Nanolattice Coupling to Single Nanoparticles

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Periodic structures are becoming increasingly common in engineering applications, particularly in the visible light regime. They can be used for wave guiding, mode conversion, and even enhancement of Q-factor for detection applications. As a result, accurate simulation of periodic structures becomes important when designing highly optimized devices that push theoretical limits. To accommodate the need for accurate field solvers, we have designed a field solver which can accurately simulate coupling between singular metallic nanoparticles to infinitely periodic nanolattices.

Our solver is based on a surface integral formulation for dielectrics. Specifically, we consider the Calderon preconditioner and the A-Phi formulation for dielectric objects. Using a dielectric formulation enables the accurate simulation of metallic nanoparticles using real loss (no PEC approximation). In order to accurately characterize dielectrics, our discretization uses the idea of primary and dual basis functions to accurately discretize the K operator. On top of all of this, we implement our own version of the periodic fast multipole method which uses Ewald summation to perform a series of lattice sums necessary to capture the field from an infinite number of mirror cells. Putting all of this together gives us a method for accurately solving the field due to a 2-D array of metallic nanoparticles under plane wave excitation.

To introduce coupling to an aperiodic nanoparticle, we consider the array scanning method and plane wave expansion approach. These two methods are used to couple a dipole to periodic structure by decomposing the dipole into a sum of phased excitations (ie. plane wave). Essentially, the coupling of an aperiodic object to a periodic array involves solving $O(10^3)$ periodic scattering problems and combining their solutions. In addition to the speedup achieved from using periodic fast multipole algorithm, we also utilize MPI to solve multiple plane wave directions simultaneously. This culminates in an accurate field solver for coupling between nanoparticles and nanolattices, which we believe will be useful for device designers seeking optimal designs.