



# Splitting Strategies for Structured Illumination Microscopy Reconstruction

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**Emmanuel Soubies**, IRIT, CNRS, Université de Toulouse

Journées Optimisation Fonctionnelle – CNES, COMET-TSI

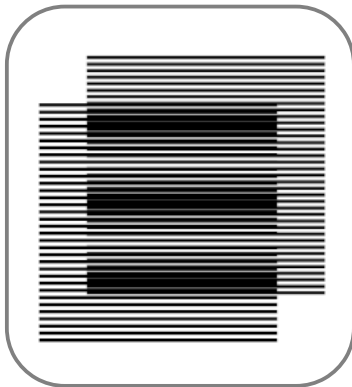
Wednesday June 26th 2024, ISAE-Toulouse



# Outline of the Talk

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**SIM Principle**



**ADMM for SIM**



**GlobalBioIm**

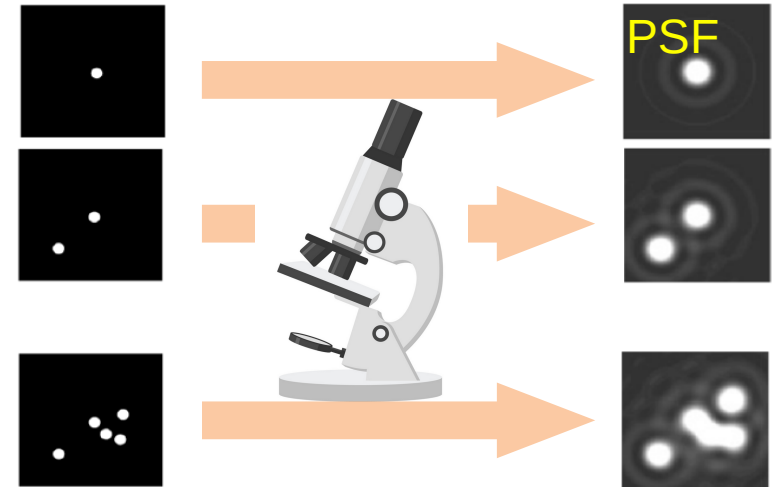


# Resolution Limit in Microscopy

## Diffraction Phenomenon

- Limited physical aperture of optical components
- Restrict the spatial extent of the wavefront

*The system response to a source point is a blurry spot*

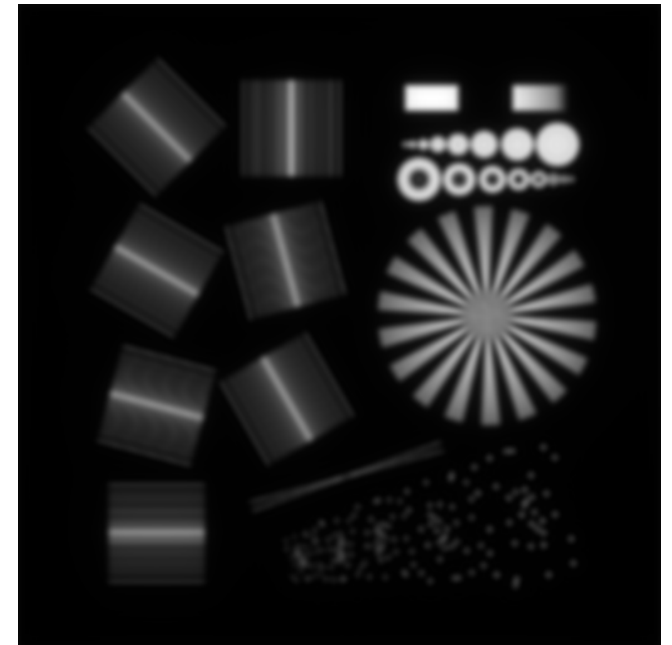
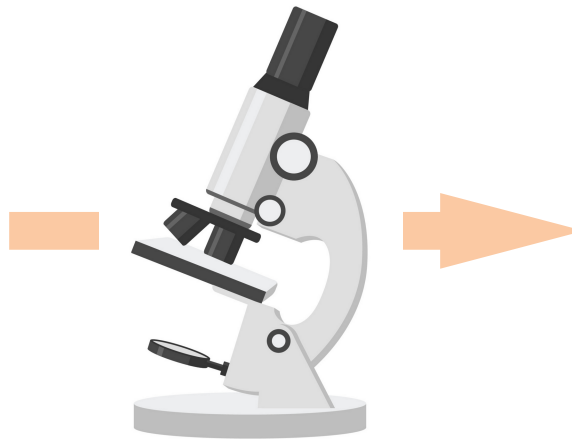
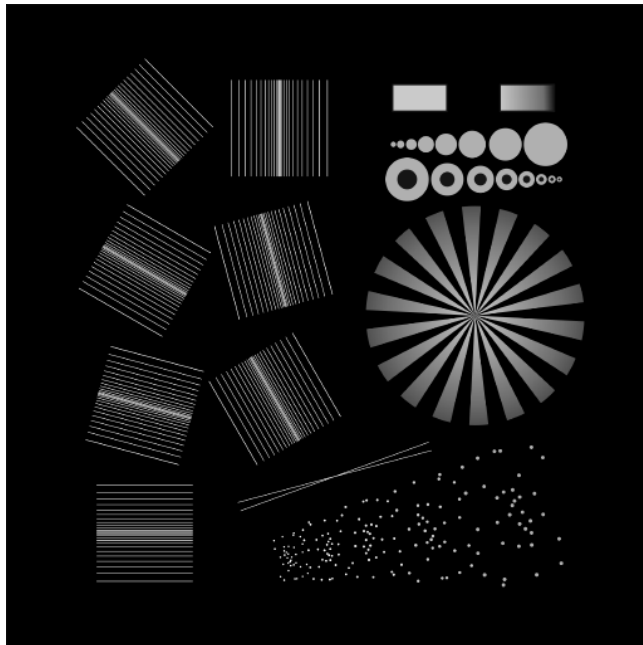
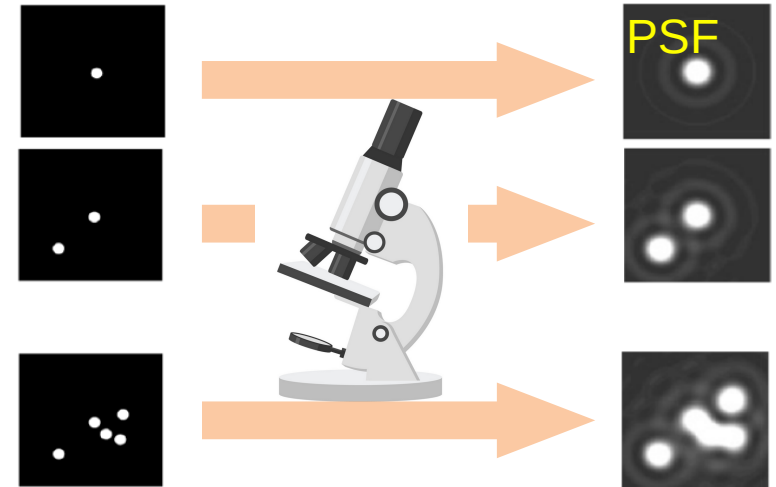


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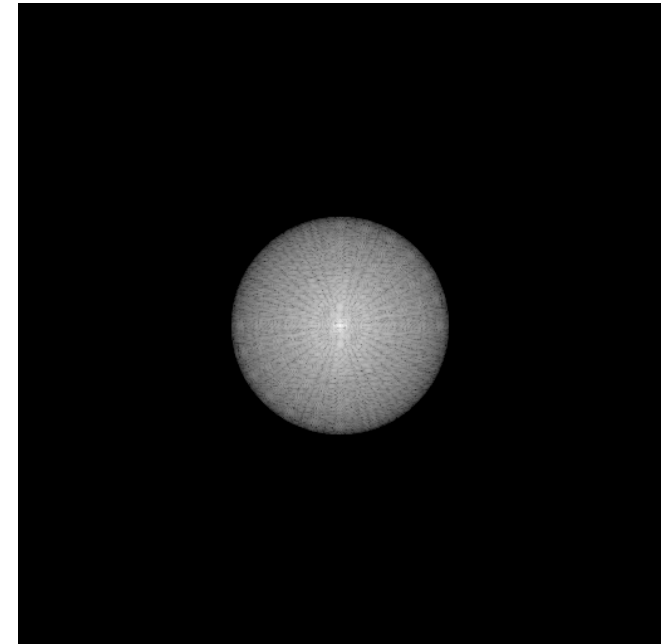
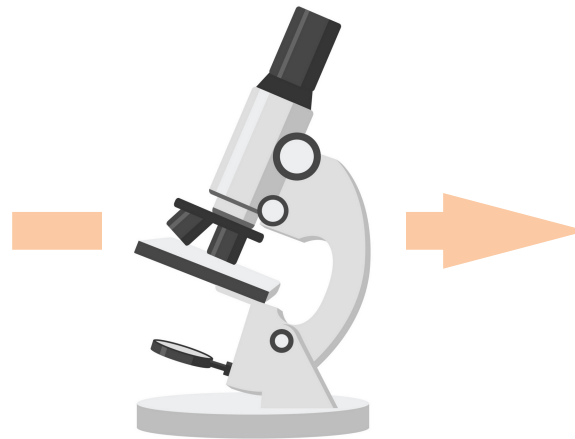
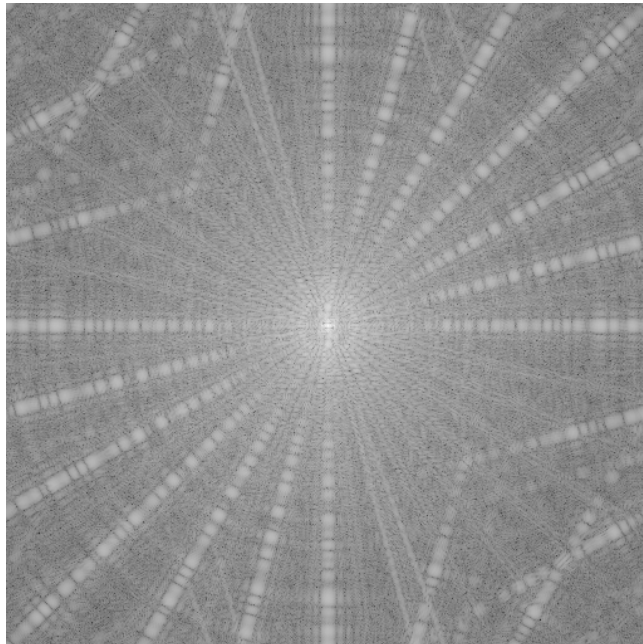
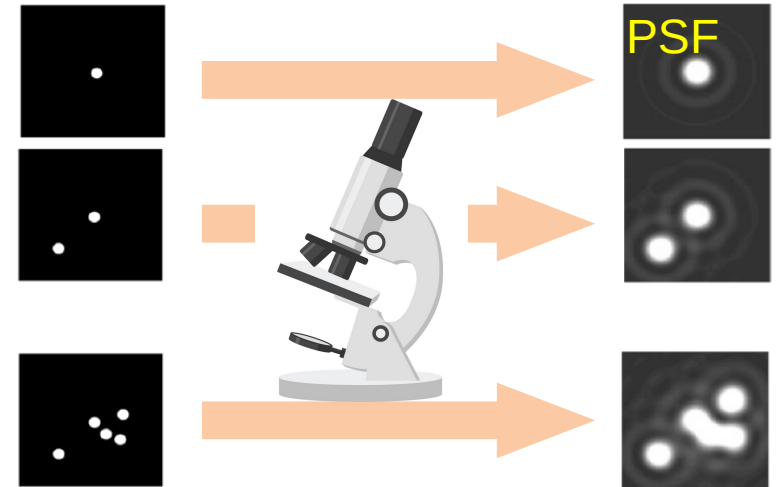


