HORUS

A detector simulation tool

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Outline

- HORUS
  - What's that?
  - Usage and simulation steps
  - Approximations, limitations, etc.
- XPCS simulations
  - XPCS what's that?
  - Simple test system
  - Parameter space
  - Data evaluation
  - Results
- Outlook on next generation of simulations

What is HORUS?

- HORUS stands for:
  Hpad **O**utput **R**esponse
  f**U**nction **S**imulator
- Collection of IDL routines
- Designed to evaluate influences of certain design choices for AGIPD
- Expanded to allow simulations of photon counting detectors (Medipix3) by D. Pennicard

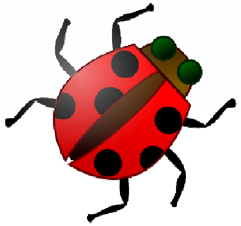
```
;HORUS program : Version 1.9b
;HPAD Output Response fUnction Simulator

function horus, original_picture, $
  no_noise=no_noise, no_electron_conversion=no_elect
  no_dead_area=no_dead_area, infinite_dynamic=infini
  energy = energy, only_center=only_center, perfect_
  no_charge_sharing=no_charge_sharing, quiet = quiet
  bypass_ASIC = bypass_ASIC, oversampling = oversamp
  add_elec=add_elec, parameters=parameters, gains=ga

;Main Program for the simulation of the detector
; Guillaume Potdevin
; Last update Apr 09
; guillaume.potdevin@desy.de
; Julian Becker
; Last update Nov 2010
; julian.becker@desy.de
;
; /no_noise                    suppress any source of
; /no_electron_conversion      to bypass the electron
; /make_mask                   simply return a mask wi
; /no_dead_area                makes the detector mono
; /infinite_dynamic            suppresses any dynamic
; /ADU_unit                    to return the image in
; /no_parallax                 to exclude any parallax
; /only_center:                shrinks the image to it
; /perfect_QE:                 no photon goes through
; /no_large_pixel_treatment    supresses larger pixels
; /no_charge_sharing           suppresses the charge s
; /no_fano                     sets the fano factor to
; /bypass_asic                 The image is returned d
; /fast                        bypass calculations for
```

What HORUS is:

- NO full scale Monte Carlo simulation
  - Pseudo analytical treatment of charge transport
  - Simplifying assumptions on sensor geometry
  - No simulation of surrounding material (Bumps/ASIC/Module mechanics)
- NOT tested with whole scale AGIPD (not there yet!)
  - Simulation results for Medipix match well
  - Test results from all recent AGIPD test chips are included
- NOT Bug free
  - Most major bugs are fixed
  - Works as designed, passed many consistency checks
  - …but you never find the last one



Design of HORUS

- HORUS is designed as a transparent end-to-end simulation tool:
  – Needs ‚input image‘ containing the number of photons in each pixel
  – Provides an output image, i.e. the number of detected photons in each pixel
  – Simulation parameters/behavior can by adjusted by the user
  – Additional functionality with special options/workarounds

The HORUS-GUI

Options | Images | Histograms

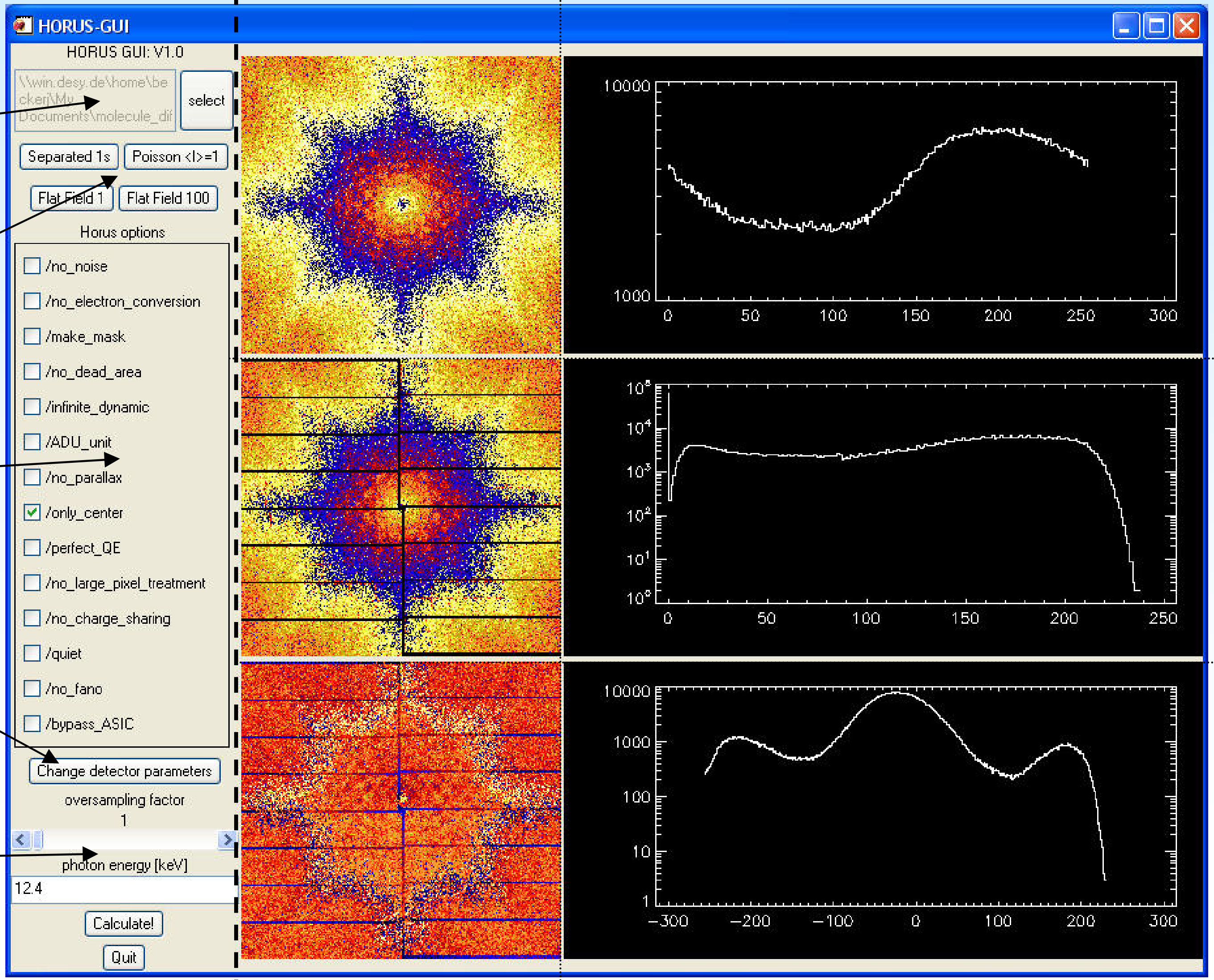
Input image selector

Generate standard patterns

Selector for simulation parameters

Change of detector parameters

Additional options



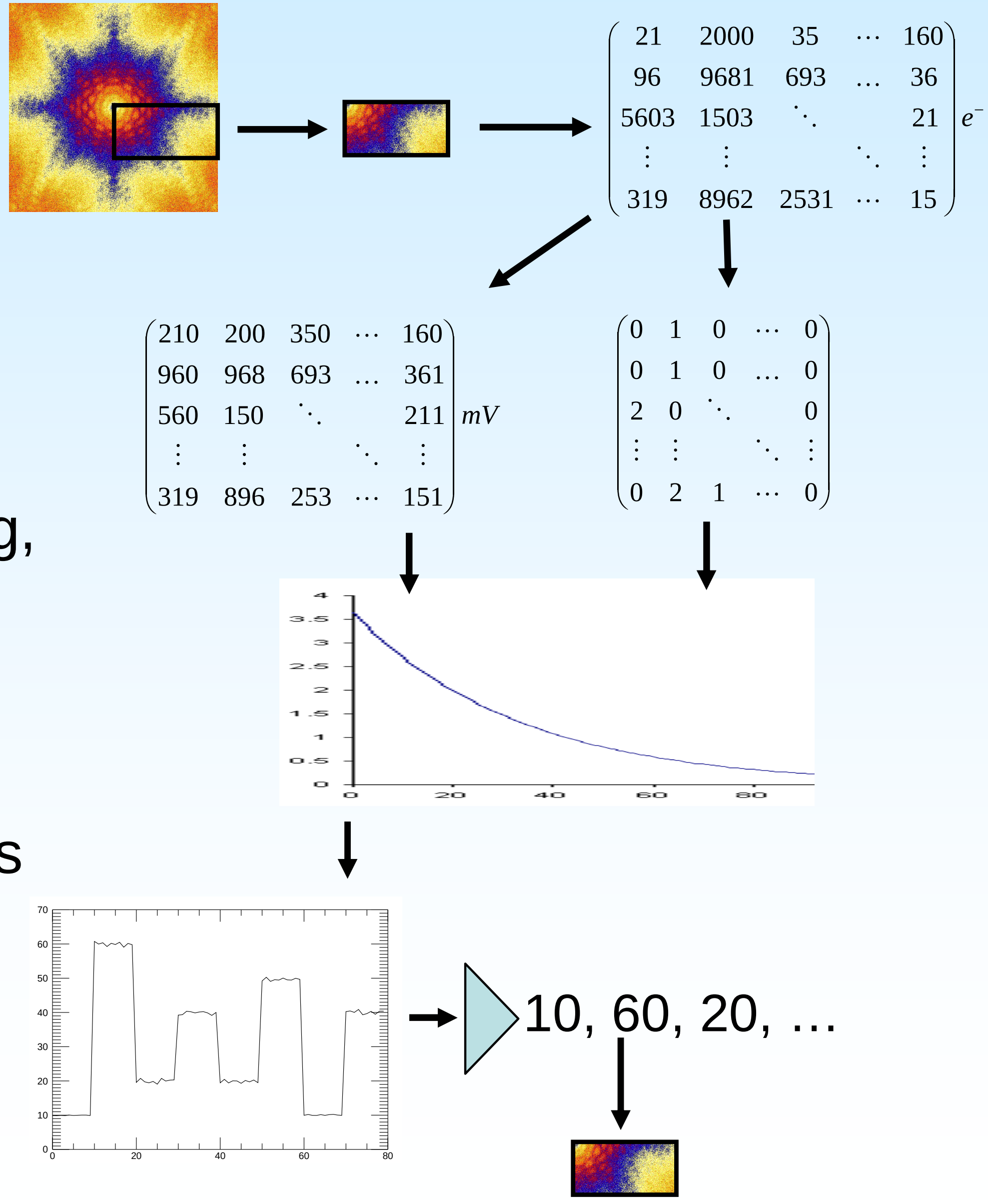
Input

Output

Difference

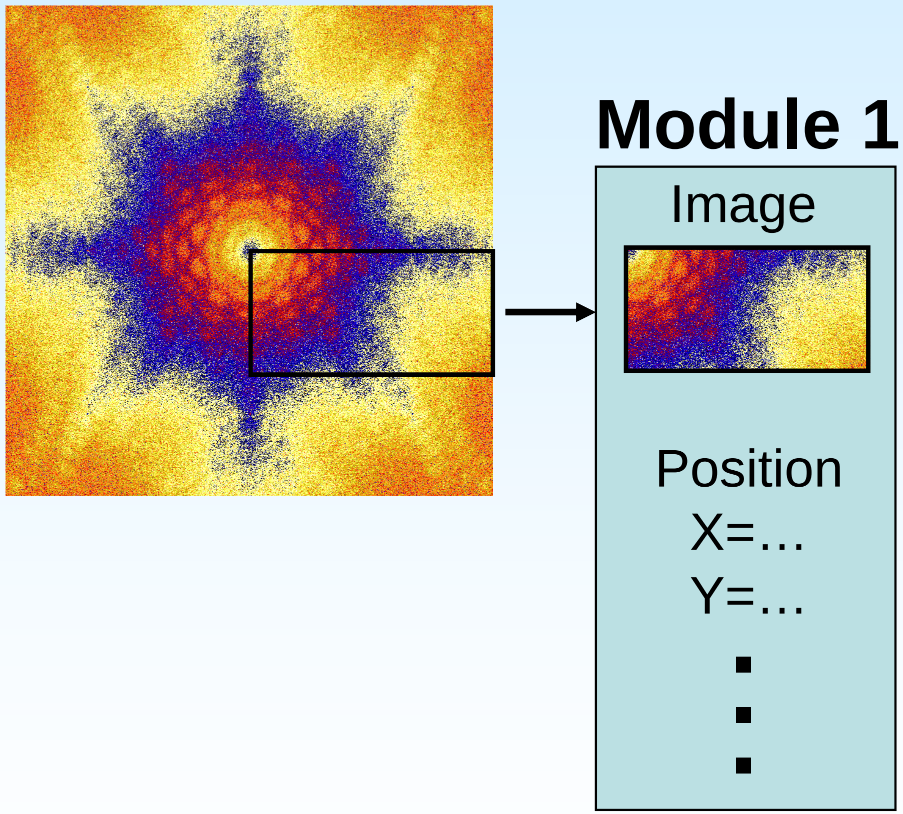
Simulation steps

- Input image processing, module definition
- Photon conversion -> generates input charge
- Amplification, gain switching, CDS simulation
- Treatment of storage cells
- ADC of voltage signals
- Requantization of ADC units
- Construction of the output image



