Final Technical Report

Grant/Contract Title: FUNDAMENTAL MODELING AND DESIGN STRATEGIES IN COMPUTATIONAL PHOTONICS- APPLICATIONS TO LASERCOM THROUGH CLOUDS AND ELECTRO-OPTICAL/NANOPHOTONICS

Grant/Contract Number: FA9550-04-1-0213

Executive Summary

This summary highlights significant advances and discoveries under the support of the above grant. Two broad non-overlapping research topic areas were addressed in the project: I. Lasercom through clouds using novel partially spatially and temporally coherent laser beams, and II. Computational nanophotonics, plasmonics and metamaterials applied to new algorithm development with applications to atom/quantum dot traps, nonlinear harmonic generation in metamaterials and novel plasmonic high density data storage.

The lasercom project focused on investigating whether partially spatially coherent beams, constructed from an array of individual emitters, would reduce the scintillation index relative to a single Gaussian beam. Our results indicated a significant reduction and this was confirmed by a follow-on collaborative experiment with AFRL personnel where multiple beams were generated by fiber lasers. The proposed end solution for a partially spatially coherent laser source was an array of Vertical External Cavity Surface Emitting semiconductor lasers (VECSEL). Funding was provided under the project to grow VECSEL wafers that could be processed into laser chips. The chip processing (mounting and etching) and VECSEL laser demonstration was carried out under parallel ongoing JTO MRI projects.

The main focus of the project was on developing novel algorithms aimed at improving on 3D finite difference time domain (FDTD) approaches existing in the literature. A number of key issues were addressed and resolved. Firstly, while it is computationally expedient to employ a fixed computational grid (Cartesian) over most of a general computational domain, mix of symmetries of objects embedded in this domain inevitably gives rise to grid stair-casing effects on surfaces on odd-shaped objects. Additionally, the large scale disparity between the wavelength of light and the nanostructured materials with which it reacts dictated the need to develop a stable, second-order adaptive space and time mesh for solving 3D vector Maxwell equations. In the study of nanophotonics, plasmonics and metamaterials, it is the near-field details on the surfaces of objects that determine the key sub-wavelength interactions. Stair-casing creates discontinuous artifacts on surfaces even though the far-field (a few nanometers away) is unaffected. We successfully studied and implemented a number of non-orthogonal grid algorithms that remove these spurious effects. Solve 3D vector Maxwell. A 3D finite element method with single cell PML absorbing boundaries was developed toOn the applications side, we developed a new theory of second harmonic generation from arrays of metallic SRRs starting from a microscopic description and successfully applied this theory to explain some new results from an experimental group at the University of Karlsrühe, Germany. Further applications involved the calculation of forces on quantum dots and/or dielectric nanospheres in the vicinity of metallic bow-tie nano-apertures and the design of a novel high-density plasmonic data storage device.

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Technical Highlights

I. Lasercomm through Clouds

In this study, we explored the concept of creating a partially coherent laser beam consisting of an array of spatially overlapping or separated Gaussian beams with possible individual control of each individual emitter's wavelength. The idea was to test whether such a transmitter array could propagate more effectively through weak or strong atmospheric turbulence. A schematic of the transmitter array is sketched in Figure 1 with the color coding indicating different colors (wavelengths) of individual beams.

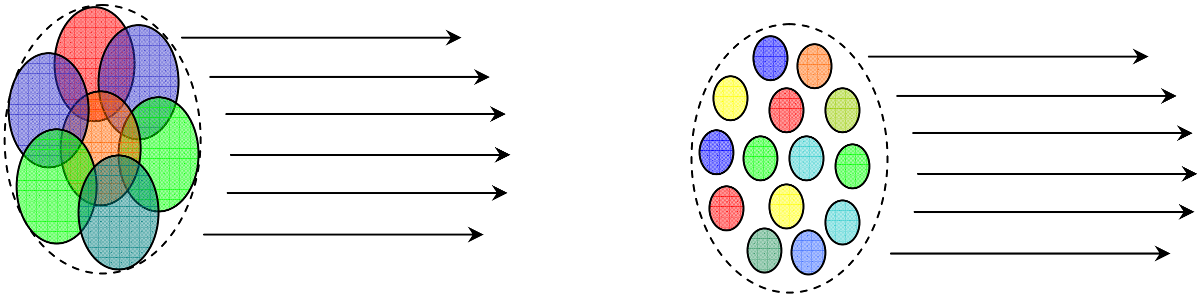


Figure 1 Schematic of an overlapping array of individual spatially overlapping transmitter beams (left) or spatially separated transmitter beams (right) individually capable of operating at different wavelengths. The center-to-center separation between individual emitters is a key control parameter in our theoretical analysis.

