Obtainment of Prototypical images and Detector performance simulations

Guillaume Potdevin for the XFEL-HPAD-Consortium

Outlook

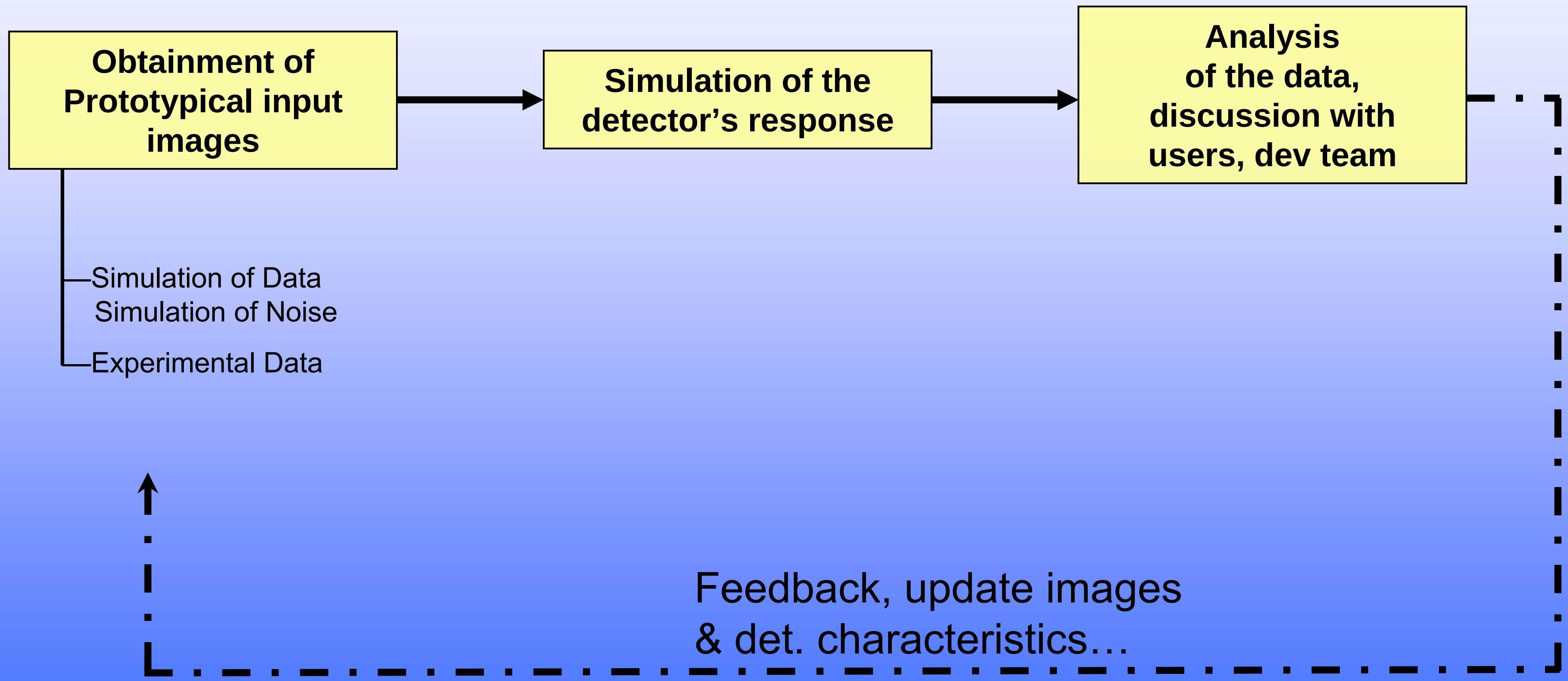
- Overview of the analysis

- Prototypical images:
  - Single object imaging & XPCS short presentation (reminder…)
  - Presentation of the data ⇒ Dynamic range analysis

- Detector Simulation Software
  - Presentation
  - Waiting for your inputs

HELMHOLTZ GEMEINSCHAFT DESY PAUL SCHERRER INSTITUT PSI universitätbonn Universität Hamburg

Overview of the Analysis



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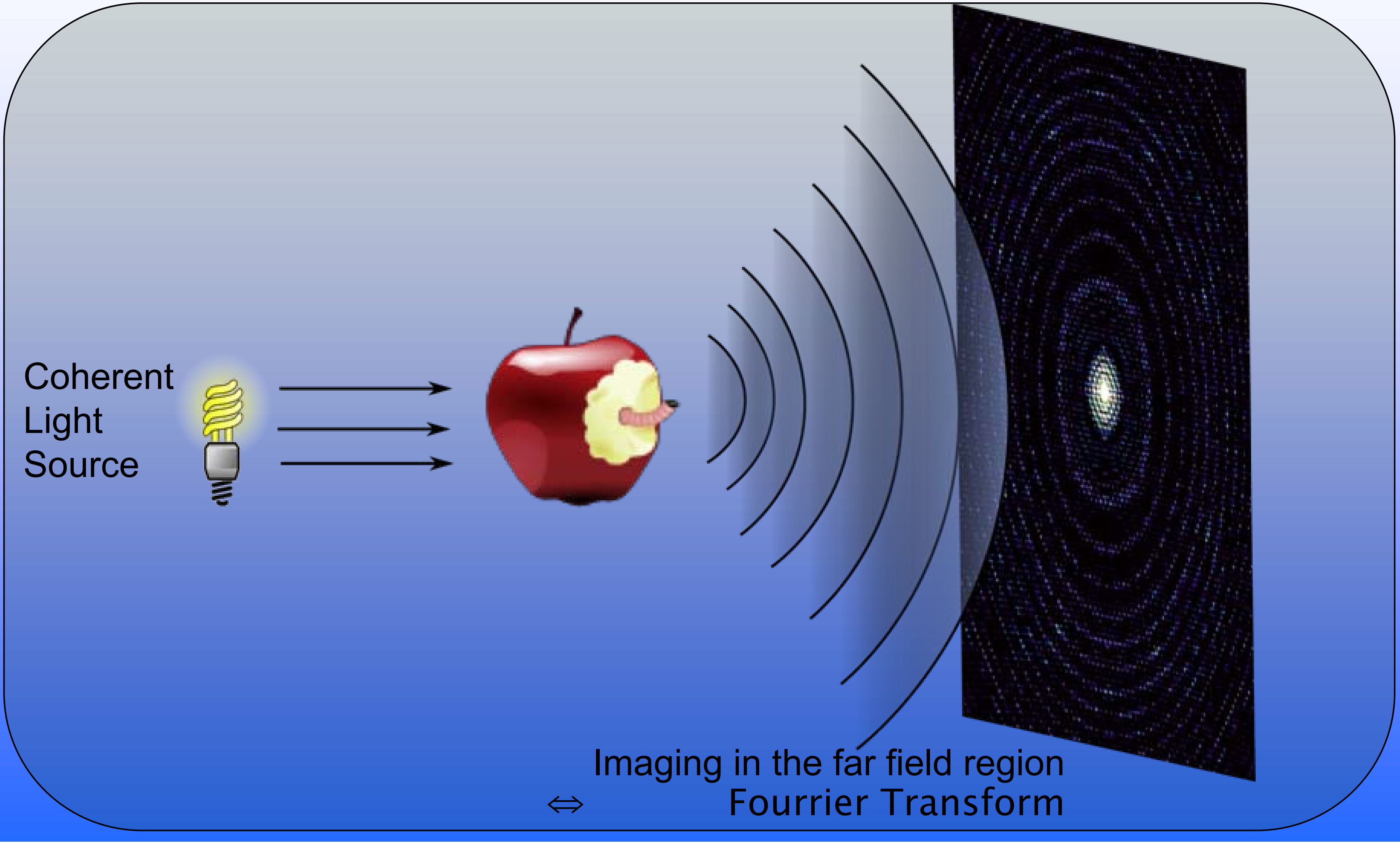
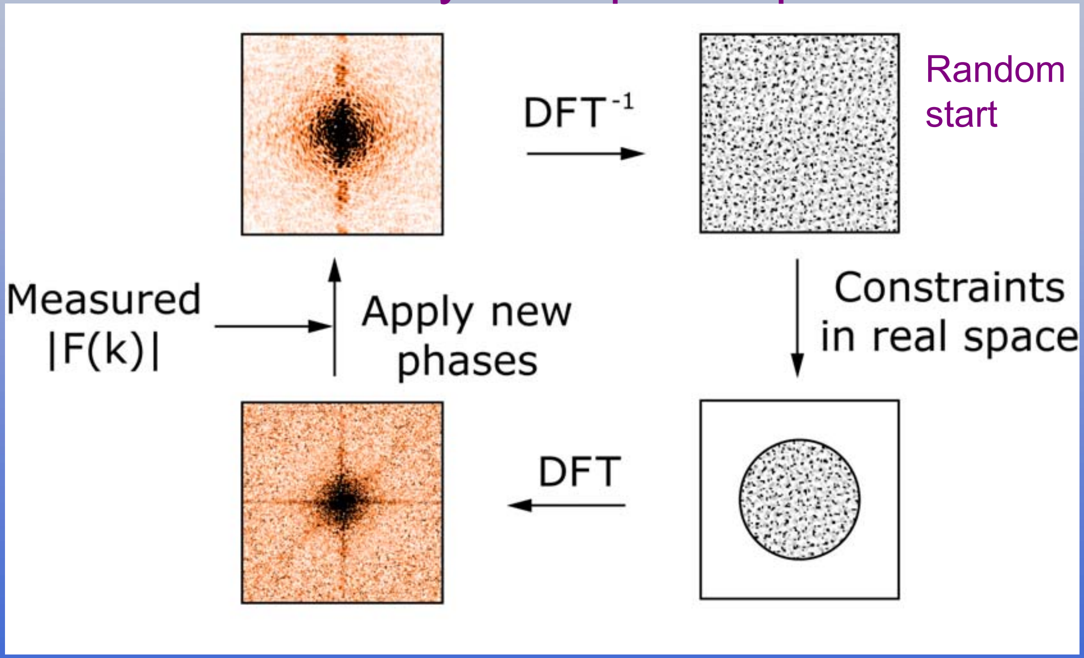
Single object Imaging



Single object Imaging, the reconstruction

- Algorithm starts with an image (random)
- Apply projections
- Iteratively modify image until converge