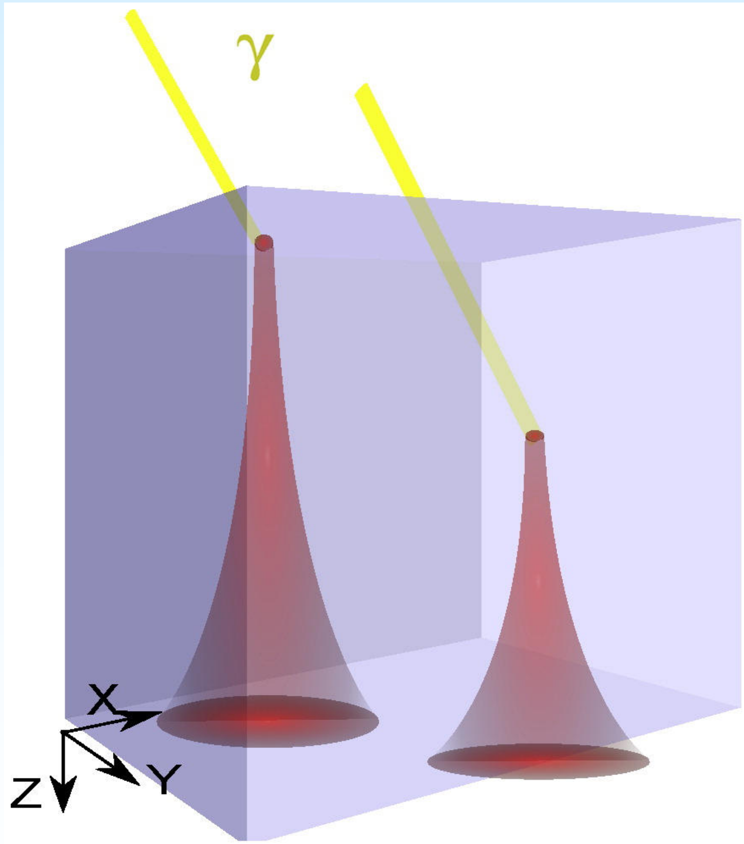
Module definition

- Simulations are performed on a ‘per module’ basis
- Input image is sliced into pieces
- Each module is an IDL struct carrying the image information of the current simulation step and additional information, like position, gains etc.
- Number of pixels/ASIC, ASICs/module and their arrangement is user definable

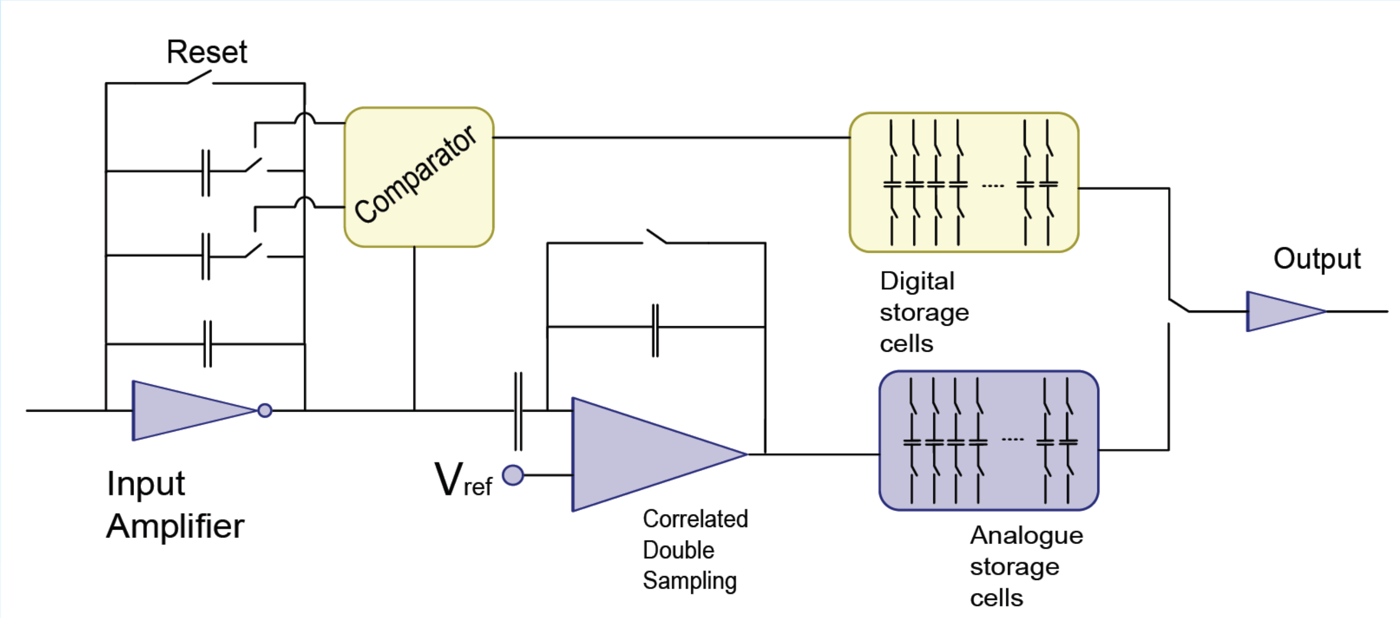


Photon conversion

- Each photon is treated separately (MC approach)
- Absorption probability taken into account (Quantum efficiency, entry window as dead layer)
- Parallax effect is modeled
- Dispersion in actual e,h pairs created is modeled taking Fano factor into account
- Charge sharing:
  - independent for each photon
  - depth dependent Gaussian
  - user-provided Cross-Coupling Matrix (allows CCE<1, non-uniform sharing etc.)



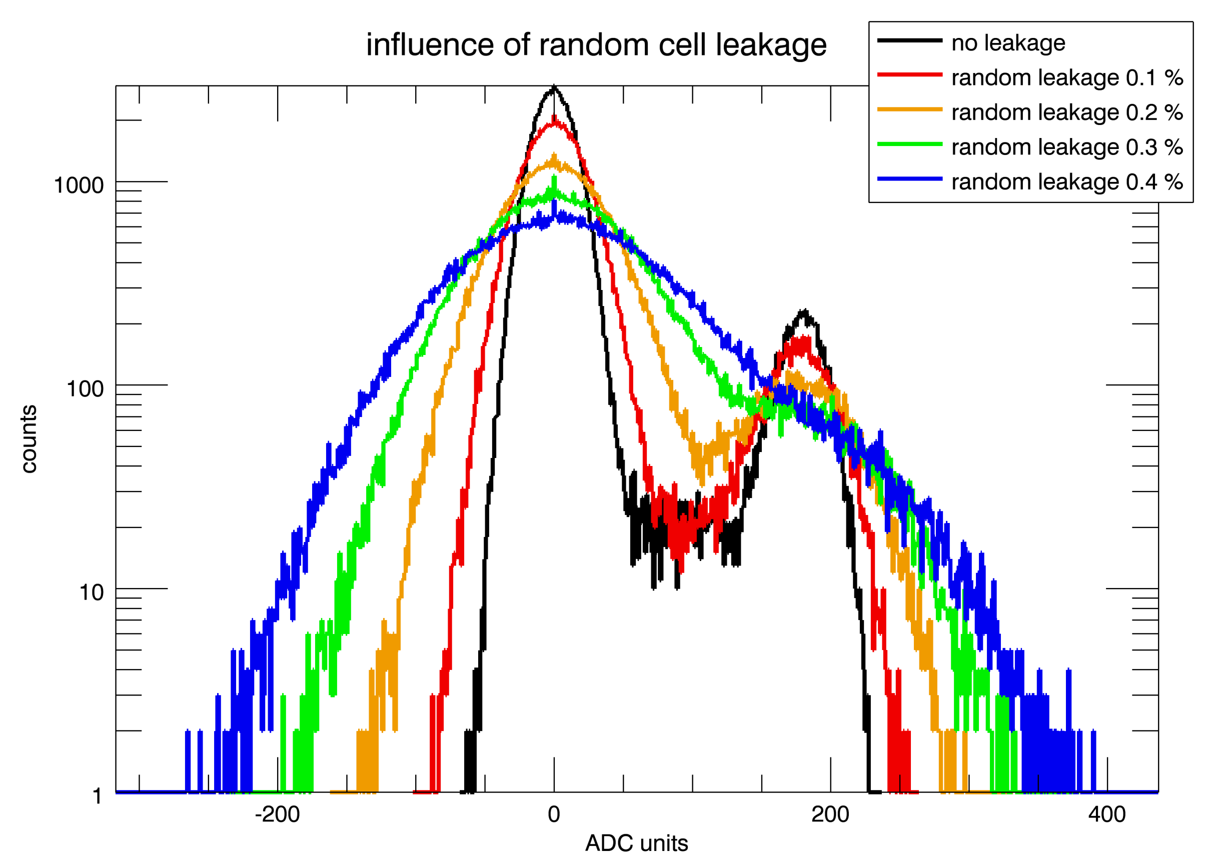
Amplification, gain switching, CDS simulation



- Noise sampled randomly according to ENC of current gain stage
- Charge injected by gain switching can be added (no data yet)
- Switching thresholds, gains and noise can be set by the user
- Fixed gain operation can be simulated by setting thresholds correspondingly
- Saturation behavior is unknown, implemented simple clipping to maximum allowed value, but code is prepared for different models

Treatment of storage cells

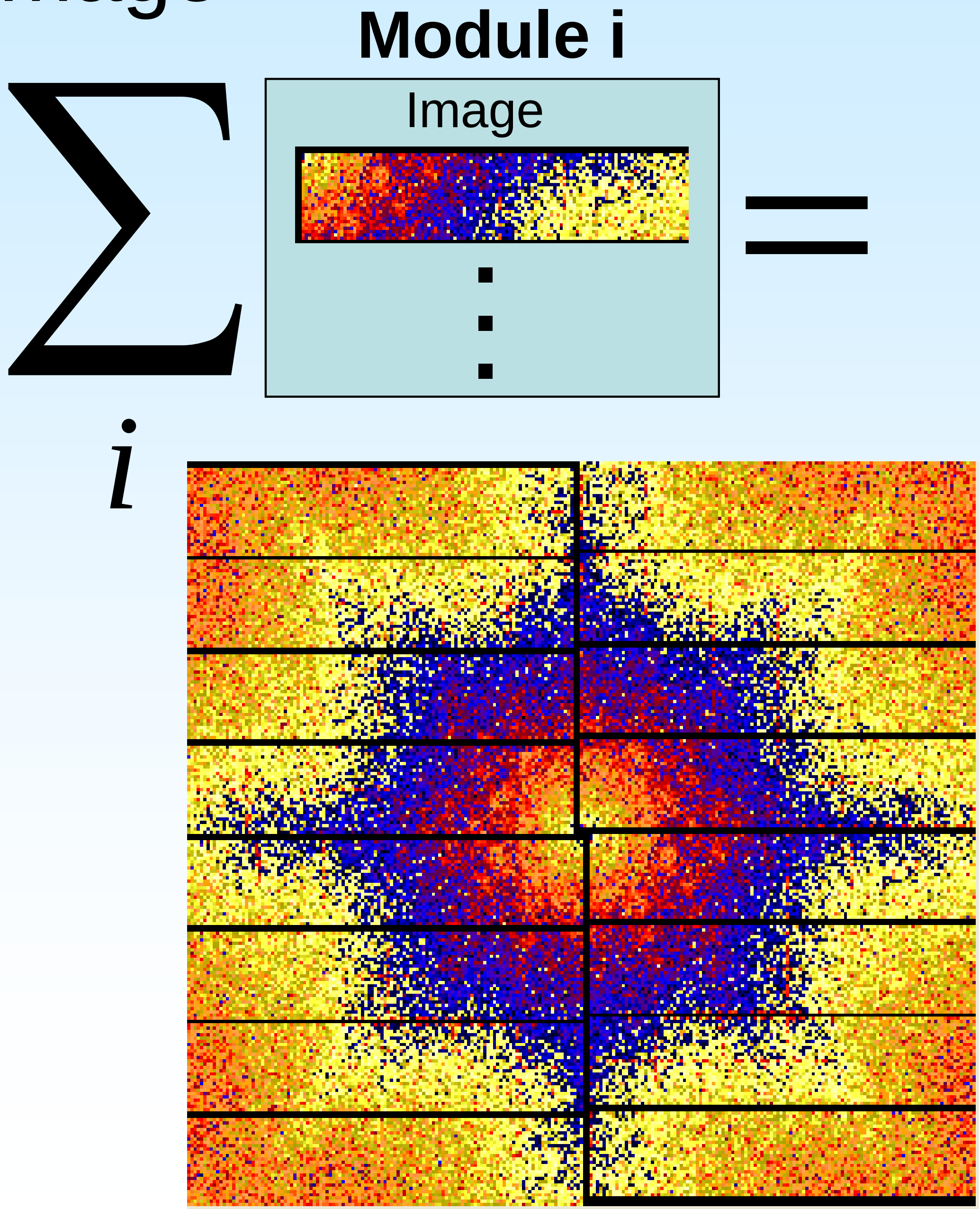
- Fixed leakage (can be corrected for): each cell the same each time it is read
- Random leakage (can not be corrected for): each cell different each time it is read
- Leakage parameters can be set by the user
- Code ready to handle more elaborate models



