A COMPUTATIONAL STOCHASTIC METHODOLOGY FOR THE DESIGN OF RANDOM META-MATERIALS

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Abstract. Nanostructured materials like thin film solar cells have opened new opportunities for light management and energy efficiency. Recently, it has been shown that structurally correlated random surfaces can drastically increase light absorption [11]. The meta-atoms used in meta-materials may have a random variation by design or due to a defective manufacturing process. Of interest is how the correlated random position of the meta-atoms affects the optical properties such as transmission and reflection coefficients of random structures [3, 12]. We shall present a computational stochastic methodology for generating and optimizing random meta-material configurations with non-overlapping geometric constraints subject to various types of covariances and distributions characterizing the randomness of the meta-material configurations [8, 9].

The methodology developed consists of three main components: (1) A deterministic solver for electromagnetic scattering from multiple objects [1, 2]. (2) The Karhunen-Loève (K-L) expansion to represent the correlated configurations of the scattering objects [5, 10]. (3) The Multi-element probabilistic collocation method (ME-PCM) to provide flexibility in achieving desired distributions of the meta-materials [4]. In the current work, we employ random fields from a Spartan family that includes covariance functions with damped oscillatory behavior [6, 10]. The algorithm is applied to study light propagation through random layered heterojunctions and random 3-D meta-materials. We found that greater transmission and reflection, compared to the uniformly spaced structures, can be achieved for a structure with an oscillatory spacing profile along the propagation direction. Optimized configurations of the heterojunctions and 3-D meta-materials have been found with larger or smaller transmission coefficients for different wave numbers of the incoming wave and different correlations [8]. We shall discuss generalizations of this methodology by using non-separable covariance functions [7] as well as by applying the adaptive ANOVA decomposition [13] to investigate the sensitivity of the reflection coefficient to different parameters and deal with dimensionality challenges.

Key words. Meta-materials, electromagnetic scattering,stochastic collocation, Karhunen-Loève expansion, Spartan spatial random fields, correlated randomness.

REFERENCES

[1] D. Chen, W. Cai, B. Zinser, and M. H. Cho, *Accurate and efficient Nyström volume integral equation method for the Maxwell equations for multiple 3-d scatterers*, J. Comput. Phys., 321 (2016), pp. 303–320.

[2] M. H. Cho and W. Cai, *A parallel fast algorithm for computing the Helmholtz integral operator in 3-d layered media*, J. Comput. Phys., 231 (2012), pp. 5910–5925.

[3] V. E. Ferry, M. A. Verschuuren, M. C. v. Lare, R. E. Schropp, H. A. Atwater, and A. Polman, *Optimized spatial correlations for broadband light trapping nanopatterns in high efficiency ultrathin film a-si: H solar cells*, Nano Lett., 11 (2011), pp. 4239–4245.

[4] J. Foo and G. E. Karniadakis, *Multi-element probabilistic collocation method in high dimensions*, J. Comput. Phys, 229 (2010), pp. 1536–1557.

[5] R. G. Ghanem and P. D. Spanos, *Stochastic Finite elements: A Spectral Approach. Revised Edition*, Dover Publications, New York, 2003.

[6] D. T. Hristopulos, *Spartan Gibbs random field models for geostatistical applications*, SIAM J. Sci. Comput., 24 (2003), pp. 2125–2162.

[7] D. T. Hristopulos and E. Porcu, *Multivariate Spartan spatial random field models*, Probab. Eng. Mech., 37 (2014), pp. 84–92.

[8] I. C. Tsantili, M. H. Cho, W. Cai, and G. E. Karniadakis, *A computational stochastic methodology for the design of random meta-materials under geometric constrains.*

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[9] I. C. Tsantili, M. H. Cho, W. Cai, and G. E. Karniadakis, *Uncertainty quantification algorithms for meta-materials*, 2017. Presented in 2nd International Conference on Uncertainty Quantification in Computational Sciences and Engineering, Rhodes, June, 1-6.
[10] I. C. Tsantili and D. T. Hristopulos, *Karhunen-Loève expansion of Spartan spatial random fields*, Probab. Eng. Mech., 43 (2016), pp. 132–147.
[11] K. Vynck, M. Burresi, F. Riboli, and D. S. Wiersma, *Photon management in two-dimensional disordered media*, Nat. Mater., 11 (2012), pp. 1017–1022.
[12] D. S. Wiersma, *Disordered photonics*, Nat. Photonics, 7 (2013), pp. 188–196.
[13] X. Yang, M. Choi, G. Lin, and G. E. Karniadakis, *Adaptive anova decomposition of stochastic incompressible and compressible flows*, J. Comput. Phys., 231 (2012), pp. 1587–1614.