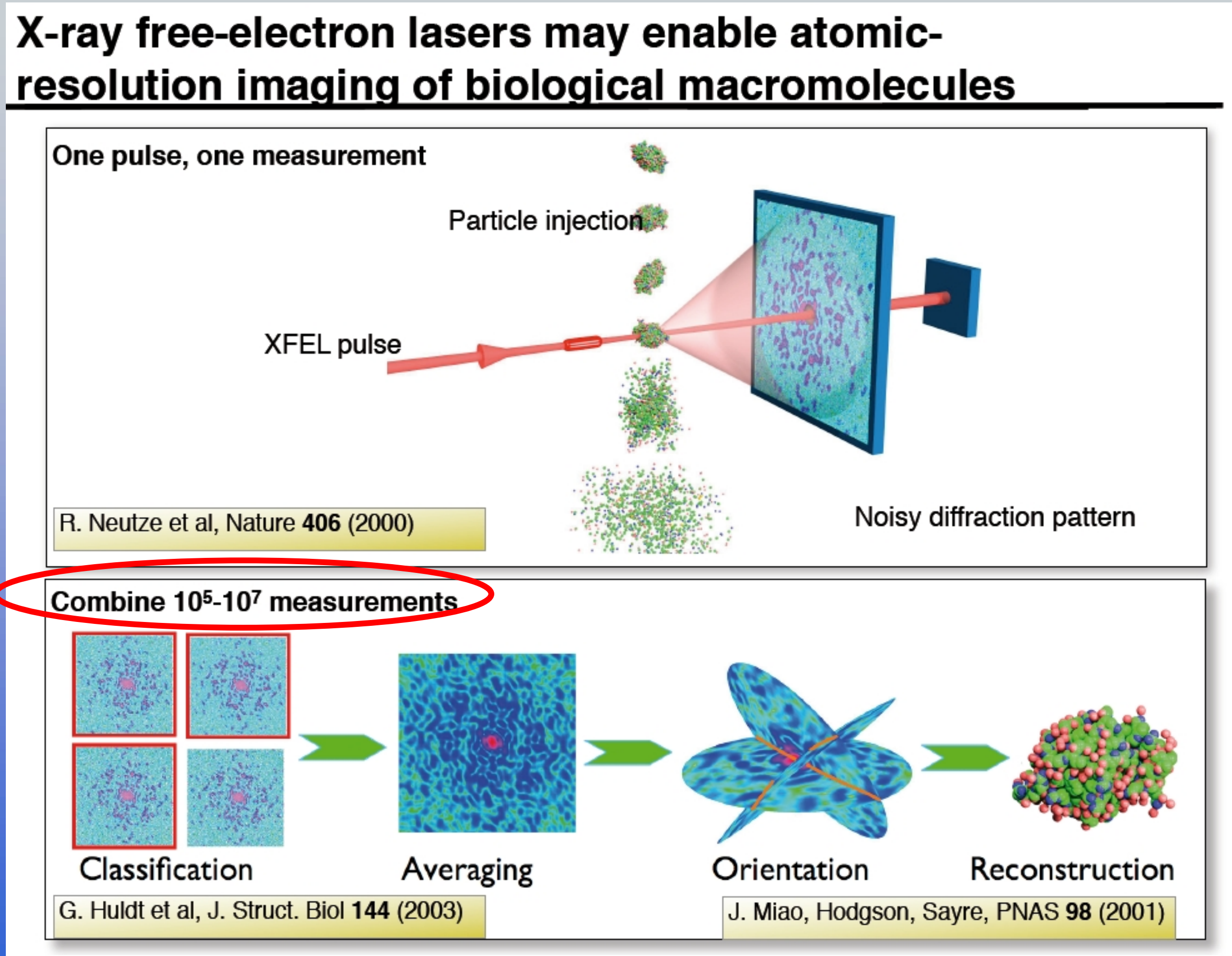
hybrid input-output (Fienup, *Appl. Opt.* **21**, 2759 (1982))



difference map: Elser, *J. Opt. Soc. Am. A* **4**, 118 (2002)

Slide robbed to J. Kirz , ALS Berkeley

Single object Imaging @XFel Sources



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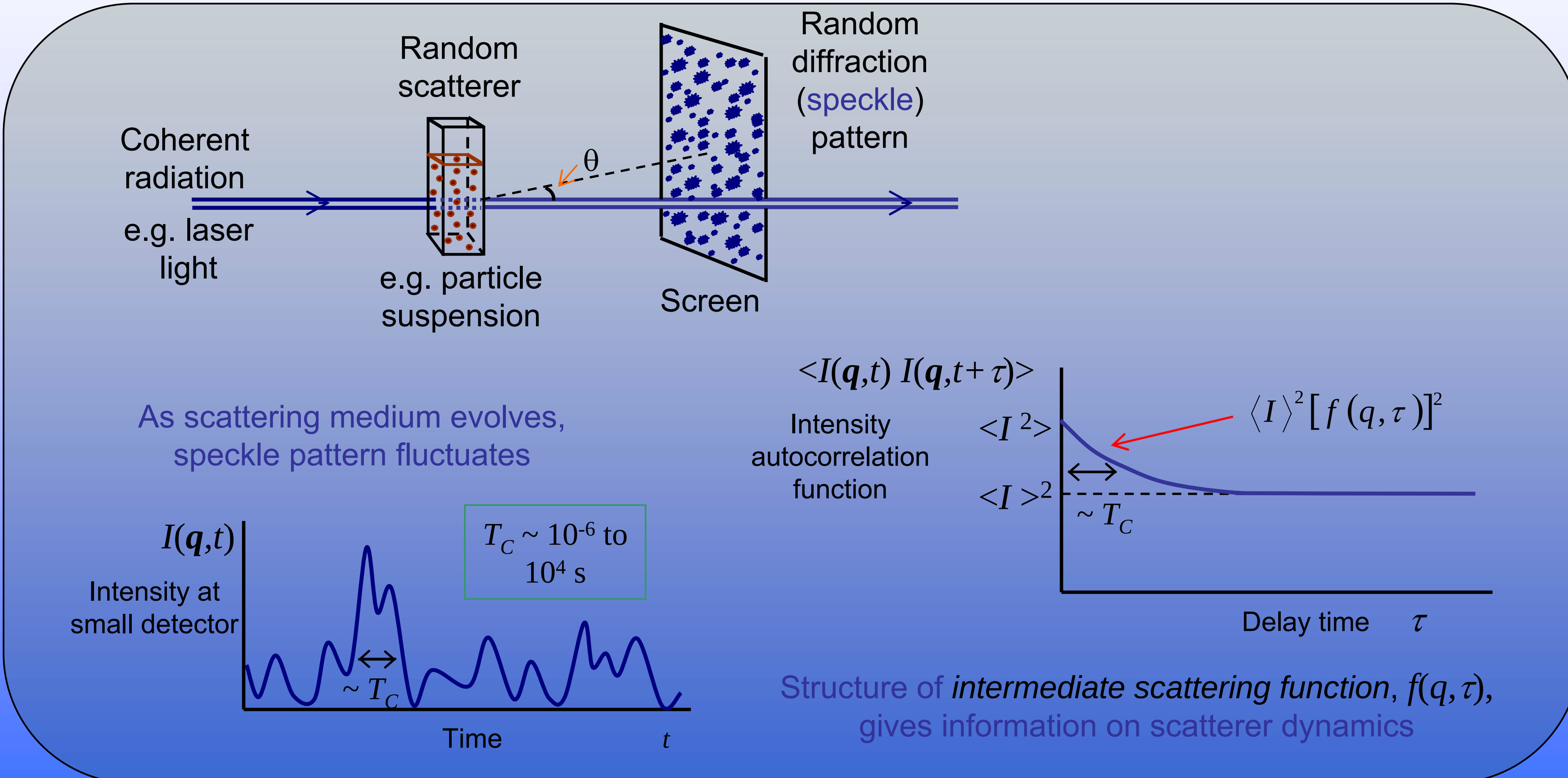
XPCS

X-ray Photon Correlation Spectroscopy



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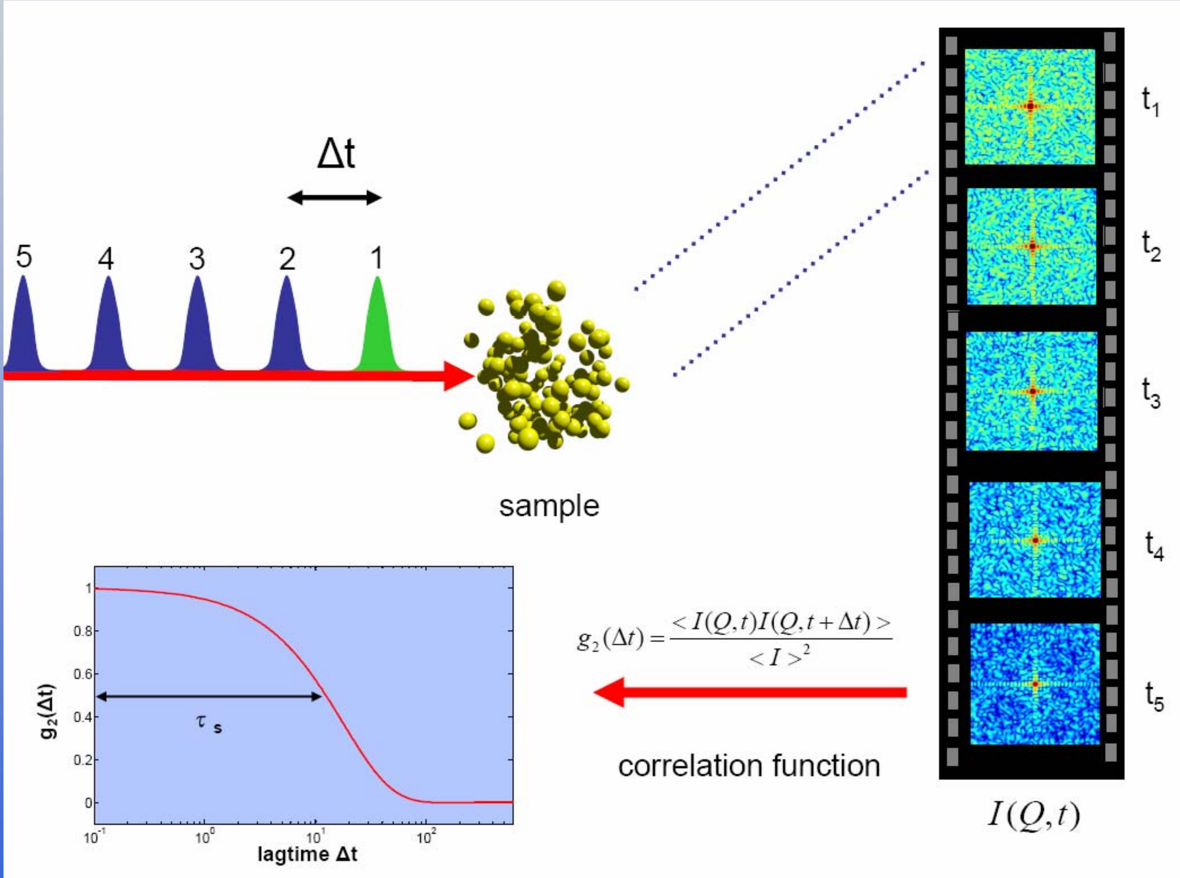
XPCS @ XFel Sources

Sequential Mode



XPCS (Sequential):

$0.1\ s \leq \tau$

$200ns \leq \tau \leq 600\ \mu s$

Desire 5 MHz frame-rate.
Eventually logarithmic time bins.
(record less than 3000 frames)

"Timing limited".

