Determination of Random Periodic Structures in Transverse Magnetic Polarization

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Abstract. Consider an inverse problem that aims to identify key statistical properties of the profile for the unknown random perfectly conducting grating structure by boundary measurements of the diffracted fields in transverse magnetic polarization. The method proposed in this paper is based on a novel combination of the Monte Carlo technique, a continuation method and the Karhunen-Loève expansion for the uncertainty quantification of the random structure. Numerical results are presented to demonstrate the effectiveness of the proposed method.

AMS subject classifications: 78A46, 65C30, 65N21

Key words: Random periodic structure, inverse scattering, Karhunen-Loève expansion, Monte Carlo-continuation-uncertainty quantification method.

1 Introduction

The direct and inverse scattering problems in periodic structures have received considerable attentions due to diverse sets of applications, especially in the design and manufacture of optical elements including correction lenses, sensors, solar cells and surface plasmons [4,13,18,19,23,32]. In this paper, we consider the

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inverse scattering of a time-harmonic electromagnetic plane wave by a periodic structure which is usually regarded as a grating in diffractive optics.

There are two fundamental polarizations for electromagnetic fields: transverse electric (TE) polarization and transverse magnetic (TM) polarization. The direct and inverse scattering problems in periodic structures for TE and TM polarization have been studied both numerically and mathematically. For the mathematical studies of the existence and uniqueness of the diffraction of a time harmonic wave modeled by a generalized Helmholtz equation in TE and TM polarization, we refer to [2, 7, 8, 27] and references therein. A comprehensive review of diffractive optics in mathematics and computation can be found in [6, 10, 30]. Numerically, most of the studies are concerned with TE polarization, for which many numerical methods have been developed in [1, 15, 24, 25, 33] to solve the inverse scattering problems. A method of coupling of finite element and boundary integral equations for the solutions of direct and inverse electromagnetic scattering in both transverse electric and magnetic polarization cases was proposed in [9, 28]. An efficient continuation method to capture the grating profile with multiple frequency data was developed in [12] and further extended to the case of phaseless data in [11]. Recently, Qu et al. [31] proposed a novel integral equation for direct and inverse scattering by a locally perturbed infinite plane on which a Neumann boundary condition is imposed.

This paper is devoted to the numerical solution of the inverse scattering by a periodic structure for TM polarization, i.e., given the incident field, determine the periodic structure from the measured diffracted field at a constant distance from the structure.

By far, most of the research in the area of diffractive optics has assumed that the periodic grating profile is deterministic and only the noise level of measurements is considered for the inverse problem. In reality, however, one has to deal with the uncertainty of grating structures, including its manufacturing defects, some possible damage due to long-term usage and so on. Actually, surface roughness measurement is of great significance for the functional performance evaluation of machined parts and the design of micro-optical components. Thus a natural question arises: in addition to the noise level of the measured data, how does one reconstruct the unknown grating profile by considering the uncertainty of gratings? The real challenge is how to characterize the grating profile with uncertainties appropriately based on the measured data. What makes the reconstruction extremely difficult is the nonlinearity between the measured diffracted field and the unknown grating structure. For the direct random scattering problem, there have been many studies in various numerical methods [3, 35]. Feng et al. [21] proposed an efficient Monte Carlo-transformed field expansion method for the
computation of electromagnetic waves scattered by randomly periodic surfaces. In mathematics, Pembery et al. [29] established the well-posedness and a priori bounds for the stochastic Helmholtz equation for arbitrarily large wavenumber.

However, for the inverse random surface scattering problem, very little is known in mathematics or computation. We have made some preliminary progress in the study of solving the inverse scattering by a random periodic structure based on a novel combination of the Monte Carlo technique, a continuation method and the Karhunen-Loève expansion for the uncertainty quantification of the random structure in TE polarization in [14]. Besides, the Monte Carlo method has been employed in [26] to calculate the statistical properties of scattered waves. B-splines have been applied in [22] to recover an unknown randomly rough surface, which is represented by some control points. A Bayesian inversion technique [17, 36] has been developed for solving some inverse problems with randomness such as the two-dimensional heat source inversion and the inferring of the diffusion coefficient in elliptic PDEs. Until now, no study is available on the inverse scattering problem by periodic random surfaces in TM polarization. It should be pointed out that the TM case is by no means a trivial extension of the TE case since the solution is less regular and the corresponding boundary condition is the Neumann boundary condition instead of the Dirichlet one. The scattering of penetrable random surfaces and more complicated biperiodic issues will be considered in a separate work.

Throughout, the medium is assumed invariant in the $x_3$-direction. Therefore, the model problem of the three-dimensional time-harmonic Maxwell equations can be reduced to the two-dimensional Helmholtz equation. For the random periodic structure, it is assumed to be a stationary Gaussian process modeled by the Karhunen-Loève (KL) expansion in this work due to the fact that the expansion is optimal in the sense that the mean-square error of the truncation of the expansion after finite terms is minimal [34]. In this scenario, an efficient numerical method is proposed to reconstruct the periodic random structure from multi-frequency scattered fields away from the structure in TM polarization, in the sense that all three critical statistical properties, namely the expectation, the root mean square (rms) height, and the correlation length of random structure may be reconstructed. Our method is based on a combination of the Monte Carlo technique for sampling the probability space, a continuation method with respect to the wavenumber, and the Karhunen-Loève expansion for the uncertainty quantification of the random structure. Since the KL expansion decomposes the random process in a bi-orthogonal fashion, after the mean reconstruction of the random structure, eigenvalues of the covariance operator may be determined by using properties of the KL expansion and the other two statistical properties of the random structure.
may be further determined by the reconstructed eigenvalues, which realizes the reconstruction of the random structure investigated in this work.

