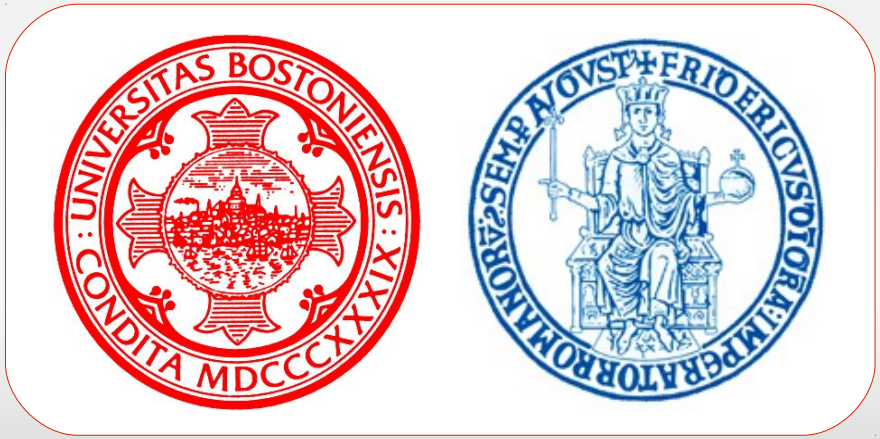
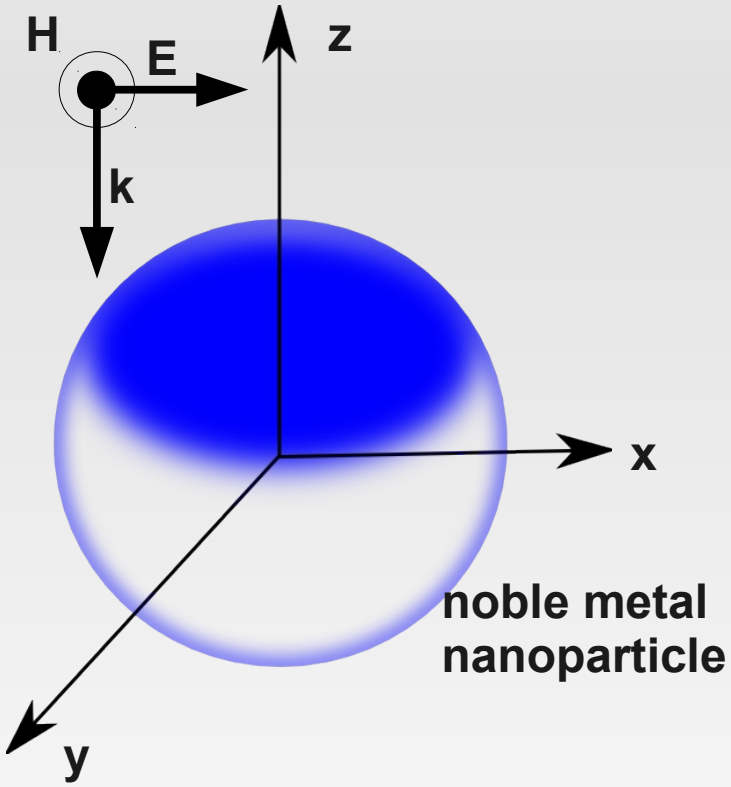
Risonanze plasmoniche in array di nanoparticelle metalliche