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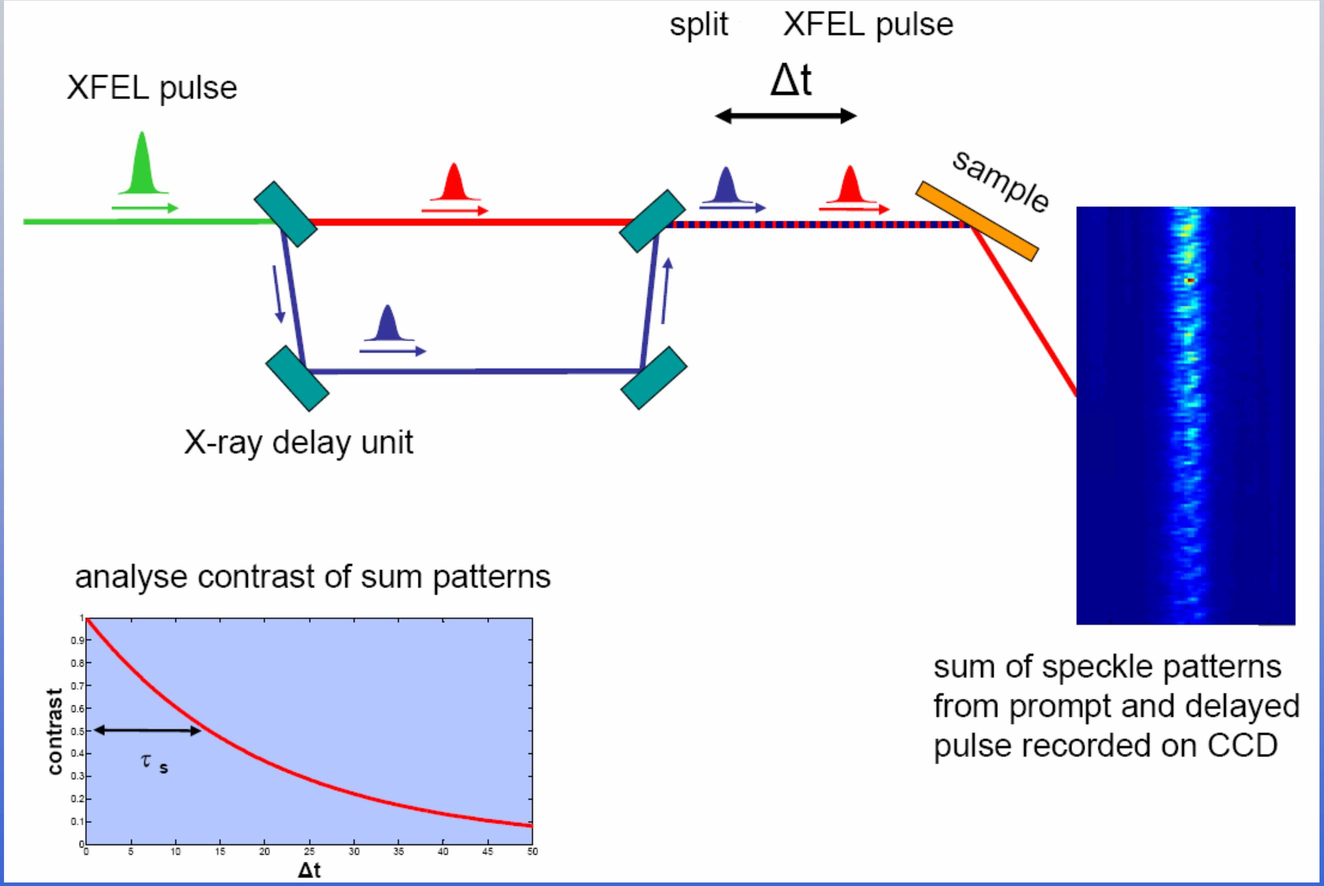
XPCS @ XFel Sources

Delay line Mode



"Delay Line" Mode:

1ps < Δt < 10ns

(1 ps ⇔ 0.3 mm; 1ns ⇔ 300 mm)

"luminosity limited".

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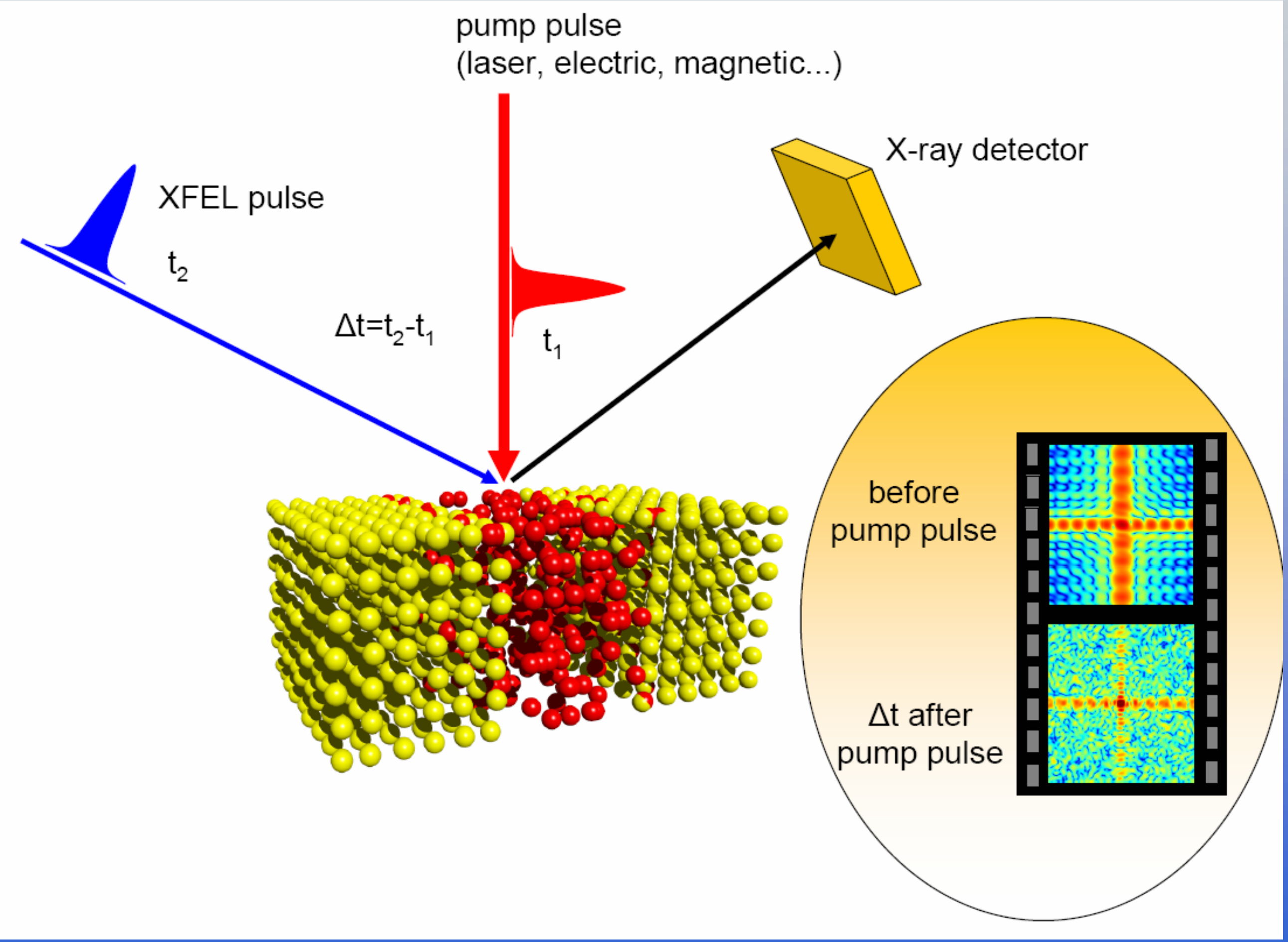
XPCS @ XFel Sources

Pump Probe Mode



Slide Robbed to *G. Gruebel, DESY*

Outlook

- Overview of the analysis

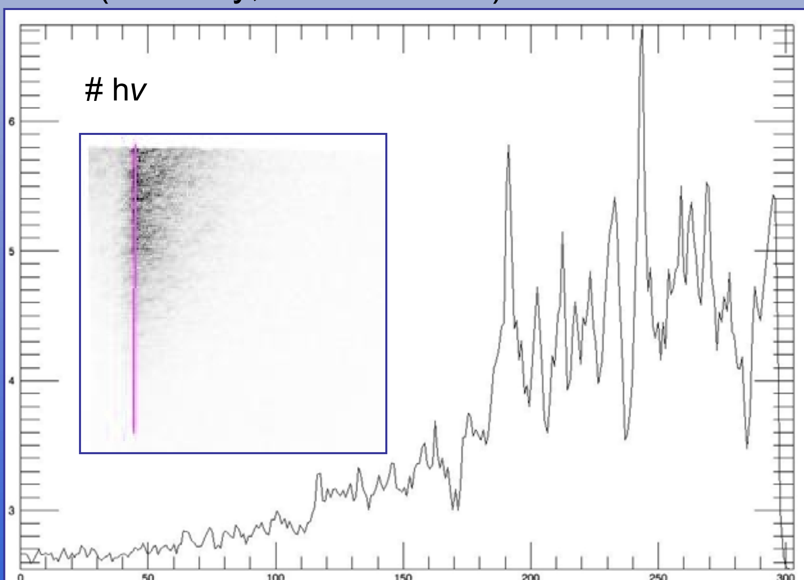
- Prototypical images:
  - Single object imaging & XPCS short presentation (reminder…)
  - Presentation of the data ⇒ Dynamic range analysis
    - Which sort of data
    - The data

- Detector Simulation Software
  - Presentation
  - Waiting for your inputs

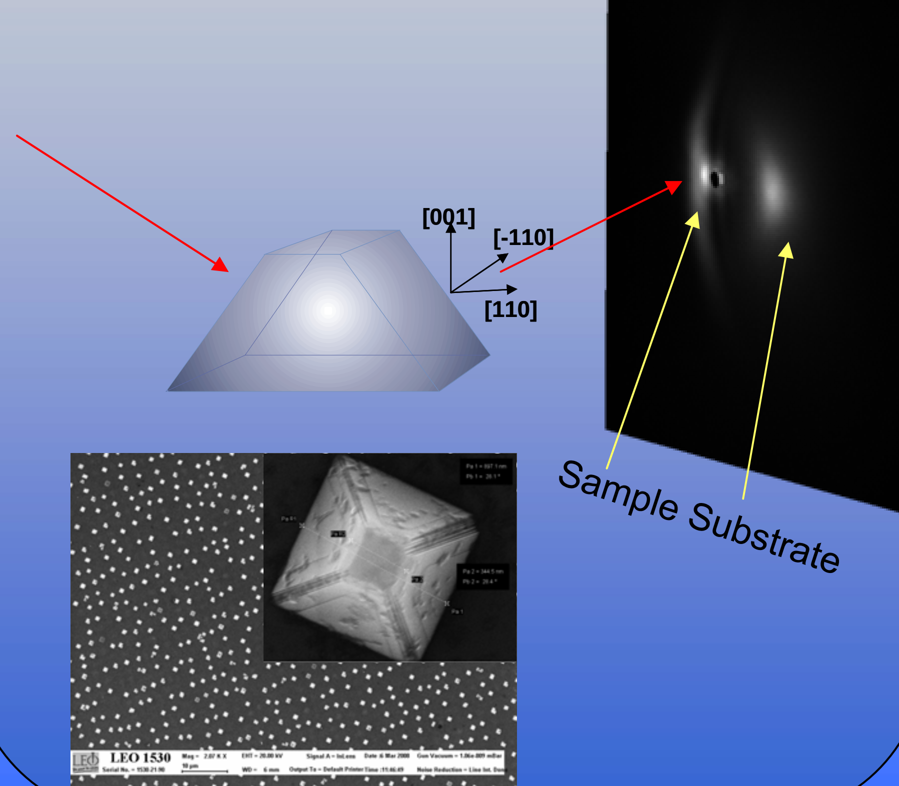
Obtainment of prototypical images :
Use of relevant experimental data