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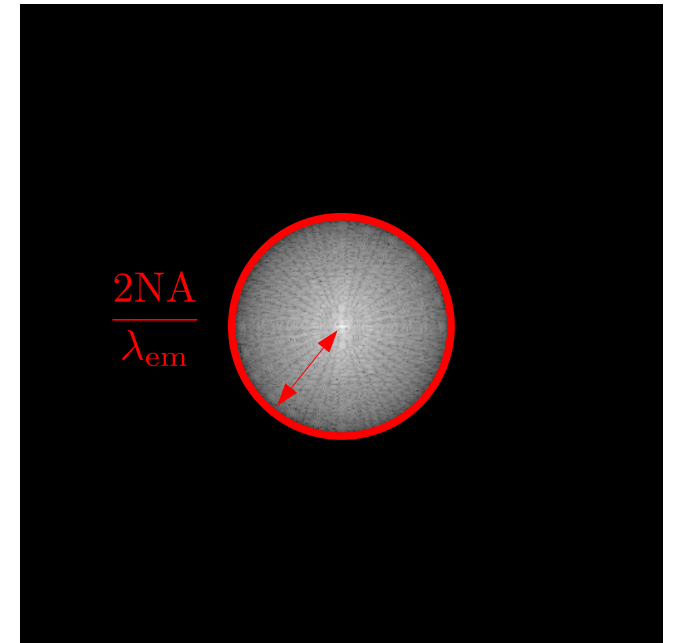
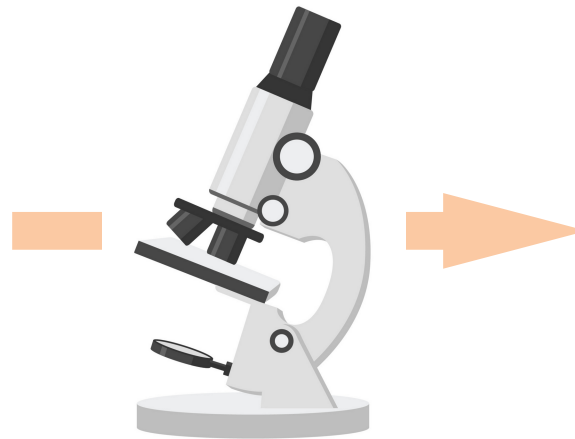
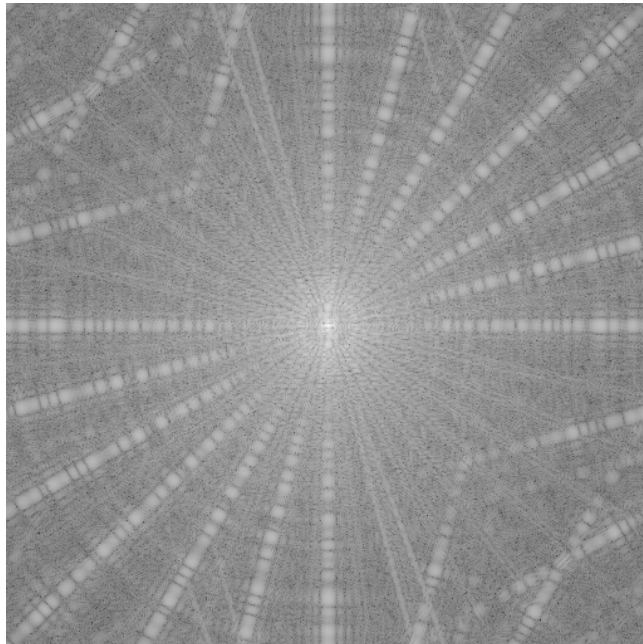
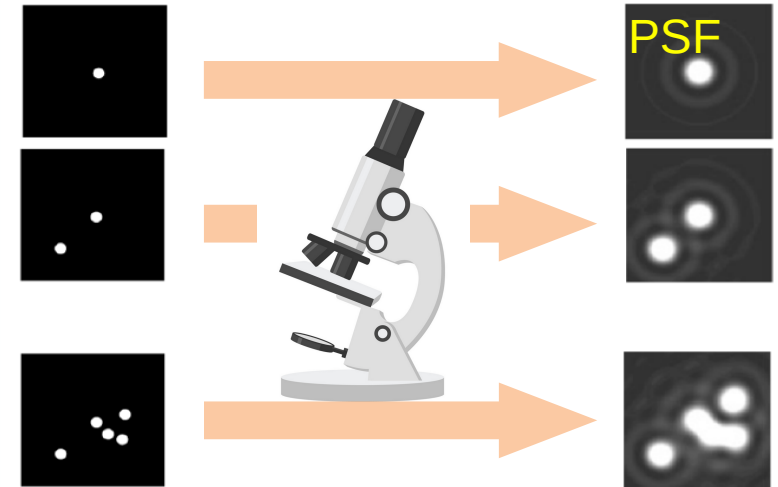


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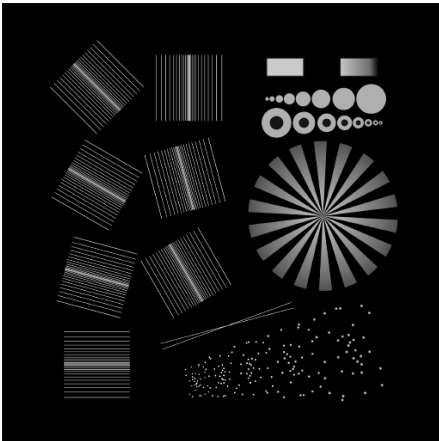
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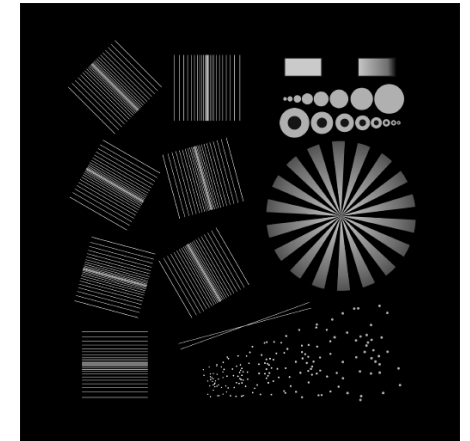
# Resolution Limit in Microscopy

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Sample



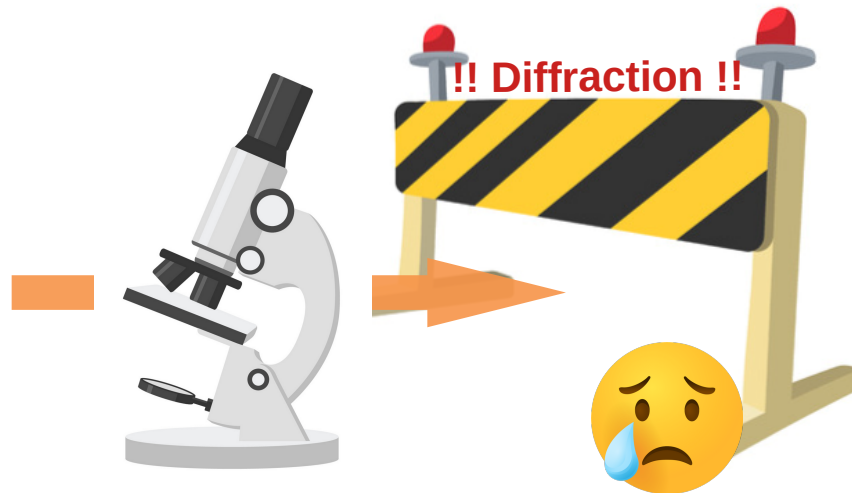
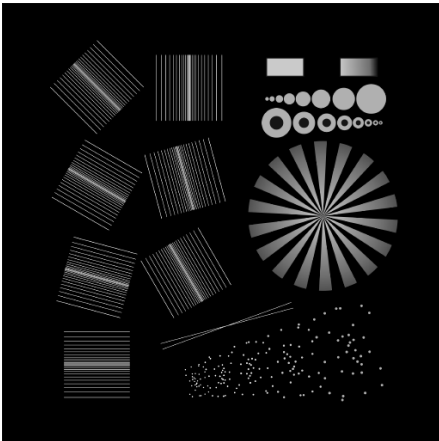
“Ideal” image



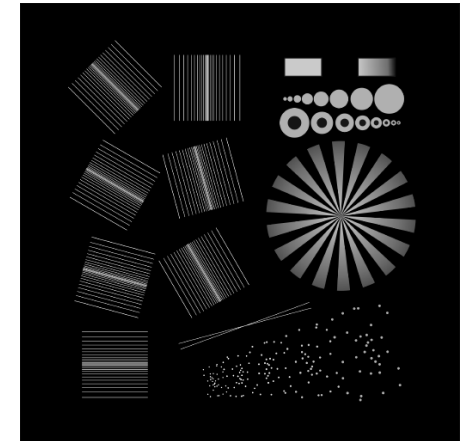
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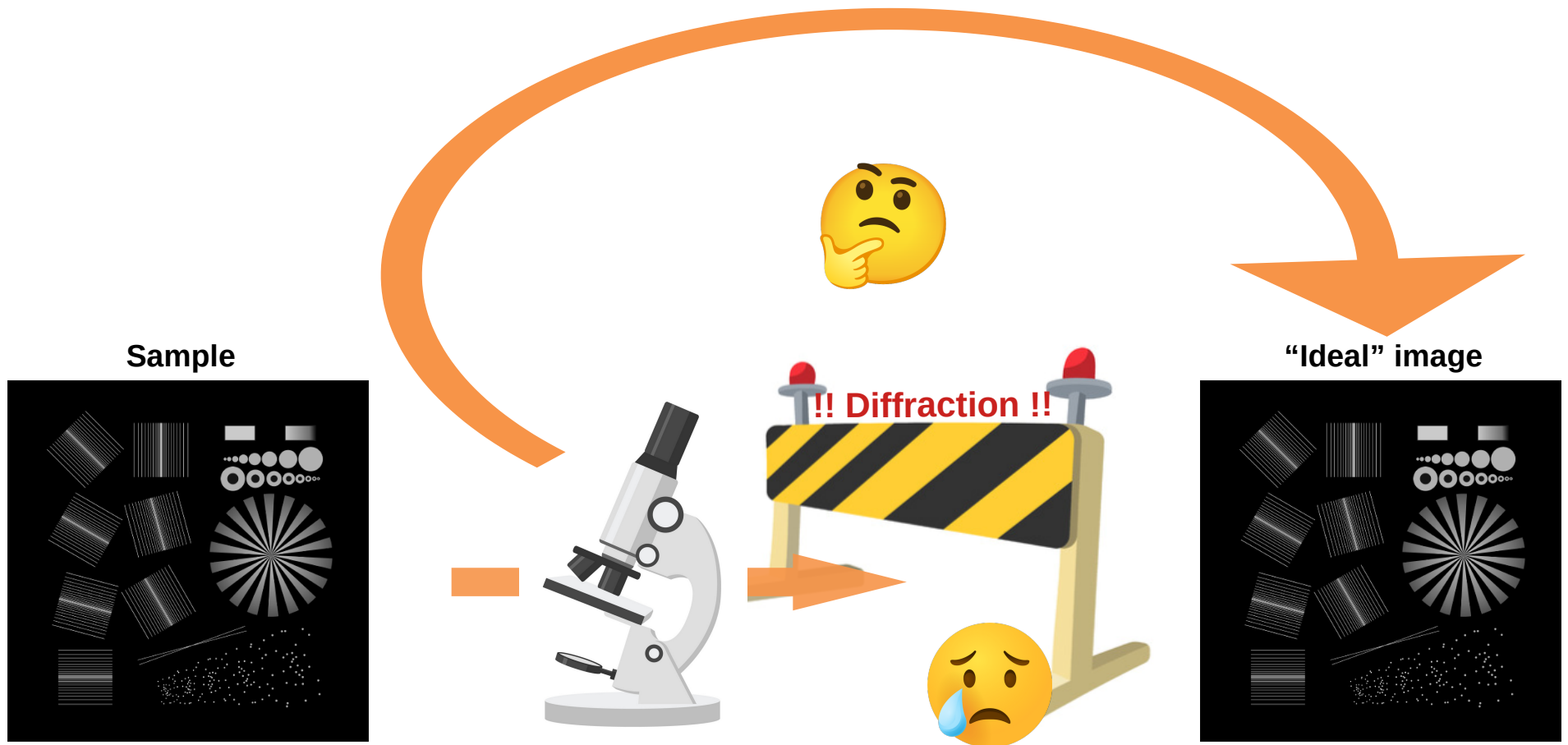
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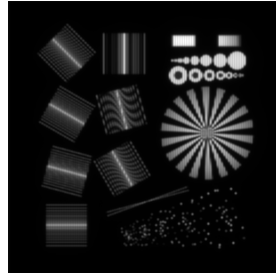
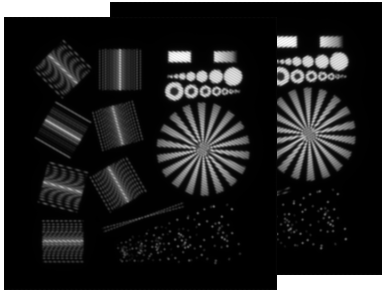
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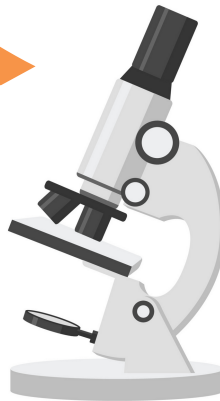
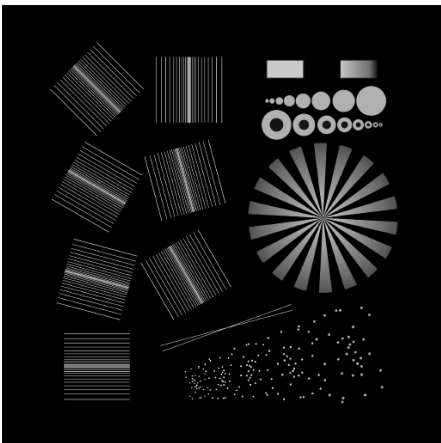
# Resolution Limit in Microscopy

## 1) Acquire a **set of diffraction limited** images

- Diversity of illuminations
- Diversity of orientations
- Diversity of “activation”
- ...



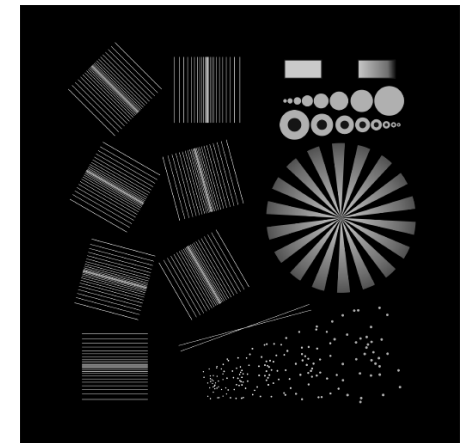
Sample



!! Diffraction !!



