Science Simulations
+
Interaction with XFEL Scientists

Julian Becker

Outline

- HORUS
  - –New features
  - –Current AGIPD performance estimates
  - –Open issues
- XPCS Simulations
- CDI Simulations
- Summary and Outlook

HORUS processing chain

- Behavior of all steps can be modified
- Intermediate results can be accessed

new in version 2.0

new in version 3.0

Incoming photon distribution

- Provided by user
- Can be oversampled with respect to pixel size
- Quantized if necessary

Photon interaction in sensor volume

- Entry window
- Mean free path of photons
- Parallax
- Compton/ Thomson scattering (3%)*
- Fluorescence (4% of events)*

Charge transport in sensor volume

- Charge sharing
- Plasma effects
- Arbitrary CCE possible

ASIC and FE electronics

- Amplifier noise
- Dynamic gain switching
- Storage cells
- AD conversion

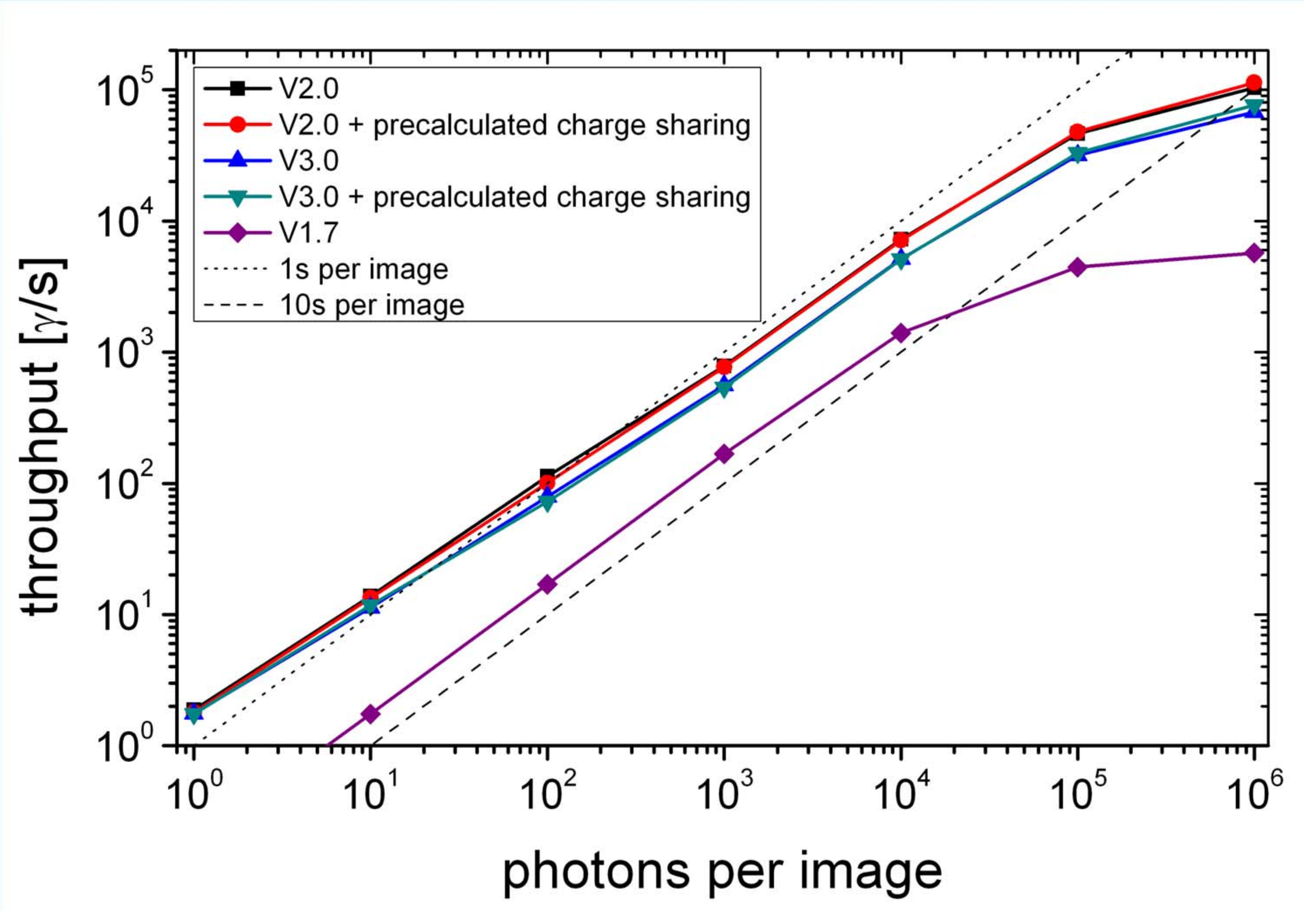
Requantized number of detected photons

- Requantization threshold

* 12.4 keV photons and 500 µm silicon

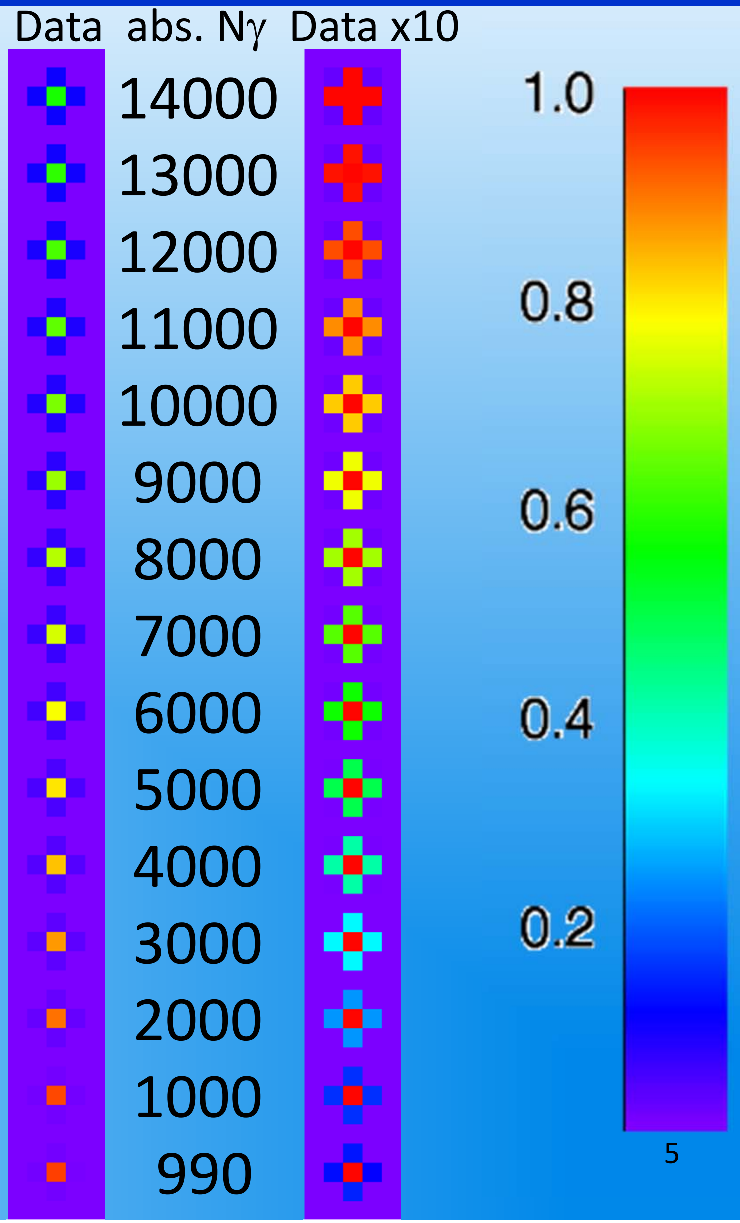
Computing speed of HORUS

- Dominated by ASIC simulation, image processing and overhead at low photon counts
- Limited by photon number only at very high photon counts
- Precalculated charge sharing increases speed only above 10^5 photons per image



Plasma effect model

- Switch from Monte Carlo to analytic treatment above a threshold of 1000 photons
- Use data from MTCT measurements as baseline
- Output most probably wrong (correct treatment required more sub-pixel information and model for interaction of neighboring pixels), but not as wrong as without plasma model



Current AGIPD performance estimate

Total noise estimate:

≈0.01% dynamic range

-> Noise Probability

Single photon sensitivity: No acceptable noise probability defined by XFEL yet (there is some talk about 5σ)