- Use relevant data:
  - *Single object scattering*
  - *XPCS patterns*

Example: Surface Colloid
(courtesy, C.Gutt DESY)



Example: single nanocrystal study (courtesy, C.Mocuta ESRF)



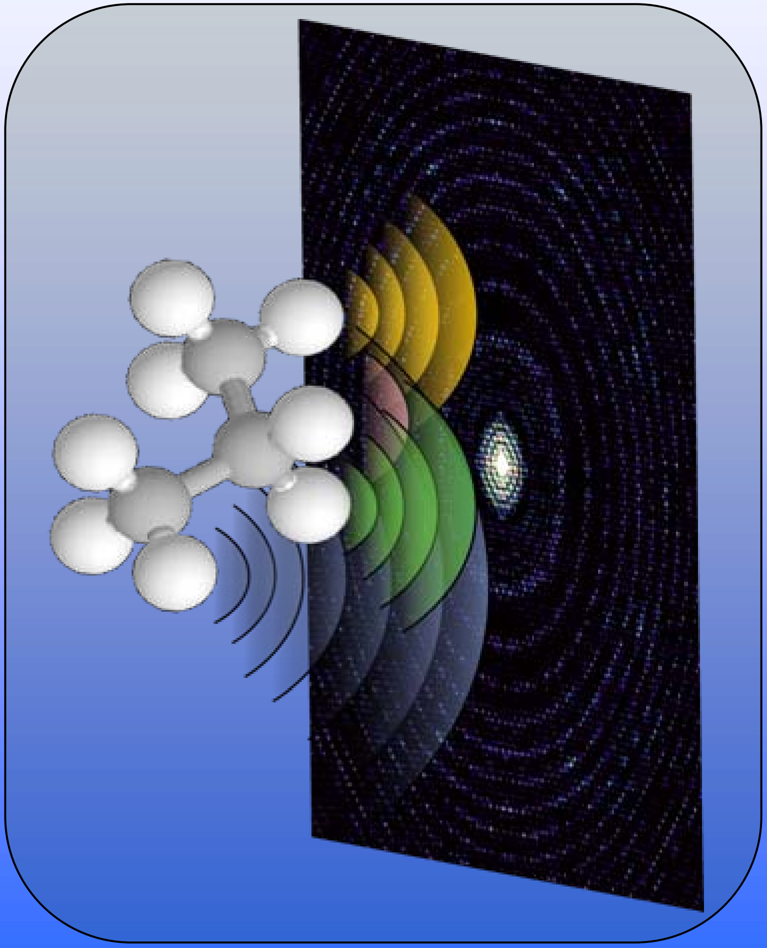
Obtainment of prototypical images :
Simulation of Small Objects Scattering

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

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

⇒ Poisson statistics analysis
Gives Intensity *(integers)*

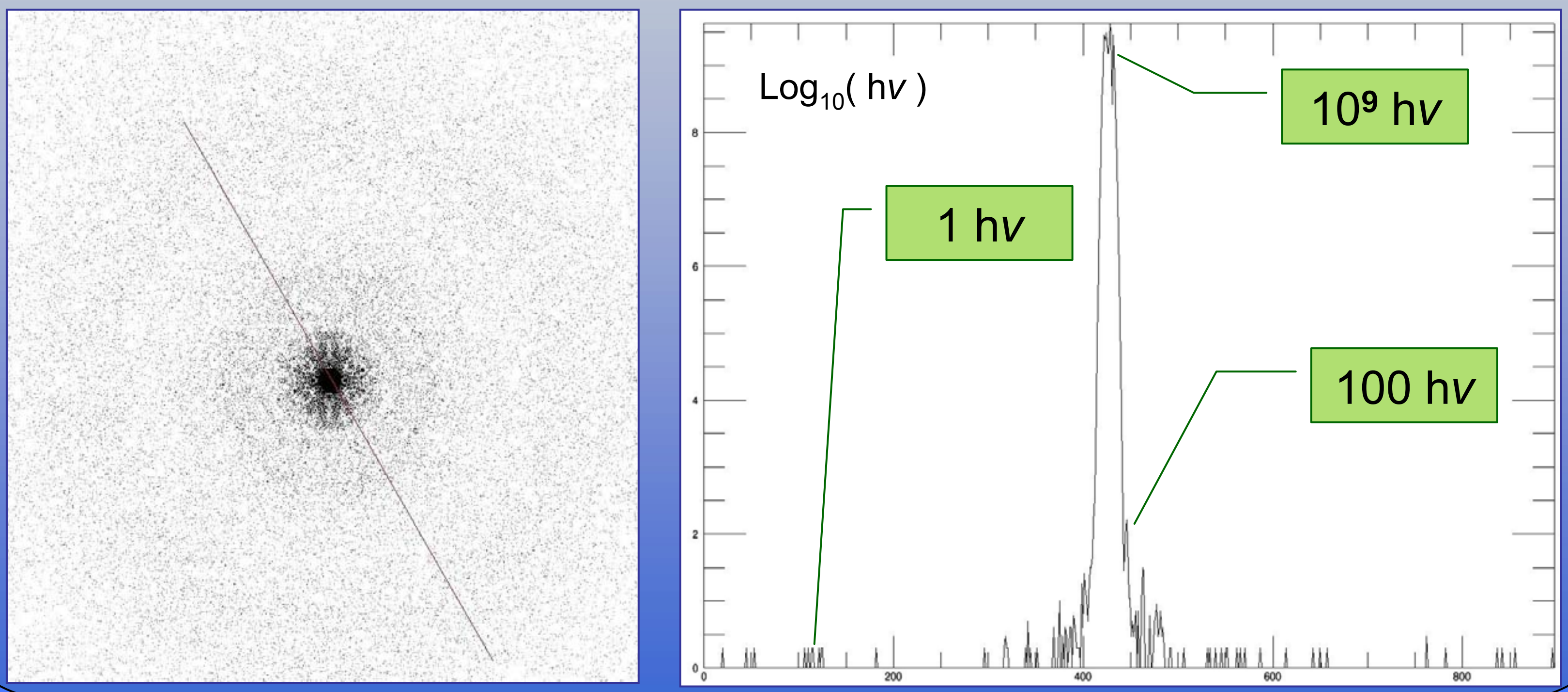
⇒ *Then Add noise…*



Data: Case of very small single object

- Simulation of a dwarf Virus

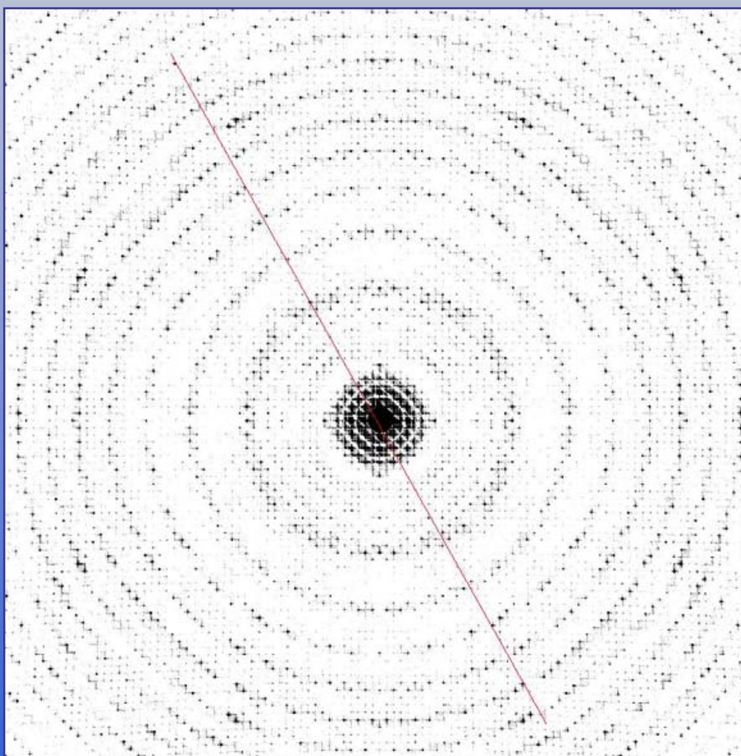
  → single virus (simulation by F.Pfeiffer, SLS)

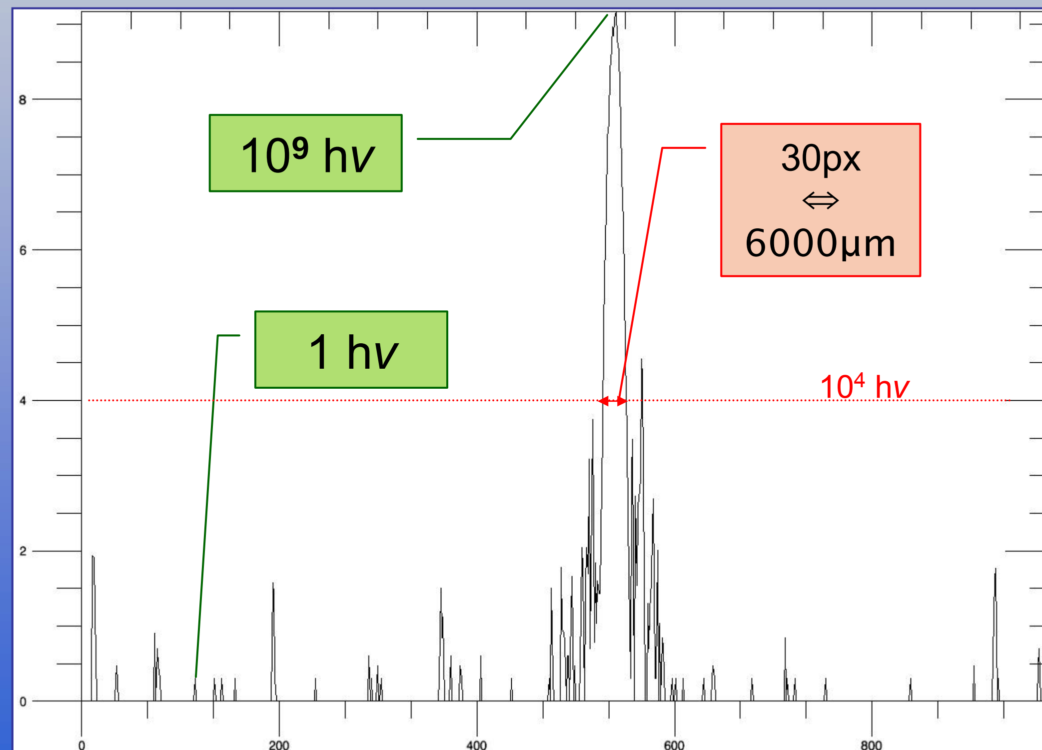


- Mostly a central peak, plus a few scattered photons.

