Direct access to the moments of scattering distributions in x-ray imaging

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The scattering signal obtained by phase-sensitive x-ray imaging methods provides complementary information about the sample on a scale smaller than the utilised pixels, which offers the potential for dose reduction by increasing pixel sizes. Deconvolution-based data analysis provides multiple scattering contrasts but suffers from time consuming data processing. Here, we propose a moment-based analysis that provides equivalent scattering contrasts while speeding up data analysis by almost three orders of magnitude. The availability of rapid data processing will be essential for applications that require instantaneous results such as medical diagnostics, production monitoring and security screening. Further, we experimentally demonstrate that the additional scattering information provided by the moments with an order of higher than two can be retrieved without increasing exposure time or dose.

In the context of phase-sensitive x-ray imaging techniques, scattering refers to the contrast channel arising from sample inhomogeneities that are smaller than the utilised pixels. The utilisation of such sub-pixel signals allows for increasing the pixel size while maintaining the signal and simultaneously decreasing dose and/or scan times significantly. The sensitivity towards sub-pixel information has been established for different x-ray imaging methods, such as analyser-based imaging (ABI)1,2, grating interferometry (GI)3-5, speckle-based imaging6-8 and edge-illumination (EI).9,10 The potential of x-ray scattering is investigated for mammography10-12, bone structure determination13 and the diagnosis of several pulmonary diseases both in small14-16 and large animals17.

Commonly used data analysis procedures provide a single contrast related to sub-pixel information, which is called the dark-field8 or the scattering signal10. An alternative deconvolution-based approach that provides multiple and complementary scattering contrasts was originally developed for GI18 and extended to tomography19 and recently translated to EI.20 In some applications, it was shown that deconvolution can provide a higher contrast to noise ratio and improved dose efficiency21,22. It was also demonstrated that the complementary contrasts can be exploited for quantitative imaging23 without the need for additional scans required by other approaches5,24,25. While the deconvolution-based analysis is suitable for ABI, GI, and EI, the approach proposed below is not directly applicable to GI due to the sinusoidal nature of the provided signal. Thus, we will introduce the approach for EI and note that all results are directly applicable to ABI.

EI is a non-interferometric, phase-sensitive x-ray imaging technique that uses a pair of apertured masks (Fig. 1). The pre-sample mask confines the incident x-rays into smaller beamlets, which are broadened by the sample due to scattering. The broadening is transformed into a detectable intensity variation by the detector mask that features apertures covering most of the detector pixels. The comparably large structure sizes of the optical elements (typically tens of microns) allows for simple mask fabrication23 and renders EI robust against vibrations and thermal variations. EI is readily compatible with laboratory-based x-ray tubes due to the achromaticity of the optical elements and the entire x-ray spectrum contributes to the signal26,27.

Accessing multiple scattering contrasts by deconvolution is based on the following approach. Scanning the pre-sample masks laterally by a fraction of its period provides a Gaussian-like intensity curve in each detector pixel. Repeating the scan with and without the sample yields the signals s(α) and f(α), respectively. Here, the scattering angle α is defined in a plane perpendicular to the line apertures of the utilised mask (Fig. 1). Scattering in the orthogonal direction does not change the detectable signal and, thus, can be omitted for the rest of the discussion. The angularly resolved scattering distribution g(α), which represents the sample’s scattering signal within one pixel, is then implicitly defined by9,10,20,28,29

\[ s(\alpha) = f(\alpha) \otimes g(\alpha), \]  

where \( \otimes \) denotes the convolution operator. The scattering distribution g(α) can be accessed from experimental

\[ g(\alpha) = \frac{s(\alpha)}{f(\alpha)} \]  

FIG. 1. Set-up for x-ray imaging based on edge-illumination. The scattering angle α is given by the geometry of the set-up.
deconvolving $s(\alpha)$ with $f(\alpha)$ and iterative Lucy-
Richardson deconvolution\cite{30,31} has been established as a
technique useful for PSF estimation in digital imaging. The 4th iteration step of the de-
convolution is performed by computing

$$g^{k+1} = g^k \times \left( \frac{s}{g^k \otimes f} \otimes \bar{f} \right),$$  \hspace{1cm} (2)

where $\bar{f}$ denotes $f$ mirrored at the origin. Usually, the
sample signal is chosen as the starting value: $g^0 = s$.
Lucy-Richardson deconvolution features an implicit posi-
tive constraint and is guaranteed to converge to the maxi-
mum likelihood solution if the experimental noise is given
by Poisson statistics, which is commonly the case in x-ray
imaging\cite{32,33}.