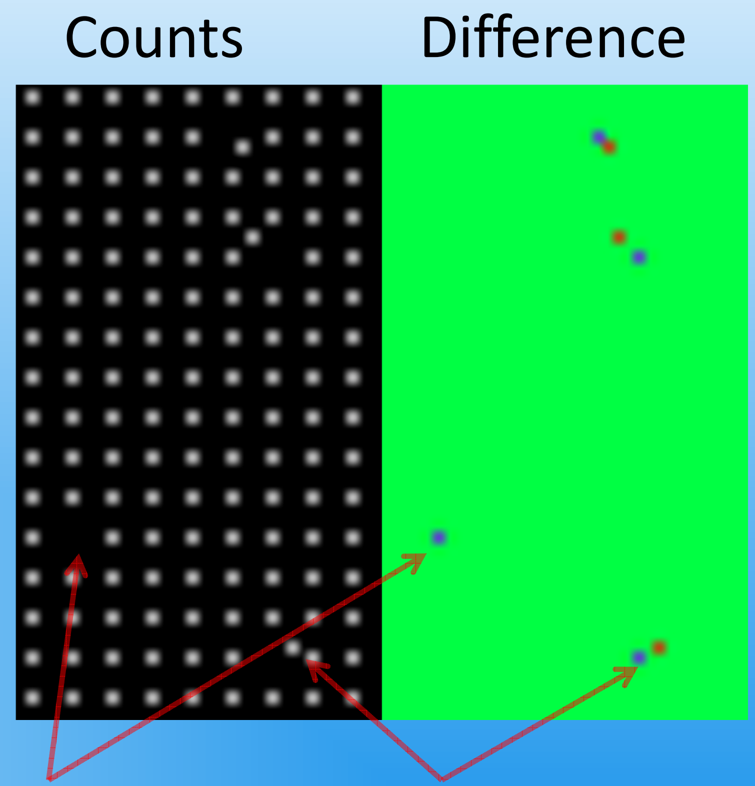
Compton/Thomson Noise

Input: standard grid of well separated ‘1’s

Additional simulation options:

- Force primary interaction in sensitive volume
- Disable charge sharing
- Disable all other noise

≈ 22 % of scattered photons leave the sensor (0.6 % in total)



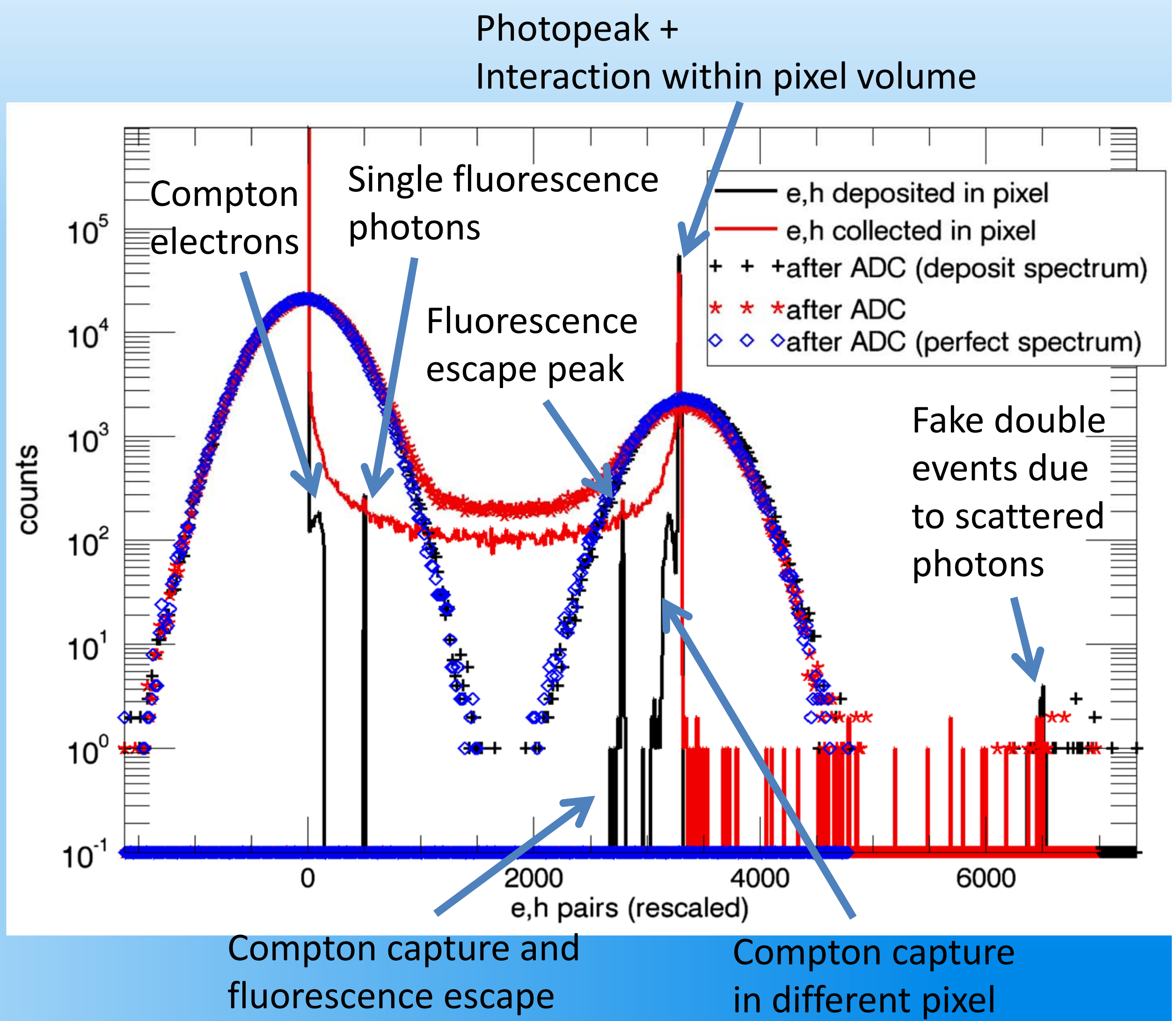
scattered photon escapes sensitive volume

scattered photon displaced by more than one pixel

Energy spectrum

Input: standard grid of well separated ‘1’s, total of ≈ 10^5 photons

- Charge sharing dominant effect in output spectrum
- Compton/Thomson scattering produces fake multiple hits
- 88.5 % quantum efficiency



Open issues

- Readout chain still rudimentary
  - No pixel-to-pixel variations
  - No charge injection
  - Saturation behavior of preamp unknown
  - No storage cell droop, noise, etc.
- Many parameters still best guess
  - Hole and gap sizes, etc.
- No effects of radiation damage included
  - Electron/hole loss close to the interface
  - Degradation of the ASIC

List of users

Name	Affiliation	Code Version	Comments
Peter Siddons	BNL/XDAC	1.8	Not installed
Anders Madsen	XFEL	1.9c	Installed
Andreas Koch	XFEL	1.9d	Installed
Ashley Joy	UCL/LPD	2.0	Not started

- No feedback beyond installation help
- LPD wants to mutilate HORUS code to do simulations for LPD

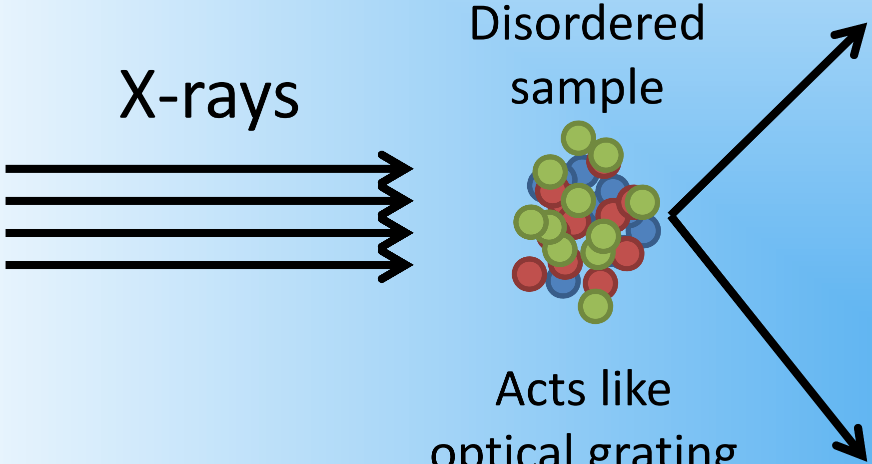
Outline (II)

- HORUS
  - –New features
  - –Current AGIPD performance estimates
  - –Open issues
- XPCS Simulations
- CDI Simulations
- Summary and Outlook

