Modifications to the EMC algorithm for orientation recovery in Single Particle Imaging experiments on X-ray free electron lasers

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Supported by HRSF-0002/18-41-06001

X-ray Free Electron Lasers

Key properties:

- Very bright radiation
- Extremely short pulses (10 fs)
- High repetition rate

European XFEL (2017)

European
XFEL

SwissFEL (2016)

PAUL SCHERRER INSTITUT
PSI

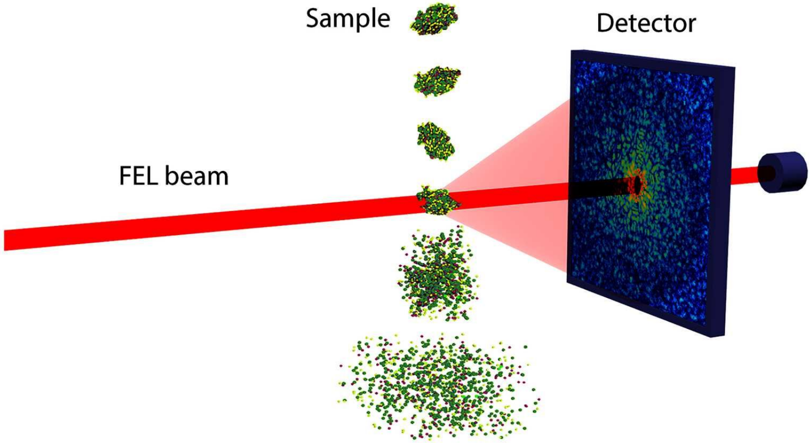
PAL XFEL (2017)

PAL
POHANG ACCELERATOR LABORATORY

LCLS (2009)

SLAC
NATIONAL ACCELERATOR LABORATORY

Single Particle Imaging



“Diffraction before destruction” principle takes care of radiation damage problem.

Destroying the sample however, makes it necessary to use many identical samples that enter the beam in an unknown orientation.

Orientation recovery problem

EMC algorithm

Set of diffraction images

$$D_i,\ i = 1 \ldots N$$

→

3d density in reciprocal space

$$W$$

Iteration t:

Expansion

Convert 3d density to tomographic representation W_j - points corresponding to image in *j-th* orientation.

Maximization

$$W_j^t \longrightarrow W_j^{t+1}$$

Compression

Convert W_j back to regular grid and impose Friedel symmetry.

Maximization step (EM)

Expectation: for each image D_i compute probability of being in *j-th* orientation $P_{ij}(W_j^t, D_i)$

Maximization: compunte new densities so that total likelihood is maximized

$$W_j^{t+1}(P_j, D) = \frac{\overbrace{\sum_i P_{ij} D_i}^{A_j^{t+1}}}{\underbrace{\sum_i P_{ij}}_{B_j^{t+1}}}$$

Online EM

Expectation: calculate the probabilities only for 1 image

$$P_{i*j}(W_j^t, D_{i*})$$

Maximization: compunte new densities so that total likelihood is maximized, based on only 1 set of updated probabilities

$$W_j^{t+1}(P_{i*j}, D)$$

Incremental EMC

Reuse the old probabilities P_{ij}^{old} for $i \neq i^*$

$$W_j^{t+1} = \frac{A_j^t + P_{i*j} D_{i*} - P_{i*j}^{old} D_{i*}}{B_j^t + P_{i*j} - P_{i*j}^{old}}$$

Stepwise EMC

Interpolate between old W_j and a new one calculated only from $P_{i*j}(W_j^t, D_{i*})$

$$W_j^{t+1} = \frac{(1-\eta_t)A_j^t + \eta_t P_{i*j} D_{i*}}{(1-\eta_t)B_j^t + \eta_t P_{i*j}}$$

Adaptive over-relaxed EMC

Maximization step:

$$W_j^t \longrightarrow W_j^{t+1}$$

Instead of using W_j^{t+1}, which maximizes total likelihood, we go in that “direction” further:

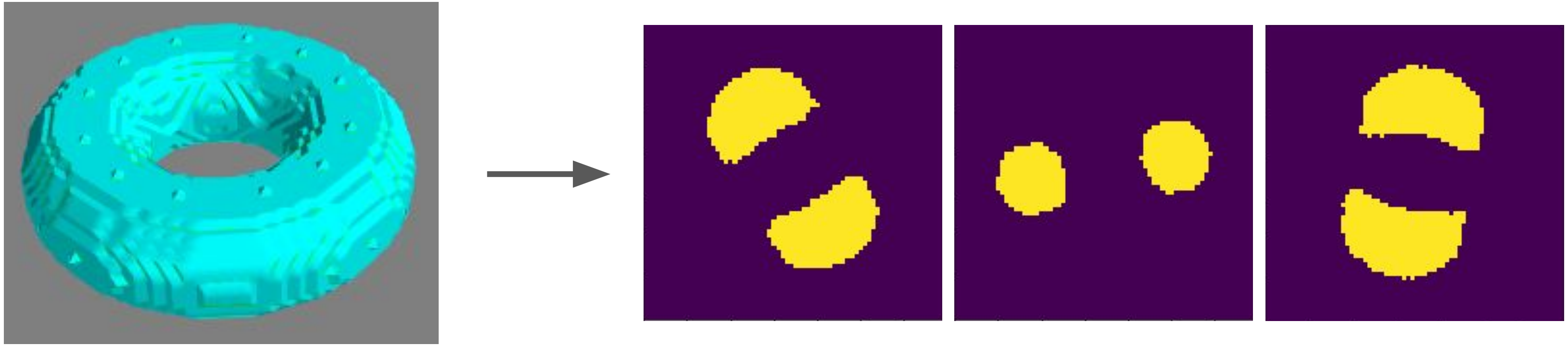
$$\overline{W_j^{t+1}} = W_j^t + \alpha(W_j^{t+1} - W_j^t),\ \alpha > 1$$

