Atomic Super-Resolution Tomography

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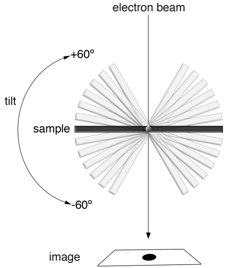
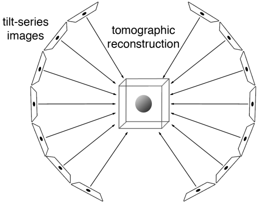
International Workshop on Combinatorial Image Analysis

Problem setting





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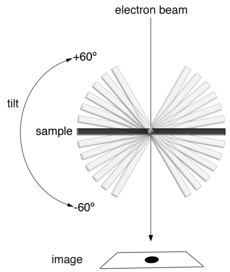

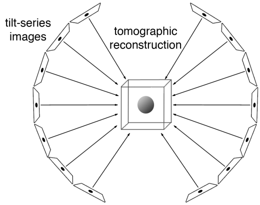

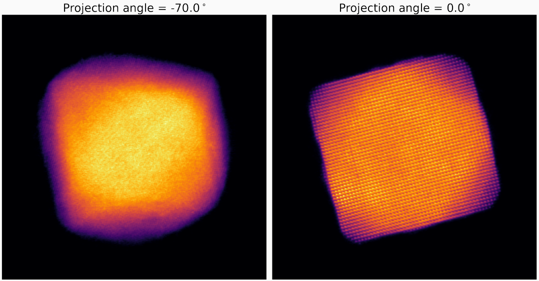

Projection images of a Pt nanoparticle

(E. A. Irmak, EMAT)

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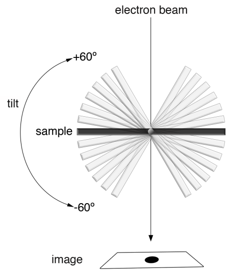

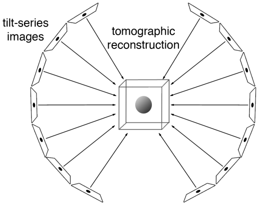

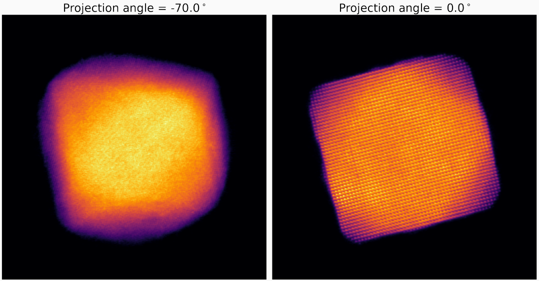

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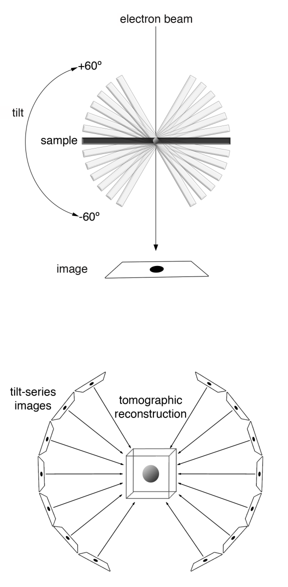

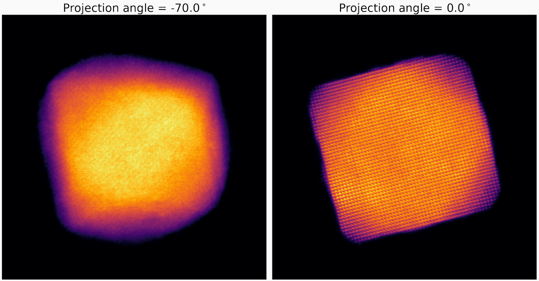

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! Infinite-dimensional optimisation

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Assume atoms lie on a fixed grid

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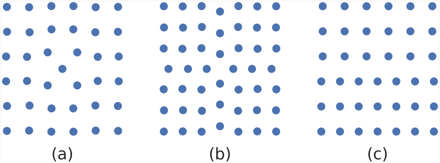
! Finer grids to resolve defects



