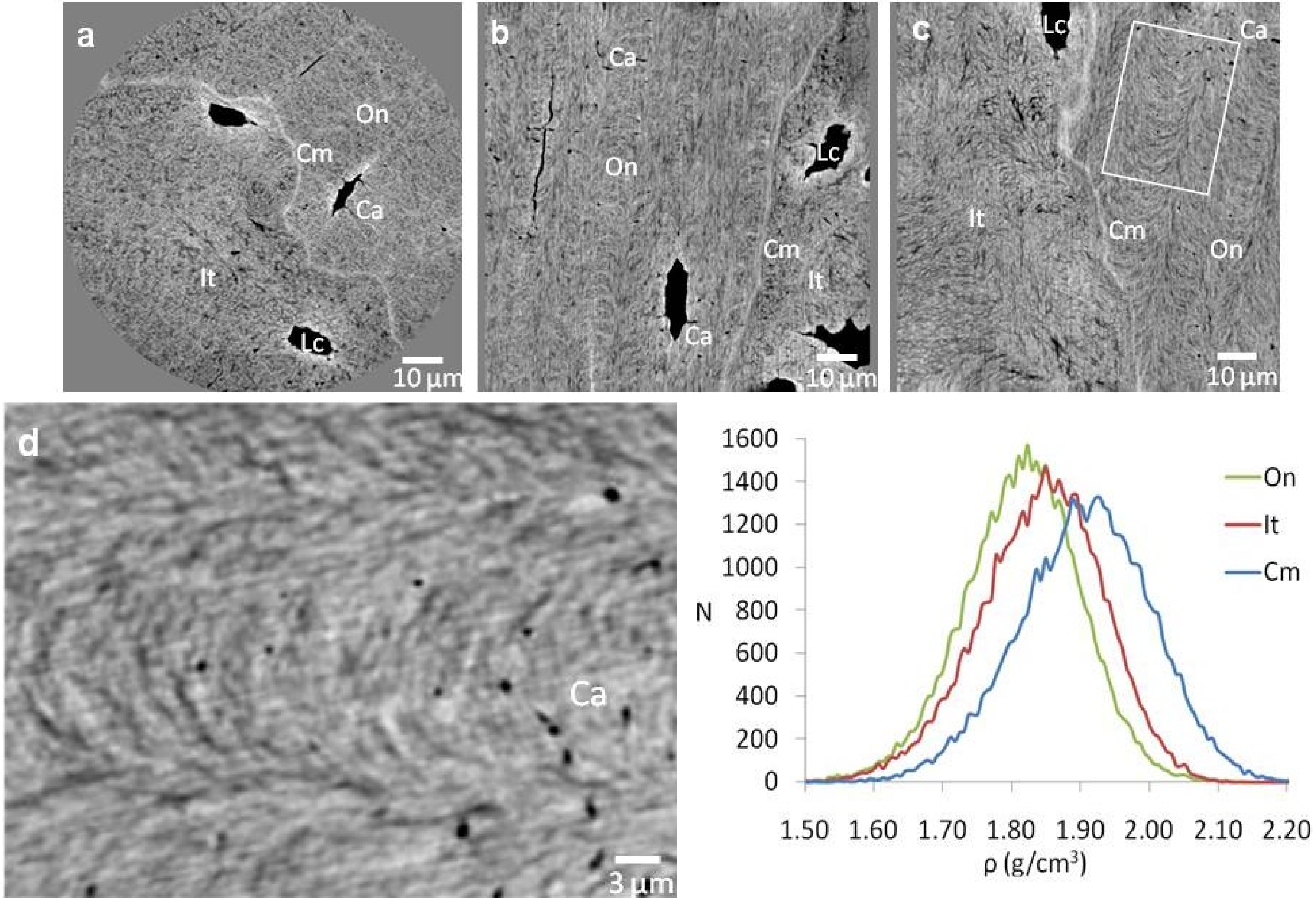


Langer et al. , *Plos one* 2012



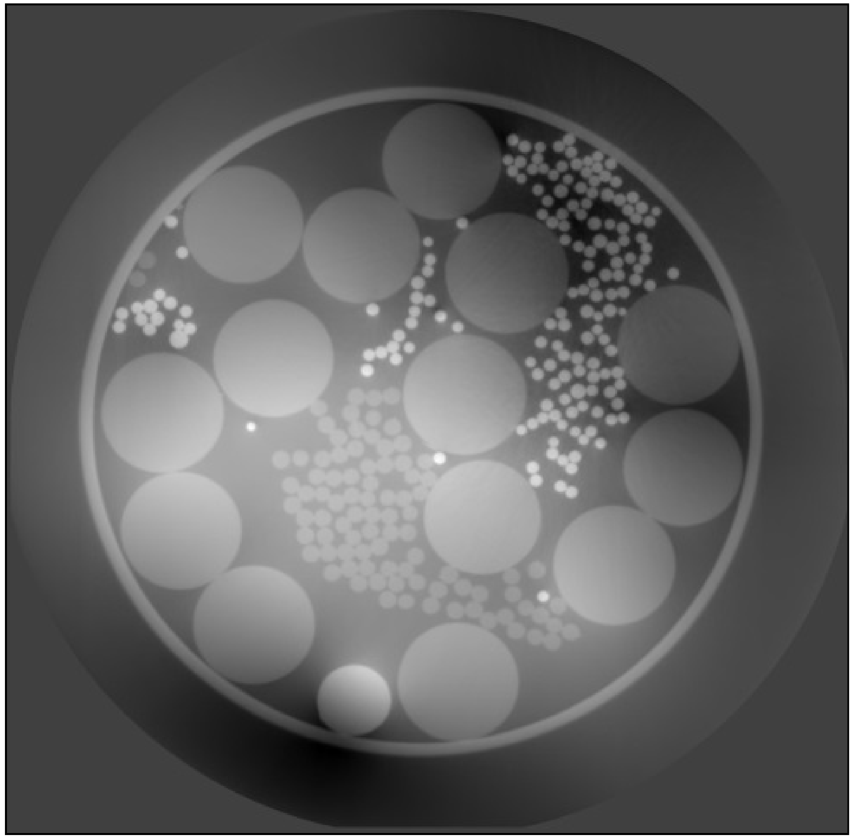


Phase nanotomography of bone



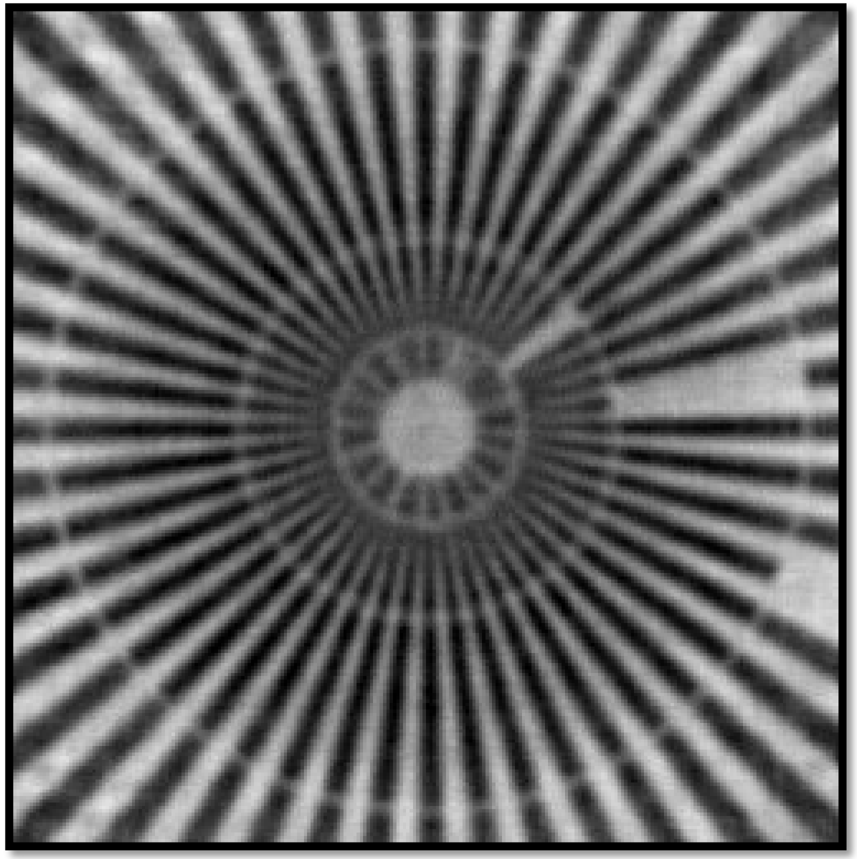
Phase Retrieval

- Low-frequency sensitivity



Regularisation, priors

- Resolution



- Non-linear refinement
  - NLCG
  - Alternating projections
  - …

Direct reconstruction : Linearized solutions

- **Transport-of-intensity equation (TIE)** [1] for **short distance**.
- **Contrast Transfer Function (CTF)** method, if **phase slowly varying** & the **absorption is weak** :

$$\widehat{I}_D(\mathbf{f}) = \delta(\mathbf{f}) - 2\cos(D\pi\lambda|\mathbf{f}|^2)\widehat{B}(\mathbf{f}) + 2\sin(D\pi\lambda|\mathbf{f}|^2)\widehat{\varphi}(\mathbf{f})$$

The CTF-linearized [2] forward model :

$$\mathbf{F}_D^{\mathrm{CTF}}(B,\varphi) = \left\{\mathscr{F}^{-1}\left(-2\cos(\pi\lambda D|\mathbf{f}|^2)\ ;\ 2\sin(\pi\lambda D|\mathbf{f}|^2)\right)\mathscr{F}\right\}(B,\varphi)$$

+ Fast	- Valid only for certain imaging conditions
	- Loss of nonlinear contribution
	- Single distance only if homogeneous assumption

1. Paganin et al., "Simultaneous phase and amplitude extraction from a single defocused image of a homogeneous object".
2. Zabler et al., "Optimization of phase contrast imaging using hard x rays".