We proposed that a versatile multi-wavelength multi-emitter configuration in Fig. 1 could be realized via an array of optically-pumped vertical external-cavity surface emitting semiconductor lasers (VECSELs). These devices at the time showed great promise as high-brightness, wavelength tunable TEM_{00} multi-Watt sources and we sought funding under the project to grow such wafers. These wafers leveraged our parallel JTO MRI project where we were able to process (mount and etch) and test them as lasers under a parallel research program. Our results to date under the JTO MRI project shows record power outputs near 40 W in a TEM_{00} mode and near 64 W multi-lateral mode. We are now confident as a result of the theoretical analysis carried out under the present project and a validation experiment using much lower power fiber lasers in a laboratory setting, that such a transmitter array is indeed feasible. The VECSEL geometry is compact, with a surface outcoupled TEM_{00} beam and is readily tunable over a 30-50nm bandwidth. Figure 2 shows a schematic of a compact VECSEL cavity where the diode pumps (at say, 808nm) are integrated onto a heat sink together with the VECSEL active mirror. At high pump power densities, the quantum wells in the resonant periodic gain stack within the VECSEL structure are inverted and emit light at the signal wavelength (for example, 1040nm). The external output coupler depicted on the left of Fig. 2 provides optical feedback and transmits the outcoupled TEM_{00} beam. The birefringent filter in the cavity acts as a tuning element to control the output signal wavelength. An array of such VECSELs can be configured to produce the transmitter beams in Fig. 1 above.

As a first step, we considered theoretically an array of Gaussian beams and carried through an analysis for propagation in both weak and strong turbulence. This work is documented in the papers [19,21]. In the transmitter-receiver geometry we assumed a slow detector and calculated the longitudinal and radial components of the scintillation index for a typical free-space communications laser setup.

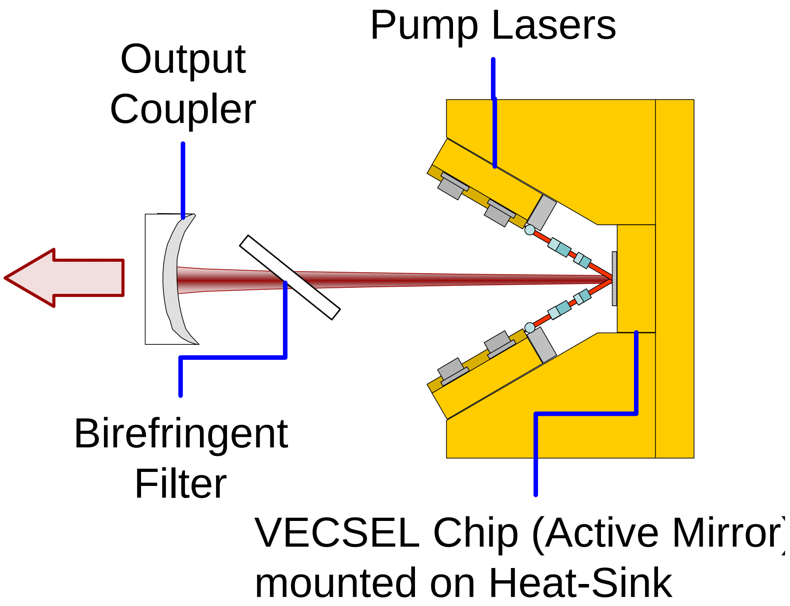


Figure 2 Schematic diagram of a compact VECSEL two-mirror cavity optically pumped by external diode lasers. The two-mirror cavity consists of an active VECSEL semiconductor chip (disk) on the right controlled by the incoherent diode pump lasers and a passive outcoupling mirror on the left to feedback and outcouple the signal beam.