ADC of voltage signals and requantization

- ADC simulation
  - Range of ADC taken into account (14 bit)
  - Noise of ADC taken into account (4.6 LSB)
  - Noise can be modified by the user
- Requantization
  - Gain stage taken into account
  - Values below 0 (due to noise) are clipped to 0

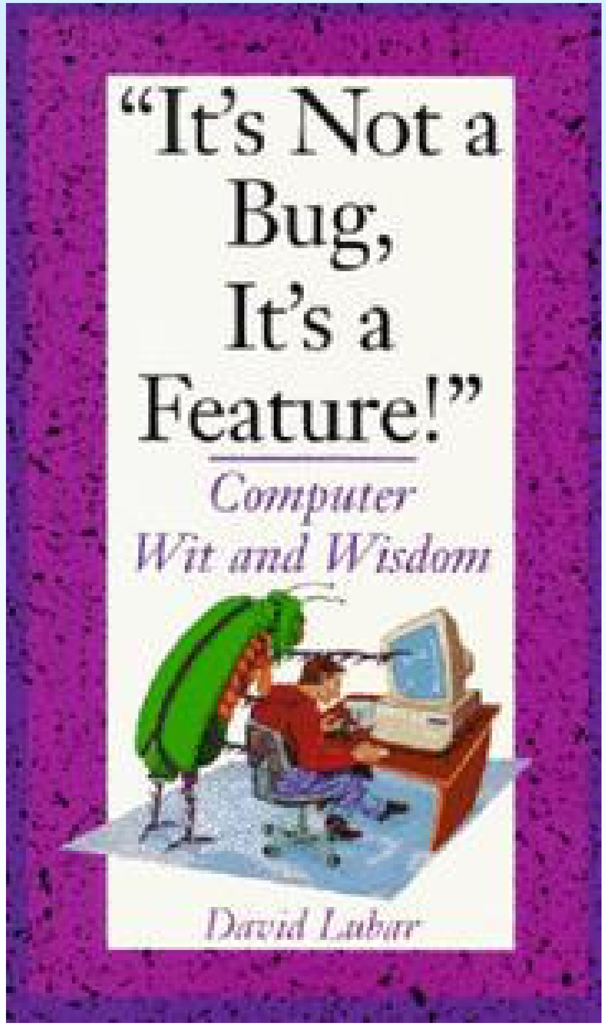
Construction of the output image



- Image data of each module is assembled into one large image
- Certain options allow to return different images (e.g. ADUs, Gains, input electrons, etc.)

Special features

- Can be used in an iterative way to calculate images for polychromatic sources (although inefficient)
- Treats parallax for any distance between detector and sample (assuming point like scattering source)
- Requantizied image, ADUs and gains are returned simultaneously



Limitations

- No treatment of plasma effects (happen with $>10^3\ \gamma$ in a pixel) so far (although some ideas are present)
- No non-centered photon sources (although there is a workaround for this)
- Fluorescence of Si not accounted for (code exists from Medipix simulations by David Pennicard)
- So far limited to silicon as sensor material
- No backscatter/fluorescence from parts behind sensor (Bumps/ASIC) (but result of a MC-simulation can be fed into HORUS)

Summary: HORUS

- Working horse of detector simulations
- Many improvements: higher speed, less bugs, more features, etc.
- Point and click interface to investigate behavior
- Less hard coded constrains
- No whole scale MC code (e.g. no fluorescence, Compton-scattering)
- Some open issues (eg. Plasma effect)

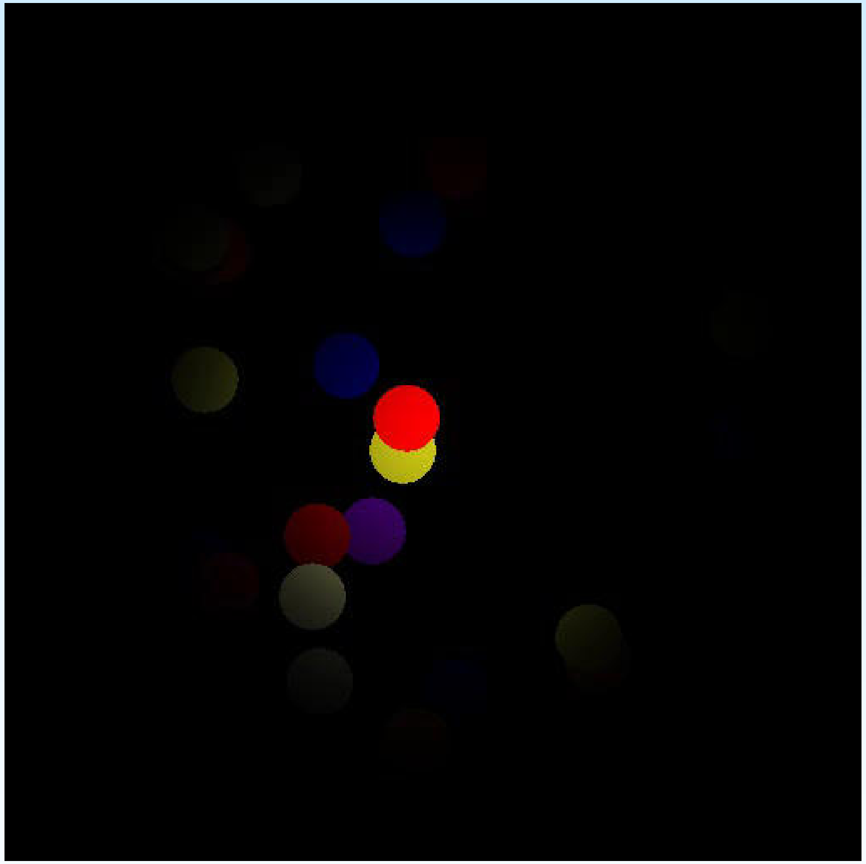
XPCS-Simulations

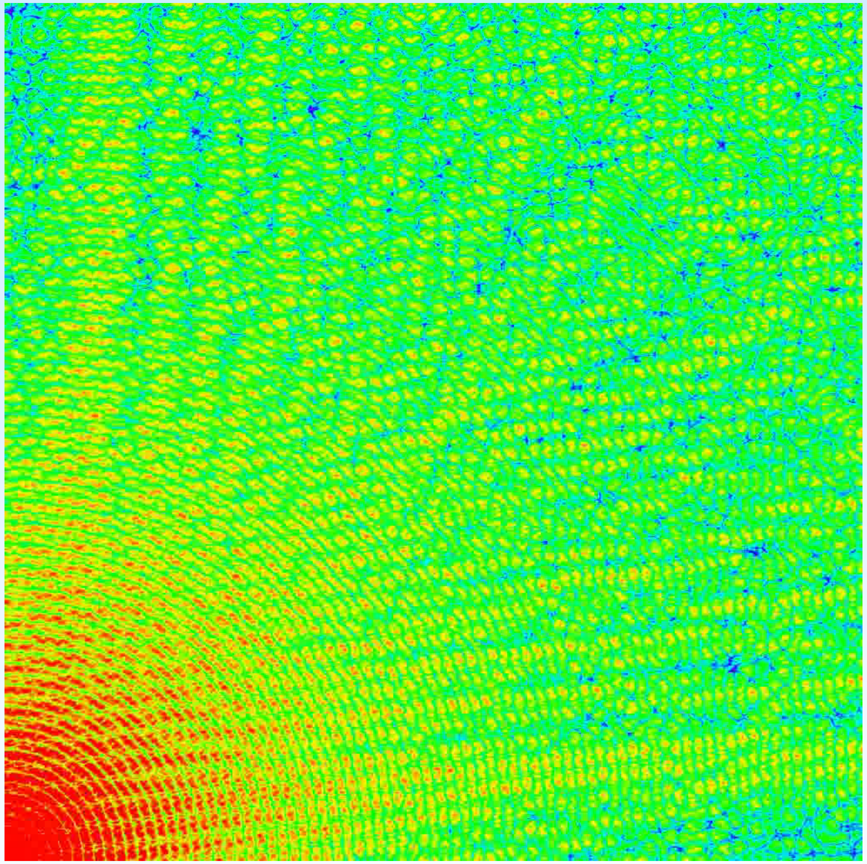
Beware: Change of topic!

XPCS-Simulations

- Strong demand from community for many (10^8!) small pixels (100µm or less)
- Sample heating/beam damage prohibits focusing -> speckles will be small (60-100µm)
- Use simple test system and evaluate influence of pixel size and aperturing as function of intensity and noise
- Show error in relevant extracted data

What XPCS does

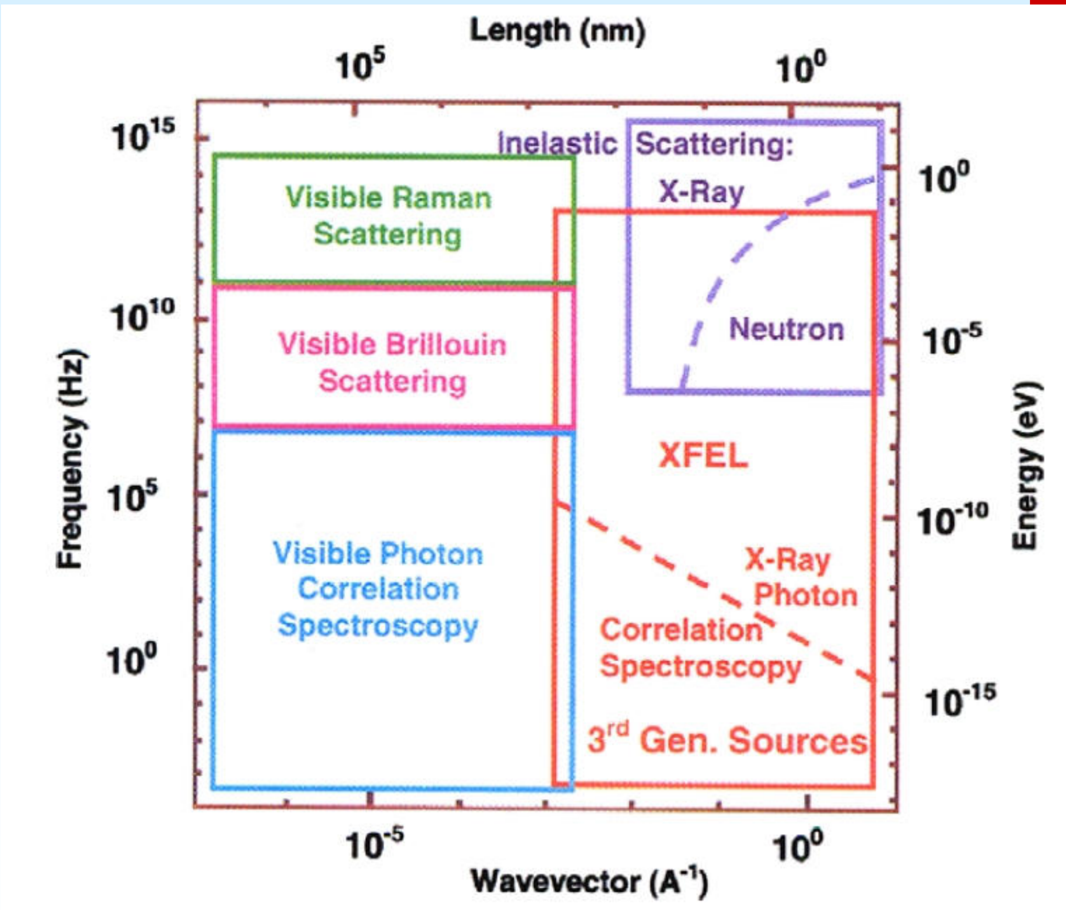




- Investigation of fluctuations in diffraction images
- Scientific case XPCS@XFEL: molecular dynamics in fluids, charge & spin dynamics in crystalline materials, atomic diffusion, phonons, pump-probe XPCS