Data: Case of small clusters

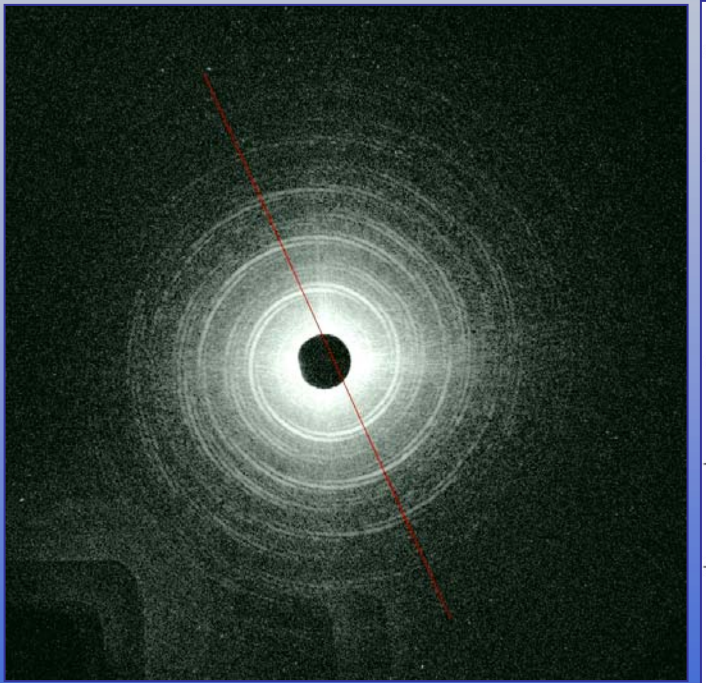
- Ex. Simulation Ferritin in 5*5*5 crystal unit crystal (large)
  →250 molecules of 20kDa each. (simulation by F.Pfeiffer, SLS)

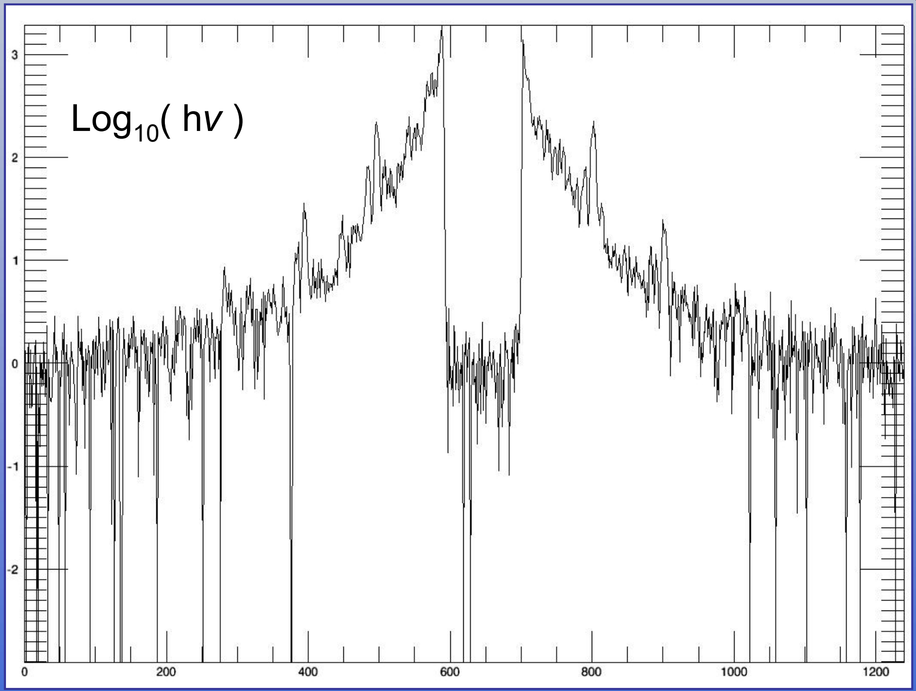




Data: The background problem

- Lithographed samples with a CCD
  (courtesy Schropp, Vartanyants @ esrf id01)

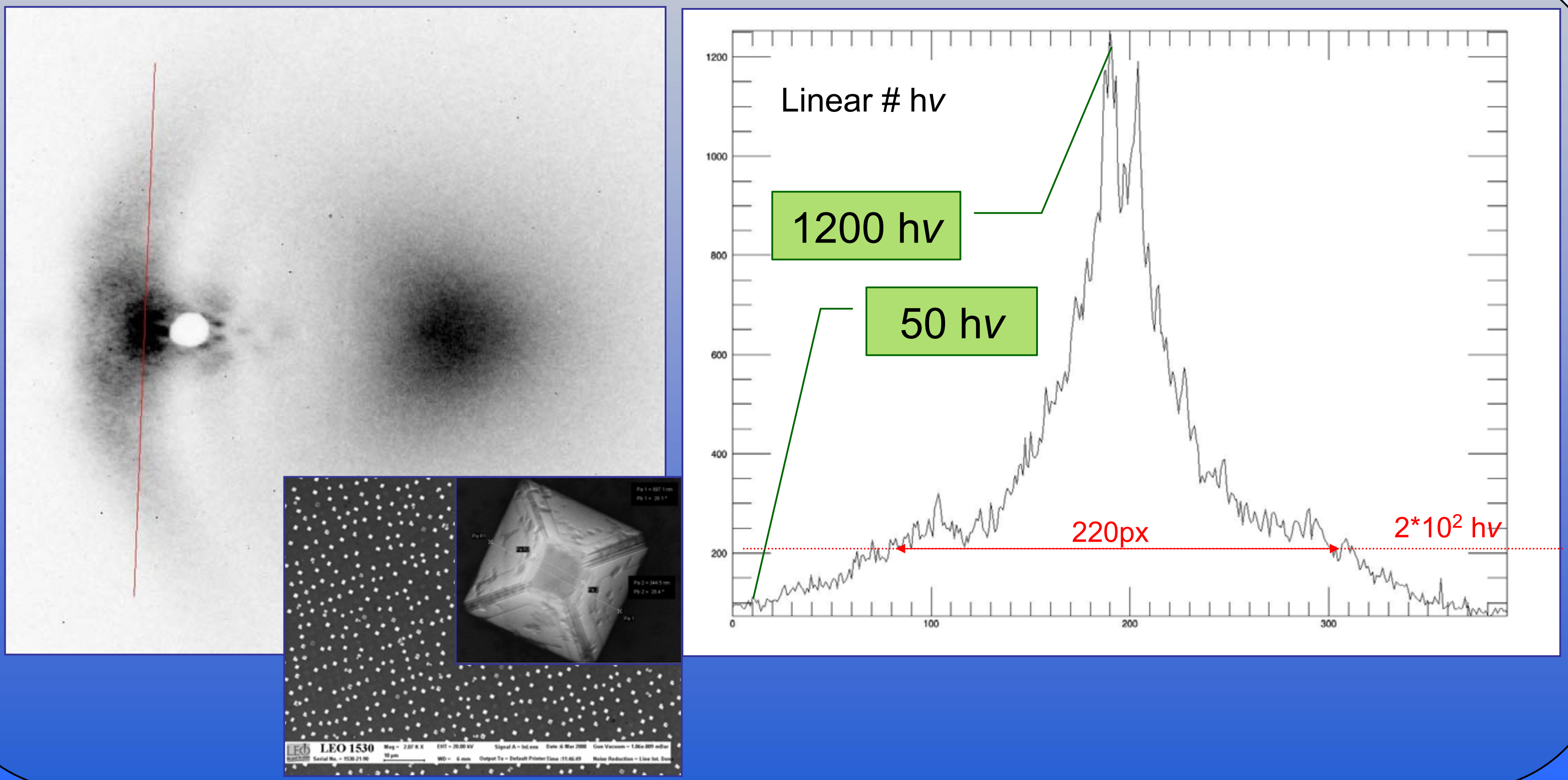




- Intensity ~ *1/q*^{3} + features.

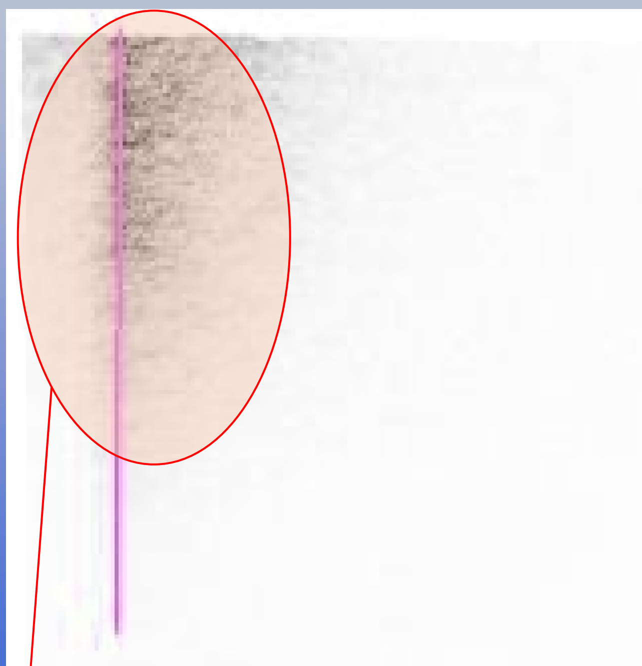
Data: An example of nano object

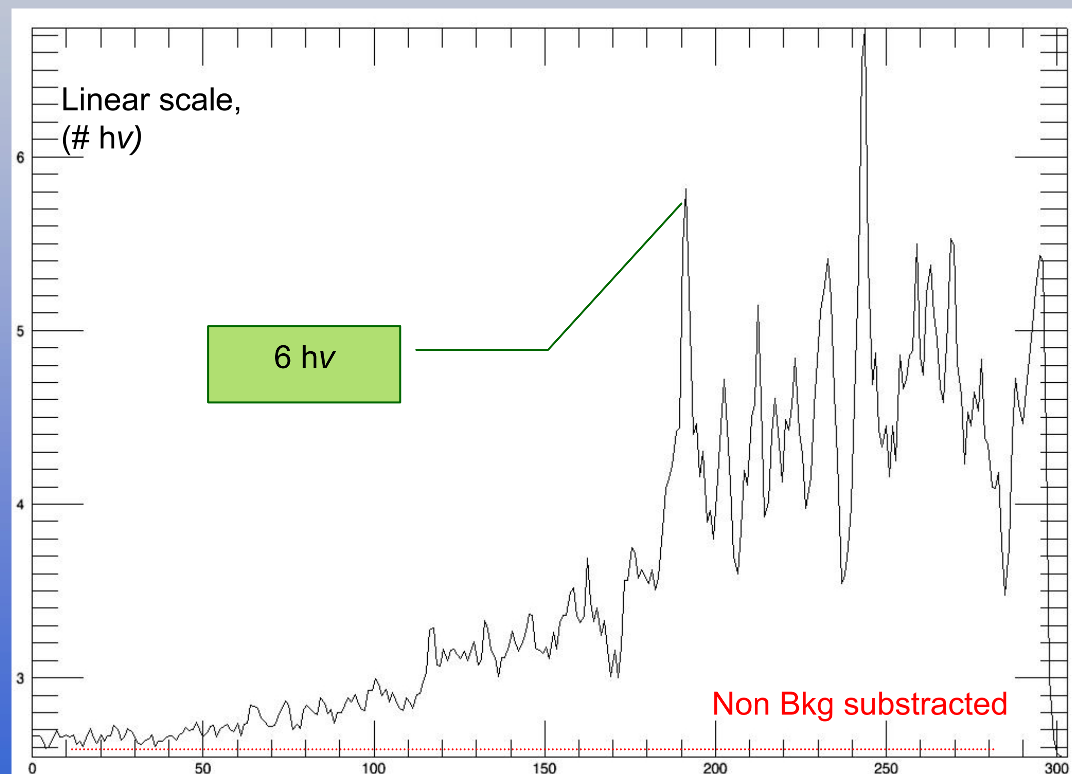
- Ex. Exp data from single object on Si Substrate
  →object : ~800nm size (courtesy of data: C.Mocutta, ESRF)



