Algorithms and Architectures for X-Ray Diffraction Tomography

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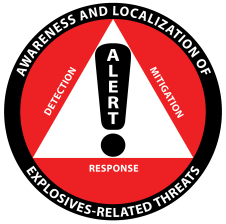

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Summary

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- Iterative reconstruction algorithms for reconstruction of XDI images
  - Good localization, characterization of materials with strong Bragg peaks
  - Harder: accurate reconstruction of liquids and other amorphous materials in the presence of stronger scatterers nearby
- XDI architectures with coded apertures and limited illumination directions leads to good reconstruction of volumetric and spectral images
  - increased scatter signal strength, better conditioned reconstruction
- Iterative reconstruction algorithms are essential in these architectures
  - Needed to mitigate artifacts from “strong” scatterers, obtain observability exploiting sparsity and spatial consistency
- Need fusion with CT or equivalent normalization for reconstruction
- Major challenges remain:
  - Computation requirements for reconstruction
  - Architecture design for improved signal/noise ratio
  - Explosives detection/classification using reconstructed signals for liquids and HME classes

Motivation

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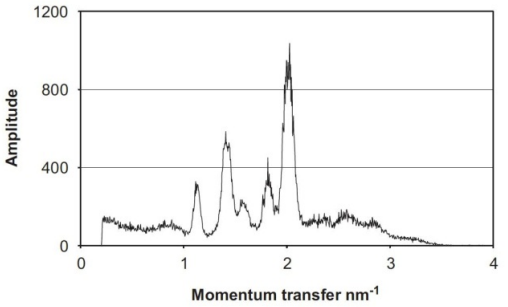
Background:

- Material identification based on conventional X-ray computed tomography (CT) images can be ambiguous
- X-ray diffraction imaging (XDI) systems identify material based on coherent-scatter form factor – New signature that depends on molecular structure



Coherent-scatter form factor of TNT (Harding '09, Morpho)

Issues:

- Weak signals may require long collection times
- What are appropriate algorithms and architectures?

Existing XDI Commercial Product:

- Single view, direct imaging

Morpho XRD 3500 ™

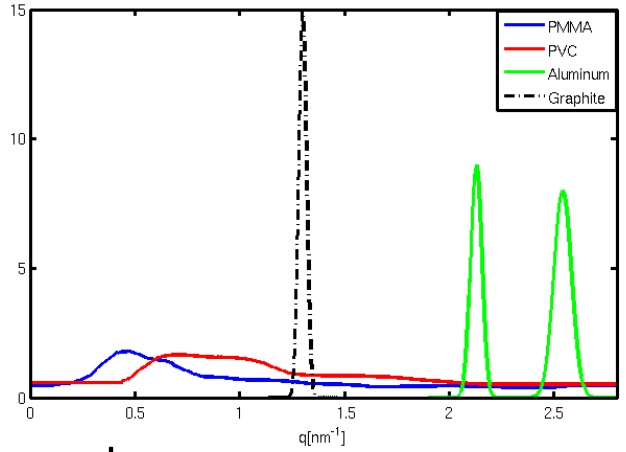
Focus of Talk: Discuss recent progress and results on algorithms for different XDI architectures

X-ray Diffraction Imaging

- Construct the *coherent-scatter form factor* $|F(q,\boldsymbol{x})|^2$ at all positions x in volume of interest: 4-dimensional function!
  - Expressed as distribution of transferred momentum q that causes the deviation of photon of wavelength λ by angle θ

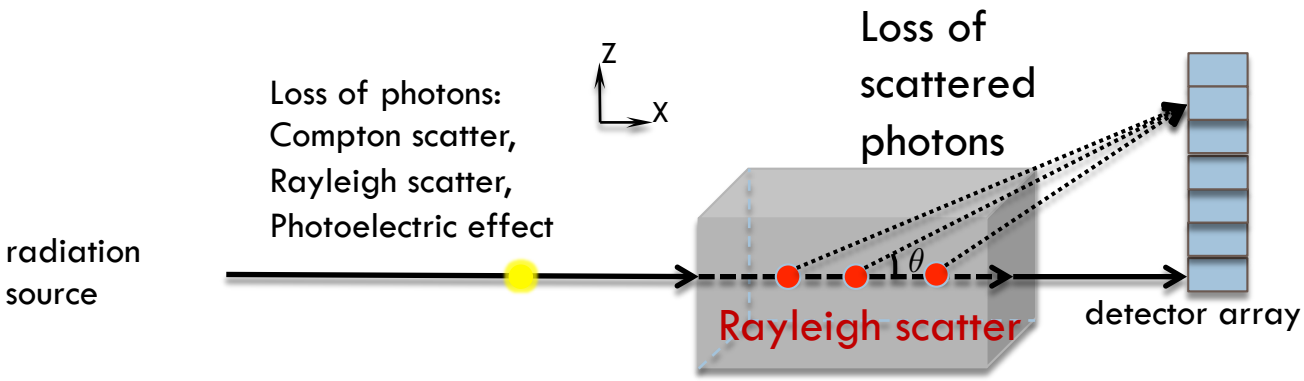
$$q = \frac{1}{\lambda}\sin(\frac{\theta}{2})$$

Form factors



  - For crystalline materials, Bragg peaks reveal molecular composition for material discrimination in terms of preferred scattering angles
  - For amorphous materials, or liquids, form factor is smoother

X-ray Diffraction Principles



Observations:

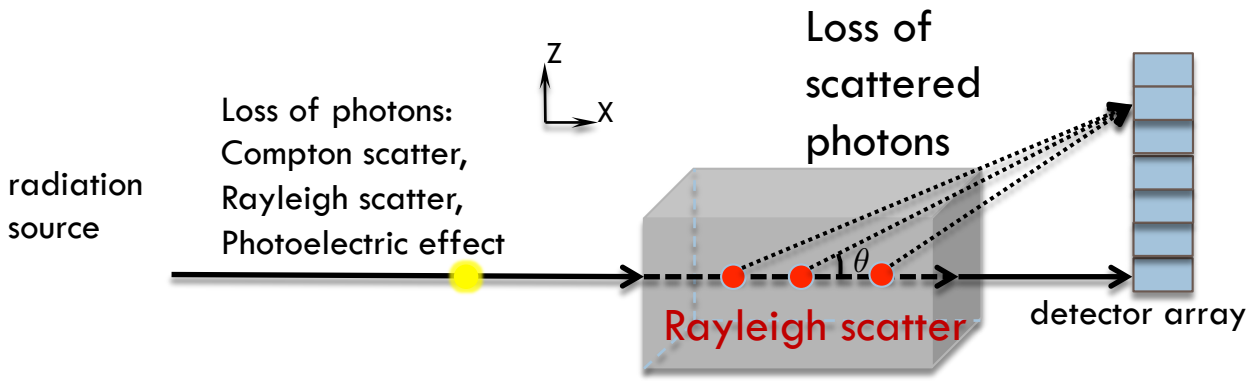
- Fraction of photons that are scattered coherently is small – fraction decreases with increasing photon energy
- Fraction of photons that are lost to photoelectric effect also decreases with increasing photon energy

