Ultra-Fast Scattering Matrix Solver for Disordered Media

Ho-Chun Lin, Zeyu Wang, and Chia Wei Hsu
Ming Hsieh Department of Electrical and Computer Engineering, University of Southern California, Los Angeles, California 90089, USA
cwhsu@usc.edu

Abstract: Using the Schur complement scattering analysis (SCSA) method, we accelerate the scattering matrix computation for large-scale disordered media by many orders of magnitude and realize full-wave simulations of classical and quantum coherent backscattering.

1. Introduction

The scattering matrix is the central object that characterizes wave transport through complex systems and is used extensively in wavefront shaping [1] and imaging [2]. However, numerical computation of the scattering matrix is a challenge, especially for large-scale disordered media which can involve thousands to millions of input and output channels.

Here, we propose the Schur complement scattering analysis (SCSA) method, which can compute the entire scattering matrix of an arbitrary complex system without looping over the input states, with no approximation beyond discretization, while utilizing the sparsity of the wave operator, the inputs, and also the outputs. For large systems, we find SCSA to be orders of magnitude faster than existing frequency-domain full-wave solvers while using less memory. As an example, we use SCSA to realize full-wave simulations of coherent backscattering in disordered media.

2. Schur complement scattering analysis (SCSA)

The scattering matrix S maps any incident wavefront β to the resulting outgoing wavefront α, as $\alpha_n = \sum_m S_{nm}\beta_m$. Each column of S corresponds to one scattering problem, defined mathematically through a system of linear equations $Ax_m = b_m$ where matrix $A = -(\omega/c)^2\varepsilon_r(\omega, r) + \nabla\times\mu_r^{-1}(\omega, r)\nabla\times$ is the electric-field Maxwell operator, and column vectors b_m and x_m are the equivalent source profile that generates the m-th incident wavefront and the resulting electric field profile $E(r)$. Solving for the m-th column of S corresponds to solving for $x_m = A^{-1}b_m$. Computing $M \gg 1$ columns of S typically requires repeating this process M times. Instead of such repetition, we directly compute S through relation $S = CA^{-1}B - D$, with $B = [b_1, \ldots, b_M]$, the n-th row of matrix C being the conjugated profile of the n-th output state on the surface, and matrix D subtracting the incident fields on the surface. Matrices A, B, C, D are all sparse.

Conventional iterative and direct solvers compute the field profile everywhere, namely $A^{-1}B$, which is redundant since the quantity of interest $CA^{-1}B$ is a much smaller matrix. To compute only what is needed, we directly evaluate $CA^{-1}B$ by constructing a new sparse matrix K and performing a partial LU factorization on it,

$$K \equiv \begin{matrix} A & B \\ C & D \end{matrix} = \begin{matrix} L & 0 \\ E & I \end{matrix} \begin{matrix} U & F \\ 0 & H \end{matrix}. \tag{1}$$

The factorization is partial as it stops after factorizing the upper-left block of K into $A = LU$ with L and U being lower-triangular and upper-triangular, and I being the identity matrix. Notably, we do not use such LU factors. By equating the middle and the right-hand sides of Eq. (1) for each of the four blocks, we can see that matrix H, called the Schur complement, satisfies $H = D - CA^{-1}B$. Using $S = CA^{-1}B - D$, we obtain the scattering matrix as $S = -H$; we call this method the "Schur complement scattering analysis" (SCSA). The Schur complement is often used in domain decomposition, but here we use it for computing the scattering matrix without looping over the inputs. SCSA is applicable to any structure, and it provides the exact full-wave solution with the only errors coming from discretization and truncation of simulation domain, which are intrinsic in all numerical methods.

The computing time of SCSA depends weakly on the number M of input states because the partial factorization time is typically dominated by matrix A which has more nonzero elements than matrices B and C. The sparsity patterns of all matrices are maintained and can be fully utilized in the partial factorization process. Furthermore, storing matrices L and U is typically the memory bottleneck for direct methods, but SCSA does not use L and U so we can drop them during the factorization process to significantly reduce memory usage and computing time.