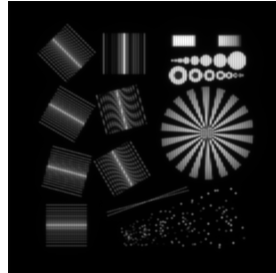
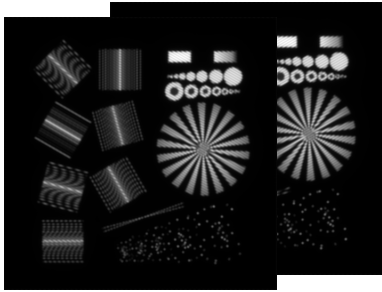
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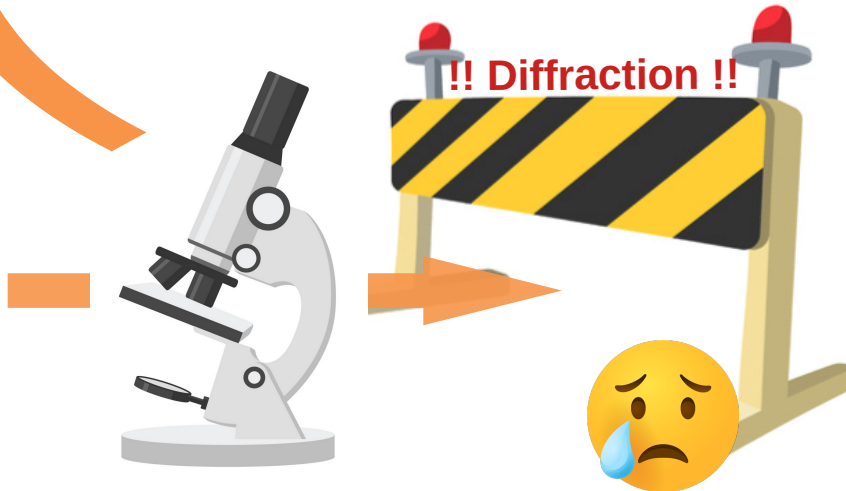
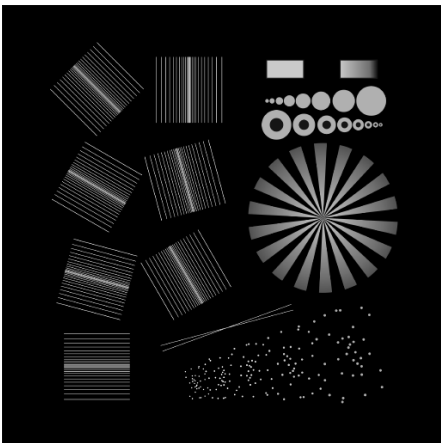
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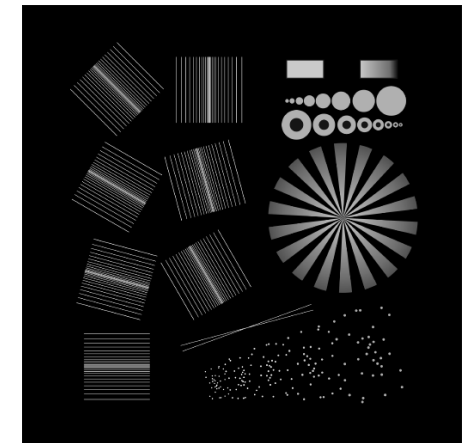
## 2) Numerical **reconstruction**



Sample

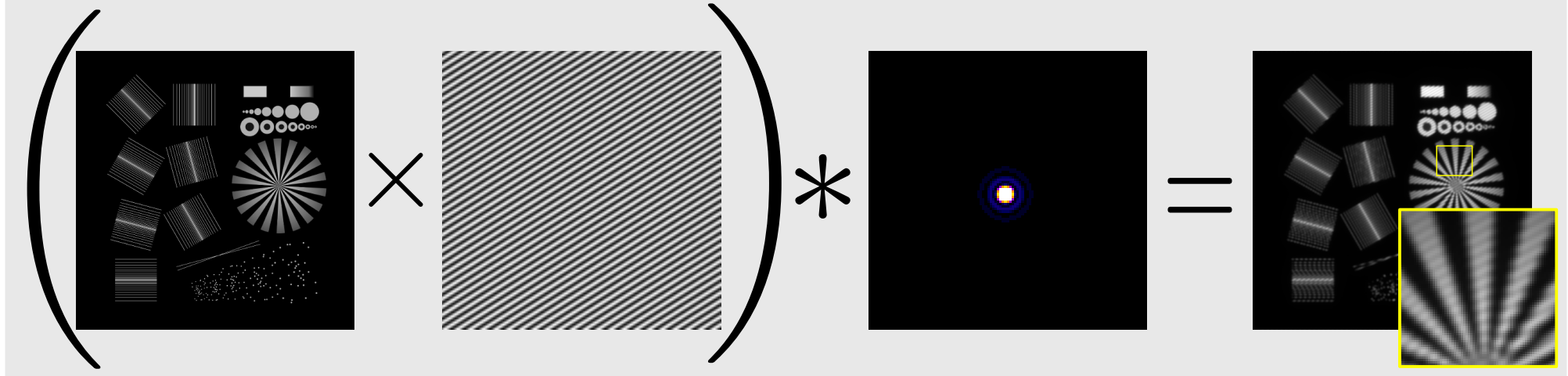


“Ideal” image



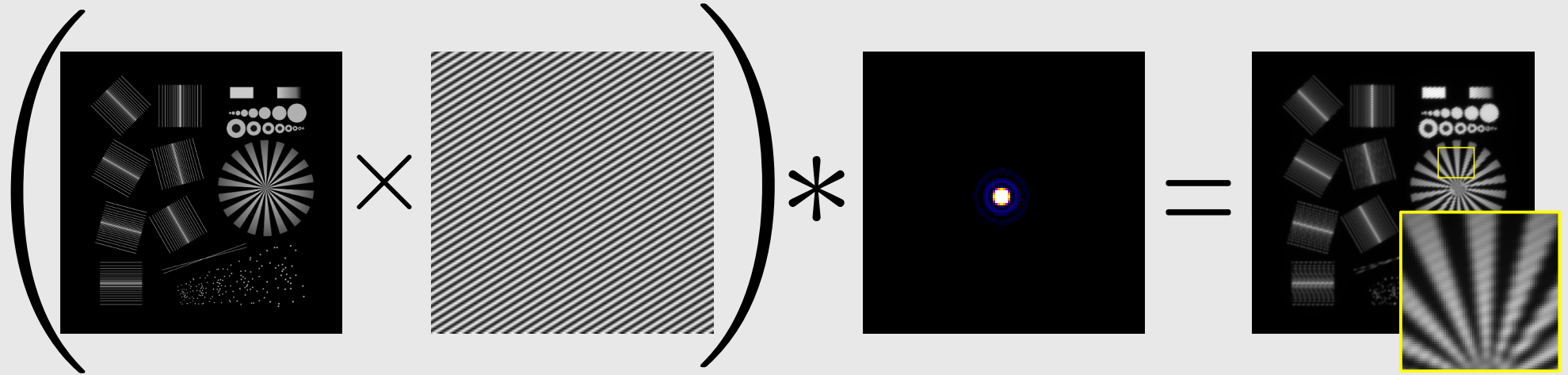
# Structured Illumination Microscopy – Image Formation

Modification of the illumination (sinusoidal pattern)



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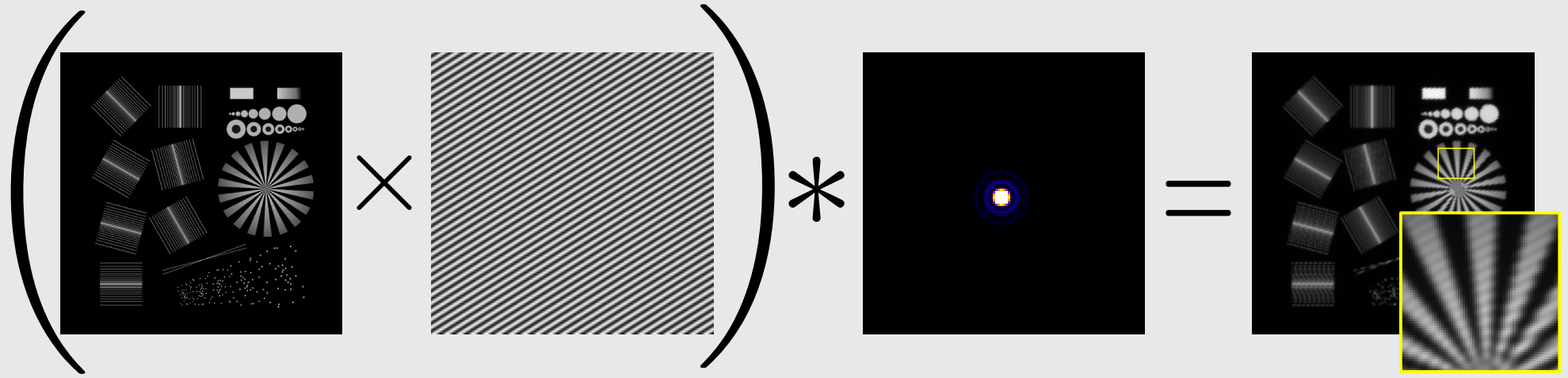
Modification of the illumination (sinusoidal pattern)



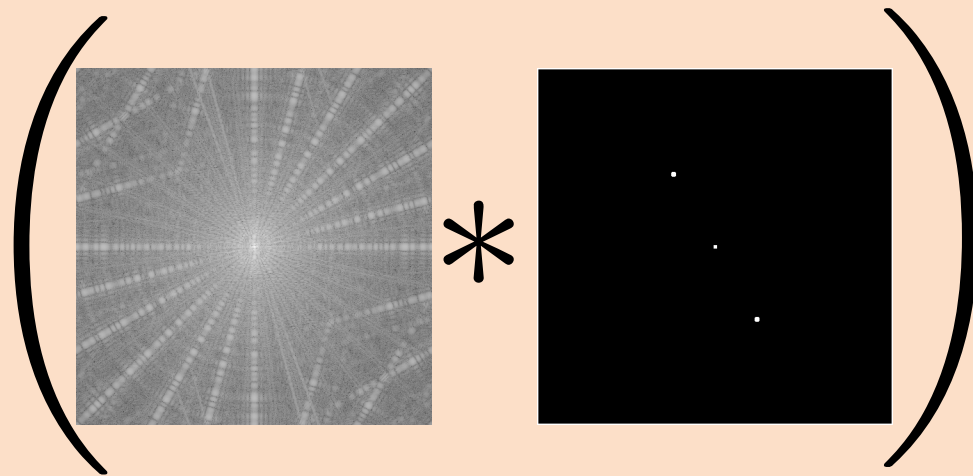
In Fourier domain...

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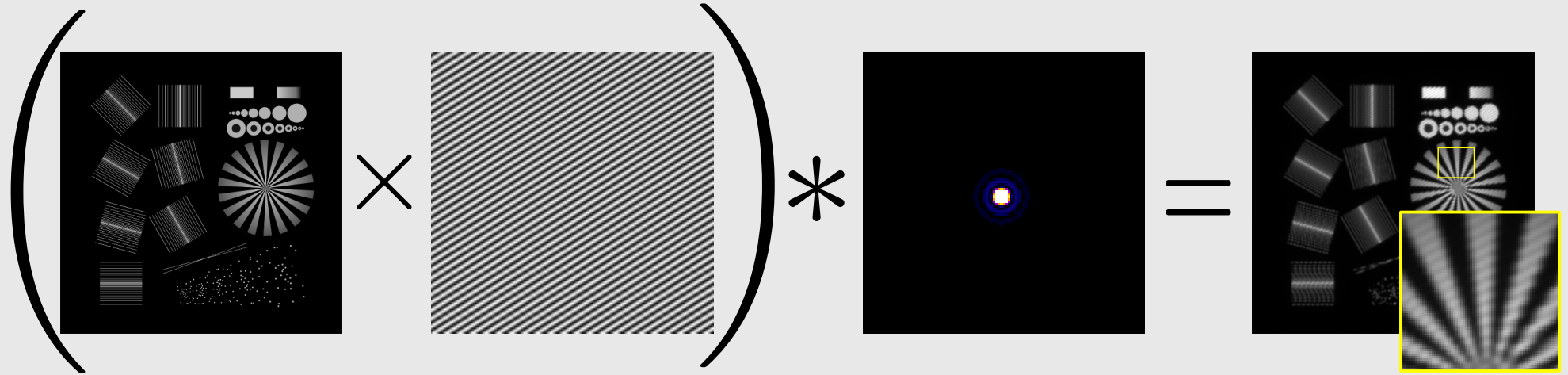


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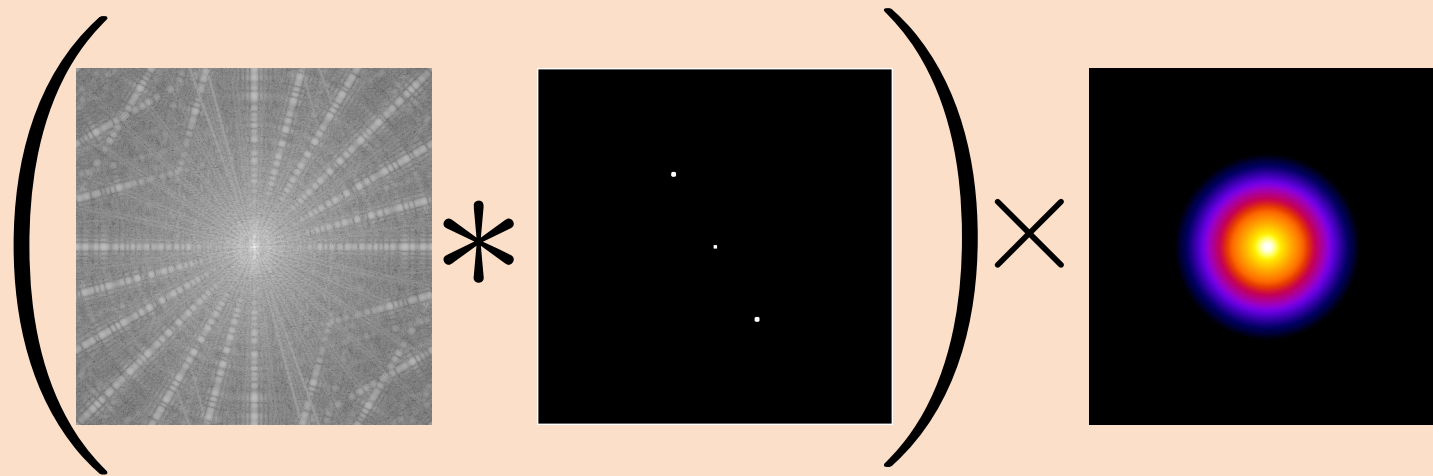