→ Low energy Rayleigh scatter will be highly attenuated

→ High energy Rayleigh scatter is less likely

Weak signals! Limit on effective energy band

X-ray Diffraction Principles - 2



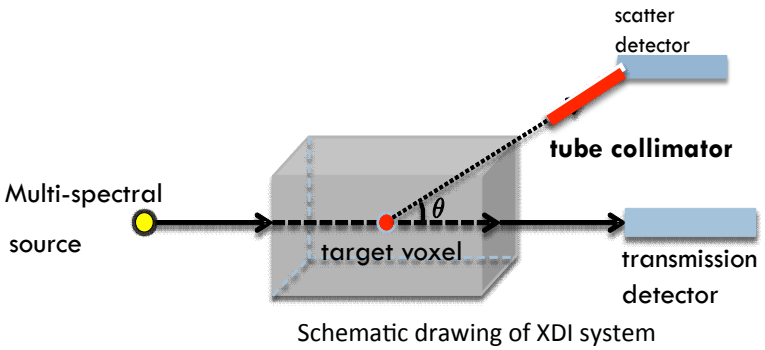
Observations 2:

- Depending on collimation scheme and source spectrum, each detector measures scatter from different locations and different energies
- Detector technology: photon counting detectors vs intensity detectors
  - Slice reconstruction: 3-D object may be easier to reconstruct from 2-D array of photon counting detectors, equivalent to 3-D measurement
  - Alternative: few views with intensity measurements (not many, though…): compressive sensing reconstruction

X-Ray Diffraction: Some Architectures

Direct imaging: tube collimators

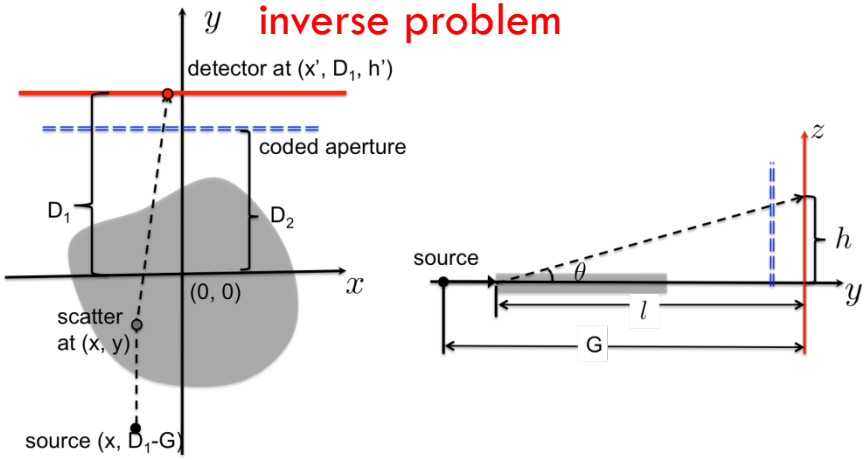
Photon-inefficient but simple algorithms



Schematic drawing of XDI system

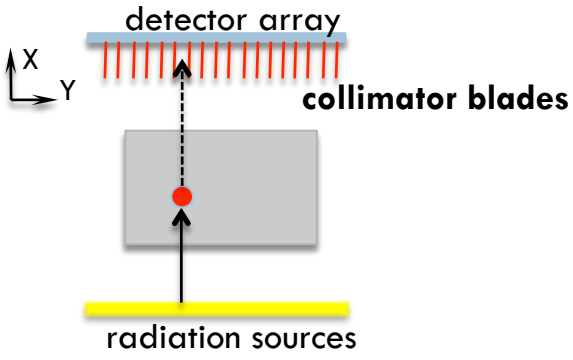
Coded aperture imaging:

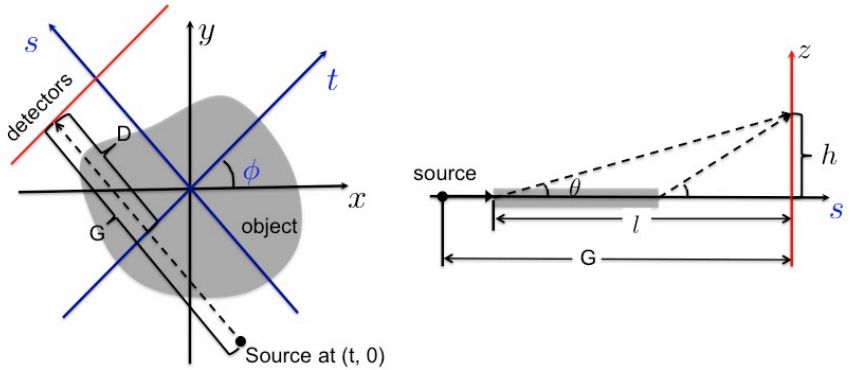
Captures more photons, complex inverse problem



Limited-angle tomography: sheet collimators

Higher SNR, often requires rotating detectors and tomography algorithms





XDI Math

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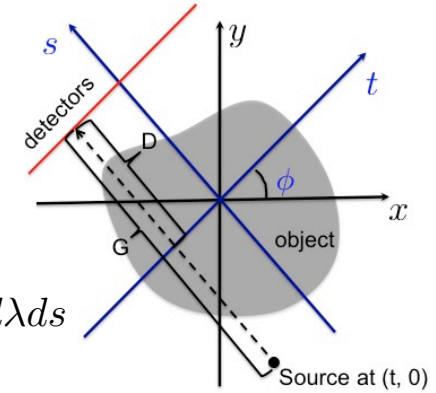
Model depends on architecture :

- Example below for intensity detectors, sheet collimators separating vertical lines of detectors



$$I_\phi(t,h) = \int_0^G \int_{\lambda_m in}^{\lambda_m ax} I_\lambda(t,0)\mathcal{A}_\lambda(t,0,s,0)\mathcal{B}_\lambda(t,s,G,h)\frac{|F(t,s,q)|^2}{[(G-s)^2+h^2]^{3/2}}d\lambda ds$$

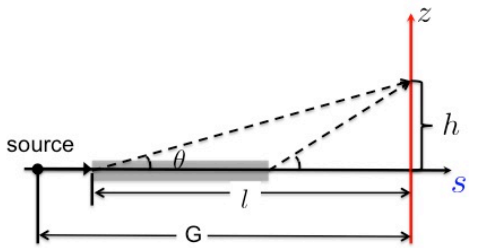
$$q = \frac{\sin(0.5\tan^{-1}(\frac{h}{G-s}))}{\lambda} \approx \frac{h}{2\lambda(G-s)}$$

$I_\lambda(t,0)$: incident x-ray intensity at λ;

$\mathcal{A}_\lambda(t,0,s,0)$:attenuation for λ along incoming ray from 0 to s;

$\mathcal{B}_\lambda(s,0,G,h)$:attenuation along the scattered ray from $(s,0)$ to (G,h).