In order to retrieve multiple contrasts relating to the
shape of $g$ a moment analysis can be applied to the scat-
tering distributions. Depending on normalisation and cen-
tralisation different definitions of the moments need
to be distinguished. The un-normalised, un-centralised
moments of an arbitrary function $h(\alpha)$ are given by

$$M_n(h) = \int \alpha^n h(\alpha) \, d\alpha,$$  \hspace{1cm} (3)

where $n$ is an integer denoting the order of the moment.
Dividing by $M_0$ yield the normalised, un-centralised mo-
ments

$$\tilde{M}_n(h) = \frac{M_n(h)}{M_0} \quad \text{for} \quad n \geq 1,$$  \hspace{1cm} (4)

and shifting by $\tilde{M}_1$ lead to the normalised, centralised
moments

$$\bar{M}_n(h) = \int (\alpha - \bar{M}_1)^n h(\alpha) \, d\alpha / M_0 \quad \text{for} \quad n \geq 2.$$  \hspace{1cm} (5)

It has been experimentally demonstrated that the first
moment of the scattering distribution $M_0(g)$ corresponds
to absorption, $\tilde{M}_1(g)$ to the differential phase signal and
$\bar{M}_2(g)$ to scattering strength\cite{20}. The relation of these
moments to sample properties are provided in\cite{23}.

Given typical noise levels in experiments, about 1000
iterations steps are required to ensure convergence of the
Lucy-Richardson deconvolution, which may lead to cun-
bersome data processing times. For example, data pro-
cessing of the dragon fly in\cite{20} took around 1 h for a 400
by 300 pixel field of view on a standard desktop PC. This
renders iterative deconvolution unsuitable for time sensi-
tive applications.

Therefore, we propose an alternative data analysis ap-
proach that uses the known moments of convolutions\cite{34},
the derivation of which is briefly sketched in the follow-
ing. The moments defined in eq. (3) appear as derivatives
at zero frequencies in Fourier space

$$M_n(s) = \frac{\sqrt{2\pi}}{(i)^n} \frac{d^n \hat{s}}{dq^n} \bigg|_{q=0},$$  \hspace{1cm} (6)

where the symbol $\hat{}$ denotes the Fourier transform and $q$
the variable in Fourier space. Since $s$ is given by a con-
volution its Fourier transform corresponds to a product:

$$s = f \otimes g \Leftrightarrow \hat{s} = \sqrt{2\pi} \hat{f} \times \hat{g}.$$  \hspace{1cm} (7)

Inserting eq. (7) into eq. (6) and dividing by $M_0$ leads to

$$\tilde{M}_n(s) = \sum_{k=0}^{n} \binom{n}{k} \tilde{M}_k(f) \tilde{M}_{n-k}(g)$$  \hspace{1cm} (8)

with the binomial coefficient $\binom{n}{k}$. Similar equations
hold true for the normalised, centralised moments $\bar{M}_n$\cite{34},
which can be solved for the moments of $g$. The result for the
first five moments are:

$$\begin{align*}
M_0(g) &= M_0(s) / M_0(f) \quad \text{(9)} \\
M_1(g) &= \tilde{M}_1(s) - \tilde{M}_1(f) \quad \text{(10)} \\
\tilde{M}_2(g) &= \tilde{M}_2(s) - \tilde{M}_2(f) \quad \text{(11)} \\
\tilde{M}_3(g) &= \tilde{M}_3(s) - 3 \tilde{M}_1(f) \tilde{M}_2(s) \quad \text{(12)} \\
\tilde{M}_4(g) &= \tilde{M}_4(s) - 6 \tilde{M}_2(f) \tilde{M}_2(s) \quad \text{(13)}
\end{align*}$$

First moment terms do not appear in equations with $n > 1$ be-
cause $\tilde{M}_1 = 0$. For the scattering width $\tilde{M}_2$ the above
equation is in agreement with published results\cite{36}. Since
the moments of $s$ and $f$ can be directly calculated from
experimental data, eqs. (9)-(13) provide direct access to
the moments of the scattering distribution $g$ without the
need for time consuming iterative deconvolution.

In order to experimentally compare the results of de-
convolution and direct moment analysis, we used an EI-
based imaging system at University College London. A
Rigaku MM007 rotating anode with a Mo target was used
as an x-ray source and operated at 25 mA current and
40 kVp voltage. The pre-sample mask consisted of a
series of Au lines on a graphite substrate with a pitch
of 79 $\mu$m and an opening of 10 $\mu$m, while the detector
mask had a pitch of 98 $\mu$m and an opening of 17 $\mu$m.
Both masks were manufactured by Creatv Microtech
(Potomac, MD). The x-ray detector was a Hamamatsu
C9732DK flat panel sensor featuring a binned pixel size
of 100 $\mu$m. The sample to detector distance was 0.32 m
and the total set-up length 2 m.