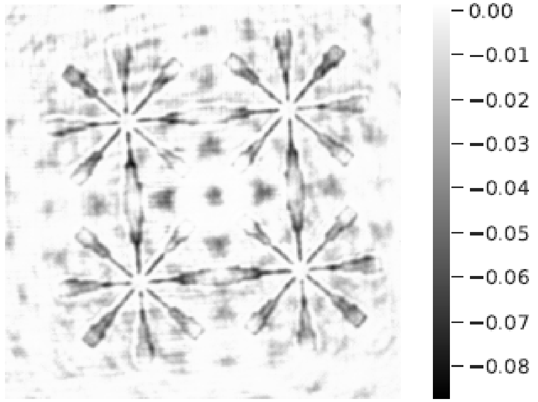
State of the art : Non-linear algorithms

Iteratively regularized Gauss-Newton (IRGN) method[3], with $f = -B + i\varphi$:

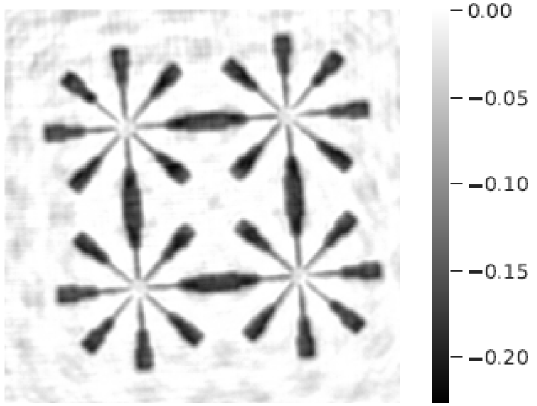
$$f_{k+1} = \underset{f}{\operatorname{argmin}} \left\{ \left|\left| \mathbf{F}_D(f_k) + \mathbf{F}'_D(f_k)^* (f - f_k) - \mathbf{I}_D^{\text{obs}} \right|\right|_2^2 + \alpha_k ||f - f_0||_X^2 \right\}$$

where :

- $\alpha_k > 0$ regularization parameter
- $\mathbf{F}'_D(f_k)^*$ is the adjoint of Fréchet dérivative at f_k
- $||f||_X = \left|\left|(1+\xi^2)^{\frac{s}{2}} \mathscr{F}(f)(\xi)\right|\right|_2$ $(s = \frac{1}{2})$



$$f_{k+1} = f_k + \left[\mathbf{F}'_D(f_k)^* \mathbf{F}'_D(f_k) + \alpha_k\right]^{-1} \left\{\mathbf{F}'_D(f_k)^* \left[\mathbf{I}_D^{\text{obs}} - \mathbf{F}_D(f_k)\right] - \alpha_k f_k\right\}$$

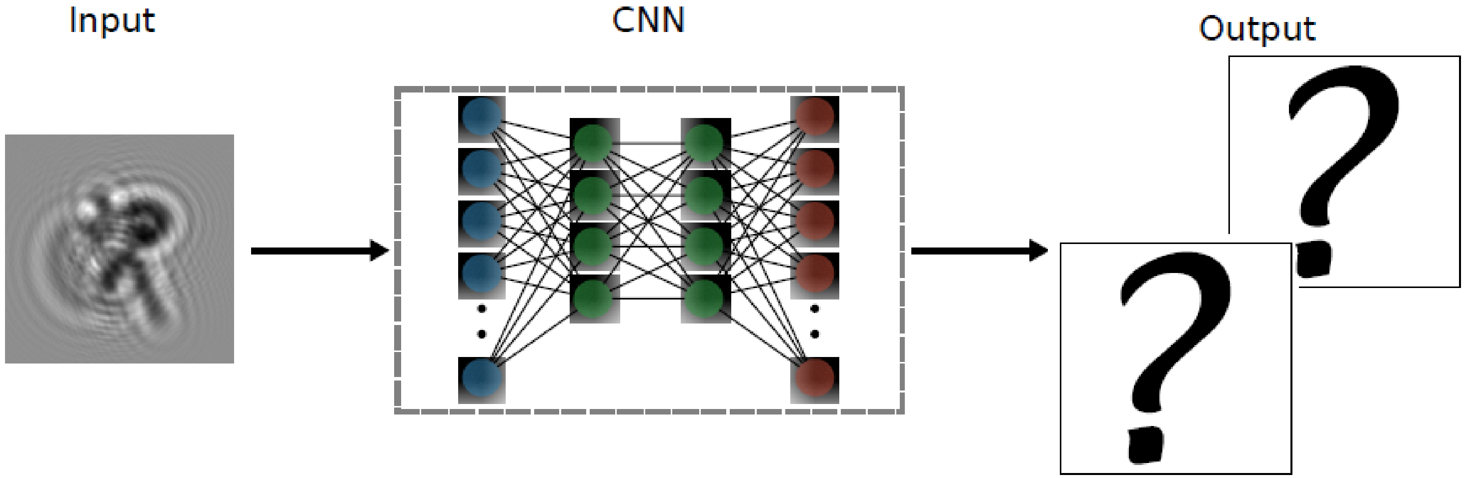


- Costly, does not overcome all artefacts, and requires parameter selection

3. Maretzke et al., "Regularized Newton methods for X-ray phase contrast and general imaging problems".

Phase retrieval using CNNs

- Direct reconstruction

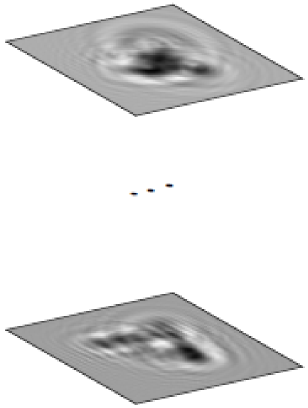


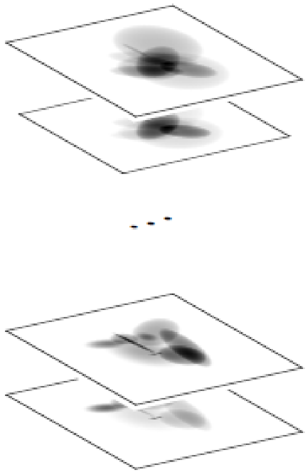
Inputs

Paired training dataset

Random projections of random compositions of ellipsoids

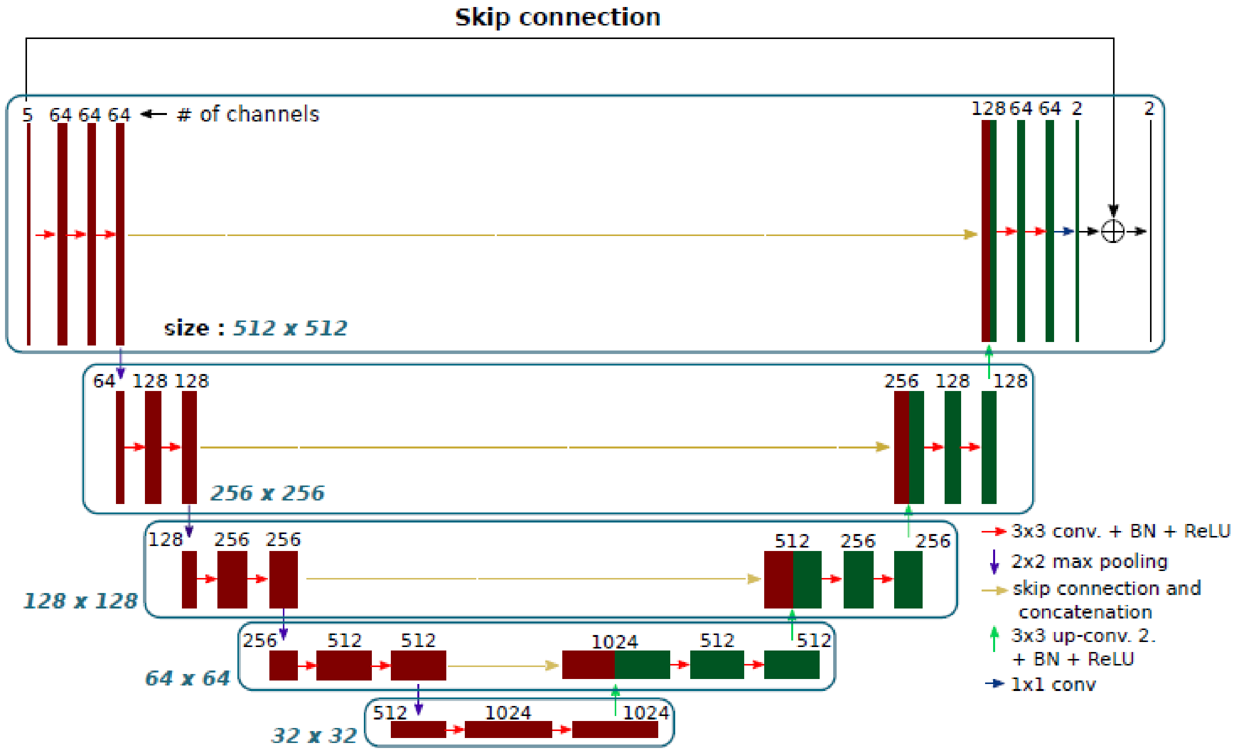
Ground truths



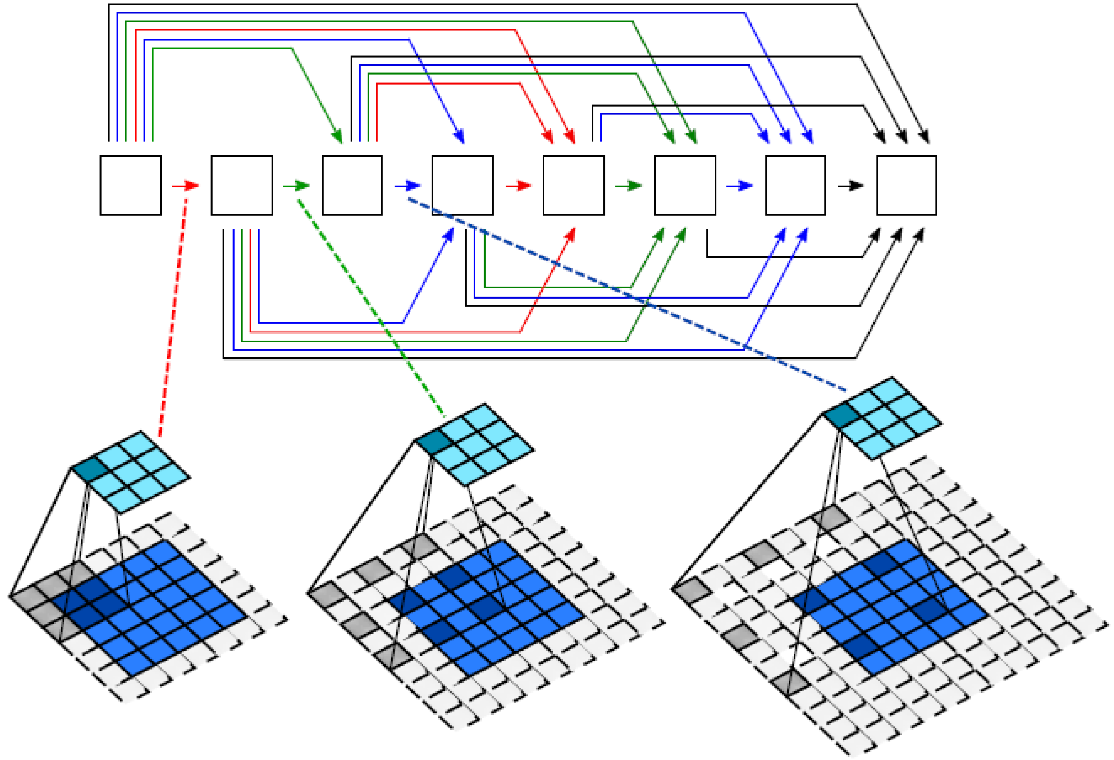


Architectures used for phase retrieval [4]