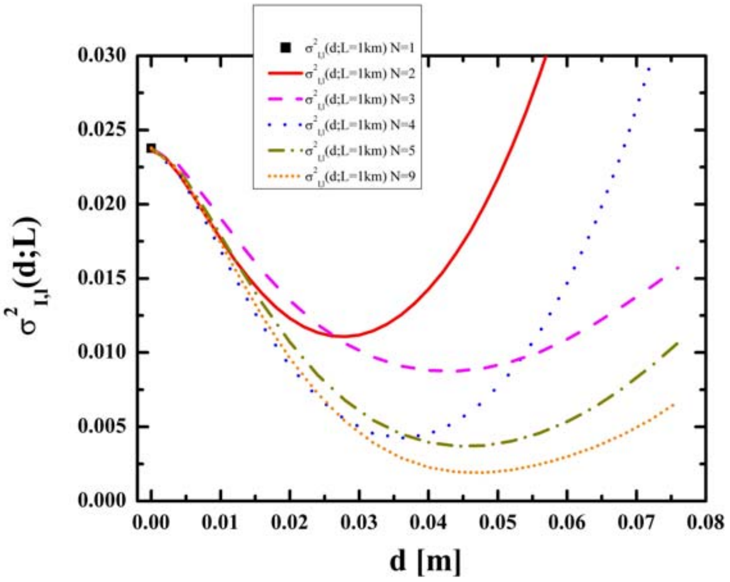


Figure 3 Calculated scintillation index at the receiver for atmospheric transmission over 1 kilometer with varying numbers of beams filling the transmitter aperture as a function of beam ceneter-to-center separation. The solid square is the reference value of the scintillation index for a single Gaussian beam.

Our calculations assuming weak optical turbulence, are detailed in references [19,21] and show a significant reduction in the scintillation index for multiple beams where we calculate this reduction as a function of different beam center-to-center spacing. Figure 3 summarizes the results of these calculations for up to 9 laser beams in the array. A reduction of longitudinal scintillation index of greater than 92% is predicted for 9 beams at the transmitter when the separation and beam spot size has been optimized.

An experiment was subsequently carried out by our research team and AFRL collaborators from AFRL Kirtland Starfire Optical Range [13]. In the laboratory experiment, the multi-emitter beam was generated by spatially combining several beams from single mode fibers. The results confirmed the theory prediction of scintillation index for weak turbulence and, moreover, showed that a similar reduction is observed under strong turbulence conditions. The experimental data are summarized in Fig 4 below. The beam diameter of the individual emitters was around 0.42 mm and a phase screen is placed in the beam path to simulate weak and strong turbulence. The total path length in the laboratory was 2 meters.

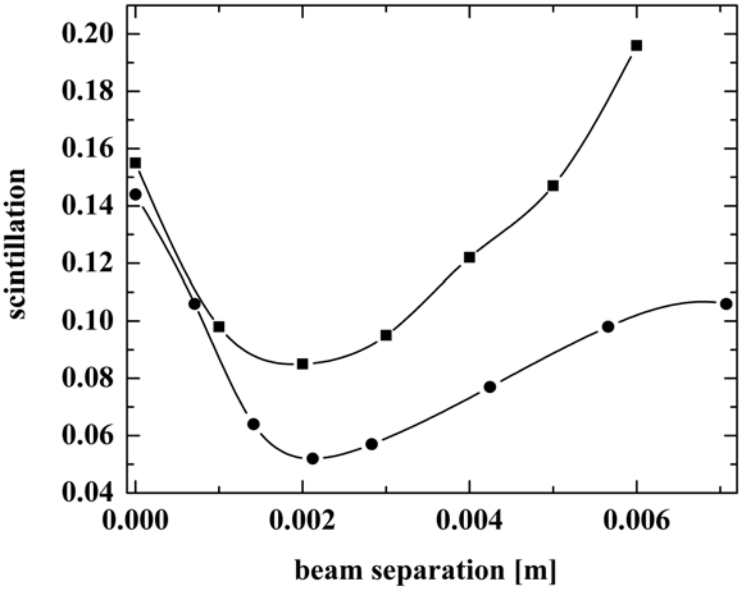


Figure 4 Experimentally measured scintillation index for two (top curve) and four (bottom curve) as a function of beam separation.

The experimental data verify the theoretical predictions and show that the partial spatial coherence was dominant over the multi-color diversity in the beam(s). This sequence of results suggests that field tests with the fiber laser array replaced by a VECSEL array, with each VECSEL outputting multi-Watts of power at selected wavelengths, is a viable modality for laser communications in a turbulent atmosphere. The VECSEL chips developed under the current parallel running JTO MRI already provide more than 25W per emitter in a TEM_{00} (and 45W multimode), are easily tunable over 30-50nm and are coincident with an atmospheric transmission window.