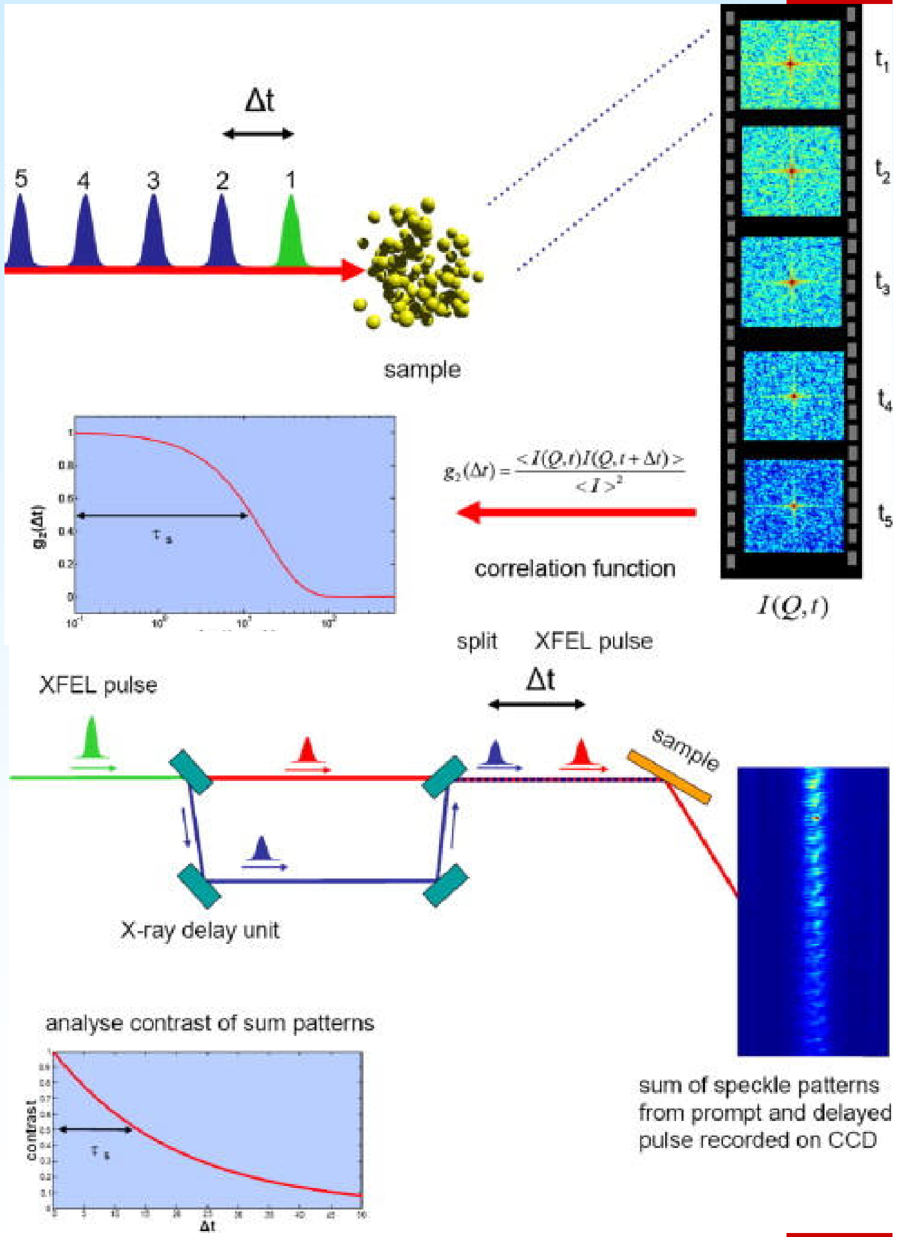
Some possible results from investigations with XPCS

- Insight into interaction type at probed length/time scales
- Determination of associated time constants
- Determination of anisotropies
- Investigation of phase transitions (esp. glassy states)
- Determination of rare symmetries (XCCS)
- … and much more



Different ways of XPCS@XFEL

- Choice of technique governed by investigated time scale τ
  - $0.22\ \mu s < \tau << 0.6\ ms$
    - intensity autocorrelation function (g2)
    - problems for low intensities, cannot correlate ‘0’ to anything
    - ‘slow’ time scale -> large particle movement -> low Q region -> SAXS
  - $\tau << 10\ ns$
    - use split pulse technique
    - problems for low intensities, offset value ~1/<I>
    - ‘fast’ time scale -> small particle movement -> large Q region -> WAXS
- For very low intensities (<I> -> 0) photon statistics have to be analyzed



Signal-to-Noise in XPCS

$$R_{sn} \propto C < I > \sqrt{N_b N_f N_{pix}}$$

C: Contrast

<I>: average intensity per speckle

N_b: number of bunches

N_f: number of frames per bunch

N_{pix}: number of Pixels

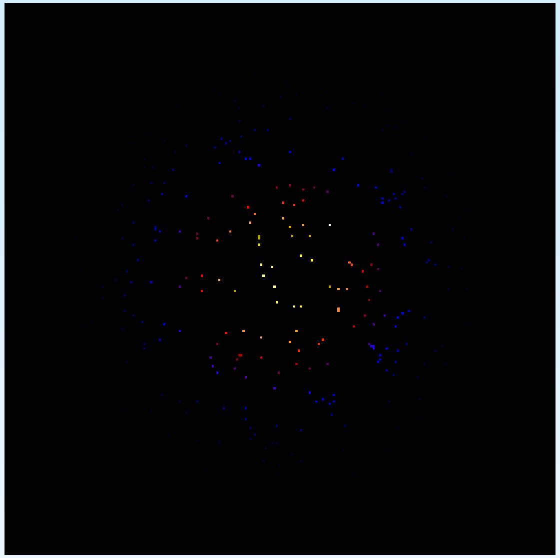
Aperturing increases C, but decreases <I>, evaluation of C*<I> by simulation

How to simulate XPCS

- Take a simple test system and generate a series of diffraction patterns
- Simulate detector response as function of relevant parameters
- Evaluate simulated detector images with established and foreseen techniques
- Quantify and compare results

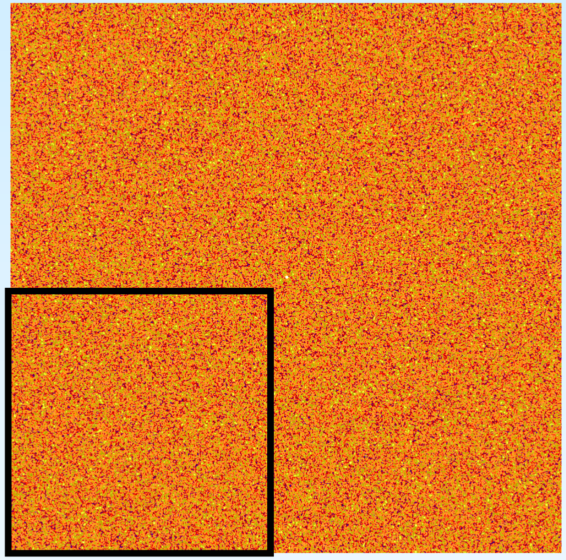
XPCS-Simulations

Real space



FFT

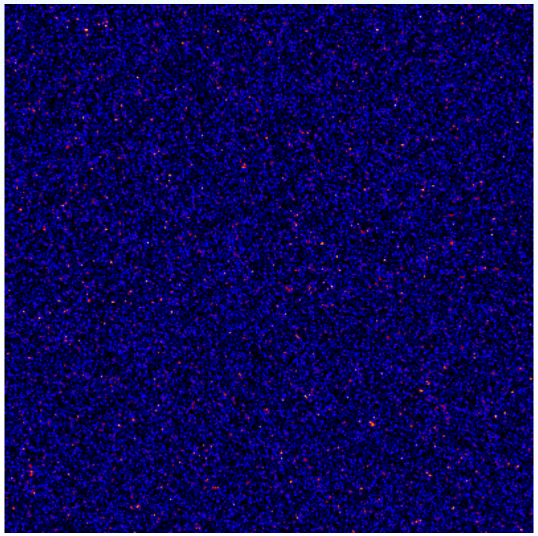
'Diffraction image'



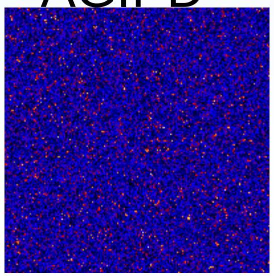
Detector response

(HORUS)

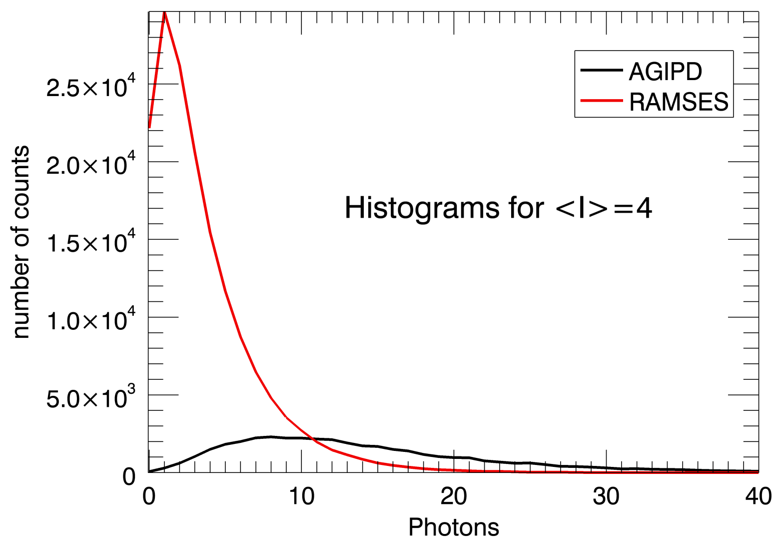
100µm AGIPD (RAMSES)



AGIPD

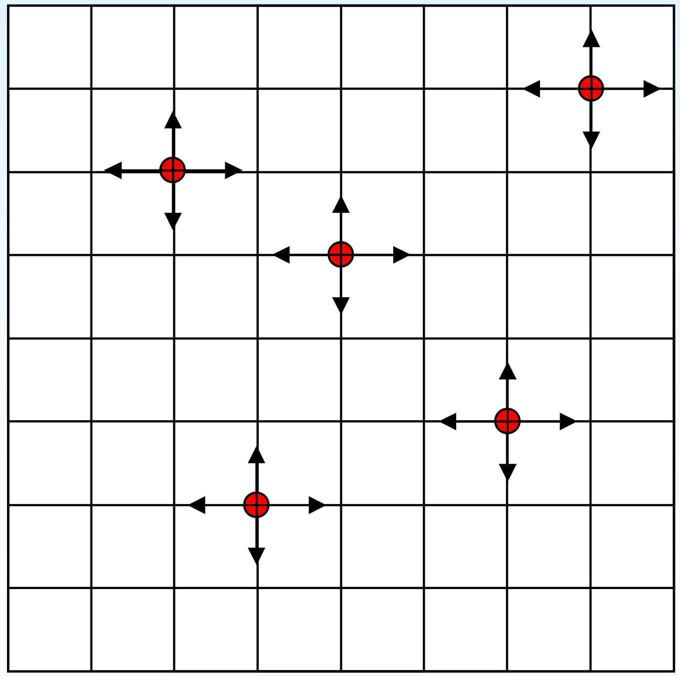


Evaluation



Simple real space system

- Points hopping on a 2D grid by ±1 position in each dimension (jump-diffusion)
- Absence of structure factor due to delta-like points
- Gaussian ‘illumination function’ producing Gaussian speckles with 4σ=2 pixels
- Oversampled ‘Diffraction’ image by Fourier transform (non-integer values)



Photon quantization

- Each image quantizized separately
- Image renormalized to given average intensity
- Each pixel value taken as average intensity individually
- Number of photons sampled randomly according to Gamma-Poisson statistics:

$$P(I)=\frac{\Gamma(I+M)}{\Gamma(M)\Gamma(I+1)}\left(1+\frac{M}{<I>}\right)^{-I}\left(1+\frac{<I>}{M}\right)^{-M}$$

