Some Applications of Sparse Modelling in Physical Measurements

13 March 2014

Shiro Ikeda , ISM

@ Today's Topics

@ X-ray diffraction imaging

Phase retrieval

@ Astronomy data analysis

Compton camera imaging

Phase Retrieval

joint work with

H. Kono (JAEA)

Background

- Fourier transform & phase
- 3D structure of biomolecule
- X-ray Free Electron Laser (XFEL)
- X-ray diffraction of single biomolecule

Proposed method

- Phase retrieval
- Standard method (HIO)
- Proposed method (SPR)
- Numerical experiments

◎ 3D structure of biomolecule

◎ 1 dimensional structure

A chain of amino acid. (There are 20 possible aminoacid)

ex) Lysozyme (a chain of 129 aminoacid)

KVFGRCE....

K : Lysine
V : Valine
F : Phenylalanine
G : Glycine

◎ 3 dimensional structure

The chain folds and forms a 3d structure

The reaction of the protein is determined by the 3d structure.

3d structure is important for medicine, biology, etc....

Protein 3D structure of Lysozyme

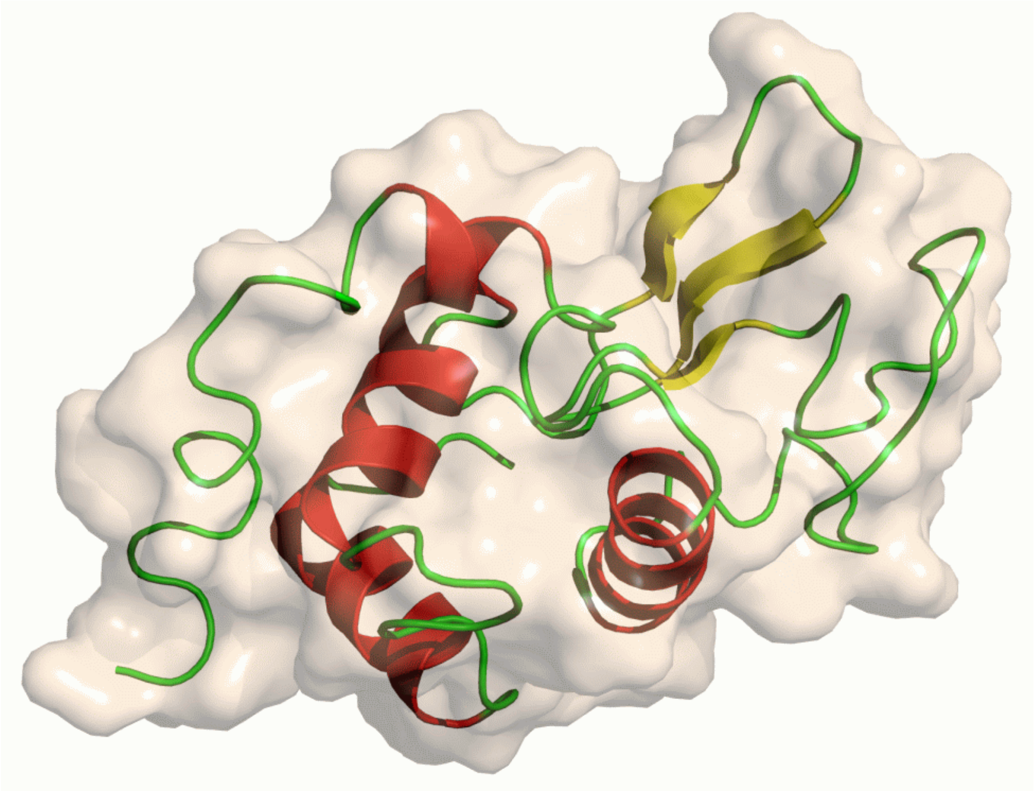


Figure: Lysozyme (wikipedia)

Protein 3D structures

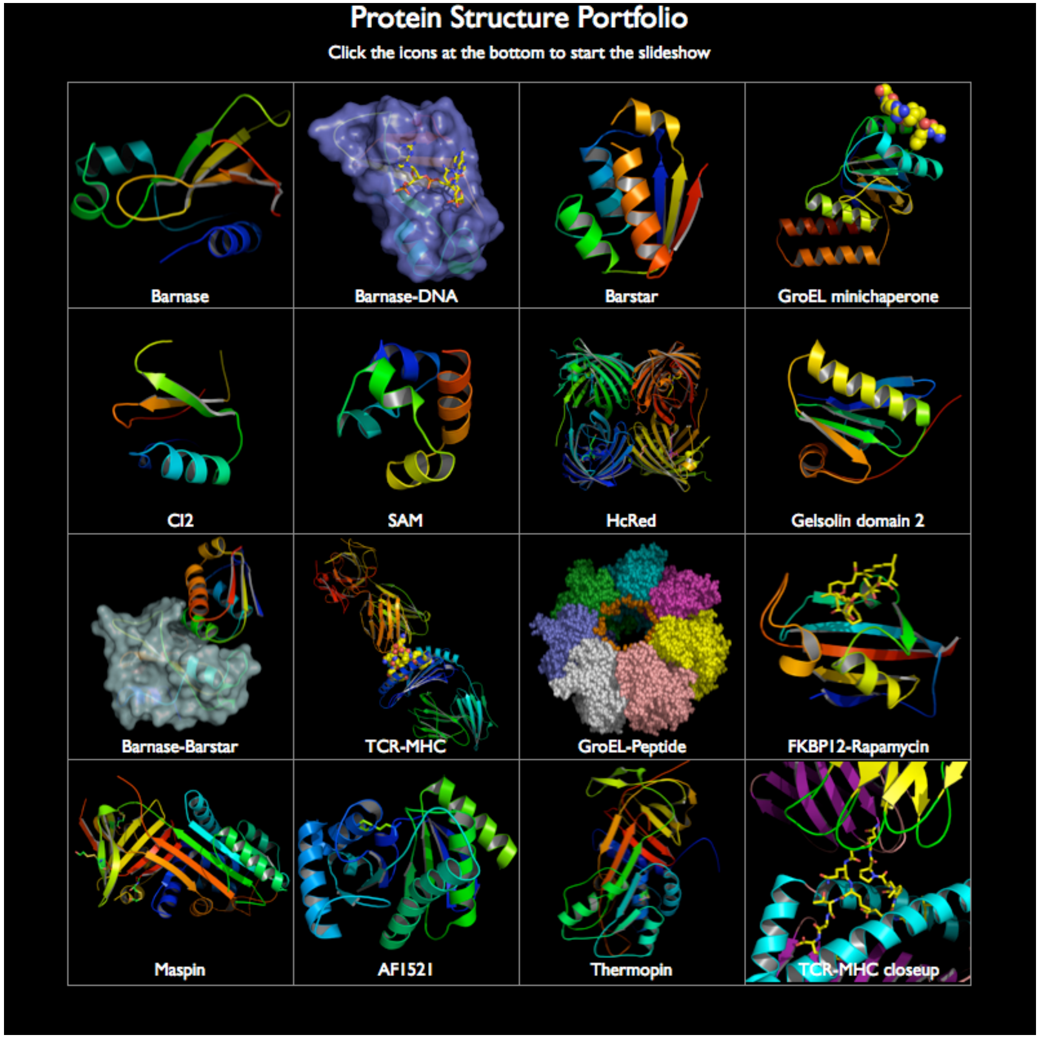


Figure: Protein structure gallery (Monash univ.)

Conventional method

- Molecular Dynamics (MD)
  - Simulate atomic dynamics with a super computer
  - Difficult for lang molecules (few μsec)
- X-ray Crystallography (from 1950's)

  Crystalization, X-ray Diffraction $\longrightarrow$ Analysis

  - Main subject is the Crystalization
  - Many protein does not become a crystal

    40% of biomolecule will not become a crystal.

Crystalization

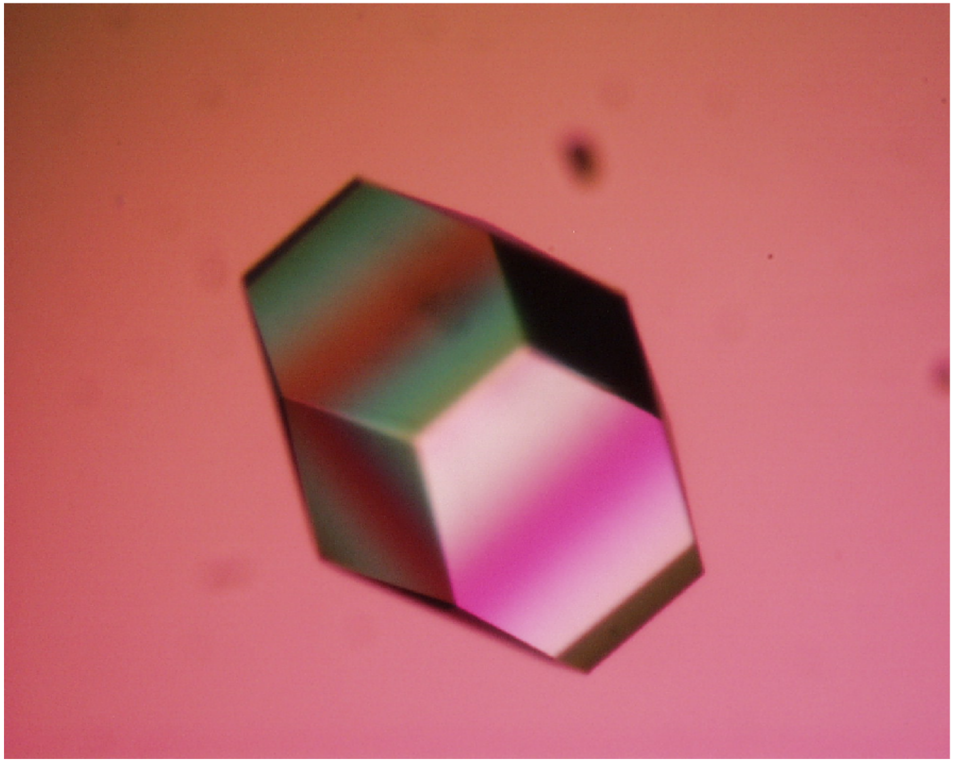


Figure: Lysozyme (wikipedia)

Crystalization

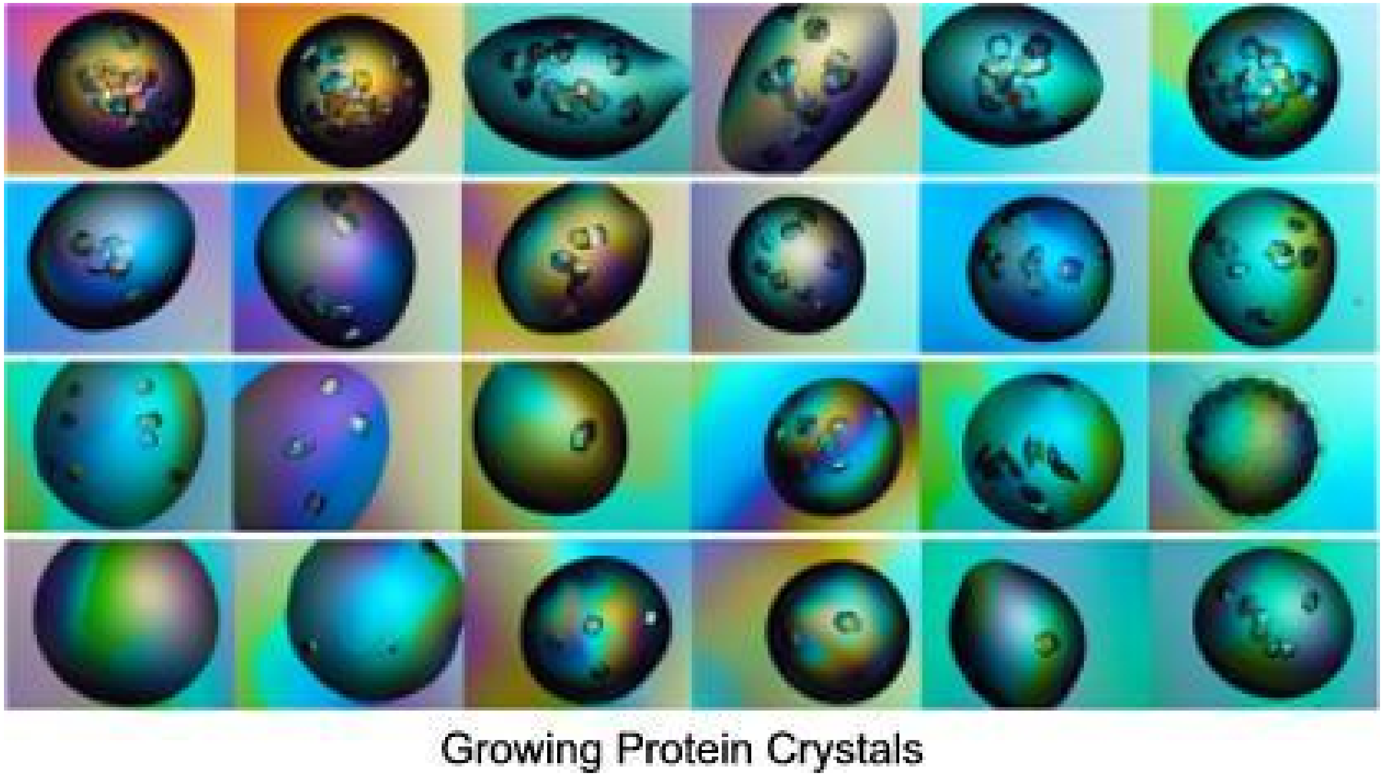


Figure: Crystalization.(Cornell Univ. CrySis)

Crystalization and protein structure identification

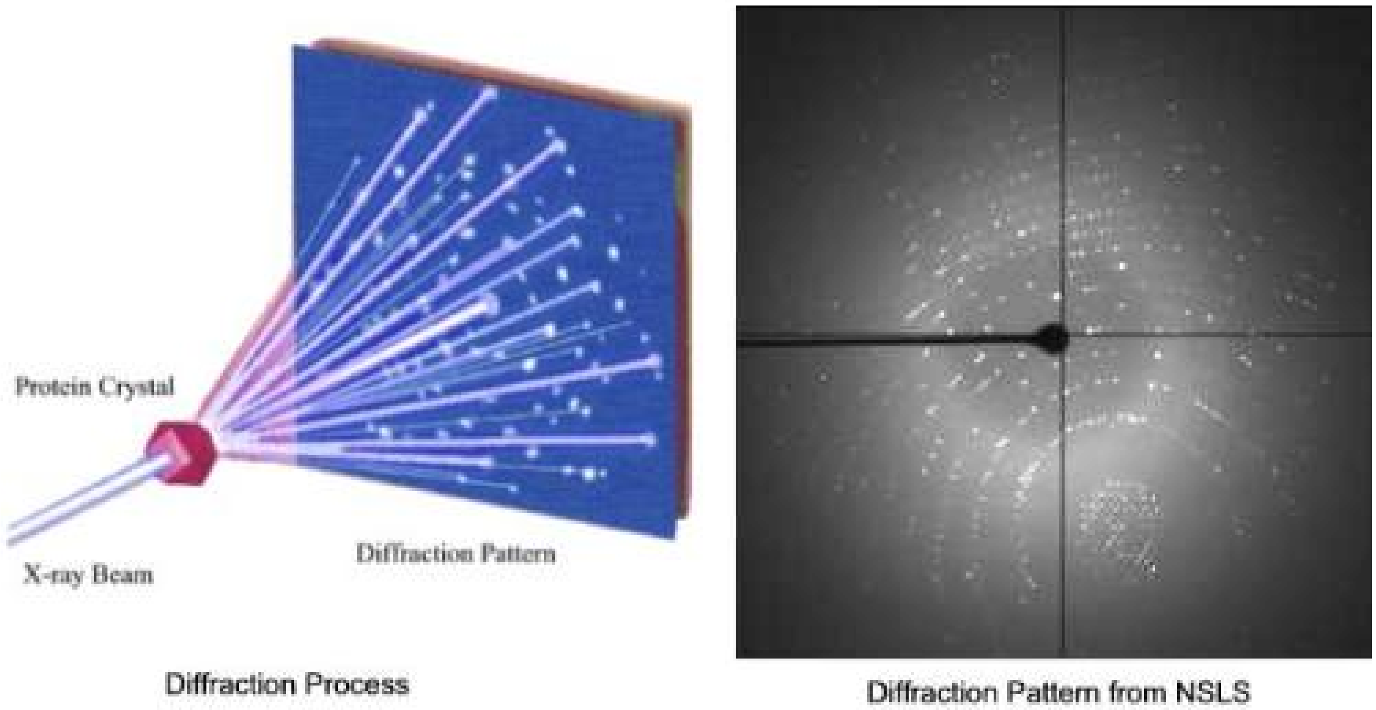


Figure: Crystalization and diffraction pattern.(Cornell Univ. CrySis)

Crystalization and protein structure identification

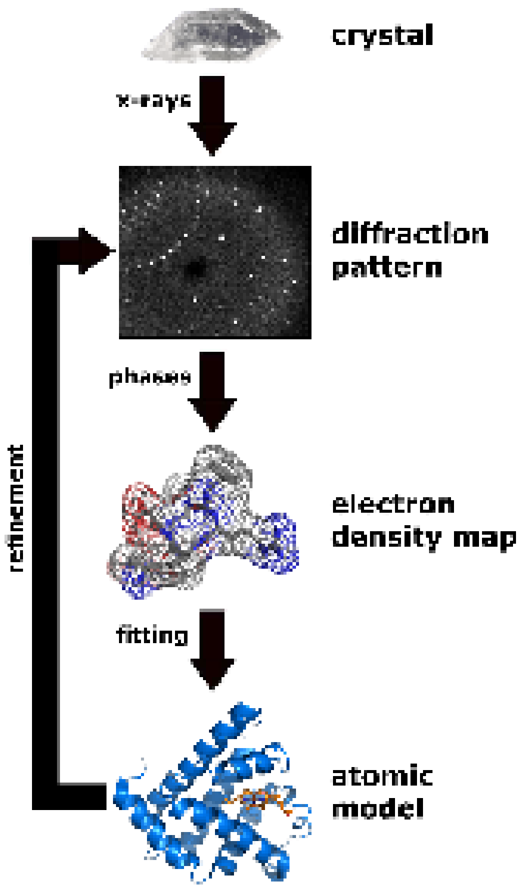


Figure: Crystalization and Structure recovery.(wikipedia)

Background

- Fourier transform & phase
- 3D structure of biomolecule
- X-ray Free Electron Laser (XFEL)
- X-ray diffraction of single biomolecule

Proposed method

- Phase retrieval
- Standard method (HIO)
- Proposed method (SPR)
- Numerical experiments

Q X-ray Free Electron Laser

IR $\rightarrow$ red $\longrightarrow$ blue $\longrightarrow$ UV $\longrightarrow$ X-ray

long $\longleftarrow$ wave length $\longrightarrow$ short

low $\longleftarrow$ Energy $\longrightarrow$ high

gas laser, solid-state laser, and semiconductor laser,

cannot emit high power X-ray laser.

