UNCERTAINTY QUANTIFICATION FOR LARGE SCALE INVERSE SCATTERING

George Biros
The University of Texas at Austin

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AIR FORCE RESEARCH LABORATORY
AF OFFICE OF SCIENTIFIC RESEARCH (AFOSR)
ARLINGTON, VIRGINIA 22203
AIR FORCE MATERIEL COMMAND
Our goal is the design of fast parallel algorithms statistical inference for scalar and wave propagation problems. We have looked at source inversion and inverse medium problem problems. We use a Bayesian approach in which the regularization appears as prior information and the data mismatch appears as a likelihood information, given known noise probability density functions. A key component of all of our algorithms is the approximation of the Hessian operator. Key components of our work are rank-revealing factorizations, fast extraction of the diagonal of the inverse, adaptivity, and integration of all of these components within a particle filter methodology. In addition, our implementations are being designed to scale on manycore and heterogeneous parallel architectures.

**Subject Terms**
Inverse problems, uncertainty quantification, fast multipole methods, electromagnetic scattering

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**Name of Responsible Person**
Fariba Fahroo

**Telephone Number**
703-696-8429
UNCERTAINTY QUANTIFICATION FOR LARGE SCALE INVERSE SCATTERING
Program Manager: Dr. Fariba Fahroo AFOSR/RTA

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George Biros
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Abstract

Our goal is the design of fast parallel algorithms statistical inference for scalar and wave propagation problems. We have looked at source inversion and inverse medium problem problems. We use a Bayesian approach in which the regularization appears as prior information and the data mismatch appears as a likelihood information, given known noise probability density functions.

A key component of all of our algorithms is the approximation of the Hessian operator. Key components of our work are rank-revealing factorizations, fast extraction of the diagonal of the inverse, adaptivity, and integration of all of these components within a particle filter methodology.

In addition, our implementations are being designed to scale on manycore and heterogeneous parallel architectures.

Figure 1: To demonstrate the effectiveness of our algorithms we have solved a multipoint illumination inverse scattering problem. Here the scatterer is an aircraft (Lockheed SR-71). The first figure from left depicts the discretization mesh; the second figure depicts the illumination due to the incoming field; the third figure depicts the scattered field (data) on a detector plane placed at a distance below the aircraft; the fourth image depicts a reconstruction of the scatterer using the algorithms developed in our group. These simulations were done using the Born approximation for the scalar Helmholtz equation using a boundary integral equation formulation accelerated using our kernel-independent Fast Multipole Method. In the inversion problem, we seek to combine multiple frequency and multiple direction illumination data (rows two and four) to reconstruct the scatterer solving the inverse medium problem. We give more details on the reconstruction in figures 2 and 3.
Introduction

Our goal is to design scalable algorithms for inverse medium and inverse source problems in wave propagation for both time-harmonic and time-domain formulations.

In inverse scattering problems, we seek to reconstruct infinite-dimensional fields by combining models of the underlying physics with observations; typically the underlying input-output (parameter-to-observable) operators are compact and result in ill-posed inverse problems. Severe computational costs of existing methods (e.g., associated with multiple forward and adjoint problem solutions, large dense operators, and strong nonlinearities even when the forward problem is linear) limit problem size and model complexity. In addition, designing effective solution methods that scale well requires application of problem-specific.

In such problems, one is given a noisy measurement of the scattered wave at certain receiver locations and seeks to reconstruct a medium inhomogeneity or an unknown source. The forward problem can be written as \( \mathbf{d} = \mathbf{K} \mathbf{z} \), where \( \mathbf{z} \) is the inversion parameter, \( \mathbf{K} \) is the input-output operator, and \( \mathbf{d} \) are the measurements in the receivers. The deterministic inverse problem is to reconstruct \( \mathbf{z} \) given \( \mathbf{d} \), that is invert \( \mathbf{K} \). The probabilistic inverse problem is to get the probability density function of \( \mathbf{z} \), given some prior knowledge and known noise characteristics.

The operator \( \mathbf{K} \) plays a key role in both deterministic and probabilistic inversions. The Hessian \( \mathbf{H} \) is defined as \( \mathbf{H} = \mathbf{K}^T \mathbf{K} \).