Data: Case of the XPCS

- Ex. XPCS data, colloids on a surface
  (courtesy of data C.Gutt, @ esrf id10)





- Speckles are localized (i.e. density of pixel matters, not only surface)

Summary of available 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 lithographed sample on SiN**	*Contribution from SiN* membrane to signal	Vartaniants, Schrupp, *et al.*
***Exp. data* of nanostructures**	Missing information for ADU→Photons conversion	C.Mocuta, *et al.*
Simulation of Pd nanocrystals	@100keV (irrelevant for now). No scaling in photons	Vartaniants, Blumes, *et al.*
***XPCS** exp. data*	8 keV, Relevant regarding intensities. For noise?	C.Gutt, *et al.*

Dynamic Range analysis

- Lots of photons at the center (not only direct beam)

⇒Central hole to let high intensities go: Hole ~ 2mm >> Central Beam
⇒Another adapted detector further (low q info)?

- "Randomly" scattered photons smaller Intensities

⇒*Per region shiftable dynamic range?*

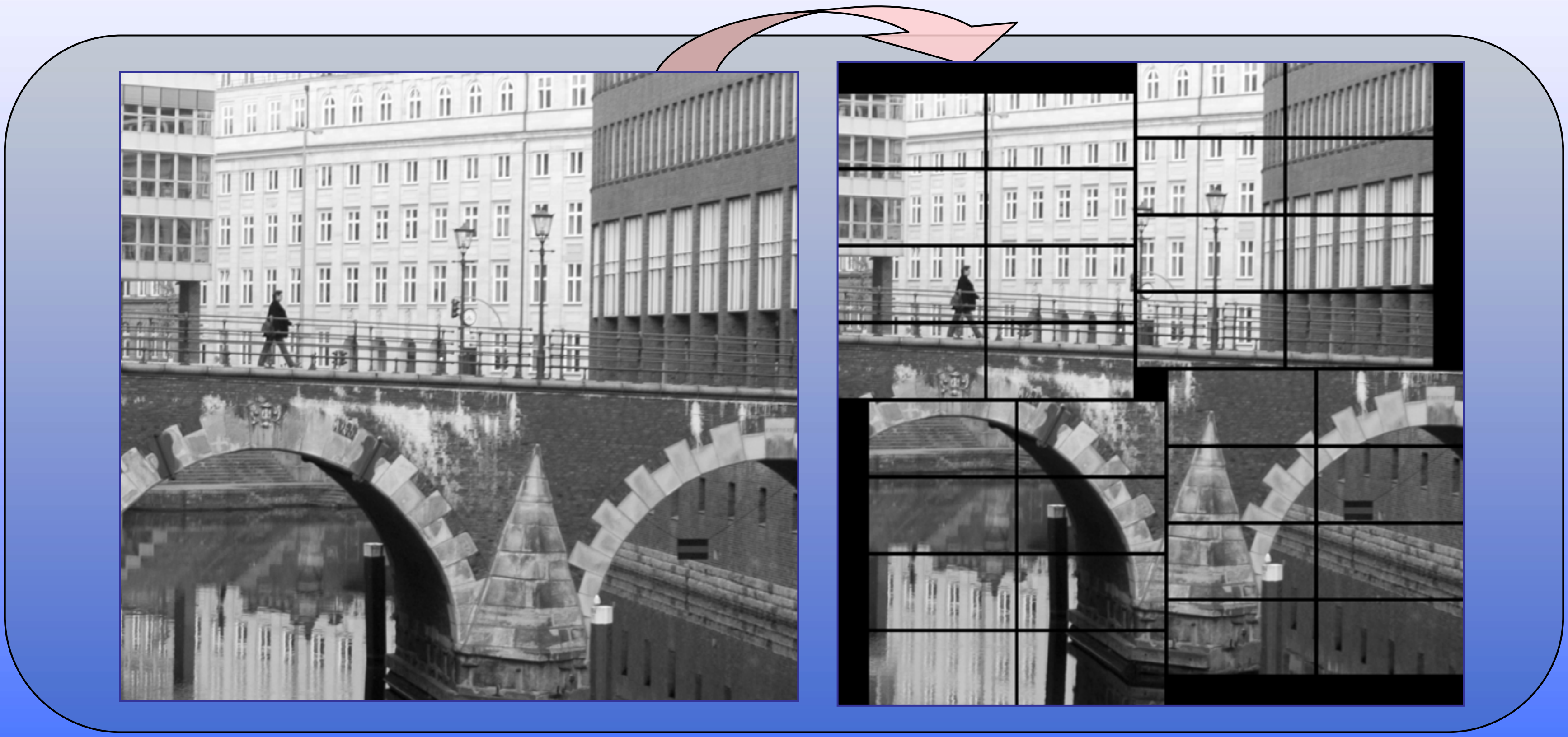
Then Add:

- Background should reinforce this tendency
- Bragg Peaks (nano-crystals) can be a problem (increased dynamics at the edge)

Case of experiments like liquid scattering (donuts shape)

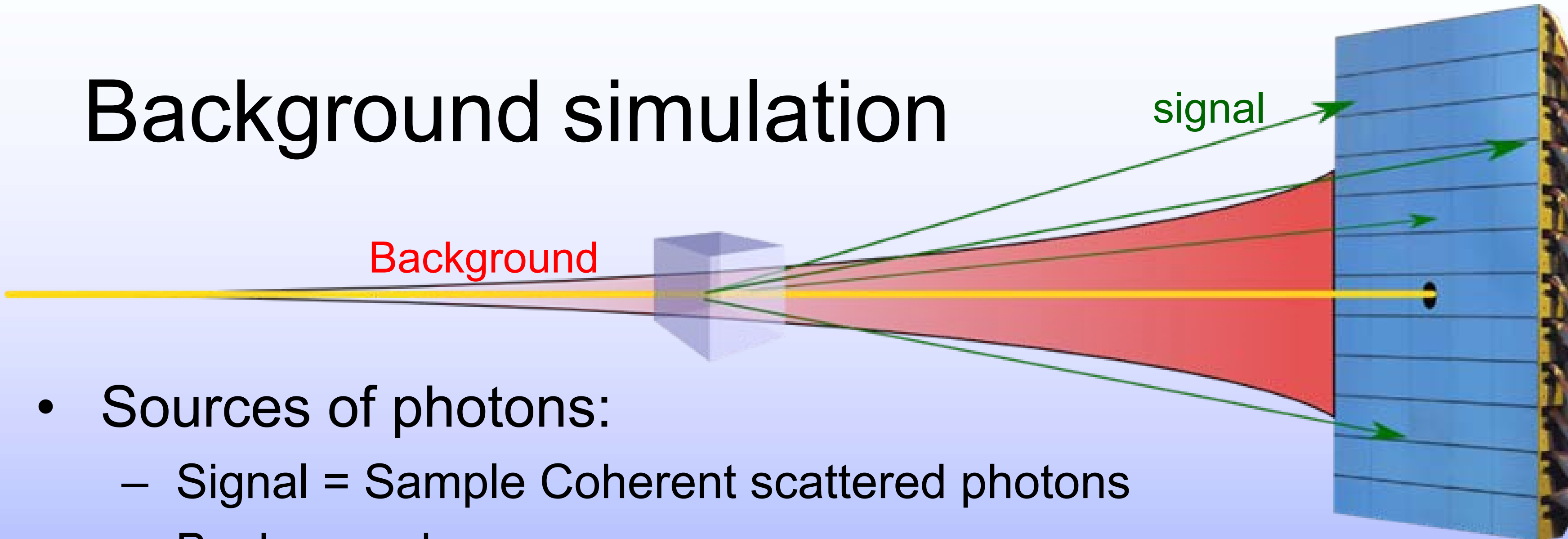
Detector Geometry

- Problem of the detector geometry: central Hole?



- For XPCS experiments, it could be interesting to split the detector in 4 (or more)

Background simulation



- Sources of photons:
  - Signal = Sample Coherent scattered photons
  - Background =
    - Sample Fluorescence + Inelastic scattering
    - Chamber Impurities inelastic & elastic scattering, fluorescence