M=1 for the fully coherent case

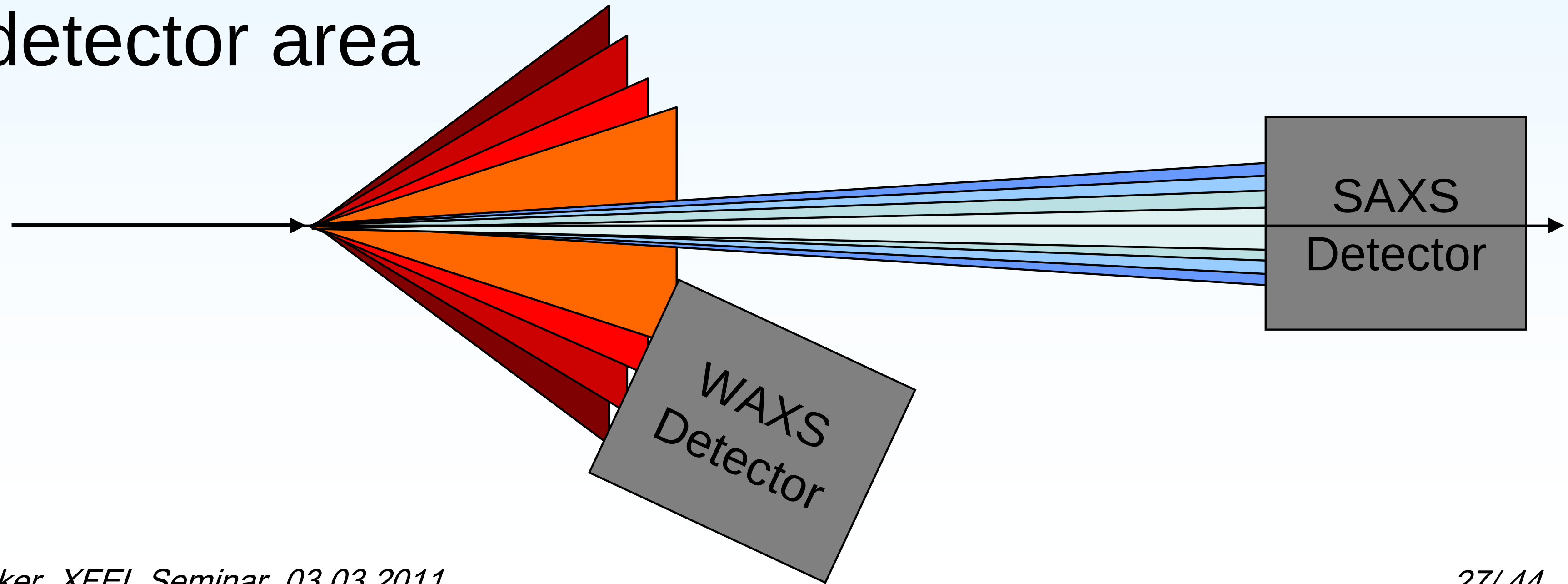
M=15 for the partially coherent case

Detector Systems

- ***Ideal***: 100µm / 200µm pixel size (no charge sharing, QE=1, no detector noise)
- ***AGIPD***: **A**daptive **G**ain **I**ntegrating **P**ixel **D**etector, 200µm pixel size
- ***MAAT***: **M**odified **A**GIPD using **A**perturing **T**echniques, 200µm pixels apertured to 100µm
- ***RAMSES***: **R**educed **AM**plitude **SE**nsing **S**ystem, AGIPD with 100µm pixel size
- WAXS/SAXS configuration for 100µm systems

Detector Geometries

- **SAXS**: interesting Q region fits on detector area -> limiting factor: pixel density
- **WAXS**: only small part of the interesting Q region can be sampled -> limiting factor: detector area



Simulated noise sources

- 10% rms (uncompensated) intensity fluctuations
  - Probably more at low intensities (inherent non-Gaussian SASE fluctuations)
  - Probably less at high intensities (can be corrected for)
- Incoherent background noise (e.g from higher harmonics, sample fluorescence, residual gas scatter, etc.): completely random, probability of 1/100 (Poisson distributed) per 100µm pixel

Parameter space

- 13 different intensities (4e-4 to 40)
- 7 detector systems
- 4 sets of noise contribution
- 2 states of coherence (M=1 and M=15)
- 300 images per set
- 5 repetitions

=> $O(10^6)$ simulations / evaluations

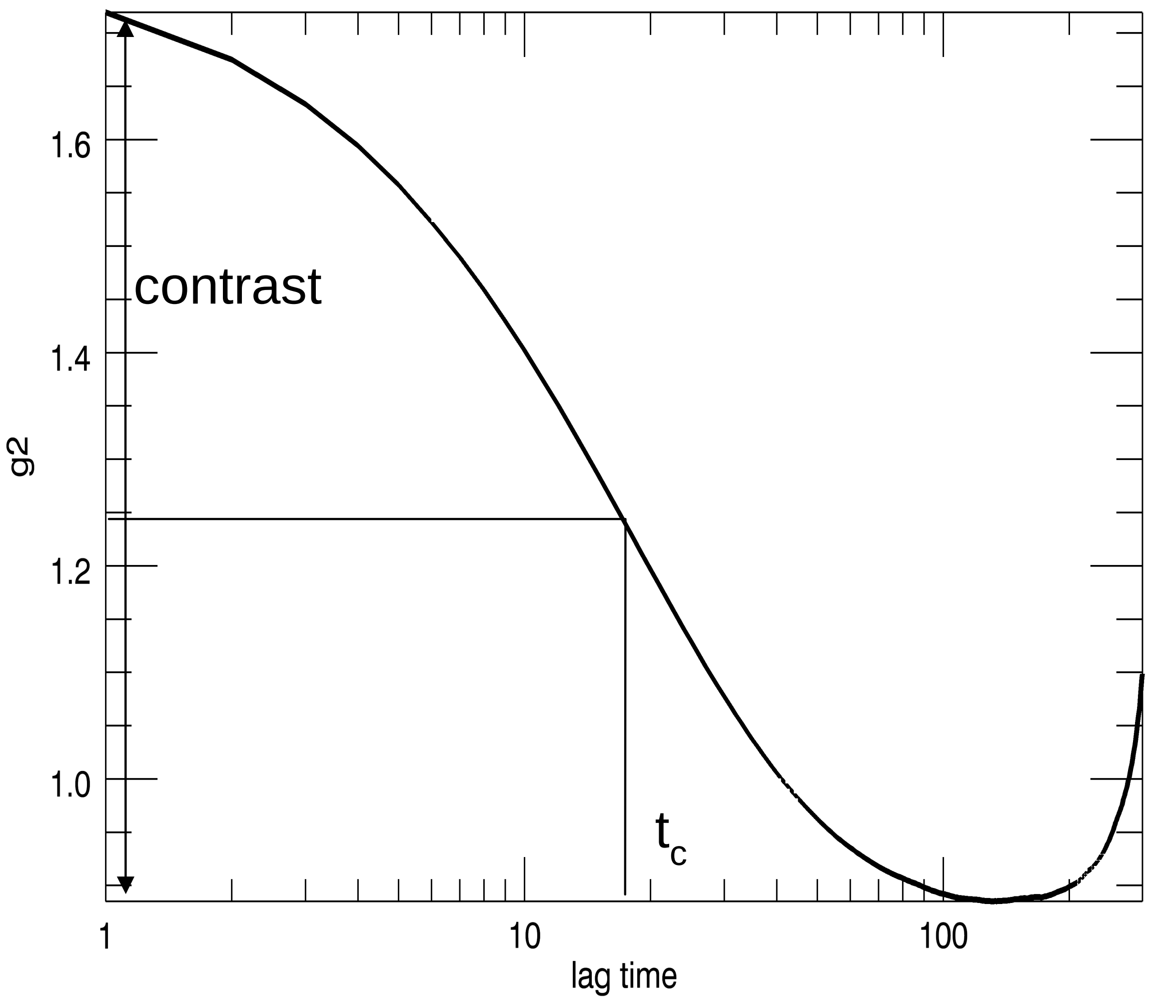
Data evaluation

- Calculate autocorrelation function (g2) per pixel
- Average values with identical Q
- Fit exponential decay to g2 function
- Extract fit parameters as function of Q
- Calculate average value and (relative) error of fit parameter

$$g2(Q,\tau) = S(Q)\left(C(Q)e^{-\frac{\tau}{\tau_c(Q)}} + 1 \right)$$

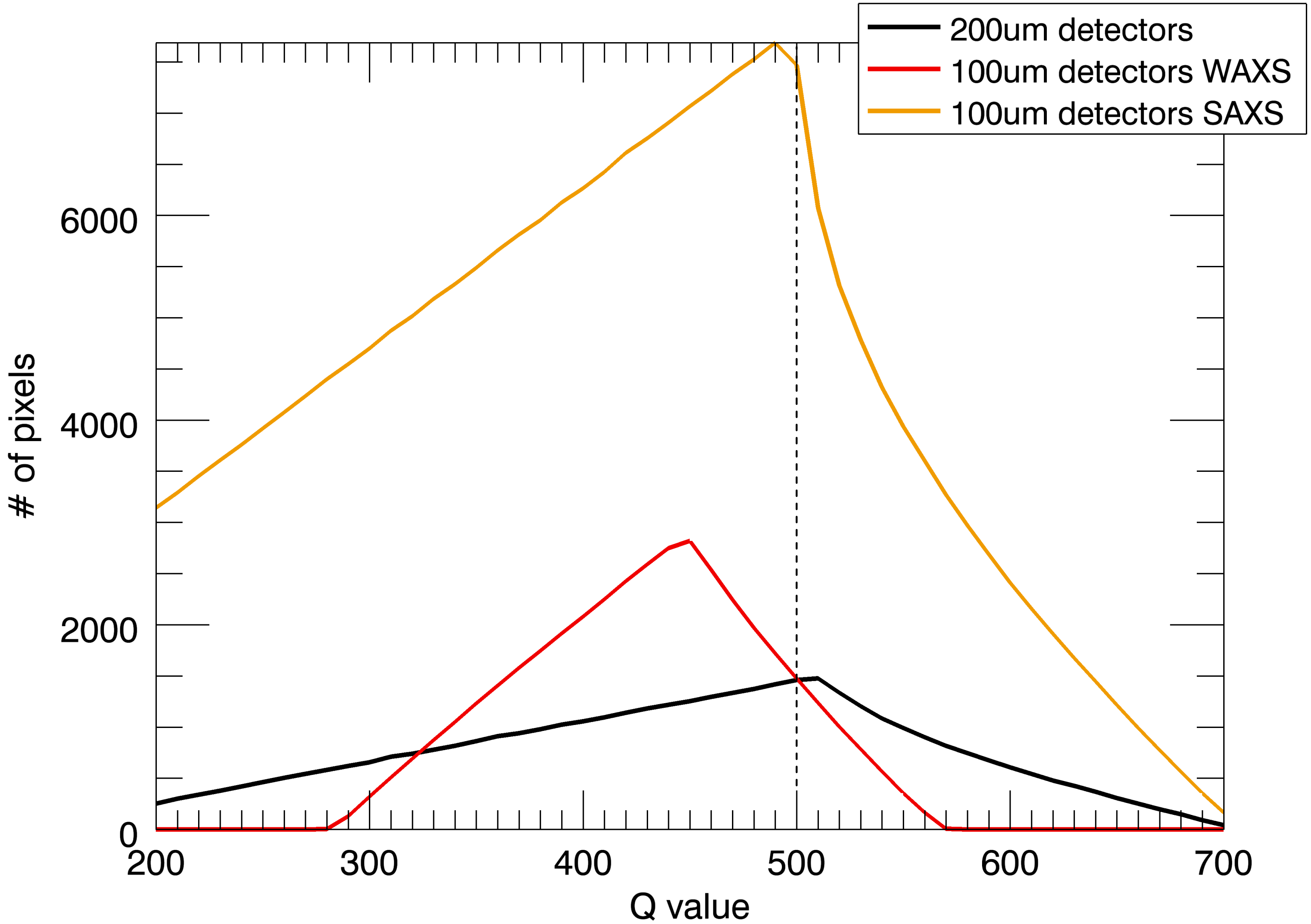
$$\Gamma(Q) = 1/\tau_c(Q)$$

G2 function



- Decaying (ideally) from contrast+1 to 1 with decay time t_c
- Artifacts toward large lag times are reduced by more frames (100x - 1000x t_c)
- Functional form determined by particle interactions

Pixel distribution

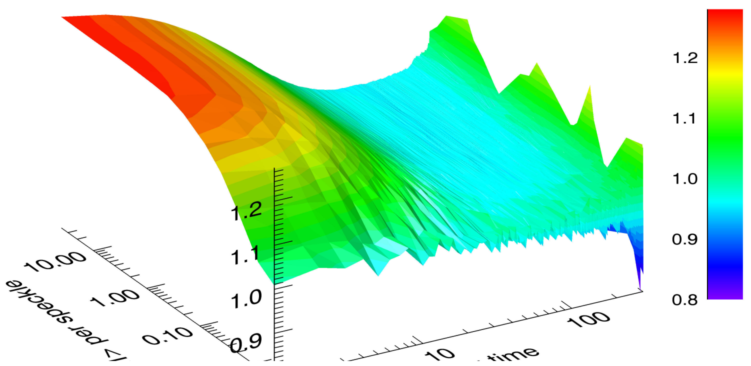


Evaluations as function of Q

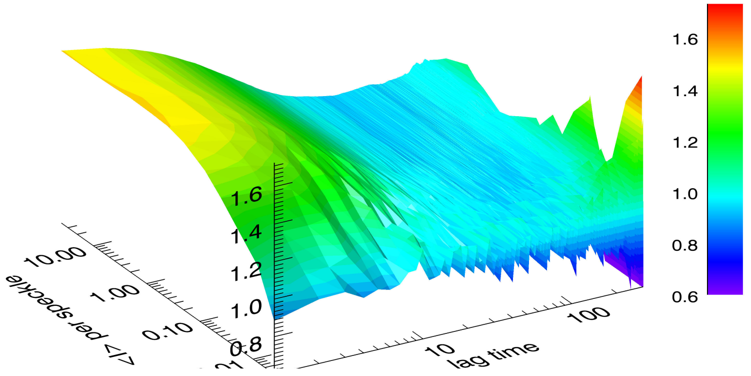
Radial symmetry in Q-space allows averaging over pixels with similar Q (±5)

