Geometric calibration in X-ray fluorescence tomography using opposite-detector consistency conditions

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A novel set of data consistency conditions (DCCs) tailored to X-ray fluorescence computed tomography (XFCT) is proposed, explicitly accounting for self-absorption. These DCCs enable estimation of the center of rotation from a single pair of projections separated by half a turn and acquired from opposing detectors. They also allow for partial rigid-motion compensation of the sample. This method offers a marker-free, analytical calibration for XFCT.

Introduction

In X-ray fluorescence computed tomography (XFCT), 3D elemental maps are reconstructed from 2D fluorescence projections, but accuracy relies on precise geometric calibration. Transmission tomography data, often collected simultaneously, can assist calibration but fails when attenuation is too low for sufficient contrast. Existing transmission-based alignment methods—such as marker tracking, reprojection motion correction, and autofocus center-of-rotation estimation—have been adapted to XFCT, yet, to the authors' knowledge, no analytical approach explicitly accounts for XFCT-specific self-absorption effects. We introduce new data consistency conditions (DCCs) for dual-detector XFCT that incorporate self-absorption and correlate opposite-detector signals, enabling center-of-rotation and motion estimation without transmission data. Simulations confirm the method's effectiveness.

Geometry and Test Phantom

In XFCT, a pencil beam is typically scanned across the sample to excite fluorescence along the incident beam path, with two detectors positioned in the $+s$ and $-s$ directions (Fig. 1).