U-Net

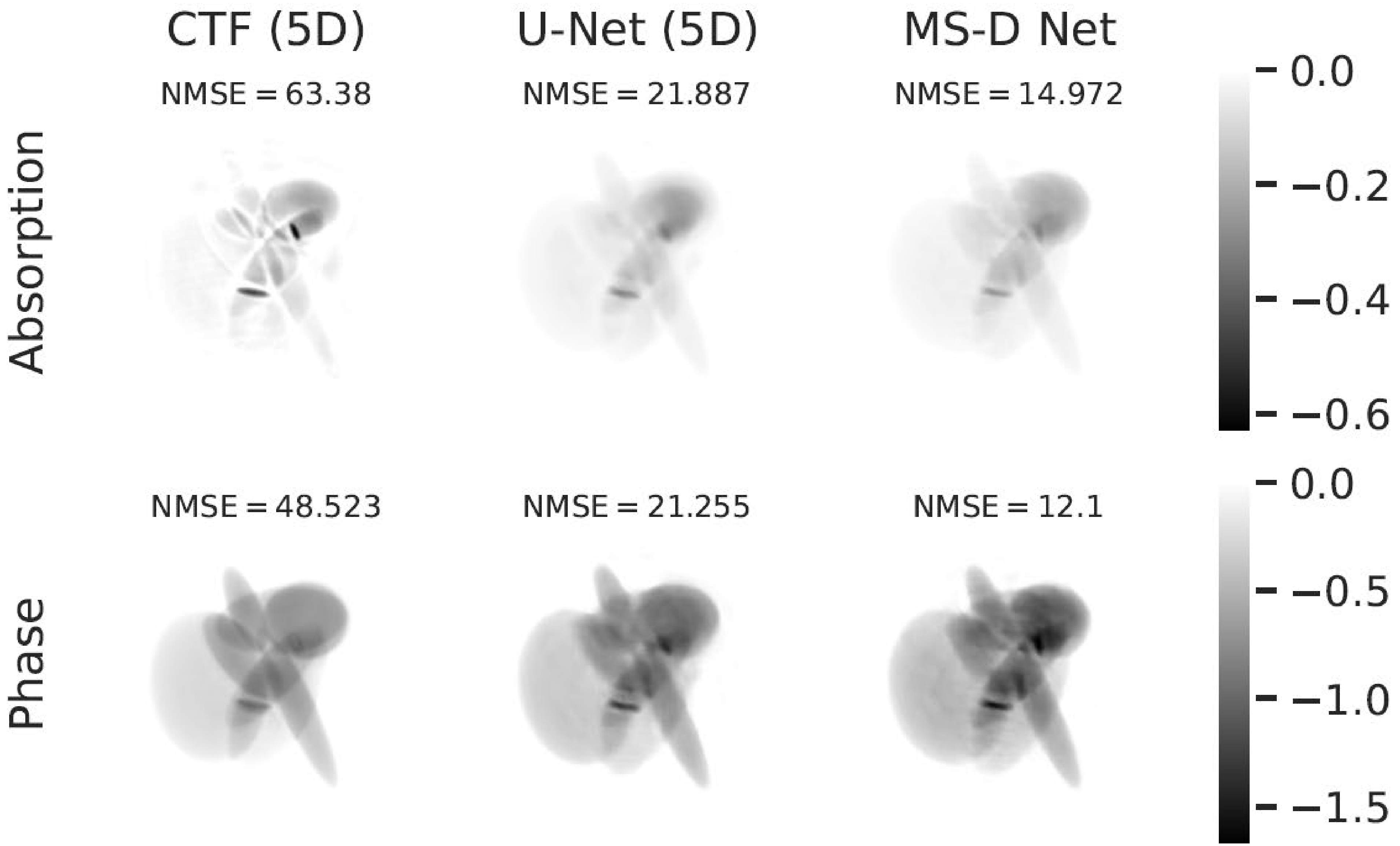


MS-D Net

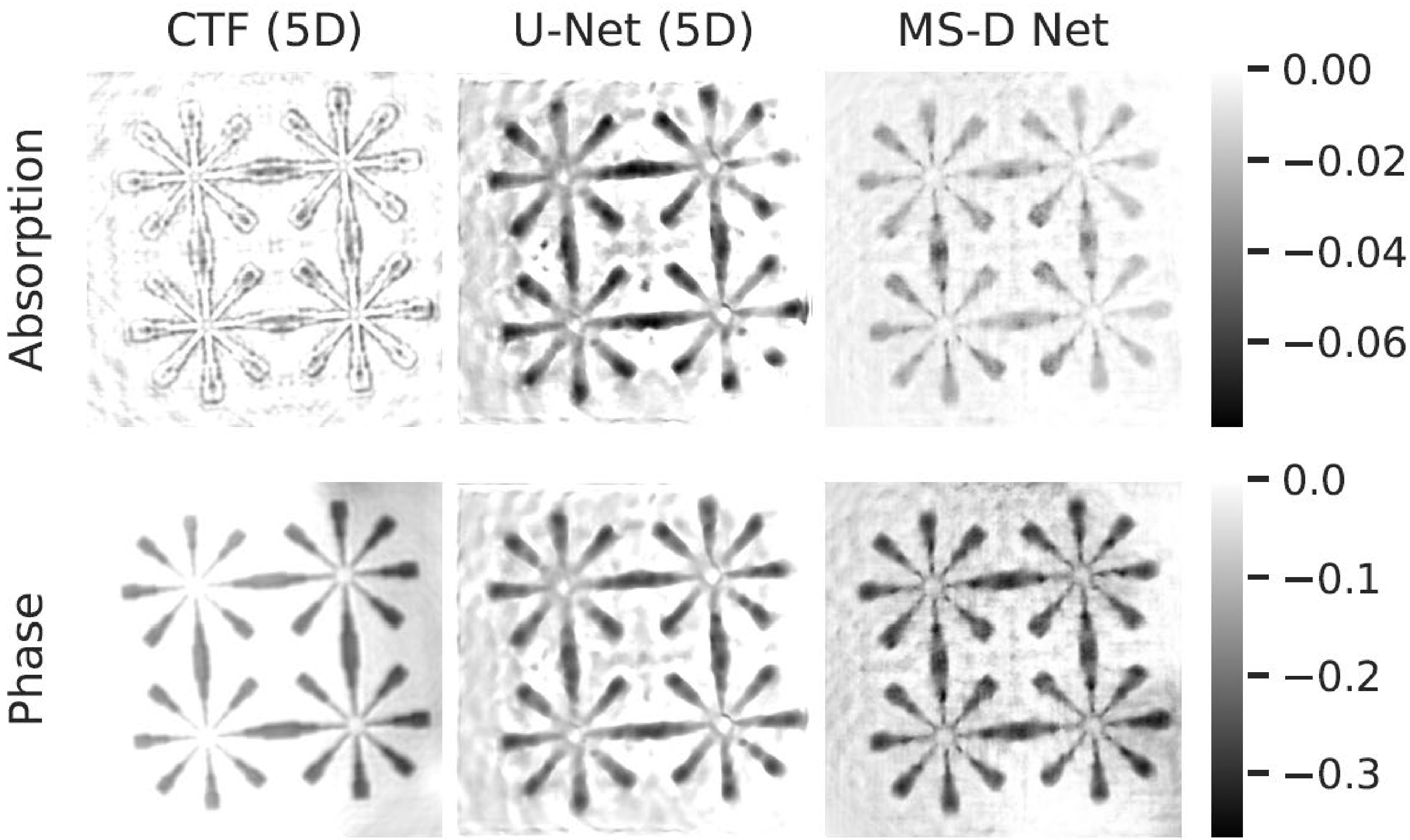


4. Jin et al., "Deep convolutional neural network for inverse problems in imaging."; Pelt, Batenburg et Sethian, "Improving tomographic reconstrucion from limited data using mixed-scale dense convolutional neural networks"; Mom, Sixou et Langer, "Mixed scale dense convolutional networks for X-ray phase-contrast imaging".

Results direct reconstruction - simulated data



Results of direct reconstruction - experimental data

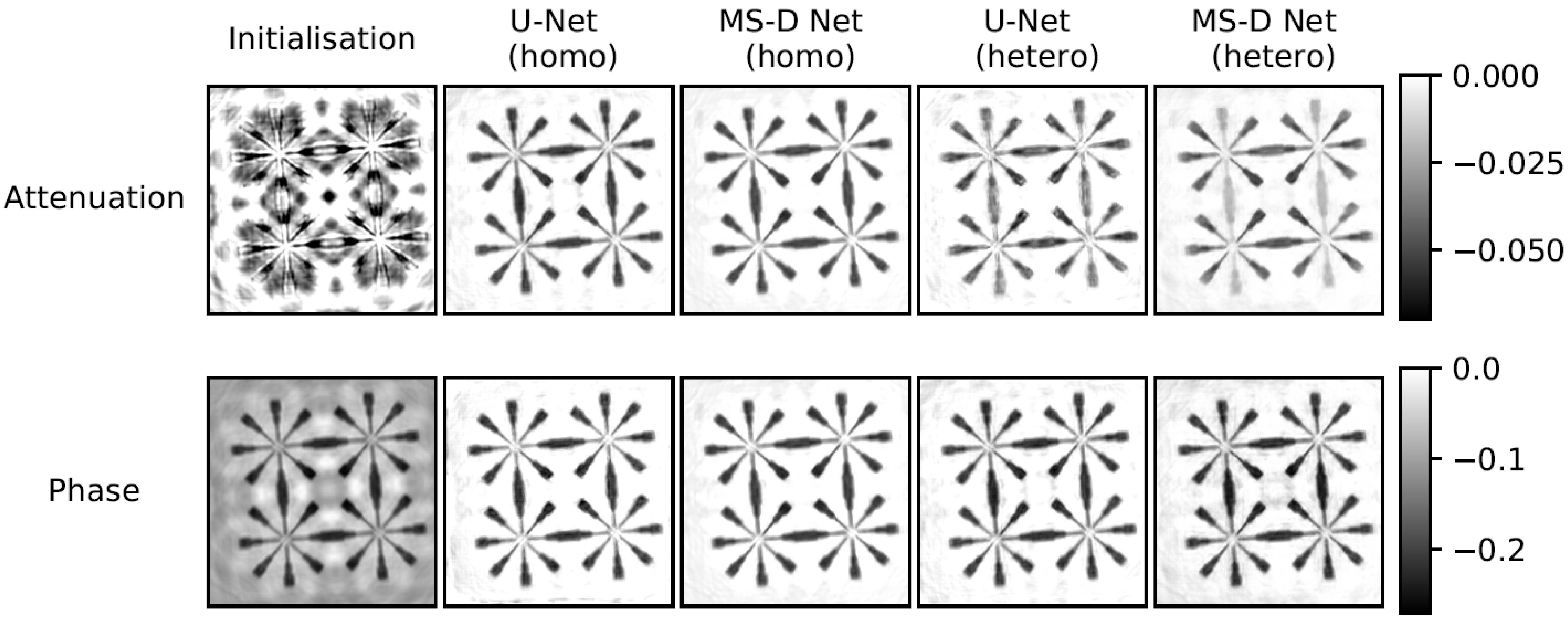


Direct reconstructions

+ Fast
+ Single distance without assumption on the object
+ Nonlinear contribution

- Doesn't generalize well to real data
- Depend on the quality of the training data
- Lack of physical knowledge

Direct reconstructions - what about the physics ?