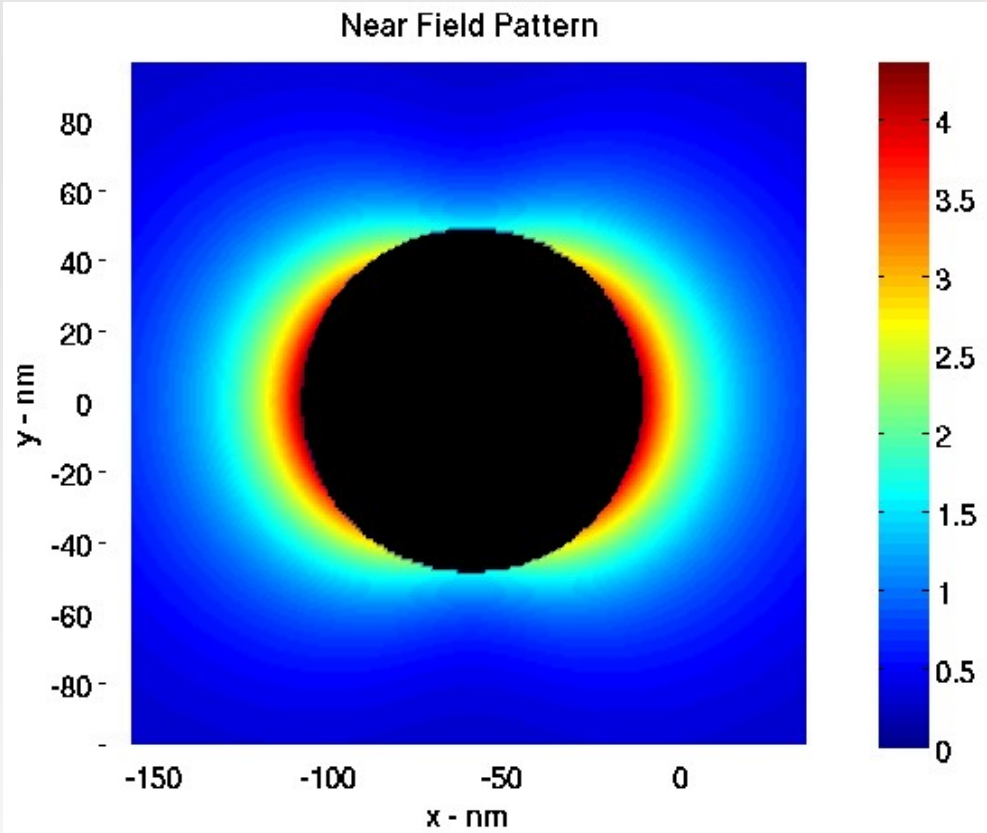
A. Capretti, L. Dal Negro, C. Forestiere,
G. Miano, A. Tamburrino



Localized surface plasmons

Localized surface plasmons (LSP) are non-propagating excitations of the conduction electrons of metallic nanostructures coupled to the electromagnetic field.





These modes arise naturally from the scattering problem of a small, sub-wavelength conductive nanoparticle in an oscillating electromagnetic field. The symmetry breaking introduced by the particle surface induces an effective **restoring force** on the driven electrons; from its competition with the inertial term a resonance can arise, leading to field amplification in the near-field zone outside the particle.

Localized surface plasmons

The actual sensors and devices are made up by **arrays** of nanoparticles (dimension of hundred of microns).

The particles can be arranged according to **periodic**, **quasi periodic**, and **random** distributions.

Our collaborator in **BU** Photonic Center can actually fabricate these devices. Some of them are shown in the picture.

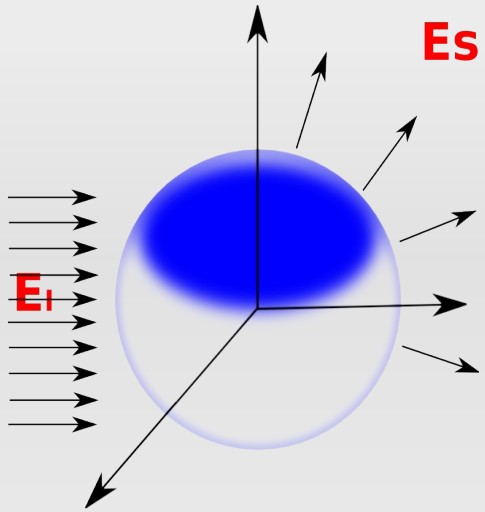
Localized surface plasmons

This field enhancement has found many applications:

- non linear effect as the production of **second harmonic generation** (SHG) in the strong field
- surface enhanced Raman scattering (**SERS**).
- Interaction of LSPs with **gain media**.
- **Ultrasensitive detection** and characterization of biomedically relevant molecules.

