Computational Approach of High Efficiency CT (HECT)™ in TEM/STEM

W. R. Jarisch

Cyber Technology, Inc., 11102 Candlelight Lane, Potomac, MD 20854

High Efficiency Computed Tomography (HECT) uses a Bayesian setup to implement an efficient new estimation technique for 3D density estimation in electron tomography. The technique structurally resembles the Kalman filter [3] and solves three key issues of present TEM/STEM CT: speed, accuracy, and constraints [1,2,7,8]. Incorporating constraints provides an extra component of efficiency by reducing the number of projections required to achieve high quality 3D images. Reducing the number of projections directly accelerates computation and may significantly reduce radiation induced sample damage.

The key to the rapid computation of HECT in TEM/STEM is the formulation of a non-linear estimation problem combined with successive linearizations. Constraints such as the requirement of positive densities are achieved by placing the pole of a logarithmic data transformation [4] at zero density during the inversion computation (typically a back-projection procedure) while updating an initial 3D density estimate in the logarithmic domain. By contrast, the forward projection is computed in true density representation and allows for residual error examination (Fig. 1). For purposes of computing updates, residual errors are defined as log-transformed ratios of the observed versus the predicted densities. These residuals are filtered over suitable projection ranges with inverse filters that represent the appropriate Wiener filter for a particular volume element (voxel). Note that these filters are generally spatially variable, even when considering parallel projection [5]. The iterative nature of the procedure, however, typically allows for the use of a single central voxel for the evaluation of a set of impulse responses and their corresponding Wiener filters. Furthermore, the iterative multi-grid nature of the procedure keeps errors small thereby providing efficient linear error correction.

In many situations [1,7] when measurement noise is present, HECT requires very few iterations to converge. Tomographic 3D reconstruction of HAADF-STEM catalyst data from 70 projections [10] requires one iteration (judged from residual errors) at the highest resolution multi-grid density estimate – the most significant computational burden. The residuals allow for overall systems evaluation. Here they show some inconsistency/imperfections in the original HAADF-STEM data (Fig. 1). The mechanism for this raw projection data inconsistency is not yet understood.

Interestingly, the reconstruction with little or no noise is considerably more difficult than that with noise. The reason for this is seen via the Bayes concept expressed in the Kalman filter variance update $R_{yy} = (H P_0 H^t + R_{vv})$, with observations y, observation noise v, prior covariance P_0 of the density, and the projection matrix H. The variance R_{yy} needs to be inverted in order to obtain the update of the density estimate. As long as the observation noise v is large, it will tend to make R_{yy} well conditioned and make related expressions involving its inverse numerically robust [9]. For 45 *noiseless* simulated views, Fig. 2 shows HECT requiring about 2 - 5 iterations for data provided by [10].

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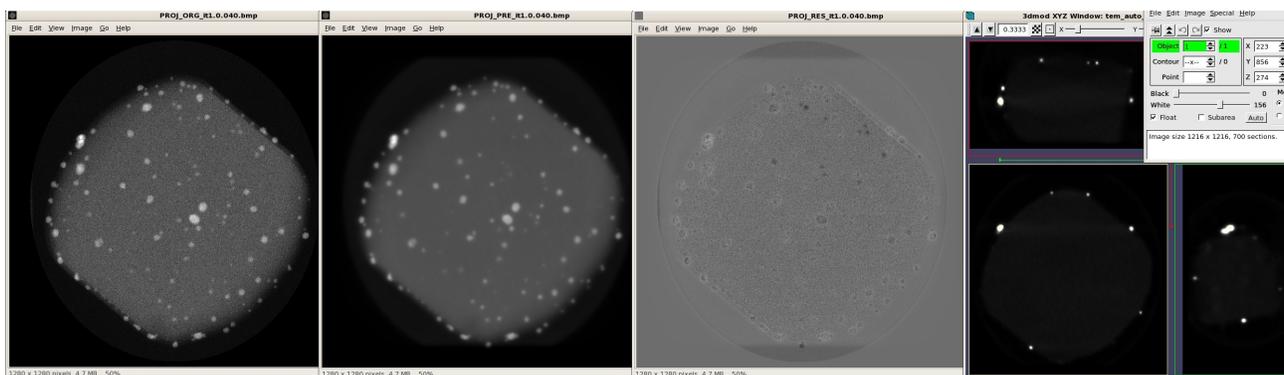
FIG. 1.   Original noisy STEM data. From left-to-right: (a) face-on projection of original catalyst data; (b) projection of the reconstructed 3D density corresponding to (a). Note the reduction of noise; (c) residuals of the reconstructed projection. Note that bead-residuals form groups that are either too dense (brighter) or have too little density (darker) when compared to the gray zero error background. The relationship of groups of beads changes gradually with changing projection directions. The gradual change is an unexplained data inconsistency that might have been missed without residual examination; (d) rendition of a slice through the 3D density with IMOD [6].
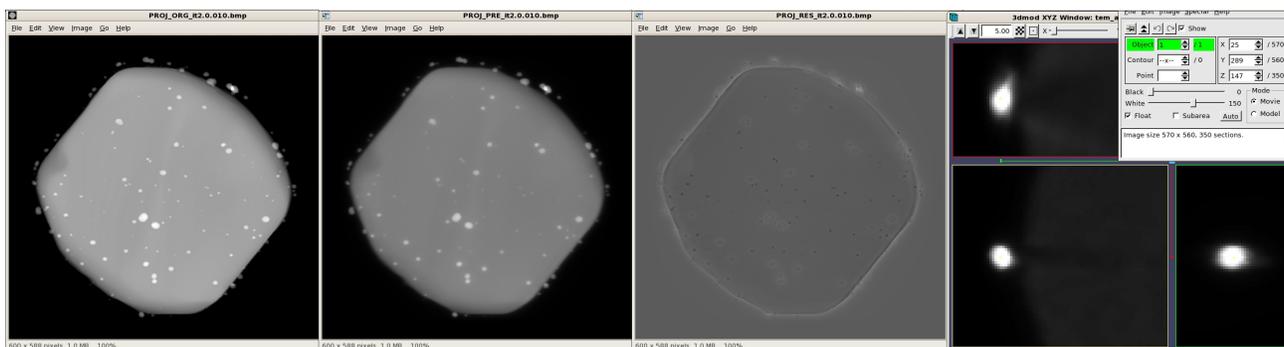

Fig. 2.   Simulated noise-free data. From left-to-right: (a) face-on projection of original data; (b) projection of the reconstructed 3D density corresponding to (a). These noise free reconstruction from 45 projections require at least 2 iterations (shown here) but more satisfying accuracy is achieved with five iterations; (c) residuals of the reconstructed projection. Note that residuals of some of the smaller beads are not yet fully eliminated; (d) rendition of a slice through the 3D density with IMOD.