XFEL (X-ray free electron laser)

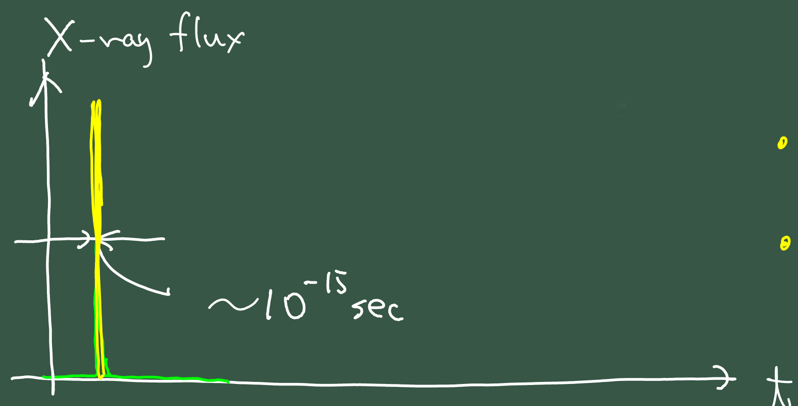
Figure: Spring8

XFEL (X-ray free electron laser)

Figure: XFEL

X-ray Free Electron Laser

- 4 projects in the world.
- Japan "lased" after USA.
  (Cheaper, More Flux, Larger Energy)



- Short pulse
- Large flux X-ray

XFEL (X-ray free electron laser)

Figure: XFEL in the world

Background

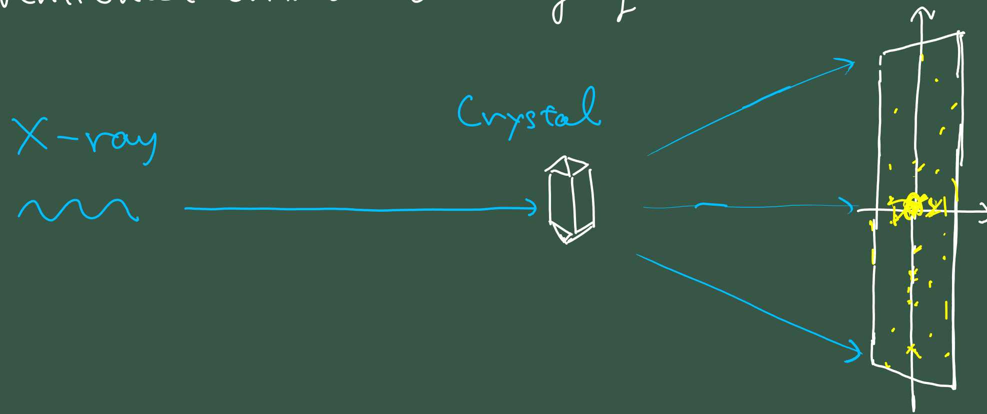
- Fourier transform & phase
- 3D structure of biomolecule
- X-ray Free Electron Laser (XFEL)
- X-ray diffraction of single biomolecule

Proposed method

- Phase retrieval
- Standard method (HIO)
- Proposed method (SPR)
- Numerical experiments

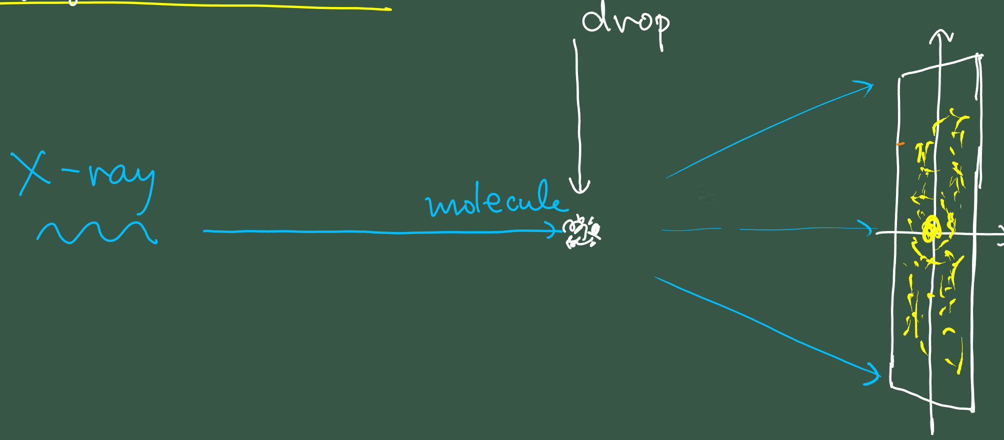
Single molecule diffraction with XFEL

Conventional diffraction imaging



- X-ray is not strong but repeat until we have good image

<u>Imaging with XFEL</u>



- hit the X-ray with free falling molecule
- <u>Experiment will start soon</u>

Protein structure identification with XFEL

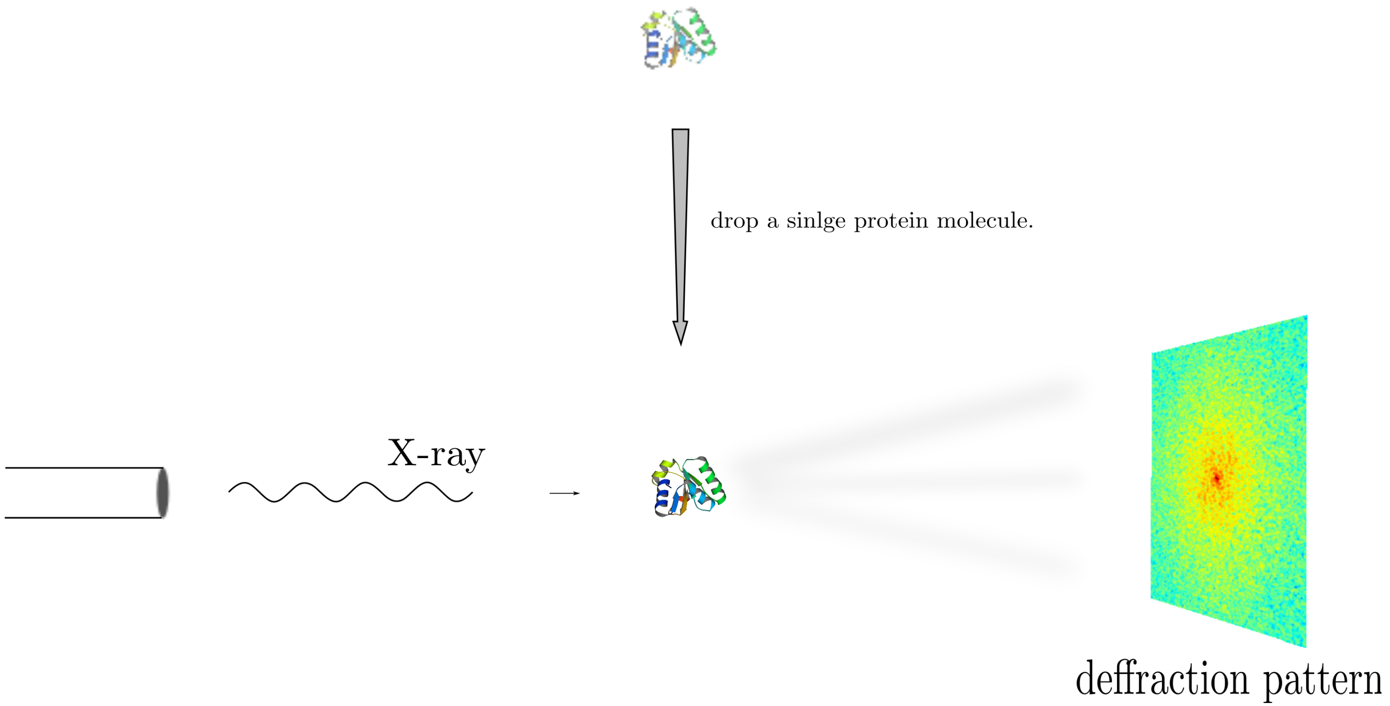


Figure: Protein diffraction pattern with XFEL.

Problems

- Hit rate
- Molecule size and flux strength
- Imaging from many angles. It is necessary to repeat measurement many times (10,000 ~ 100,000)
- Relative angles between images.
- Phase Retrieval

Protein structure identification with XFEL

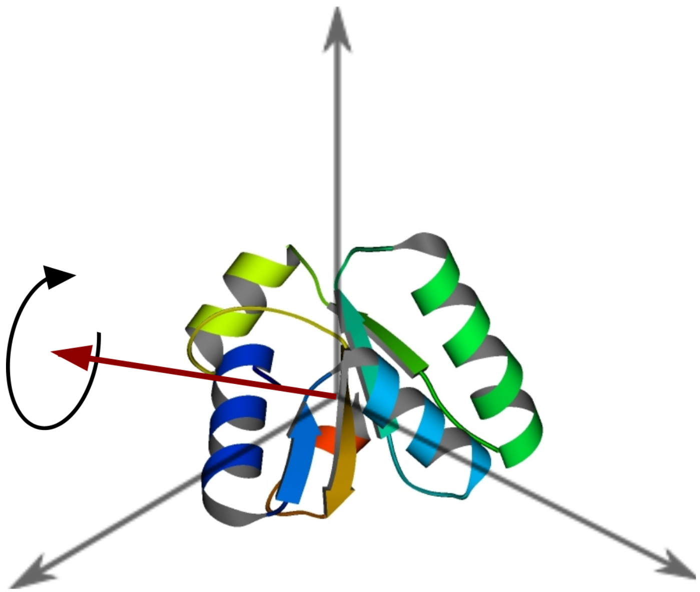


Figure: Angle retrieval problem.

Background

- Fourier transform & phase
- 3D structure of biomolecule
- X-ray Free Electron Laser (XFEL)
- X-ray diffraction of single biomolecule

Proposed method

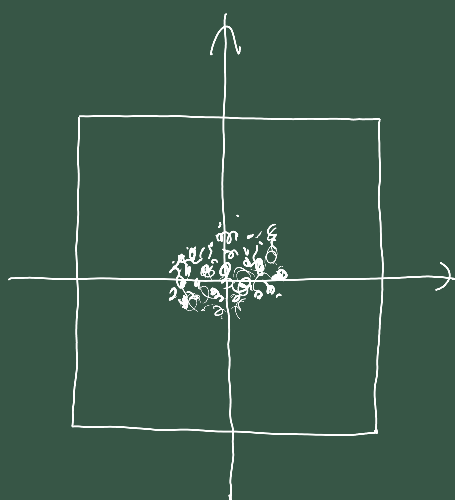
- Phase retrieval
- Standard method (HIO)
- Proposed method (SPR)
- Numerical experiments

ⓐ Phase Retrieval

Molecule $\xrightarrow{\text{X-ray imaging}}$ Diffraction image

Electron density f_{xy} $\xrightarrow[\text{Fourier trans.}]{\text{Fresnel diffraction}}$ Power Spectrum $|F_{uv}|^2$

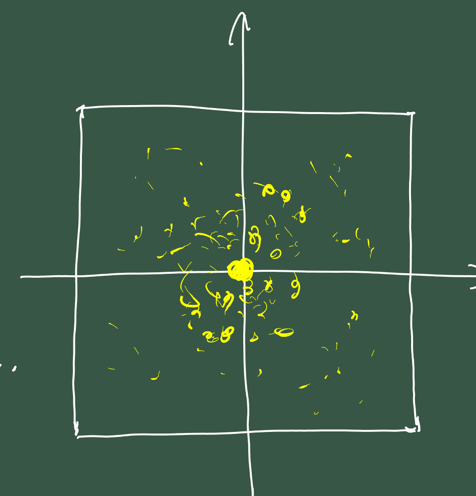
$$F = \mathcal{F}(f)$$



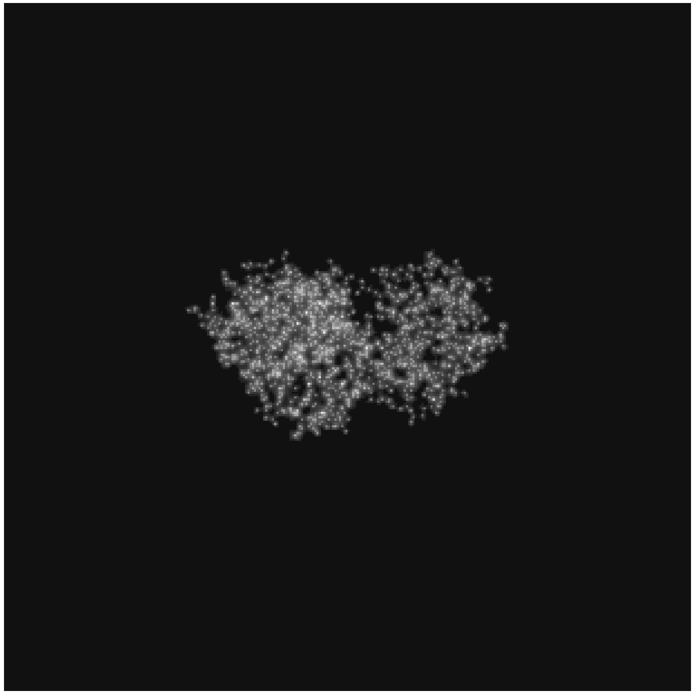
Inverse Fourier trans ?

$\longleftarrow$

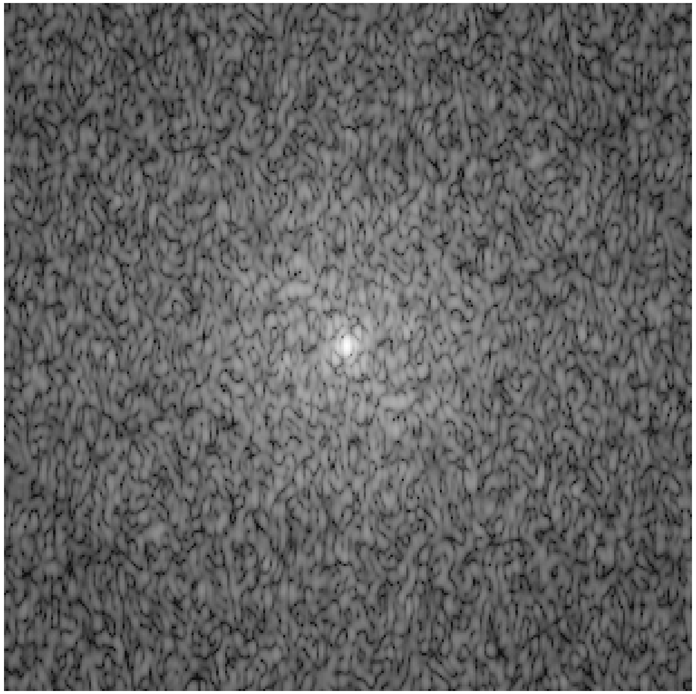
Phase is not known.



Protein structure identification with XFEL



(a) Electron density.



(b) Ideal diffraction pattern.

Figure: Electron density and ideal diffraction pattern.