$|F(t,s,q)|^2$:coherent-scatter form factor at location (t,s)



- For photon counting detectors, model changes:

$$I_\phi(t,h,\lambda_0) = \int_0^G \int_{\lambda_0}^{\lambda_0+\Delta} I_\lambda(t,0)\mathcal{A}_\lambda(t,0,s,0)\mathcal{B}_\lambda(t,s,G,h)\frac{|F(t,s,q)|^2}{[(G-s)^2+h^2]^{3/2}}d\lambda ds$$

XDI Math 2

- Easy extensions to include other architectures
  - Different collimators or coded aperture masks, fan beams, …
- Important issue: Need to account for attenuation in both the excitation path and the scatter path
- Two approaches possible
  - Estimate attenuation using dual-energy conventional CT reconstruction and incorporate into image reconstruction process -- general
  - Normalize path loss using direct path observation
    - Small angle assumption: attenuation along the path of scattered radiation is approximately same as on transmitted path
    - More appropriate for photon-counting detectors (small energy range per measurement)

$$J_\phi(t,h) = \frac{I_\phi(t,h)}{I_\phi(t,0)} \approx \int_0^G \int_{\lambda_m in}^{\lambda_m ax} \frac{|F(t,s,q)|^2}{[(G-s)^2+h^2]^{3/2}} d\lambda ds$$

Iterative Reconstruction

- Algorithm 1 (IRL1):
  - Iterative reconstruction, slice by slice
  - Look for spatial coherence in form factor reconstructions among nearby voxels
  - Sparsity in form factors representation
- Convex optimization formulation

$$\min_{\underline{\mathbf{x}}} (\mathbf{y} - C\underline{\mathbf{x}})^T W(\underline{\mathbf{y}})(\mathbf{y} - C\underline{\mathbf{x}}) + \alpha^2 \sum_{m=1}^{M} ||D\underline{\mathbf{x}}||_1$$

  - **y** : measurements, stacked by voxels and momentum transfer
  - **x** : reconstructed form factors over voxels
  - C : Discretized observation matrix
  - D : Spatial derivative operator
  - M : Number of form factor bins
- Solve using standard convex techniques

Iterative Reconstruction

- Algorithm 2 (IREP):
  - Iterative reconstruction, slice by slice
  - Look for spatial coherence in form factor reconstructions among
  - Simultaneous segmentation/image formation avoiding smoothing across edges (Ambrosio-Tortorelli)

$$\min_{(\mathbf{x},\mathbf{s})} ||\mathbf{y} - C\mathbf{x}||^2_{W(\mathbf{y})} + \alpha_1^2 \sum_{m=1}^{M} ||\mathbf{D}\mathbf{x}_\mathbf{m}||^2_{\mathbf{W_s}} + \varphi_\mathrm{S}(\mathbf{s},\gamma)$$

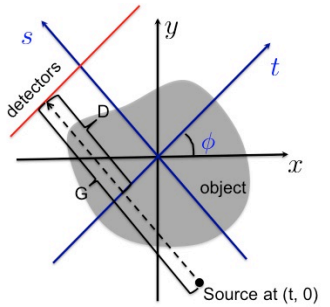
$$W_s = \mathrm{Diag}\left[(1 - [\mathbf{s}]_i)^2\right], \quad \varphi_\mathrm{S}(\mathbf{s},\gamma) = \gamma^2 \|\mathcal{D}\mathbf{s}\|^2 + \frac{1}{\gamma^2}\|\mathbf{s}\|^2$$

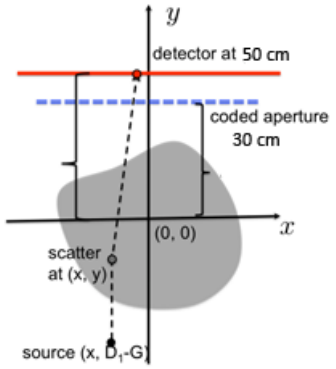
- Solve using biquadratic iterative optimization

- Other algorithms investigated (overcomplete basis representations, …) with similar results.

Experiments

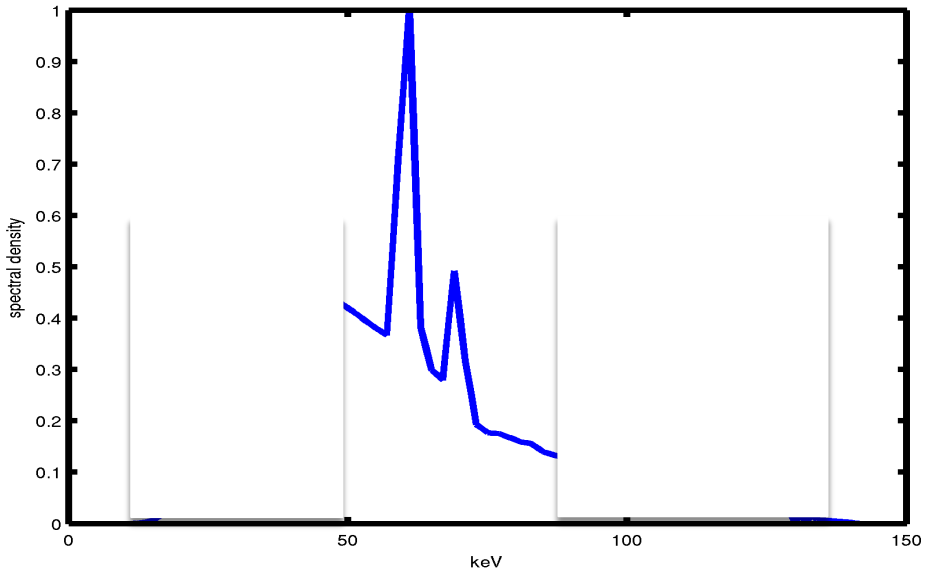
- Architecture 1: Limited angle tomography with vertical collimation
  - 7 views, from -60 to 60 degrees, 20 degrees apart
- Architecture 2: Coded aperture, single view
- Architecture 3: Coded aperture, 3 views (-60,0,60)
  - Simple coded aperture design (Brady et al '12)
  - Focus on reconstruction
- Detectors
  - Intensity detectors
  - Photon counting detectors, 6 keV resolution
- Issues:
  - 3-D slice reconstructions from very few 2-D views





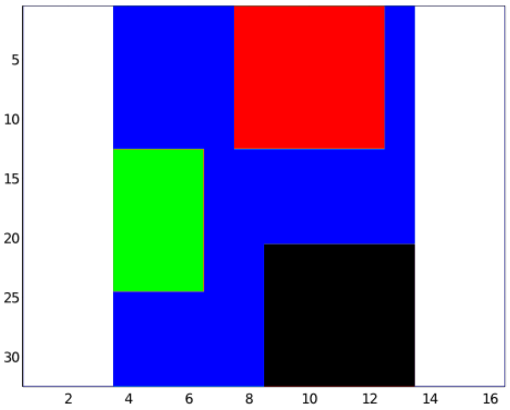
Illumination Variations

- Monochromatic source at 72 keV
- Polychromatic source from 50 keV to 80 keV with basic spectra
- Simulated Monte Carlo photon sources

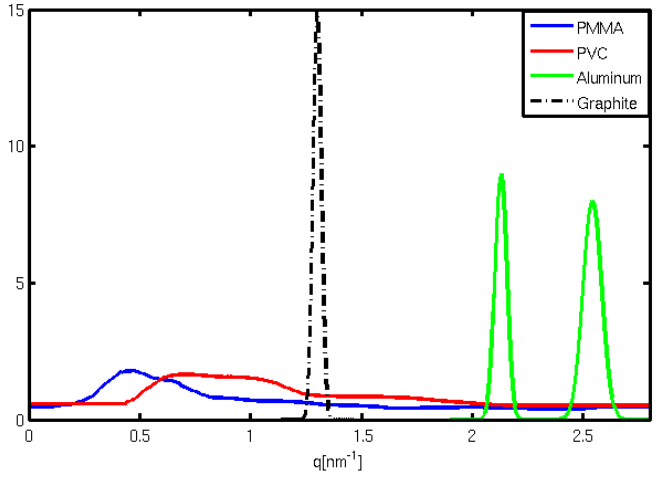


Experiment Phantom

- Object of size 8*4cm, composed of 4 elements (PMMA, PVC, Aluminum, Graphite)
- Two phantoms: a flat plate, 1 cm tall, and a tall rectangular solid, 40 cm tall
- Focus on clutter, interference, attenuation
  - Different attenuation of scatter