Where coefficient α is adaptively changed:

If $\overline{W_j^{t+1}}$ increases likelihood compared to W_j^t, then we increase α, otherwise we set α to 1 and use W_j^{t+1} instead of $\overline{W_j^{t+1}}$ as our current approximation.

Testing the algorithms

Generating data

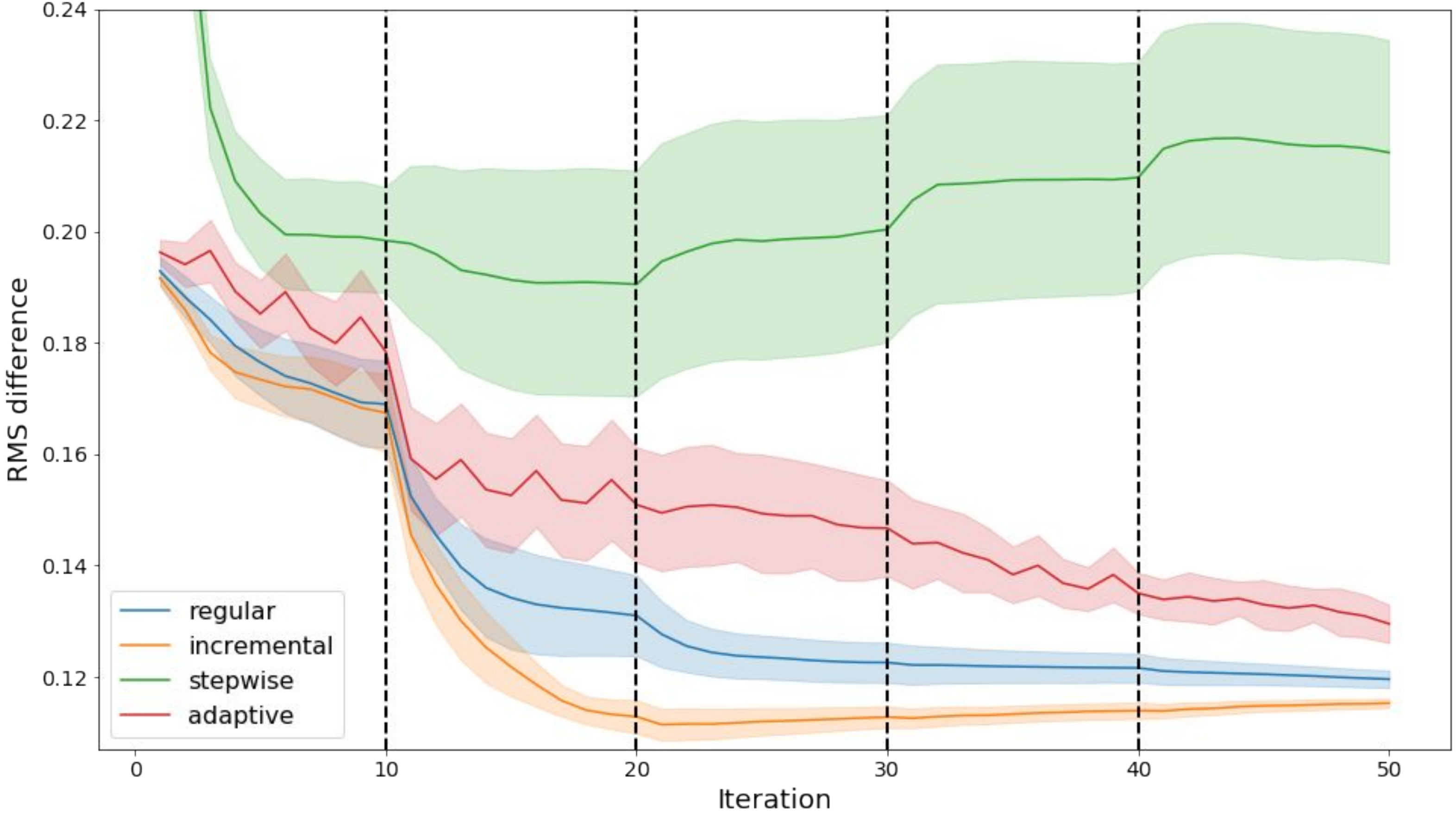


1380 images
50 (10x5) iterations

Iterations	1-10	11-20	21-30	31-40	41-50
# of orientations	420	1380	3240	6300	10360

Assessing the results - RMS difference between initial model and the reconstruction.

RMS difference between model and reconstructions



Thanks for your attention!