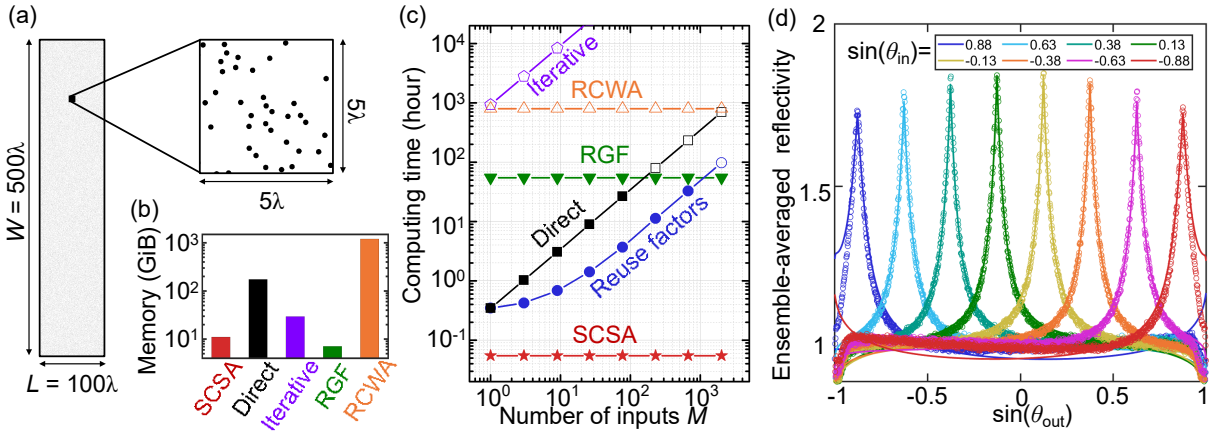

Fig. 1: (a) A $500\lambda \times 100\lambda$ disordered medium. (b) The memory usage of SCSA and other methods. (c) The computation time of SCSA and other methods when solving for M columns of the scattering matrix. Solid symbols are raw data, and open symbols are extrapolated from smaller M or smaller systems. (d) Reflectivity profiles at eight incident angles θ_{in} averaged over 40,000 realizations of disorder (open circles), in comparison to analytical prediction (solid lines).

3. Results

We implement SCSA for 2D transverse-magnetic waves under finite-difference discretization, using the MUMPS package [3] with AMD ordering to compute the Schur complement. As an example, we compute the full scattering matrix of a large-scale disordered medium with discretization size $\Delta x = \lambda/15$ (Fig. 1a), with up to $M = 2000$ inputs. The system consists of 75,000 randomly positioned cylinders with refractive index $n = 2$ and diameter $D = 0.2\lambda$ in air, with scattering mean free path $l_s = 1.5\lambda$. Periodic boundary condition is used in the trans-verse direction, and perfectly matched layers are used in the longitudinal direction. Figure 1b-c shows the mem-ory usage and computation time of SCSA in comparison to (1) a conventional direct solver implemented in MaxwellFDFD [4] where the full computation is repeated M times, (2) MaxwellFDFD modified to have the LU factors stored and reused, (3) an iterative solver implemented in FD3D [5], (4) the recursive Green's function method (RGF) implemented in [6], and (5) RCWA implemented in S4 [7]. SCSA achieves an M-independent computation time and is over 1000× faster than all of the other methods while also using less memory.

We use SCSA to realize full-wave modeling of coherent backscattering (CBS) [8] in disordered media. CBS is a hallmark of coherent effects in mesoscopic physics, where constructive interference between time-reversed paths leads to enhanced reflection in the backscattering direction. To observe CBS, it is crucial to average over many disorder realizations to suppress the speckle fluctuations that would otherwise overwhelm the CBS signal. Restricted by the efficiency of existing numerical methods, prior CBS simulations resorted to few realizations with coarse discretization [9] or point-scatterer approximation in small systems [10] and did not provide quantitative predictions of the CBS enhancement. With SCSA, we compute CBS averaged over 40,000 realizations for all incident angles for the above system. This allows, for the first time, quantitative and fitting-free validation of the exact solution of CBS [11], as shown in Fig. 1d, with an incident-angle-dependent reduction of the CBS enhancement. We also use SCSA to predict, for the first time, CBS of entangled photon pairs in disordered media [12].

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