Learned regularization

$$(B^*, \varphi^*) = \underset{B,\varphi}{\operatorname{argmin}} \left\{ ||\mathbf{F}_D(B,\varphi) - \mathbf{I}_D^{\text{obs}}||_2^2 + \mathbf{R}(B,\varphi) \right\}$$

Data fidelity term

Regularization term

Instead of using choosing $\mathbf{R}$ a priori, is it better to learn $\mathbf{R}$ from training data ?

Proximal Gradient Descent as example

$$(B^*, \varphi^*) = \underset{B,\varphi}{\operatorname{argmin}} \left\{ \left\| \mathbf{F}_D(B,\varphi) - \mathbf{I}_D^{\text{obs}} \right\|_2^2 + \mathbf{R}(B,\varphi) \right\}$$

Initialisation (B_0, φ_0) and step-size τ.

for $k = 1, \ldots, \ldots$ **do**

$\mathrm{d}_k = (B_k, \varphi_k) - \tau \mathbf{F}_D'(B_k, \varphi_k)^* \left(\mathbf{F}_D(B_k, \varphi_k) - \mathbf{I}_D^{\text{obs}} \right)$ — **Data Consistency**

$(B_{k+1}, \varphi_{k+1}) = \operatorname{prox}_{\tau \mathbf{R}}(d_k)$ — **Denoising**

end

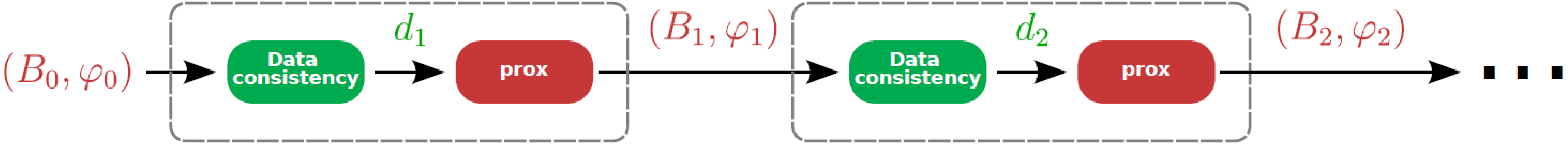


Figure – Proximal Gradient Descent

Plug-and-Play approach

$$(B^*, \varphi^*) = \underset{B,\varphi}{\operatorname{argmin}} \left\{ \left\| \mathbf{F}_D(B,\varphi) - \mathbf{I}_D^{\mathrm{obs}} \right\|_2^2 + \mathbf{R}(B,\varphi) \right\}$$

Initialisation (B_0, φ_0) and step-size τ.

for $k = 1, \ldots, \ldots$ **do**

$\quad d_k = (B_k, \varphi_k) - \tau \mathbf{F}'_D(B_k, \varphi_k)^* \left(\mathbf{F}_D(B_k, \varphi_k) - \mathbf{I}_D^{\mathrm{obs}}\right)$ — **Data Consistency**

$\quad (B_{k+1}, \varphi_{k+1}) = \mathbf{CNN}(d_k)$ — **Denoising**

end

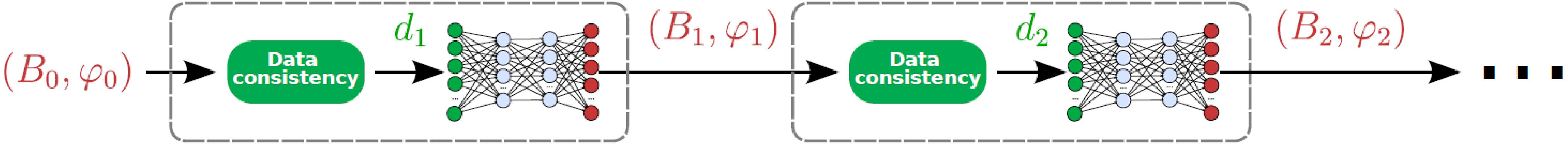
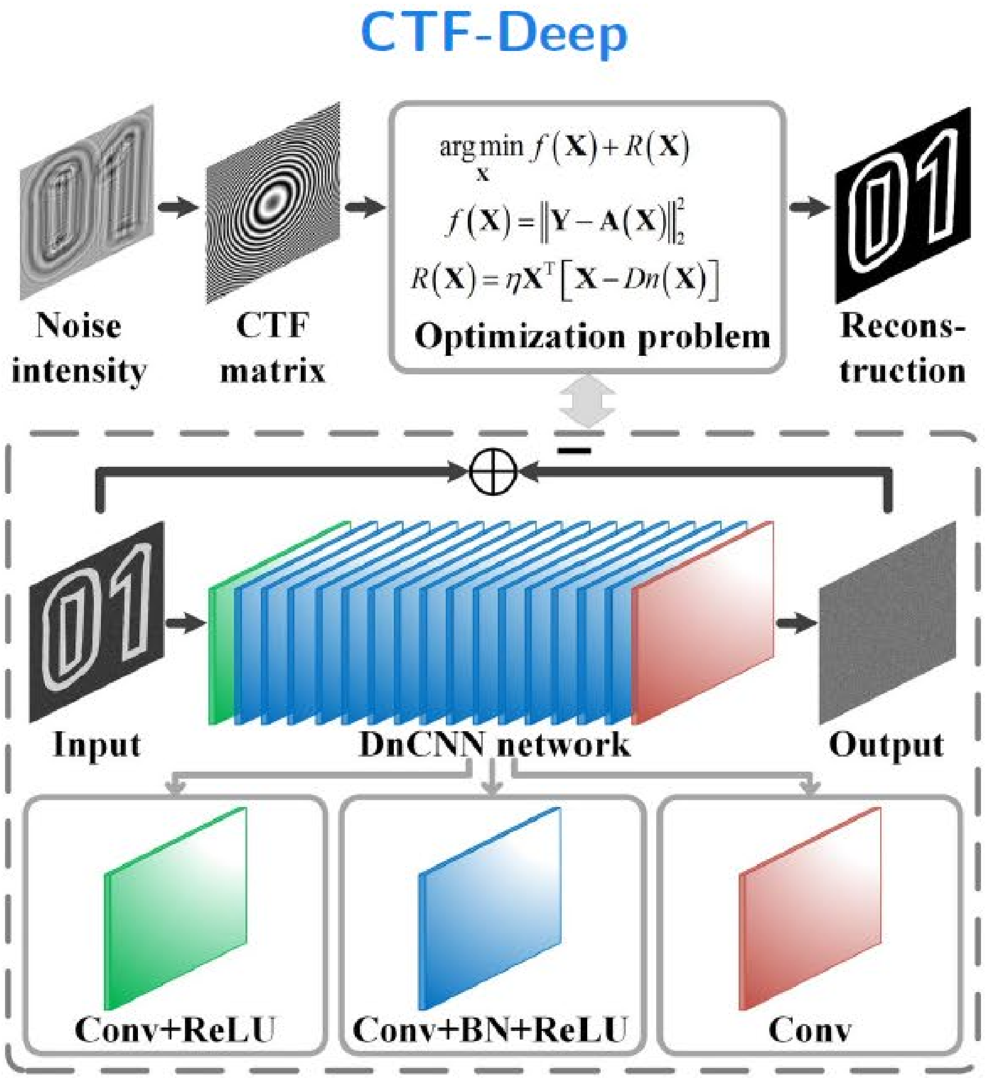
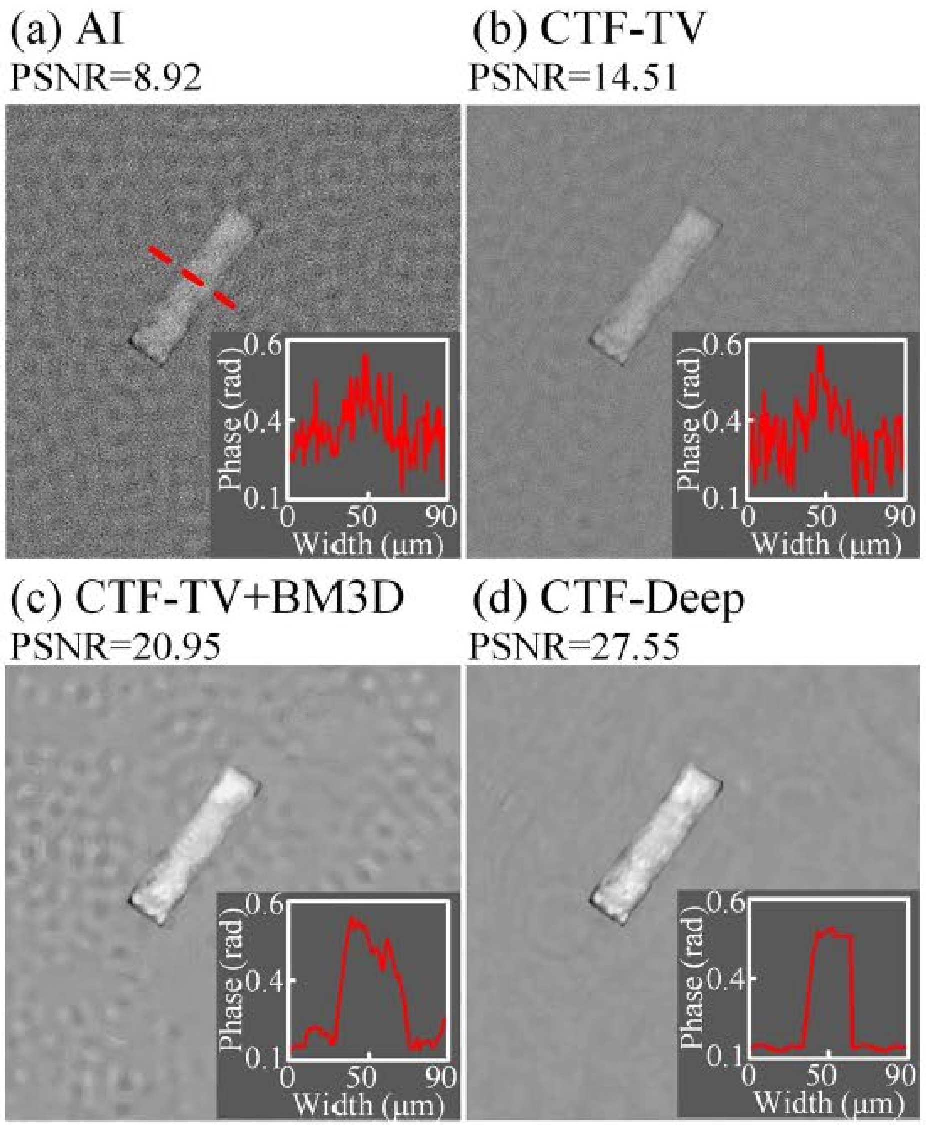


