

The Fluence-Resolution Relationship in Holographic and Coherent Diffractive Imaging: Supplement Information

Johannes Hagemann, Tim Salditt (tsaldit@gwdg.de)

Universität Göttingen
Institut für Röntgenphysik,
Friedrich-Hund-Platz 1
37077 Göttingen Germany

March 14, 2017

1 Simulation Details and Implementation

Here we want to give a short overview of the numerical implementation of the simulation using MATLAB (2016a). When the numerical experiments have been set up different phase retrieval algorithms have been tested as alternating projections (e.g. Gerchberg-Saxton and error-reduction algorithm) and the hybrid-input-output algorithm. The results have shown that for our setup, the number of iterations and constraints in use RAAR yielded the best results. Listing 1 shows the minimal implementation of RAAR, which lacks for example the error control. The simulations are sped-up by the use of GPUs. In order to use GPUs more efficiently some data is moved explicitly in the RAM of the GPU e.g. lines 9 and 10. Listing 2 shows the near-filed implementation of RAAR. Only the main differences are shown, these are (i) an additional call parameter \mathbf{F} (ii) the modified P_M for which we use 2 `PropagatorGPU` objects, for forward and backward propagation.

Lsting 3 shows the wrapper function which generates the test data and carries out resolution analysis. The structure of this script is the following first we set some parameters L. 6-20, then the phantom is chosen and set up L. 21-44. Then the NFH reconstruction and FRC calculation is carried out L. 46-67 followed by the CDI reconstruction L. 70-93. We note that CDI reconstructs the object somewhere in the support thus it is necessary to align the reconstruction with the phantom in order to get correct resolution and error measurements. NFH is in this aspect much more indulgent. The code and helper functions can be found on GitHub: <https://github.com/JHoahg/Resolution-and-Fluence>.

Listing 1: Implementation of RAAR for the far field (RAAR_ff.m).

```

function [result] = RAAR_ff(M, psi, iterations, p)
2 % inputs:
% M           - measurement (amplitudes)
4 % psi       - initial guess
% iterations  - number of iterations
6 % p         - parameters

8 h = waitbar(0, 'progress');

10 % get input arrays and put them on GPU
M = gpuArray(M);
12 supp = gpuArray(logical(p.supp));

14 % Amp_valid can be used to discriminate bad pixels
Amp_valid = gpuArray(p.Amp_valid);
16 psi = gpuArray(psi);

18 % algorithm parameters from data struct p
b_0 = p.b_0;
20 b_m = p.b_m;
b_s = p.b_s;

22 for ii = 1:iterations
24     waitbar(ii / iterations, h, ...
        sprintf('%d / %d',ii, iterations));

26     % relaxation parameter for current iteration cf. Eq. (??)
28     b = exp(-(ii/b_s)^3)*b_0 + (1 - exp(-(ii/b_s)^3))*b_m;

30     psi_old = psi;

32     % P_M
psi = DFT(psi);
34     psi(Amp_valid) = psi(Amp_valid) ./ abs(psi(Amp_valid)) ...
        .* M(Amp_valid);
36     P_M = IDFT(psi);

38     % R_M
R_M = 2* P_M - psi_old;

40     % P_S
42     % pure phase constraint
psi(supp) = exp(1i .* angle(R_M(supp)));
44     % support and negativity constraint
psi(~supp | angle(psi) > 0) = 1;

46     % R_S
48     psi = 2*psi - R_M;

50     % new RAAR iterate cf. Eq. (??)
% psi = R_S(R_M(Psi_n)) , psi_old = Psi_n
52     psi = (b/2) * (psi + psi_old) + (1-b)*P_M;

54 end
%final projection on M
56 result = gather(psi);
58 close(h);
end

```

Listing 2: RAAR near field implementation, only differences are shown (RAAR_nf.m).

```

function [result] = RAAR_nf(M, psi, iterations, F, p)
2 % ... Same as in RAAR_ff.

4 % Propagator objects
prop = PropagatorGPU(F, F, size(M,2), size(M,1));
6 prop_back = PropagatorGPU(-F, -F, size(M,2), size(M,1));

8 % ...
for ii = 1:iterations
10 % ...
    %  $P_M$ 
12     psi = prop.propTF(psi);
    psi(Amp_valid) = psi(Amp_valid) ./ abs(psi(Amp_valid)) .* M(
        Amp_valid);
14     P_M = prop_back.propTF(psi);
    % ...
16 end
18 end

