COMPUTATIONAL NANOPHOTONICS

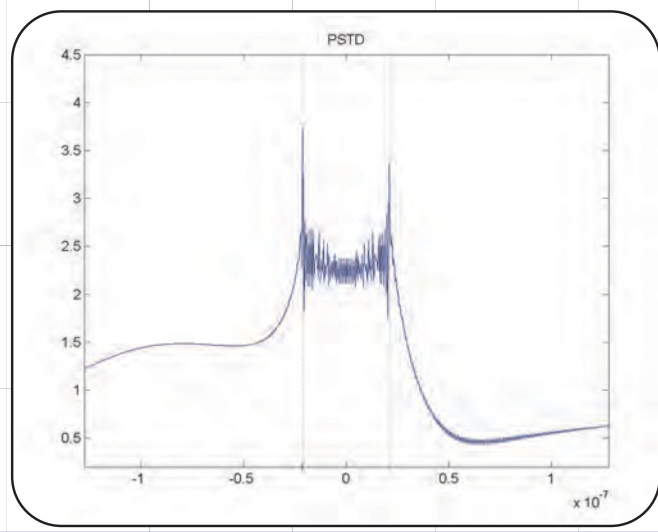
THE MULTI-INSTITUTION COMPUTATIONAL NANOPHOTONICS PROJECT AT ARGONNE AIMS TO DEVELOP REALISTIC THEORY, MODELING, AND SIMULATIONS OF LIGHT INTERACTING WITH TAILORED ARCHITECTURES OF METAL NANOPARTICLES AND HYBRID SYSTEMS. AN IMPORTANT CONTRIBUTION OF THESE EFFORTS WILL BE A COMPREHENSIVE SUITE OF SIMULATION SOFTWARE TOOLS, NSTOP (NANOSCALE STRUCTURE, TRANSPORT, AND OPTICAL PROPERTIES), WHICH WILL BE OPEN AND AVAILABLE TO THE COMMUNITY.

Our goal within the Computational Nanophotonics project is to enhance existing and develop new numerical approaches for simulating interactions of light with metal nanoparticles, as well as provide software engineering expertise and aid in the component development of the codes that constitute the NSTOP suite.

A central component of our numerical modeling is the use of multidomain spectral methods, which are capable of treating complex domains, variable coefficients, and a variety of boundary conditions, all with a maximum of efficiency.

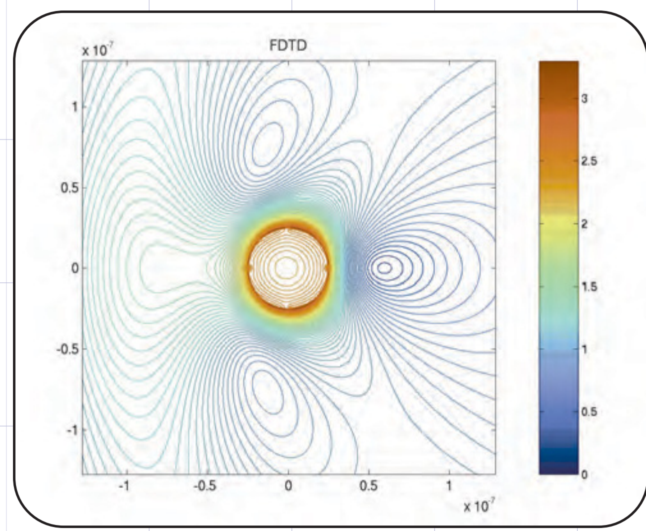
We are also developing a block-structured, adaptively refined grid implementation of the popular finite-difference time-domain methods for solving Maxwell's equations. Our novel implementation is based on the Chombo package developed at LBL. Perfectly matched layer-absorbing boundary conditions are provided to eliminate unwanted reflections off the domain boundary.

Since nanophotonics is a relatively new area, it is not clear which models and numerical approaches will be most efficacious. Thus, a flexible and extensible software design is essential. The software design approach of the new numerical approaches is based on component development principles, such as those defined by the Common Component Architecture. Our ultimate goal is to provide component implementations of the methods developed in the course of this project, which can then be assembled into nanophotonic simulations and extended with new models and algorithms.