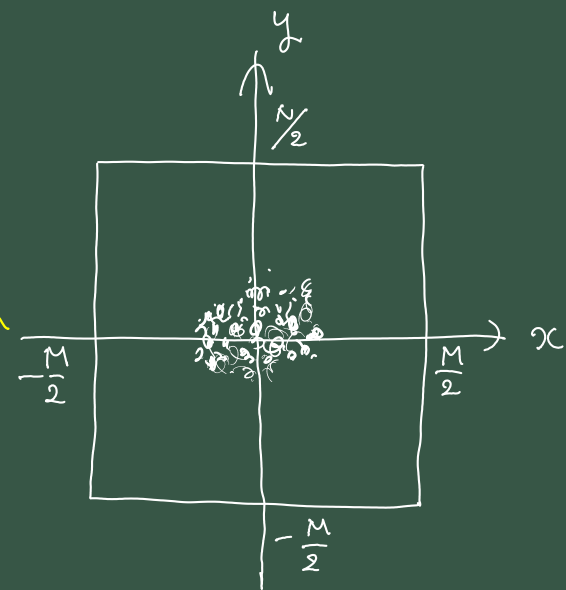
Electron density & Diffraction image

Electron density (3 dim → 2 dim. projection)

each pixel of electron density

$$\mathbb{f} = \{ f_{xy} \} \qquad -\frac{M}{2} \le x, y \le \frac{M}{2}$$

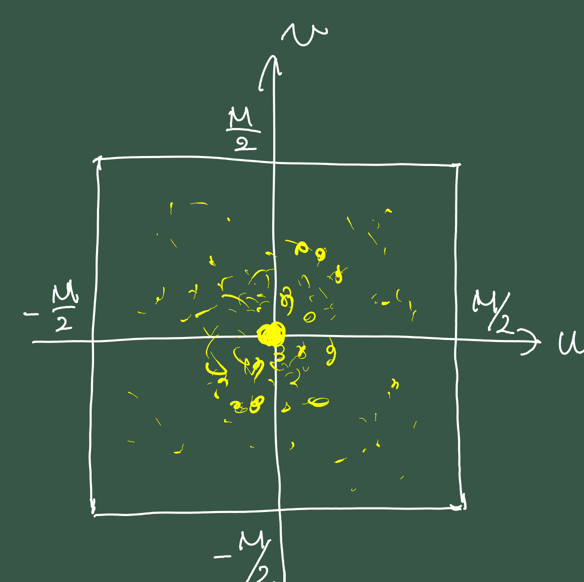
$$f_{xy} \ge 0 \ , \ f_{xy} \in \mathrm{Re}$$



Fourier Transform

$$\mathbb{F} = \{ F_{uv} \} \qquad -\frac{M}{2} \le u, v \le \frac{M}{2}$$

$$F_{uv} = \mathcal{F}(\mathbb{f}) = \frac{1}{M} \sum_{x,y} f_{xy} \exp\left(\frac{2\pi i (ux+vy)}{M} \right)$$



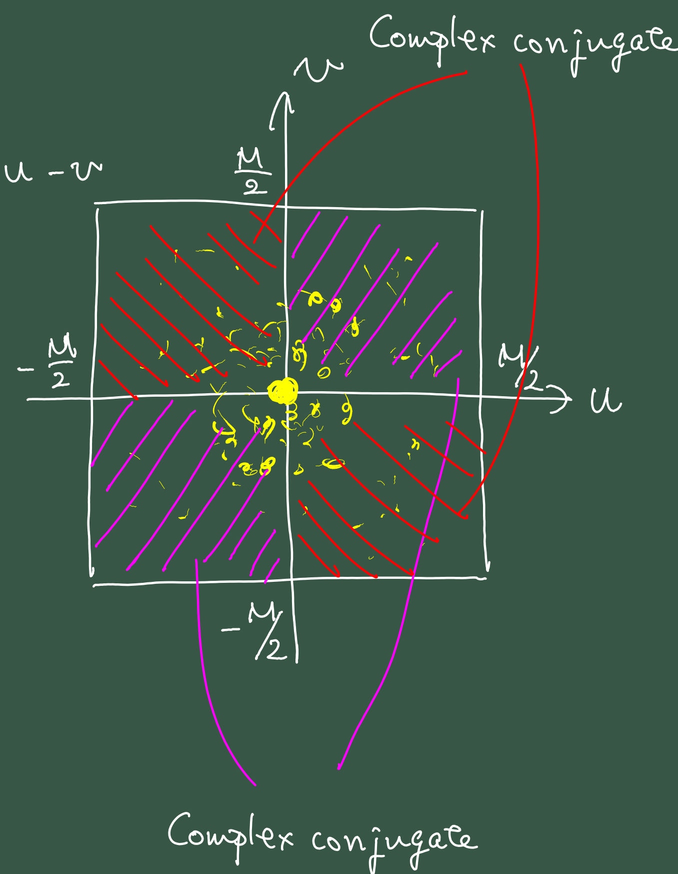
① f_{xy} is real number

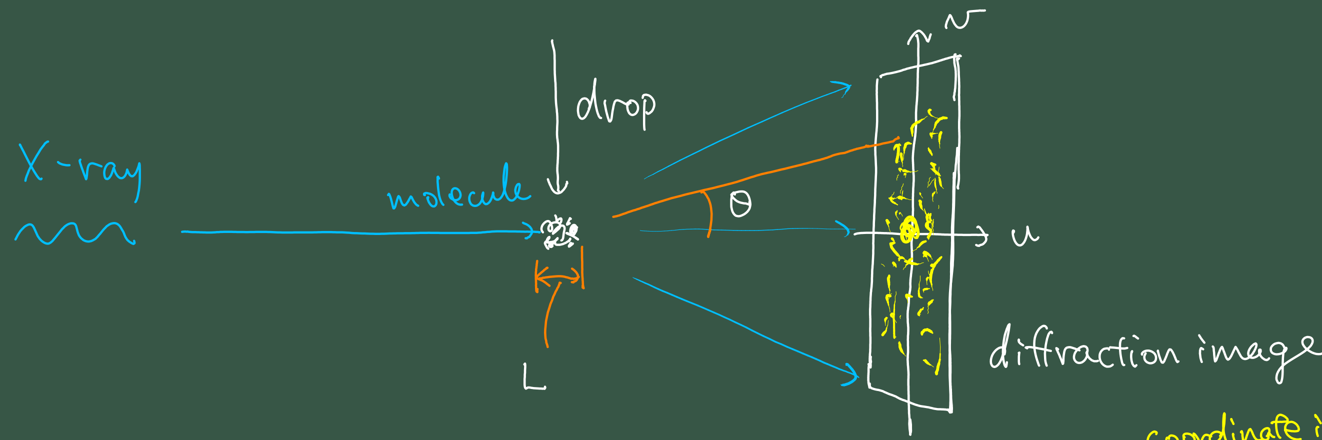
F_{uv} is the complex conjugate of F_{-u-v}

$$\because \; F_{uv} = \frac{1}{M} \sum_{x,y} f_{xy} \exp\left(\frac{2\pi i (ux+vy)}{M}\right)$$

$$\mathrm{Re}(F_{uv}) = \mathrm{Re}(F_{-u-v})$$

$$\mathrm{Im}(F_{uv}) = -\mathrm{Im}(F_{-u-v})$$





coordinate index of electron density

The relation between diffraction image S_{uv} and electron density f_{xy} is written as follows

pixel index of diffraction image

$$S_{uv} = \alpha \, |F_{uv}|^2 \cos^3\theta$$

$F_{uv} = (\mathcal{F}(f))_{uv}$: Fourier transform

$\alpha = I r_c^2 \left(\frac{\lambda}{2L}\right)^2$, I : X-ray flux (photons/pulse/mm^2)

λ : wave length

r_c : electron radius

θ, L : see the figure

$\mathbb{S}_{uv}$ corresponds to the power spectrum of f_{xy}

$\mathbb{f} \rightarrow \mathbb{S}$ is easy $\left(|(\mathcal{F}(\mathbb{f}))_{uv}|^2 \cos^3\theta \right)$

$\mathbb{S} \longrightarrow \mathbb{f}$ is difficult (Phase is not known)

$\mathbb{f}$: $M \times M$ real matrix

$\mathbb{S}$: $\frac{M \times M}{2}$ real matrix

) ill-posed proplem

- $\mathbb{S} \rightarrow \mathbb{f}$: Phase retrieval method

J. Fienup, Applied Optics (1982)

HIO (Hibrid Input Output) method is widely used.

Background

- Fourier transform & phase
- 3D structure of biomolecule
- X-ray Free Electron Laser (XFEL)
- X-ray diffraction of single biomolecule

Proposed method

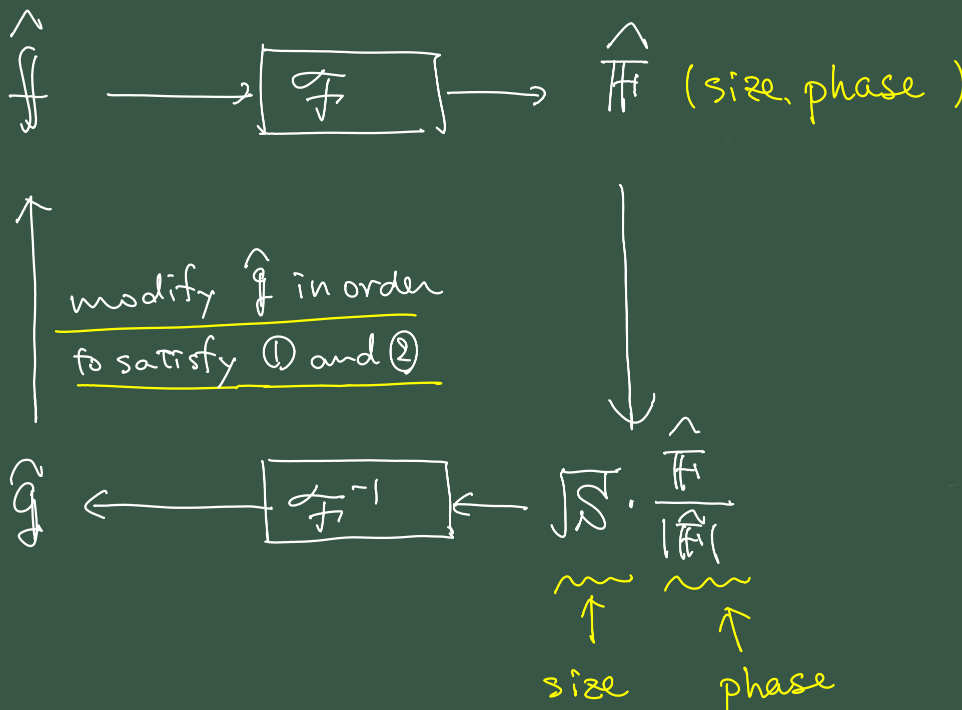
- Phase retrieval
- Standard method (HIO)
- Proposed method (SPR)
- Numerical experiments

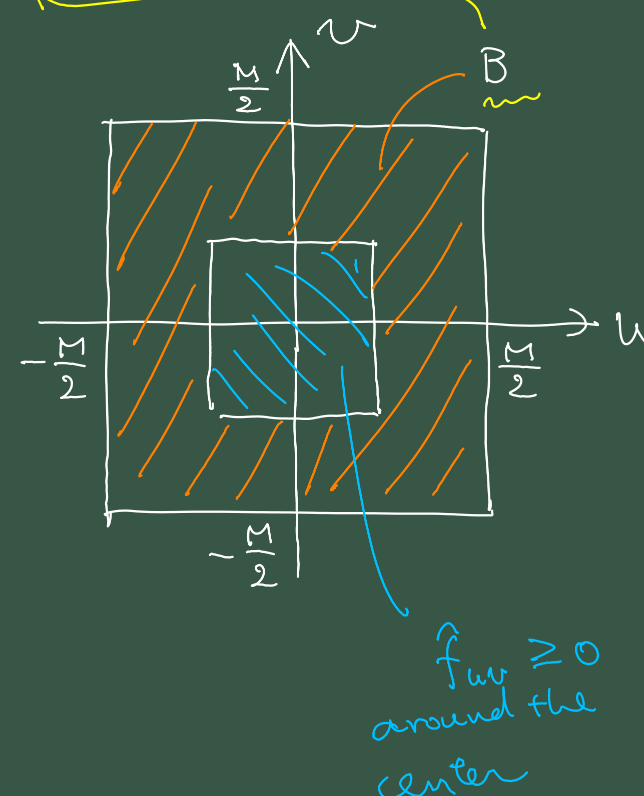
HIO method

Let $\hat{f}$ be the estimate of f. $\hat{f}$ satisfies the followings

① $\hat{f}_{xy} \geq 0$; non-negative

② $\hat{f}_{xy} = 0$ for $(x, y) \in B$; concentrate around center.





Background

- Fourier transform & phase
- 3D structure of biomolecule
- X-ray Free Electron Laser (XFEL)
- X-ray diffraction of single biomolecule

Proposed method

- Phase retrieval
- Standard method (HIO)
- Proposed method (SPR)
- Numerical experiments

From HIO to SPR (Sparce Phase Retrieval)

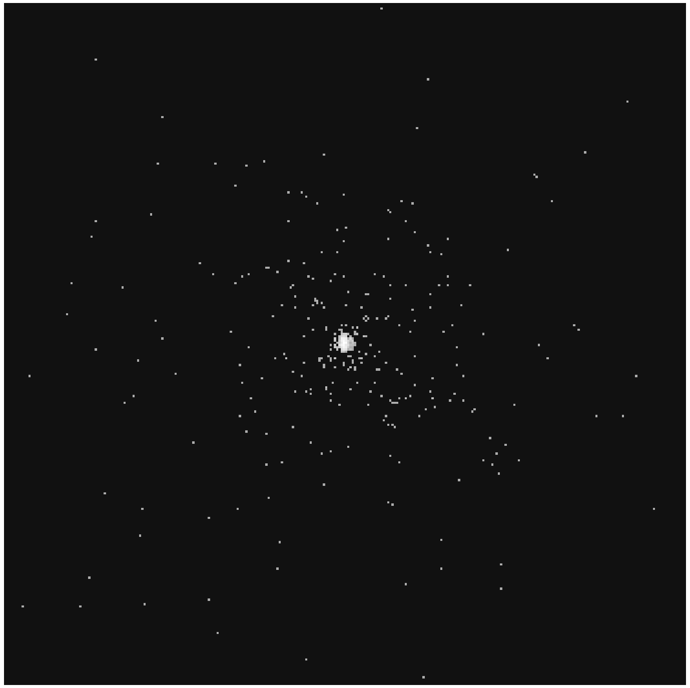
- HIO works wel for noiseless data.
- For a large particle, diffraction patterns are strong and HIO works well.
- The target of XFEL is small particles and HIO will not work well.

$\Downarrow$

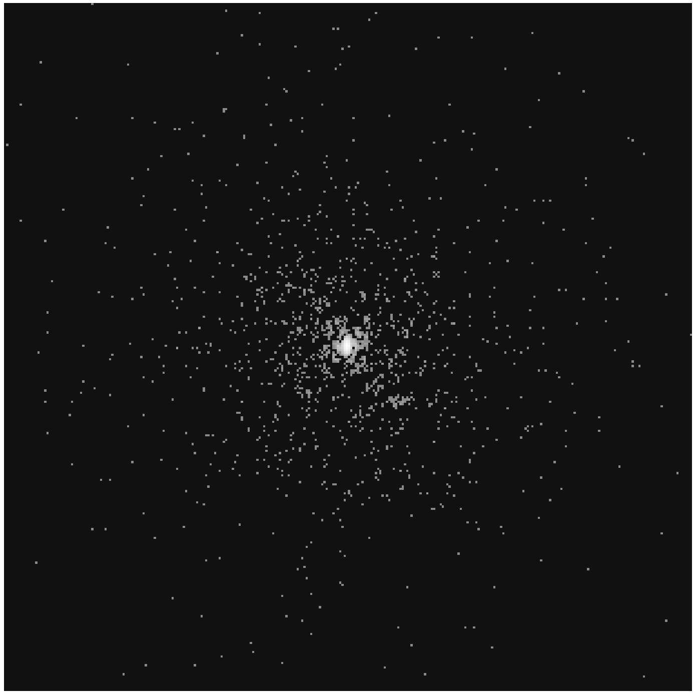
New method is needed.

- Assume f is <u>sparse</u>
- Make noise model and use the sparse prior. Estimate base on Bayesian statistics.

Protein structure identification with XFEL

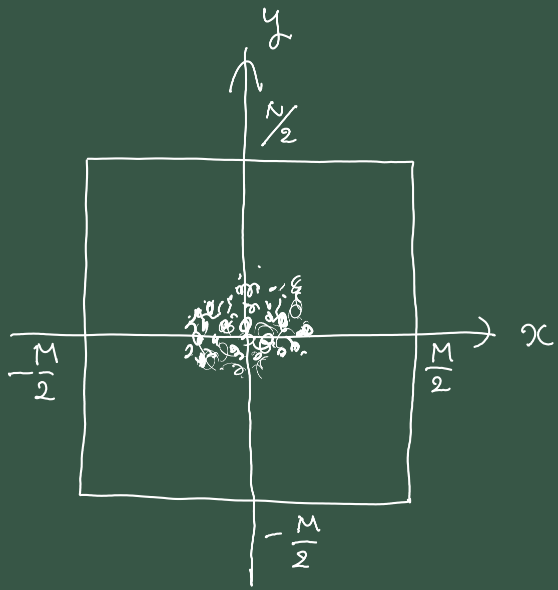


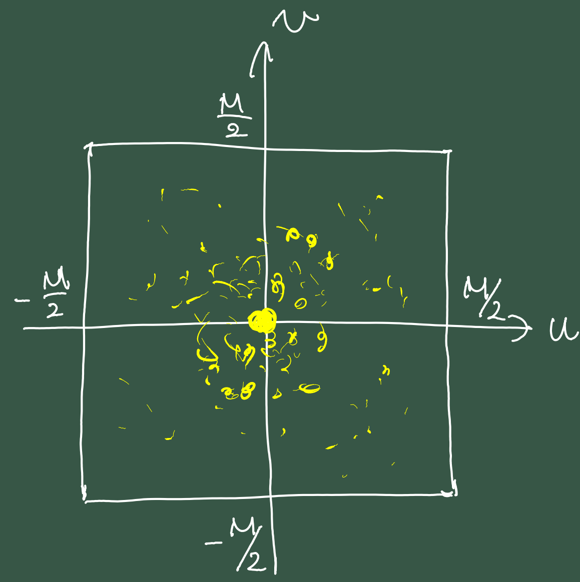
(a) X-ray fluxes $1.0 \times 10^{21}(\mathrm{photons/pulse/mm^2})$.