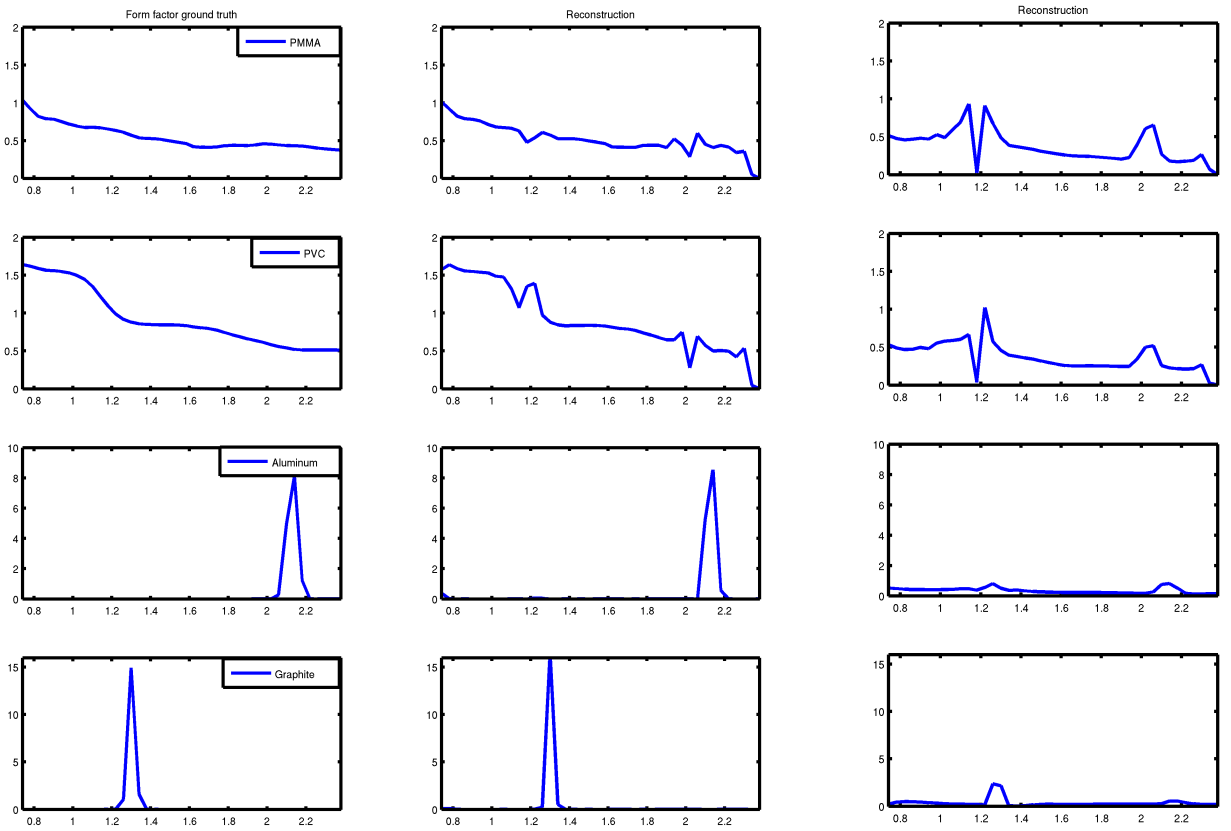
Plan view of object in Illumination plane



Form factors for the elements

Experiment 1: Why Coded Aperture

- Phantom: Thin plate
- Architecture: with and without coded aperture, 3 views (-60, 0, 60) degrees, with intensity detectors, single energy illumination (72 keV), no noise, IRL1 algorithm

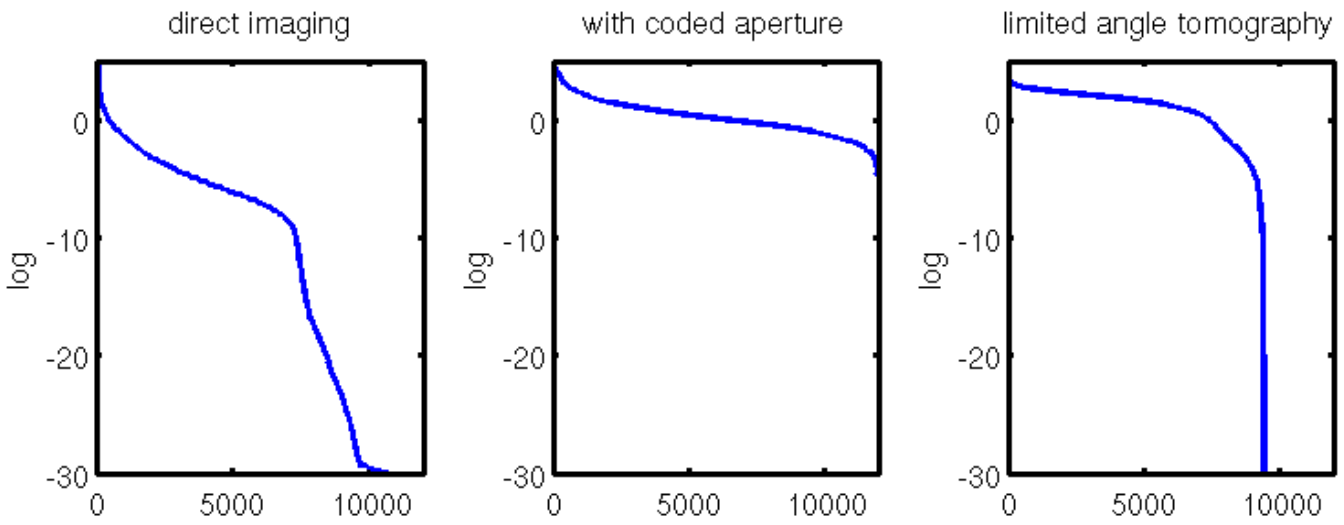


Truth | With coded aperture | Without coded aperture

Explanation

- Without coded aperture, limited angle tomography results in ill conditioned inverse problem
  - Hard to separate different material contributions