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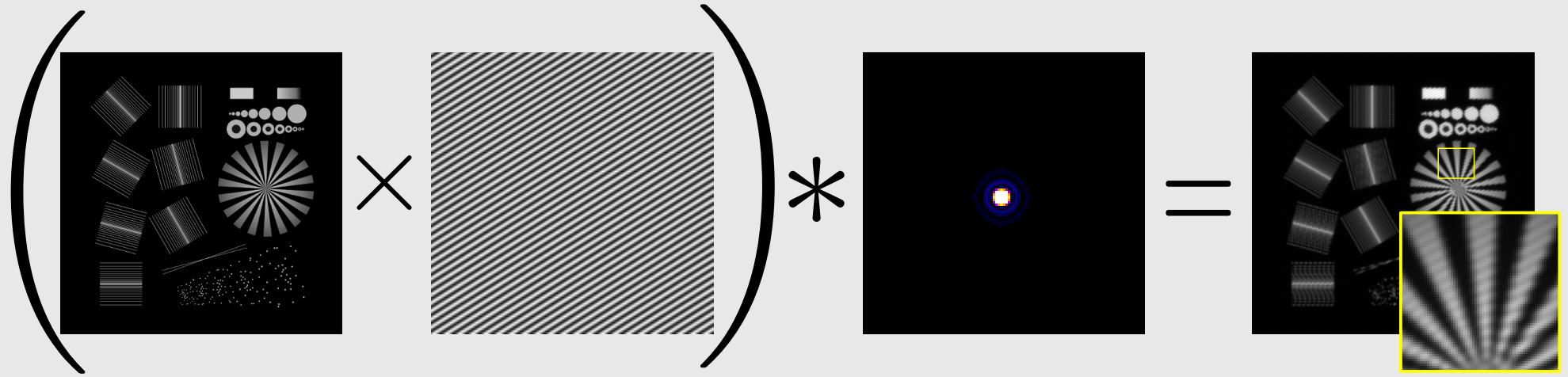


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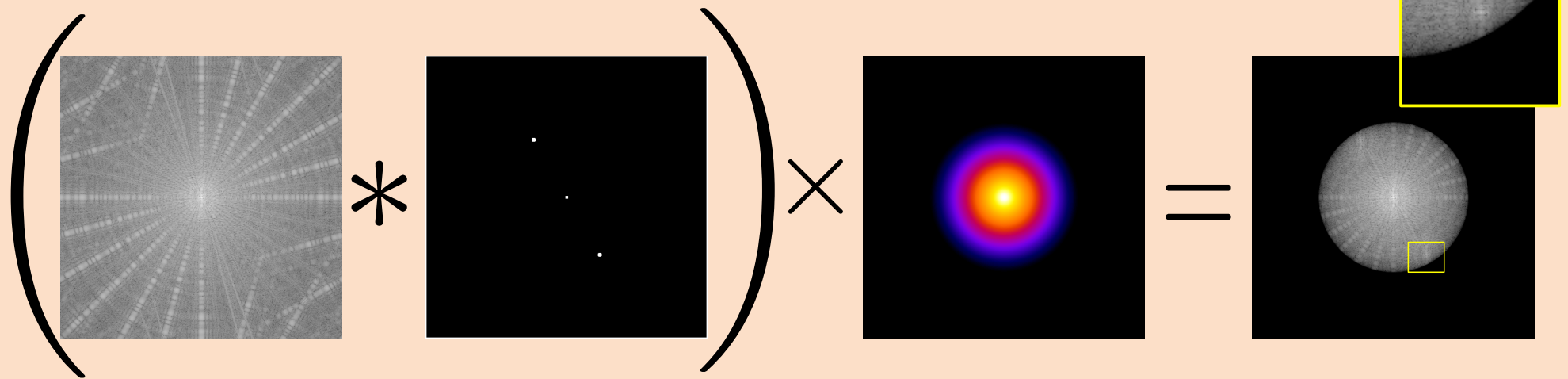


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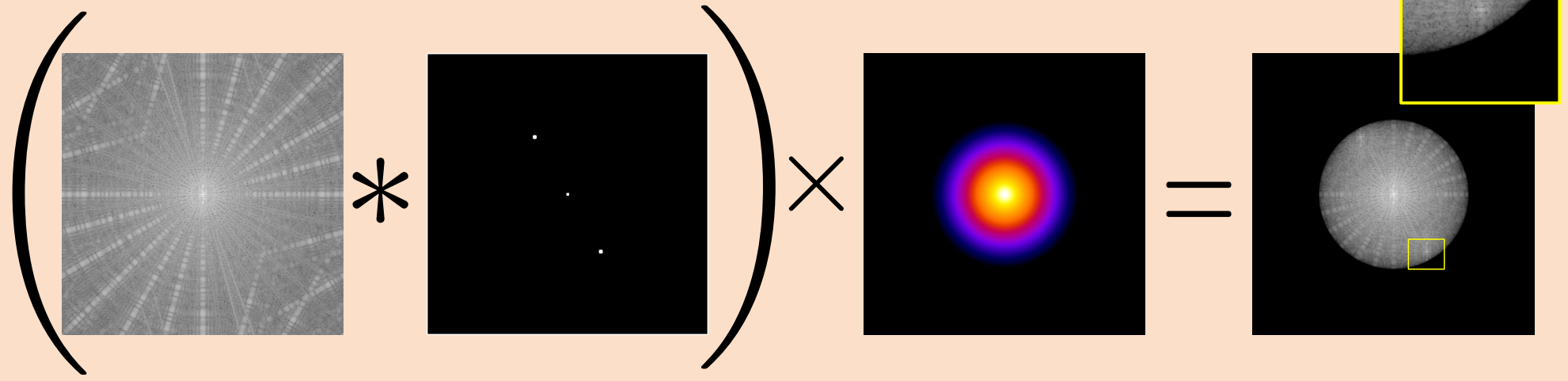