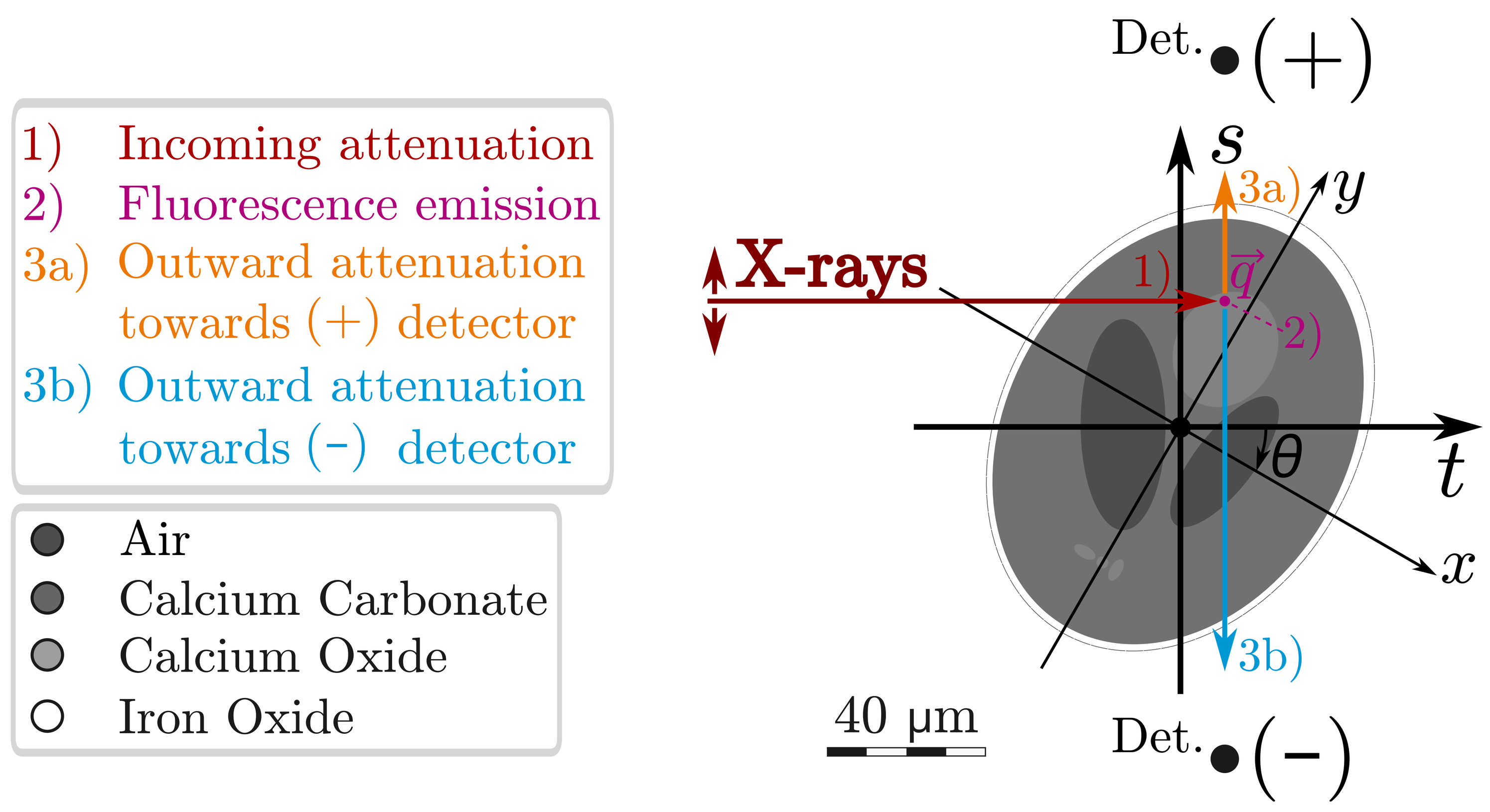

Fig. 1: Typical XFCT geometry with a fluorescence phantom.

The fluorescence tomography projection for a given element depends on the incident beam intensity (I_0), the fluorescence probability (f) and the inward (T_{in}) and outward ($T^{(\pm)}_{\text{out}}$) transmission, as defined in Eq. (1).

$$p^{(\pm)}(s,\theta) = I_0 \int_{-\infty}^{\infty} T_{\text{in}}(\vec{q},\theta) f(\vec{q},\theta) T^{(\pm)}_{\text{out}}(\vec{q},\theta)\Big|_{\vec{q}=s\hat{s}+t\hat{t}} dt \quad (1)$$

Half-Turn Symmetry

Under a half-turn $\mathcal{R}_\pi$, $T^{(+)}$and $T^{(-)}$, are interchanged and the projection $\mathcal{P}$ of every point on s is mirrored about the center of rotation s_c (Fig. 2).