Figure – Plug-and-Play *Prox-grad*

Plug-and-Play for phase retrieval [8]



$$\arg\min_{\mathbf{X}} f(\mathbf{X}) + R(\mathbf{X})$$
$$f(\mathbf{X}) = \|\mathbf{Y} - \mathbf{A}(\mathbf{X})\|_2^2$$
$$R(\mathbf{X}) = \eta \mathbf{X}^T[\mathbf{X} - Dn(\mathbf{X})]$$



8. Bai et al., "Robust contrast-transfer-function phase retrieval via flexible deep learning networks".

Deep unrolling

- **Unrolling** : Fix number of iterations and transform iterations to sequence of CNNs
- Train end-to-end
- Informed not only by physics but how to find solution

$$(B^*, \varphi^*) = \underset{B,\varphi}{\operatorname{argmin}} \left\{ \left\| \mathbf{F}_D(B,\varphi) - \mathbf{I}_D^{\mathrm{obs}} \right\|_2^2 + \mathbf{R}(B,\varphi) \right\}$$

Initialisation (B_0, φ_0) and step-size τ.

for $\boxed{k = 1, \ldots, N}$ **do**

$\mathrm{d}_k = (B_k, \varphi_k) - \tau \mathbf{F}_D'(B_k, \varphi_k)^* \left(\mathbf{F}_D(B_k, \varphi_k) - \mathbf{I}_D^{\mathrm{obs}}\right)$ **Data Consistency**

$(B_{k+1}, \varphi_{k+1}) = \mathbf{CNN}(d_k)$ **Denoising**

end

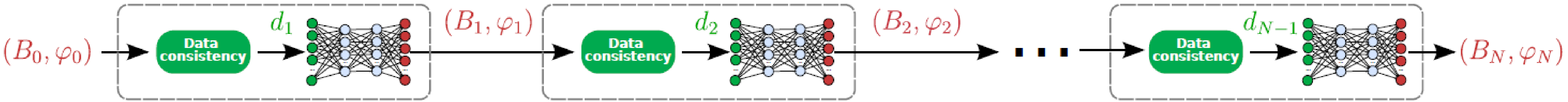


Figure – Deep unrolling Prox-grad

Unrolling in image and signal processing [9]

TABLE I
SUMMARY OF RECENT METHODS EMPLOYING ALGORITHM UNROLLING IN PRACTICAL SIGNAL PROCESSING AND IMAGING APPLICATIONS.

Reference	Year	Application domain	Topics	Underlying Iterative Algorithms
Hershey *et al.* [30]	2014	Speech Processing	Signal channel source separation	Non-negative matrix factorization
Wang *et al.* [26]	2015	Computational imaging	Image super-resolution	Coupled sparse coding with iterative shrinkage and thresholding
Zheng *et al.* [31]	2015	Vision and Recognition	Semantic image segmentation	Conditional random field with mean-field iteration
Schuler *et al.* [32]	2016	Computational imaging	Blind image deblurring	Alternating minimization
Chen *et al.* [16]	2017	Computational imaging	Image denoising, JPEG deblocking	Nonlinear diffusion
Jin *et al.* [27]	2017	Medical Imaging	Sparse-view X-ray computed tomography	Iterative shrinkage and thresholding
Liu *et al.* [33]	2018	Vision and Recognition	Semantic image segmentation	Conditional random field with mean-field iteration
Solomon *et al.* [34]	2018	Medical imaging	Clutter suppression	Generalized ISTA for robust principal component analysis
Ding *et al.* [35]	2018	Computational imaging	Rain removal	Alternating direction method of multipliers
Wang *et al.* [36]	2018	Speech processing	Source separation	Multiple input spectrogram inversion
Adler *et al.* [37]	2018	Medical Imaging	Computational tomography	Proximal dual hybrid gradient
Wu *et al.* [38]	2018	Medical Imaging	Lung nodule detection	Proximal dual hybrid gradient
Yang *et al.* [14]	2019	Medical imaging	Medical resonance imaging, compressive imaging	Alternating direction method of multipliers
Hosseini *et al.* [39]	2019	Medical imaging	Medical resonance imaging	Proximal gradient descent

9. MONGA, LI et ELDAR, "Algorithm Unrolling: Interpretable, Efficient Deep Learning for Signal and Image Processing".

Deep Gauss-Newton (DGN) [11]

$$(B_{k+1},\varphi_{k+1}) = (B_k,\varphi_k) + \left[\mathbf{F}'_D(B_k,\varphi_k)^*\mathbf{F}'_D(B_k,\varphi_k) + \alpha_k\right]^{-1}\left\{\mathbf{F}'_D(B_k,\varphi_k)^*\left[\mathbf{I}_D^{\mathrm{obs}} - \mathbf{F}_D(B_k,\varphi_k)\right] - \alpha_k(B_k,\varphi_k)\right\}$$