The rest of the paper is organized as follows. In Section 2, we introduce a mathematical model for the inverse scattering problem of a time-harmonic plane wave incident on a periodic perfectly reflecting random surface in TM polarization. In Section 3, the Monte Carlo-continuation-uncertainty quantification reconstruction method for TM polarization is presented and discussed. Several numerical experiments are presented in Section 4 to demonstrate the efficiency and reliability of the method, followed by some general concluding remarks.

2 Model problem

Consider the scattering of a time-harmonic plane wave incident from a set of incident angles on a periodic structure

\[ \Gamma_f := \{(x_1, x_2) \in \mathbb{R}^2 | x_2 = f(\omega; x_1), \omega \in \Omega \}, \]

which is characterized by the wavenumber \( \kappa \) ruled on a perfect conductor as shown in Fig. 1. Here, \((x_1, x_2) \in \mathbb{R}^2\) are the spatial variables, \(\omega \in \Omega\) denotes the random sample, and the random surface \(f(\omega; x_1)\) is the sum of a deterministic \(\Lambda\)-periodic function \(\tilde{f}(x_1)\) and a stationary Gaussian process with a continuous and bounded covariance function \(c(|x_1 - y_1|)\). It is assumed that the medium and the material are invariant in the \(x_3\)-direction and periodic in the \(x_1\)-direction with a period of \(\Lambda\). Throughout, the medium above the structure is assumed to be homogeneous. There are two fundamental polarizations for electromagnetic fields:
transverse electric (TE) polarization and transverse magnetic (TM) polarization. Here, we consider the inverse scattering problem on periodic perfectly conducting random surfaces in TM polarization.

More precisely, as shown in Fig. 1, the scattering is illuminated from above by a time-harmonic plane wave \( u^{inc} = e^{i\alpha x_1 - i\beta x_2} \), where \( \alpha = \kappa \sin \theta \), \( \beta = \kappa \cos \theta \), \( \kappa = \rho \sqrt{\varepsilon \mu} \) is the wavenumber, \( \rho > 0 \) is the angular frequency, \( \varepsilon > 0 \) is the constant electric permittivity, \( \mu > 0 \) is the constant magnetic permeability, and \( \theta \in (-\frac{\pi}{2}, \frac{\pi}{2}) \) is the incident angle with respect to the positive \( x_2 \)-axis. Denote \( D_f^+ = \{ x_2 > f(\omega; x_1) \} \).

Let the total field

\[ u^{total}(\omega; x) = u^{inc} + u(\omega; x) \quad \text{in} \quad D_f^+ , \]

where \( u \) is the diffracted field. Then, since both \( \varepsilon \) and \( \mu \) are constants, the scattering on a periodic perfectly conducting random surface in TM polarization can be reduced to the two-dimensional Helmholtz equation with the Neumann boundary condition as follows [8]:

\[
\begin{align*}
\Delta u(\omega; x) + \kappa^2 u(\omega; x) &= 0 \quad \text{in} \quad D_f^+ , \\
\partial_\nu u(\omega; x) + \partial_\nu u^{inc} &= 0 \quad \text{on} \quad \Gamma_f , \\
\end{align*}
\]

(2.1)

where \( \nu \) is the unit normal vector on \( \Gamma_f \) directed into \( D_f^+ \). Due to the uniqueness consideration, we seek for the quasi-periodic solutions as usual, i.e., a solution \( u(\omega; x) \) such that \( u(\omega; x) e^{-i\alpha x_1} \) is \( \Lambda \) periodic in \( x_1 \).

For the representation of the random structure, the Karhunen-Loève (KL) expansion is adopted here among different kinds of spectral decomposition for uncertainty quantifications in that it decomposes the stochastic process in a bi-orthogonal fashion, i.e., both orthogonal over the domain \( \mathcal{X}_1 \) and the probability space \( \Omega \), and the mean-square error of the truncation of the KL expansion after finite terms is minimal [34]. Specifically, define the covariance operator \( C_f : L^2(\mathcal{X}_1, dx_1; \mathbb{R}) \to L^2(\mathcal{X}_1, dx_1; \mathbb{R}) \) of the random surface \( f \) by

\[
(C_f \psi)(x_1) := \int_{\mathcal{X}_1} c(|x_1 - y_1|) \psi(y_1) dy_1
\]

with \( \mathcal{X}_1 = [-\frac{L}{2}, \frac{L}{2}] \). Note that \( c(|x_1 - y_1|) \) is a continuous and bounded covariance function interpreted as providing some information on the root mean square (rms) height and correlation length of the stochastic process \( f \). Here, the covariance function [34] is taken as the following Gaussian form:

\[
c(|x_1 - y_1|) = \sigma^2 \exp\left(-\frac{|x_1 - y_1|^2}{l^2}\right), \quad 0 < l \ll \Lambda,
\]
where \( \sigma \) is the rms height and \( l \) is the correlation length of the structure. In some literatures, there is a Gaussian auto-correlation function related with the correlation length defined by

\[
w(|x_1 - y_1|) = \exp\left(-\frac{|x_1 - y_1|^2}{l^2}\right), \quad 0 < l \ll \Lambda. \tag{2.4}\]

Let \( \{\varphi_j, \lambda_j\}_{j \in \mathbb{N}} \) be an orthonormal set of eigenvectors/eigenvalues for the covariance operator \( C_f \) defined by

\[
\varphi_j(x_1) = \begin{cases} 
\sqrt{\frac{1}{\Lambda}}, & j = 0, \\
\sqrt{\frac{2}{\Lambda}} \cos\left(\frac{2j\pi x_1}{\Lambda}\right), & j > 1, \text{ even}, \\
\sqrt{\frac{2}{\Lambda}} \sin\left(\frac{2j\pi x_1}{\Lambda}\right), & j > 1, \text{ odd}, 
\end{cases} \tag{2.5}
\]

and ordered so that \( \lambda_0 \geq \lambda_1 \geq \lambda_2 \geq \cdots \).