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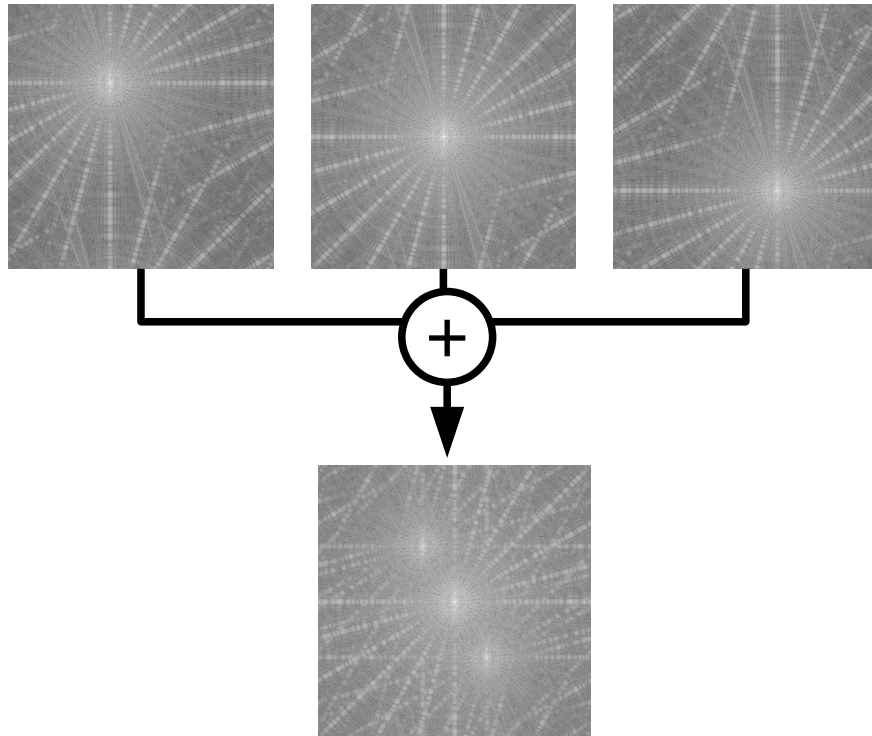
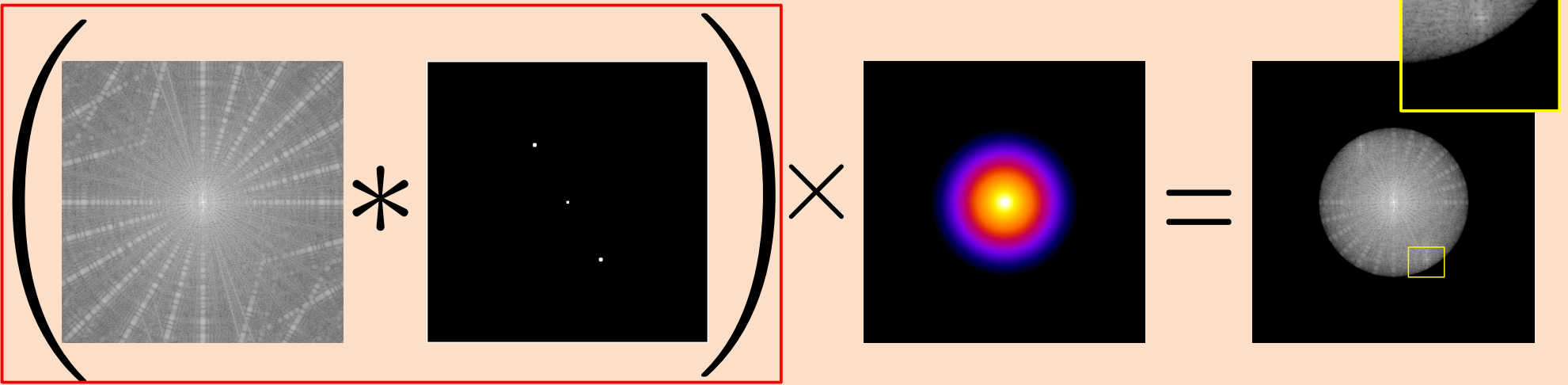
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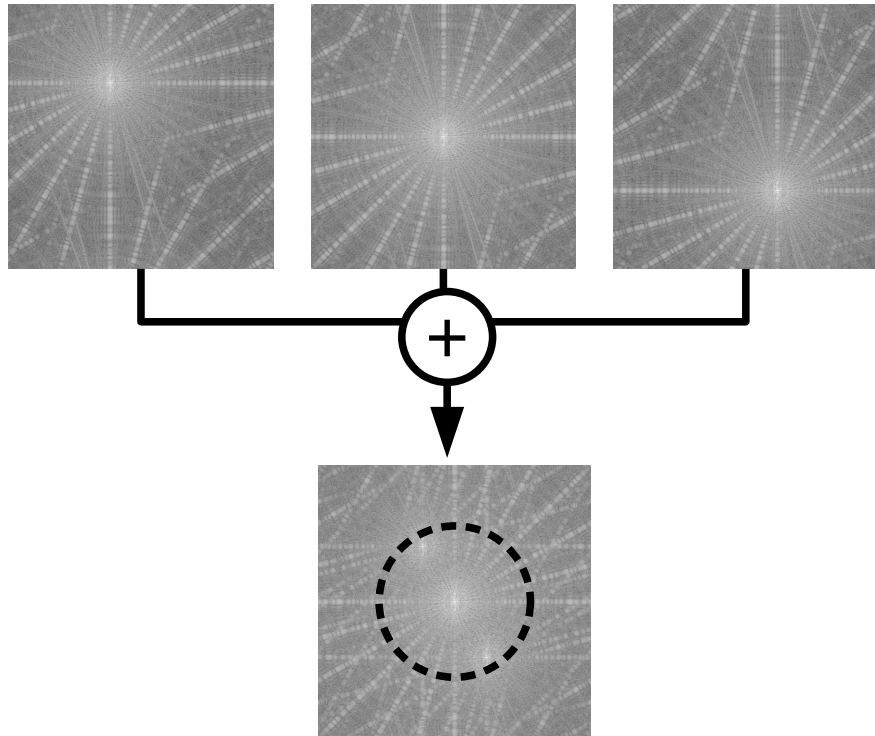
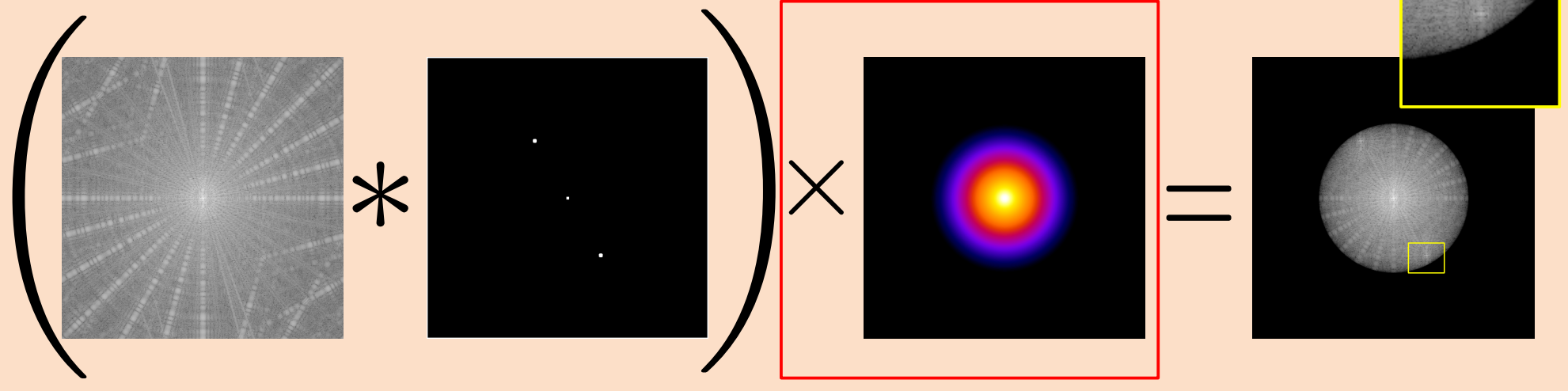
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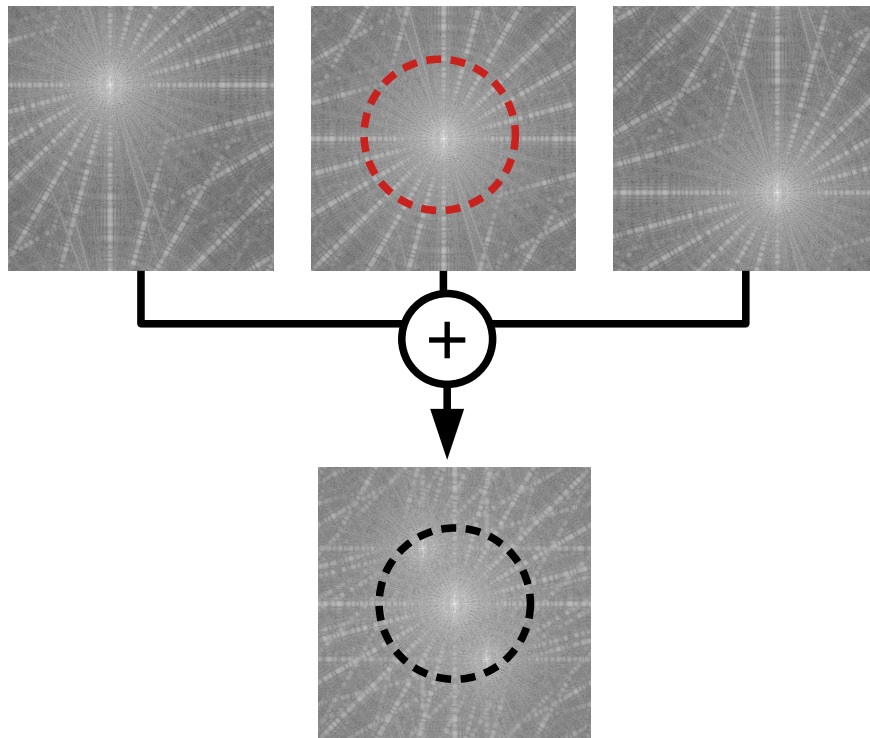
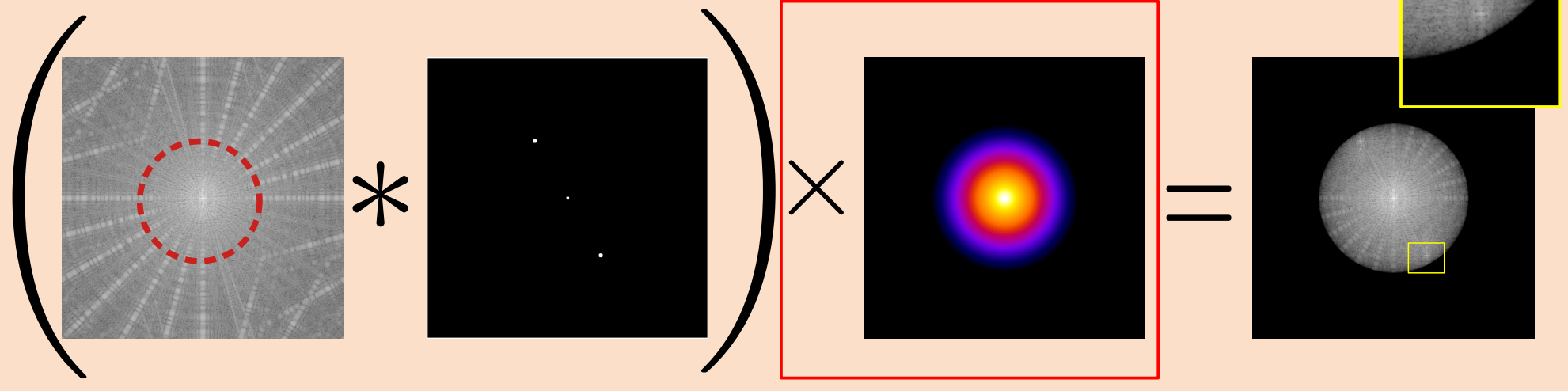
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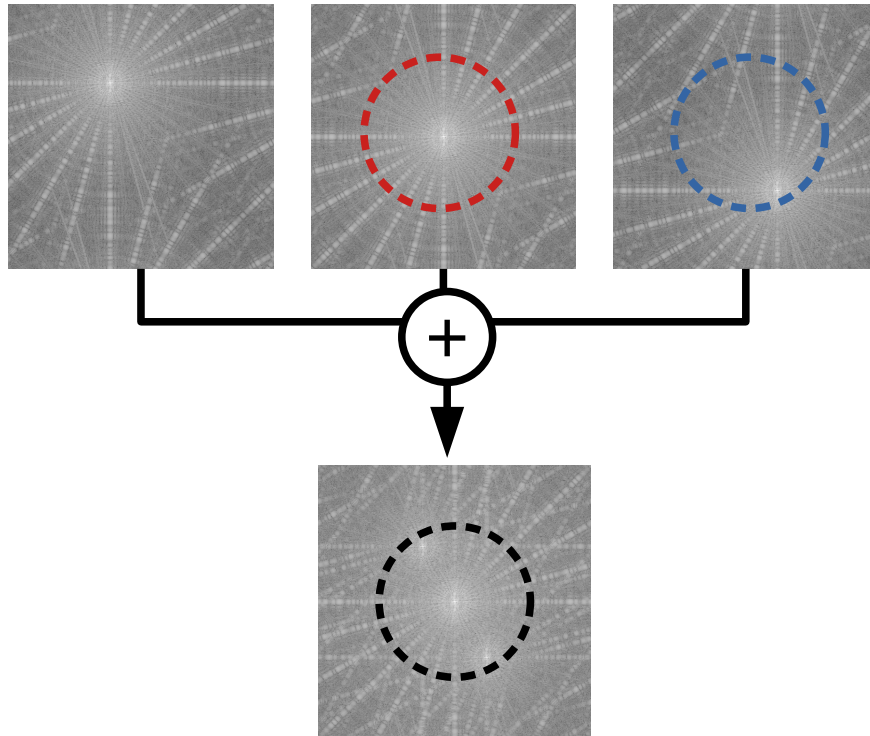
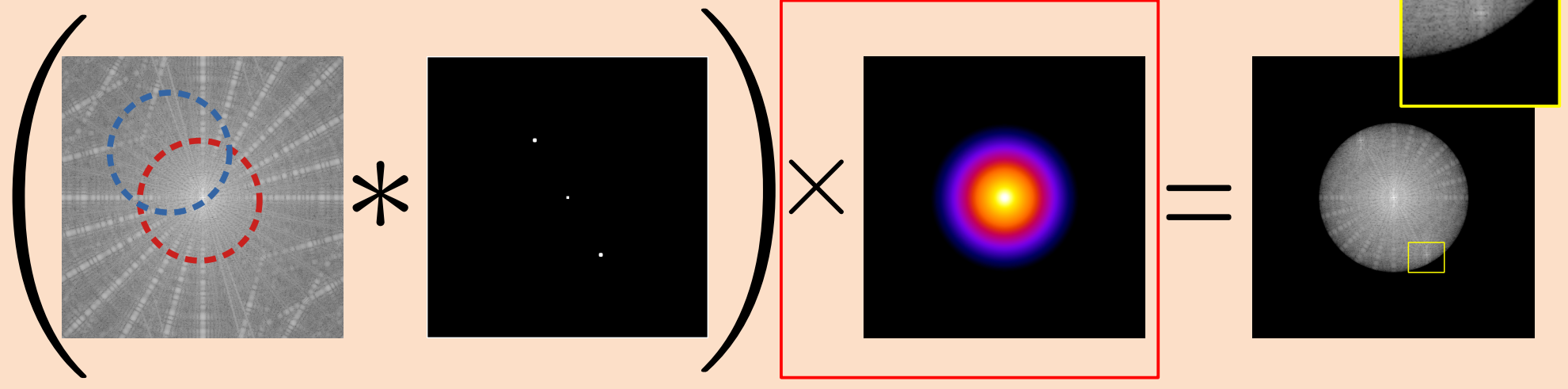
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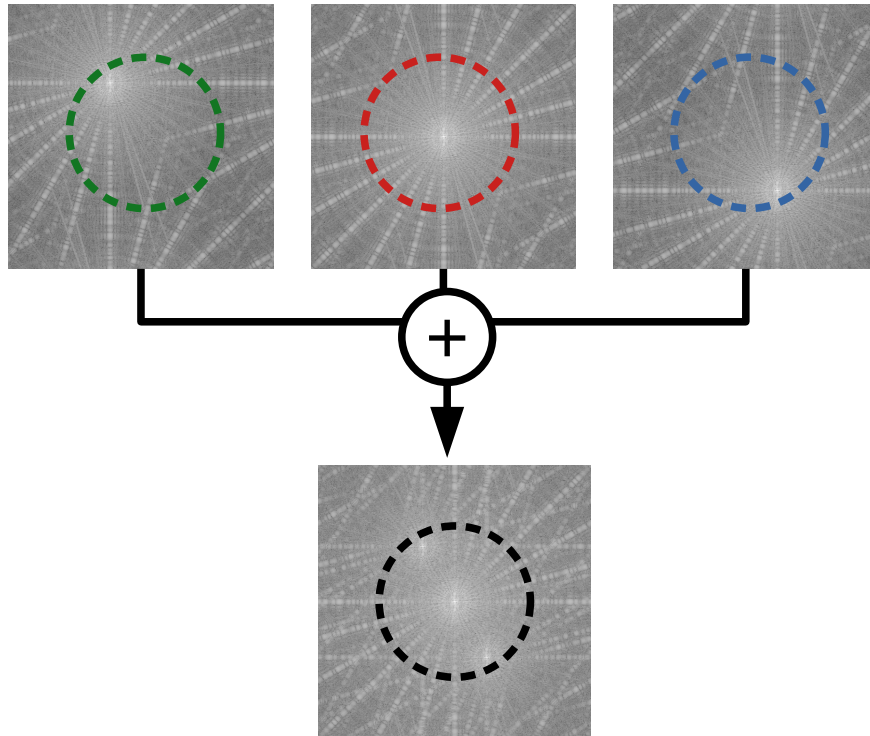
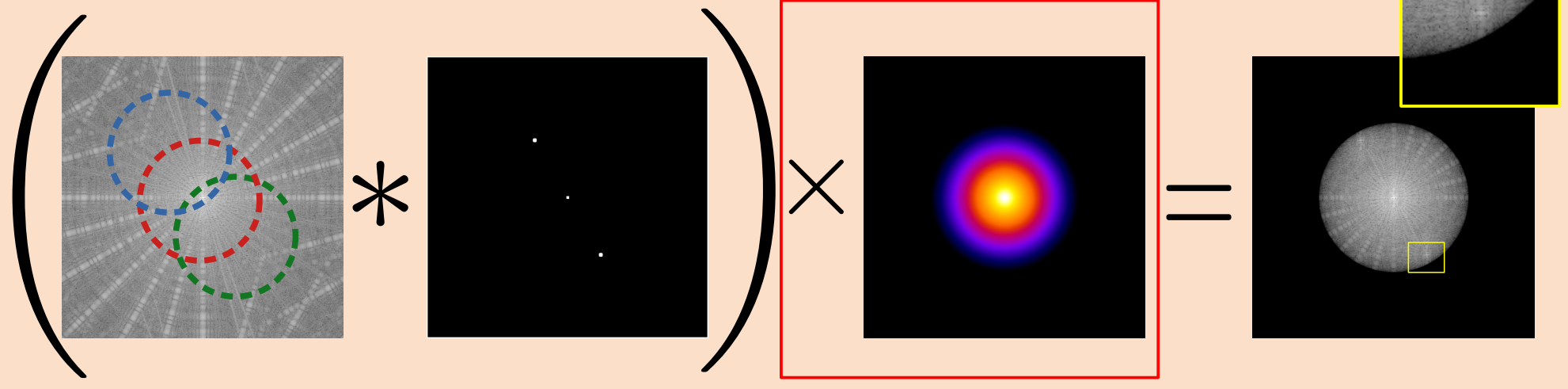
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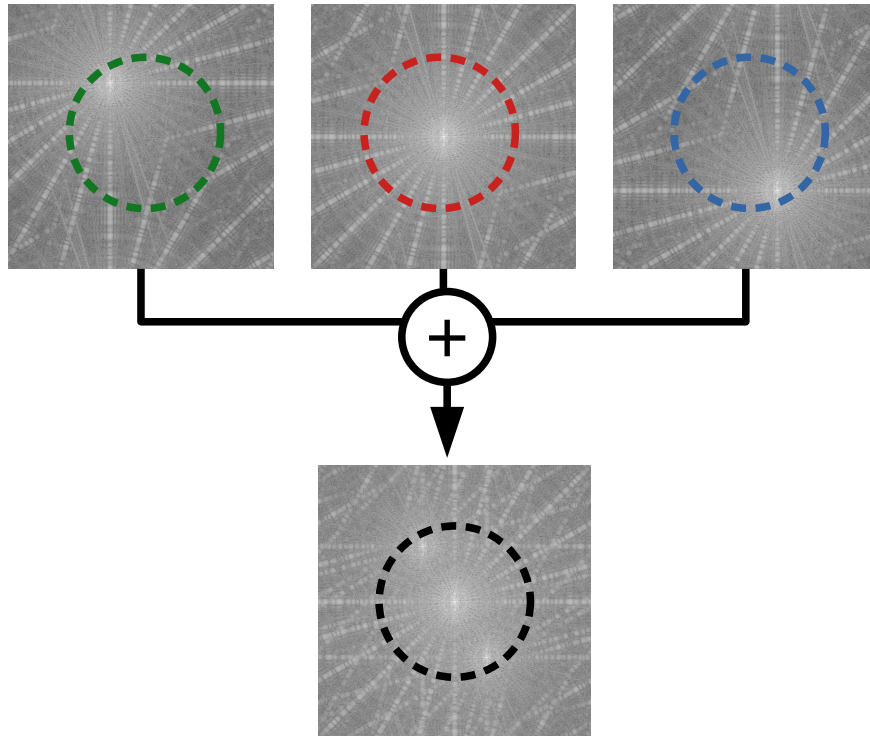
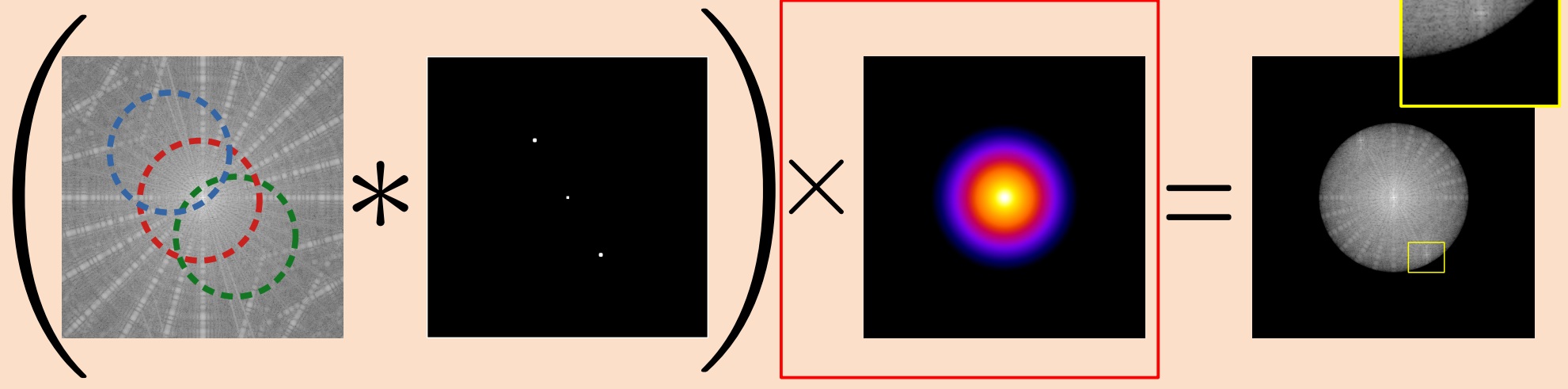
# Structured Illumination Microscopy – Image Formation

