Science Requirements and Sensor Update

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4th XDAC Meeting, 13-15 Oct.

Science requirements:
Available tools for simulations

- Simulation of coherent diffraction pattern

Prototypical images

Scattering of residual gas molecules

- Detector simulations

Detector transfer function

Detector impact on reconstruction algorithms

Coherent diffraction simulation

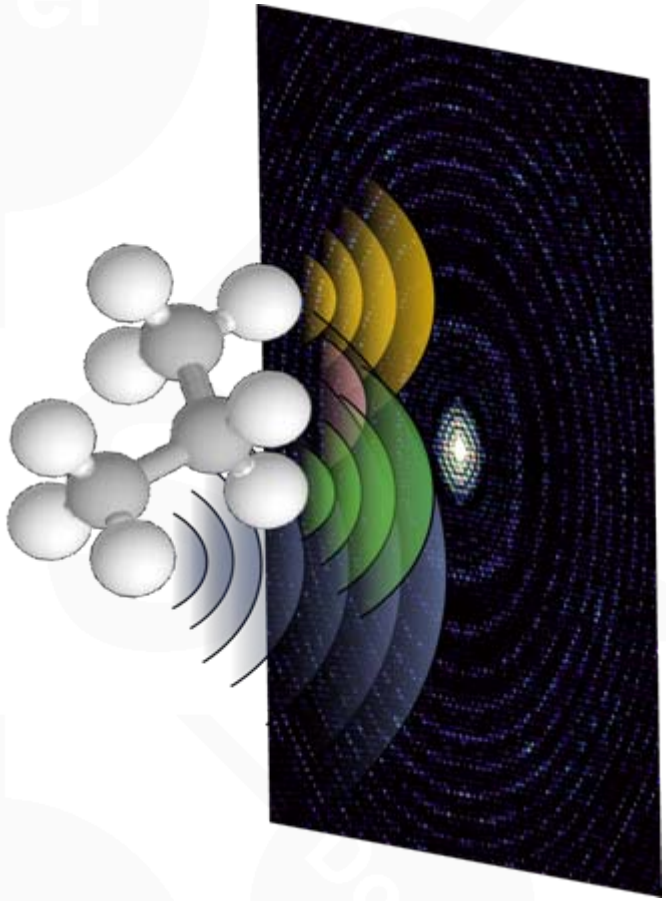
- Compute the contribution of each atom for each pixel
- Sum the intensities *(complex)*

⇒ Map of Most Likely intensities for each pixels *(real numbers)*

⇒ Correct for Solid Angle, Polarization…

⇒ Poisson statistics analysis Gives Intensity *(integers)*

⇒ *Then Add noise…*

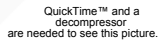


Detector simulation model

Monte Carlo approach

Charge sharing

Soon Charge explosion



Basic amplifier model +

Charge storage leak

$$Q_n^2 = \frac{\exp(2)}{8}\left[\left(2eI_d + \frac{4kT}{R_p} + i_{na}^2\right)\tau + \left(4kTR_s + e_{na}^2\right)\frac{C^2}{\tau} + 4A_f C^2\right]$$

Science requirements:
Coherent diffraction imaging techniques

Variety of prototypical images

- Simulations (F.Pfeiffer, self made)
- Experimental data (C.Mocuta, I.Vartaniants)

Some work on the photon background simulation

- Simulation of the residual gas scattering
- Need to understand more the contribution of the optics

Phase retrieval algorithms, impact of the detector geometry?