Then the KL expansion of the random process \( f(\omega; x_1) \) may be written as

\[
f(\omega; x_1) = \tilde{f}(x_1) + \sqrt{\lambda_0} \xi_0(\omega) \sqrt{\frac{1}{\Lambda}}
+ \sum_{j=1}^{\infty} \sqrt{\lambda_j} \left( \tilde{\xi}_{j, e}(\omega) \sqrt{\frac{2}{\Lambda}} \sin\left(\frac{2j\pi x_1}{\Lambda}\right) + \tilde{\xi}_{j, s}(\omega) \sqrt{\frac{2}{\Lambda}} \cos\left(\frac{2j\pi x_1}{\Lambda}\right) \right), \tag{2.6}
\]

where \( \tilde{f}(x_1) \) is a deterministic \( \Lambda \)-periodic function, \( \xi_0, \tilde{\xi}_{j, e} \) and \( \tilde{\xi}_{j, s} \) are independent and identically distributed (iid) random variables with zero mean and unit covariance.

Denote

\[
D_f = \{(x_1, x_2) \in \mathbb{R}^2 \mid f(\omega; x_1) < x_2 < d, \forall \omega \in \Omega\}
\]

with the boundary given by

\[
\Gamma_0 = \{(x_1, x_2) \in \mathbb{R}^2 \mid x_2 = d\}
\]

and

\[
d > \max_{\omega \in \Omega, x_1 \in (0, \Lambda)} f(\omega; x_1).
\]

It follows from Eq. (2.1) that the scattering of time-harmonic electromagnetic waves in TM polarization by a periodic perfectly reflecting random surface may
be stated as the following value problem: to find the quasi-periodic solution \( u(\omega; x) \) such that
\[
\begin{align*}
\Delta u(\omega; x) + \kappa^2 u(\omega; x) &= 0 \quad \text{in} \quad \Omega \times D_f, \\
\partial_\nu u(\omega; x) + \partial_\nu u^{inc} &= 0 \quad \text{on} \quad \Omega \times \Gamma_f.
\end{align*}
\]
Correspondingly, the inverse problem for a periodic perfectly reflecting random structure may be stated as follows: for each sample \( \omega \), given the incident plane wave \( u^{inc} \), determine the KL expansion random structure \( x_2 = f(\omega; x_1) \) along with all certain statistical properties of the structure, i.e., the expectation \( \bar{f} \), the rms height \( \sigma \) and the correlation length \( l \), from multiple frequency measurements of the diffracted fields \( u(\omega; x_1, d) \).

3 Reconstruction method

To get the relation between the measurements and the random structure, consider the single-layer potential representation for the diffracted field at the measured horizontal line
\[
u(\omega; x) = \int_0^\Lambda \phi(\omega; y_1) G(x_1, f(\omega; x_1); y_1, 0) dy_1, \quad \omega \in \Omega, \quad x \in \Gamma_f, \tag{3.1}
\]where \( \phi \) is an unknown periodic density function and \( G \) is a quasi-periodic Green function with the following form
\[
G(x_1, x_2; y_1, y_2) = \tilde{G}(x, y) := i \frac{1}{4} \sum_{n \in \mathbb{Z}} H_0^{(1)}(\kappa \tau_n) e^{in\alpha k}. \tag{3.2}
\]Here, \( H_0^{(1)} \) is the Hankel function of the first kind with order zero and \( \tau_n = |x_1 - y_1 - n\Lambda| \).

Define the operator
\[
T_f : L^2(\Omega; L^2(0, \Lambda)) \to L^2(\Omega; L^2(0, \Lambda))
\]by
\[
(T_f \phi)(\omega; x) = \int_0^\Lambda \phi(\omega; y_1) G(x_1, f(\omega; x_1); y_1, 0) dy_1, \quad x \in \Gamma_f. \tag{3.3}
\]Expand the quasi-periodic solution \( u(\omega; x_1, d) \) and the periodic function \( \phi \) as
\[
u(\omega; x_1, d) = \sum_{n \in \mathbb{Z}} u_n(\omega) e^{in\alpha x_1}, \quad \phi(\omega; y_1) = \sum_{n \in \mathbb{Z}} \phi_n(\omega) e^{in\alpha y_1}. \tag{3.4}
\]
respectively. Then, a combination of Eqs. (3.1)-(3.4) yields
\[
(T_f \phi)(\omega; x) = \sum_{n \in \mathbb{Z}} \psi_n(\omega) e^{i\alpha_n x_1 + i\beta_n f(\omega; x_1)}, \quad x \in \Gamma_f,
\]
(3.5)
where
\[
\psi_n(\omega) = u_n(\omega) e^{-i\beta_n d}, \quad \alpha_n = \alpha + \frac{2\pi n}{\Lambda} \quad \text{for} \quad n \in \mathbb{Z},
\]
and
\[
\beta_n = \begin{cases} \sqrt{\kappa^2 - \alpha_n^2}, & |\kappa| > |\alpha_n|, \\ i\sqrt{\alpha_n^2 - \kappa^2}, & |\kappa| < |\alpha_n|. \end{cases}
\]
Note that the operator \( T_f \) gives the relation between the measured data and the grating profile. Actually, if \( \kappa > |\alpha_n| \), then \( \beta_n = (\kappa^2 - \alpha_n^2)^{1/2} \) is a positive real number and the term \( \exp(-i\beta_n d) = \exp((-i(\kappa^2 - \alpha_n^2)^{1/2})d) \) represents an incoming plane wave; if \( \kappa < |\alpha_n| \), then \( \beta_n = i(\alpha_n^2 - \kappa^2)^{1/2} \) is a pure imaginary number and the term \( \exp(-i\beta_n d) = \exp((\alpha_n^2 - \kappa^2)^{1/2})d) \) is an exponentially increasing term. Since the error of the measured data may cause an exponential increase in noise, the regularization [20] needs to be taken here to suppress the exponential growth of the noise and obtain a stable reconstruction, i.e.,
\[
\psi_n(\omega) = \begin{cases} u_n(\omega) e^{-i\beta_n d} & \text{for} \quad \kappa > |\alpha_n|, \\ u_n(\omega) e^{i\beta_n d} & \text{for} \quad \kappa < |\alpha_n|, \\ u_n(\omega) e^{2i\beta_n d + \gamma} & \text{for} \quad \kappa = |\alpha_n|, \end{cases}
\]
(3.6)
where \( \gamma \) is some positive regularization parameter.