Scattering on many particles

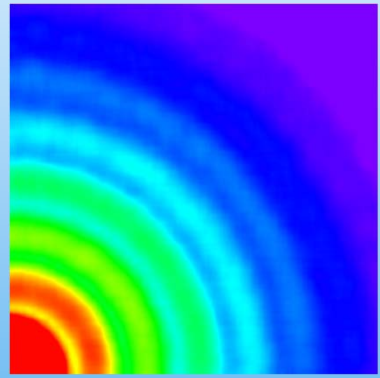
X-rays

Disordered sample



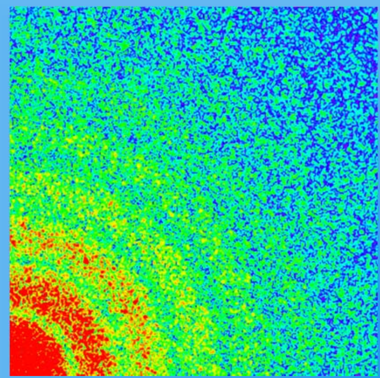
Acts like optical grating

Incoherent beam



Encodes average properties of the particles

Coherent beam

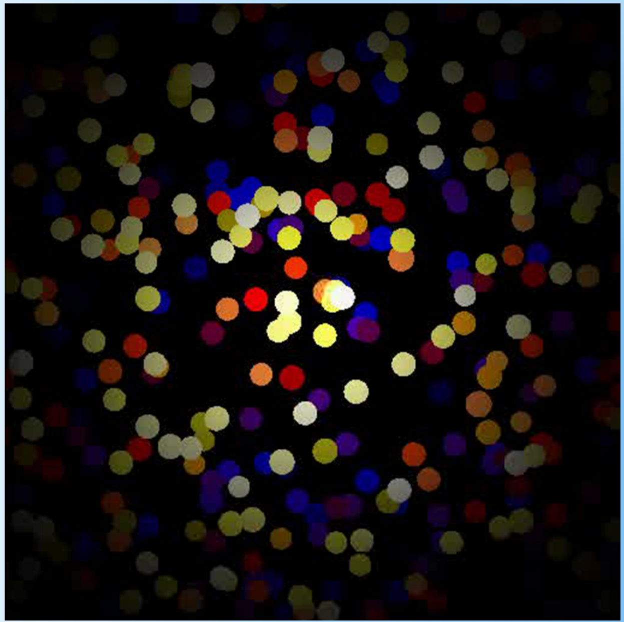


Additionally encodes position of each particle as 'speckles' on the average value

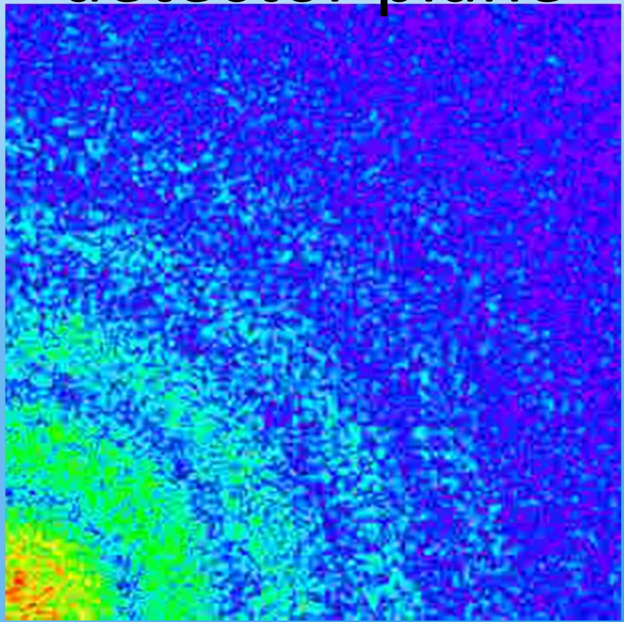
Changes in the positions of the scattering particles change the positions of the speckles

What is XPCS?

Real space



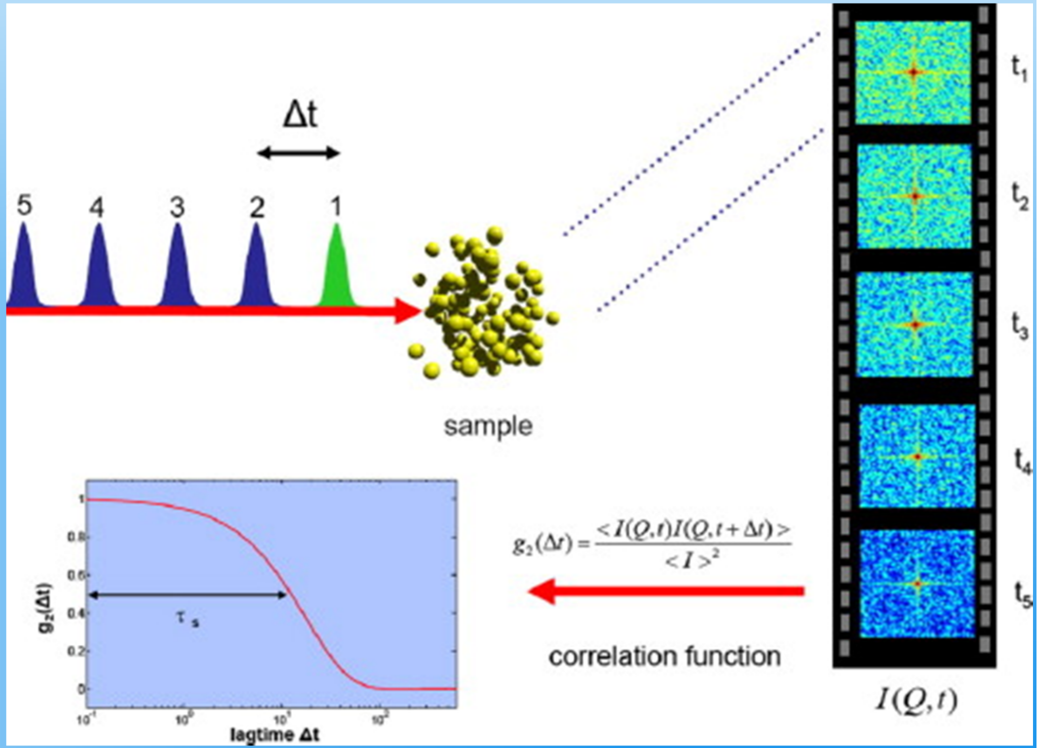
Log(Intensity) in detector plane



- Investigation of fluctuations in diffraction images
- Scientific case XPCS@XFEL: molecular dynamics in fluids, charge & spin dynamics in crystalline materials, atomic diffusion, phonons, pump-probe XPCS

How XPCS is performed

- Probe sample sequentially with non-destructive XFEL pulses
- Analyze image series using intensity autocorrelation (g_2 function)
- Functional form determined by interaction mechanism
- Extract time constant



Non-destructiveness requires large low intensity XFEL pulses
-> resulting speckles will be small

XPCS Simulations

1. Generate and evolve real space system
2. Calculate complex wave form in the detector plane (Fourier transform)
3. Scale and quantize wave form to produce discrete photon distribution
4. Use the photon distribution in the detector simulation
5. Evaluate output data and derive a figure of merit

Key simulation parameters

- Linear sequence of 300 images
- 5 independent bunches
- Infinite coherence length (long./lat.)
- Incoherent noise of 10^{-2} γ/pixel/frame
- Speckle size of ≈ 150 µm FWHM

→ At 20m distance: ≈ 13 µm FWHM beam

Figures of merit (I)

Signal to noise ratio of the g_2 function

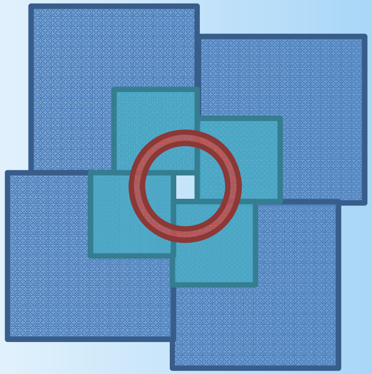
- Analytic expression available for low intensities
- Has been successfully used for many years

Relative error of the correlation constant

- Relevant physical parameter
- Essential for error determination on derived parameters like hydrodynamic functions etc.