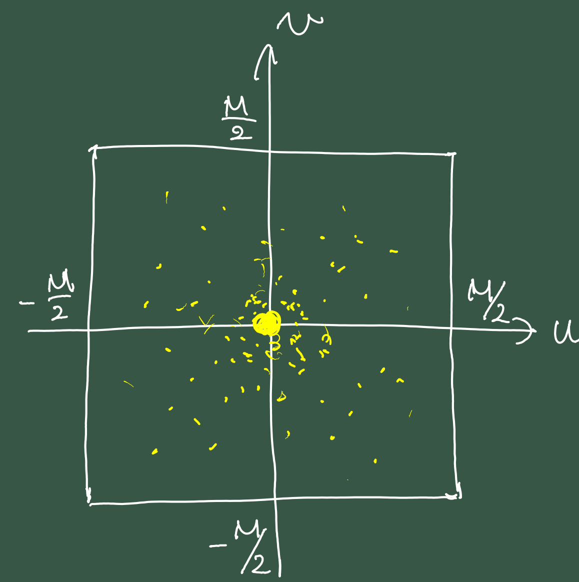


(b) X-ray fluxes $5.0 \times 10^{21}(\mathrm{photons/pulse/mm^2})$.

Figure: Diffraction patterns in experimental situation.







Electron density

$f = \{f_{xy}\}$

Ideal diffraction pattern

$S = \{S_{uv}\}$

$S_{uv} = |F_{uv}|^2 \cos^2\theta$

$F_{uv} = (\mathcal{F}(f))_{uv}$

Measurement.

$N = \{N_{uv}\}$

The number of photons at each pixel.

What is the relation between S_{uv} and N_{uv}?

Measurement of each pixel is the number of photons which is a integer. Denoted as N_{uv}

N_{uv} : Nonnegative integer $\quad -\frac{M}{2} \le u, v \le \frac{M}{2}$.

N_{uv} follows a Poisson distribution whose expected value is S_{uv}

$$p(N_{uv} \mid S_{uv}) = \frac{S_{uv}^{N_{uv}} \exp(-S_{uv})}{N_{uv}!}$$

$$\boxed{p(\mathbb{N} \mid \mathbb{f}) = \prod_{uv} \frac{\left(|F_{uv}|^2 C_{uv}\right)^{N_{uv}} \exp\left(-|F_{uv}|^2 C_{uv}\right)}{N_{uv}!}}$$

($\underline{C_{uv} = \cos^3\theta}$ and $S_{uv} = \alpha |F_{uv}|^2 C_{uv}$ where we set $\underline{\alpha = 1}$)

$p(\mathbb{N} \mid \mathbb{f})$ is modelled. How to estimate $\mathbb{f}$.

$\Downarrow$

Statistical Estimation Problem

@ Maximum Likelihood Estimate (MLE)

Compute $\mathbb{f}$ which maximizes $p(\mathbb{N} \mid \mathbb{f})$

$\Longrightarrow$ Ill posed problem (phase)

@ Bayesian Statistics

Assume the prior of $\mathbb{f}$ as $\pi(\mathbb{f})$

$$\pi(\mathbb{f}) \cdot p(\mathbb{N} \mid \mathbb{f}) = p(\mathbb{f}, \mathbb{N}) \quad \text{-- Joint dist}$$

$$p(\mathbb{f} \mid \mathbb{N}) = \frac{p(\mathbb{f}, \mathbb{N})}{\int p(\mathbb{f}, \mathbb{N})\, d\mathbb{f}}$$

posterior prob.

$\Longrightarrow$ Maximize

MAP estimate

$$\underbrace{p(\mathbf{f} \mid \mathbf{N})}_{\text{Posterior}} \propto \underbrace{p(\mathbf{N} \mid \mathbf{f})}_{\substack{\text{Poisson model} \\ \text{Likelihood}}} \cdot \underbrace{\pi(\mathbf{f})}_{\substack{\text{Sparsity} \\ \text{Prior dist}}} \quad (\text{Bayes Theorem})$$

MAP (Maximum a Posterior) estimate $\hat{\mathbf{f}}$ maximize above $p(\mathbf{f} \mid \mathbf{N})$

- maximize $p(\mathbf{N} \mid \mathbf{f}) \cdot \pi(\mathbf{f}) \Longrightarrow$ maximize $\log p(\mathbf{N} \mid \mathbf{f})\, \pi(\mathbf{f})$

- $\log p(\mathbf{N} \mid \mathbf{f}) + \log \pi(\mathbf{f})$

$$\underbrace{\sum_{uv} \left(N_{uv} \ln |F_{uv}|^2 - |F_{uv}|^2 C_{uv} \right)}_{\text{likelihood}} + \underbrace{\log \pi(\mathbf{f})}_{\text{Prior}}$$

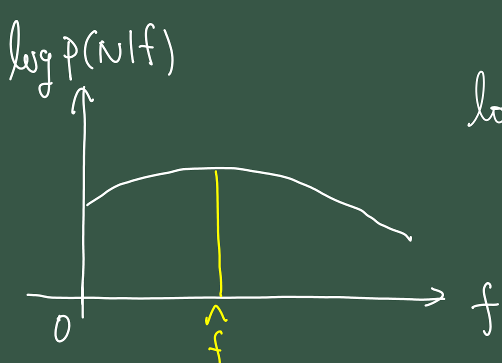
How to define $\pi(f)$?

- $\pi(f)$ reflects the prior knowledge of f.
- f has a lot of 0 components. $\Longrightarrow$ sparse

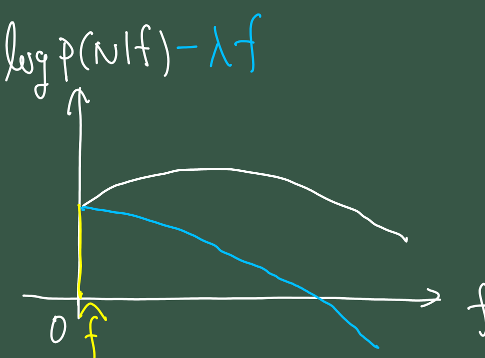
$$\pi(f) = \lambda \exp(-\lambda f) \qquad (f \geq 0)$$

If we use above $\pi(f)$, a lot of f_{xy} become 0.

(LASSO: statistics 1996
Compressed Sensing: Inform. Th. 2000 ~)



$$\log p(N|f) \underbrace{- \lambda f}_{(\log \pi(f))} \quad \Longrightarrow$$



Define prior $\pi(\mathbb{f})$ as follows

$$\pi(\mathbb{f}) = \rho_{xy} \exp\left(-\rho_{xy} f_{xy}\right), \quad f_{xy} \geq 0.$$

$$\rho_{xy} = \mu \cdot w_{xy} = \mu \cdot \frac{2}{M^2}\left(x^2+y^2\right)$$

$\rho_{xy} \rightarrow$ large means f_{xy} is more likely to be 0.

μ is a hyper parameter

Collect $\mathbb{f}$ related terms from $\log p(\mathbb{f} \mid \mathbb{N})$,

$$l(\mathbb{f} \mid \mathbb{N}) = \overbrace{\sum_{uv}\left(N_{uv} \ln |F_{uv}|^2 - |F_{uv}|^2 C_{uv}\right)}^{\text{likelihood term}} \overbrace{- \mu \sum_{xy} w_{xy} f_{xy}}^{\text{prior term}}$$

$$\boxed{\hat{\mathbb{f}} = \arg\max_{\mathbb{f}} l(\mathbb{f} \mid \mathbb{N}) \quad \text{is the problem}}.$$

SPR

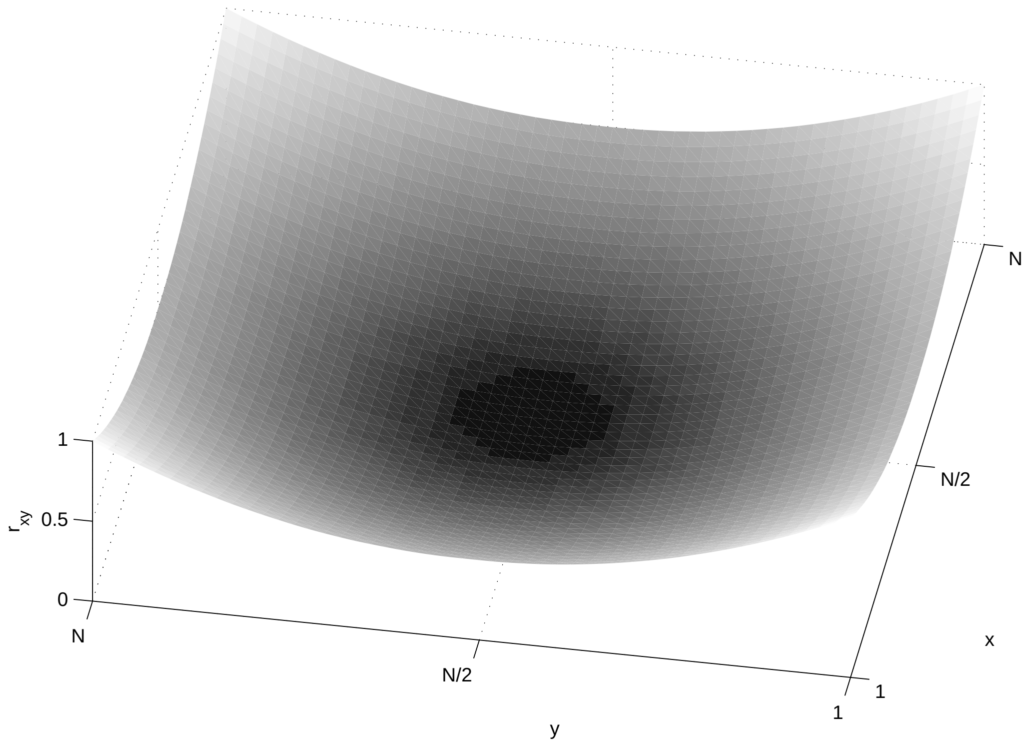


Figure: Sparsity prior w_{xy}.

$$l(f|N) = \overbrace{\sum_{uv}\left(N_{uv}\ln|F_{uv}|^2 - |F_{uv}|^2 C_{uv}\right)}^{\text{Likelihood term}} - \overbrace{\mu\sum_{xy} w_{xy} f_{xy}}^{\text{prior}}$$

frequency domain

real domain

mixed

Optimizing with a gradient-based method.

Phase retrival is an ill-posed problem. It is necessary to use additional information

HIO method ---- active region

SPR method ----- sparsity

準備

$$\frac{\partial |F_{uv}|^2}{\partial f_{xy}} = \frac{2}{M} \mathrm{Re}\left(F_{uv} \exp\left(-\frac{2\pi i (ux+vy)}{M}\right)\right)$$

Inverse Fourier trans. $\mathcal{F}^{-1}(\mathbb{F}) = \frac{1}{M} \sum_{uv} F_{uv} \exp\left(-\frac{2\pi i (ux+vy)}{M}\right)$

$$\frac{\partial \ell(\mathbb{f} \mid \mathbb{N})}{\partial f_{xy}} = 2\,\mathrm{Re}\left(\mathcal{F}^{-1}(g(\mathbb{F};\mathbb{N}))\right)_{xy} - \mu w_{xy}$$

$$,\quad g_{uv}(\mathbb{F};\mathbb{N}) = \left(\frac{N_{uv}}{|F_{uv}|^2} - C_{uv}\right) F_{uv}$$

$$\boxed{f_{xy}^{t+1} = \max\left(0,\ f_{xy}^{t} + \eta_t \frac{\partial \ell(\mathbb{f}^t \mid \mathbb{N})}{\partial f_{xy}^t}\right)}$$

Each $\mathbb{f}^t \to \mathbb{f}^{t+1}$ needs a Fourier & inverse Fourier trans.

η_t controls the step size. A simple line search speeds up the convergence.

Background

- Fourier transform & phase
- 3D structure of biomolecule
- X-ray Free Electron Laser (XFEL)
- X-ray diffraction of single biomolecule

Proposed method

- Phase retrieval
- Standard method (HIO)
- Proposed method (SPR)
- Numerical experiments

Numerical experiments.

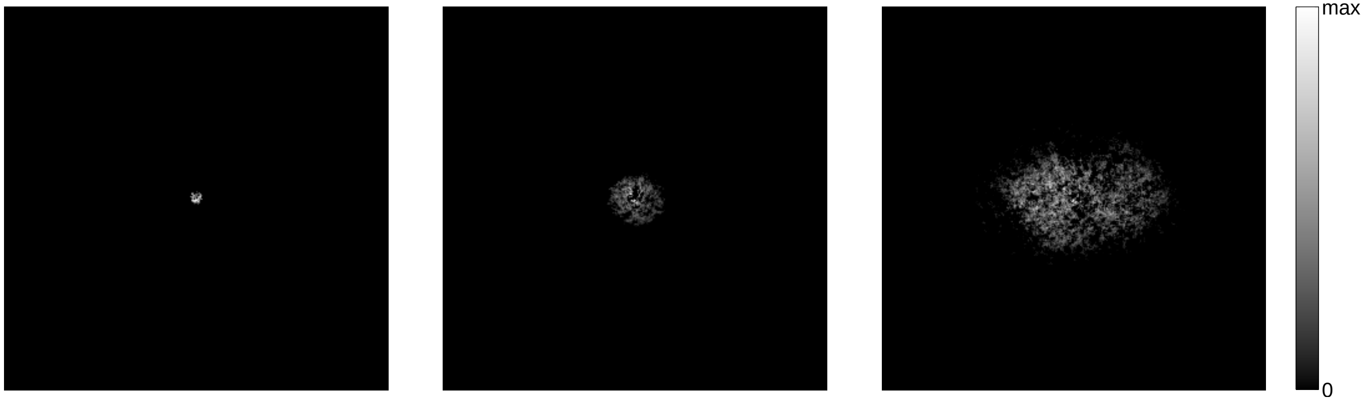
When μ is large, many f_{xy} become 0 and the optimization is easy.

Starting with a large μ, shrink it. For each μ, compute $\hat{f}$ and the following error(μ). the μ which minimizes the error is the optimal μ.

$$\mathrm{error}(\mu) = \frac{\sum \left(|F_{uv}| \, C_{uv}^{1/2} - N_{uv}^{1/2} \right)^2}{\sum_{u'v'} N_{u'v'}}$$

(widely used error in optics)

SPR



(a) Reconstructed electron density with $\mu = 10000$.

(b) Reconstructed electron density with $\mu = 100$.

(c) Reconstructed electron density with $\mu = 1$.

Figure: SPR results with different μ for true diffraction data.

SPR

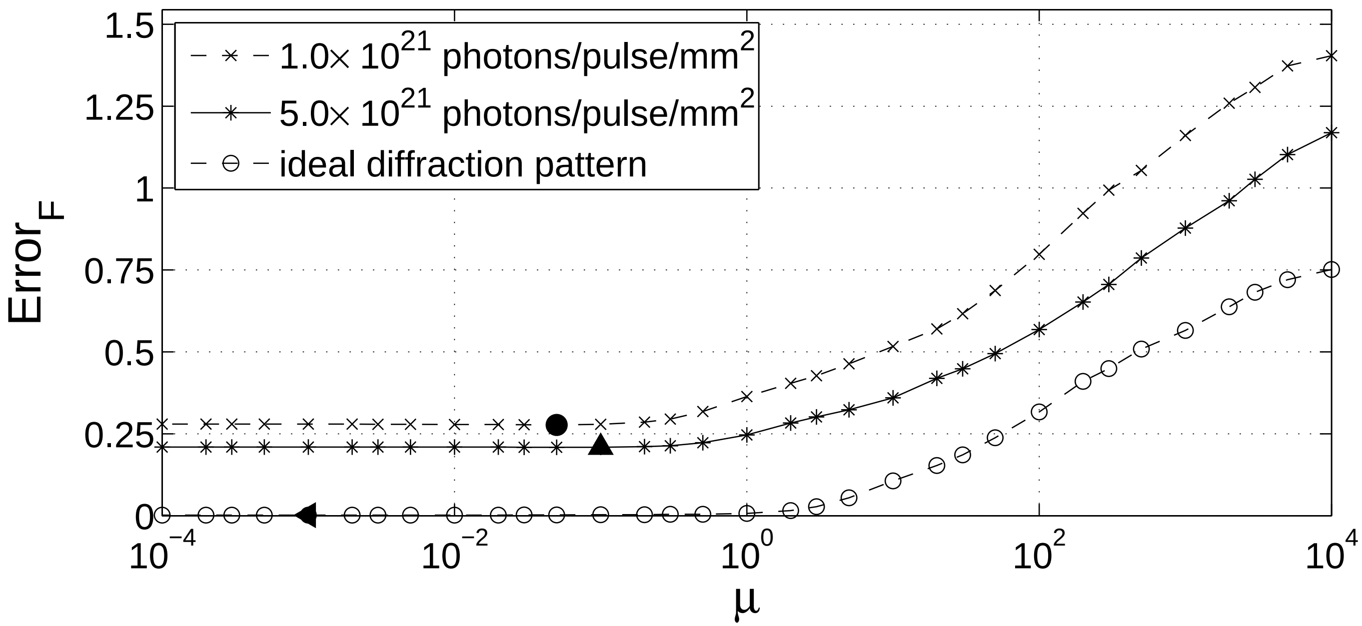
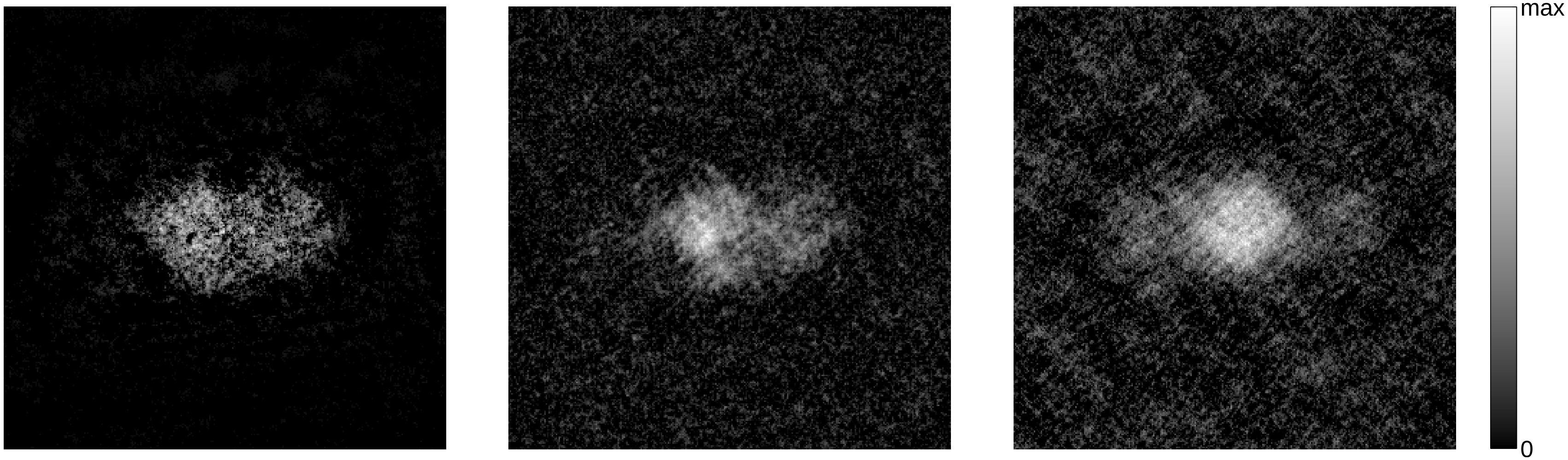


Figure: Error and μ.