Since the diffracted field \( u \) satisfies the Neumann boundary condition
\[
\partial_v u(\omega; x) + \partial_v u^{inc} = 0 \quad \text{on} \quad \Gamma_f
\]
in Eq. (2.1), we get the nonlinear problem
\[
\left\| \partial_v (T_f \phi)(\omega; x) + \partial_v u^{inc}(x_1, f(\omega, x_1)) \right\|_{L^2(\Omega; L^2(0, \Lambda))}^2 = 0
\]
for reconstructing the random grating profile. Substituting the expansion (3.5) for the operator \( T_f \), the nonlinear equation for TM polarization may be truncated into a finite summation due to the fact that the summation exponentially decreases with respect to \( |n| \), i.e.,
\[
\left\| \sum_{n=-N}^{N} \frac{i\alpha_n f' - i\beta_n}{\sqrt{1 + f'^2}} \psi_n(\omega) e^{i \alpha_n x_1 + i\beta_n f} + \frac{i\alpha f' + i\beta}{\sqrt{1 + f'^2}} e^{i\alpha x_1 - i\beta f} \right\|_{L^2(\Omega; L^2(0, \Lambda))}^2 = 0,
\]
(3.7)
where \( f' \) is the derivative of \( f(\omega, x_1) \) with respective to \( x_1 \).
In order to reconstruct important statistical properties of the unknown random structure from boundary measurements of the diffracted fields away from the structure, we propose the Monte Carlo-continuation-uncertainty quantification (MCCUQ) reconstruction method based on a novel combination of the Monte Carlo technique, a continuation method, and the properties of the Karhunen-Loève expansion for the uncertainty quantification of the random structure. We remark that our MCCUQ follows the general procedure of the method first proposed for solving the inverse problem for TE polarization in [14]. However, necessary modifications must be made due to the differences between the models, boundary conditions, and regularities of the respective solutions.

For the approximation of the solution of the nonlinear equation (3.7), the Monte Carlo technique is employed to sample the probability space. Let $M$ be a positive integer which denotes the number of realizations. For each sample $\omega_m$, $m = 1, \ldots, M$, denote the reconstructed random surface by $f_m(x_1), m = 1, \ldots, M$. Thus an approximation of the expectation and the standard deviation may be given by

$$\bar{f}(x_1) = \frac{1}{M} \sum_{m=1}^{M} f_m(x_1), \quad s_f(x_1) = \sqrt{\frac{1}{M} \sum_{m=1}^{M} (f_m(x_1) - \bar{f})^2},$$

respectively. The expectation of the standard deviation may be regarded as an approximation of the rms height of the random structure.

First, reconstruct the expectation of the random structure. The main idea for the reconstruction of the mean grating profile is to reconstruct the Fourier coefficients from the smaller wavenumber, increase the wavenumber again and again until the prescribed wavenumber $\kappa_0$ is reached. Specifically, it follows immediately from the KL expansion of the random process in Eq. (2.6) that the profile $\tilde{f}(x_1)$ is a real $\Lambda$-period function, and $E(\tilde{\xi}_0) = E(\tilde{\xi}_{j,c}) = E(\tilde{\xi}_{j,s}) = 0$ provided that the sample size $M$ is large enough. Without loss of generalities, the period $\Lambda$ is taken as $2\pi$ from now on. Hence the mean grating profile $\bar{f}$ admits a Fourier series expansion, i.e.,

$$\bar{f}(x_1) = \bar{c}_0 + \sum_{p=1}^{\infty} [\bar{c}_{2p-1}\cos(px_1) + \bar{c}_{2p}\sin(px_1)],$$

where $\bar{c}_p = \frac{1}{M} \sum_{m=1}^{M} c_{m,p}$.

It is obvious that the finite expansion of Eq. (3.8) can reasonably approximate the periodic random grating profile for TM polarization. By choosing a prescribed wavenumber $\kappa_0$ not exceeding the wavenumber $\kappa$, taking the number of
Fourier expansion modes not larger than the prescribed wavenumber, and considering the finite expansion of Eq. (3.8), our first goal is to determine each coefficient $\bar{c}_p$ ($p = 0, 1, \ldots, 2k_{\text{max}}$) to reconstruct the mean profile of the random structure. For each sample $\omega_m$, $m = 1, \ldots, M$, the procedure for the reconstruction of each Fourier coefficient $c_{m,p}$ ($p = 0, 1, \ldots, 2k_{\text{max}}$) in TM polarization is summarized as the following four steps:

**Step 1.** Initialization. Set the initial approximation $c_{m,0} = y_0$ and $c_{m,p} = 0$, $p = 1, \ldots, 2k_{\text{max}}$, where $k_{\text{max}}$ is taken to be the largest integer that is smaller than or equal to the prescribed wavenumber, i.e. $k_{\text{max}} = \lfloor \kappa_0 \rfloor$. Denote the vector $c_{m,k_{\text{max}}} = \begin{bmatrix} c_{m,0} & c_{m,1} & \cdots & c_{m,2k_{\text{max}}} \end{bmatrix}^T$.