Applying \( \mathbf{K} \) to a vector involves the solution of wave propagation problems and applying \( \mathbf{K}^T \) involves the adjoint operator. In fact, for problems that involve multiple illuminations and multiple frequencies then a matrix-vector multiplication with the Hessian involves numerous forward and adjoint wave propagations. Finally, the Hessian is typically a compact operator and thus, is not invertible in a stable manner.

Status/Progress

In this report we discuss progress on several related fronts together aimed at developing and applying fast scalable methods for quantification of uncertainty in the solution of inverse wave propagation problems:

- **FaIMS**: It is a fast approximation scheme for time-harmonic problems with multiple illuminations. But it can be integrated with the time-domain solvers developed by Prof. Ghattas’s group. In fact the solver can be used for any problem in which two properties are necessary, the existence of a fast method to evaluate the Green’s function of the underlying differential operator, and smoothness of this Green’s function, which is required in order to compress long-range interactions.
• **Adaptivity for inverse medium problems:** We are developing algorithms specific to the inverse medium problem. We are exploring uncertainty-based adaptivity and jump-localization techniques. The hardest problem in adaptivity is the interplay between the regularization and the discretization. Indeed, discretization corresponds to some form of regularization. We have developed a scheme that shows promising results for simple examples.

FaIMS.
Our recent contribution is the development of **FaIMS**, an algorithm for the inverse medium problem for the scalar wave equation. We consider the inverse medium problem for the time-harmonic wave equation with broadband and multi-point illumination in the low frequency regime. Such a problem finds many applications in geosciences (e.g. ground penetrating radar), non-destructive evaluation (acoustics), and medicine (optical tomography). We use an integral-equation (Lippmann-Schwinger) formulation, which we discretize using a quadrature method. We consider only small perturbations (Born approximation). To solve this inverse problem, we use a least-squares formulation. We present a new fast algorithm for the efficient solution of this particular least-squares problem. Let us emphasize that

![Figure 2: In this figure, we demonstrate the problem of a multipoint illumination inverse scattering problem. In the first row (from the top), we depict the plane-wave illumination of the scatterer for different frequencies (which correspond to a scatterer size equal to 1, 4, 16, and 64 wavelengths respectively). In the second row, we show the corresponding amplitude of the scattered field due to the illumination. The observations are made on a plane at a distance below the scatterer and detector resolution is sufficient to resolve the minimum wavelength. In the third row, we show multiple...](image-url)
illuminations using the same wavelength but different illumination directions; in the fourth row we show the corresponding scattered field on the detector plane. The results of the inversion are given in Figure 3.

If $N_f$ is the number of excitation frequencies, $N_s$ the number of different source locations for the point illuminations, $N_d$ the number of detectors, and $N$ the parametrization for the scatterer, a dense singular value decomposition for the overall input-output map will have $[\min(N_sN_fN, N)]^2 \times \max(N_sN_fN_d, N)$ cost. We have developed a fast SVD-based preconditioner that brings the cost down to $O((N + N_s + N_f + N_d) \log N)$ thus, providing orders of magnitude improvements over a black-box dense SVD and an unpreconditioned linear iterative solver.

![Figure 3: In this figure, we depict reconstructions for different illumination and maximum frequency regimes using our FAIMS inverse medium solver. We use data created by the simulations and the scatterer (SR-71) described in Figure 2. The scatterer is modeled as an unknown medium perturbation (point scatterers). In the top row from left, the first reconstruction was done using a single sub-wavelength illumination, the second using an incoming wave whose frequency corresponds to the true scatterer being one wavelength long and 8 illuminations, the third using a four-wavelength frequency and 8 illuminations, and the last one using a four-wavelength frequency and 32 illuminations. In the second row we depict different views (top, side, front, and angled) of a high resolution reconstruction using four different illumination frequencies (the maximum illumination frequency corresponds to eight wavelengths) and 128 illumination directions (for each frequency). As we increase the illumination frequency, the rank of the Hessian increases and the reconstructions become computationally demanding. Nevertheless, we are able to reconstruct the target scatterer quite accurately.]