SPR



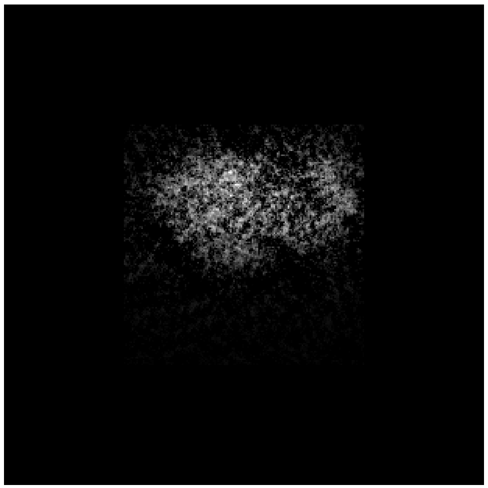
(a) Reconstruction from diffraction image Fig.2b by the SPR method with $\mu = 0.001$. Error$_F$ is 1.60×10^{-3}.

(b) Reconstruction from diffraction image Fig.2c by the SPR method with $\mu = 0.1$. Error$_F$ is 0.209.

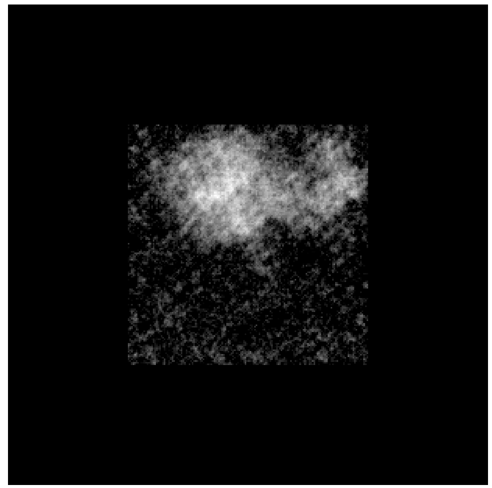
(c) Reconstruction from diffraction image Fig.2d by the SPR method with $\mu = 0.05$. Error$_F$ is 0.277.

Figure: Reconstruction with SPR.

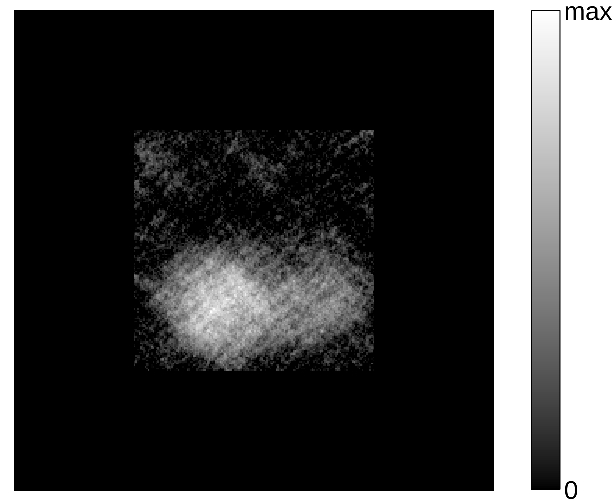
HIO



(a) Reconstruction from diffraction image Fig.2b by the HIO method. Error_F is 3.30×10^{-3}.



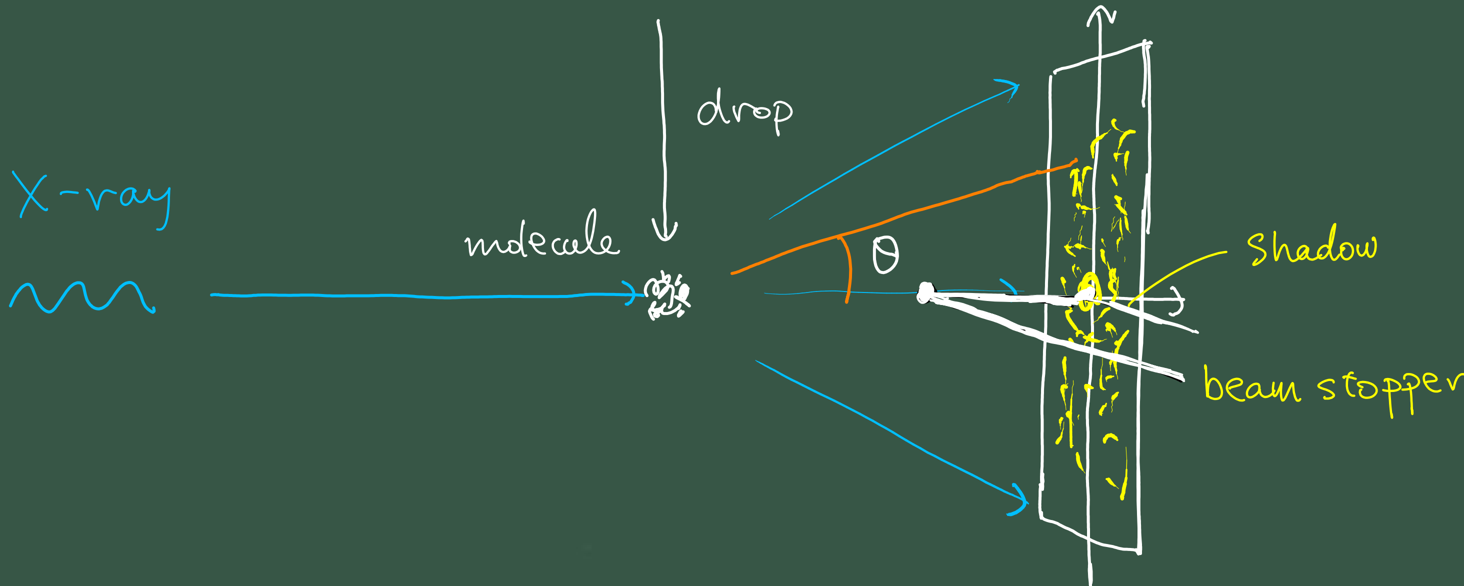
(b) Reconstruction from diffraction image Fig.2c by the HIO method. Error_F is 0.220.



(c) Reconstruction from diffraction image Fig.2d by the HIO method. Error_F is 0.291.

Figure: Reconstruction with HIO.

Another Problem



There is a beam-stopper around the center.

308×308 diffraction image of Lysozyme

1 center pixel	$\longrightarrow$ 5%	photons are blocked
3×3 "	$\longrightarrow$ 35%	
5×5 "	$\longrightarrow$ 54%	

$$l(\mathbb{f}\mid\mathbb{N}) = \underbrace{\sum_{uv\in A}\left(N_{uv}\ln|F_{uv}|^2 - |F_{uv}|^2 C_{uv}\right)}_{\text{Likelihood}} - \underbrace{\mu\sum_{xy} W_{xy} f_{xy}}_{\text{prior}}$$

A: visible pixel set.

- The same algorithm can be used.
- More robust against photons loss than the HIO method.

SPR without 1 center pixel

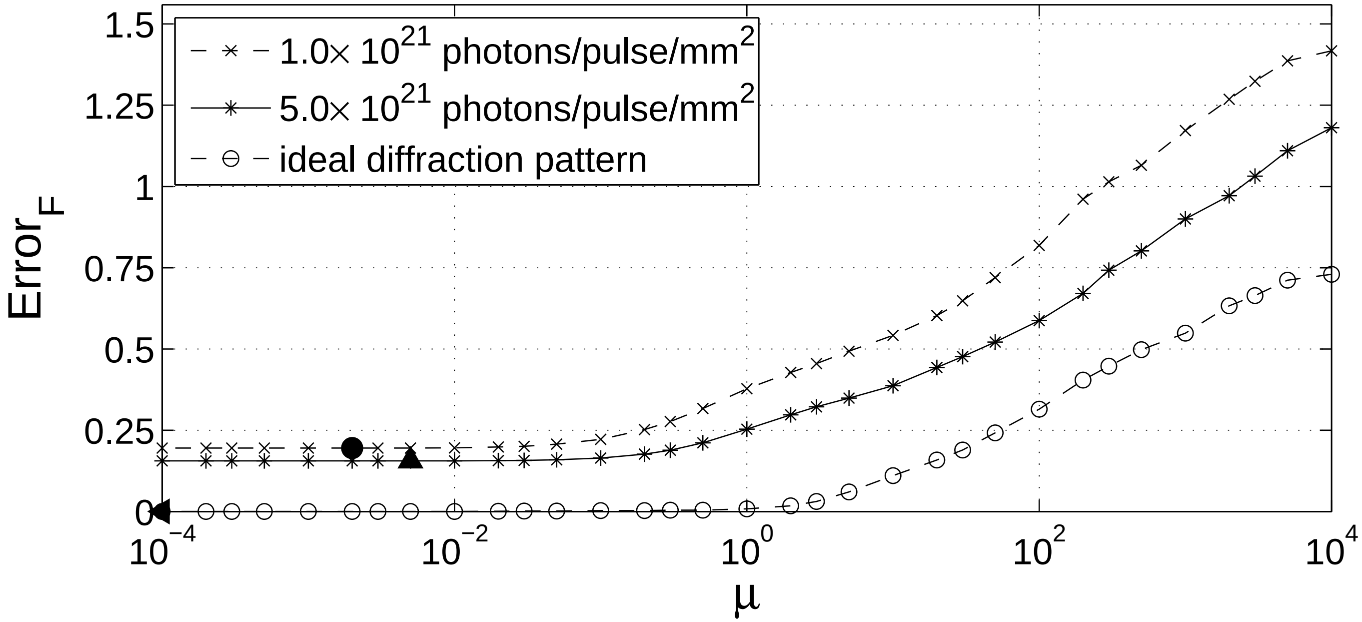
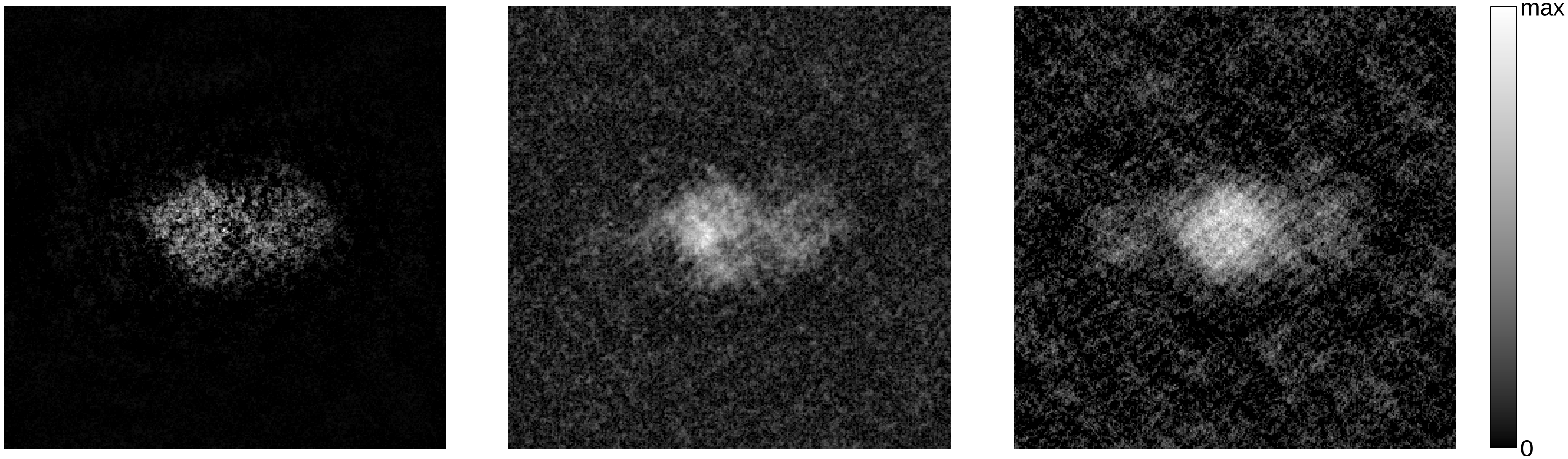


Figure: Error and μ.

SPR without 1 center pixel



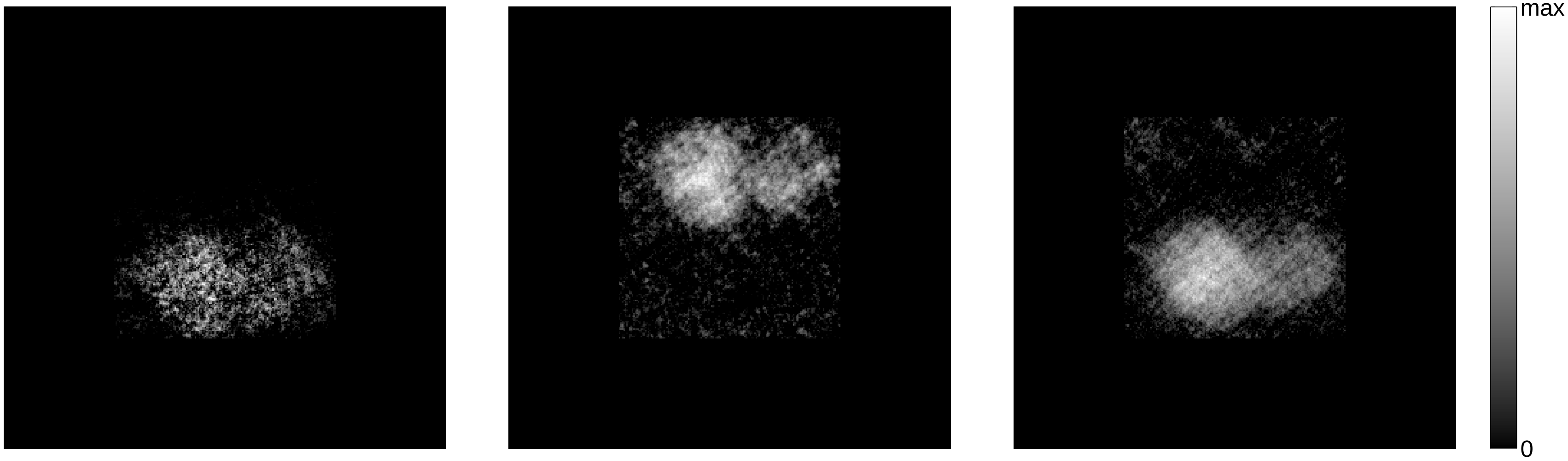
(a) Reconstruction from diffraction image Fig.2b without the central pixel by the SPR method with $\mu = 0.0001$. Error_F is 1.78×10^{-6}.

(b) Reconstruction from diffraction image Fig.2c without the central pixel by the SPR method with $\mu = 0.002$. Error_F is 0.156.

(c) Reconstruction from diffraction image Fig.2d without the central pixel by the SPR method with $\mu = 0.005$. Error_F is 0.195.

Figure: Reconstruction with SPR.

HIO without 1 center pixel



(a) Reconstruction from diffraction image Fig.2b without the central pixel by the HIO method. Error_F is 1.01×10^{-2}.

(b) Reconstruction from diffraction image Fig.2c without the central pixel by the HIO method. Error_F is 0.245.

(c) Reconstruction from diffraction image Fig.2d without the central pixel by the HIO method. Error_F is 0.318.

Figure: Reconstruction with HIO.