**Step 2.** Choose an initial value for the wavenumber $\kappa_1$ smaller than the prescribed wavenumber, and seek for an approximation to the profile $f(\omega_m; x_1)$ by the Fourier series

$$f_{m,k}(x_1) = c_{m,0} + \sum_{p=1}^{k} \left[ c_{m,2p-1}\cos(px_1) + c_{m,2p}\sin(px_1) \right],$$  

where $k = \lfloor \kappa_1 \rfloor$. Denote $c_{m,k}$ the first $2k+1$ terms of $c_{m,k_{\text{max}}}$, i.e.,

$$c_{m,k} = \begin{bmatrix} c_{m,0}, c_{m,1}, \ldots, c_{m,2k} \end{bmatrix}^T$$

with $c_{m,0} = y_0$ and $c_{m,p} = 0$, $p = 1, \ldots, 2k$.

For the incident angle $\theta_l \in (-\frac{\pi}{2}, \frac{\pi}{2})$, $l = 1, 2, \ldots, L$, $\alpha = k\sin(\theta_l)$, $\beta = k\cos(\theta_l)$, define

$$J_l(c_{m,k}) = \left\| \sum_{n=-N}^{N} \frac{i\alpha_{n} f'_{m,k}(x_1) - i\beta_{n}}{\sqrt{1 + f'_{m,k}(x_1)^2}} \psi_{n,l}(\omega_m) e^{i\alpha_{n} x + i\beta_{n} f_{m,k}(x_1)} + i\frac{\alpha_{n} f'_{m,k}(x_1) + i\beta}{\sqrt{1 + f'_{m,k}(x_1)^2}} e^{i\alpha_{n} x - i\beta f_{m,k}(x_1)} \right\|_{L^2(0,\Lambda)}^2,$$

where $f'_{m,k}(x_1)$ is the derivative of $f_{m,k}(x_1)$. Denote

$$J(c_{m,k}) = \begin{bmatrix} J_1(c_{m,k}), \ldots, J_L(c_{m,k}) \end{bmatrix}^T,$$

then the nonlinear problem (3.7) may be written as

$$J(c_{m,k}) = 0,$$  

(3.10)
where $J : \mathbb{R}^{2k+1} \to \mathbb{R}^L$. Consider the nonlinear Landweber iteration [20]

$$
\mathbf{c}^{(t+1)}_{m,k} = \mathbf{c}^{(t)}_{m,k} - \eta_k \mathbf{D}J^T\left( \mathbf{c}^{(t)}_{m,k} \right) \mathbf{J}\left( \mathbf{c}^{(t)}_{m,k} \right), \quad t = 0, 1, \ldots, \tag{3.11}
$$

where $\eta_k$ is a relaxation parameter dependent on the wavenumber, the initial vector $\mathbf{c}^{(0)}_{m,k} = \mathbf{c}_{m,k}$, and the Jacobi matrix

$$
\mathbf{D}J = \left( \frac{\partial J_l}{\partial \mathbf{c}_{m,p}} \right), \quad l = 1, 2, \ldots, L, p = 0, 1, \ldots, 2k
$$

may be computed explicitly.

**Step 3.** Increase the wavenumber $\kappa_1$ to $\kappa_2$ ($\kappa_2 < \kappa_0$), seek for a new approximation to the profile $f(\omega_m; x)$ by the Fourier series

$$
f_{m,k'}(x_1) = c_{m,0} + \sum_{p=1}^{k'} \left[ c_{m,2p-1} \cos(px_1) + c_{m,2p} \sin(px_1) \right] \tag{3.12}
$$

with $k' = \lfloor \kappa_2 \rfloor$, and determine the coefficients $\mathbf{c}_{m,k'}$. Denote

$$
\mathbf{c}_{m,k'} = \left[ c_{m,0}, c_{m,1}, \ldots, c_{m,2k'} \right]^T,
$$

where

$$
c_{m,p} := \begin{cases} 
    c_{m,p} & \text{for } 0 \leq p \leq 2k, \\
    0 & \text{for } 2k < p \leq 2k'.
\end{cases}
$$

Repeat the above Landweber iteration described in Step 2 with the starting point given by the resulting coefficients obtained at the previous smaller wavenumber, i.e. $\mathbf{c}^{(0)}_{m,k'} = \mathbf{c}_{m,k'}$.

**Step 4.** Repeat Step 3 until the prescribed wavenumber $\kappa_0$ is reached.

The resulting coefficients $\mathbf{c} = [\bar{c}_0, \bar{c}_1, \ldots, \bar{c}_{2k_{\text{max}}}]^T$ are computed by taking the expectation of $\mathbf{c}_{m,p}$ ($m = 1, \ldots, M$), i.e.,

$$
\mathbf{c} = \frac{1}{M} \sum_{m=1}^{M} \mathbf{c}_{m,p}.
$$

Hence, the mean grating profile of the periodic randomly rough structure is reconstructed as the following finite Fourier series expansion

$$
\bar{f}(x) = \bar{c}_0 + \sum_{p=1}^{k_{\text{max}}} \left[ \bar{c}_{2p-1} \cos(px_1) + \bar{c}_{2p} \sin(px_1) \right] \tag{3.13}
$$
with $\bar{c}_p = \frac{1}{M} \sum_{m=1}^{M} c_{m,p}$, $p = 0, 1, \ldots, 2k_{\text{max}}$. Note that since all of the samples in the probability space are chosen iid, the Monte Carlo sampling process can be executed well in parallel.

It is known that solutions for TM polarization converge much more slowly than TE polarization. The reconstruction algorithm for TM polarization differs from that for TE polarization in the following aspects: the prescribed wavenumber in TM polarization should be chosen larger than that in TE polarization, and the relaxation parameter $\eta_k$ in TM polarization should be much smaller than that in TE polarization. Since our algorithm seems to be convergent and stable, a good approximation to the unknown periodic random rough structure at a larger wavenumber may be obtained at each recursion.