Cannot distinguish from Signal

- Shape of the background:
  - Probably an exp or $1/q^n$ decay

Simulations are on the way

Use of Penelope Monte Carlo code

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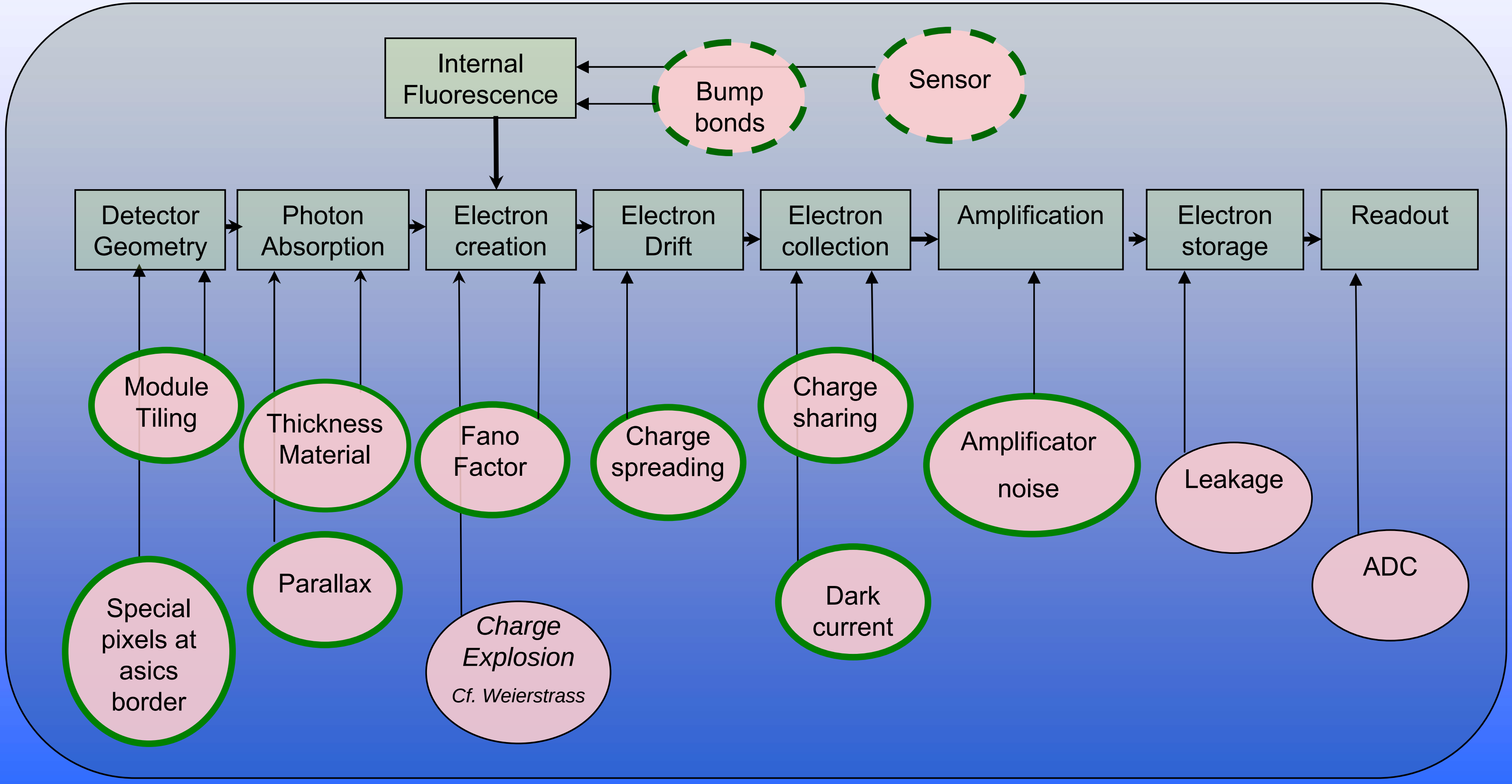
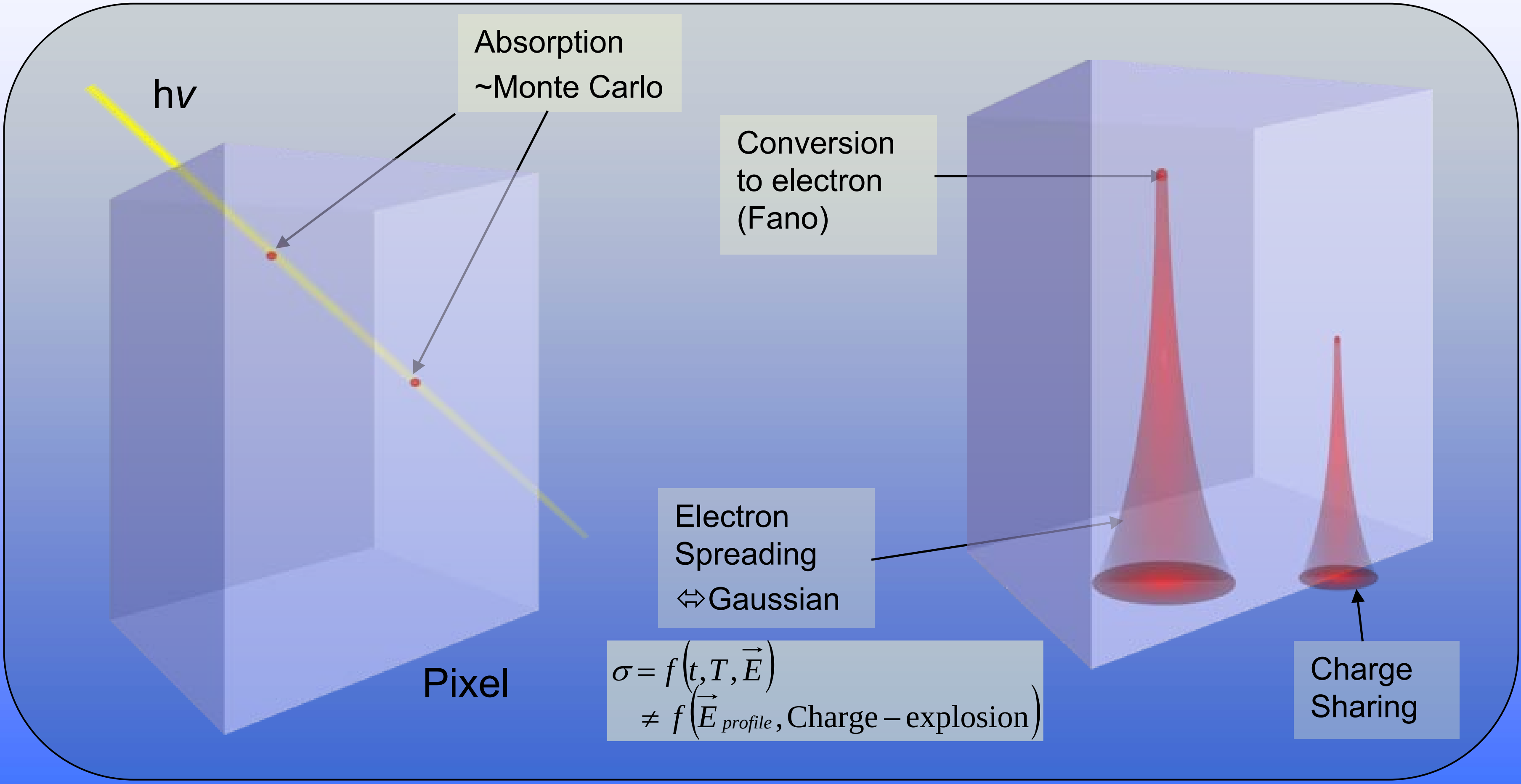
- Detector Simulation Software
  - Presentation
    - Sensor
    - Asic noise
  - Waiting for your inputs

Simulation of the detector Performances

The code is built on a modular structure



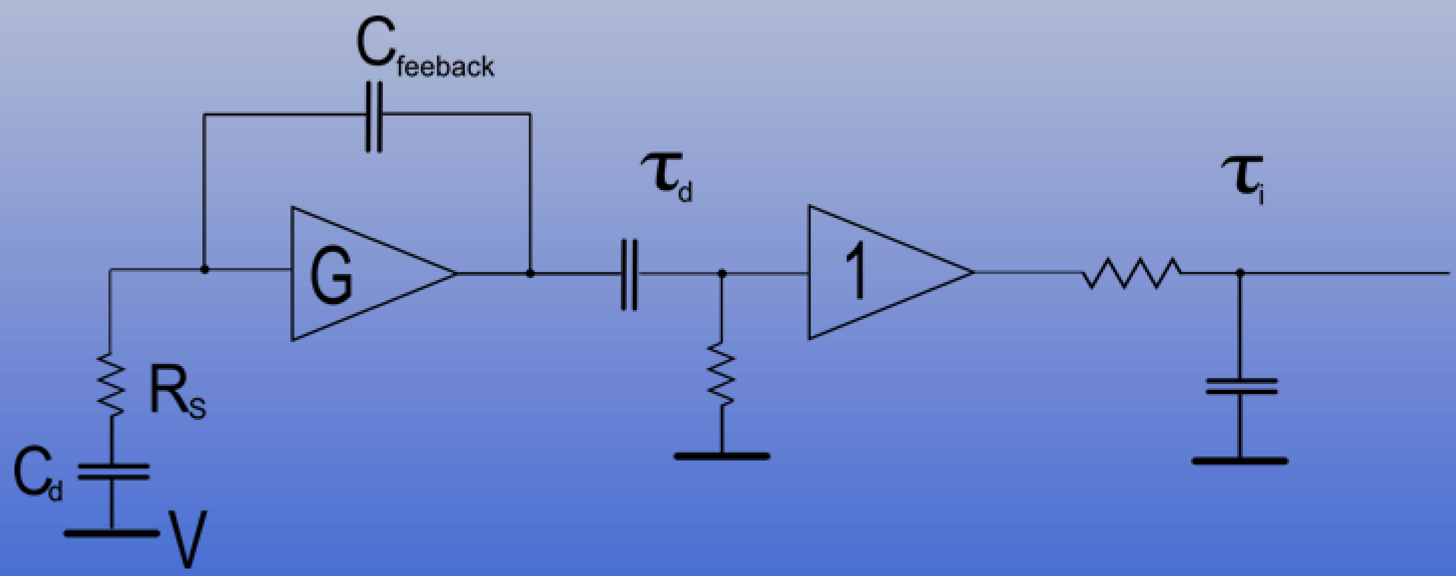
Sensor Absorption simulation



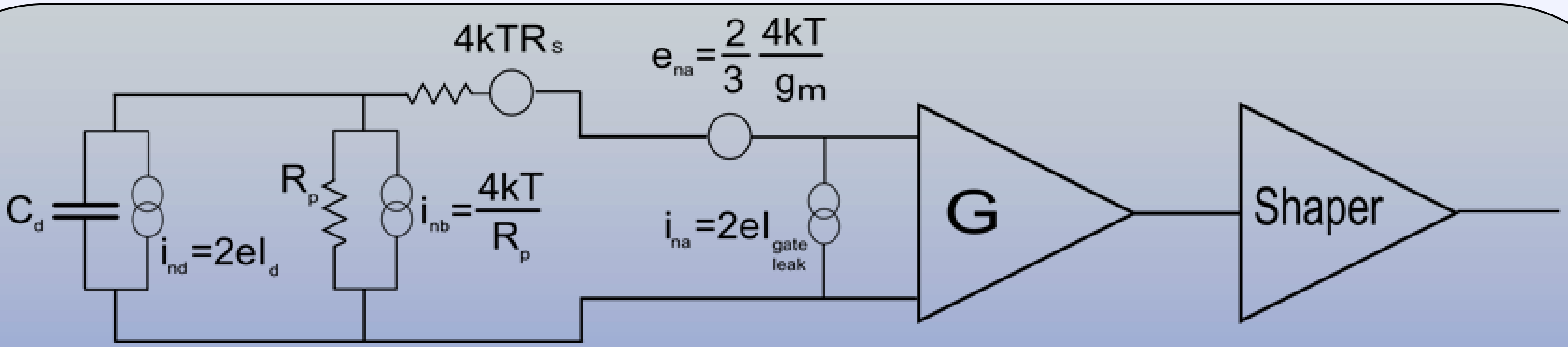
$$\sigma = f\left(t, T, \vec{E}\right)$$
$$\neq f\left(\vec{E}_{profile}, \text{Charge} - \text{explosion}\right)$$

ASIC noise simulation

Basic Charge amplifier coupled to CR-RC pulse shaper



ASIC noise simulation: Model[1]



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

$\frac{\exp(2)}{8}$	Normalization of noise to signal gain
$2eI_d$	Shot Noise in Sensor
$\frac{4kT}{R_p}$	Shunt resistances noise
i_{na}^2	Amplifier noise current
$4kTR_s$	Serie resistances noise
e_{na}^2	Amplifier voltage noise
$4A_f C^2$	1/f noise