II. Computational Methods Applied to Nanophotonics, Plasmonics and Metamaterials

This component of the project became the focus of research in years 3-5 of the project. Our goal here was two-fold:

A. Develop robust 3D vector Maxwell solvers that could be applied to realistic situations and,

B. Apply the developed computer codes to important problems involving the interaction of light with sub-wavelength structures.

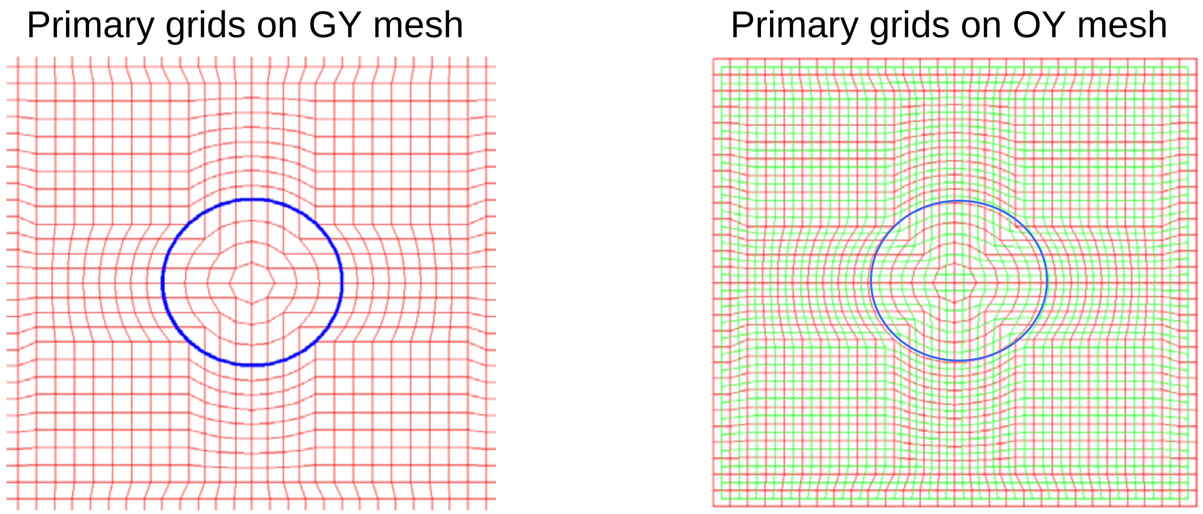
A. Computational Methods

We wanted to extend the already successful and extensively applied Finite Difference Time Domain (FDTD) method to nanofeatured structures with irregular geometries. The large separation of scales between the wavelength of the incident light and individual nano features led us to implement an adaptive space and time FDTD algorithm [24,25]. Many attempts have been made over the past few decades, by the microwave research community, to develop stable, second order accurate adaptive space-time FDTD schemes. To our knowledge, the result in reference [25] is the only such stable and second order accurate 3D space and time mesh refinement FDTD scheme published in the literature. We employ this code in many of the simulations carried out in the present project. The challenge in maintaining algorithm stability and second order accuracy was in implementing appropriate extrapolation schemes between fine and coarse time and space mesh boundaries. Details are presented in reference 25.

Another issue that we addressed was that of avoiding stair-casing effects on surfaces due to the fact that the global coarse grid on the large computation domain does not generally conform to the shape of an arbitrary surface. In realistic simulations, one does that have the luxury of assuming an ideal numerical grid that satisfies a specific symmetry as we encounter objects with arbitrary complex shapes within the computational domain. We explored a number of schemes involving nonorthogonal grids to achieve smooth transitioning between our global Cartesian and a numerical grid that conforms to the surface of interest. The latter grid would avoid numerical artifacts associated with staircasing on surfaces – for example, the surface plasmonic modes generated on a metallic nanostructure. As stressed above, these near-fields profoundly influence objects (atoms, quantum dots, etc) that may be attached to the surface of only a few nanometers away.