Next, reconstruct the two critical statistical properties of the random structure, i.e., the rms height and the correlation length. Based on the properties of the KL expansion for the uncertainty quantification of the random process $f(\omega; x_1)$ in Eq. (2.6) and as shown in Fig. 2 with period $\Lambda = 2\pi$, rms height $\sigma = 0.1$ and correlation length $l = 0.8$ for an example, eigenvalues in the KL expansion decrease exponentially and thus it is appropriate to truncate the KL expansion with $\{\lambda_j\}_{j \in \mathbb{N}}$ arranged in a descending order and only use the first several terms to represent the random profile with an accuracy of $10^{-2}$ or even much higher.

Therefore, we can truncate the KL expansion and only use the first several terms for further reconstruction. Since the eigenfunctions $\{\varphi_j\}_{j \in \mathbb{N}}$ of the covariance operator are orthonormal and $\zeta_0, \zeta_j, \zeta_{j\sigma}, \zeta_{j\rho}$ are iid random variables with zero mean and unit covariance, eigenvalues of the covariance function are those of the

![Figure 2: Eigenvalues of the covariance when $\Lambda = 2\pi, \sigma = 0.1$ and $l = 0.8$.](image-url)
corresponding covariance matrix $C = (c_{ij})$ where
\[
c_{ij} = \mathbb{E} \left( \langle f - \mathbb{E}(f), \varphi_i \rangle \langle f - \mathbb{E}(f), \varphi_j \rangle \right) \\
= \frac{1}{M} \left( \sum_{m=1}^{M} \langle f_m(x_1) - \bar{f}(x_1), \varphi_i(x_1) \rangle \langle f_m(x_1) - \bar{f}(x_1), \varphi_j(x_1) \rangle \right)
\]
with
\[
f_m(x_1) = c_{m,0} + \sum_{p=1}^{k_{\text{max}}} [c_{m,2p-1}\cos(px_1) + c_{m,2p}\sin(px_1)], \\
\bar{f}(x_1) = \bar{c}_0 + \sum_{p=1}^{k_{\text{max}}} [\bar{c}_{2p-1}\cos(px_1) + \bar{c}_{2p}\sin(px_1)].
\]

Note that the profile of a periodic random rough grating structure in our MCCUQ method is reconstructed in the form of the sum of a finite Fourier series expansion and a truncated KL expansion represented by the reconstructed eigenvalues. Moreover, it may be deduced after simple calculation that the eigenvalues has the following correlation with the rms height $\sigma$ and the correlation length $l$:
\[
\lambda_j \approx \sqrt{\pi \sigma^2 l e^{-j^2/4}}, \quad j = 0, 1, \ldots
\]
provided that the correlation length $l$ is much smaller than the period $\Lambda$. Hence only the two eigenvalues are needed to approximate the two critical statistical properties which are usually used to describe a random process. Specifically, the recovery formula by the two eigenvalues $\lambda_1$ and $\lambda_2$ may be reduced to
\[
l' = \sqrt{\frac{4}{3} \ln \left( \frac{\lambda_1}{\lambda_2} \right)}, \quad \sigma' = \sqrt{\frac{\lambda_1}{\sqrt{\pi l' e^{-l'^2/4}}}}.
\]

In fact, the correlation length $l$ and rms height $\sigma$ may be determined by any two eigenvalues, which fully realizes the reconstruction of the random structure.

4 Numerical results

In this section, two numerical experiments are presented to test the reliability and efficiency of the proposed method. Both experiments are implemented on MATLAB.
In order to test the stability of our method, some random noise is added to all of the measured data, that is, for each given sample, the measured data takes the following form:

$$u(\omega; x_1, d) = u(\omega; x_1, d)(1 + \tau \text{rand}),$$  \hspace{1cm} (4.1)

where \( \text{rand} \) is a uniformly distributed random variable in \([-1,1]\) and \( \tau \) is the noise level of the measured data. All the measurements \( u(\omega; x_1, d) \) are simulated by using an adaptive finite-element method with a perfectly-matched-layer technique [5, 16]. Since all of the samples are chosen iid, our numerical method can be executed in parallel.

For all numerical examples given below, the number of eigenvalues determined by the covariance operator \( C_f \) is selected to satisfy a random surface with an accuracy of \( 10^{-6} \); the noise level \( \tau \) is taken as \( 0.1\% \); the regularization parameter \( \gamma \) is chosen as \( 10^{-6} \); the relaxation parameter \( \eta_k \) dependent on the wavenumber \( \kappa \) for the continuation method are selected as \( \eta_k = 2 \times 10^{-6} / k^3 (k \leq \kappa) \); and the truncation of infinite summation in Eq. (3.7) is set to \( N = 8 \).

To test the accuracy of our algorithm, we first show certain realizations of periodic random rough surfaces with different rms heights and correlation lengths as seen in Fig. 3. Specifically, each realization is a sum of a \( 2\pi \)-periodic deterministic function \( \tilde{f}(x_1) = 0.9 + 0.2 \cos(x_1) + 0.2 \sin(2x_1) \) and a stationary Gaussian
process with the rms height $\sigma = 0.06, 0.1$ and the correlation length $l = 1.2, 0.8$, respectively, modeled by the KL expansion with the Gaussian covariance function $c(x - y) = \sigma^2 \exp(-|x - y|^2 / l^2)$ described above. It can be seen from Fig. 3 that when the rms height $\sigma$ increases, the deviation of the sample profile from the center profile becomes larger, and as the correlation length $l$ decreases, the random surface becomes rougher.

4.1 Reconstruction of the mean unknown periodic random rough structure

Let us consider two periodic random rough surfaces both of which are described as a sum of a deterministic function and a stationary Gaussian process with the Gaussian covariance function. We default the rms height $\sigma = 0.06$ and the correlation length $l = 1.2$ in Example 4.1, and consider the periodic random rough surface with different rms heights and correlation lengths in Example 4.2 to discuss the influence of changes of the rms height and the correlation length on our proposed MCCUQ reconstruction method.