SPR without 3×3 center pixels

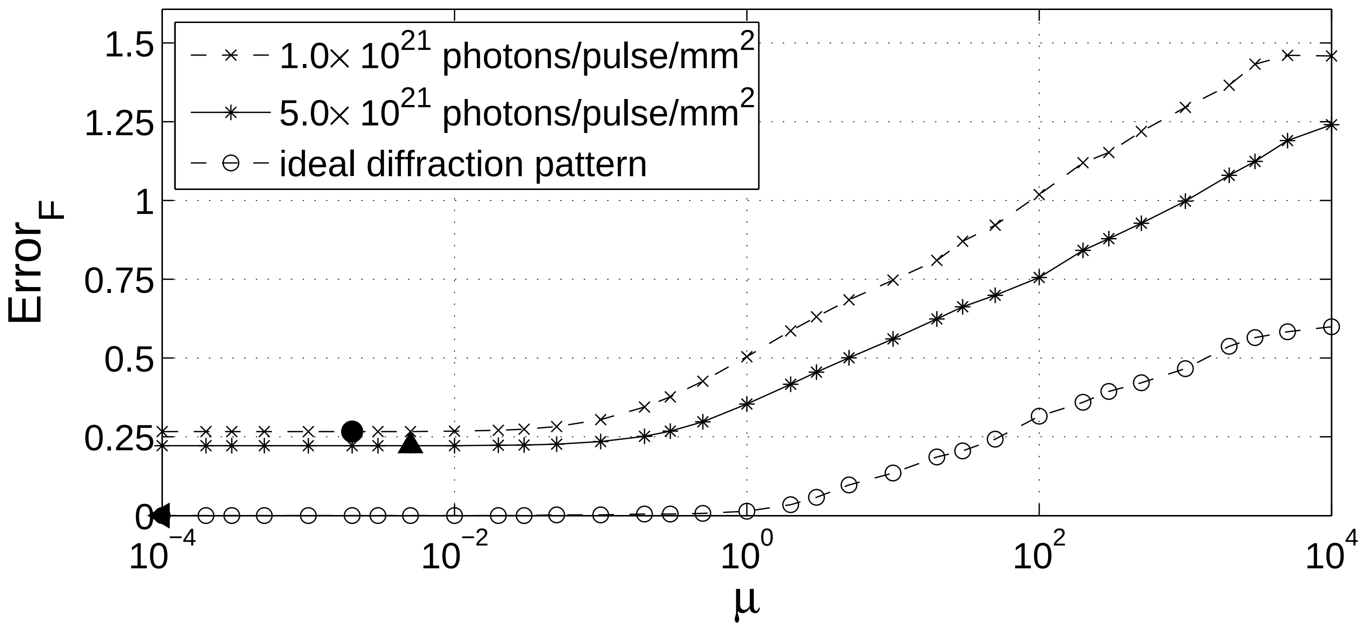
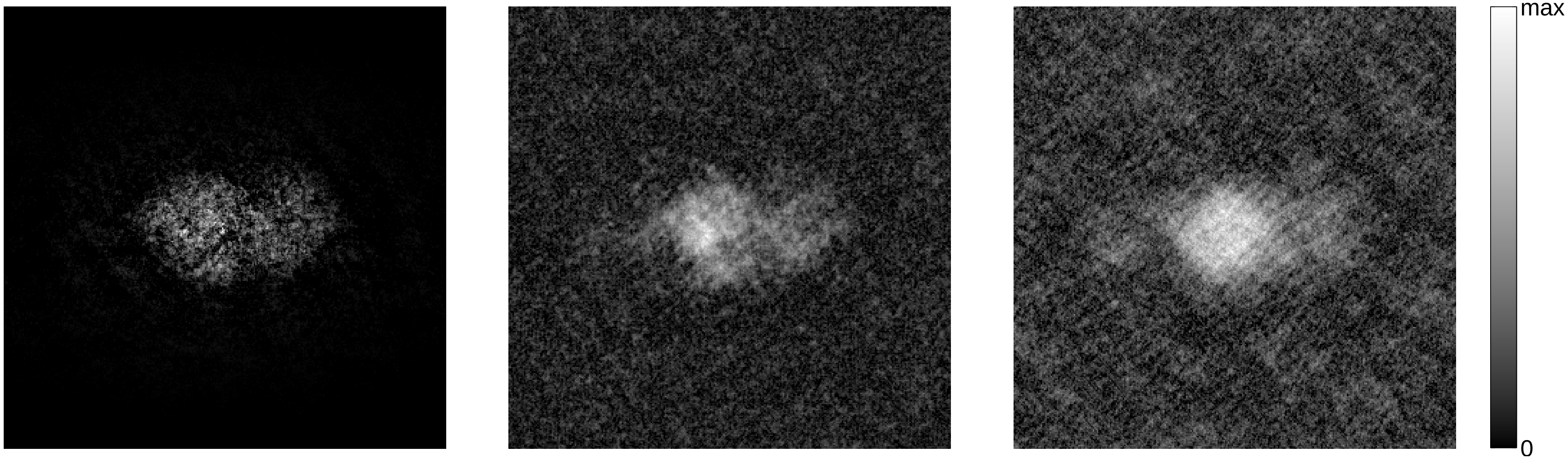


Figure: Error and μ.

SPR without 3×3 center pixels



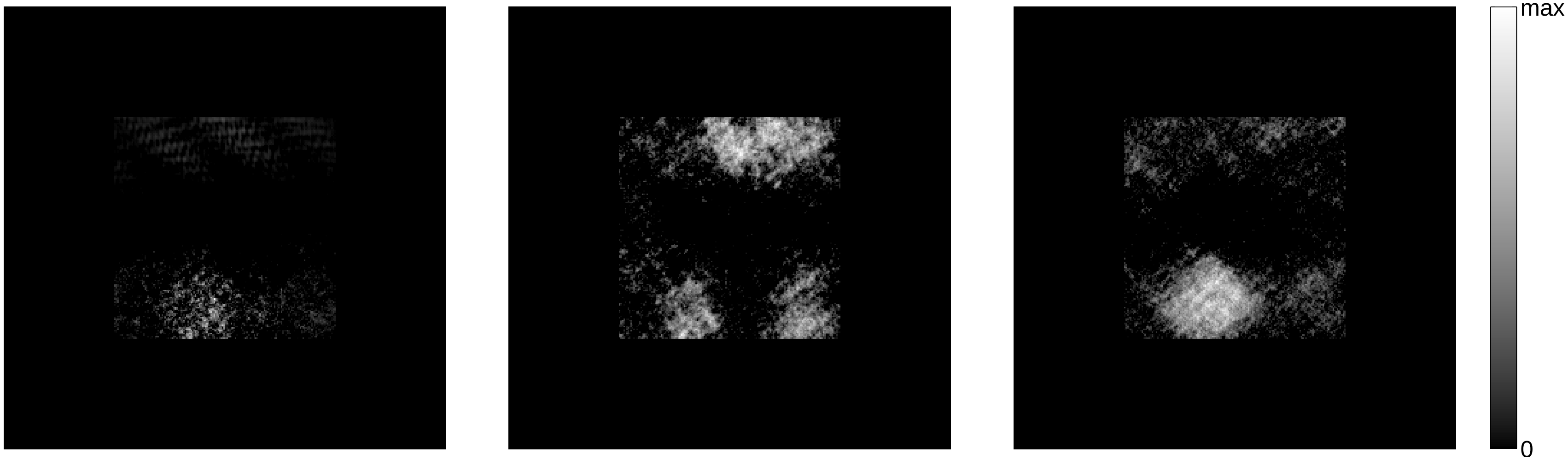
(a) Reconstruction from diffraction image Fig.2b without the central 3×3 pixels by the SPR method with $\mu = 0.0001$. Error_F is 2.34×10^{-6}.

(b) Reconstruction from diffraction image Fig.2c without the central 3×3 pixels by the SPR method with $\mu = 0.002$. Error_F is 0.222.

(c) Reconstruction from diffraction image Fig.2d without the central 3×3 pixels by the SPR method with $\mu = 0.005$. Error_F is 0.267.

Figure: Reconstruction with SPR.

SPR without 3×3 center pixels



(a) Reconstruction from diffraction image Fig.2b without the central 3×3 pixels by the HIO method. Error_F is 0.128.

(b) Reconstruction from diffraction image Fig.2c without the central 3×3 pixels by the HIO method. Error_F is 0.487.

(c) Reconstruction from diffraction image Fig.2d without the central 3×3 pixels by the HIO method. Error_F is 0.557.

Figure: Reconstruction with HIO.

Conclusion

- Proposed a new SPR method for phase retrieval
  - Based on sparsity of electron density.
  - Works well with small number of photons
  - Works well even some center pixels are blocked.
  - SPR method can be used instead of HIO.

Compton Camera Imaging

joint work with

H. Odaka[*], M. Uemura[+]

T. Takahashi[*], S. Watanabe[*]

& T. Takeda[*]

[*] JAXA

[+] Hiroshima Univ.

- Compton camera

- Compton camera imaging
  - measurement process.
  - estimation method
  - improvement

- Conclusion

Compton Camera

Visualize γ-rays

Wide range of applications

- Astronomy (ASTRO-H)
- Medical application
- Visualize the contamination of soil (Fukushima)

Astro-H project.

smartphone with a radiation detector

LONGFORM VIDEO REVIEWS TECH SCIENCE CULTURE DESIGN BUSINESS US & WORLD FORUMS

LOG IN OR JOIN

9 COMMENTS

SoftBank Pantone 5 107SH hands-on: radiation detection comes to Android

By Sam Byford on May 29, 2012 02:24 am Email @345triangle

DON'T MISS STORIES *FOLLOW THE VERGE* Like 243k Follow 335K followers

PART OF THIS STORYSTREAM 1

16 UPDATES TO

Japan's summer 2012 phone lineup

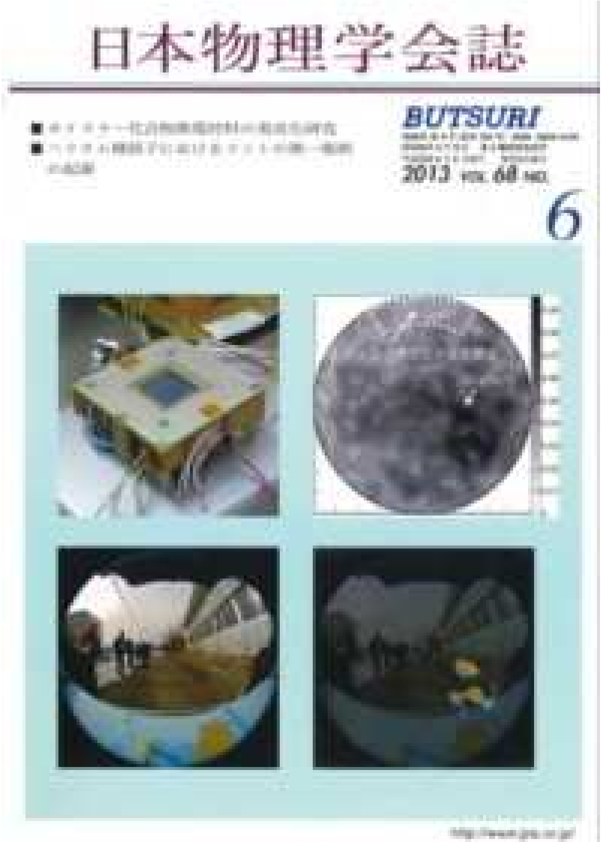
JUN 19 Frog redesigns the Android user experience with Feel_UX

MAY 29 SoftBank's summer 2012 Android lineup: better signal, faster downloads

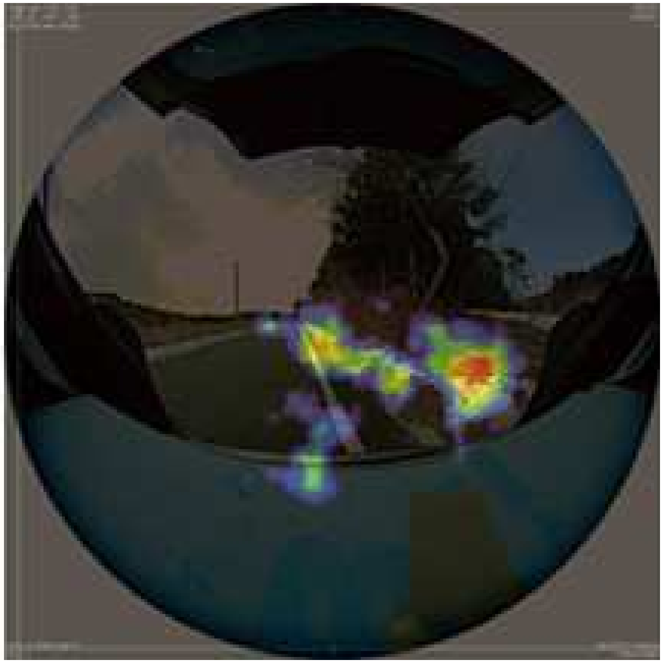
MAY 29 'Fastest ever' 110Mbps SoftBank 4G mobile router out in Japan this fall

SoftBank's Pantone 5 107SH will make headlines in the global press for one reason and

福島での応用(JAXA, 日本物理学会の HP より).



福島での応用(JAXA の HP より).



γ-rays: Electromagnetic radiation with wavelength ($< 10\,\mathrm{pm}$)

- Difficult to detect.

- Measurement techniques

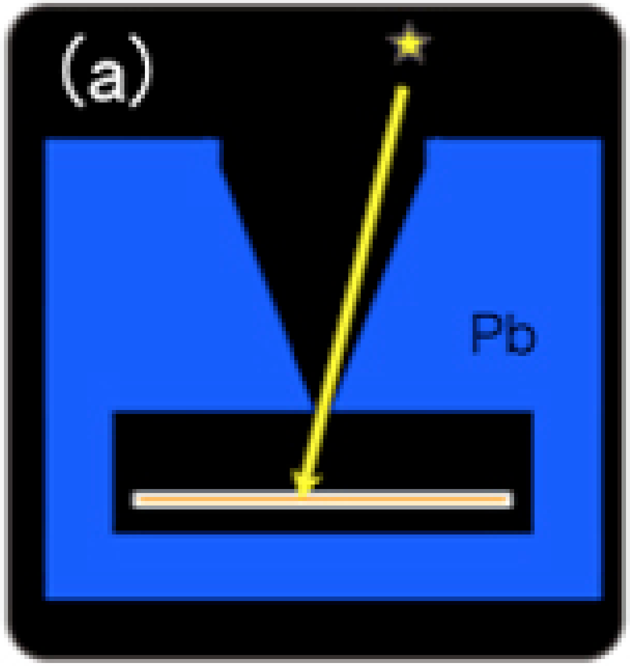
  - Geiger-counter
  - Scintillation detector

  Cannot measure direction of arrival

  - Compton camera ---- use Compton scattering

    can be used for imaging

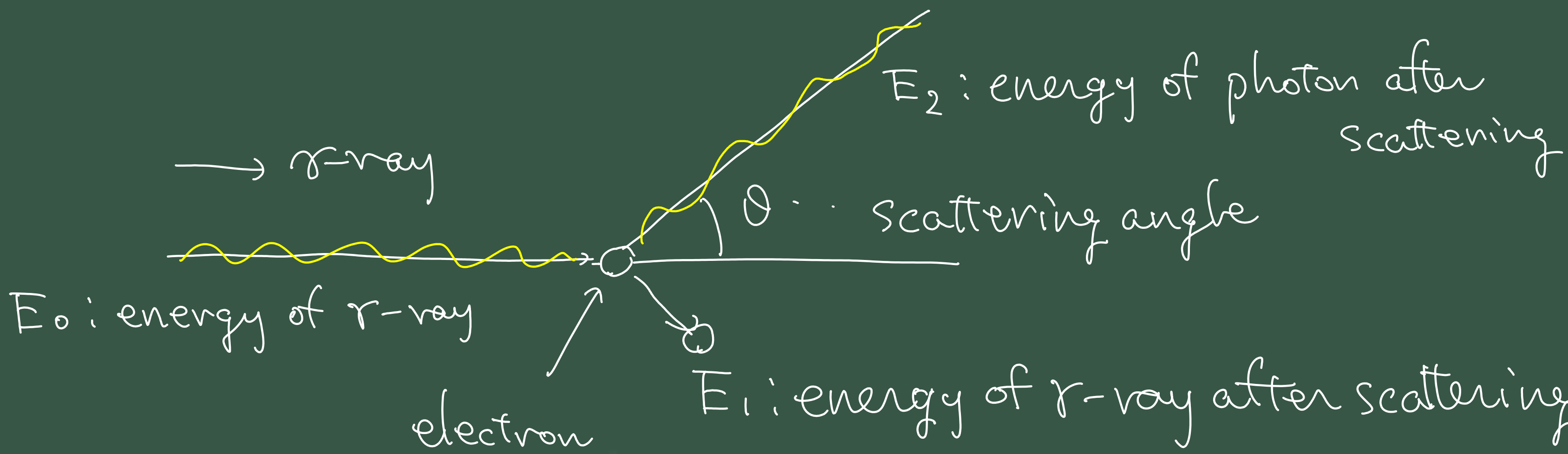
gamma-ray camera as a pinhole camera



- Compton camera
- Compton camera imaging
  - measurement process.
  - estimation method
  - improvement
- Conclusion