We proposed and evaluated two nonorthogonal grid schemes, which we call “Generalized Yee (GY)” and “Overlapping Yee (OY). The first GY scheme is based on earlier results of Gedney (1996) and others in the literature and on the Discrete Surface Integral (DSI) method due to Marsden (1995). The scheme when implemented for vector Maxwell preserved second order accuracy, is divergence free, avoids staircasing and reduces to the standard FDTD when grids are orthogonal. A picture of an OY grid is shown on the left of Figure 5 below. Unfortunately this scheme exhibits a late time instability typically after tens of thousands of time steps and we did not pursue it further. The overlapping YEE scheme preserves all of the above mentioned favorable properties and moreover, exhibits no late time instability [7]. This scheme however comes at the cost of doubling the mesh (the base mesh and a companion mesh as shown on the right of Figure 5 below). This adds memory and CPU execution costs but is still manageable.

Two manuscripts are under review [L. Lu et al: Manuscripts under Review below] on further improvements in 3D FDTD algorithms.


Primary grids on GY mesh

Primary grids on OY mesh

Figure 5 Left: Grid layout for the Generalized Yee FDD scheme applied to a 2D dielectric cylinder. Right: The Overlapping Yee dual grid applied to the same problem.

We also developed a companion 3D frequency domain Finite Element vector Maxwell solver with the adding novel feature of a single cell absorbing boundary (PML) layer that dramatically reduces memory requirements in 3D simulations [34, Mohan-Gundu Ph.D thesis, Arizona]. This scheme has been applied to mode calculations and scattering problems. PML absorbing layers generally extend over many cells surrounding the computational domain of interest. In 3D this adds a huge computational overhead requiring inversion of a very large matrix. The single cell PML involves utilizing a higher-order polynomial within a singe cell to reduce the reflectivity for outward propagating waves in 3D [Mohan-Gundu, Ph.D thesis Arizona].

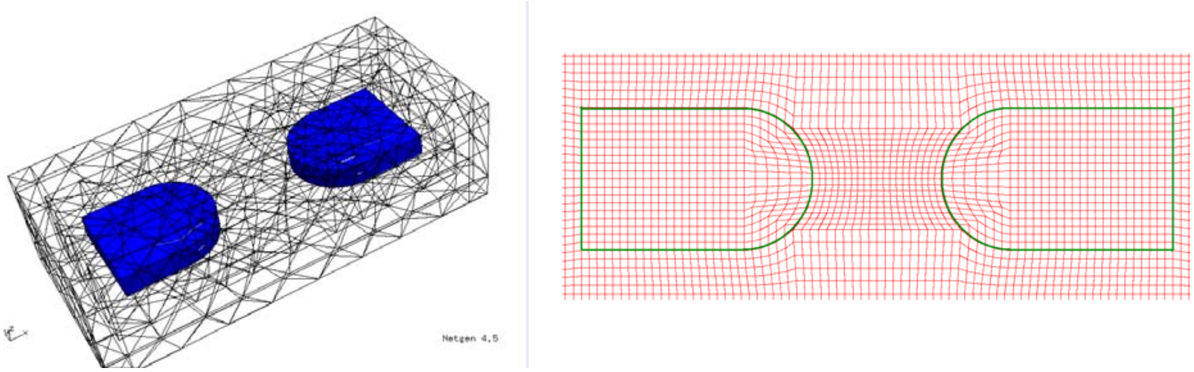


Figure 6 Left: FEM grid for scattering from a nanostructured bow-tie aperture. Right: Nonorthogonal GY grid (2D slice) for the same scattering problem.

Figure 6 shows the 3D FEM grid on the left and a slice through the center of the Generalized Yee grid on the right in the study of scattering of an incident plane wave from a metal bowtie nano-aperture. We have used this physical problem extensively in the calculation of forces on and trapping of individual quantum dots and dielectric nanospheres. A comparison of FEM and GY FDTD with the adaptive space and time FDTD shows as expected, significant deviations of the electric field on the surface of the metallic bowtie.