Comparison of log of singular values for different architectures



Experiment 2: Coded aperture vs vertical collimation

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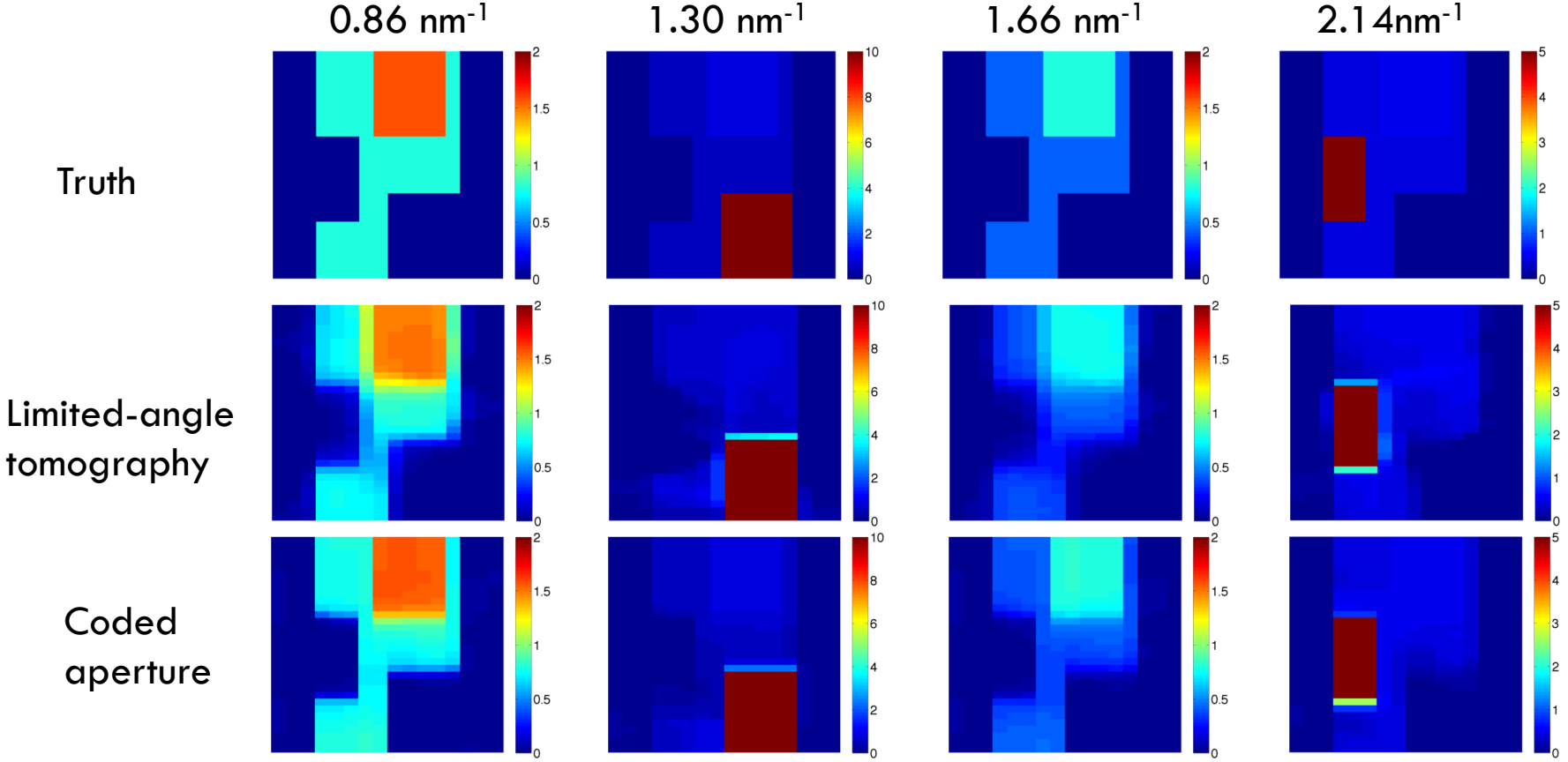
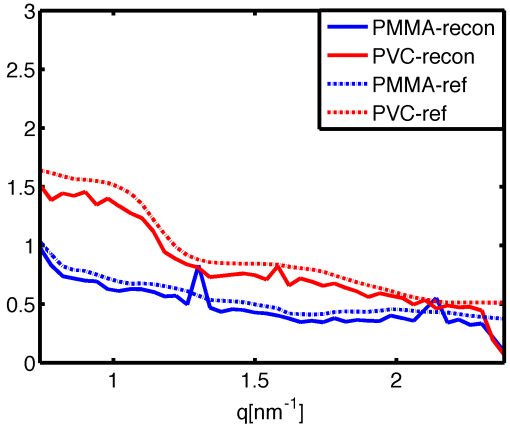
- Phantom: **thin plate**
- Architectures: Coded aperture, 3 views (-60, 0, 60) degrees and limited angle tomography with vertical collimators, 7 views, intensity detectors, single-energy at 72 keV, IRL1 algorithm

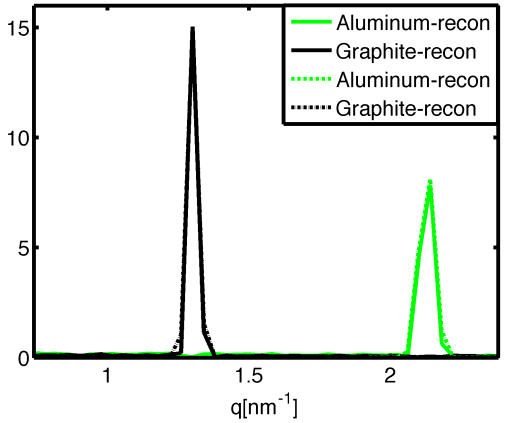


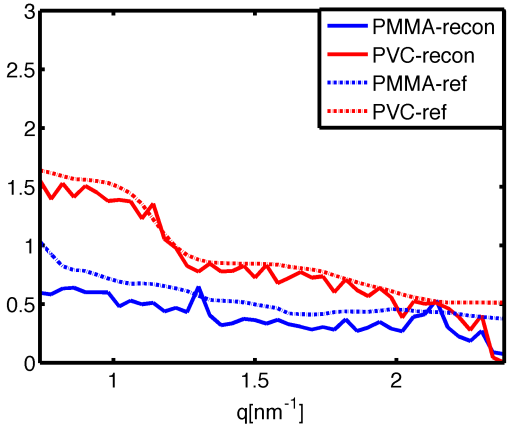
Main difference: More efficient collection of scattered photons in coded aperture – Increased signal strength