Example 4.1. To reconstruct a periodic random grating structure which is a sum of a deterministic function $\tilde{f}(x_1) = 0.9 + 0.2\cos(x_1) + 0.2\sin(2x_1)$ and a stationary Gaussian process with the covariance function $c(x_1 - y_1) = 0.06^2 \exp(-|x_1 - y_1|^2 / 1.2^2)$.

Example 4.2. To reconstruct a periodic random surface that is a sum of a deterministic function $\tilde{f}(x_1) = 1.5 + 0.2\cos(\pi(x_1 - \pi))\exp(-(x_1 - \pi)^2 / 2)$ and a stationary Gaussian process with the covariance function $c(x_1 - y_1) = \sigma^2 \exp(-|x_1 - y_1|^2 / l^2)$, where $\sigma = 0.06, l = 1.2; \sigma = 0.06, l = 0.8; \sigma = 0.1, l = 0.8$.

By choosing the total number of realizations $M = 1000$ and performing our numerical method in parallel, graphs of the original profile and evolutions of the reconstructed profiles of the random process with the rms height $\sigma = 0.06$ and the correlation length $l = 1.2$ at different wavenumbers in Example 4.1 and Example 4.2 are shown in Fig. 4 and Fig. 5, respectively. It is obvious that the reconstructions are getting better as the wavenumber $\kappa$ increases, and the mean random profile can be reconstructed as a finite Fourier series expansion with at least an accuracy of $10^{-2}$, which is a wonderful mean reconstruction of the unknown periodic random rough grating structure.

By doing more simulations, it can be concluded that whether it is a smoother random process with smaller rms height or a rougher random process with larger
Figure 4: Evolutions of the reconstructions in Example 4.1. The solid curve: the reconstructed profile; the dotted curve: the given deterministic profile $\tilde{f}(x_1)$. From left to right, from top to bottom are the reconstructions at $k=1,2,3,4,5,6$. Here, $\sigma=0.06, l=1.2$, and the number of realizations is $M=1000$.

Figure 5: Evolutions of the reconstructions in Example 4.2. The solid curve: the reconstructed profile; the dotted curve: the given deterministic profile $\tilde{f}(x_1)$. From left to right, from top to bottom are the reconstructions at $k=1,2,3,4,5,6,7,8,9$. Here, $\sigma=0.06, l=1.2$, and the number of realizations is $M=1000$. 
Figure 6: Evolutions of the reconstructions of a certain realization in Example 4.2 by the continuation method. The solid curve: the reconstructed profile; the dotted curve: the given profile. From the top to the bottom are the reconstructions at $k=2,4,6,8$. The first column is reconstructions of the deterministic profile; The next three columns from left to right are reconstructions of a certain realization of the random process with $\sigma = 0.06, l = 1.2$; $\sigma = 0.06, l = 0.8$; and $\sigma = 0.1, l = 0.8$, respectively.

rms height, the proposed method has the convergence and stability for the periodic random rough profile, which confirms that our method is reliable and efficient.

Specifically, Fig. 6 gives the experimental results in Example 4.2 with different rms heights and correlation lengths. Each shows the evolutions of the reconstructions of the deterministic profile and a particular realization of different random surfaces at different wavenumbers. As seen in Fig. 6, our continuation method
has the convergence for each realization of the periodic random rough structures with the rms height in the range of 0.06-0.1 and the correlation length in the range of 0.8-1.2. Since all of the samples in the probability space are chosen iid, our Monte Carlo sampling process can be performed well in parallel and all of these mean unknown periodic structures with different rms heights and correlation lengths can be reconstructed by our method.

4.2 Reconstruction of rms height and correlation length of the random structure

As presented in Section 3, based on the mean profile $\bar{f}(x)$ reconstructed above, the rms height $\sigma$ and the correlation length $l$ can be further reconstructed. Specifically, we can calculate the two critical statistical properties of the periodic random rough surface from the reconstructed eigenvalues by the recovery formula (3.14).

Still consider the two periodic random rough surfaces in Example 4.1 and Example 4.2 mentioned above.

Fig. 7 shows the reconstructions of the eigenvalues, the covariance function and the random profile in Example 4.1 when $\sigma = 0.06, l = 1.2$. Then it can be calculated directly from the reconstructed eigenvalues that $\sigma' = 0.057, l' = 1.33$ in Example 4.1, which is a good evaluation of the rms height and the correlation length of the random structure. Note that the random profile reconstructed by our MCCUQ method is in the form of the sum of a finite Fourier series expansion and a truncated KL expansion.

More detailed results including reconstructions of the rms height, the eigenvalues, the covariance function and the random profile with different rms heights and correlation lengths for Example 4.2 are presented in Figs. 8-12.

Figure 7: From the left to the right: reconstructions of the eigenvalues, the covariance function and the random profile in Example 4.1 by our MCCUQ method. Here, $\sigma = 0.06, l = 1.2, M = 1000$. 
Fig. 8 shows the evolution of the evaluation of the rms height $\sigma$ of the random structure as the wavenumber increases. As shown in Fig. 8, evaluation of the rms height $\sigma$ is getting better with the wavenumber increasing.

It can be seen from Fig. 9 that the reconstructions of the eigenvalues have a very high accuracy by our MCCUQ method.

Since the recovery formula (3.14) can reconstruct the rms height and the correlation length of the random structure, we can calculate the two statistical properties by the recovery formula from the reconstructed eigenvalues. Specifically, it can be calculated directly that $\sigma' = 0.057$, $l' = 1.251$ when $\sigma = 0.06$, $l = 1.2$; $\sigma' = 0.057$, $l' = 0.820$ when $\sigma = 0.06$, $l = 0.8$; and $\sigma' = 0.094$, $l' = 0.859$ when $\sigma = 0.1$, $l = 0.8$ in Example 4.2. The conclusion can be deduced that no matter the rougher or smoother random structure with larger or smaller rms height, all the evaluations of the two critical statistical properties of the periodic random rough surfaces by
Figure 10: Reconstructions of the covariance function in Example 4.2 by our MCCUQ method. Blue solid curve: the reconstructed covariance function; red dotted curve: the original covariance function. From left to right are $\sigma = 0.06, l = 1.2$; $\sigma = 0.06, l = 0.8$; and $\sigma = 0.1, l = 0.8$, respectively.

our MCCUQ method is excellent. Fig. 10 shows the corresponding reconstructed Gaussian covariance function in Example 4.2.