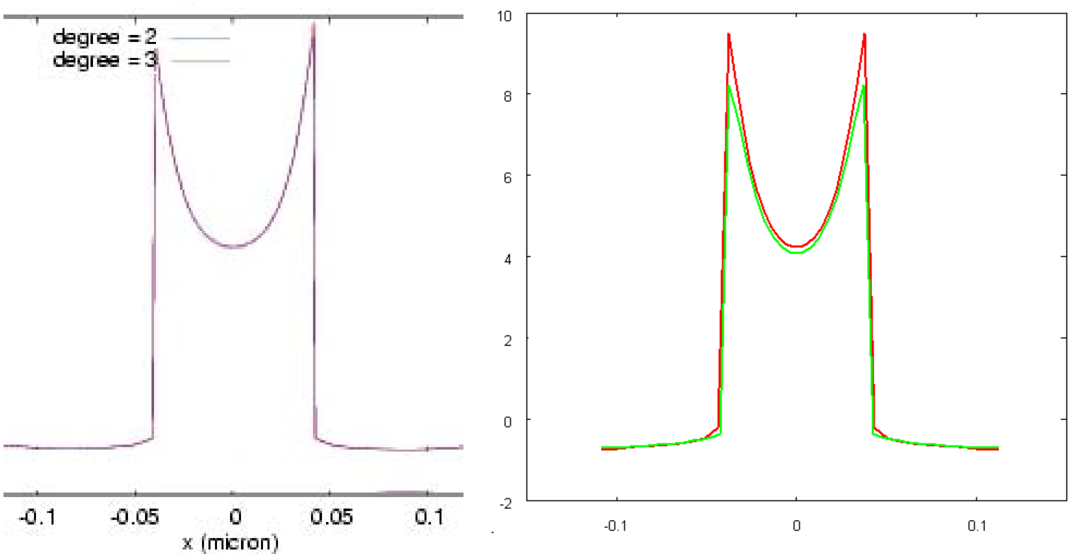


Figure 7 1D slice of the electric field through the center line of the bowtie aperture. Left: 3D FEM solution using a degree 2 and degree 3 polynomial in the single cell PML layer. Right: Comparison of the GY FDTD (red) and the adaptive space-time FDTD green for the same problem.

Figure 7 compares full 3D simulations of scattering of an incident plane wave (on nanoscales, there is no difference between a plane wave and a Gaussian beam) from a nanoscale bowtie aperture. Parameters used in this simulation are: Bowtie Metal (Gold): length=145nm; Gap between tips=80nm; thickness=20nm; Tip: semi-disk with radius=43.3nm and an incident x-polarized plane wave at 800nm. The left picture shows the superposition of two 3D FEM vector Maxwell calculations where the single cell PML is modeled with a degree 2 and a degree 3 polynomial. The solutions are essentially identical. The right picture compares two FDTD simulations. The green curve is the adaptive space and time FDTD and the red curve the nonorthogonal mesh Generalized Yee method. The red curve agrees with the FEM calculations but the red curve shows a significant difference at both bowtie tips due to staircasing artifacts. A manuscript is in preparation on these results.

II. Applications to Nanophotonics, Plasmonics and Metamaterials

Application of the above computational schemes to problems in nanophotonics, plasmonics and metamaterials are fully detailed in the publications below. Here we present a brief overview and point the reader to the appropriate papers.

Our earlier research in this area focused on photonic crystal structures (in fibers or thin films) where we explored the near-field coupling between the defect mode of the PC grown on a nearby quantum well [29], multimode interference based PCs [36], enhanced coupling in 1D semiconductor based PCs [35], polarizing beam splitters [31], intersecting PC waveguides [30] and fabrication of 2D PCs with embedded defects [26]. Our study of surface plasmon modes in thin metallic films with periodic nanostructured air holes, shed light on the role of surface plasmons in enhancing the experimentally observed extraordinary transmission of light through such sub-wavelength apertures [16,27, 28] and the excitation of the latter on metallic surfaces [15]. A second focus of the project was on the study of force on and trapping of microbeads in light fields [23], fundamental properties of radiation pressure [17,18] and trapping of quantum dots in metallic bowtie apertures [10]. A highlight of this work was the recent discovery of a novel scheme for utilizing plasmonic nanostructures for high density optical data storage [1].

In reference [2], we employed a cold-plasma model for the interaction of light with a metallic structure, derived from a microscopic theory, to explain the origin of second harmonic generation in metallic split-ring resonators (SRR). This was experimentally confirmed in joint work with a group at the University of Karlsrühe, Germany [8]. The remaining publications in the list below cover such diverse topics as improved numerical schemes for solving vector Maxwell [4-6], applications to light strings [32,12] and modeling vertical external cavity semiconductor lasers (VECSELs) [11].