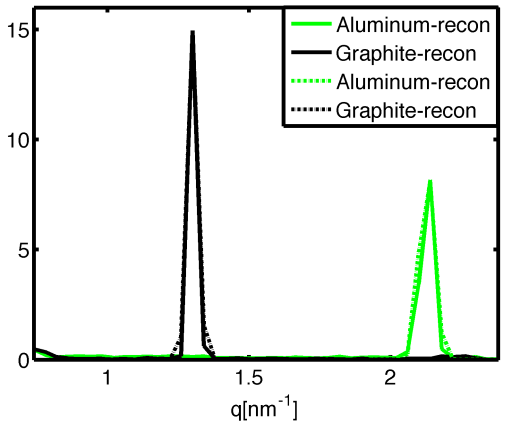
Form Factor Reconstructions

- Average over region of the materials



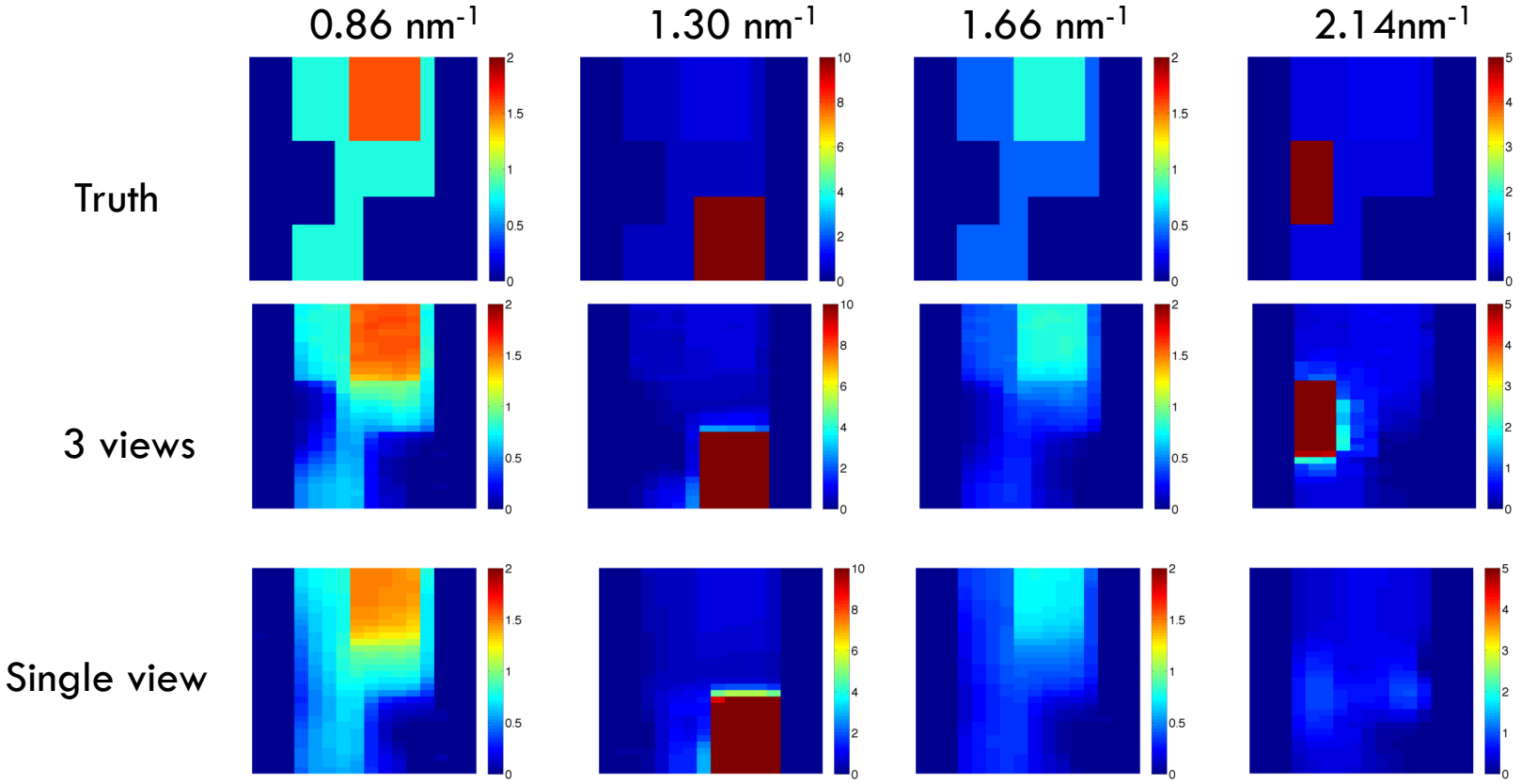






Experiment 3: Why Multiview?

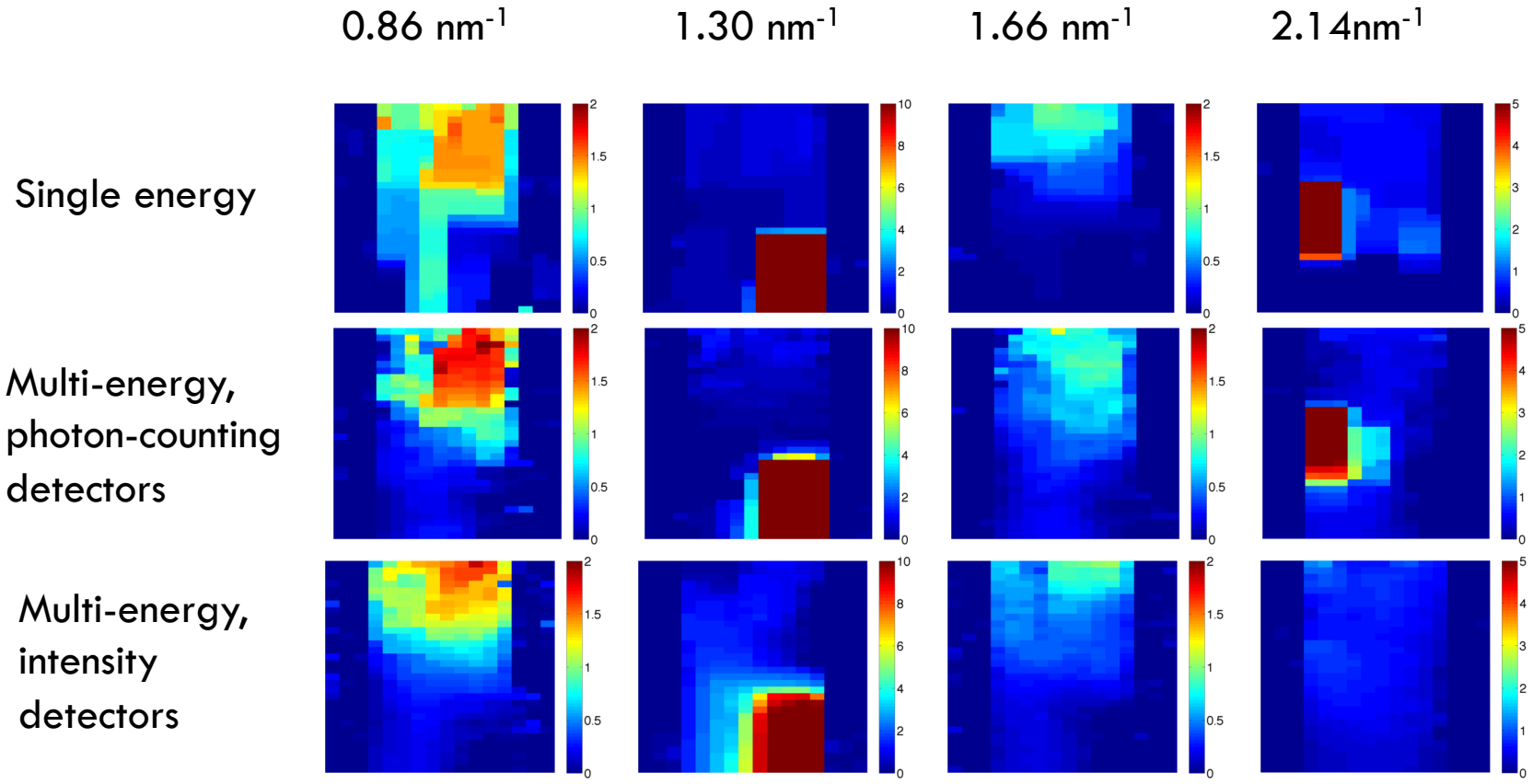
- Phantom: **Tall rectangular solid**
- Architecture: Coded aperture, 3 views (-60, 0, 60) degrees, vs single view, 0 degrees, with photon-counting detectors, multi-energy illumination, IRL1



Strong absorption from a single view can reduce scatter signal (no aluminum…)