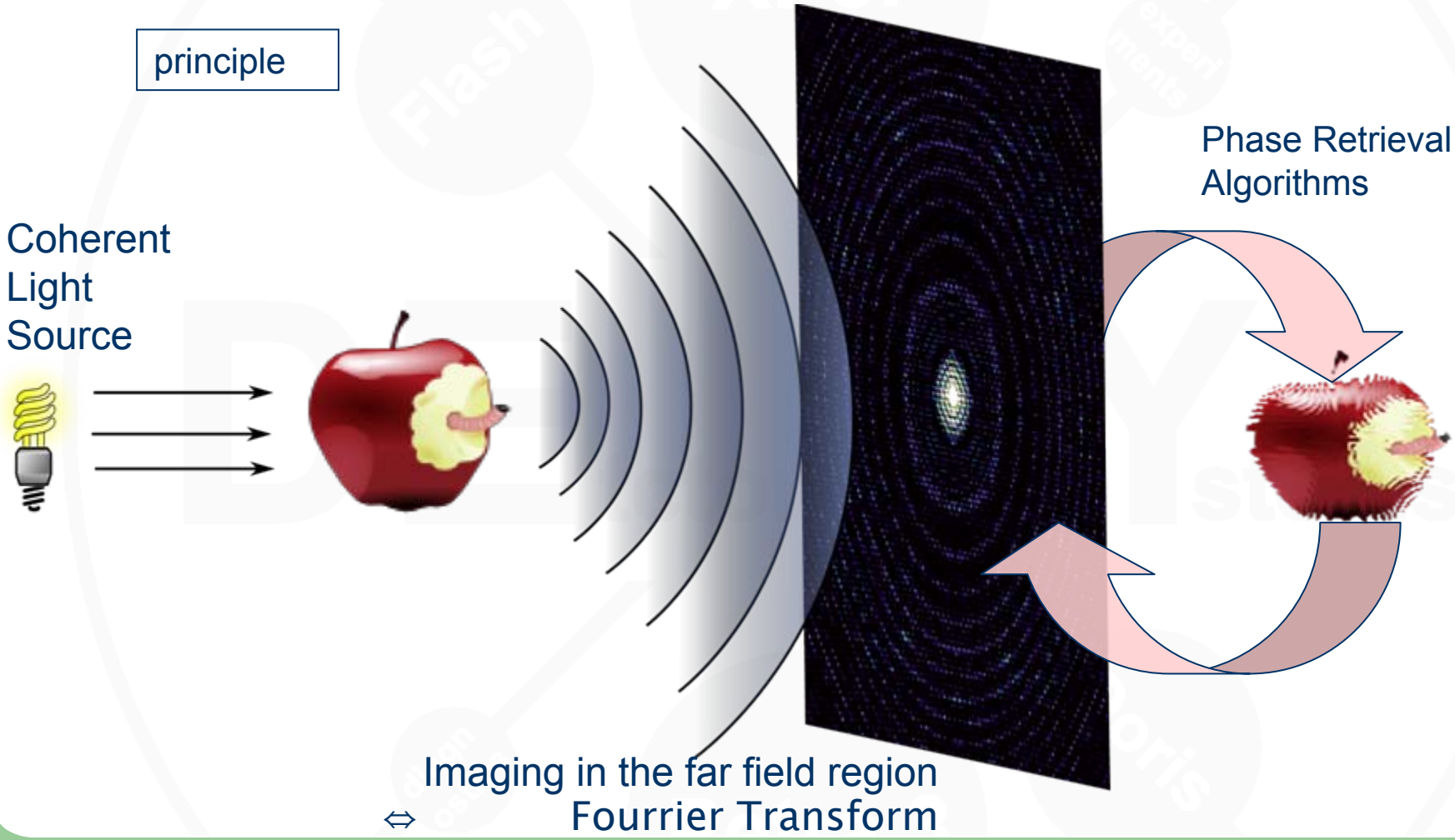
Science requirements:
Available prototypical images

Sample	Remark	Contributor
***Simulation* of Ferritin**	Single Mol, 1, 3, 5, crystal units	Pfeiffer, *et al.*
***Simulation* of Dwarf Virus**	Standalone	Pfeiffer, *et al.*
***Exp. data* of nanostructures**	Single objects	C.Mocuta, *et al.*
Oversampled *Simulation* of biomolecules	Enable study of expected peak shape	Potdevin

Science requirements:
Detectors Geometry

- It is evident that we need a central hole. But what size??

principle



Science requirements: Biomolecules

Coherent diffraction imaging techniques

- Single molecules are a challenge (not everybody believes in it):

PAUL SCHERRER INSTITUTE

„Generative Topographic Mapping“

Classifying individual shots makes poor use of photons.
Must use correlations in entire diffracted ensemble.

Diffraction Pattern

Diffraction Pattern Vector

p-Dimensional Space

p = # pixels

Intensities depend on molecular orientation θ, φ ⇒

vectors on a 3D manifold

Mapping

p-Dimensional Space

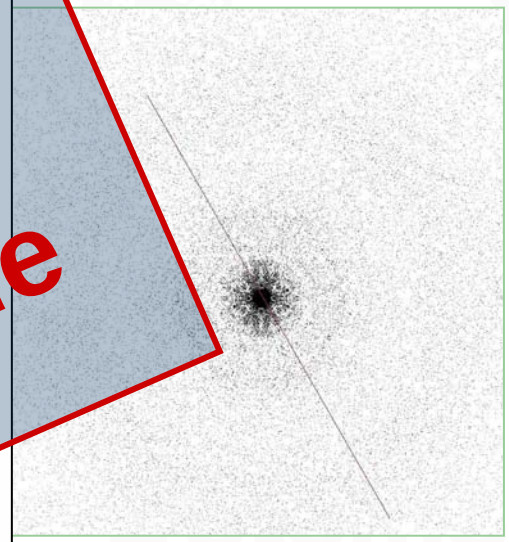
θ

Analyze total data set to find mapping function.

