

Abstract: The aim of this thesis is to investigate applicability of regularization by Krylov subspace methods to discrete inverse problems arising in single particle analysis (SPA). We start with a smooth model formulation and describe its discretization, yielding an ill-posed inverse problem $Ax \approx b$, where A is a linear operator and b represents the measured noisy data. We provide theoretical background and overview of selected methods for the solution of general linear inverse problems. Then we focus on specific properties of inverse problems from SPA, and provide experimental analysis based on synthetically generated SPA datasets (experiments are performed in the Matlab environment). Turning to the solution of our inverse problem, we investigate in particular an approach based on iterative Hybrid LSQR with inner Tikhonov regularization. A reliable stopping criterion for the iterative part as well as parameter-choice method for the inner regularization are discussed. Providing a complete implementation of the proposed solver (in Matlab and in C++), its performance is evaluated on various SPA model datasets, considering high levels of noise and realistic distribution of orientations of scanning angles. Comparison to other regularization methods, including the ART method traditionally used in SPA, clearly shows various advantages of the proposed approach.