```

Listing 3: Usage example of data generation, algorithms and analysis (fluence_cdi_vs_nfh.m).

```

2 % Setup directories, paths, standard settings...

4 %% Simulation parameters
% sizes of image and surrounding frame
6 p.width = 512;
p.height = 512;
8 p.width2 = 1024;
p.height2 = 1024;
10 p.rec_width = 1024;
p.rec_height = 1024;

12
14 p.F = 1e-3;
p.num_photons = 200;
p.b_0 = 0.99;
16 p.b_m = 0.75;
p.b_s = 150;
18 p.num_iterations = 200;
p.Amp_valid = logical(true(p.rec_height, p.rec_width));

20
%% Sample Setup - choose dicty or bitmap
22 if(1) %dicty sketch
    %prepare probe reads the images and scales gray values to desired
    phase/amplitude values.
24     sample = prepare_probe('dicty_sketch.png', 'dicty_sketch.png',
        0, 1, 1, 1, p);
    sample = abs(sample) .* exp(1i.*(angle(conj(sample))));
26     p.supp = load('support_dicty_ff.mat');
    p.supp = p.supp.supp.I_supp;
28     p.supp = imresize(p.supp, (p.height/256), 'box');
end

```

```

30
31 if(0) % use binary bitmap
32     upscale = 10;
33     sample = binary_bitmap(10, 10, -1, upscale, p.rec_height, p.
34         rec_width);
35     p.supp = ones(10*upscale, 10*upscale);
36     p.supp(1:floor(10*upscale/2), 1:ceil(10*upscale/2)) = 0;
37 end
38 p.supp = pad_to_size(p.supp, p.rec_height, p.rec_width, 'zero');
39
40 figure()
41 imagesc(angle(mid(sample,p)));
42
43 figure()
44 imagesc(mid(p.supp, p));
45
46 %% NFH data setup, as described in the recipe in Sec. 2
47 prop = Propagator(p.F, p.F, p.width2, p.height2,1);
48 id_holo = abs(prop.propTF(sample)).^2;
49 id_holo = id_holo ./ sum(id_holo(:));
50 figure; imagesc(id_holo)
51
52 if(1) % use RAAR
53     holo = imnoise((id_holo*p.num_photons.* numel(id_holo))*1e-12, '
54         poisson')*1e12;
55     % set 0 to epsilon, otherwise we get NaNs
56     holo(holo == 0) = 2*eps;
57     % this rescaling is necessary to get float numbers again, the
58     reconstruction did not work (also for CDI) for integer numbers
59     in the measurement.
60     holo = holo ./ sum(holo(:)) .* numel(holo);
61
62     holo_rec{1} = RAAR_nf(sqrt(double(holo)), ones(p.rec_height), p
63         .num_iterations,...
64         p.F, p);
65 end
66
67 %% compare with frc
68 p.beta = 7;
69
70 % FSC is a general function to calculate the Correlation in 2d and
71 3d
72 frc_holo_to_ori = FSC(angle((sample)), angle((holo_rec{1})), p);
73
74 %% CDI data setup
75 id_FT = abs(DFT(sample)).^2;
76 id_FT = id_FT ./ sum(id_FT(:));
77 figure; imagesc(log10(abs(id_FT)));
78 %%
79 if(1)
80     FT = imnoise((id_FT*p.num_photons.* numel(id_FT))*1e-12, 'poisson
81         ')*1e12;
82     FT(FT == 0) = 2*eps;
83     FT = FT ./ sum(FT(:)) .* numel(FT);

```

```

80     [CDI_rec{1}] = RAAR_ff(sqrt(FT),...
81         exp(1i .* rand(p.rec_height)), p.num_iterations, p);
82 end
83
84 %% compare with frc
85 p.beta = 7;
86
87 % in CDI we have to align the reconstruction with the original,
88 % since the reconstruction can be shifted in the reconstruction
89 % array
90 [err, aligned_sample] = dftregistration(fft2(angle(CDI_rec{1})),...
91     fft2(angle(sample)), 5);
92 % err
93 aligned_sample = (ifft2(aligned_sample));
94 frc_CDI_to_ori = FSC(angle((CDI_rec{1})), aligned_sample, p);
95
96 %% compare both
97 % make nice pictures of results

```