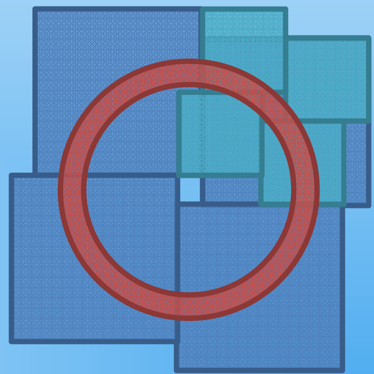
Region of interest

Small ROI

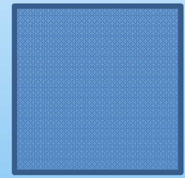


Limited by pixel density

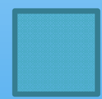
Large ROI



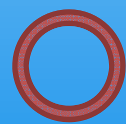
Limited by total area



Quadrant of 200 µm pixels (AGIPD, MAAT)



Quadrant of 100 µm pixels (RAMSES)



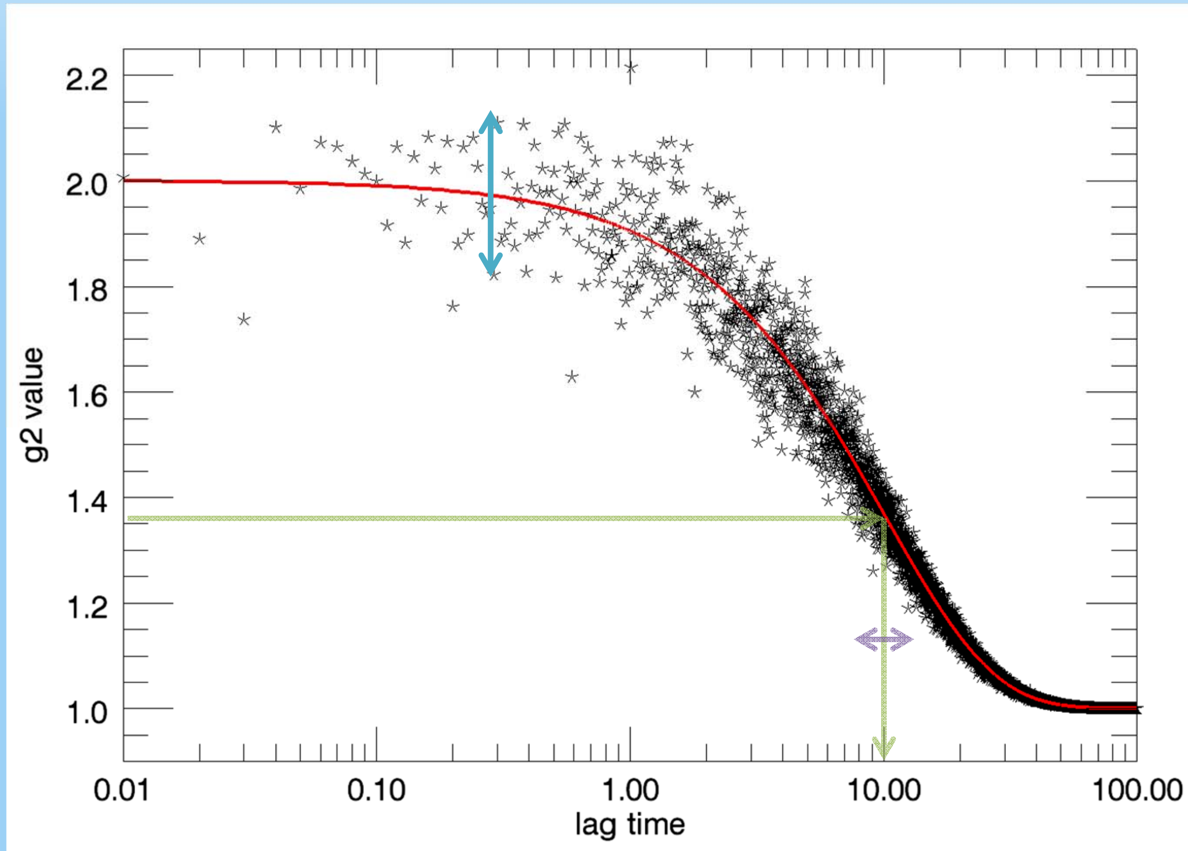
Region of Interest

MAAT = AGIPD + aperturing to 100 µm effective pixel size

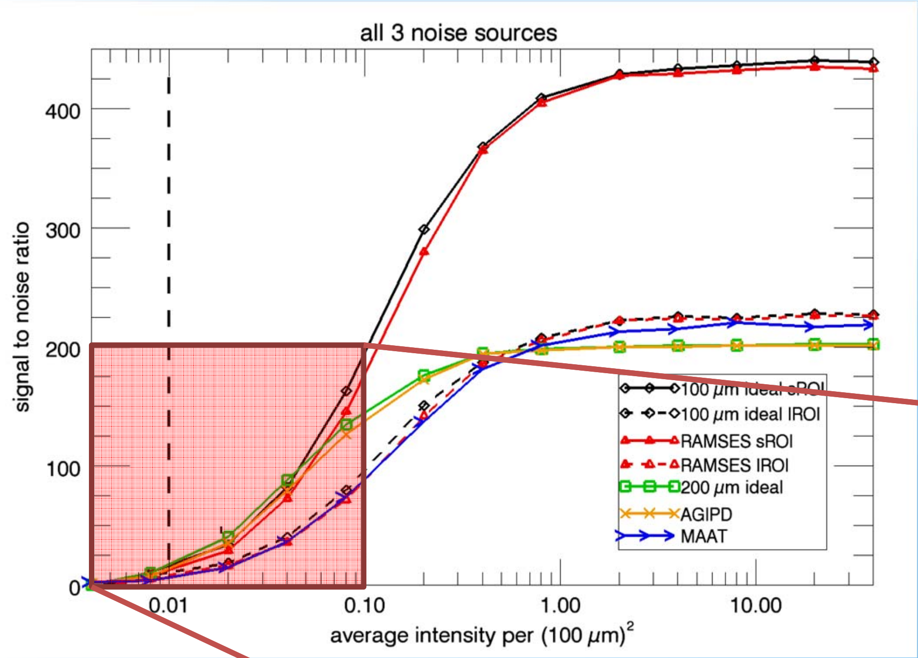
Figures of merit (II)

The signal to noise ratio is derived from the dispersion of g2 values (blue arrow)

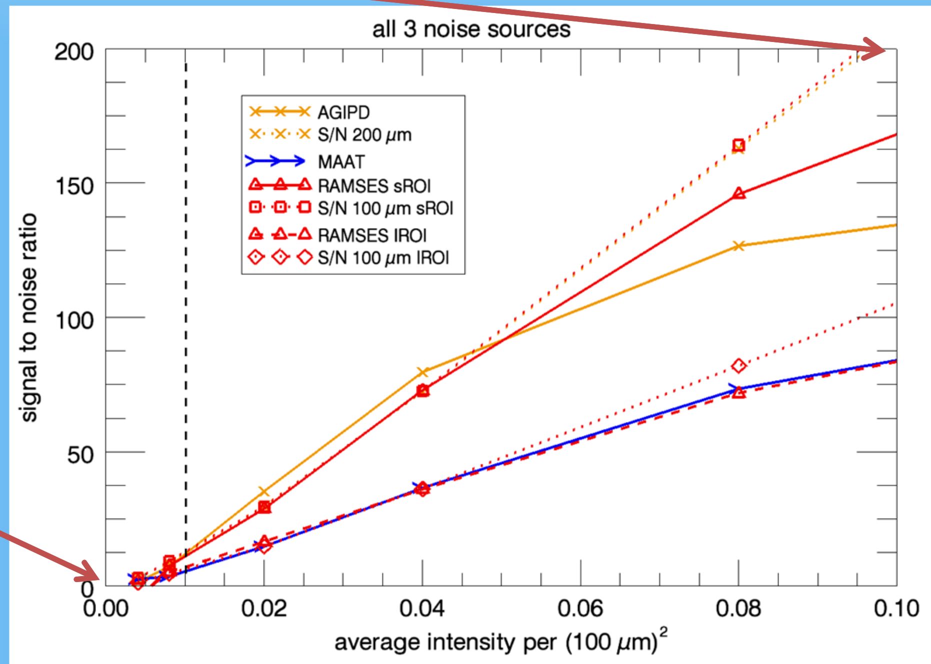
The relative error of the correlation constant is the error of fit result (violet arrow)



Signal to noise ratio



- Higher values indicate better quality
- Noise level at dashed vertical line
- S/N saturates around <I> ≈ 1
- At low intensities 200 μm pixel systems have higher S/N than 100 μm systems