A. Ourmazd

12 keV
slicing (τ<20 fs)
maximum brightness

Requirements are mostly on the storing server side



Single Virus

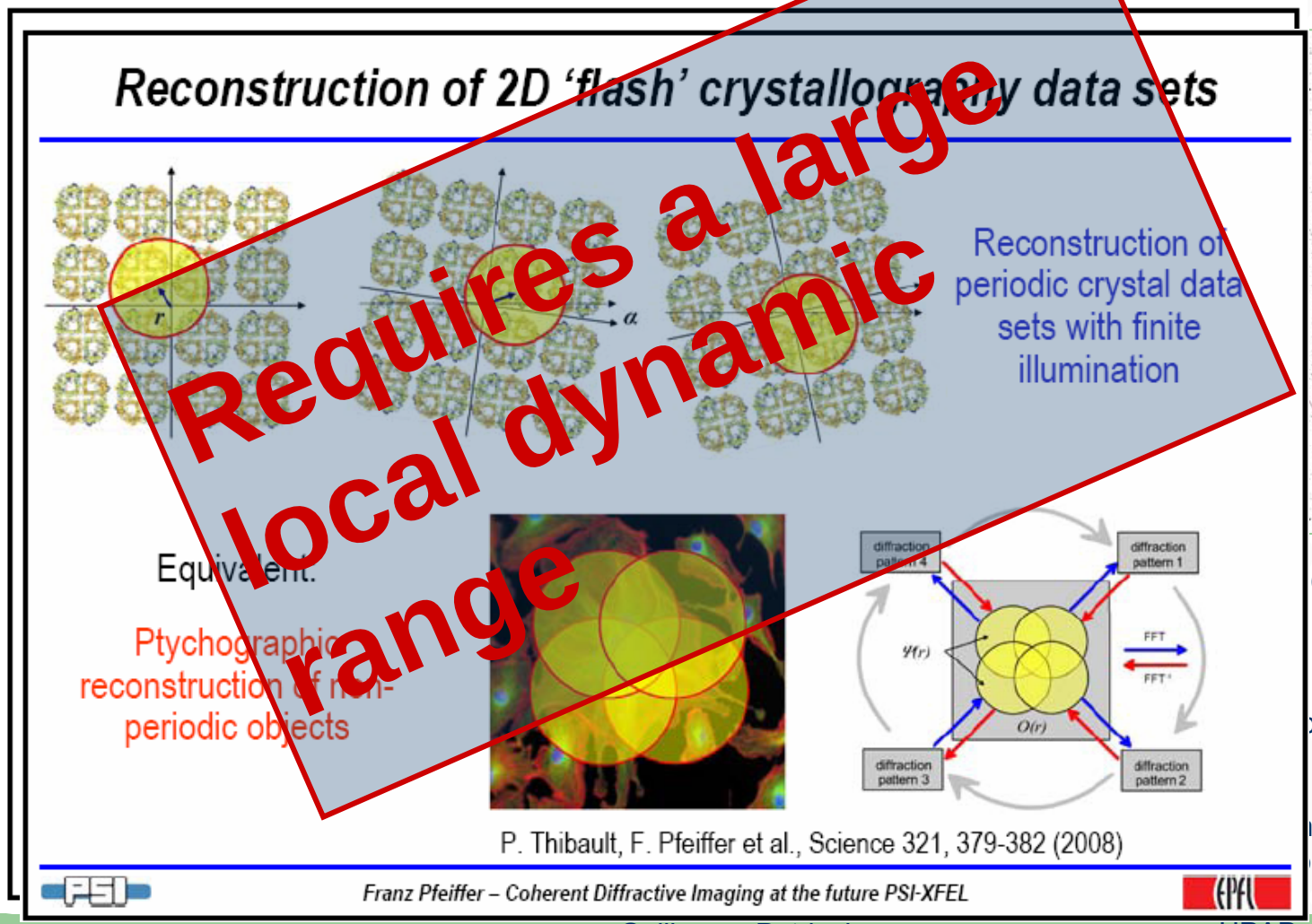
(big molecule)

Total intensity – central peak
= 80 000 photons

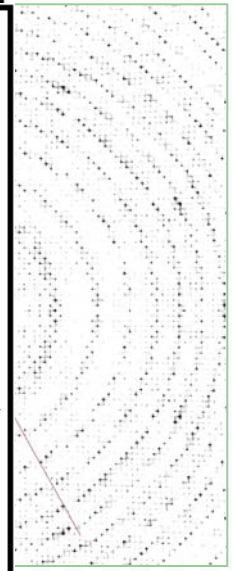
Among pixels with intensity
96.7% pixels < 4 photons

Science requirements: Nanocrystals
Coherent diffraction imaging techniques

- 2D and 3D crystals are promising



Requires a large local dynamic range



o-crystal

peak

case)

sity
ns

Science requirements: Nanocrystals
Coherent diffraction imaging techniques

Peak extension

Science requirements:
Can we count on the background to help us?