This work has been completed and a paper has been submitted to SISC. Our next step is to extend it to nonlinear inverse medium problems and to introduce adaptivity. Also, we are developing a parallel library that implements FaIMS. In the application domain, we are extending FaIMS to the Maxwell and Navier equations (time-harmonic) and we are integrating with the massively parallel Fast Multipole Methods developed in our group.

Adaptivity.
We are investigating adaptive methods for the inverse medium for the Helmholtz equation. The medium is represented using an octree data-structure and piecewise Chebyshev polynomials. We are investigating two approaches, one is based on the Hessian information and the second one is based on Tadmor concentration kernels.

In the first approach, the diagonal of the inverse of the Hessian gives us the diagonal of the covariance matrix, which in turn indicates the uncertainty (variance) of our estimate. If this uncertainty is high, we do not refine otherwise
we do. The diagonal of the inverse we will be built by a randomization method that only requires matrix-vector multiplications.

Figure 4: LEFT: Settings of the simplified configuration considered in this example. The detectors (blue circles) are located on a plane ($Nd = 100$). The sources (red circles) are located on a sphere ($Ns = 12$). We assume a line singularity of the scatterer, with strength given by the inset at the lower left. We use Chebyshev polynomials for the discretization of the forward problem, along with a direct evaluation of the The discretization is 1D (along the dashed line). The number of frequencies is set to $Nf = 3$. The size of the box is $5\lambda$. RIGHT: We report results for our adaptive scheme in the absence of noise.

In the second approach, is computationally cheaper as it is entirely local. It uses edge detection using the spectral coefficients of a discontinuous function. This estimator will be based on the work of Anne Gelb and Eitan Tadmor, Acta Numerica 1999. The basic idea, is that upon inversion the Chebyshev coefficients of every octree leaf are examined with the help of a concentration kernel, and if the resulting jump is sufficiently large (this is an application-dependent parameter), then we proceed with refinement. This process will be combined with multiscale sampling techniques for Bayesian inversion schemes.

Eventually, the two adaptivity approaches will be combined as the uncertainty-based one does not use information from the reconstructed field and the jump-detection one does not address the ill-posedness of the inverse problem. The work has not been completed yet, but we continue our work with funding by other resources. Preliminary results are reported below.

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Personnel Supported During Duration of Grant
Stephanie Chaillat  
Research Associate, Georgia Tech  
George Biros  
Associate Professor, Georgia Tech  
Professor, The University of Texas at Austin

Publications

• S. Chaillat and G. Biros, An adaptive algorithm for the nonlinear inverse medium problem for the Helmholtz equation, in preparation
• S. Chaillat and G. Biros, FalMS: A fast algorithms for the inverse medium problem with multiple frequencies and multiple sources for the scalar Helmholtz equation. Journal of Computational Physics, 231 (20), 2012
• S.S. Adavani and G. Biros, Fast algorithms for inverse problems with parabolic PDE constraint, SIAM Journal on Imaging Sciences, SIAM Journal on Imaging Sciences, to appear
• S.S. Adavani and G. Biros, Fast algorithms for source identification problems with elliptic PDE constraints, SIAM Journal on Imaging Sciences, 3 (4), 2010
• I. Lashuk, G. Biros et al, A massively parallel adaptive fast-multipole method on heterogeneous architectures, Proceedings of SC 2009

Honors and Awards Received

• The paper I. Lashuk, A. Rahimian, G. Biros et al. “Petascale direct numerical simulation of blood flow on 200K cores and heterogeneous architectures,” received the 2010 Gordon Bell Prize.
• The paper I. Lashuk, G. Biros et al, A massively parallel adaptive fast-multipole method on heterogeneous architectures, Proceedings of SC 2009, was a Best Technical Paper finalist.
• Biros gave a plenary talk on fast elliptic solvers at the 2010 Parallel Matrix Algorithms and Applications Conferences, in Basel, Switzerland, July 2010
• Biros gave a plenary talk on inverse problems at the Applied Inverse Problems, Conference in Vienna, July 2009

AFRL Point of Contact: None  
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New Discoveries: Fast algorithms for inverse medium solvers