Analytic expression (dotted)

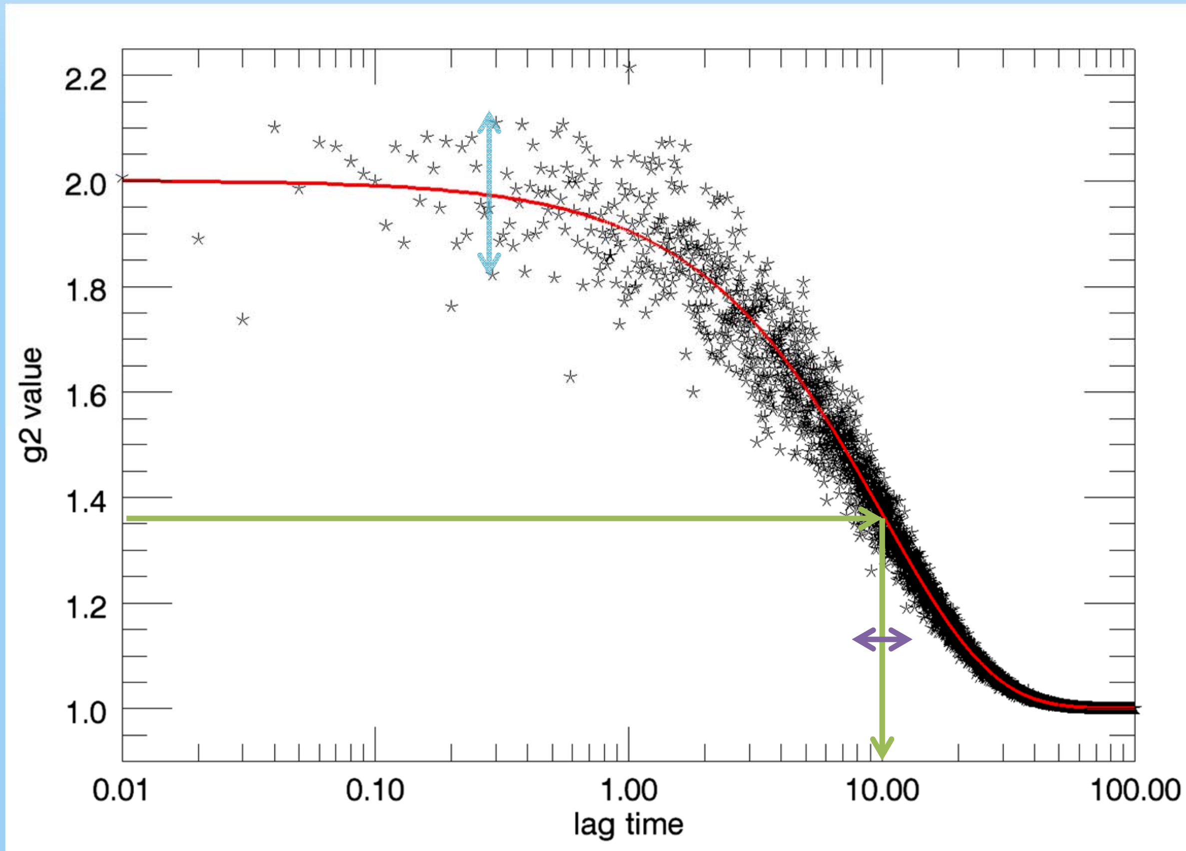
( ) √

valid for low intensities

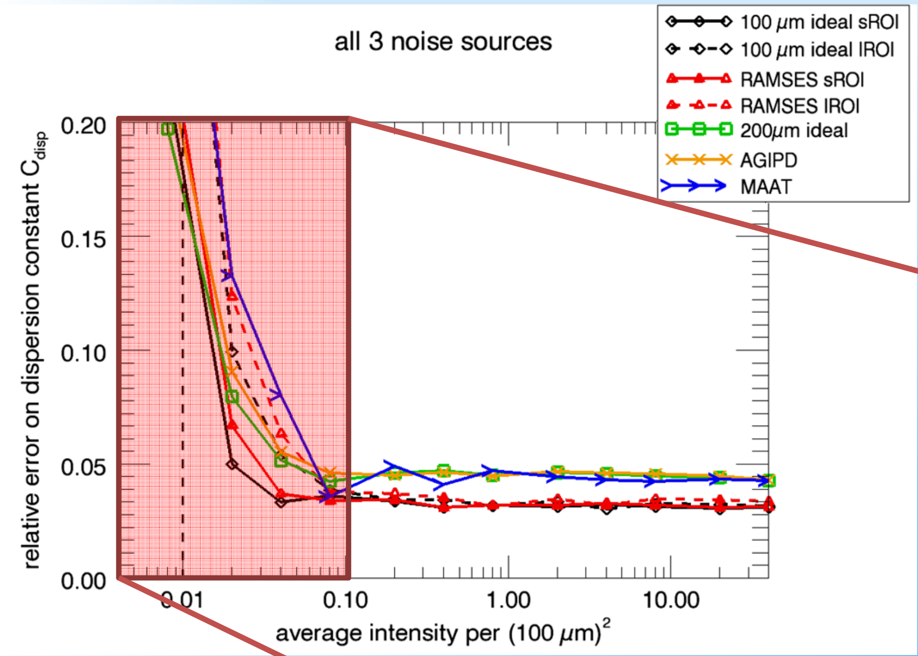
Figures of merit (III)

The signal to noise ratio is derived from the dispersion of g2 values (blue arrow)

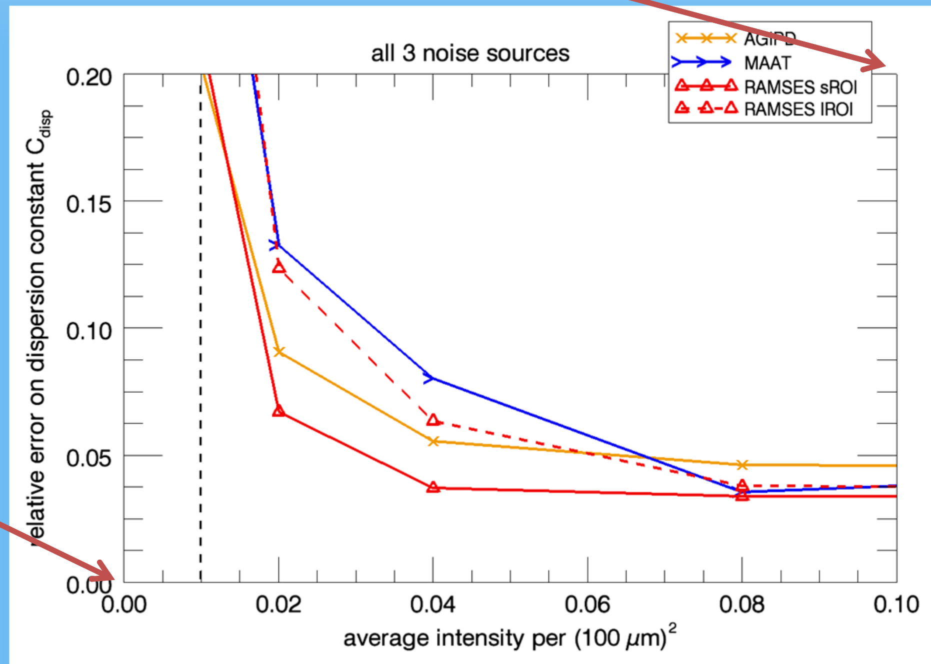
The relative error of the correlation constant is the error of fit result (violet arrow)



Relative error



- Lower values indicate better quality
- Noise level at dashed vertical line
- Error saturates around <I> ≈ 0.1
- Lower saturation value for small pixels
- AGIPD lower than RAMSES for large ROI and low intensity



- No analytic expression available
- Relevant quantity for further data evaluation (diffusion constants, hydrodynamic functions, etc)

Conclusions for XPCS

- XPCS insensitive to FEL fluctuations (not shown)
- Aperturing not beneficial at low intensities
- S/N and relative error behave differently
- Both saturate, but at different intensities
- Better performance of AGIPD at low intensities comp. to 100 µm pixel version

Outlook XPCS

- Paper under review
  preprint: http://arxiv.org/abs/1108.2980
- 3D data set under analysis
  - Realistic Q dependence
  - Lin/log bunch filling schemes
- Cooperation shifting from C. Gutt (DESY) to A. Madsen (XFEL)

Outline (III)