Compton camera imaging

Compton scattering

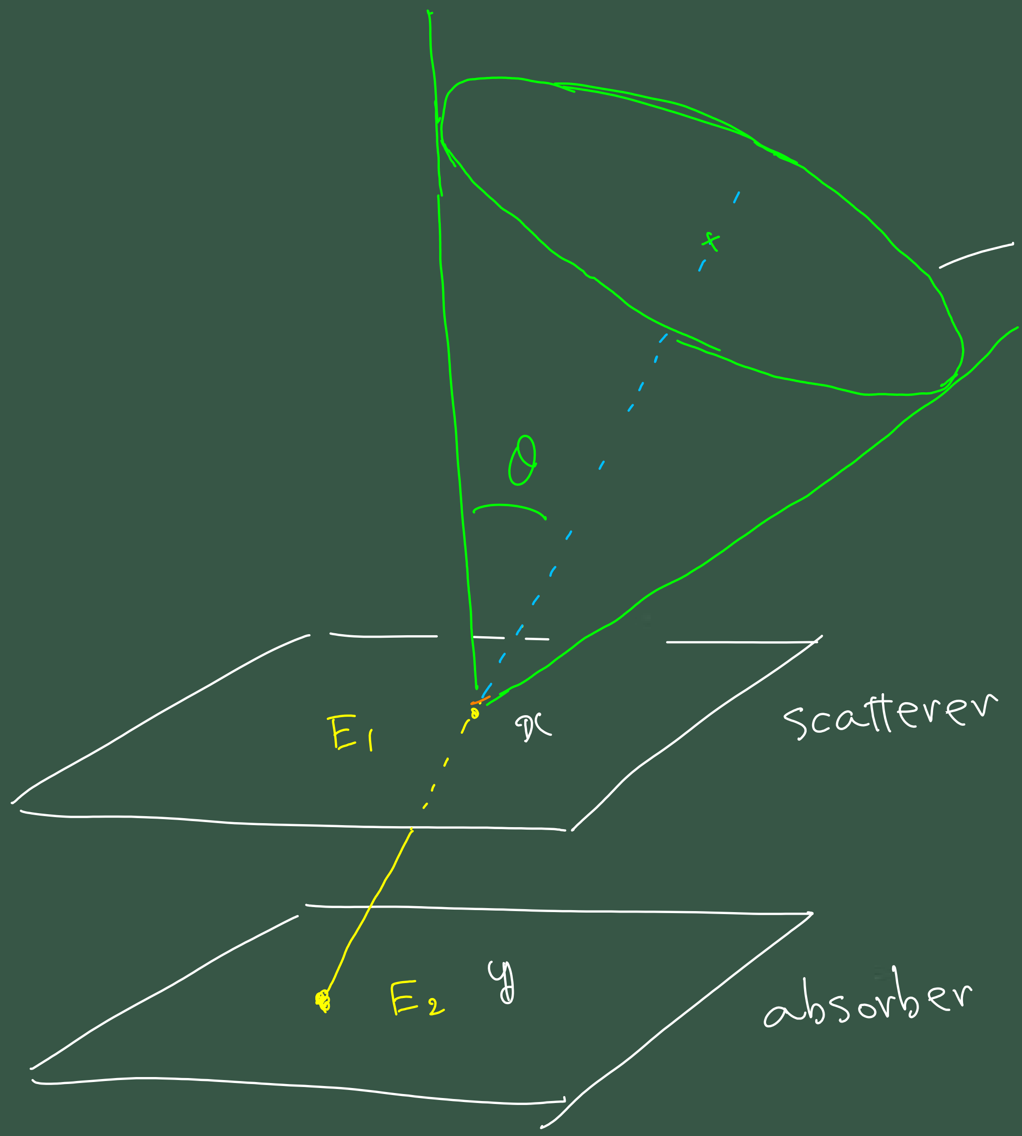


$$\frac{1}{E_2} - \frac{1}{E_0} = \frac{1}{E_2} - \frac{1}{E_1 + E_2} = \frac{1}{m_e c}(1 - \cos\theta)$$

m_e : mass of electron

c : speed of light

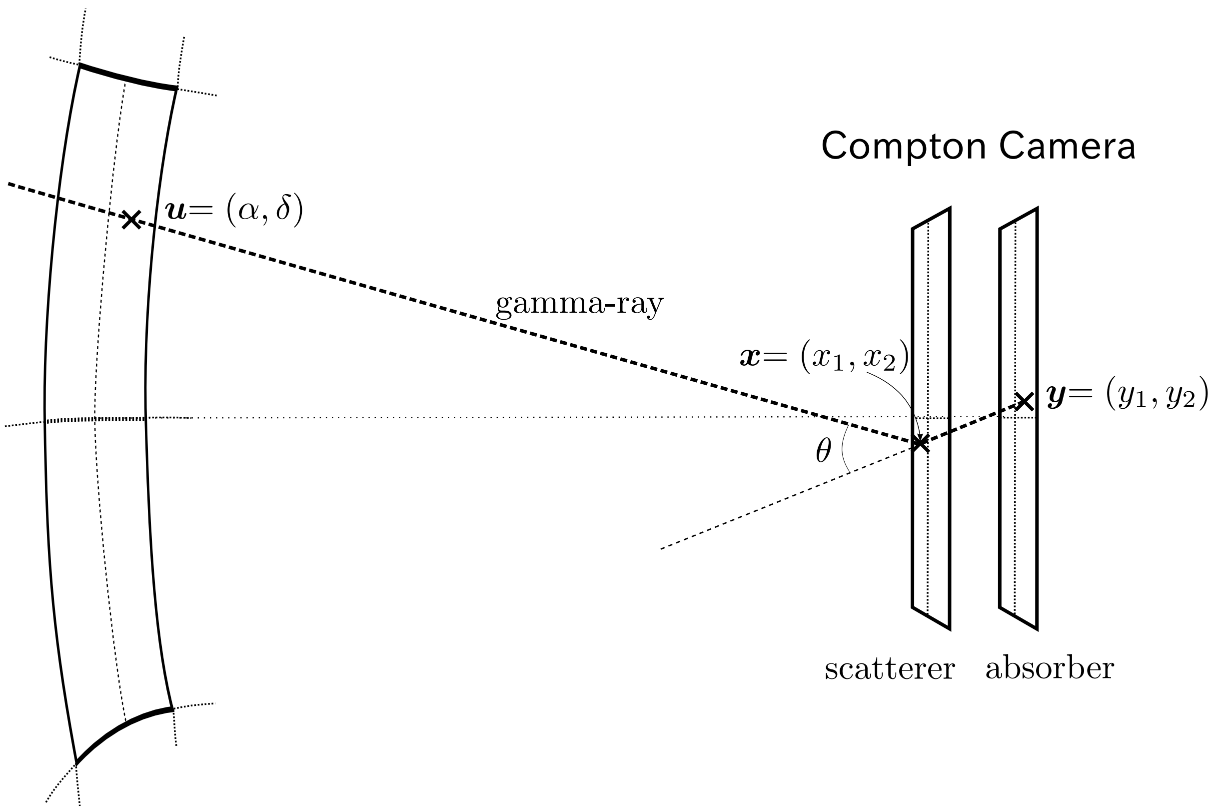
Q Compton camera imaging



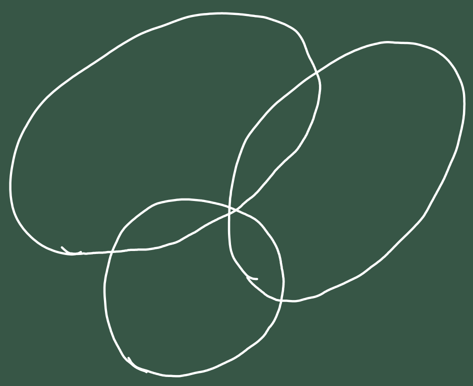
Photon came from a point on this cone

Observing many photons and γ-ray intensity map can be reconstructed.

Compton camera imaging.



Conventional method for Compton camera imaging.



Back projection.

- Draw an ellipsoid for each observation
- Simple and fast

$\Downarrow$

Image becomes blurred.

Physical parameters of the simulated semi-conductor.

		density	energy resolution
		[g cm^{-3}]	FWHM[keV]
scatterer	Si	2.33	2.0
absorber	CdTe	5.86	2.0

- Compton camera
- Compton camera imaging
  - measurement process.
  - estimation method
  - improvement
- Conclusion

Probabilistic framework for Compton camera imaging

γ-ray

- DOA : u
- γ-ray strength from u : $\lambda(u)$

Compton camera

- Probability of scattering : $s(u)$

position of scattering on scatterer : x

" absorbtion on absorber : y

- For large distance sources: $w = x - y$
- Scattering angle : $\cos\theta$

$\rightarrow v = (z, \cos\theta)$

- model : $p(v \mid u)$

(Scattering angle θ follows Klein-Nishina formula)

☆ Observation Process

$Y(v)$: The number of photons observed at position $v=(w, \cos\theta)$ follows a Poisson dist.

$$Y(v) \sim \mathrm{Poisson}\left(\sum_u p(v \mid u)\, \lambda(u) s(u)\right).$$

re-parameterization

$$q(v) = \frac{Y(v)}{\sum_{v'} Y(v')} , \quad \rho(u) = \frac{\lambda(u) s(u)}{\sum_{u'} \lambda(u') s(u')}$$

$$q(v) = \sum_u p(v \mid u)\, \rho(u)$$

$q(v)$: Prob. that absorbed photons is observed at v

$\rho(u)$: 〃 came from u

- $p(v \mid u)$, $s(u)$

- Theoretically, Klein-Nishina formula can be used to compute $p(v \mid u)$, but we use a Monte Carlo simulation

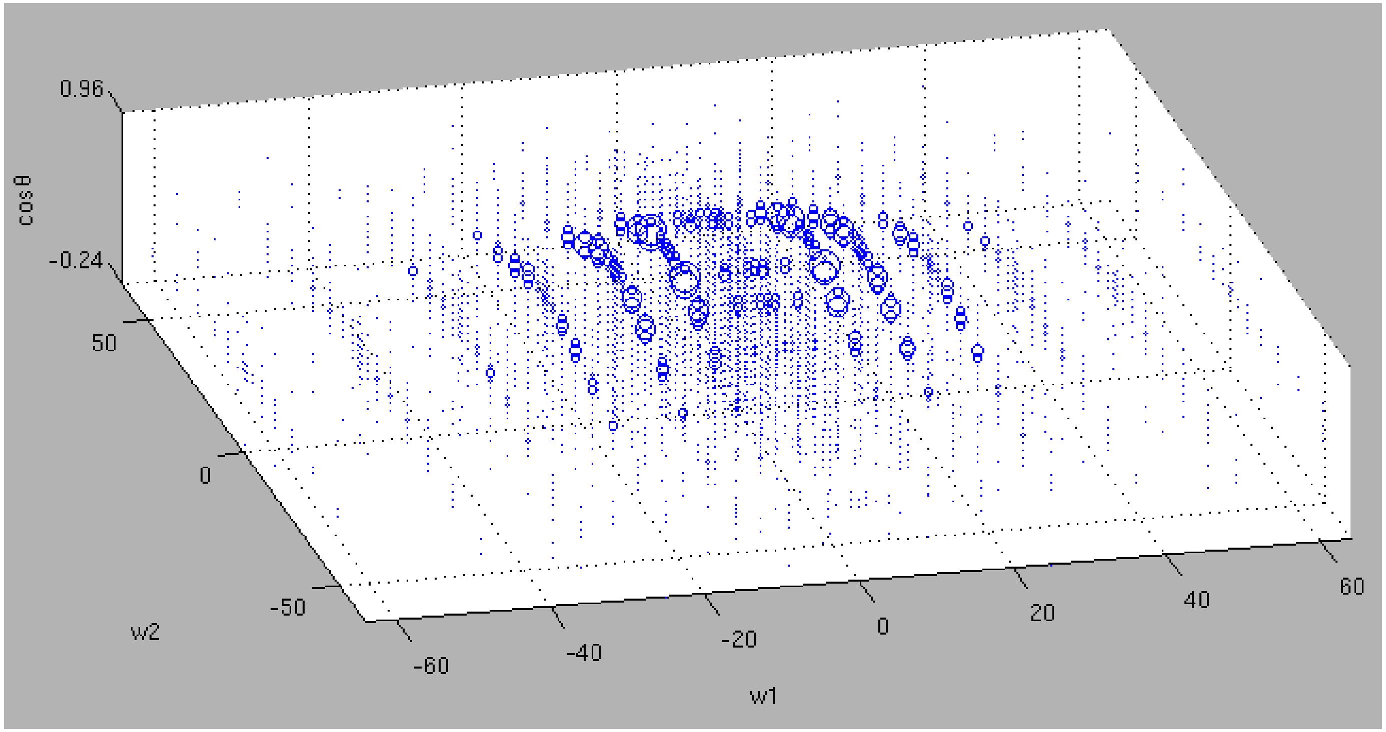
- Well-designed physical simulation with real camera can be used to measure $p(v \mid u)$ physically.

- $p(v \mid u)$ and $s(u)$ must be prepared for each energy level E_0. This should be done off-line beforehand.

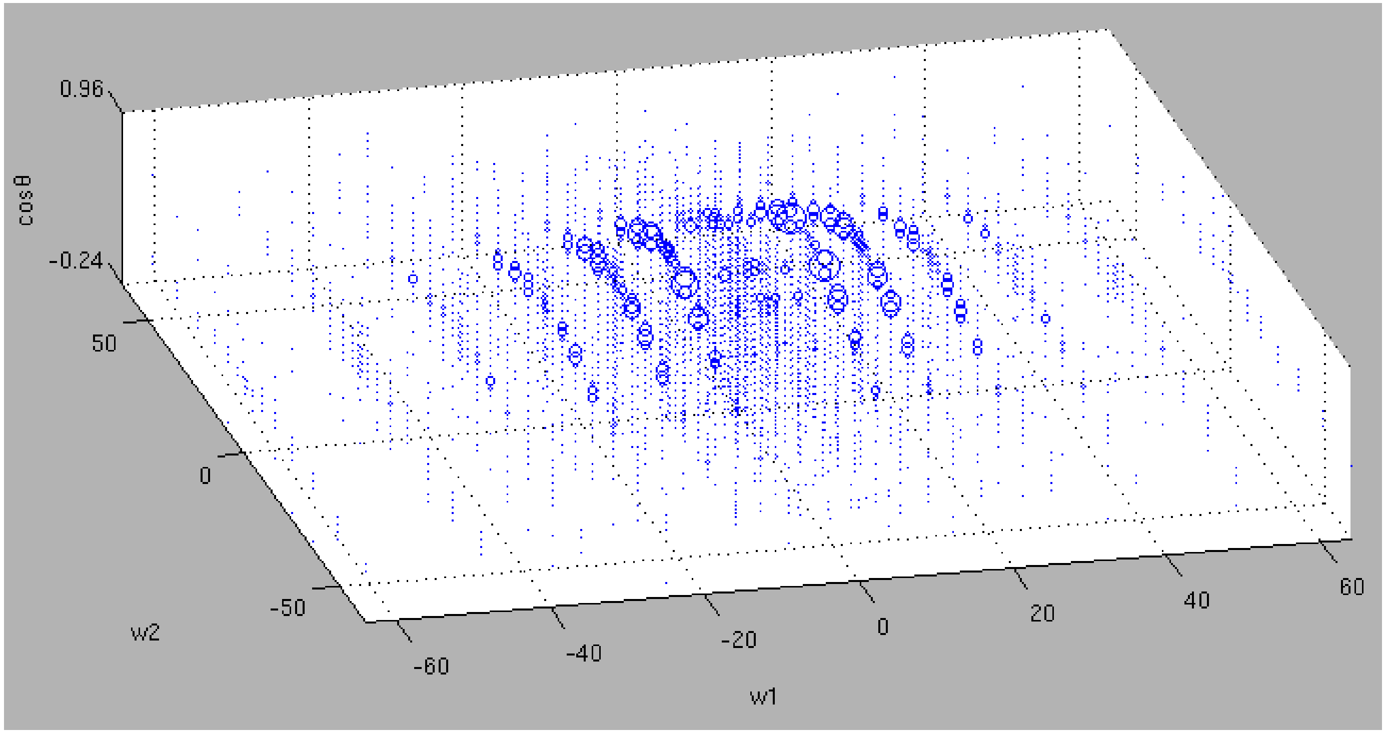
Design of bins of $\boldsymbol{u}$ and $\boldsymbol{v}$.

	$\boldsymbol{u}$		$\boldsymbol{v}$		
	α	δ	$\dfrac{w_1}{\sqrt{\lvert w_1\rvert}}$	$\dfrac{w_2}{\sqrt{\lvert w_2\rvert}}$	$\cos\theta$
	[degree]		$[\mathrm{mm}^{1/2}]$		
min	-30	-30	-8.2	-8.2	$-.24$
max	30	30	8.2	8.2	$.96$
# of bins	21	21	17	17	24

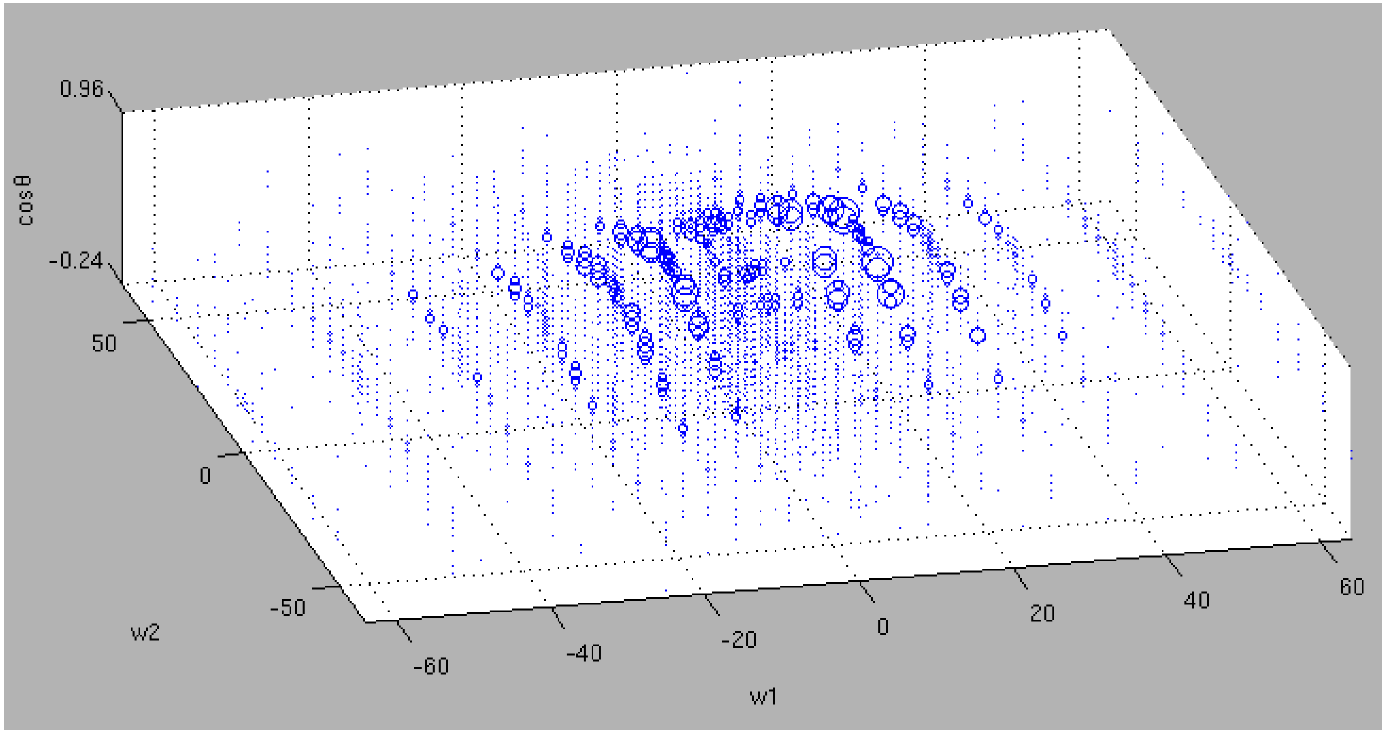
Distribution of the received photon from center.