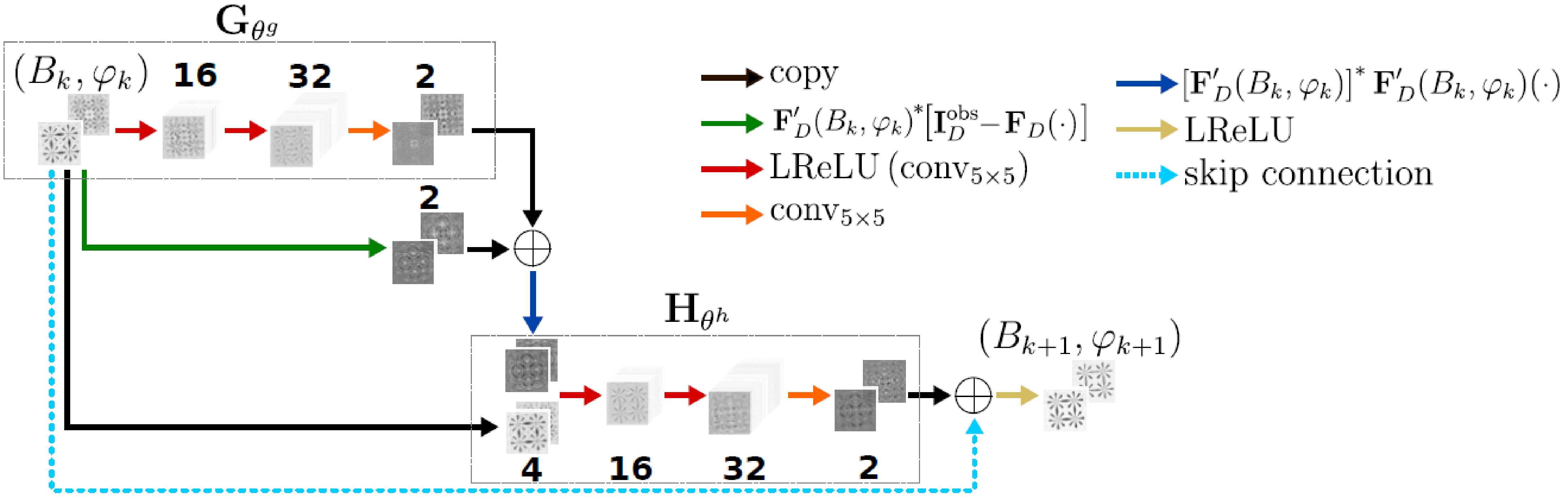


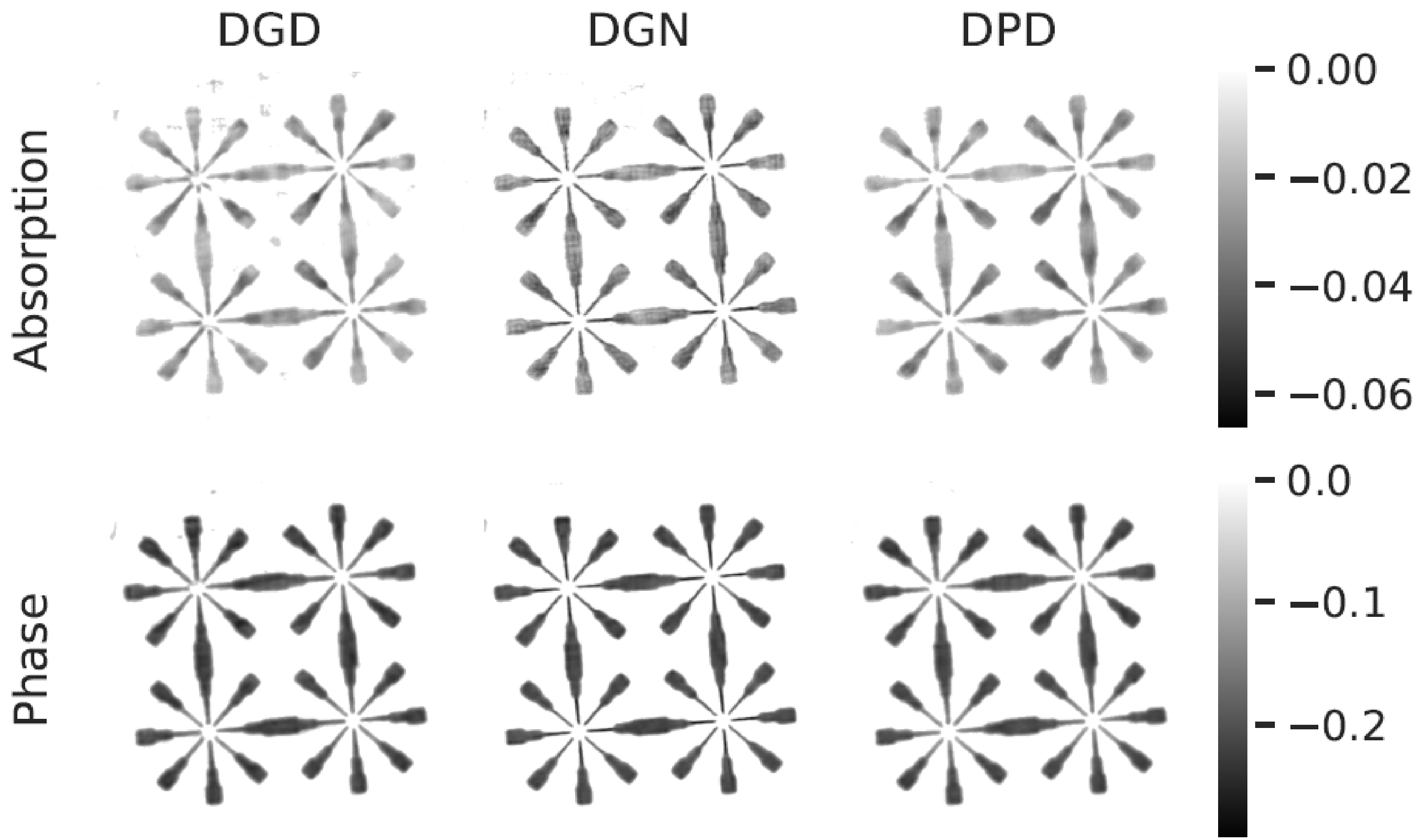
Figure – Architecture proposed for one iteration.

$$\Gamma_\theta = \mathrm{Id} + \mathbf{H}_{\theta^h}\left[(B_k,\varphi_k),\mathbf{F}'_D(B_k,\varphi_k)^*\mathbf{F}'_D(B_k,\varphi_k)\left\{\mathbf{F}'_D(B_k,\varphi_k)^*\left[\mathbf{I}_D^{\mathrm{obs}} - \mathbf{F}_D(B_k,\varphi_k)\right] + \mathbf{G}_{\theta^g(B_k,\varphi_k)}\right\}\right]$$

11. Mom, Langer et Sixou, "Deep Gauss-Newton for phase retrieval".

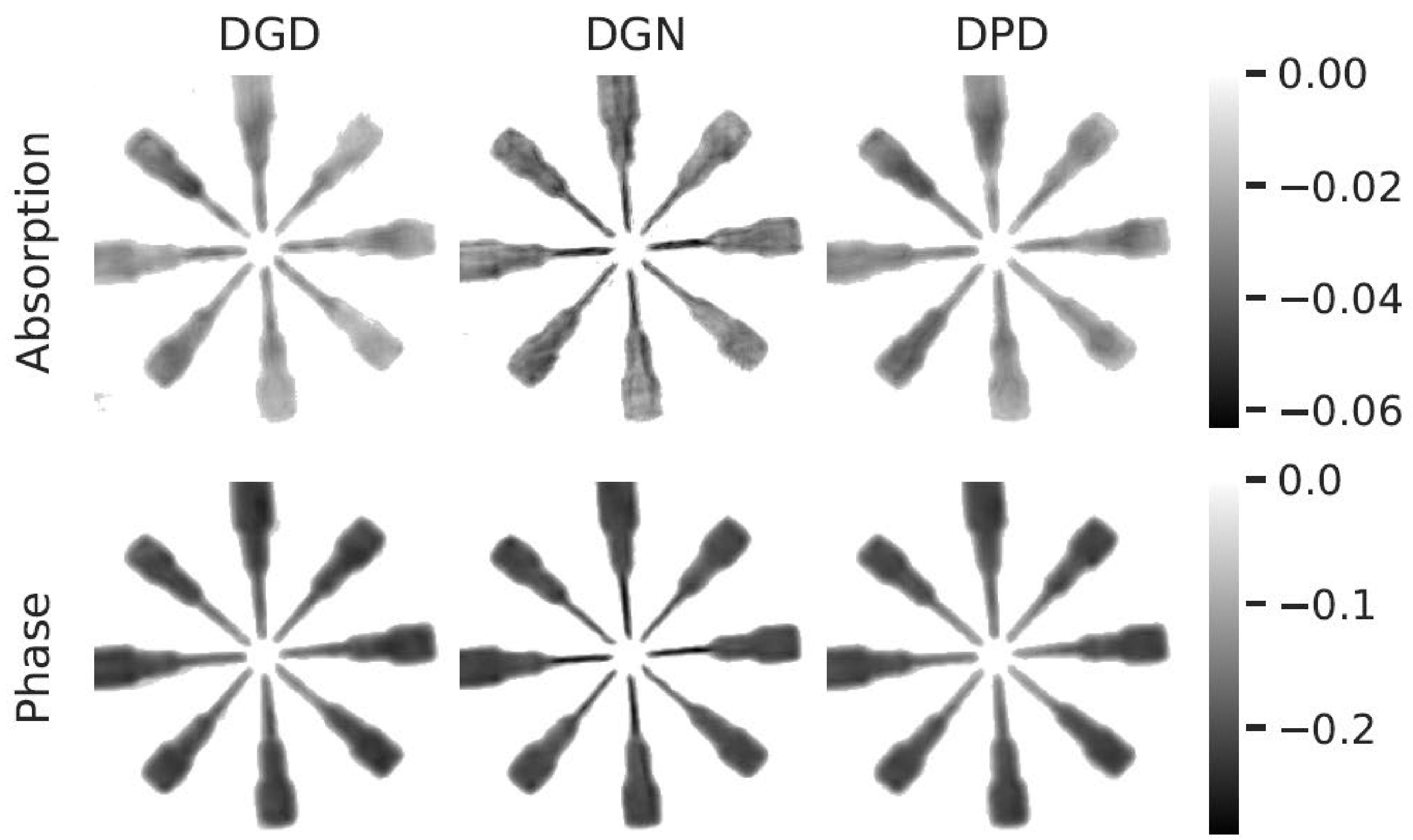
Comparison with other unrolling schemes [13] [14]

- Deep Gradient-Descent (DGD), Deep Primal-Dual (DPD)



13. Hauptmann et al., "Model-Based Learning for Accelerated, Limited-View 3-D Photoacoustic Tomography".
14. Adler et Oktem, "Learned Primal-Dual Reconstruction".

Comparison with other unrolling schemes



Quantitative evaluation

- Average Quality over 1000 simulated images

Method	NMSE (in %) Absorption	NMSE (in %) Phase	FRCM Absorption	FRCM Phase	Resolution (in nm) Absorption	Resolution (in nm) Phase	#Parameters	Time (s)
MS-D Net	13.6 (12.8)	10.6 (10.8)	48.8 (13.8)	47.8 (13.3)	102 (77.4)	98.5 (135)	45×10^3	**2.60**
U-Net	12.8 (17.4)	10.4 (15.9)	45.9 (17.9)	45.9 (18.0)	94.5 (91.7)	96.6 (158)	31×10^6	2.85
GD-TV$^\epsilon$	37.5 (17.4)	36.4 (18.2)	61.8 (12.2)	57.7 (13.2)	214 (101)	139 (78)	–	145
IRGN	85.5 (40.7)	39.3 (15.0)	71.2 (9.95)	68.1 (5.45)	238 (136)	154 (43)	–	116
NL-PDHG	29.19 (14.8)	23.6 (12.6)	58.4 (9.08)	50.7 (8.28)	146 (85.2)	99.7 (26.5)	–	147
DGD	13.2 (17.3)	4.74 (6.99)	37.6 (13.2)	23.8 (15.7)	82.2 (116)	64.3 (62.6)	41×10^3	4.85
DPD	12.5 (15.5)	**4.48 (6.2)**	39.2 (14.4)	24.3 (16.5)	107 (138)	75.5 (66.7)	31×10^3	5.63
DGN	**12.1 (13.5)**	4.61 (6.20)	**35.7 (15.7)**	**23.0 (16.6)**	**72.2 (55.2)**	**62.3 (37.0)**	31×10^3	5.88

Table – Comparison of different methods applied on the test dataset containing 1 000 images, according to different metrics.

Comparison with other unrolling schemes

+ Fast
+ Take knowledge of the physical model into account
+ More robust and better generalization

- A lot of memory required
- Lack of convergence proof
- Model need to be accurate

PyPhase - a Python package for phase retrieval

- Motivation : facilitate access to phase retrieval codes and permit development, testing, comparison and deployment of different algorithms

- A library of phase retrieval algorithms
- High level of modularity to facilitate the integration of different functionality, e.g., registration, tomography, reading and writing data, and visualization.
- Tools for deployment on different computing infrastructures
- Tools for implementation and development of phase retrieval algorithms
- available on PyPI

- Repository : https ://gitlab.in2p3.fr/mlanger/pyPhase
- Publication Journal of Synchrotron Radiation (May 2021) : https ://journals.iucr.org/s/issues/2021/04/00/gy5024/gy5024.pdf

Deep learning for phase retrieval in propagation-based X-ray phase contrast imaging

