Shape calculus in nano optics

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Nano optics is the study of the interaction of light with structures of size in the order of a wavelength or less. In particular we are interested in nano antennae, consisting of plasmonic nano structures (gold or other noble metals). Thanks to plasmonic resonances, nano antennae may resonate even when they are considerably smaller than the wavelength and they localize the field in sub-wavelength regions. Such hotspots can be exploited for sensing applications, for novel light sources and for enhancing solar cells.

Despite of the fast progress of fabrication methods in this field, production inaccuracies cannot be avoided. Especially in the case of nano antennae, these perturbations can amount more than 10 deviation from the initially designed structure, which can drastically affect its optical behavior.

The sensitivity of a design can be mathematically investigated using shape gradients. The behavior of the optical response in a region of interest can be modeled by introducing an objective functional. Its Eulerian derivative can then be computed by assuming a shape perturbation caused by the flow of a vectorfield. Sokolowsky showed that, under some assumptions on the regularity of the shape, the Eulerian derivative is a linear continuous functional on a proper space of vector fields. Its Riesz representative, the shape gradient, expresses the sensitivity of the design.

Currently there are two approaches for computing the shape gradient. A continuous one is based on a mathematical derivation of the shape gradient, whose formula involves the solution of two PDEs. In the continuous approach the shape gradient is thus recovered with a post-processing on a Galerkin discretization of these PDEs. The discrete approach relies on a discretization with a mesh of the shape design. The Eulerian derivative of the objective functional is computed with respect to the variation of the position of the mesh nodes. The shape gradient is then recovered by computing its L2-representative on the surface of the designed structure. In our work we investigate (both in theory and experimentally) the convergence properties of these two methods with respect to the discretization level.

Another important aspect in the fabrication of nano-structures is to detect shape perturbations. Different kinds of imaging methods, like SNOM, are able to measure the strongly localized field. The imaging of the fabricated structure is then an inverse problem with respect to these measurements and can be reformulated in terms of shape optimization. We study an algorithm for solving this inverse problem with a steepest descent method based on shape gradients. Since this inverse problem is ill-posed, we investigate its regularization by discretization and by means of penalty functionals on the surface curvature of the shape.

References:

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