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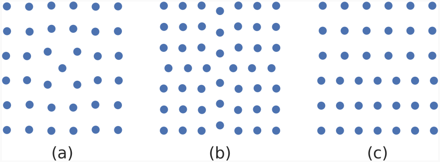

✗ More ill-posed problem

✗ Higher computational times

Super-resolution tomography

- Remove requirement for atoms to lie on a grid
- Keep assumption of discrete weights
- Add potential energy of the configuration as a physical prior

$$\underset{\boldsymbol{x}\in\mathcal{C},\, w\in\{0,1\}^n}{\text{minimise}} \quad \left\| \sum_{i=1}^{n} w_i \psi(\boldsymbol{x}_i) - y \right\|_2^2 + \alpha V_{\text{tot}}(\boldsymbol{x}), \tag{4}$$

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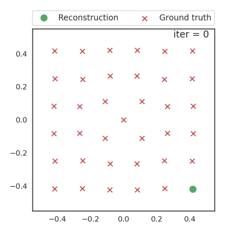
Solve using modified alternating descent conditional gradient (ADCG) algorithm[1]

[1]Boyd, Nicholas, Geoffrey Schiebinger, and Benjamin Recht. "The alternating descent conditional gradient method for sparse inverse problems." (2017)

Reconstruction results



One reconstruction run
using ADCG + energy

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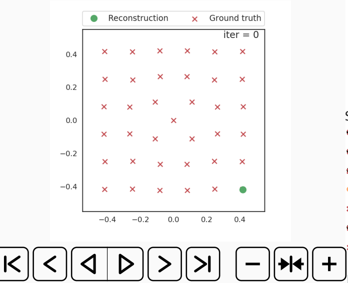

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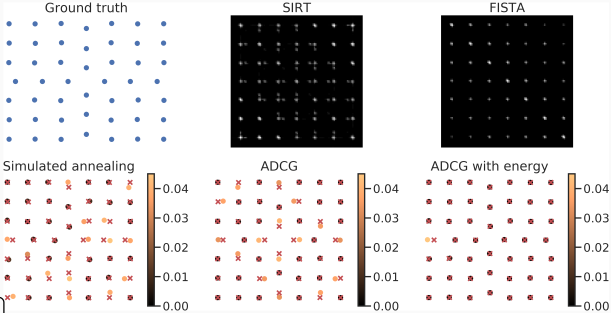
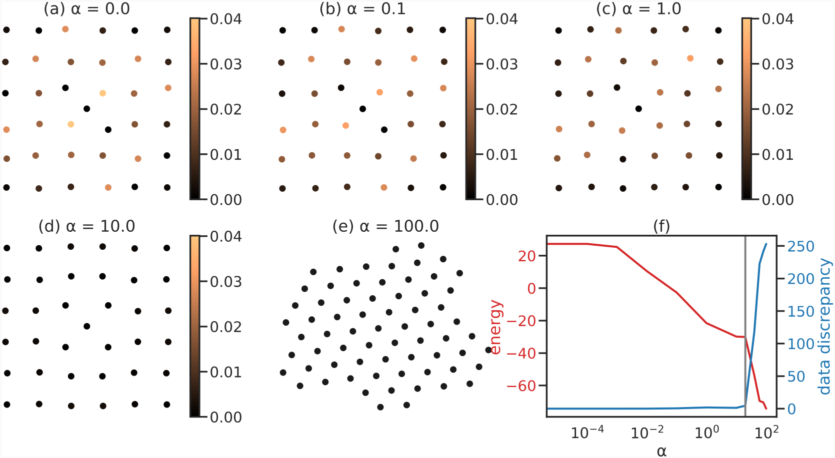


Reconstructions of a vacancy defect from 3 projections. For simulated annealing, ADCG and ADCG with energy, the atoms are coloured according to the distance from the ground truth (red crosses)

Effect of adding energy



Increasing the weighting of the potential energy term amounts to moving from data-optimal to energy-optimal configurations

Thank you for your attention!

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