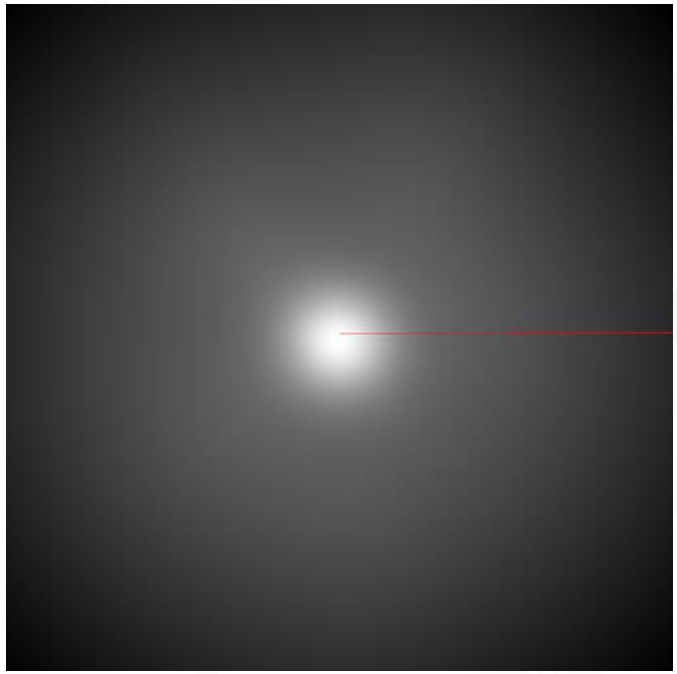
The main sources of photon background are:

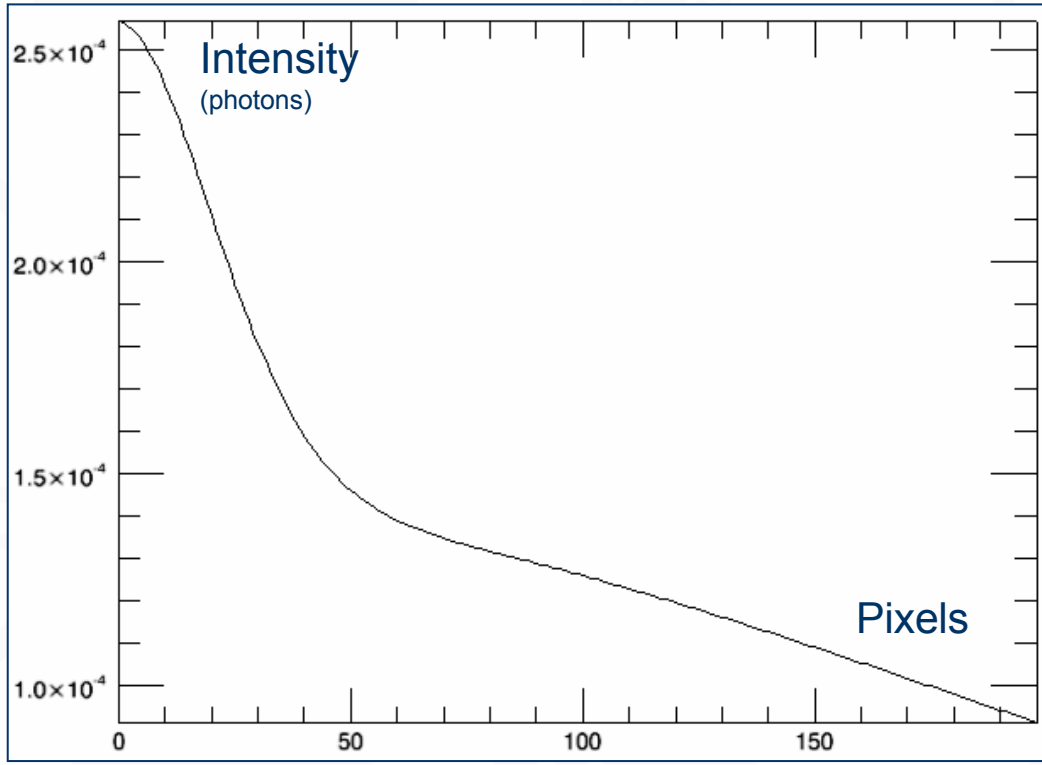
- Residual gas scattering ("*The scattering of vacuum*")
- Inelastic scattering (sample and residual gas)
- Optics imperfection

Science requirements:
Residual gas coherent scattering

Simulation of the photon background of a chamber:

- 10m long
- Pressure 10^{-3}mBar
- Only H_2O molecules

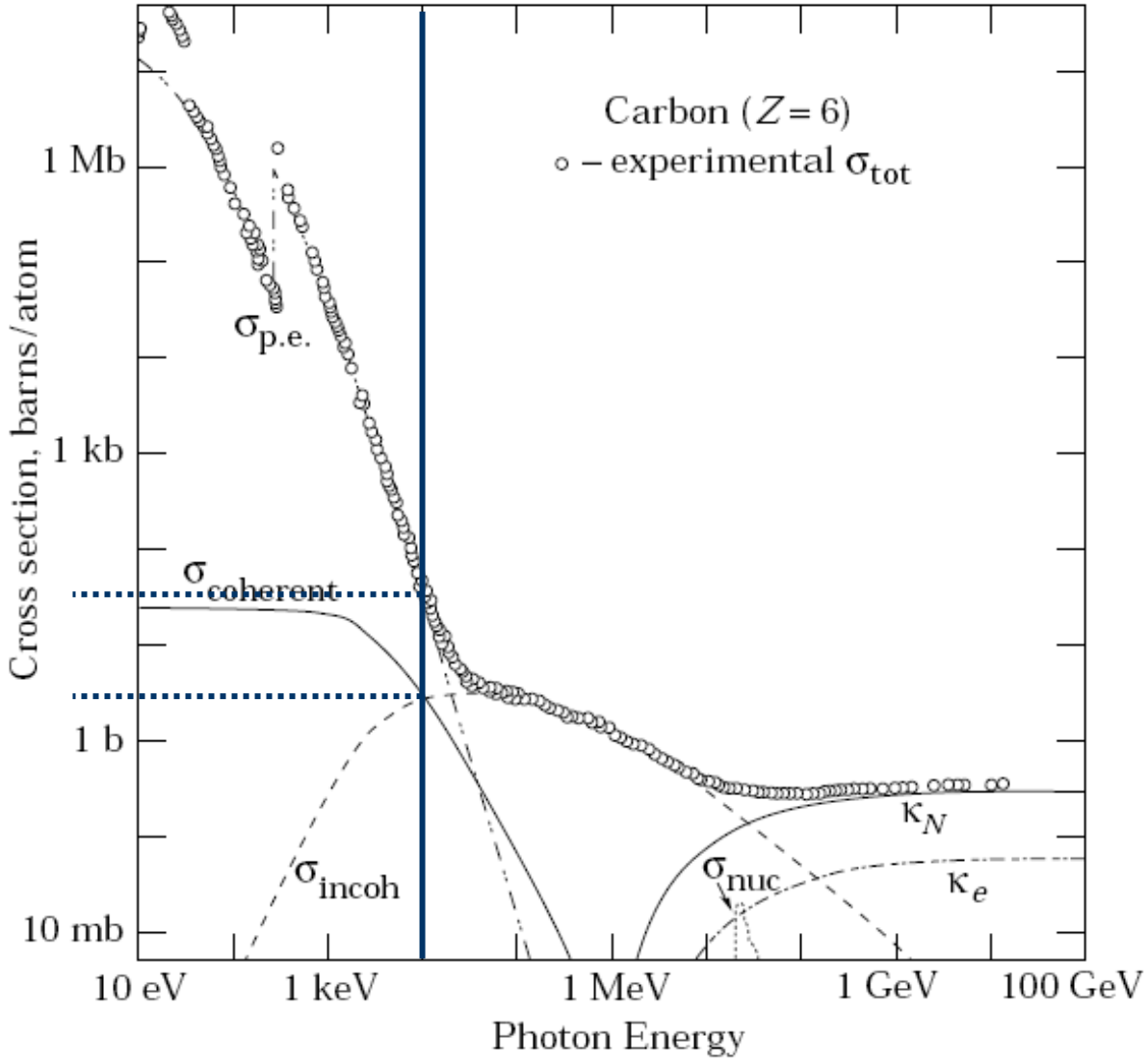




ie. On average 18 photons on detector.

Science requirements:
Inelastic scattering

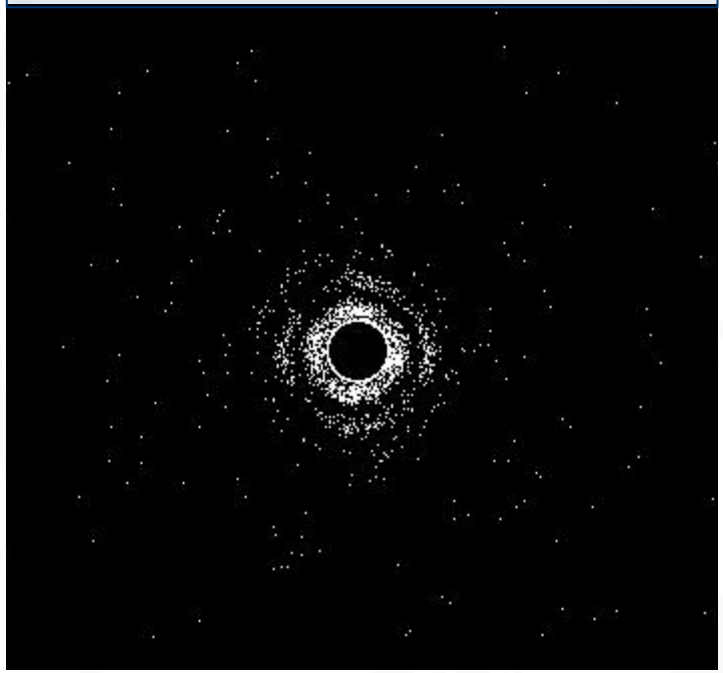
Inelastic is 10x smaller for organic compounds