Detector is a square, thus the number of pixels as function of Q shows a distinctive shark fin shape

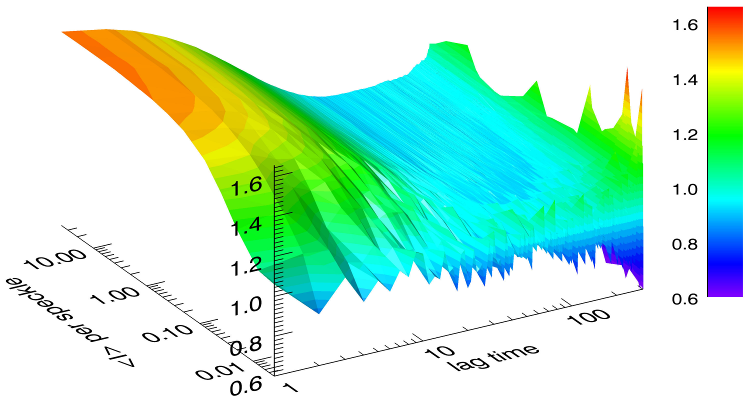
G2 function, AGIPD, incoherent noise and intensity fluctuations



G2 function, RAMSES WAXS, incoherent noise and intensity fluctuations



G2 function, MAAT, incoherent noise and intensity fluctuations



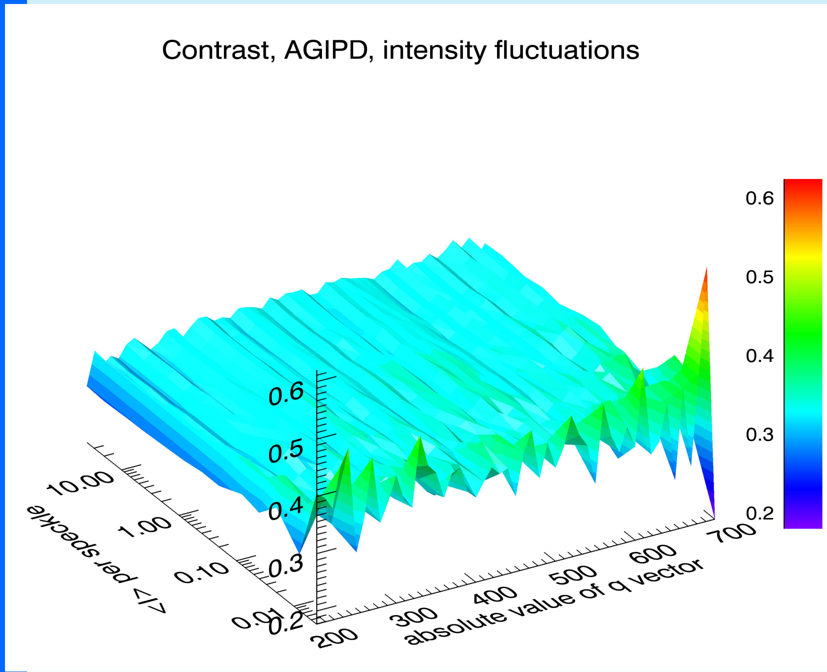
G2 at Q=500

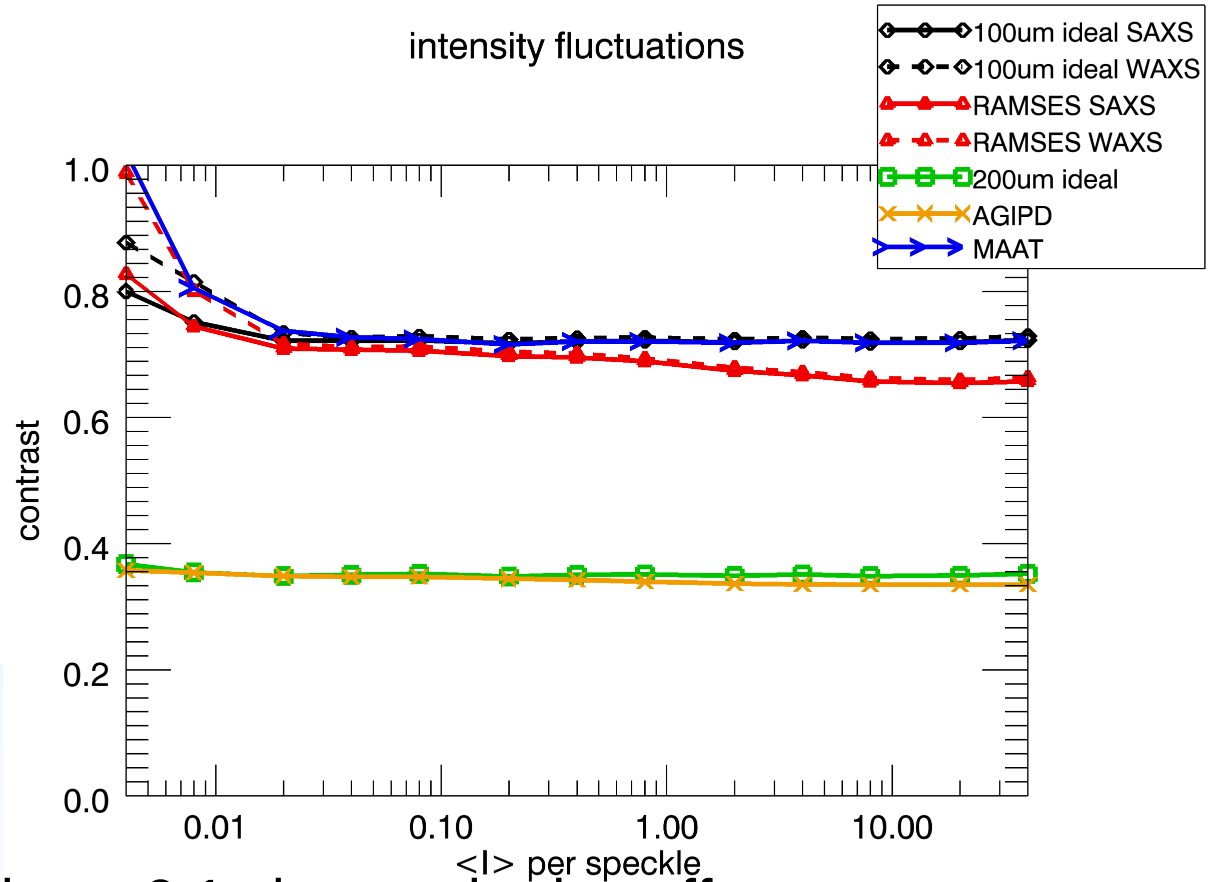
Basic data set to be fitted

- For AGIPD contrast is low, but lowest noise
- RAMSES in WAXS shows higher contrast and higher noise
- For MAAT contrast is as high as for RAMSES with similar noise

In the following slides only the results of the fit will be shown

Contrast with fluctuations



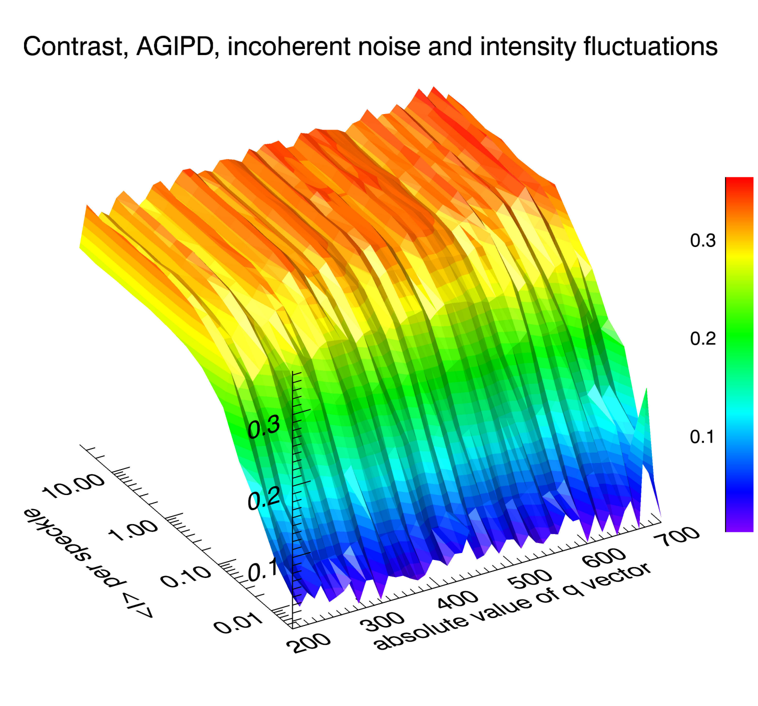


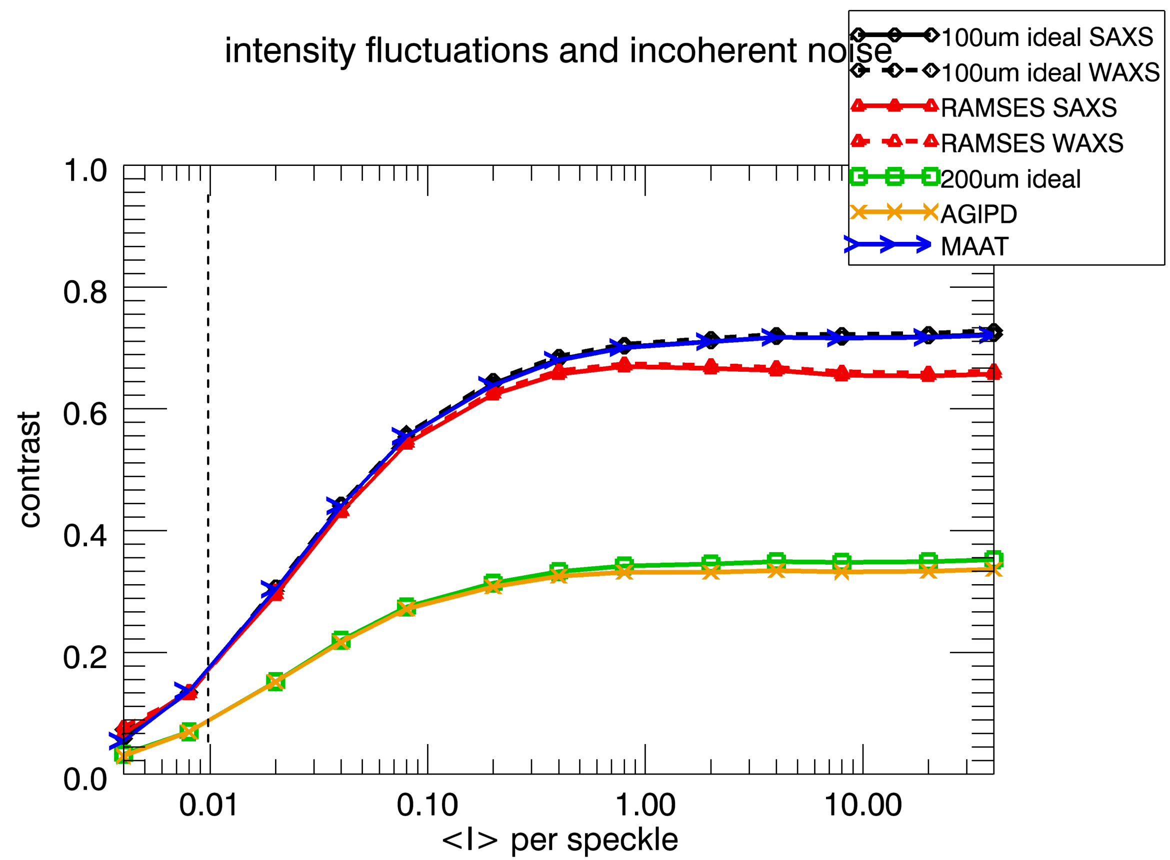
At average intensities above 0.1 charge sharing effects decrease the contrast, less strong for bigger pixels

At very low intensities the number of pixels/frames/bunches is not high enough for reliable results