Distribution of the received photon from 8° off center.



Distribution of the received photon from 12° off center.



☆ Estimation method

$$\sum_v q(v) = 1, \quad \sum_u p(u) = 1 \quad \sum_v p(v|u) = 1,$$

$$\underbrace{q(v)}_{\text{mixture dist.}} = \sum_u \underbrace{p(v|u)}_{\text{given}} \underbrace{p(u)}_{\text{dist. to estimate}}$$

samples from a mixture dist. are observed.

Each mixture component is known ($\underline{p(v|u)}$)

we want to estimate the mixing coefficient ($\underline{p(u)}$).

Estimation method (EM algorithm)

Observation: v_t $(t=1,\cdots,N)$

Starting from $\rho^{(0)}(u)$, update $\rho^{(\ell)}(u)$ as follows.

E-step

$$q^{(\ell)}(v_t) = \sum_u p(v_t|u)\,\rho^{(\ell)}(u)$$

M-step

$$\rho^{(\ell+1)}(u) = \frac{1}{N}\sum_{t=1}^{N}\frac{p(v_t|u)}{q^{(\ell)}(v_t)}\,\rho^{(\ell)}(u)$$

Two problems

- $\hat{\rho}(u)$ is not sparse $\longrightarrow$ MAP estimate with Dirichlet prior
- Slow convergence $\longrightarrow$ Approximate Fisher's scoring.

- Compton camera
- Compton camera imaging
  - measurement process.
  - estimation method
  - improvement
- Conclusion

(a) MAP estimation (Bayesian approach)

In astronomy approximation, $p(u)$ should be sparse (lot of 0's)

$p(u)$ is a multinomial dist. Its conjugate prior is Dirichlet dist.

$$\pi_\alpha(p) = \frac{\Gamma(\alpha M)}{\Gamma(\alpha)^M} \prod_u p(u)^{\alpha-1}, \quad (M \text{ is the \# of } u)$$

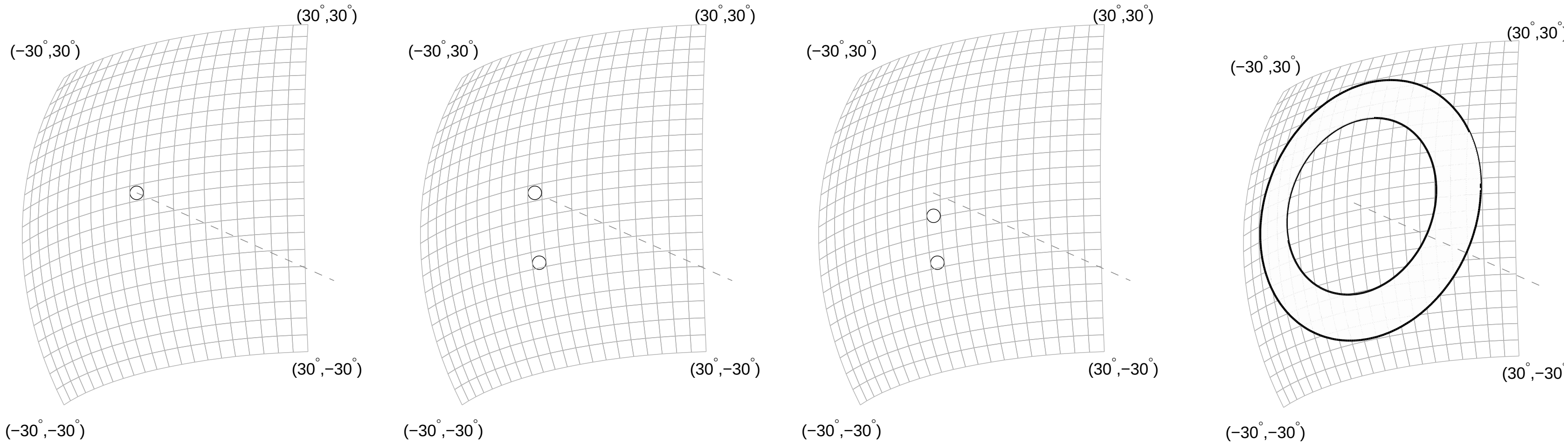
MAP estimate

$$\hat{p}_{MAP} = \arg\max \left[\log P(p \mid v_1, \cdots, v_N)\right]$$

$$= \arg\max \Big[\underbrace{(\alpha-1)\sum_u \log p(u)}_{\text{prior distribution}} + \underbrace{L(p)}_{\text{log-likelihood}}\Big]$$

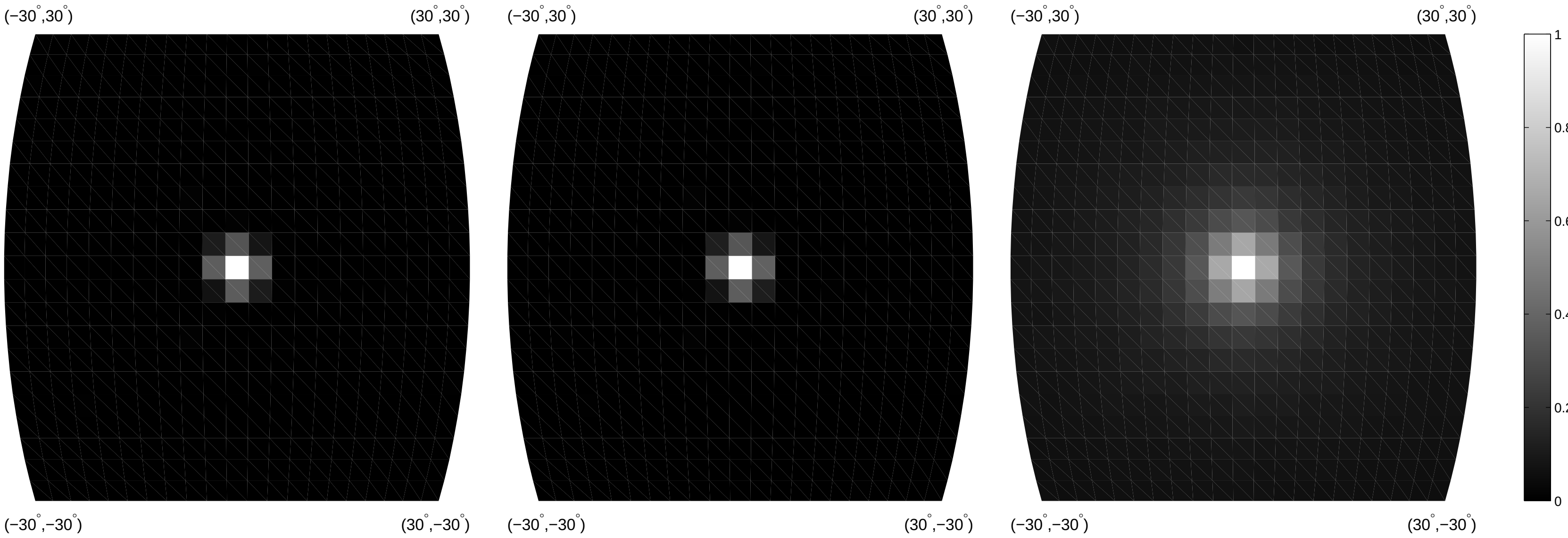
for $\alpha < 1$, $\hat{p}_{MAP}$ generally becomes sparse.

Gamma-ray sources used for numerical simulations.



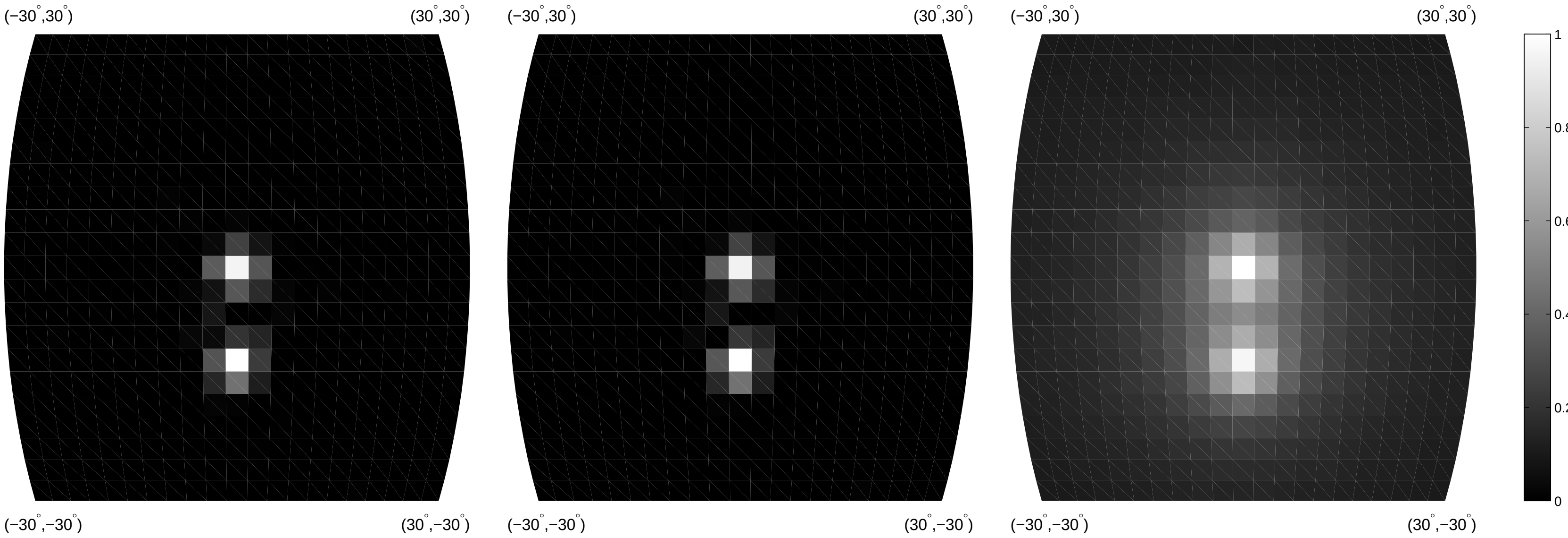
(a) single point source. (b) two point source. (c) two point source. (d) distributed source.

Reconstructed images for data from (a) sigle point source.



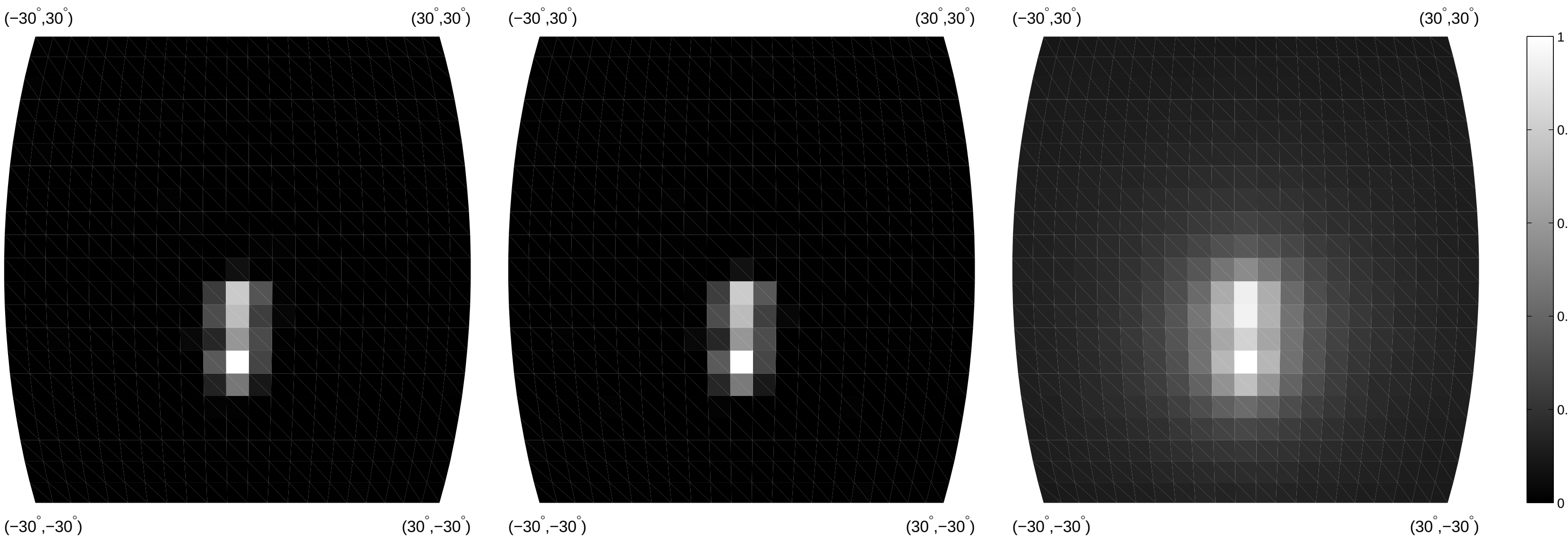
MLE reconstruction. MAP reconstruction. Back projection reconstruction.

Reconstructed images for data from (b) two point source.



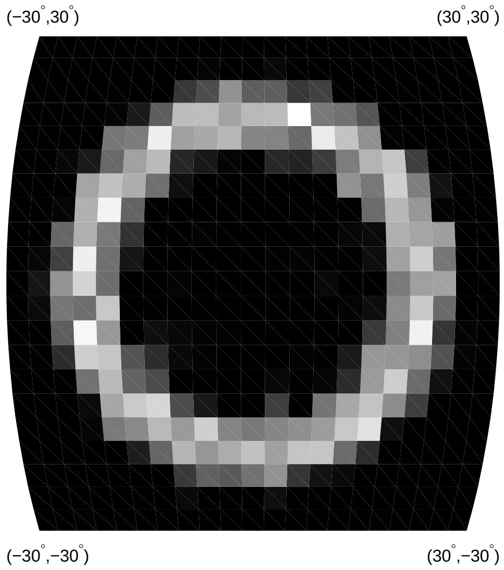
MLE reconstruction. MAP reconstruction. Back projection reconstruction.

Reconstructed images for data from (c) two point source.

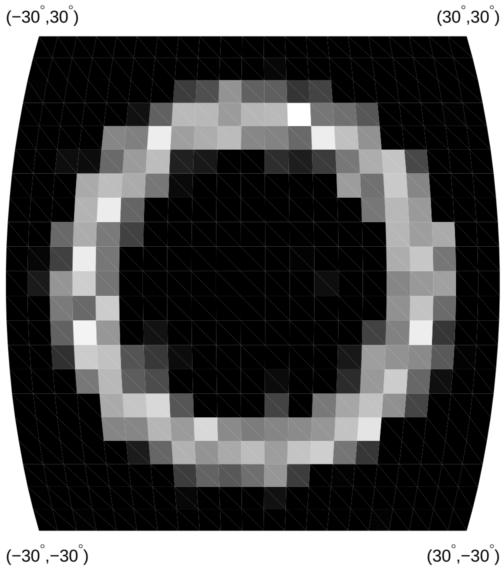


MLE reconstruction. MAP reconstruction. Back projection reconstruction.

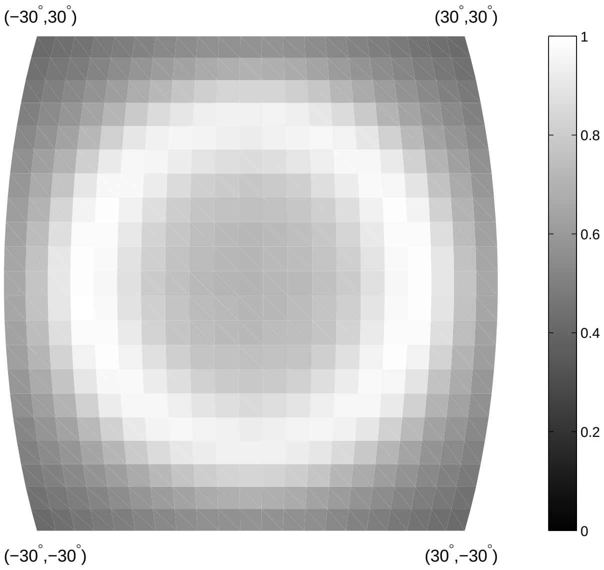
Reconstructed images for data from (d) distributed source.



MLE reconstruction.



MAP reconstruction.



Back projection reconstruction.

- Compton camera
- Compton camera imaging
  - measurement process.
  - estimation method
  - improvement
- Conclusion

Conclusion

- Probabilistic framework for Compton camera imaging
- MAP estimation for sparse solution
- Speed up version of the EM algorithm.

Ongoing projects

- multi-layered camera
- other applications, such as Fukushima soil contamination