Ph.D Degrees Supported

1. Liu, Tao (2005) Optical Sciences, Arizona “Photonic Crystals and Optical Devices”
2. Xie, Yong (2006) Optical Sciences, Arizona, “Transmission Properties of Sub-Wavelength Metallic Slits and their Applications”
3. Mohan-Gundhu, Krishna Optical Sciences, Arizona “hp-Finite Element method for Photonic Applications”

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Undergraduate Student
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LASERCOM PUBLICATIONS
AFOSR FA9550-04-1-0213

Fundamental modeling and design strategies in computational photonics

1. M. Mansuripur, A. R. Zakharian, A. Lesuffleur, Sang-Hyun Oh, R. J. Jones, N. C. Lindquist, Hyungsoon Im, A. Kobyakov, and J. V. Moloney, "Plasmonic nano-structures for optical data storage", *Optics Express*, **17**, 14001 (2009).

2. C. Dineen, M. Reichelt, S. W. Koch, and J. V. Moloney, "Optical trapping of Quantum dots in a metallic nano-trap", *Journal of Optics A: Pure and Applied Optics*, **11**, 114004, (2009).
Y. Zeng, W. Hoyer, J. Liu, S. W. Koch, and J. V. Moloney, "Classical theory for second-harmonic generation from metallic nanoparticles", *Physical Review B*, **79**, 2009.

3. Yong Zeng, Walter Hoyer, Jinjie Liu, Stephan W. Koch, and Jerome V. Moloney, "Classical theory for second-harmonic generation from metallic nanoparticles", *Physical Review B*, **79**, 235109 (2009).

4. Yong Zeng and Jerome V. Moloney, "Polarization-current-based, finite-difference time-domain, near-to-far- field transformation", *Optics Letters*, **34**, 1600 (2009).

5. Shuqi Chen, Weiping Zang, Axel Schulzen, Jinjie Liu, Lin Han, Yong Zeng, Jianguo Tian, Feng Song, Jerome V. Moloney, and Nasser Peyghambarian, “Implicit high-order unconditionally stable complex envelope algorithm for solving the time-dependent Maxwell’s equations”, *Optics Letters*, **33**, 2755 (2009).

6. Shuqi Chen, Lin Han, Axel Schülzgen, Hongbo Li, Li Li, 1, Jerome V. Moloney, and N. Peyghambarian1 “Local electric field enhancement and polarization effects in a surface-enhanced Raman scattering fiber sensor with chessboard nanostructure”, *Optics Express*, **16**, 13016 (2008).

7. Jinjie Liu, Moysey Brio, Jerome V. Moloney, “Overlapping Yee FDTD Method on Nonorthogonal Grids”, *J Sci Comput*, **39**, 129 (2008).

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10. M. Reichelt, C. Dineen, S.W. Koch, J.V Moloney, "Optical Forces on a Quantum Dot in Metallic Bowtie Structures", *IEEE Photonics Technology Letters,* **20**, 431 (2008).

11. M. Kolesik and J.V. Moloney, “Time-Domain Vertical External Cavity Semiconductor Laser Simulation”, *IEEE Journal of Quantum Electronics*, **43**, 588 (2007).

12. D.E. Roskey, E.M. Wright, M. Kolesik, J.V. Moloney, “The role of linear power partitioning in beam filamentation”, *Applied Physics B*, **86**, 249 (2007).

13. P. Polynkin, A. Peleg, L. Klein, T. Rhoadarmer, and J.V. Moloney, “Optimized multiemitter beams for free-space optical communications through turbulent atmosphere”, *Optics Letters*, **32**, 885 (2007).

14. Krishna Mohan Gundu, M. Kolesik and J.V., Moloney, “Mode shaping in multicorefibers”, *Optics Letters*, **32**, 763 (2007).

15. A. R. Zakharian, J. V. Moloney, and M. Mansuripur, “Surface plasmon polaritons on metallic surfaces,” *IEEE Transactions on Magnetics*, **43**, 845 (2007).

16. F. Kalkum, G. Gay, O. Alloschery, J. Weiner, H. J. Lezec, Y. Xie, and M. Mansuripur, “Surface-wave interferometry on single subwavelength slit-groove structures fabricated on gold films,” *Optics Express*, **15**, 2613 (2007).

17. M. Mansuripur, “Radiation pressure on submerged mirrors: Implications for the momentum of light in dielectric media,” *Optics Express*, **15**, 13502 (2007).

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19. Avner Peleg and Jerome V. Moloney, “Scintillation reduction by use of multiple Gaussian laser beams with different wavelengths”, *IEEE Photonics Technology Letters*, **19**, 883 (2007).

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22. Krishna M. Gundu, Miroslav Kolesik, Kyung Shik Lee, and Jerome V. Moloney “Ultra-flattened-dispersion selectively liquid-filled photonic crystal fibers”, *Optics Express*, **14**, 2870 (2006).