In Fourier domain...



# Structured Illumination Microscopy – Image Formation

In Fourier domain...



Using structured illuminations, *high-frequency* components of the sample are *shifted* into the *OTF bandwidth*.

Reconstruction is needed to “unmix” the three frequency components



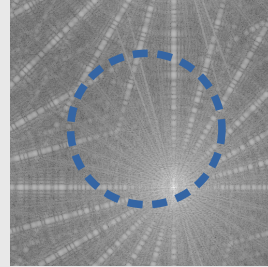
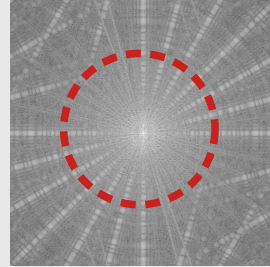
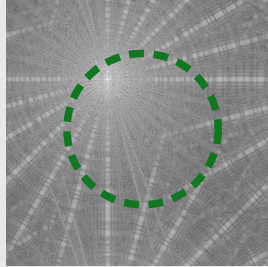
... and *shift them back* to their correct location in the Fourier plane.

# Structured Illumination Microscopy – Reconstruction

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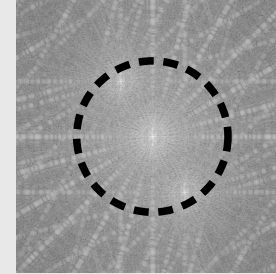
For a single SIM image:

*3 unknown components to unmix*



*with*

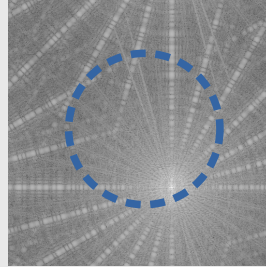
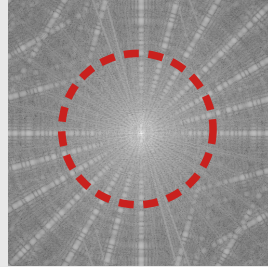
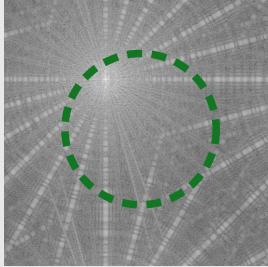
*1 “measure”*



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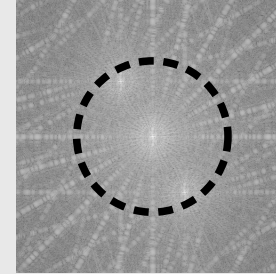
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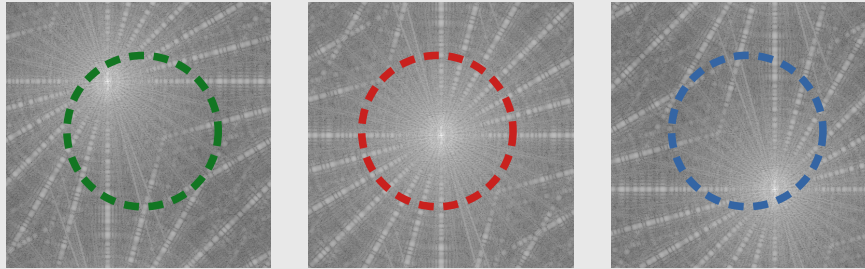


→ Need for additional measures to “close” the system of equations

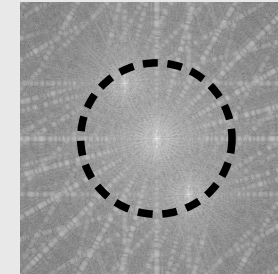
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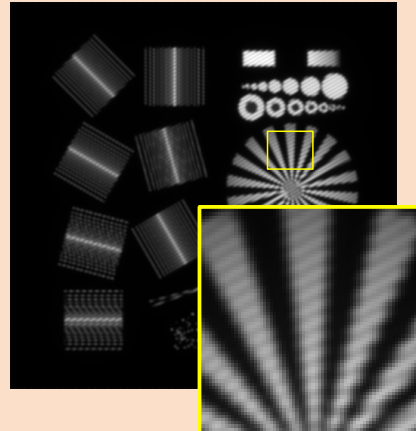
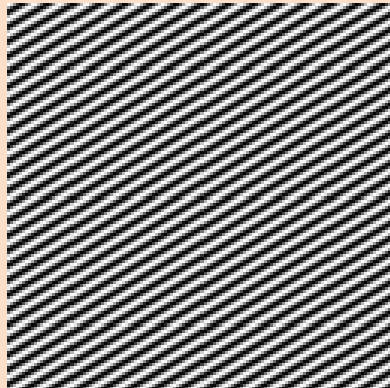
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*with*

—► Need for additional measures to “close” the system of equations

Take 3 SIM images with different illumination phases

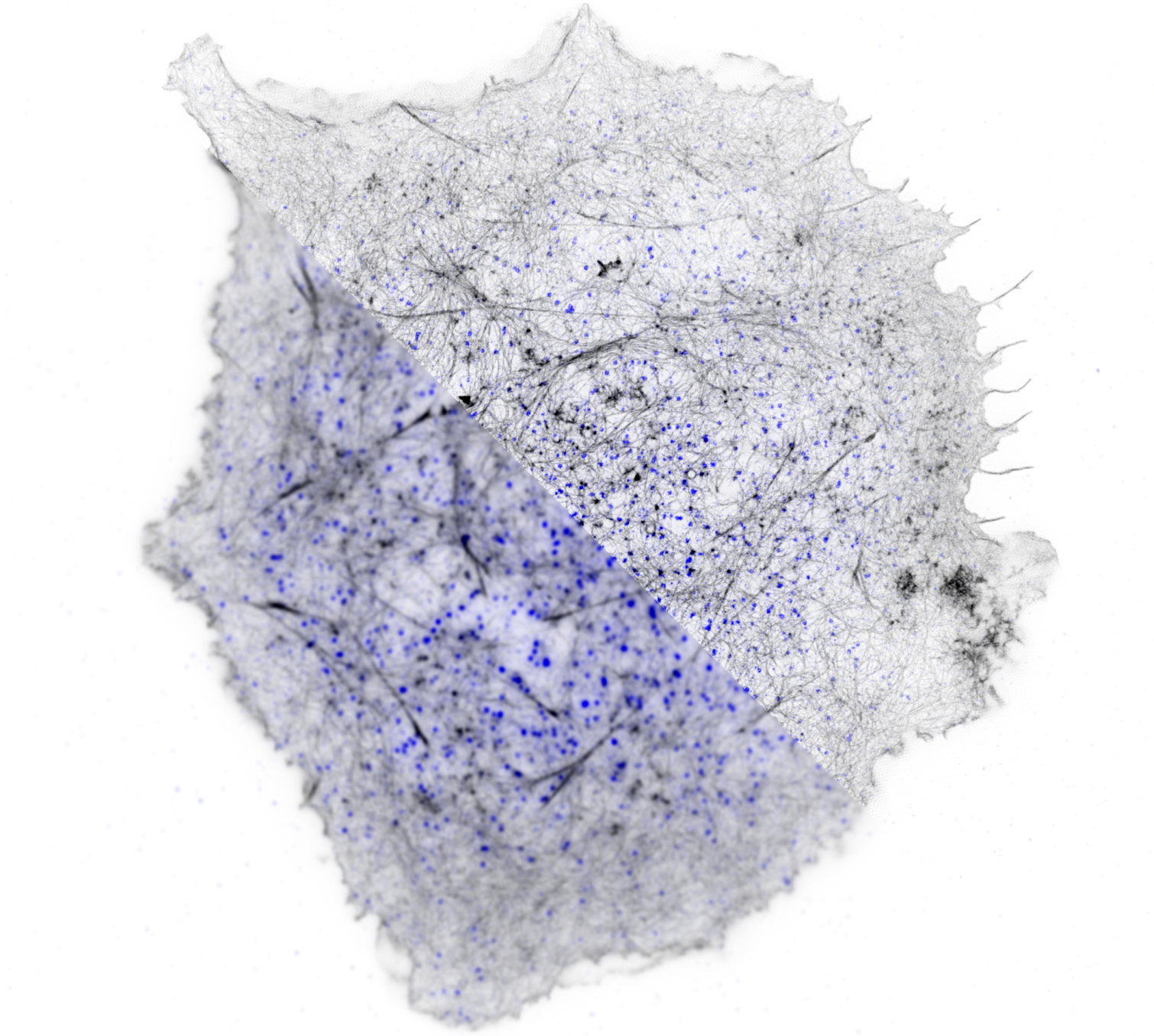


For  $n = 0, 1, 2$

$$w_n(x) = 1 + \cos\left(fx + \frac{2n\pi}{3}\right)$$

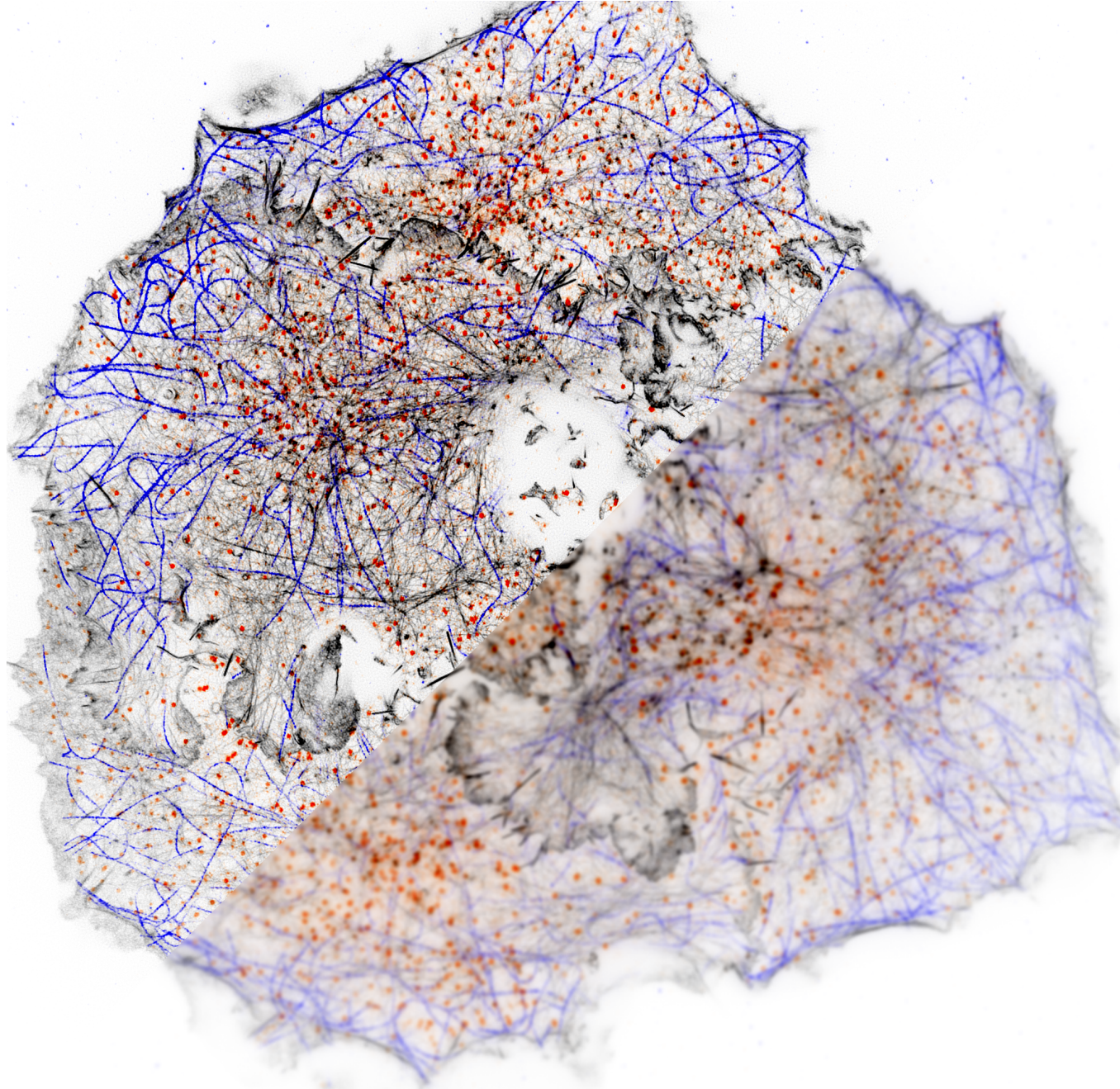
# Examples of SIM reconstructions

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# Examples of SIM reconstructions

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# Outline of the Talk

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SIM Principle



ADMM for SIM



GlobalBioIm



# Variational Formulation for SIM Reconstruction

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## Image formation model

$$\mathbf{y} = \mathbf{S}_d \mathbf{H} \mathbf{W} \mathbf{x} + \mathbf{n},$$

- where
- $\mathbf{x} \in \mathbb{R}^N$  the 3D biological sample,
  - $\mathbf{W} = \text{diag}(\mathbf{w})$  with  $\mathbf{w} \in \mathbb{R}_{\geq 0}^N$  an illumination pattern,
  - $\mathbf{H} : \mathbb{R}^N \rightarrow \mathbb{R}^N$  the convolution operator with the PSF,
  - $\mathbf{S}_d : \mathbb{R}^N \rightarrow \mathbb{R}^M$  a decimation operator with downsampling factor  $\mathbf{d} \in \mathbb{N}_{\geq 0}^3$ .