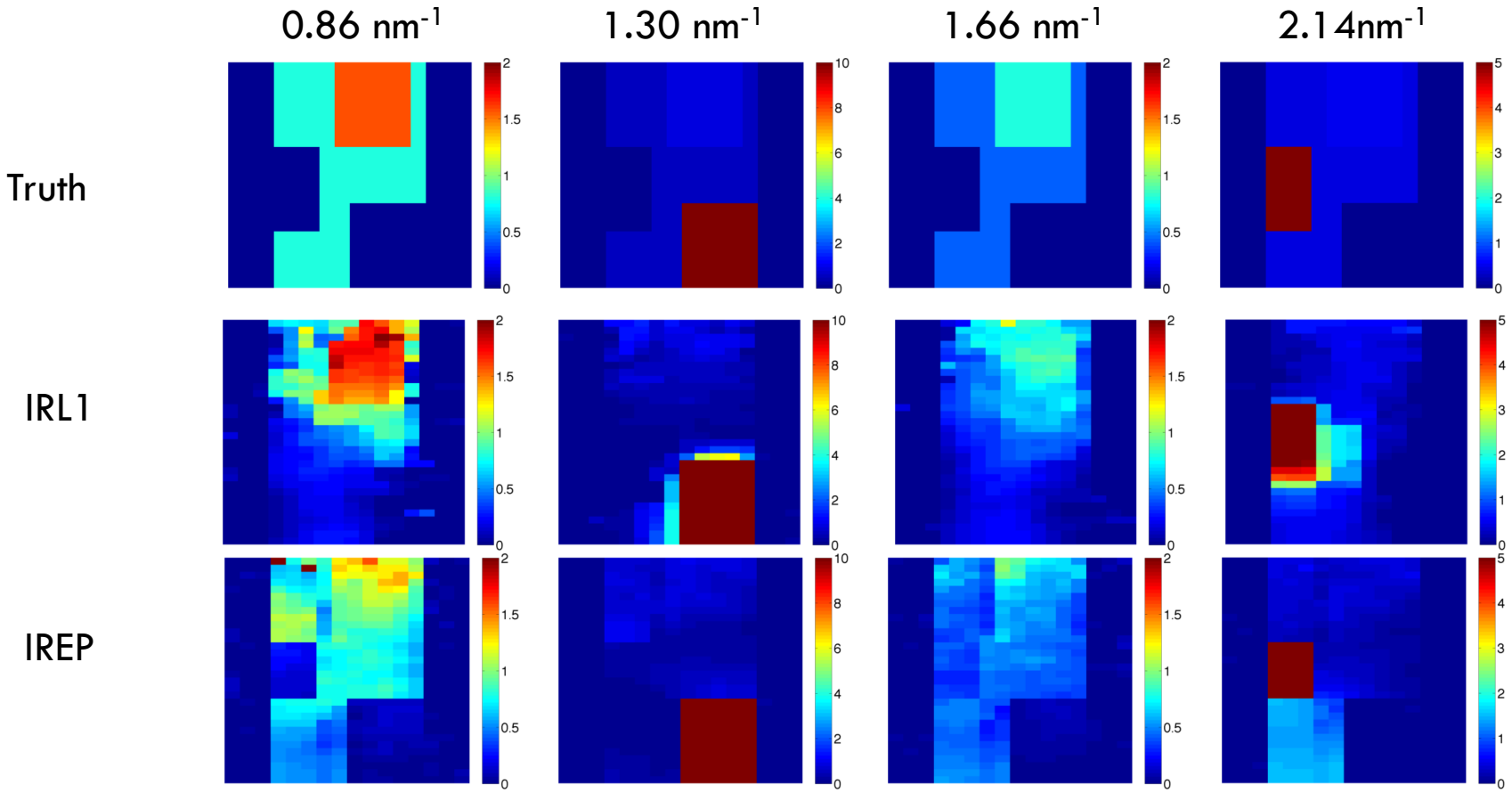
Experiment 4: Photon-counting detectors help

- Phantom: **Tall rectangular solid**
- Architecture: Coded aperture, 3 views (-60, 0, 60) degrees, with intensity detectors and photon-counting detectors , monochromatic vs multi-energy illumination, IRL1



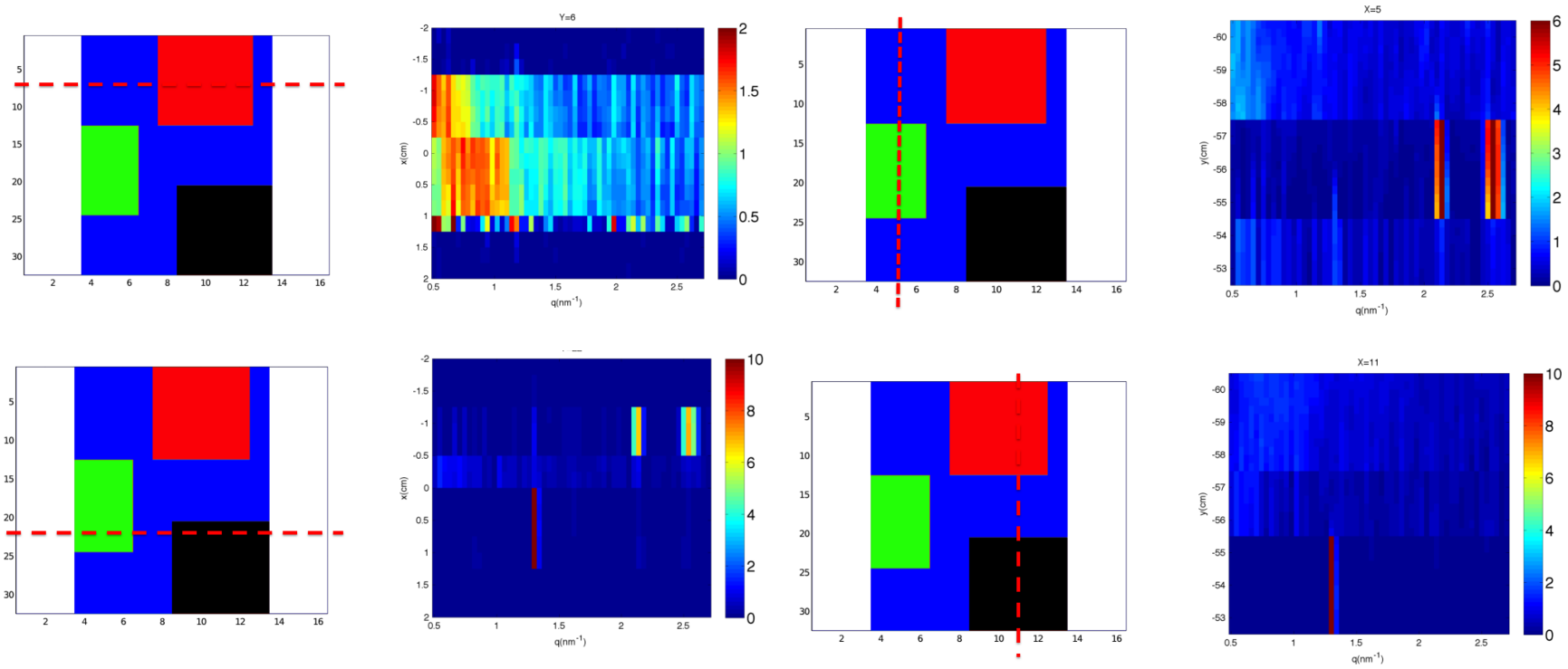
Experiment 5: Algorithm choices

- Phantom: Tall rectangular solid
- Architecture: Coded aperture, 3 views (-60, 0, 60) degrees, with photon-counting detectors, multi-energy illumination, IRL1 and IREP algorihms