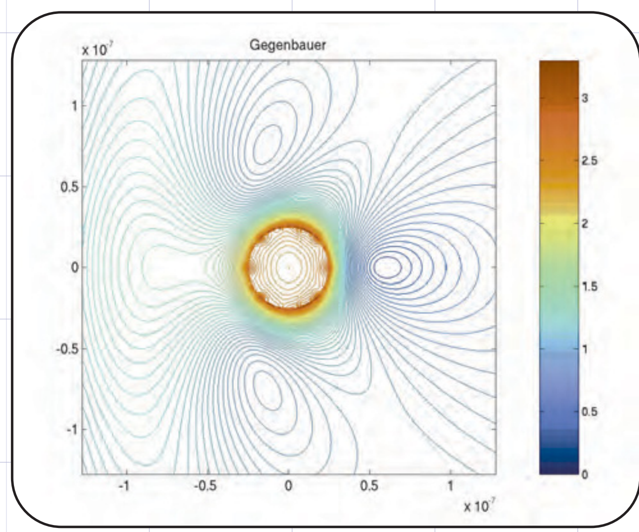


Frequency-domain field distributions of the electric field |E|:

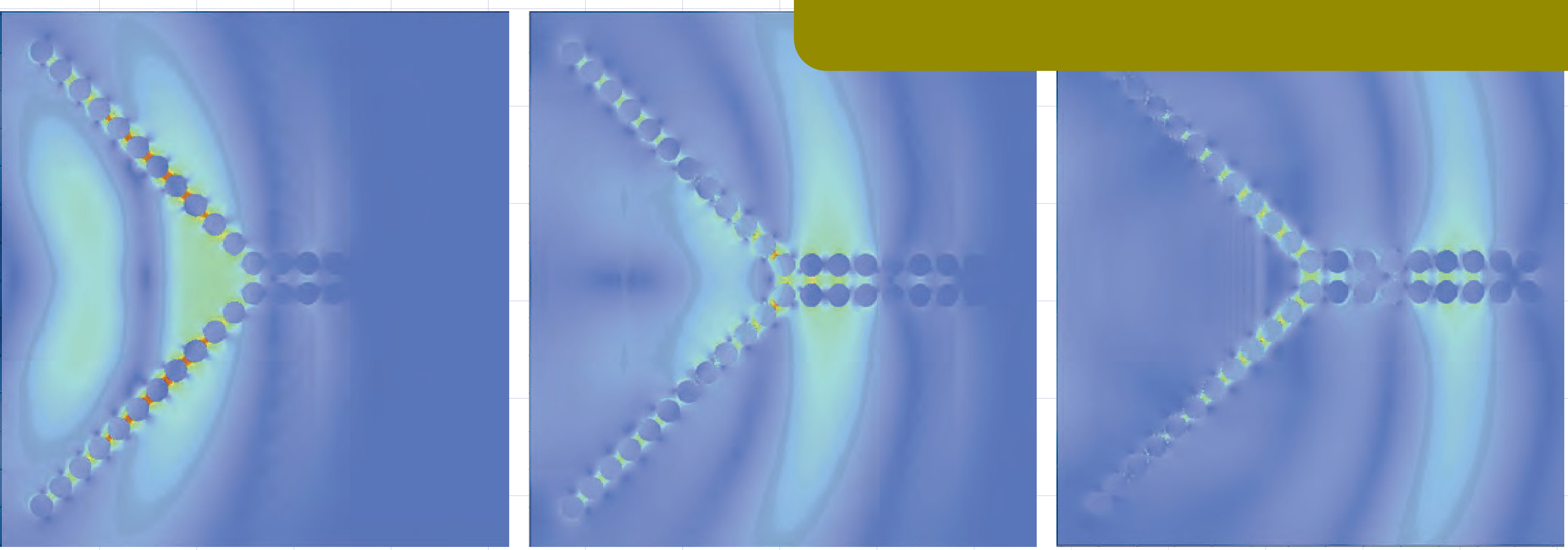
(a) Pseudospectral time-domain (PSTD) method with 0.5 nm mesh resolution



(b) PSTD and G-reconstruction with 0.5 nm mesh resolution



(c) Finite-difference time-domain method with 0.1 nm mesh resolution



600 nm

Funnel configuration of Ag nanowires [Gray and Kupka, Phys. Rev. B 68, 045415 (2003)], showing E field at 0.5 fs time intervals. The illustration demonstrates achieving 100 nm nanoscale localization of light.

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