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## Inverse problem: Variational formulation

$$\hat{\mathbf{x}} \in \left\{ \arg \min_{\mathbf{x} \in \mathbb{R}^N} \left( \sum_{p=1}^P \frac{1}{2} \|\mathbf{S}_d \mathbf{H} \mathbf{W}_p \mathbf{x} - \mathbf{y}_p\|_2^2 + \mu \mathcal{R}(\mathbf{L} \mathbf{x}) + i_{\geq 0}(\mathbf{x}) \right) \right\},$$

- with
- $\mathcal{R}(\mathbf{L} \cdot)$  a regularization term (e.g. Total variation, Hessian-Schatten-norm),
  - The regularisation parameter  $\mu > 0$ ,
  - Nonnegativity constraint  $i_{\geq 0}(\mathbf{x}) = \{0 \text{ if } \mathbf{x} \in \mathbb{R}_{\geq 0}^N, +\infty \text{ otherwise}\}$ .

# Alternating Direction Method of Multipliers (ADMM)

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**ADMM** [*Boyd et al., 2011, Combette and Pesquet, 2011, Setzer et al, 2010*]

$$\mathcal{J}(\mathbf{x}) = \sum_{q=1}^Q \mathcal{F}_q(\mathbf{A}_q \mathbf{x}), \quad \left| \begin{array}{l} \mathcal{F}_q : \mathbb{R}^{N_q} \rightarrow \mathbb{R} \text{ convex} \\ \mathbf{A}_q \in \mathbb{R}^{N_q \times N} \end{array} \right.$$

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## Principle

- Variable splitting

$$\arg \min_{\mathbf{x}, \mathbf{u}_q} \sum_{q=1}^Q \mathcal{F}_q(\mathbf{u}_q) \quad \text{s.t.} \quad \mathbf{u}_q = \mathbf{A}_q \mathbf{x}$$

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- Alternating optimization on augmented Lagrangian formulation

$$\mathcal{L}(\mathbf{x}, \mathbf{u}_q, \mathbf{v}_q) = \sum_{q=1}^Q \mathcal{F}_q(\mathbf{u}_q) + \langle \mathbf{v}_q, \mathbf{A}_q \mathbf{x} - \mathbf{u}_q \rangle + \frac{\rho_q}{2} \|\mathbf{A}_q \mathbf{x} - \mathbf{u}_q\|_2^2$$

# Alternating Direction Method of Multipliers (ADMM)

**ADMM** [*Boyd et al., 2011, Combette and Pesquet, 2011, Setzer et al, 2010*]

$$\mathcal{J}(\mathbf{x}) = \sum_{q=1}^Q \mathcal{F}_q(\mathbf{A}_q \mathbf{x}), \quad \left| \begin{array}{l} \mathcal{F}_q : \mathbb{R}^{N_q} \rightarrow \mathbb{R} \text{ convex} \\ \mathbf{A}_q \in \mathbb{R}^{N_q \times N} \end{array} \right.$$

## Principle

- Variable splitting

$$\arg \min_{\mathbf{x}, \mathbf{u}_q} \sum_{q=1}^Q \mathcal{F}_q(\mathbf{u}_q) \quad \text{s.t.} \quad \mathbf{u}_q = \mathbf{A}_q \mathbf{x}$$

- Alternating optimization on augmented Lagrangian formulation

$$\mathcal{L}(\mathbf{x}, \mathbf{u}_q, \mathbf{v}_q) = \sum_{q=1}^Q \mathcal{F}_q(\mathbf{u}_q) + \langle \mathbf{v}_q, \mathbf{A}_q \mathbf{x} - \mathbf{u}_q \rangle + \frac{\rho_q}{2} \|\mathbf{A}_q \mathbf{x} - \mathbf{u}_q\|_2^2$$

- Proximal operator

$$\text{prox}_f(\mathbf{z}) = \arg \min_{\mathbf{x}} \left( \frac{1}{2} \|\mathbf{x} - \mathbf{z}\|_2^2 + f(\mathbf{x}) \right)$$

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**Require:**  $\mathbf{x}^0 \in \mathbb{R}^N$ ,  $(\rho_q)_{q \in [1 \dots Q]} \in \mathbb{R}_{\geq 0}^Q$

1:  $\mathbf{u}_q^0 = \mathbf{A}_q \mathbf{x}^0$ ,  $\forall q \in [1 \dots Q]$

2:  $\mathbf{v}_q^0 = \mathbf{u}_q^0$ ,  $\forall q \in [1 \dots Q]$

3:  $k = 0$

4: **while** (not converged) **do**

5:  $\mathbf{u}_q^{k+1} = \text{prox}_{\frac{1}{\rho_q} \mathcal{F}_q}(\mathbf{A}_q \mathbf{x}^k + \mathbf{v}_q^k / \rho_q)$ ,  $\forall q \in [1 \dots Q]$   $\leftarrow$  **Prox Step**

6:  $\mathbf{x}^{k+1} = \left( \sum_{q=1}^Q \rho_q \mathbf{A}_q^* \mathbf{A}_q \right)^{-1} \left( \sum_{q=1}^Q \rho_q \mathbf{A}_q^* (\mathbf{u}_q^{k+1} - \mathbf{v}_q^k / \rho_q) \right)$   $\leftarrow$  **Linear Step**

7:  $\mathbf{v}_q^{k+1} = \mathbf{v}_q^k + \rho_q (\mathbf{A}_q \mathbf{x}^{k+1} - \mathbf{u}_q^{k+1})$ ,  $\forall q \in [1 \dots Q]$

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**Which splitting should we adopt?**

# Splitting Strategies for SIM

$$\hat{\mathbf{x}} \in \left\{ \arg \min_{\mathbf{x} \in \mathbb{R}^N} \left( \sum_{p=1}^P \frac{1}{2} \left\| \underbrace{\mathbf{S}_d \mathbf{H} \mathbf{W}_p \mathbf{x}}_{\substack{\text{red} \\ ?}} - \mathbf{y}_p \right\|_2^2 + \mu \mathcal{R}(\underbrace{\mathbf{L} \mathbf{x}}_{\substack{\text{blue} \\ \mathbf{u}_1}}) + i_{\geq 0}(\underbrace{\mathbf{x}}_{\substack{\text{green} \\ \mathbf{u}_2}}) \right) \right\}$$

	Prox Step	Linear Step
$\mathbf{A}_q = \mathbf{S}_d \mathbf{H} \mathbf{W}_q$	$\text{prox}_{\frac{\gamma}{2} \ \cdot - \mathbf{y}\ _2^2}(\mathbf{z})$ $\rightarrow (1 + \gamma)^{-1} \mathbf{I}$ Component-wise division	$\left( \sum_{p=1}^P \mathbf{W}_p^* \mathbf{H}^* \mathbf{S}_d^* \mathbf{S}_d \mathbf{H} \mathbf{W}_p + \mathbf{L}^* \mathbf{L} + \mathbf{I} \right)^{-1}$ $\rightarrow$ CG: 4xP (i)FFTs / Iter
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\*CG: Conjugate-gradient

# Proximal Operator of $\|\mathbf{S}_d \mathbf{H} \cdot - \mathbf{y}\|_2^2$

**Proposition 1** *The proximal operator of  $f = \frac{\gamma}{2} \|\mathbf{S}_d \mathbf{H} \cdot - \mathbf{y}\|_2^2$  can be efficiently computed at the expense of **2 (i)FFTs** as*

$$\text{prox}_f(\mathbf{z}) = \mathbf{F}^* (\mathbf{I} - \gamma \mathbf{\Lambda}^* \mathbf{P}_d \mathbf{D}^{-1} \mathbf{P}_d^* \mathbf{\Lambda}) \mathbf{F} \mathbf{r},$$

- where
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  - $\mathbf{\Lambda} = \text{diag}(\mathbf{F} \mathbf{h})$  with  $\mathbf{h}$  the kernel of  $\mathbf{H}$ ,
  - $\mathbf{P}_d$  is a periodization operator,
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## Quick Proof

1) Woodbury matrix identity

$$(\mathbf{I} + \gamma \mathbf{H}^* \mathbf{S}_d^* \mathbf{S}_d \mathbf{H})^{-1} = (\mathbf{I} - \gamma \mathbf{H}^* \mathbf{S}_d^* (\mathbf{I} + \gamma \mathbf{S}_d \mathbf{H} \mathbf{H}^* \mathbf{S}_d^*)^{-1} \mathbf{S}_d \mathbf{H})$$

2) We can write  $\mathbf{I} + \gamma \mathbf{S}_d \mathbf{H} \mathbf{H}^* \mathbf{S}_d^*$  as a convolution

$$\begin{aligned} \mathbf{I} + \gamma \mathbf{S}_d \mathbf{H} \mathbf{H}^* \mathbf{S}_d^* &= \mathbf{I} + \gamma \mathbf{S}_d \mathbf{F}^* \mathbf{\Lambda} \mathbf{\Lambda}^* \mathbf{F} \mathbf{S}_d^* \\ &= \mathbf{I} + \frac{\gamma}{\bar{d}} \mathbf{F}^* \mathbf{P}_d^* \mathbf{\Lambda} \mathbf{\Lambda}^* \mathbf{P}_d \mathbf{F} \\ &= \mathbf{I} + \frac{\gamma}{\bar{d}} \mathbf{F}^* \text{diag}(\mathbf{P}_d^* \mathbf{\Lambda} \mathbf{\Lambda}^* \mathbf{1}_N) \mathbf{F} \end{aligned}$$

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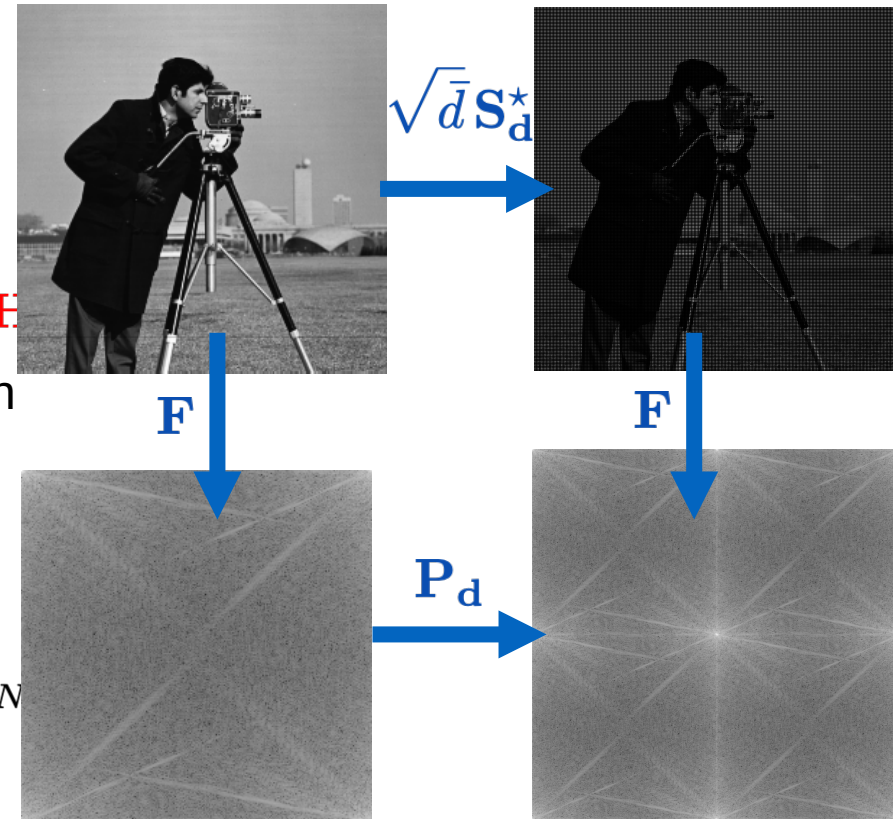
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# (Re)formulation of the Problem

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**Definition 1** *Let  $\mathbf{T} \in \mathbb{R}^{N \times N}$ . We say that  $\mathbf{T} \in \mathcal{N}_{\geq 0}$  if and only if*

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where  $\mathbf{T} = \left( \alpha \mathbf{I} - \mathbf{diag} \left( \sum_{p=1}^P \mathbf{w}_p \odot \mathbf{w}_p \right) \right)$  with  $\alpha > \left\| \sum_{p=1}^P \mathbf{w}_p \odot \mathbf{w}_p \right\|_{\infty}$ .