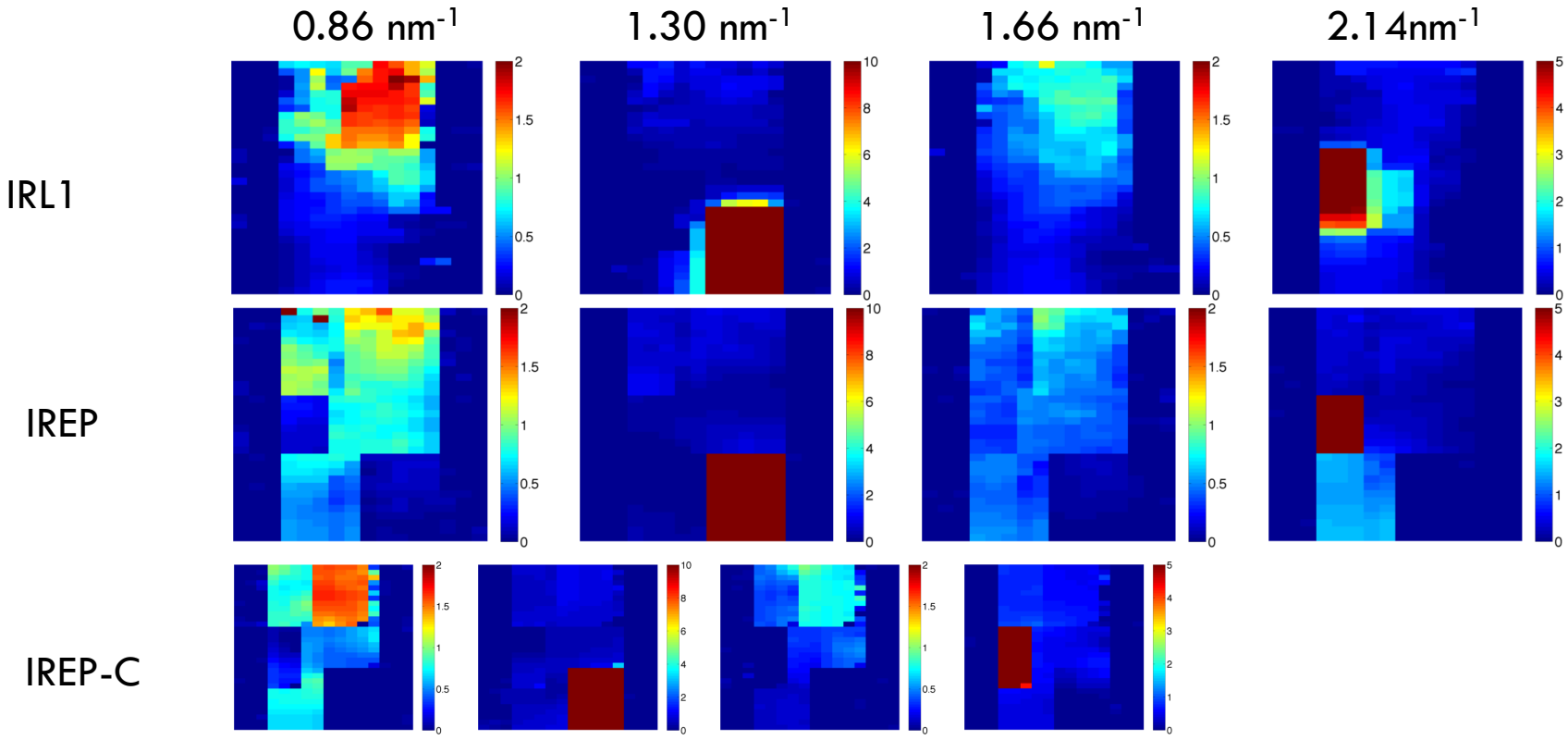
A Different View: Segmentation

- Showing form factors of X, Y slices: Can segment, approximately…



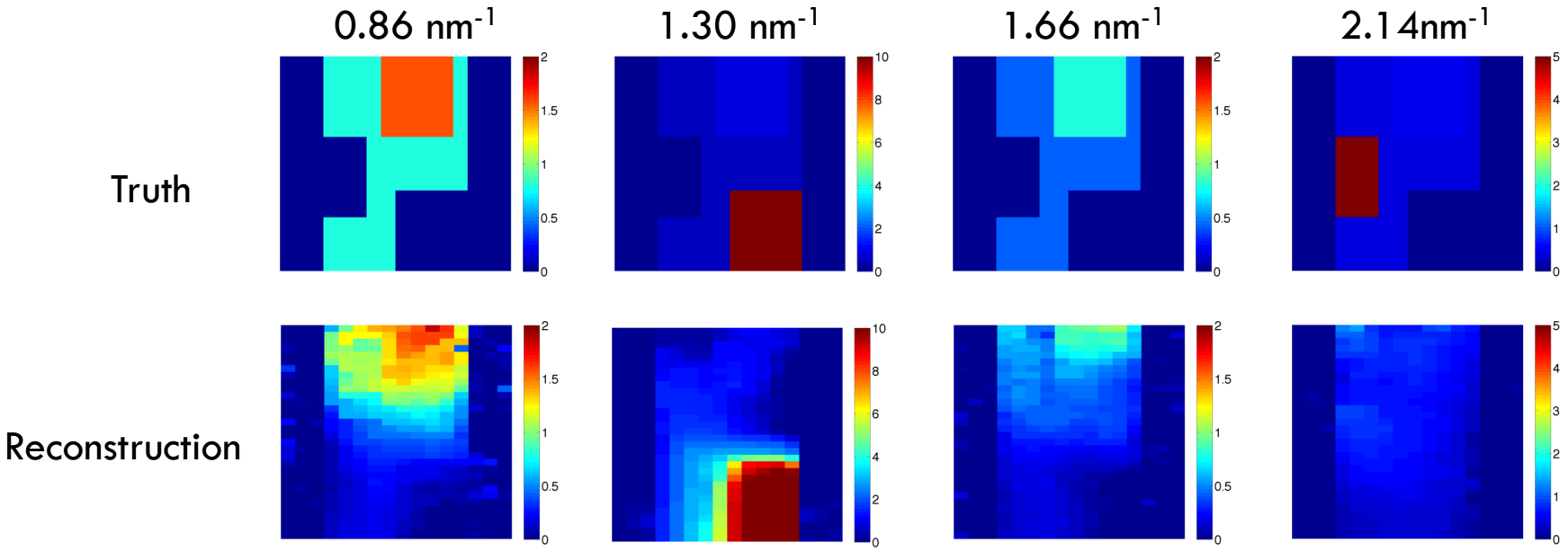
Avoiding Local Minima

- Initialize IREP after Segmentation

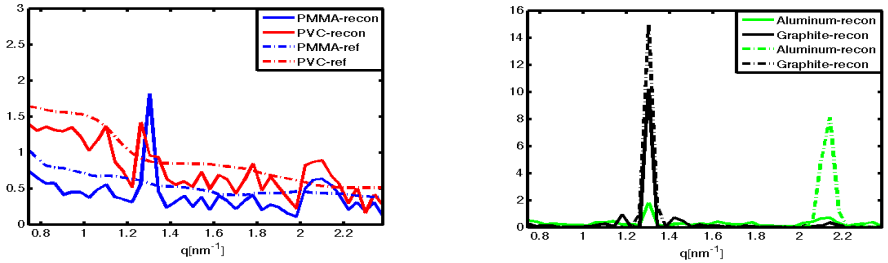


Experiment 6

- Phantom: Tall rectangular solid, reconstructing a slice
- Architecture: Coded aperture, 3 views (-60, 0, 60) degrees, with intensity detectors, multi-energy illumination, ideal noiseless case



Estimated form factors, averaged over true region



Summary

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- Iterative reconstruction algorithms are promising for reconstruction of XDI images
  - Good localization and characterization of materials with well-defined Bragg peaks
  - Harder to get accurate reconstruction of liquids and other amorphous materials in the presence of stronger scatterers nearby
- Architectures with photon-counting detectors offer improved reconstruction
  - Higher dimensional measurement, better conditioned reconstruction
- Attenuation correction requires fusion with CT or equivalent normalization for different architectures
- Major challenges remain:
  - Computation requirements for reconstruction
  - Architecture design for improved signal/noise ratio
  - Explosives detection/classification using reconstructed signals for liquids and HME classes