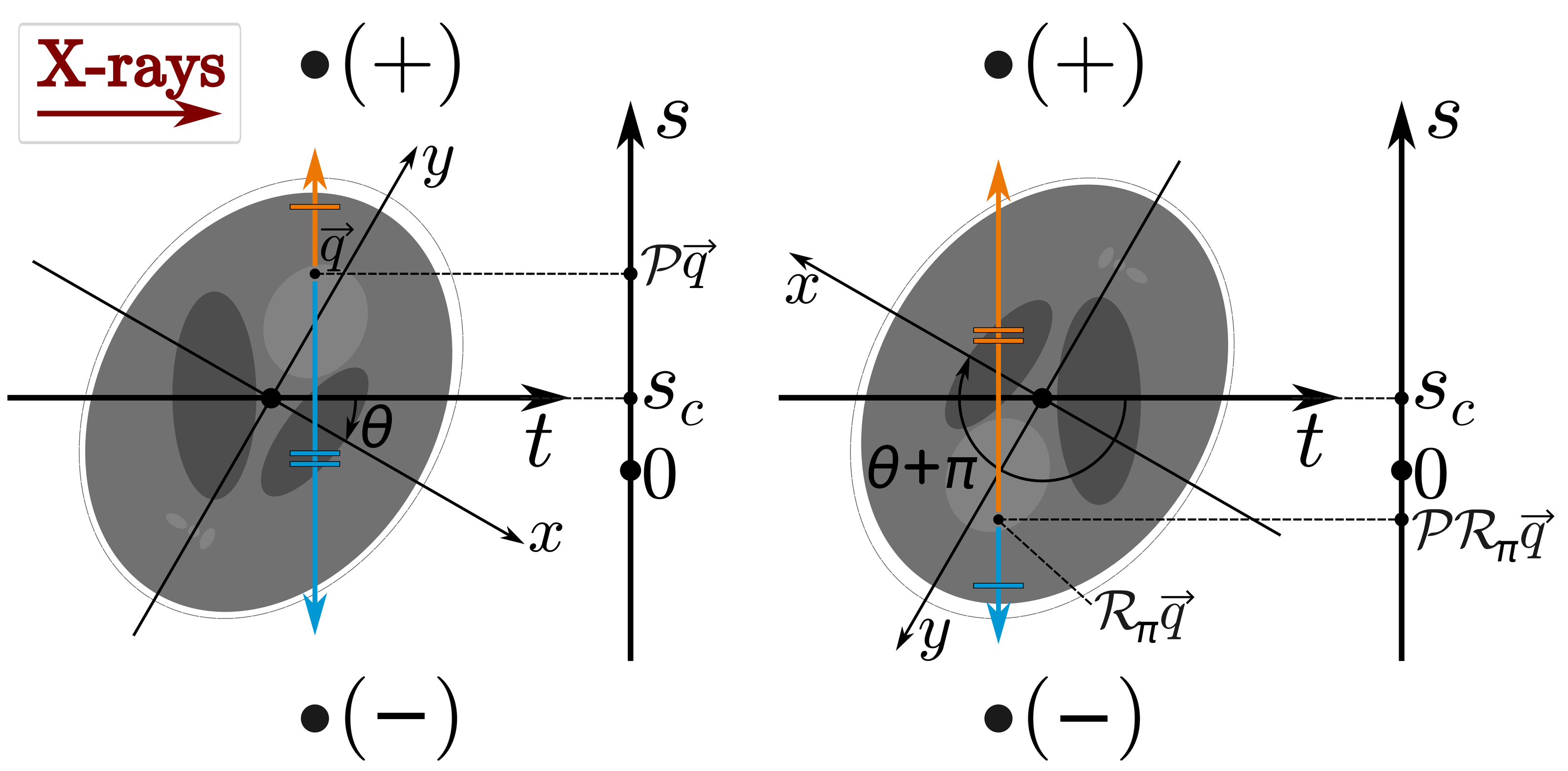

Fig. 2: Rotational symmetry in transmission under a π-rotation.

Neglecting the attenuation of the high-energy incident beam, this then gives the projection DCC stated in Eq. (2).

$$p^{(\pm)}(s,\theta) = p^{(\mp)}(2s_c - s, \theta+\pi) \quad (2)$$

Substituting Eq. (2) into the definition of the n-th order moment yields the set of moment-relation DCCs given in Eq. (3).

$$\begin{aligned} J_n^{(\pm)}(\theta) &:= \frac{\int_{-\infty}^{\infty} s^n p^{(\pm)}(s,\theta) ds}{\int_{-\infty}^{\infty} p^{(\pm)}(s,\theta) ds} \\ &= (-1)^n \sum_{k=0}^{n} \binom{n}{k} (-2s_c)^k J_{n-k}^{(\mp)}(\theta+\pi) \end{aligned} \quad (3)$$

Center-of-Rotation Determination

Using the first-order case in Eq. (3), the center of rotation s_c can be expressed as in Eq. (4). Simulation with the known phantom [1] at an incident beam energy of 20 keV shows that the s_c estimated via Eq. (4) closely matches the true value, with only minor deviations from neglecting incident-beam attenuation (Fig. 3). Averaging s_c over all angles further reduces this discrepancy.

$$s_c = \frac{1}{2}\left[J_1^{(+)}(\theta) + J_1^{(-)}(\theta+\pi)\right] \quad (4)$$