$C = C_d + C_{parasitic}$ $\qquad i_{na}^2 = 2\,e\,I_{gate\ leakage}$

[1] from H.Spieler, Semiconductor detector system, oxford science publication

ASIC noise simulation: Values

$I_d = 1nA$

R_p = 100MΩ
T = 345 K

$i_{na}^2 = 2eI_{gate\,leakage} = 2e \cdot 134pA$

$\tau = 50ns$

$R_s = 50\Omega$

$e_{na}^2 = \frac{2}{3}\frac{4kt}{gm}$

$gm = 300\mu A/V$

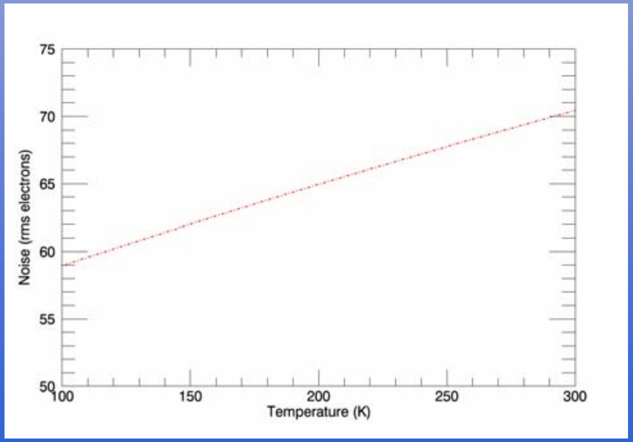
$C = 150\,fF$

$A_f = 10^{-12}V^2$

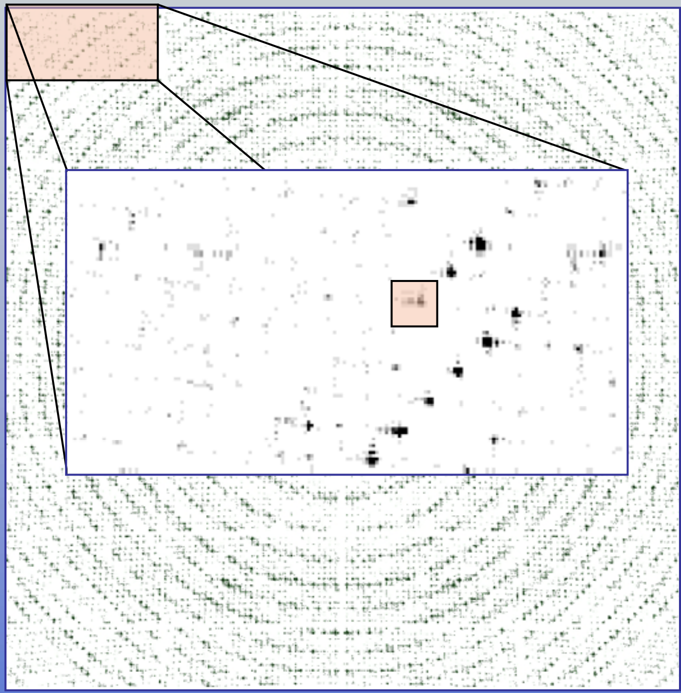
$$Q_n^2 = \frac{\exp(2)}{8}\left[\left(2eI_d + \frac{4kT}{R_p} + i_{na}^2\right)\tau + \left(4kTR_s + e_{na}^2\right)\frac{C^2}{\tau} + 4A_f C^2\right]$$

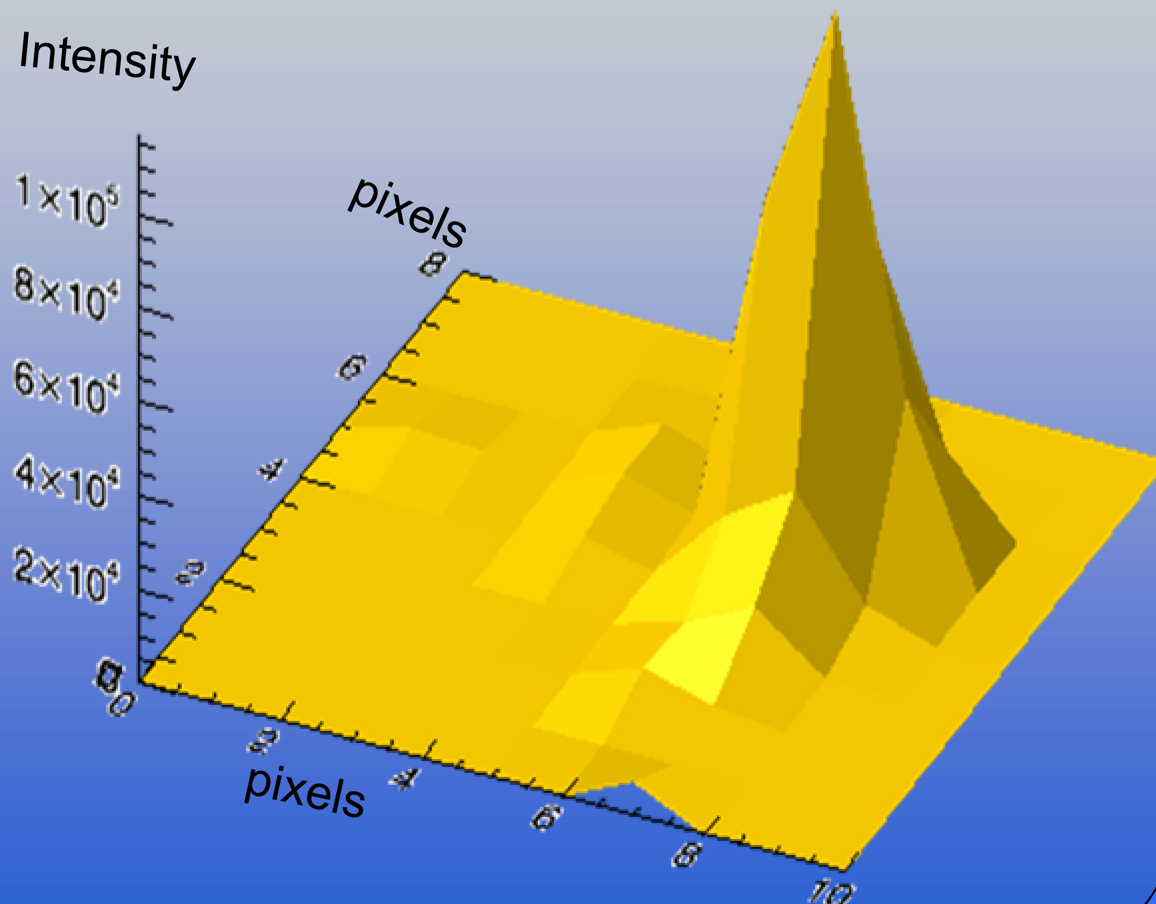
Normalization of noise to signal gain	Shot Noise in Sensor	Shunt resistances noise	Amplifier noise current	Series resistances noise	Amplifier voltage noise	1/f noise
	46 e-	46 e-	23 e-	9 e-	2 e-	4 e-

$$Q_n(Basic\ \ parametters) = 70\ e^-$$



Code Test





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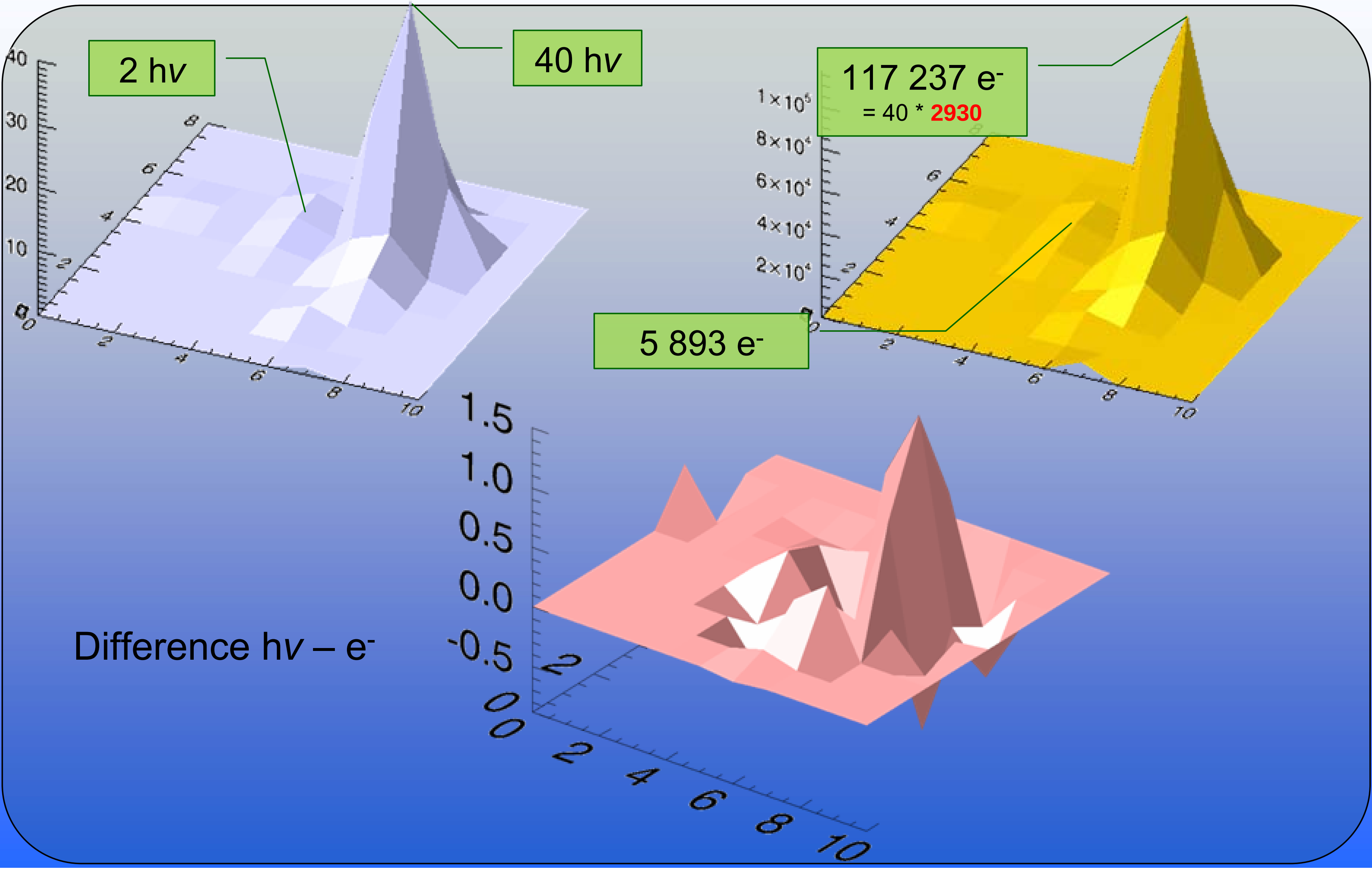

Future

- Finish the whole simulation code
- Develop Background simulation tool
- Get more images
- Loop back, ex. Try reconstruction algorithms with various parameters (hole size, Sensor Thickness…)