MAAT yields contrast of an ideal 100um system

Contrast with noise



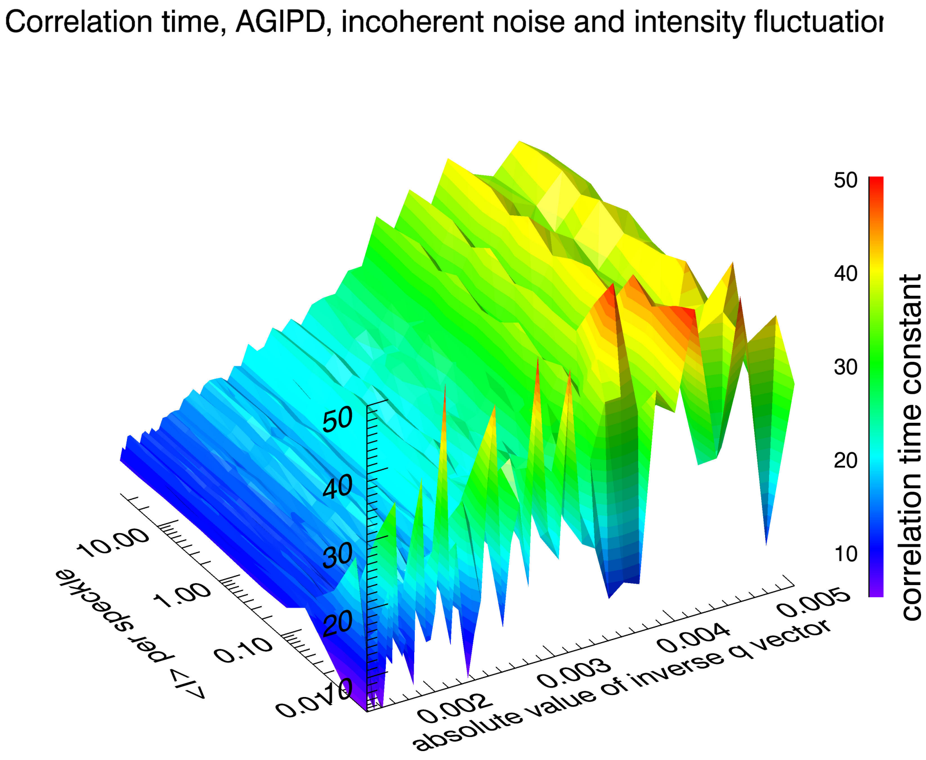


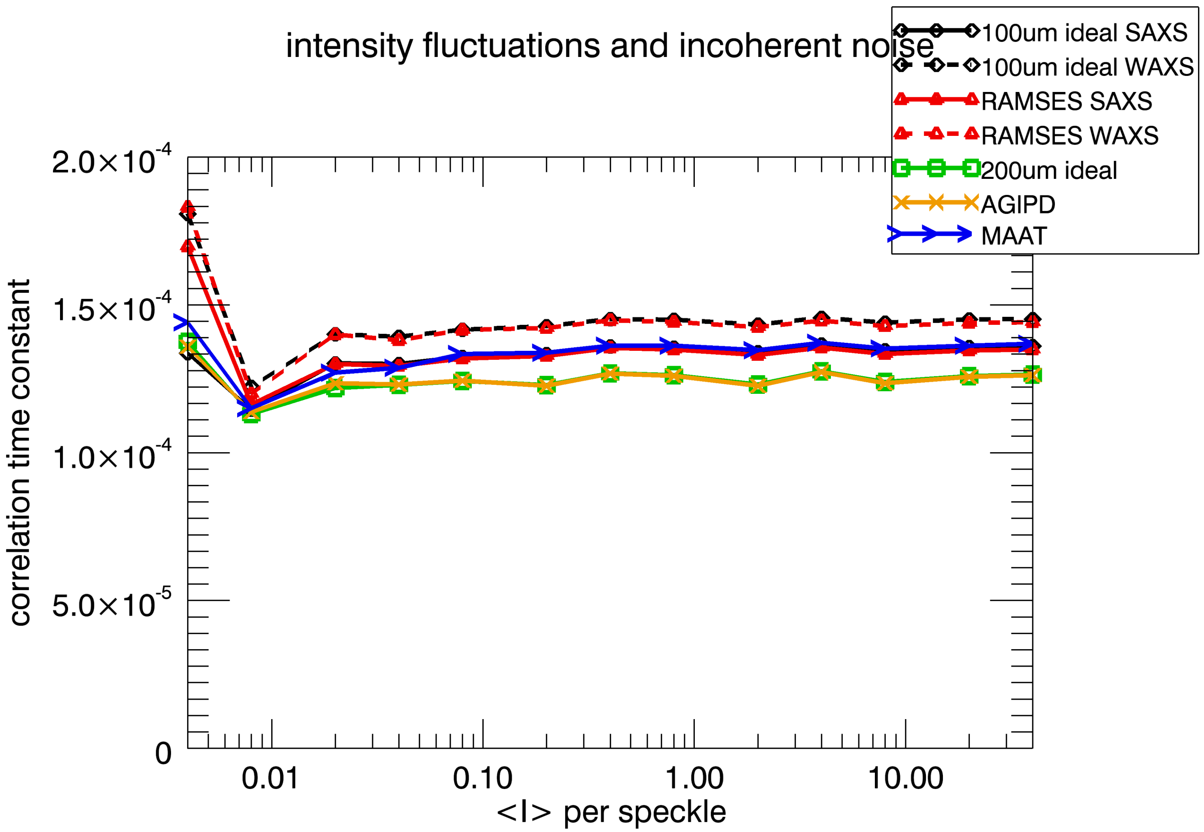
Charge sharing independent of noise

Contrast significantly decreases around the average intensity of the incoherent noise ($<I_{noise}>=0.01$)

MAAT still yields contrast of an ideal 100um system

Correlation time





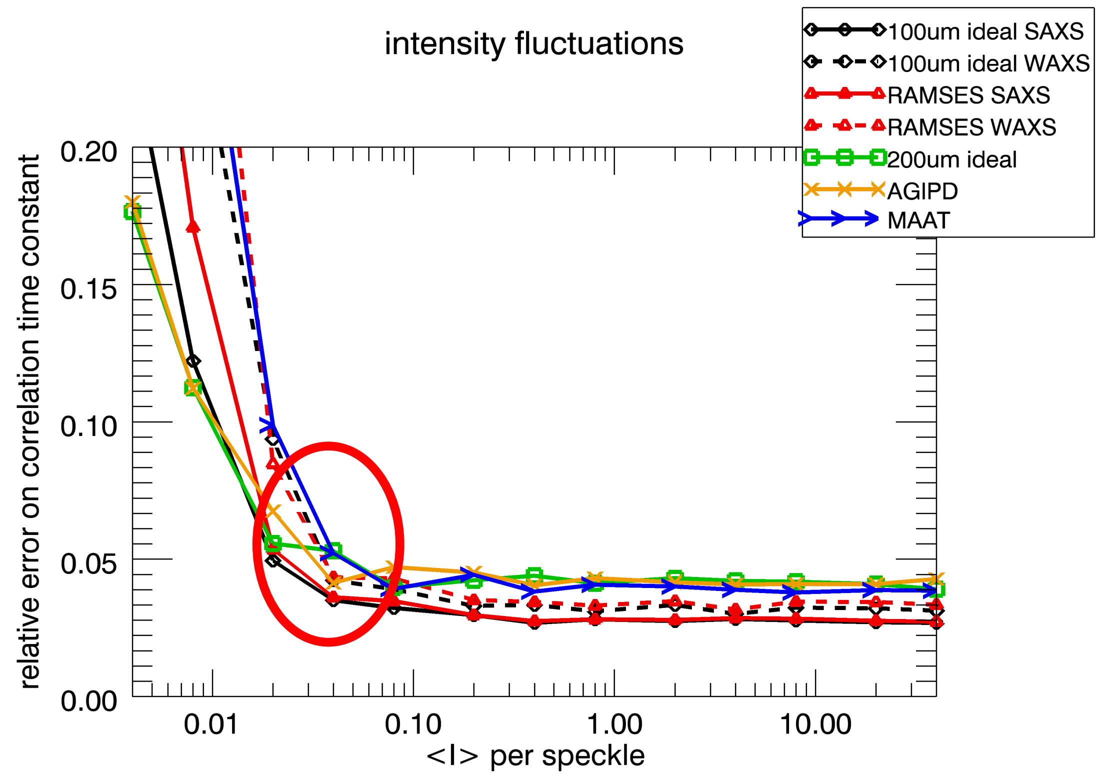
$\Gamma(Q)=(1/t_c)$ should be proportional to Q^2 for small Q and show distinct deviations from this when Q is in the region of the inverse lattice size

Correlation time is linear in 1/Q (crude approximation for this case)

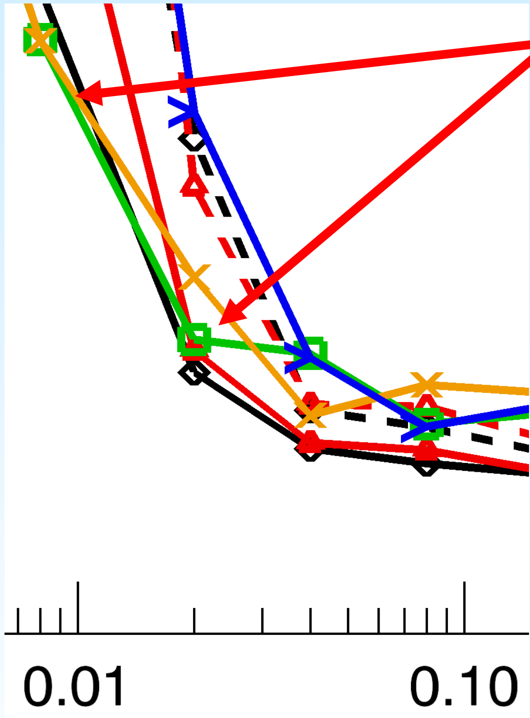
Slightly different slope for different systems (due to crude approximation)

Error on correlation time only fluctuations

Optimum Q range for each system



Zoom



Green/Yellow below other lines!

Bigger pixels win!

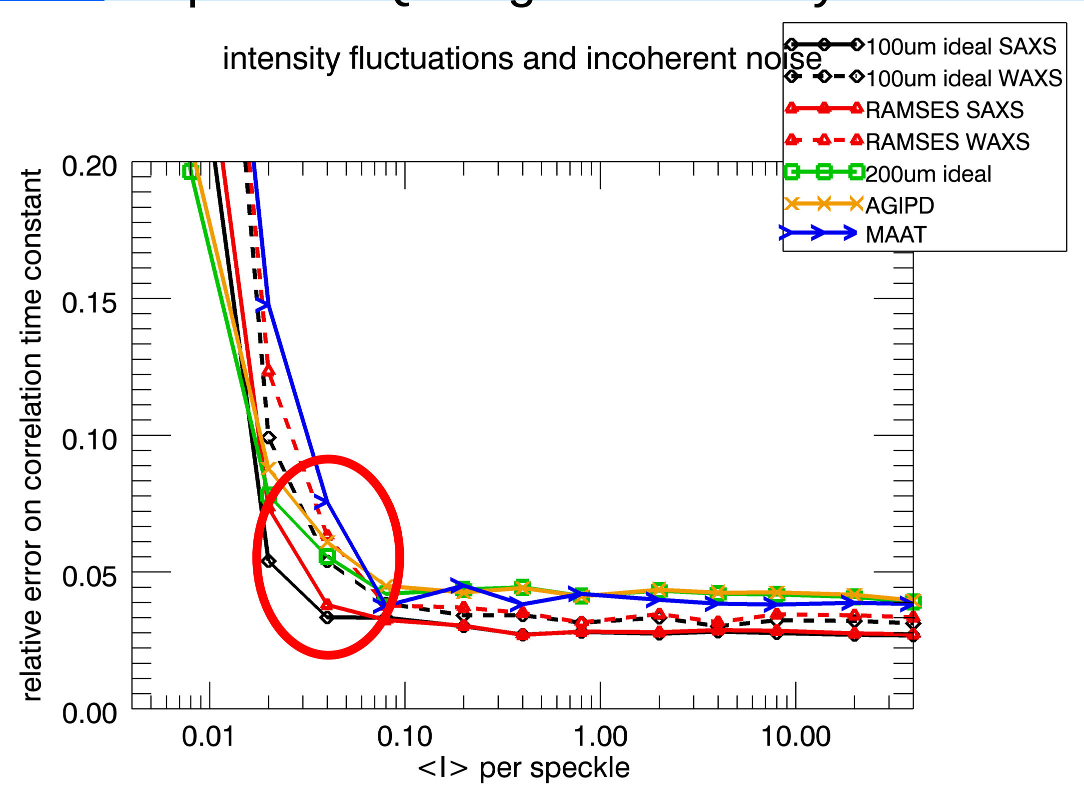
Intensities below <I>=0.01 require more images/bunches/pixels (seen from contrast)