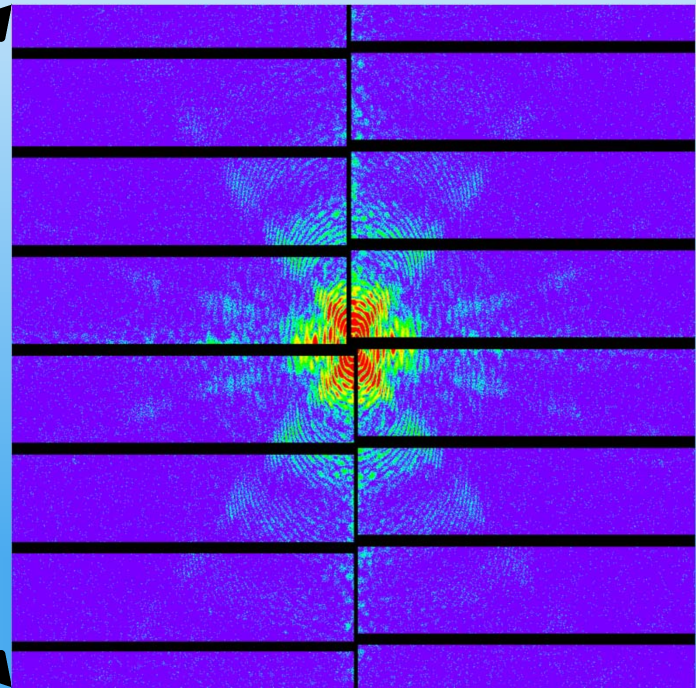
- HORUS
  - –New features
  - –Current AGIPD performance estimates
  - –Open issues
- XPCS Simulations
- CDI Simulations
- Summary and Outlook

Scattering on small samples

Focused coherent x-rays

Sample

Acts like optical grating



- High number of photons usually destroys the sample (Coulomb explosion)
- Short pulses allow for imaging before that

Very large dynamic range in the image

Phase information is lost

Coherent diffraction imaging

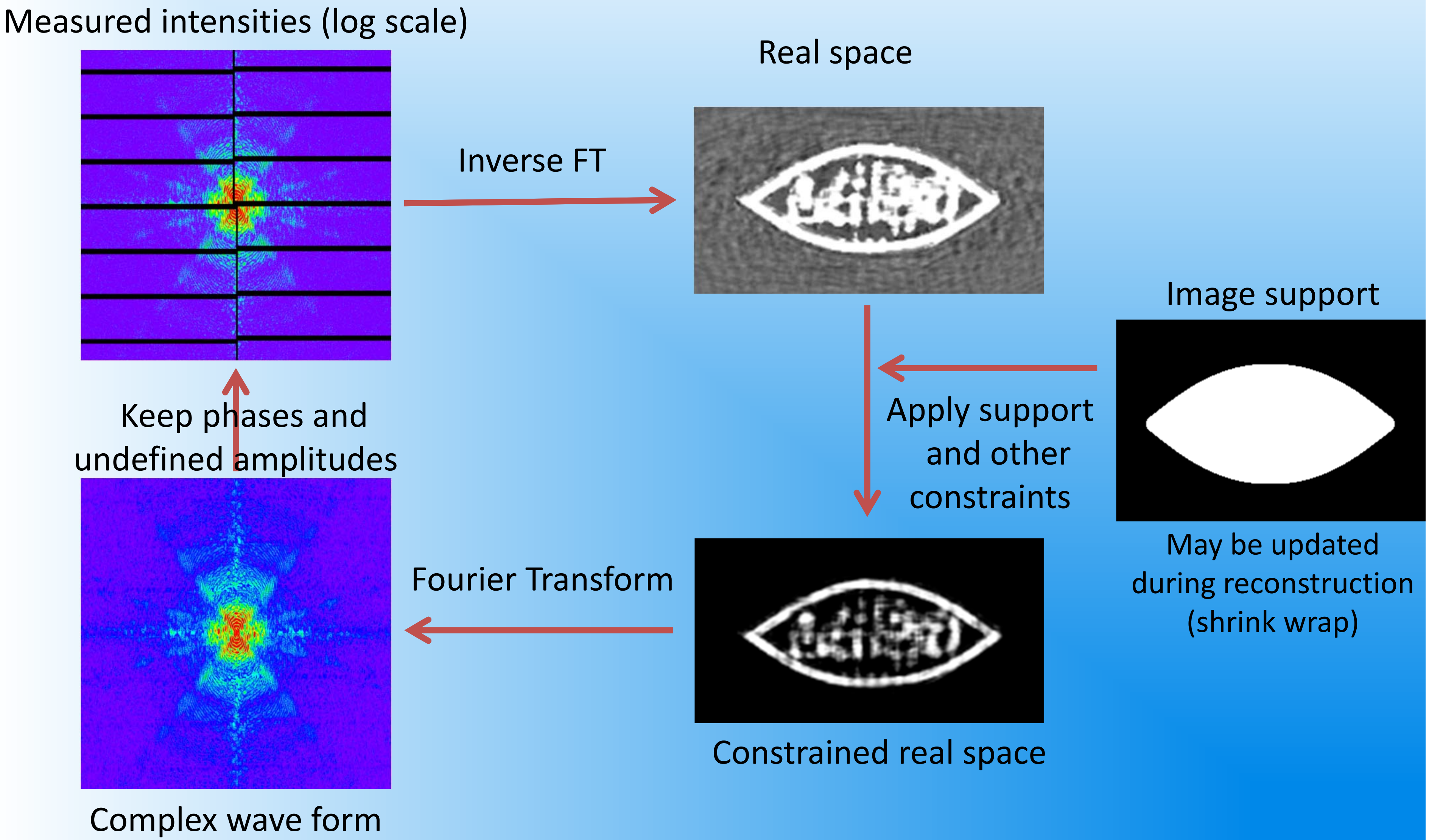
- Extended unique objects
  - Large dynamic range

True single shot experiments

- Identical small objects
  - Single photon sensitivity
  - Low noise
- Nano-crystals
  - Large dynamic range
  - Radiation hardness
  - Bright peaks

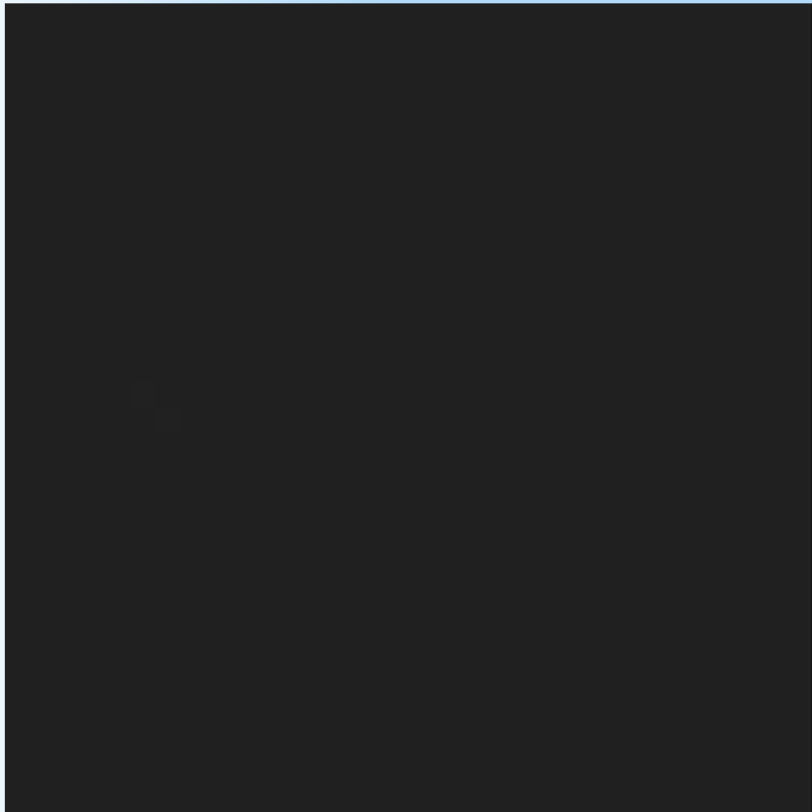
Need as many images as possible $O(10^6)$, but not necessarily in sequence

HIO algorithm



HIO image reconstruction

Reconstructed
real space image



Support mask

CDI Simulations

1. Define ‘realistic’ 2D real space object
2. Calculate complex wave form in the detector plane (Fourier transform)
3. Scale and quantize wave form to produce discrete photon distribution
4. Use this in the detector simulation
5. Sum output images if necessary
6. Do image reconstruction on output data and derive a figure of merit