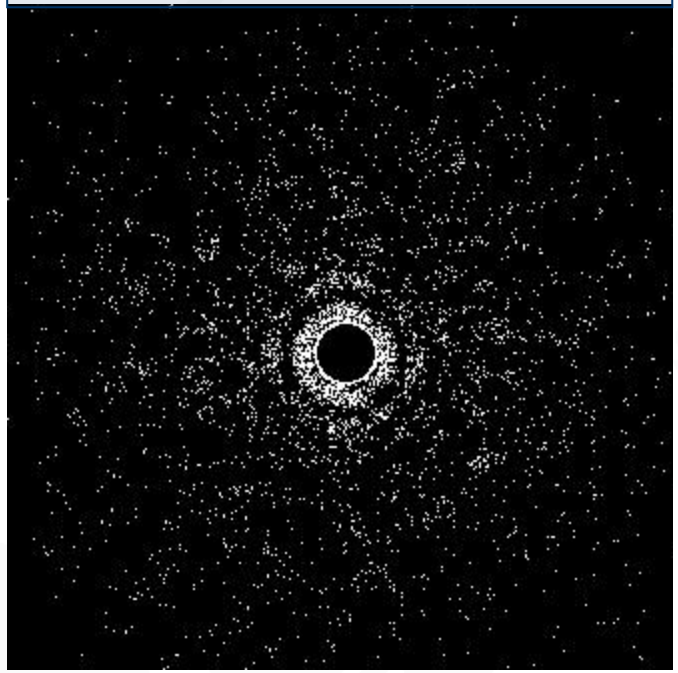
Science requirements:
Impact of the optics

- Optical elements are probably the strongest source of photon background
  - Surface roughness
  - Slits scattering
  - …

Single Ferritin molecule
Without optics background



Single Ferritin molecule
With optics background



"Trivial attempt" by F.Pfeiffer

Science requirements:
Detectors Geometry

Geometry is determined by:

- Object Size $2d \sin\Theta = \lambda$
- Focusin optics

BIG OBJECTS:

- Small Θ
- Good scattering power

Long distance, no lens

Small hole

Small objects:

- Large Θ
- Poor scattering power

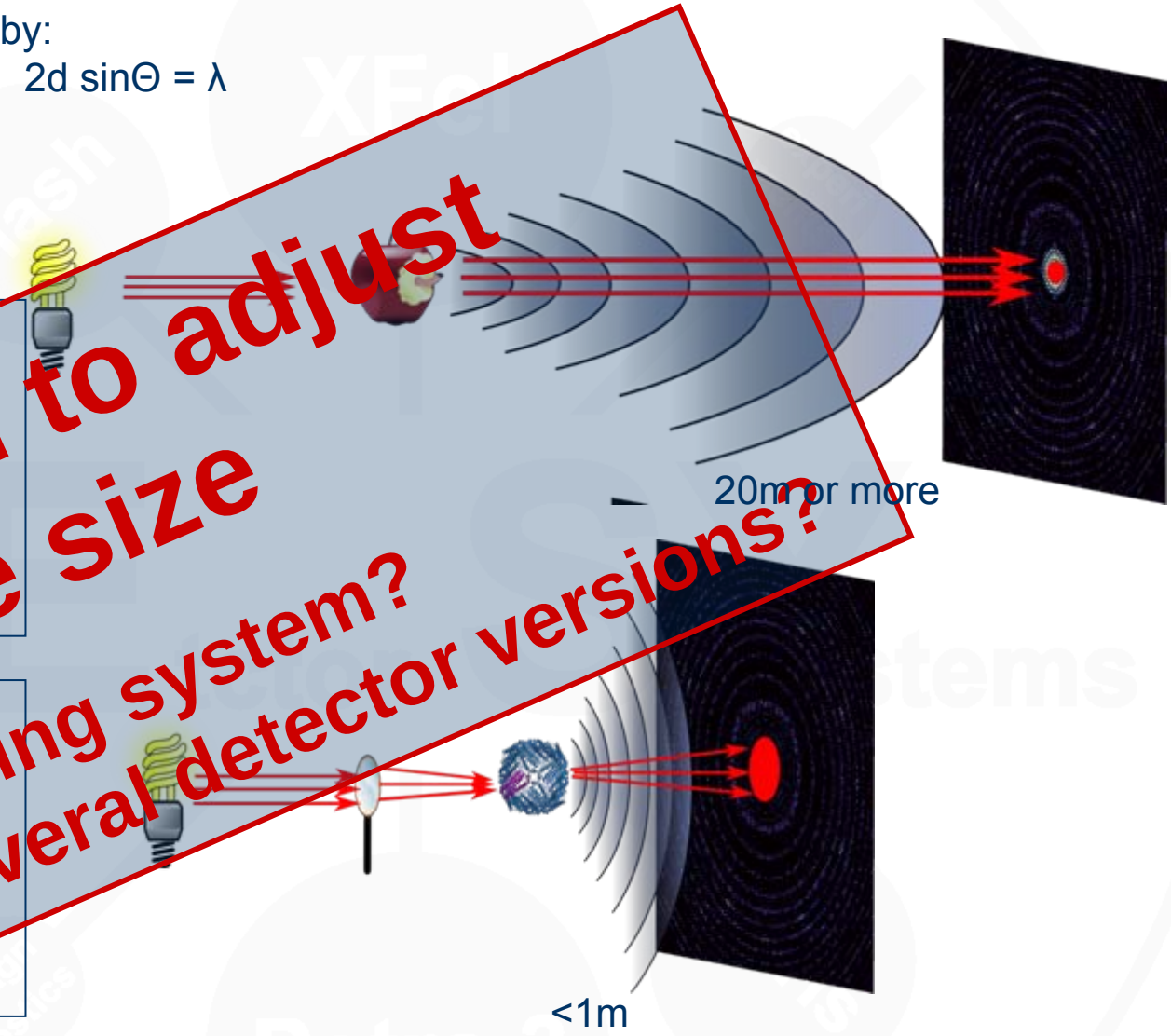
short distance, need lens

Big hole

Need to adjust hole size

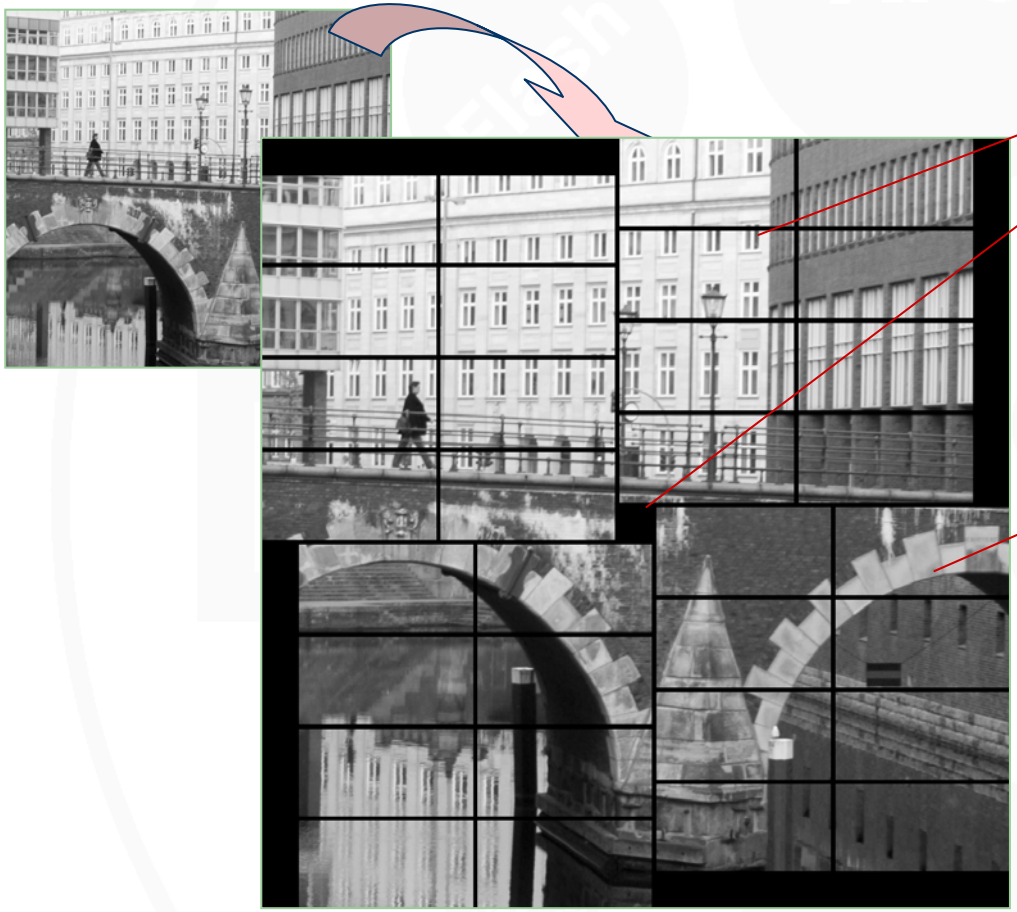
Sliding system?