The sample was a dragon fly, which was known to pro-
vide a sufficient signal for the first five moments. The
sample mask was scanned over one pitch with 32 steps
and an exposure time of 25 s per step. The same data
set was used for the deconvolution (eq. 2) and moment
analysis (eqs. 9-13). The resulting scattering contrasts
(Fig. 2) show an excellent visual agreement between the
two approaches, while data processing for direct moment
analysis was about 600 times faster than for deconvo-
lation. Furthermore, direct moment analysis eliminates
the number of iteration steps as a necessary parameter for
deconvolution.

Table I presents a performance comparison of decon-
volution and moment analysis. The high degree of visual
agreement between the approaches is confirmed by the correlation factors ($\geq 0.9$ for all contrasts). Columns 3 and 4 compare the standard deviation of the signals in a 50x50 pixel background area as a measure of the noise level in the two analysis approaches. With the exception of $M_2$ (details discussed below), both approaches deliver the similar noise levels.

For the 2nd moment, the scatter plot of values retrieved by deconvolution and moment analysis (Fig. 3) reveals a discrepancy for scattering strengths that are small compared to the width of the flat-field scan ($\tilde{M}_2(g) \leq 0.05 \times \tilde{M}_2(f)$). In this case, the deconvolution approach (eq. 2) does not retrieve the correct $\delta$-shaped signal for $g$ due to the presence of noise, but will retrieve a signal with $\tilde{M}_2(g) > 0$. The moment analysis, on the other hand, is not subject to such a restriction. The difference in bias between the two approaches is also reflected in the mean of the background areas, which are 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 $\tilde{M}_2$ from deconvolution / $\tilde{M}_2$ (flat)
-0.1 0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0 $\tilde{M}_2$ from moment analysis / $\tilde{M}_2$ (flat)

TABLE I. Performance comparison of the two data analysis approaches for the first five moments shown in Fig. 2. 2nd column: correlation between the results of deconvolution and moment analysis. 3rd and 4th column: standard deviation of the signals in the background. The additional entry for $M_2$ relates to the standard deviation of larger scattering values (see text for explanation).

<table>
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<th>$M_0$</th>
<th>$M_1$</th>
<th>$M_2$</th>
<th>$M_3$</th>
<th>$M_4$</th>
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<td>0.99</td>
<td>0.90</td>
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<tr>
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<td>6.5 x 10^{-8} rad</td>
<td>8.3 x 10^{-12} rad^2</td>
<td>3.1 x 10^{-16} rad^3</td>
<td>4.4 x 10^{-20} rad^4</td>
</tr>
<tr>
<td>(6.7 x 10^{-11} rad^2)</td>
<td>(6.7 x 10^{-11} rad^2)</td>
<td></td>
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</tbody>
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FIG. 2. Comparison of four moments retrieved by deconvolution (left column) and moment analysis (right column). The sample was a dragonfly and the two data analysis approaches deliver practically identical results. Pixel size is 100 $\mu$m and scale bars are 5 mm.

FIG. 3. Scatter plot of $\tilde{M}_2$ as retrieved by deconvolution and moment analysis. The $M_2$ values have been normalised by the mean of $\tilde{M}_2$ in the flat scan ($\tilde{M}_2(f) = 7 \times 10^{-10}$ rad^2). For small values of $M_2(g)$ there is a noticeable discrepancy between the results of the algorithms, which is due to the inability of the deconvolution approach to retrieve a scattering distribution with zero width in the presence of noise.
points are required for the linear independence of 5th moment, increasing the number of scan points increases the number of accessible and complementary scattering information.

To this end, we acquired an additional data set, where we varied the number of scan points from 4 to 11, while keeping the total exposure time constant (200 s). We used the standard deviation of the different scattering contrasts in a background area retrieved by direct moment analysis to quantify the dependency. As can be seen in Fig. 4 the noise levels vary within a small 15% interval, which implies that the sensitivity of the different contrasts does not change significantly with the number of scan points. In essence, this means that moment analysis provides the additional scattering contrasts (i.e., moments with order higher than 2) without the need to increase total exposure time or dose.

In conclusion, we have established a direct moment analysis as an alternative approach for retrieving multiple scattering contrasts for EI. We also suggest that this approach can be readily extended to ABL. Direct moment analysis delivers results equivalent to previously utilised deconvolution, while speeding up data processing by almost three orders of magnitude and providing unbiased values for small or absent scattering signals. Furthermore, we have experimentally demonstrated that increasing the number of scan points while keeping total exposure time and dose constant provides additional scattering information without losing sensitivity. Fast data processing that provides reliable scattering contrasts will be crucial for applications demanding rapid feedback, such as medical diagnostics, production monitoring and security screening.

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$\tilde{M}_2$ from moment analysis / $\tilde{M}_2$ (flat)

$v$ from deconvolution / $v$ (flat)

$y=x$