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Computational modeling of Plasmon coupled gold nanoparticles for biomedical applications

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There has been a recent increase in the use plasmonic nanoparticles for biomedical applications, such photothermal therapy, optical and optoacoustic imaging, and biosensors. Gold nanoparticles (GNPs) are of particular interest due to their strong plasmon resonances, stability and biocompatibility. Plasmon coupling occurs when GNPs aggregate resulting in a shift of the resonance wavelength. GNPs can be designed to self-assemble under certain biological conditions such as low PhD or elevated temperature. Aggregation can also occur when GNPs are endocytosed and compartmentalized in intracellular vesicles. Coating GNPs with peptides that cause them to bind to cell surface receptors, a process known as receptor-mediated endocytosis, enables this. Therefore the optical behavior of GNPs ensembles can be sensitive to biological conditions, opening up a large possibility of new medical imaging modalities and therapies.

The presentation will outline a finite element method based computational model of the optical behavior of GNPs that includes plasmon coupling. The model has been used to study the application of plasmon coupled GNPs for several biomedical applications. The results from some of these studies will be presented.

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