Several detector versions?



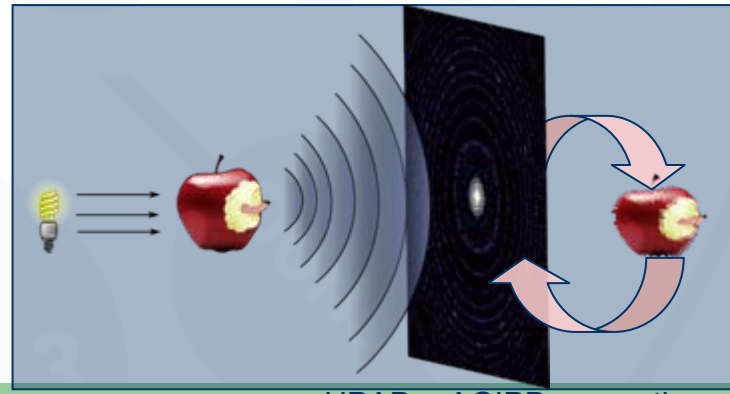
Science requirements:
Detectors Geometry

- Reconstruction



Hole and dead areas
impact on reconstruction?

Distortion impact
(doping profile, mechanics)

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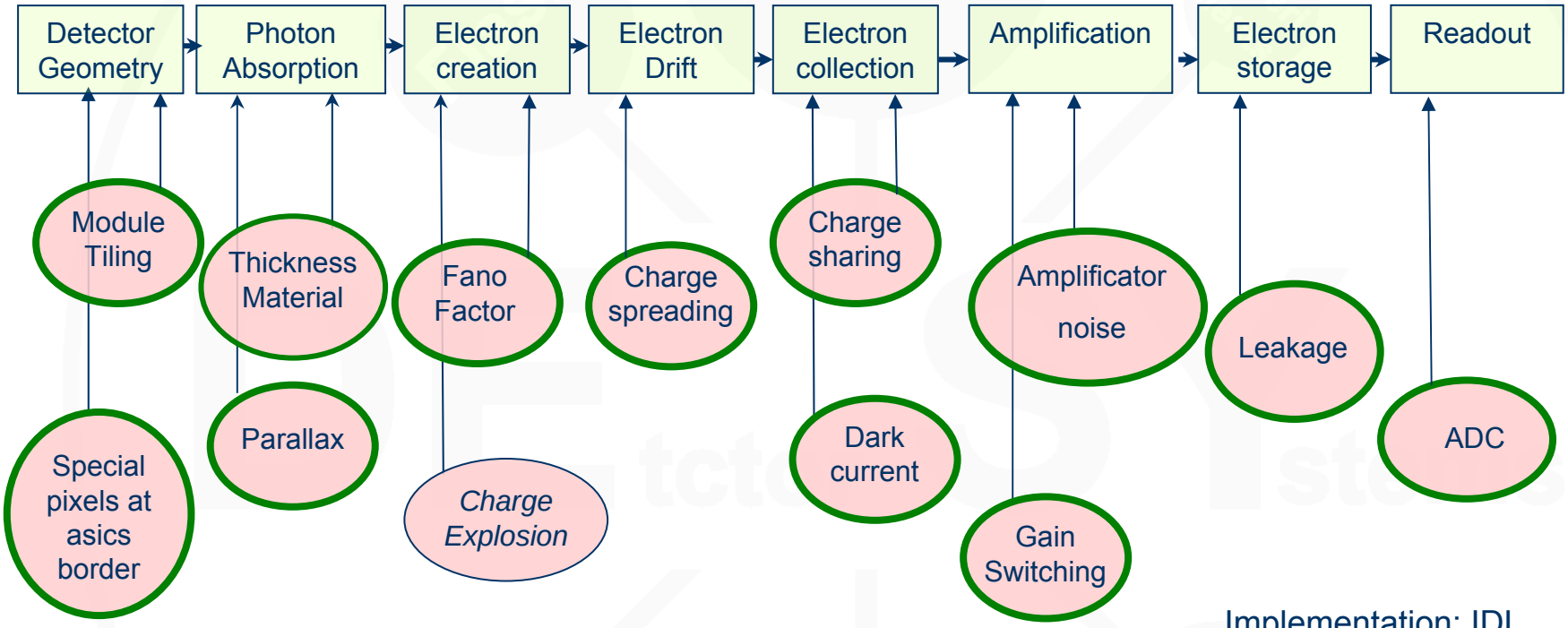
Detector simulation software



Implementation: IDL