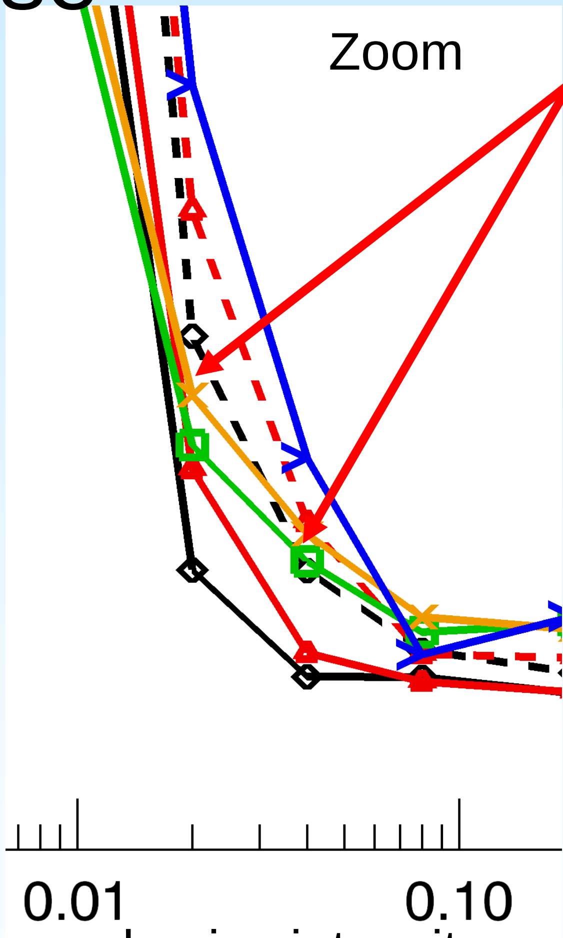
Crossing behavior -> statistical effect: cannot correlate 0 photons to anything, higher fraction of non-zero pixels for larger pixel size

For low intensities MAAT (blue) performs as good/bad as small pixel systems in WAXS geometry

Error on correlation time with incoherent noise

Optimum Q range for each system





Green/Yellow below WAXS lines

Bigger pixels win, but noise ruins the game

Error increases significantly around noise intensity

Crossing behavior only in WAXS geometry

For low intensities MAAT performs as good/bad as small pixel systems in WAXS geometry

Reduced Coherence / Split pulse technique

- Data evaluation for reduced coherence quantization (m=15) is underway, preliminary results look similar to full coherence
- Data for split pulse technique has been calculated and evaluated, however calculation of 5 images each at 300 different Δt is not enough statistics to evaluate performance of the different systems (even at high intensities)
- Evaluation using photon statistics (# of 0’s, 1’s, 2’s, etc.) underway

Summary: XPCS

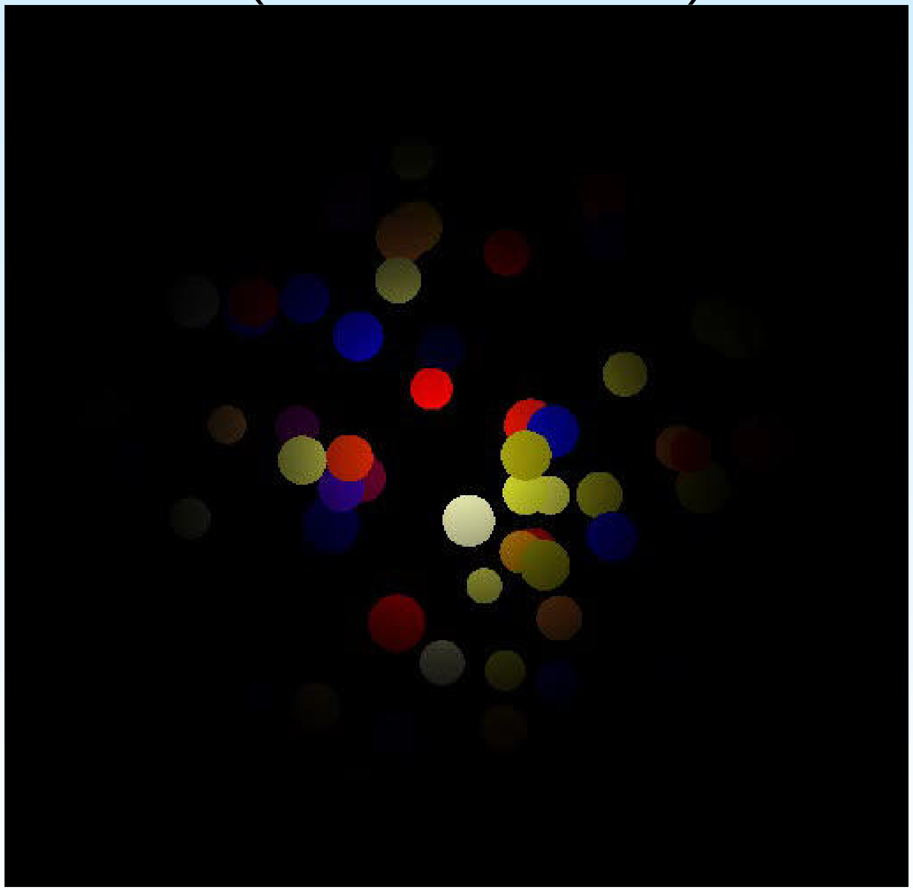
- Whole simulation chain set-up and tested
- Extraction of parameters allows comparison of different systems
- At high intensities (SAXS, lim. by pixel density):
  - MAAT yields higher contrast compared to AGIPD
    - smaller speckles
    - less focused x-rays
    - less beam damage
    - can cope with high intensities
  - RAMSES shows superior performance
    - amplitude limitation
- At low intensities (WAXS, lim. by detector area):
  - AGIPD outperformes other systems
    - larger area (Q-space) coverage
    - better statistics due to higher non-zero probability
  - RAMSES and MAAT show equal performance

Next Generation XPCS simulations

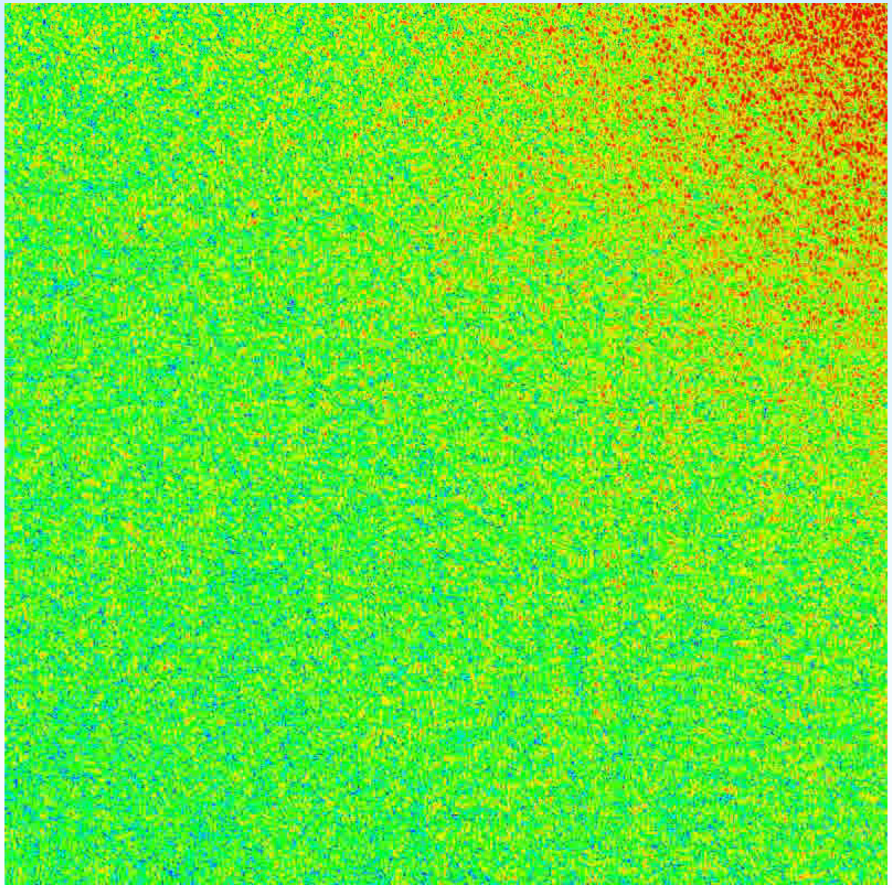
- Simulate a more realistic system
  - Charge stabilized colloids
    - 3D Diffusion
    - 3D Volume -> path length difference
    - Repulsive screened Coulomb force (Yukawa potential)
    - Finite extend of particles -> Structure factor
  - Based on PhD Thesis of Fabian Westermeier
- Concentrate on interesting region of phase space (high intensities take long to calculate)
- Calculate enough statistics to evaluate split pulse technique

Next generation XPCS simulations

Real space
(z axis color coded)



Detector plane
($\log_{10}$(intensity) color coded)



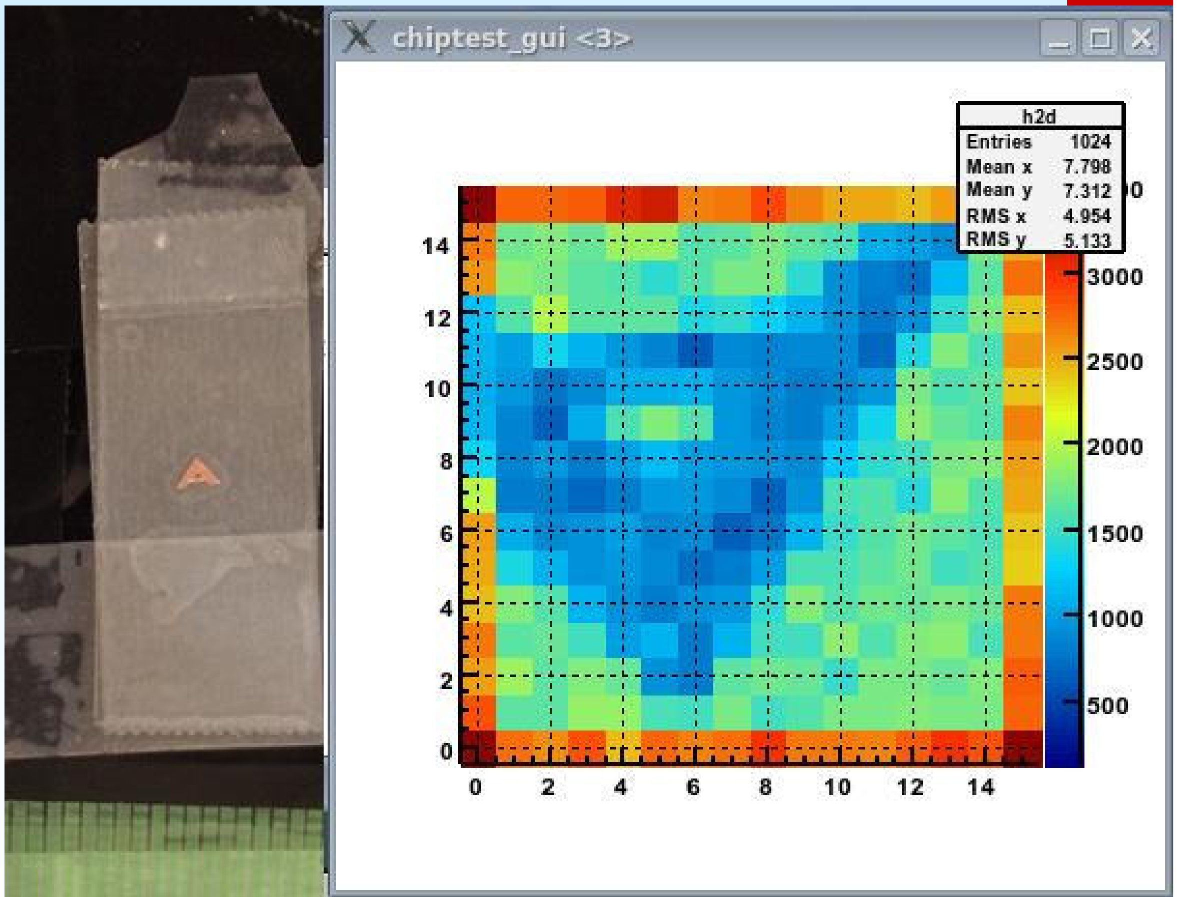
- All simulations in arbitrary units -> normalization constants
- Need to find right parameters to simulate a realistic system

CDI simulations

- In principle all tools to calculate CDI are there
- Proper input systems are needed (Lysosyme?)
- Reconstruction algorithms need to be implemented and some automation added
- No progress so far due to lack of knowledge (and time)
- Next big topic on the list

Thank you for your attention

There surely are a lot of questions



'A' first image acquired with an AGIPD02 assembly bump bonded to a sensor