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24. A.R. Zakharian, M. Brio, C. Dineen, and J.V. Moloney, “Stability of 2D FDTD Algorithms with Local Mesh Refinement for Maxwell’s Equations”, *Comm. Math Sci.*, **4**, 345 (2006).

25. A.R. Zakharian, M. Brio, C.Dineen and J.V. Moloney, "Second-Order Accurate FDTD Space and Time Grid Refinement Method in Three Space Dimensions", *IEEE Photonics Technology Letters*, **18**, 1237 (2006).

26. Tao Liu, M. Fallahi, J. V. Moloney, and M. Mansuripur, “Fabrication of two-dimensional photonic crystals with embedded defects using blue-laser-writer and optical holography,” *IEEE Photonics Technology Letters*, **18**, 1100 (2006).

27. Y. Xie, A. R. Zakharian, J. V. Moloney, and M. Mansuripur, “Transmission of light through periodic arrays of sub-wavelength slits in a metallic host,” *Optics Express*, **14**, 6400 (2006).

28. Y. Xie, A. R. Zakharian, J. V. Moloney, and M. Mansuripur, “Optical transmission at oblique incidence through a periodic array of sub-wavelength slits in a metallic host,” *Optics Express*,**14**, 10220 (2006).

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32. M. Kolesik, E. Wright, and J. Moloney, "Interpretation of the spectrally resolved far field of femtosecond pulses propagating in bulk nonlinear dispersive media," *Optics Express*, **13**, 10729 (2005).

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35. Bernhard Pasenow, Matthias Reichelt, Tineke Stroucken, Torsten Meier, Stephan W. Koch, Aramis R. Zakharian, Jerome V. Moloney, "Enhanced light-matter interaction in semiconductor heterostructures embedded in one-dimensional photonic crystals" *JOSA B*, **22**, 2039 (2005).

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Manuscripts under Review

Jinjie Liu, Moysey Brio, Jerome V. Moloney, "A Diagonal Split-cell Model for the Overlapping Yee FDTD Method", Acta Mathematica Scientia, submitted.

Jinjie Liu, Moysey Brio, Yong Zeng, Armis Zakharian, Walter Hoyer, Stephan W. Koch, Jerome V. Moloney, "Generalization of the FDTD algorithm for simulations of hydrodynamic nonlinear Drude model", J. Comput. Phys., submitted.

Conference Talks (invited and contributed):

J.V. Moloney, Ultrafast Nonlinear Optics: Manipulating plasma channels using Bessel and Airy beams" colloquium talk at San Francisco State University, 2009.

J.V. Moloney, “Ultrafast nonlinear optics: Manipulating plasma channels using Bessel and Airy beams”, invited seminar at the Tyndall national Institute, Cork, Ireland, 2009.

J.V. Moloney, “Computational Nanophotonics/Plasmonics and Metamaterials”, invited seminar at the Tyndall National Institute Cork, Ireland, 2009.

C. Dineen, “Time Domain Simulation and Visualization of the Near-Field Electromagnetic Distribution Around Dielectric and Metal Nano-Structures”, International Workshop on Theoretical and Computational Nano-Photonics, TaCoNa-Photonics, Physikzentrum, Bad Honnef, Germany, 2009.

C. Dineen, M. Reichelt, S. W. Koch, and J. V. Moloney, "A Plasmonic Nano-Trap for the Optical Confinement of Quantum Dots," in Optical Trapping Applications, OSA Technical Digest, Optical Society of America Conference on Optical Trapping Applications, Vancouver, Canada, 2009.

J.V. Moloney, Invited talk at NLO contractor’s meeting, “Fundamental Modeling and Design Strategies in Computational Photonics: Applications to Lasercom through clouds and Electro-optical/ Nanophotonics”, Dayton, Ohio, 2009.

J.V. Moloney, “Ultrashort Intense Pulse Propagator: Light Strings, Higher Harmonic Generation and Extreme NLO”, invited talk at NLO contractor’s meeting, Dayton, Ohio, 2009.

M. Mansuripur, A. Zakharian, Sang-Hyun Oh, R. J. Jones, A. Lesuffleur, N. C. Lindquist, Hyungsoon Im, A. Kobyakov, and J. V. Moloney, "Plasmonic optical data storage" Optical Data Storage Conference, Lake Buena Vista, Florida, 2009.

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