Kannara Mom, Bruno Sixou, Max Langer

Université Grenoble Alpes, CNRS, UMR 5525, VetAgro Sup, Grenoble INP, TIMC, 38000 Grenoble, France

max.langer@univ-grenoble-alpes.fr

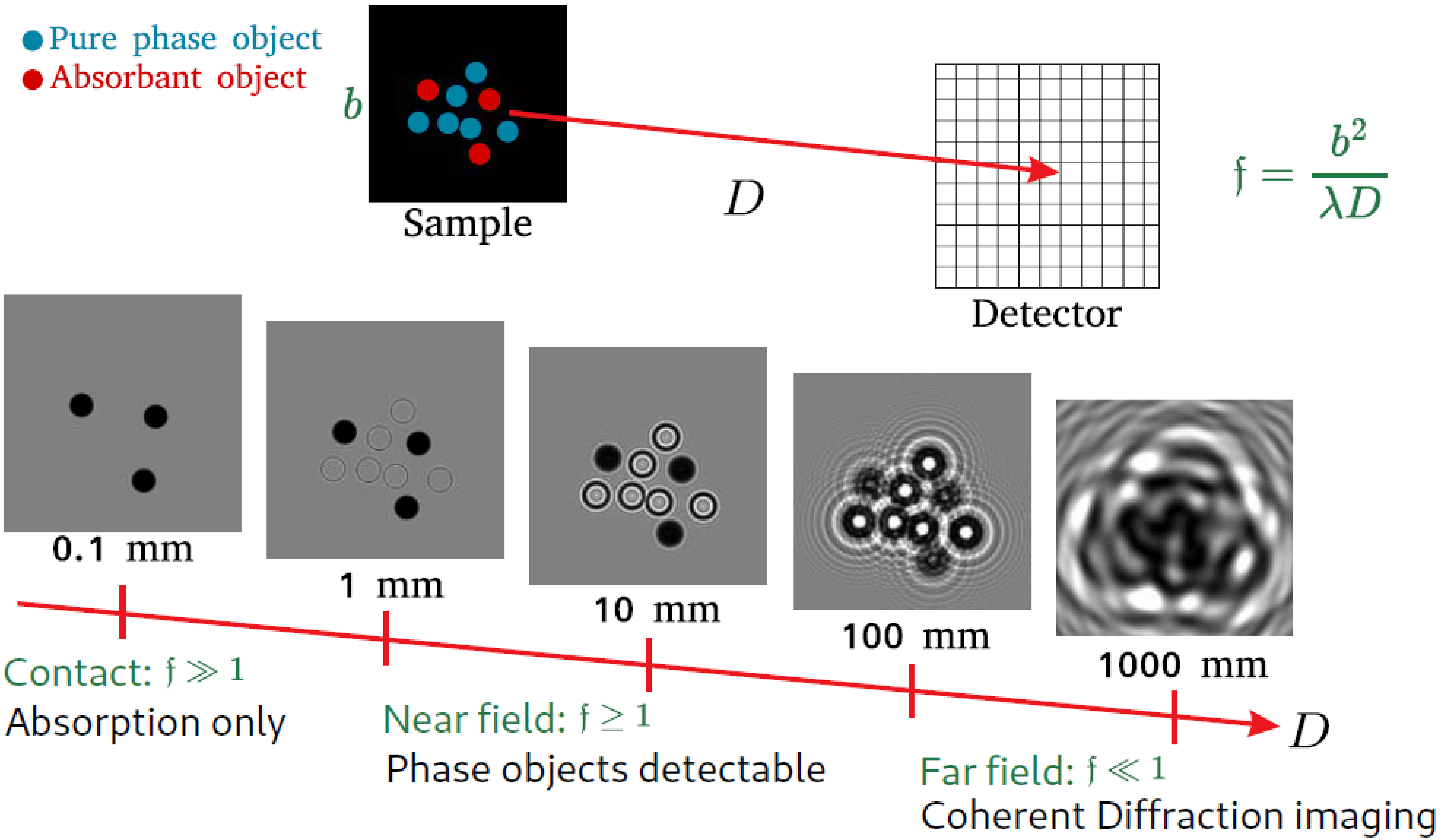
Simulation of X-ray phase contrast using the Wigner Distribution Function

Emilie Pietersoone, Jean Michel Létang, Simon Rit, Emmanuel Brun, Max Langer

Université Grenoble Alpes, CNRS, UMR 5525, VetAgro Sup, Grenoble INP, TIMC, 38000 Grenoble, France

max.langer@univ-grenoble-alpes.fr

Simulation of phase contrast



[Nielsen, McMorrow (2011)]

Simulation of phase contrast

- Origin of artefacts – LF problem due to scatter?
- Preparation of synchrotron experiments
- Training data for CNN methods
- Address validity of Fresnel/Fraunhofer model
- Combine contributions from “all” physical processes
- Idea: calculate interference at the exit plane instead of the detector plane using the Wigner Distribution Function (WDF)
    - Generate photon trajectories by sampling the WDF
    - Combine with MC simulation for incoherent effects
    - Simulate a coherent imaging system photon by photon

Wigner Distribution Function

T. Pfau, Phys. Today 1998

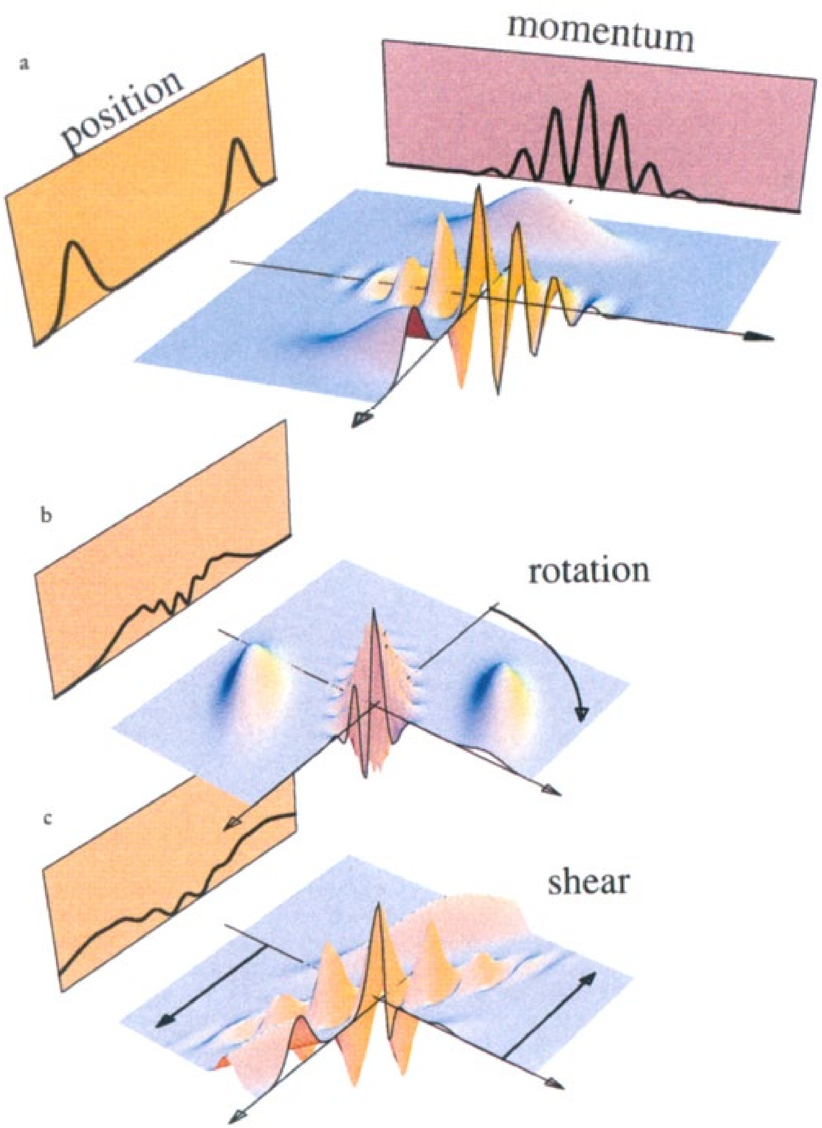
- WDF: $W_f(x,\phi) = \int f\left(x+\frac{y}{2}\right) f^*(x-\frac{y}{2}) e^{i\frac{2\pi}{\lambda}x\phi}$

- Quasi-probability (real but can be negative)

- Projection property

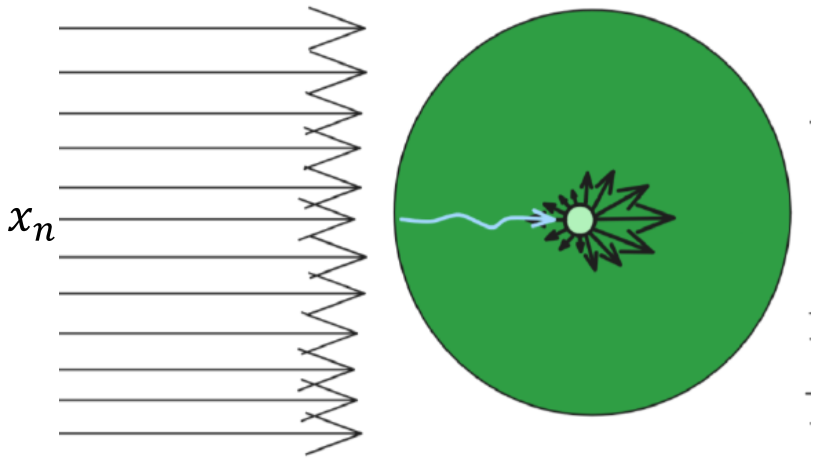
$$|f(x)|^2 = \int W_f(x,\phi)\, d\phi \quad \left|\tilde{f}\,(\phi)\right|^2 = \int W_f(x,\phi)\, dx$$

- Independent of (but related to) contrast model
    - Fraunhofer: rotation of WDF by π/2
    - Fresnel: shear of WDF by λD



Proposed algorithm

- Generate a photon with random position x_n
- Simulate scattering through Monte Carlo particle transport
  - If scattered, ray-trace to detector and record a hit



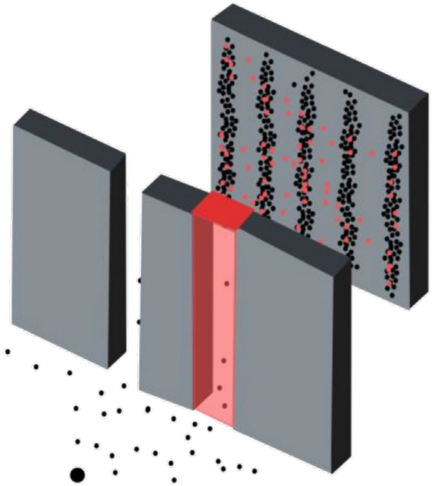
- If not scattered, check absorption with

$$P(x_n) = \int \left|W_f(x_n, \phi)\right| d\phi$$

- If not absorbed, get diffraction angle and sign according to $W_f(x_n, \phi)$
  - Ray-trace to detector.
  - If sign negative, increase negative potential +1
  - If sign positive, decrease negative potential and record a hit if <0
  - Signed particle formulation of quantum physics (Sellier 2018)