In some scenarios, a random process is characterized by its mean, rms height, and an auto-correlation function which is defined as $w(x_1 - y_1) = \exp(-|x_1 - y_1|^2/l^2)$. Reconstructions of the auto-correlation function in Example 4.2 are shown in Fig. 11. It is easily seen that the reconstructions of the auto-correlation function in Example 4.2 are great.

Finally, Fig. 12 shows the reconstruction of the KL expansion random profile by our MCCUQ method in Example 4.2 which is in the form of the sum of a finite Fourier series expansion and a truncated KL expansion. We can see that the reconstructions of the periodic random rough surfaces with the rms height $\sigma = 0.06, 0.1$ and the correlation length $l = 1.2, 0.8$ in Example 4.2 shown in Fig. 12 reach an accuracy of $10^{-3}$.

Figure 11: Reconstructions of the auto-correlation function in Example 4.2 by our MCCUQ method. Blue solid curve: the reconstructed auto-correlation function; red dotted curve: the original auto-correlation function. From left to right are $\sigma = 0.06, l = 1.2$; $\sigma = 0.06, l = 0.8$; and $\sigma = 0.1, l = 0.8$, respectively.
Numerical results show that our MCCUQ reconstruction method has the convergence and stability for periodic random rough surfaces. We can reconstruct the mean unknown periodic random rough structure with at least an accuracy of $10^{-2}$ or even higher, and give a good evaluation of the rms height and correlation length to certain degree, which realizes the characterization of the periodic random rough structure, and shows a better reconstruction than that of the deterministic issues which only considers the noise level of data measurement. The conclusion can also be deduced that under the condition that $l$ is much smaller than the period $\Lambda$, the larger the correlation length $l$ is or the smaller the rms height $\sigma$ is, the more accurate the evaluation of the statistics is.

### 4.3 Comparison with the reconstruction in TE polarization

Finally, discuss about the reconstruction in TM polarization in comparison with that in TE polarization. Still consider the periodic random rough surface in Example 4.2 mentioned above. The rms height and the correlation length are defaulted as $\sigma=0.1, l=0.8$, and the total number of the realizations for sampling the probability space is $M=1000$.

Graphs of the original profile and evolutions of the reconstructed profiles of the periodic random rough structure at different wavenumbers in Example 4.2 are shown in Fig. 13. It is obvious that the reconstruction by our MCCUQ method in TM polarization has a slower convergence than that in TE polarization. Thus, in order to get the same accuracy, the reconstruction in TM polarization requires larger wavenumber, i.e., higher frequency.

Specifically, the relative errors of the reconstruction in TM and TE polarization in Fig. 14 are illustrated to give further comparison. On the left of Fig. 14, the
Figure 13: Evolutions of the reconstructions of the periodic random structure in Example 4.2 by our proposed method. Blue solid curve: the reconstructed profile; red dotted curve: the given deterministic profile $\tilde{f}(x)$. The left column is the reconstruction in TM polarization, from top to bottom are the reconstructions at $k = 2, 4, 6, 8$; the right column is the reconstruction in TE polarization, from top to bottom are the reconstructions at $k = 1, 2, 3, 4$. Here $\sigma = 0.1, l = 0.8$.

Relative errors of the mean unknown profile at different wavenumbers in TM and TE polarization in Example 4.2 are presented. We can see that all of the reconstructions in TM and TE polarization have an accuracy of $10^{-2}$. Moreover, higher frequency is required in TM polarization to reach the same accuracy as that in TE polarization. Specifically, the relative error of the mean unknown profile at $k = 4$ in TE polarization is $1.18 \times 10^{-2}$. To reach the same level of the relative error, the reconstruction in TM polarization requires a larger wavenumber, at least $k = 6$. 
The larger the wavenumber is, the more accurate reconstruction we achieve. The reconstructions in TM polarization in Example 4.2 have an accuracy of $10^{-3}$ provided that the wavenumber is greater than 7. On the right of Fig. 14, the relative errors of the rms height at different wavenumbers in TM and TE polarization in Example 4.2 are shown. The relative error of the rms height at $k=4$ in TE polarization is 6.05%, while the relative error of the rms height at $k=4$ in TM polarization is 24.65%. With the wavenumber increasing, the relative error of the rms height in TM polarization decreases gradually and becomes 6.98% at $k=8$ and 6.05% at $k=9$, which is close to that in TE polarization at $k=4$. It can be deduced that the reconstruction in TM polarization needs higher frequency than that in TE polarization.

5 Concluding remarks

We have developed an efficient numerical method for solving the inverse problem of determining periodic perfectly conducting random grating surfaces for TM polarization. Numerical results show the reliability and efficiency of the proposed method. In comparison to the TE case, with less regular solutions in the TM case, much smaller relaxation parameter should be chosen and higher frequency should be used for the TM reconstruction. Note that the reconstruction by our MCCUQ method reach a certain accuracy for both TE and TM cases, including the reconstruction of the expectation, rms height and correlation length.
of the random structure. There are many open problems along this direction. Although our numerical examples illustrate the convergence of MCCUQ, there is no rigorous analysis of convergence and stability. Other interesting future directions include solving the inverse scattering problems by penetrable random rough surfaces, non-periodic random rough surfaces, or bi-periodic random surfaces in higher dimensional scenarios.

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