Realistic 2D object

Real space image

Initial support

- Diatom cell (phytoplankton)
- Studied by A. Mancuso et. al.
  New Journal of Physics **12** (2010) 035003

Figure of merit

Define a pseudo-χ^2 as figure of merit:

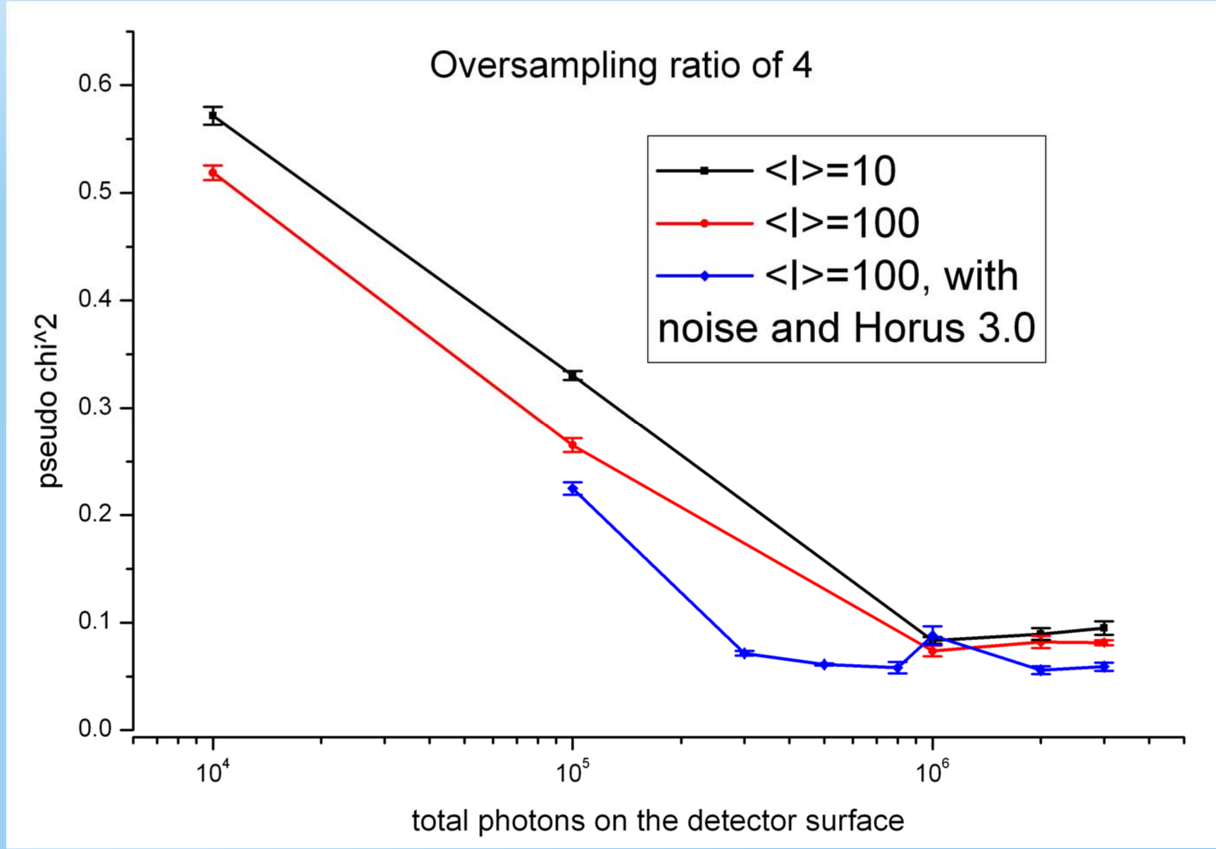
$$\frac{(\qquad\qquad)}{}$$

Lower values indicate better reconstructions

Then vary parameters and study effect on figure of merit

Total intensity

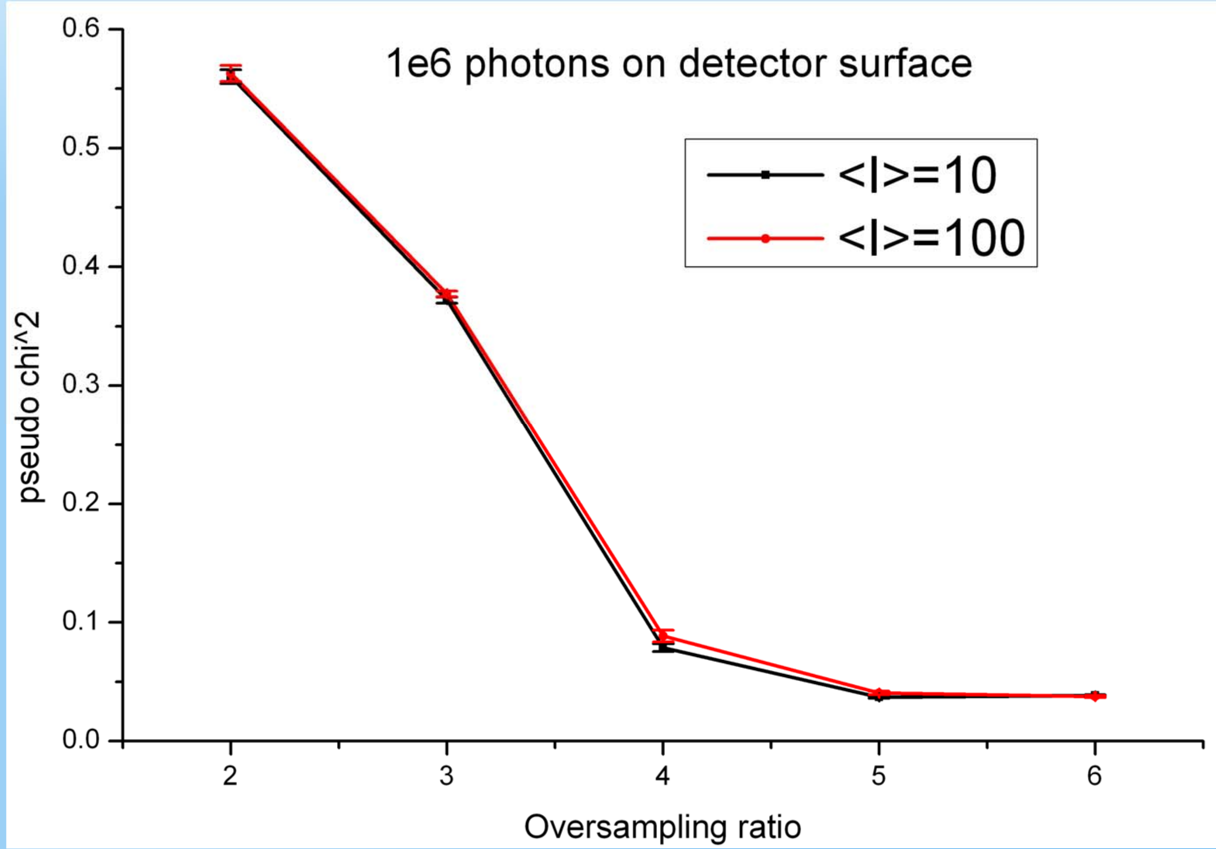
- Single objects are usually weak scatters
- Sum images of low intensities and reconstruct the sum image
- Assume all RS images are identical



<I>: Average number of photons per image

Oversampling ratio

- Loosely defined as 'pixels per fringe'
- Proportional to detector distance
- Inversely proportional to obtainable resolution