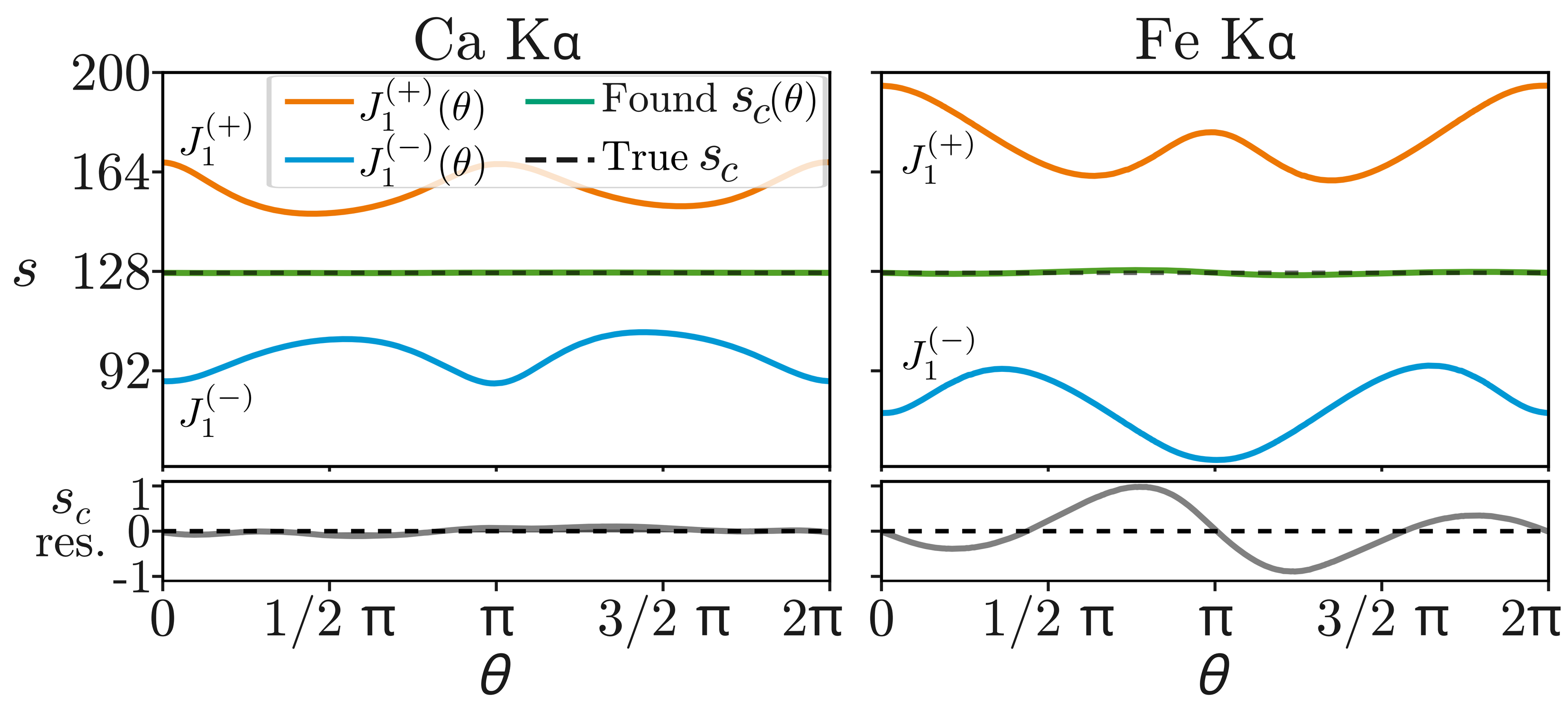

Fig. 3: Comparision between estimated and true s_c.

Motion Estimation

In the presence of motion, perturbed moments J_1^* are recorded, exhibiting angle-dependent shifts $\delta s(\theta)$. By adjusting Eq. (4), the sum of two shifts separated by a half-turn can be obtained, as expressed in Eq. (5).

$$\delta s(\theta) + \delta s(\theta+\pi) = J_1^{*(+)}(\theta) + J_1^{*(-)}(\theta+\pi) - 2s_c \quad (5)$$

Approximating the error as equally distributed over pairs enables shift estimation (Fig. 4). For purely random motion, this yields a 50% reduction in mean squared error, with performance varying across motion types.

