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Design Optimizations Simulation of Wave Propagation in Metamaterials

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Final Report

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14. ABSTRACT
Metametarials are scientifically engineered materials that are designed to interact with and control mechanical and electromagnetic waves in ways that cannot be achieved with conventional materials. For instance, metamaterials can be designed to bend electromagnetic waves around an object so that the object appears invisible to surrounding observers, focus light to create a subwavelength image of a source, and mitigate blast waves to protect structures and humans from explosion. Among the many research fronts we have been working on under this grant, one highlight is the introduction of a fundamentally new modeling paradigm that incorporates fabrication issues in the optimal design of metamaterials. Another highlight of our work under this grant is our successful development of full 3D topology optimization (in which every voxel of the unit cell is a degree of freedom) of photonic-crystal structures in order to find optimal omnidirectional band gaps for various symmetry groups, including fcc (including diamond), bcc, and simple-cubic lattices.

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Final Report for AFOSR Grant:
Design Optimization and Simulation of Wave Propagation in Metamaterials

Metametarials are scientifically engineered materials that are designed to interact with and control mechanical and electromagnetic waves in ways that cannot be achieved with conventional materials. For instance, metamaterials can be designed to bend electromagnetic waves around an object so that the object appears invisible to surrounding observers, focus light to create a subwavelength image of a source, and mitigate blast waves to protect structures and humans from explosion.

Among the many research fronts we have been working on under this grant, one highlight is the introduction of a fundamentally new modeling paradigm that incorporates fabrication issues in the optimal design of metamaterials. This new modeling method is motivated by the observation that the computed optimal solution of an optimization problem often cannot be implemented directly, irrespective of data accuracy, due to either (i) technological limitations (such as physical tolerances of machines or processes), (ii) the deliberate simplification of a model to keep it tractable (by ignoring certain types of constraints that pose computational difficulties), and/or (iii) human factors (getting people to "do" the optimal solution). We have developed a modeling paradigm called "fabrication-adaptive optimization" for treating issues of implementation/fabrication. We develop computationally-focused theory and algorithms, and we present computational results for incorporating considerations of implementation/fabrication into constrained optimization problems that arise in photonic crystal design. The fabrication-adaptive optimization framework stems from the robust regularization of a function (see A. Lewis (2002) "Robust regularization," Technical Report, Simon Fraser University, Burnaby, British Columbia, Canada). When the feasible region is not a normed space (as typically encountered in application settings), the fabrication-adaptive optimization framework typically yields a non-convex optimization problem. (In the special case where the feasible region is a finite-dimensional normed space, fabrication-adaptive optimization can be re-cast as an instance of modern robust optimization.) We study a variety of problems with special structures on functions, feasible regions, and norms, for which computation is tractable, and develop an algorithmic scheme for solving these problems in spite of the challenges of non-convexity. We apply our methodology to compute fabrication-adaptive designs of two-dimensional photonic crystals with a variety of prescribed features. The fabrication-adaptive methodology together with the convex optimization formulations we proposed before integrate into a systematic design framework for the metamaterials applications that are of direct and practical interest to the Air Force.

Another highlight of our work under this grant is our successful development of full 3D topology optimization (in which every voxel of the unit cell is a degree of freedom) of photonic-crystal structures in order to find optimal omnidirectional band gaps for various symmetry groups, including fcc (including diamond), bcc, and simple-cubic lattices. Even without imposing the constraints of any fabrication process, the resulting optimal gaps are only slightly larger than previous hand designs, suggesting that current photonic crystals are nearly optimal in this respect. However, optimization can discover new structures, e.g. a new fcc structure with the same symmetry but slightly larger gap than the well-known inverse opal, which may offer new degrees of freedom to future fabrication technologies. Furthermore, our band-gap optimization is an illustration of a computational approach to 3D dispersion engineering which is applicable to many other problems in optics, based on a novel semidefinite program formulation for non-convex eigenvalue optimization combined with other techniques such as a simple approach to impose symmetry constraints. We also demonstrate a technique for robust topology optimization, in which some uncertainty is included in each voxel and we optimize the worst-case gap, and we show that the resulting band gaps have increased robustness to systematic fabrication errors.

Publications for AFOSR Grant:
Design Optimization and Simulation of Wave Propagation in Metamaterials

[] "Functional Gaussian processes for regression with linear PDE models," Ngoc-Cuong Nguyen and Jaime Peraire, submitted.

[] "A model and variance reduction method for computing statistical outputs of stochastic elliptic partial differential equations" by Ferran Vidal-Codina, Ngoc-Cuong Nguyen, Mike Giles, Jaime Peraire, submitted.

[] "Robust topology optimization of three-dimensional photonic-crystal band-gap structures," with H. Men, K. Y. K. Lee, J. Peraire, and S. G. Johnson, *Optics Express* 22 (19), pp. 22632-22648, September 2014.

[] "Designing Phononic Crystals with Conic Convex Optimization" with Han Men, N.-C. Nguyen, Joel Saa-Seoane, and Jaime Peraire, ASME2013 International Mechanical Engineering Congress and Exposition, pp. V014T15A047, San Diego, November 2013.

[] "New Analysis and Results for the Frank-Wolfe Method," (formerly titled "New Analysis and Results for the Conditional Gradient Method") Robert Freund and Paul Grigas, conditionally accepted in *Mathematical Programming*.

[] "AdaBoost and Forward Stagewise Regression are First-Order Convex Optimization Methods," Robert Freund, Paul Grigas, and Rahul Mazumder, MIT Operations Research Center working paper OR 397-14.

[] "Bandwidth optimization of single-polarization single-mode photonic crystal fibers," with N.-C. Nguyen, H. Men, and J. Peraire, Technical Report.

[] "Fabrication-Adaptive Optimization, with an Application to Photonic Crystal Design," Robert Freund, J. Saa-Seoane, N.-C. Nguyen, H. Men, and J. Peraire, *Operations Research* 62 (2), pp. 418-434, 2014.

[] "A Binary Optimization Method for Linear Metamaterial Design Optimization," with J. Saa-Seoane, N.-C. Nguyen, H. Men, and J. Peraire, *Journal of Applied Physics A 109* (4), pp. 1023-1030, 2012.

[] “An Accelerated First-Order Method for Solving Unconstrained SOS Polynomial Optimization Problems”, with Dimitris Bertsimas and Xu Andy Sun, *Optimization Methods and Software 28* (3), pp. 424-441, 2013.