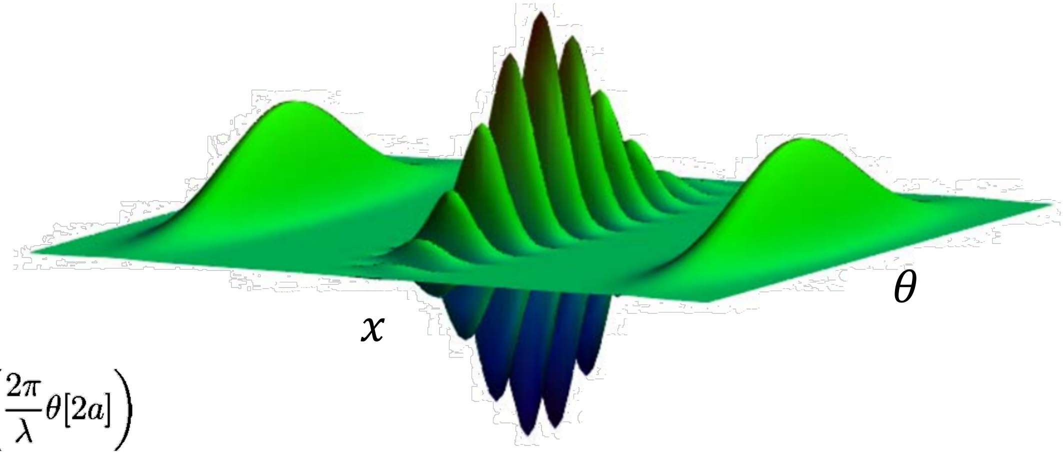
Proof of concept – Double-slit with scatterer

- Keep everything analytical to avoid numerical problems for now

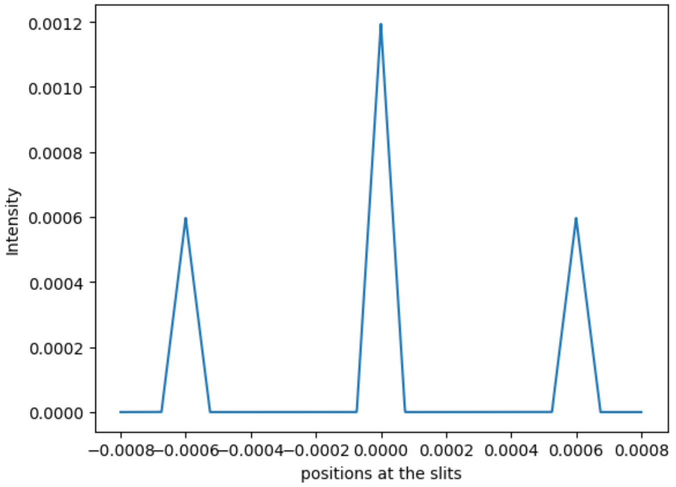


$$\Psi(x) = B_1 \prod\left(\frac{x-a}{A}\right) + B_2 \prod\left(\frac{x+a}{A}\right)$$

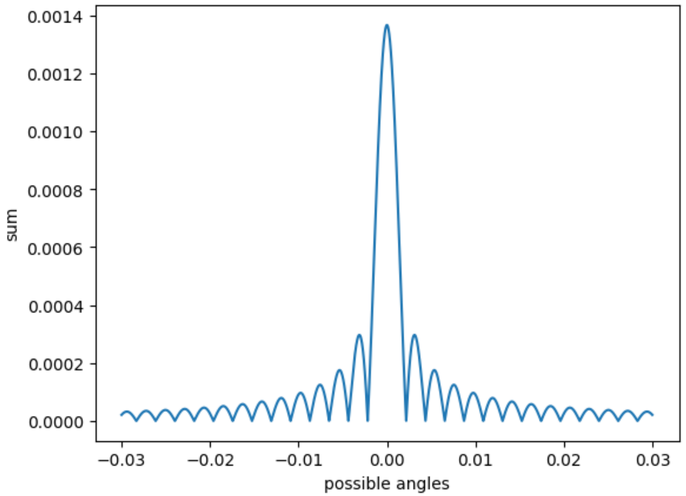
$$W_\Psi(x,\theta) = 2AB_1 \wedge\left(\frac{x-a}{A/2}\right) \mathrm{sinc}\left([2A-4|x-a|]\frac{\theta}{\lambda}\right) + 2AB_2 \wedge\left(\frac{x+a}{A/2}\right) \mathrm{sinc}\left([2A-4|x+a|]\frac{\theta}{\lambda}\right) + 4 * A(B_1 * B_2) \wedge\left(\frac{x}{A/2}\right) \mathrm{sinc}\left([2A-4|x|]\frac{\theta}{\lambda}\right) \cos\left(\frac{2\pi}{\lambda}\theta[2a]\right)$$



$$P(x) = \int \left|W_f(x,\phi)\right| d\phi$$



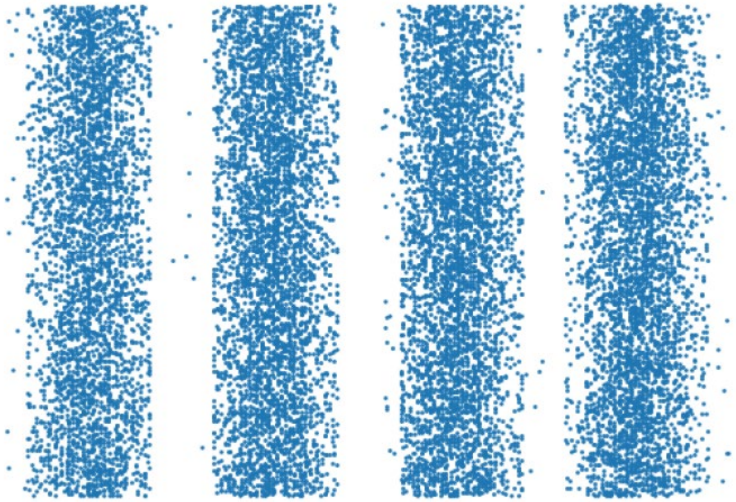
$$W_f(x_n,\phi)$$



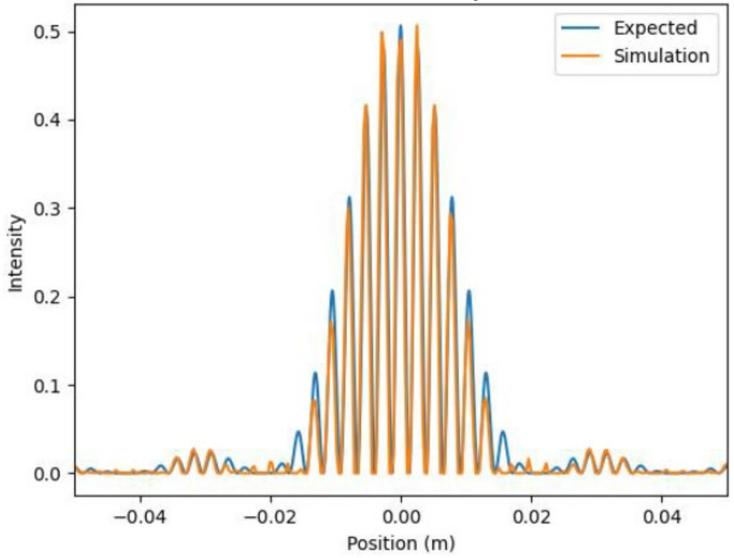
Results

No scattering

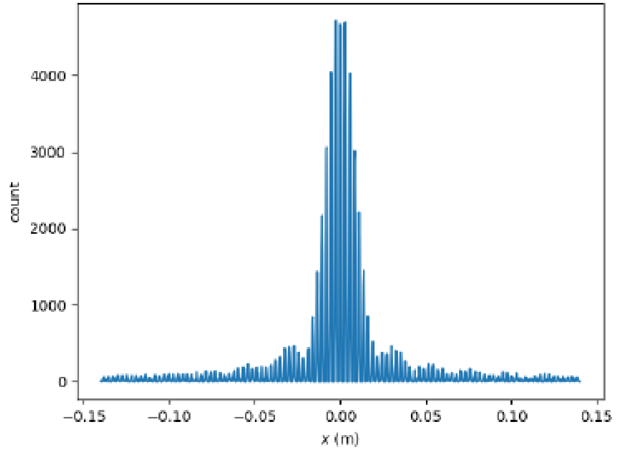
Individual hits on the detector



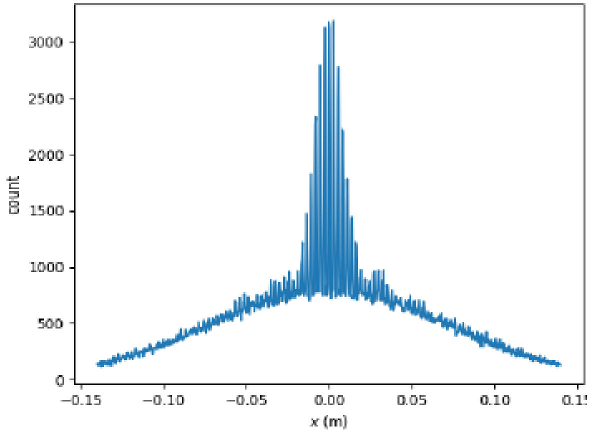
Intensity



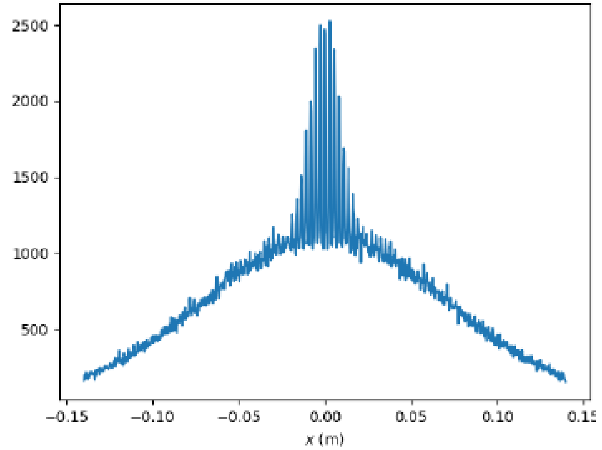
With scattering



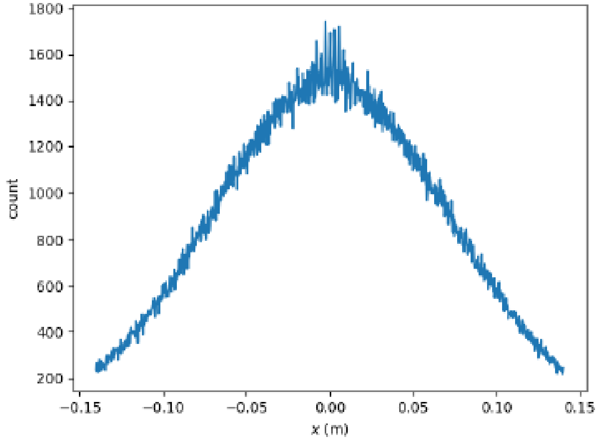
0% scattering



50% scattering



70% scattering



95% scattering

Wigner Approach - conclusion

- Simple successful proof of concept, but…
- Numerical calculation of $P(x_n) = \int \left|W_f(x_n, \phi)\right| d\phi$ and $W_f(x_n, \phi)$

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