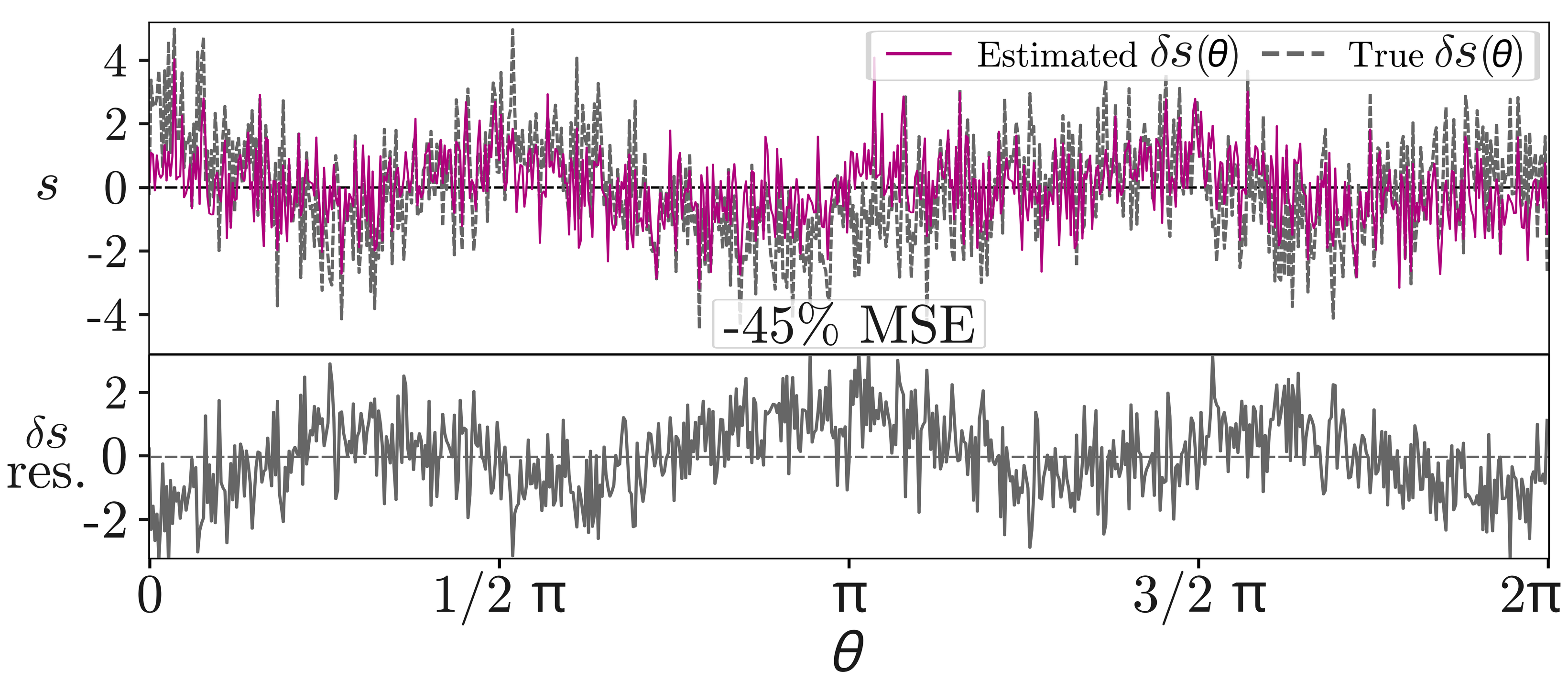

Fig. 4: Example comparison of estimated and ground-truth motion.

Conclusion

A novel set of XFCT-specific data consistency conditions (DCCs) is proposed and validated through simulation, accounting for self-absorption and applicable when transmission contrast is insufficient. These DCCs enable determination of the center of rotation using a single pair of projections acquired from opposing detectors and separated by half a turn. Additionally, the DCCs can be used to estimate and correct for sample motion.

[1] N. Viganò and V. A. Solé. Physically corrected forward operators for induced emission tomography: a simulation study. Measurement Science and Technology, Advanced X-Ray Tomography:1–26, November 2017.