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The linear step in ADMM amounts to invert

$$\mathbf{B} = \sum_{p=1}^P \mathbf{W}_p^* \mathbf{W}_p + \mathbf{L}^* \mathbf{L} + \mathbf{T}^* \mathbf{T} = \mathbf{L}^* \mathbf{L} + \alpha \mathbf{I}$$

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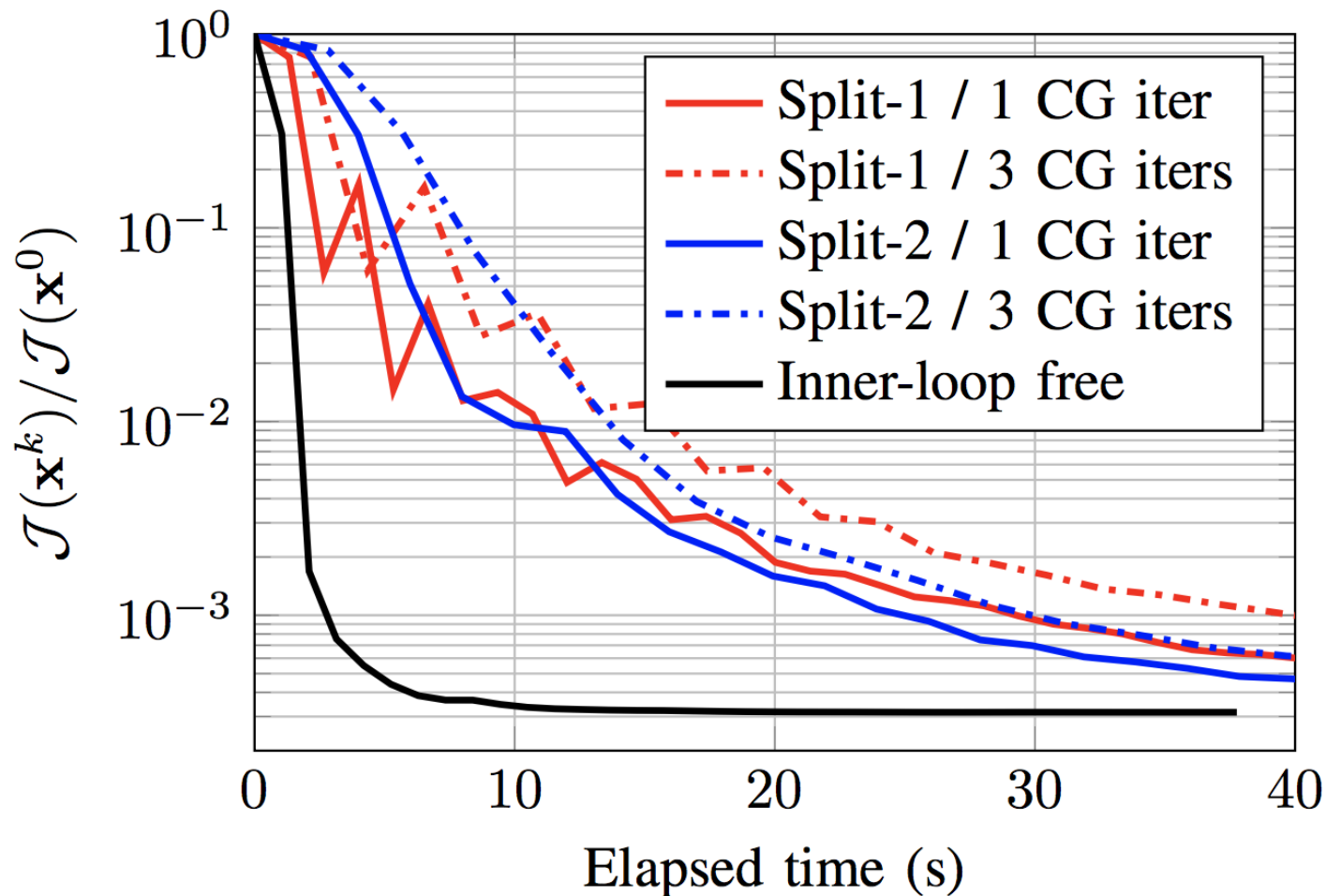
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**Inner-loop-free ADMM: 2x(P+1) (i)FFTs / iter !**

# Numerical Comparisons

- (512 x 512) size problem
- Lagrangian multipliers tuned empirically to get fastest convergence



# Outline of the Talk

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SIM Principle



ADMM for SIM



GlobalBioIm



## Objectives

- Unification of inverse problems solving
- Decompose the problem in small reusable modules
- Capitalises on the commonalities between image formation models

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### Cost Functions:

- *Evaluate*
- *Compute Gradient*
- *Compute Prox*
- ...

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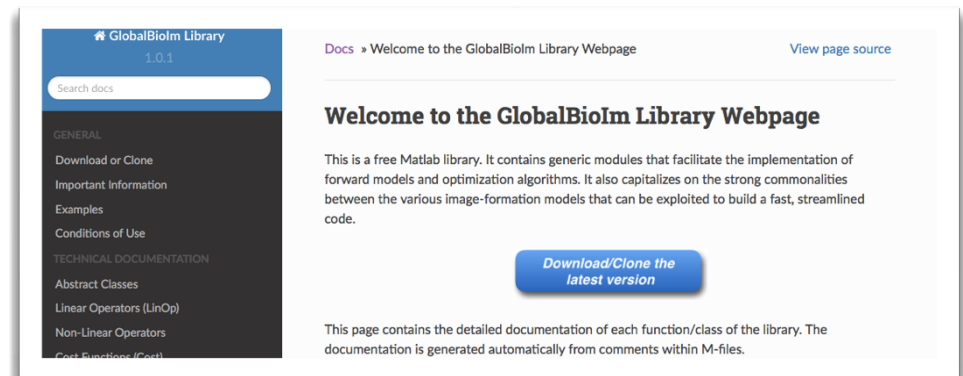
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<http://bigwww.epfl.ch/algorithms/globalbioim/>

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## Three classes of modules

### Cost Functions:

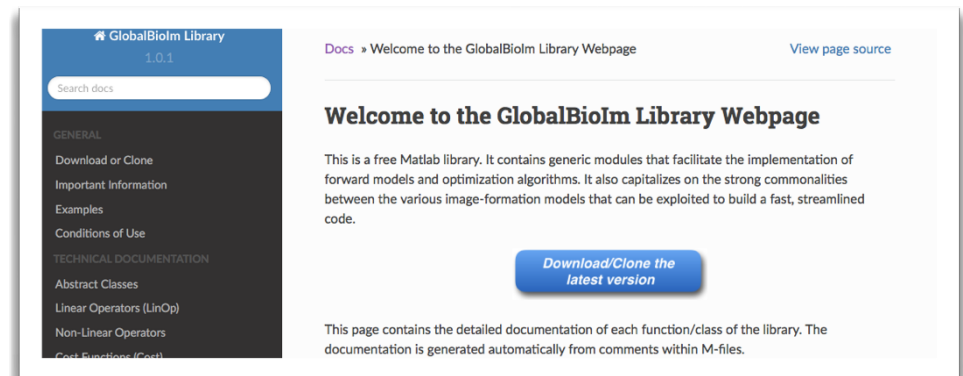
- *Evaluate*
- *Compute Gradient*
- *Compute Prox*
- ...

### Operators:

- *Apply forward*
- *Apply Jacobian*
- ...

### Optimizers

- *Minimize a cost*
- ...



<http://bigwww.epfl.ch/algorithms/globalbioim/>

## Python alternatives

- Deep Inverse
- Pyxu

# ADMM for SIM Reconstruction with GlobalBioIm

## Splitting 1

$$\hat{\mathbf{x}} \in \arg \min_{\mathbf{x} \in \mathbb{R}^N} \left( \sum_{p=1}^P \frac{1}{2} \|\mathbf{S}_d \mathbf{H} \mathbf{W}_p \mathbf{x} - \mathbf{y}_p\|_2^2 + \mu \mathcal{R}(\mathbf{L} \mathbf{x}) + i_{\geq 0}(\mathbf{T} \mathbf{x}) \right)$$

%- Data fidelity

```
H=LinOpConv(fftn(psf),1);
```

```
S=LinOpDownsample([szUp,H.sizeout(3)],[downFact,H.sizeout(3)]);
```

```
Fn={};Hn={};F0=[];
```

```
for i=1:size(patt,3)
```

```
    L2=CostL2([],y(:, :, i));
```

```
    Fn{i}=L2; Fn{i}.doPrecomputation=true;
```

```
    Hn{i}=S*H*LinOpDiag(H.sizein,patt(:, :, i));
```

```
end
```

%- Regularization

```
Opreg=LinOpHess(H.sizein,'circular',[1 2]);
```

```
Freg=CostMixNormSchatt1(Opreg.sizeout,1);
```

```
T=LinOpIdentity(H.sizein);
```

```
pos=CostNonNeg(H.sizein);
```

%- ADMM

```
FF=[Fn,{pos},{lamb*Freg}];
```

```
HH=[Hn,{OpD},{Opreg}];
```

```
rho=[ones(size(Fn))*rhoDTNN,rhoDTNN,rhoReg];
```

```
Opt=OptiADMM([],FF,HH,rho);
```

```
Opt.CvOp=TestCvgStepRelative(1e-5);
```

```
Opt.maxiter=500;
```

```
Opt.run(zeros(H.sizein));
```

# ADMM for SIM Reconstruction with GlobalBioIm

## Splitting 2

$$\hat{\mathbf{x}} \in \arg \min_{\mathbf{x} \in \mathbb{R}^N} \left( \sum_{p=1}^P \frac{1}{2} \|\mathbf{S}_d \mathbf{H} \mathbf{W}_p \mathbf{x} - \mathbf{y}_p\|_2^2 + \mu \mathcal{R}(\mathbf{L} \mathbf{x}) + i_{\geq 0}(\mathbf{T} \mathbf{x}) \right)$$

%- Data fidelity

**H**=LinOpConv(fftn(psf),1);

**S**=LinOpDownsample([szUp,**H**.sizeout(3)],[downFact,**H**.sizeout(3)]);

Fn={};Hn={};F0=[];

for i=1:size(patt,3)

**L2**=CostL2([],y(:, :, i));

    Fn{i}=**L2**\***S**; Fn{i}.doPrecomputation=true;

    Hn{i}=**H**\*LinOpDiag(**H**.sizein,patt(:, :, i));

end

%- Regularization

**Opreg**=LinOpHess(**H**.sizein,'circular',[1 2]);

**Freg**=CostMixNormSchatt1(**Opreg**.sizeout,1);

**T**=LinOpIdentity(**H**.sizein);

**pos**=CostNonNeg(**H**.sizein);

%- ADMM

FF=[Fn,{pos},{lamb\*Freg}];

HH=[Hn,{OpD},{Opreg}];

rho=[ones(size(Fn))\*rhoDTNN,rhoDTNN,rhoReg];

**Opt**=OptiADMM([],FF,HH,rho);

**Opt**.CvOp=TestCvgStepRelative(1e-5);

**Opt**.maxiter=500;

**Opt**.run(zeros(**H**.sizein));



# ADMM for SIM Reconstruction with GlobalBioIm

## Inner-loop free ADMM

$$\hat{\mathbf{x}} \in \arg \min_{\mathbf{x} \in \mathbb{R}^N} \left( \sum_{p=1}^P \frac{1}{2} \|\mathbf{S}_d \mathbf{H} \mathbf{W}_p \mathbf{x} - \mathbf{y}_p\|_2^2 + \mu \mathcal{R}(\mathbf{L} \mathbf{x}) + i_{\geq 0}(\mathbf{T} \mathbf{x}) \right)$$

%- Data fidelity

**H**=LinOpConv(fftn(psf),1);

**S**=LinOpDownsample([szUp,**H**.sizeout(3)],[downFact,**H**.sizeout(3)]);

Fn={};Hn={};F0=[];

for i=1:size(patt,3)

**L2**=CostL2([],y(:, :, i));

    Fn{i}=**L2**\*(**S**\***H**); Fn{i}.doPrecomputation=true;

    Hn{i}=LinOpDiag(**H**.sizein,patt(:, :, i));

end

%- Regularization

**Opreg**=LinOpHess(**H**.sizein,'circular',[1 2]);

**Freg**=CostMixNormSchatt1(**Opreg**.sizeout,1);

**T**=LinOpDiag(**H**.sizein,sqrt(alpha-sum(patt.^2,3)));

**pos**=CostNonNeg(**H**.sizein);

%- ADMM

FF=[Fn,{pos},{lamb\*Freg}];

HH=[Hn,{OpD},{Opreg}];

rho=[ones(size(Fn))\*rhoDTNN,rhoDTNN,rhoReg];

**Opt**=OptiADMM([],FF,HH,rho);

**Opt**.CvOp=TestCvgStepRelative(1e-5);

**Opt**.maxiter=500;

**Opt**.run(zeros(**H**.sizein));



### Take home message

- ADMM is a very flexible method
- Offers several choices of splitting
- Can be tailored to each individual problem

#### **Computational Super-Sectioning for Single-Slice Structured-Illumination Microscopy**

IEEE Transactions on Computational Imaging, vol 5, pp. 240-250, 2019.

E. Soubies and M. Unser.

#### **Pocket Guide to Solve Inverse Problems with GlobalBioIm,**

Inverse Problems, vol. 35, no. 10, 2019.

E. Soubies, F. Soulez, M. T. McCann, T-A. Pham, L. Donati, T. Debarre, D. Sage, and M. Unser.

**Thank you !**