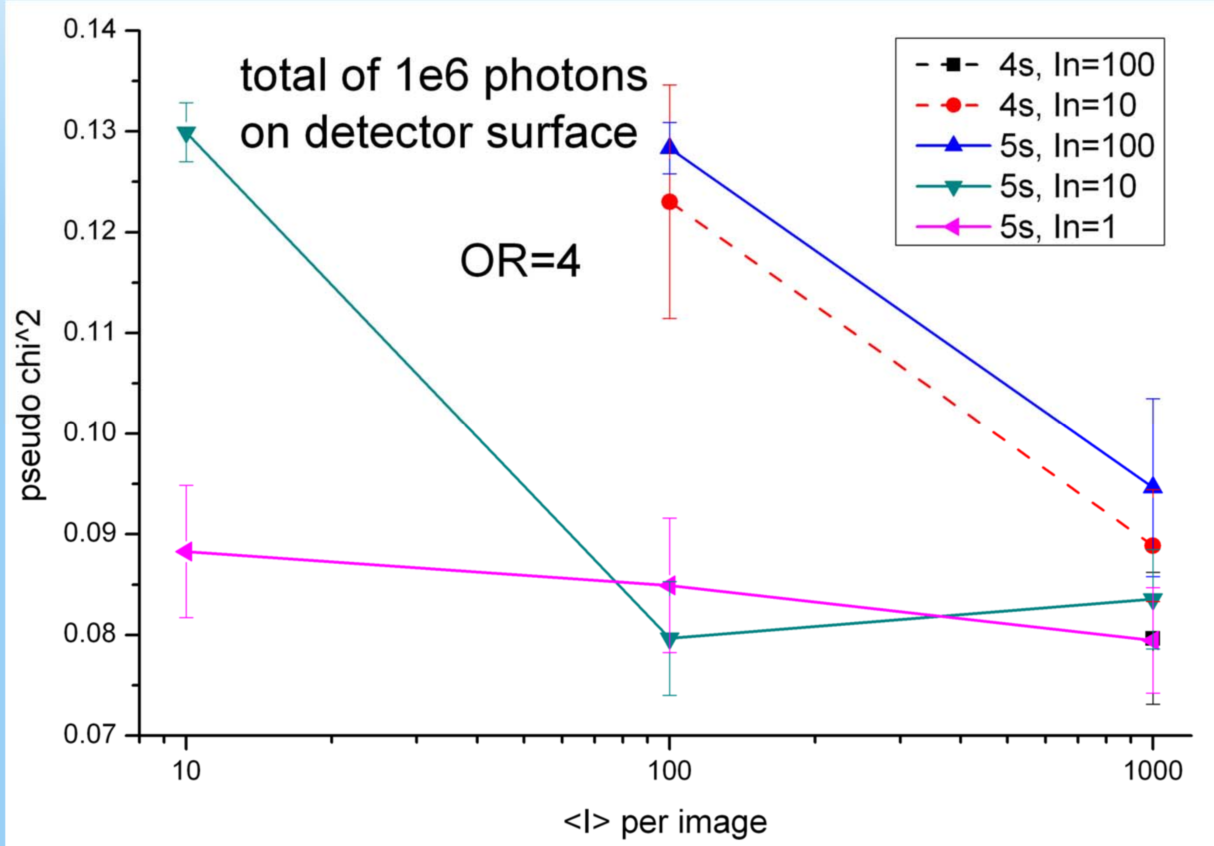
<I>: Average number of photons per image

Parameter study

Multi parameter space including:

- Oversampling ratio
- Total accumulated intensity
- Useful photons per image
- Background photons per image
- Detector noise

Defining the point from which ‘good’ reconstructions are possible



The point additionally depends on the image to reconstruct

Summary CDI

- Different requirements for different experimental approaches/samples
- Investigations of nano-crystals need large dynamic range but no single photon resolution
- Reconstruction algorithm available and working
- AGIPD is a suitable detector for CDI
- Simple tests confirmed ‘magic’ numbers for good reconstructions of OR ≥ 4 and $I_{total} \geq 10^6$ photons

Outlook CDI

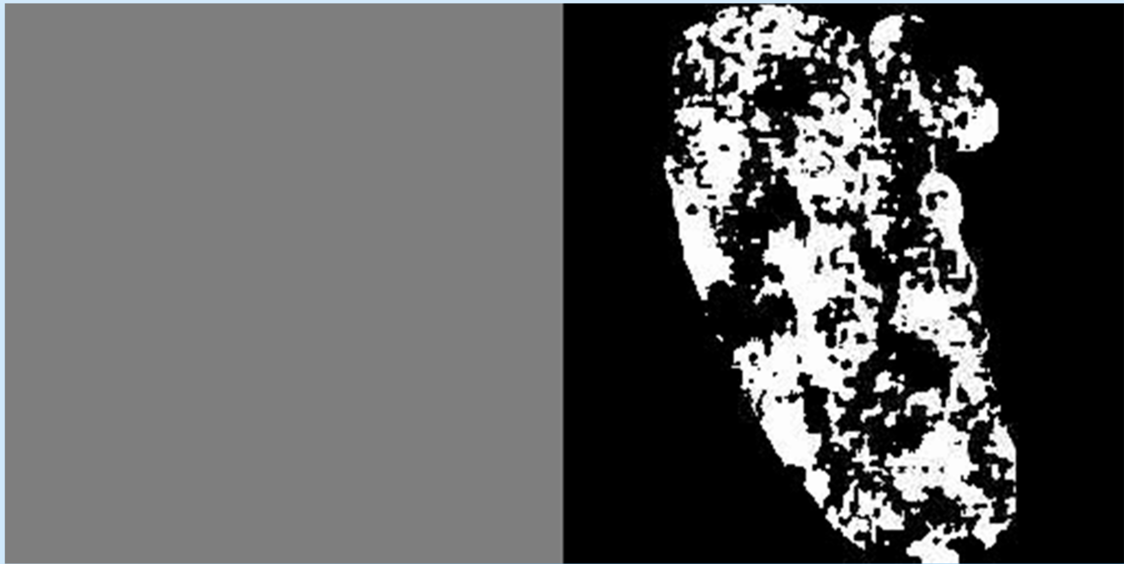
- Ongoing study using HORUS 3.0 and a more realistic noise estimate
- Simulation/Reconstruction of nano-crystal data is complicated but on the roadmap
- Cooperation with A. Mancuso (XFEL) is successful and so far fruitful

Summary

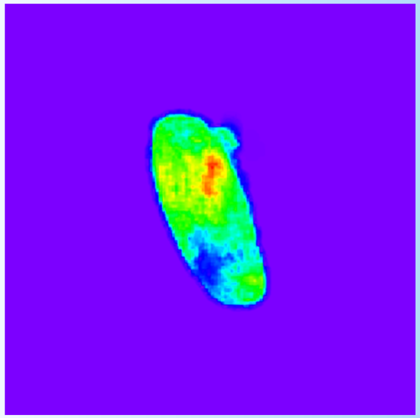
- Progress on HORUS code
- Published first results on XPCS
  - AGIPD suitable for XPCS
- Work on CDI simulations progressing
  - AGIPD shown to be suitable

BACKUP

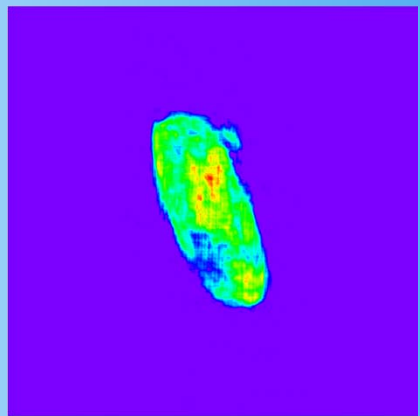
Reconstruction OR4



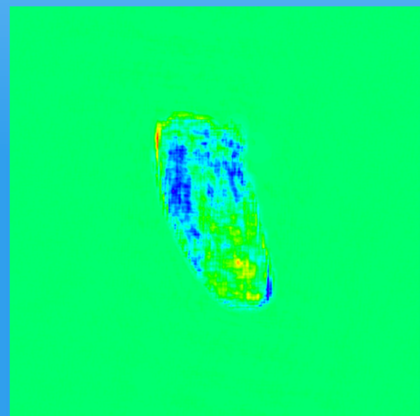
input



output

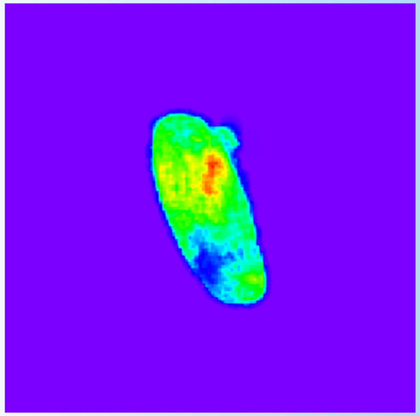


difference

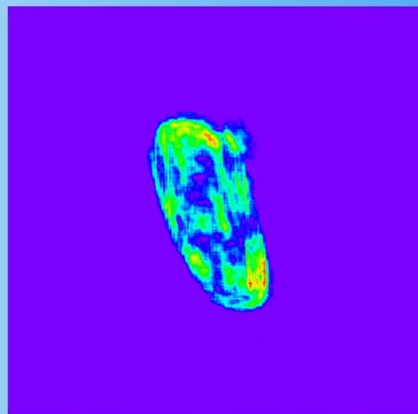


Reconstruction OR2

input



output



difference