Figures of merit

- Near Field Enhancement
- Scattering cross section



$$\mathbf{S_{scat}} = \frac{1}{2} Re\left[\mathbf{E_s} \times \mathbf{H_s^*}\right] \quad \mathbf{S_{inc}} = \frac{1}{2} Re\left[\mathbf{E_{inc}} \times \mathbf{H_{inc}^*}\right] \quad \mathbf{S_{ext}} = \frac{1}{2} Re\left[\mathbf{E_S} \times \mathbf{H_{inc}^*} + \mathbf{E_{inc}} \times \mathbf{H_S^*}\right]$$

$$W_{scat} = -\int_{S_C} \mathbf{S_{scat}} \cdot \mathbf{n} \quad W_{inc} = \int_{S_C} \mathbf{S_{inc}} \cdot \mathbf{n} \quad W_{ext} = -\int_{S_C} \mathbf{S_{ext}} \cdot \mathbf{n}$$

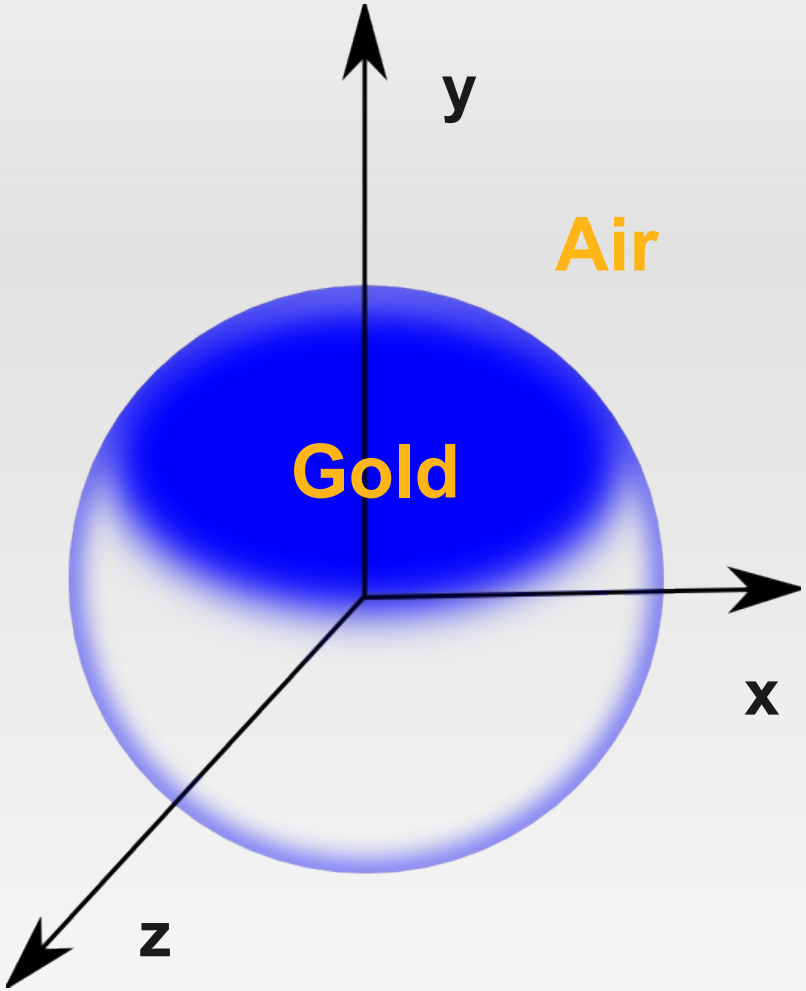
$$Wext = Wscat + Wabs$$

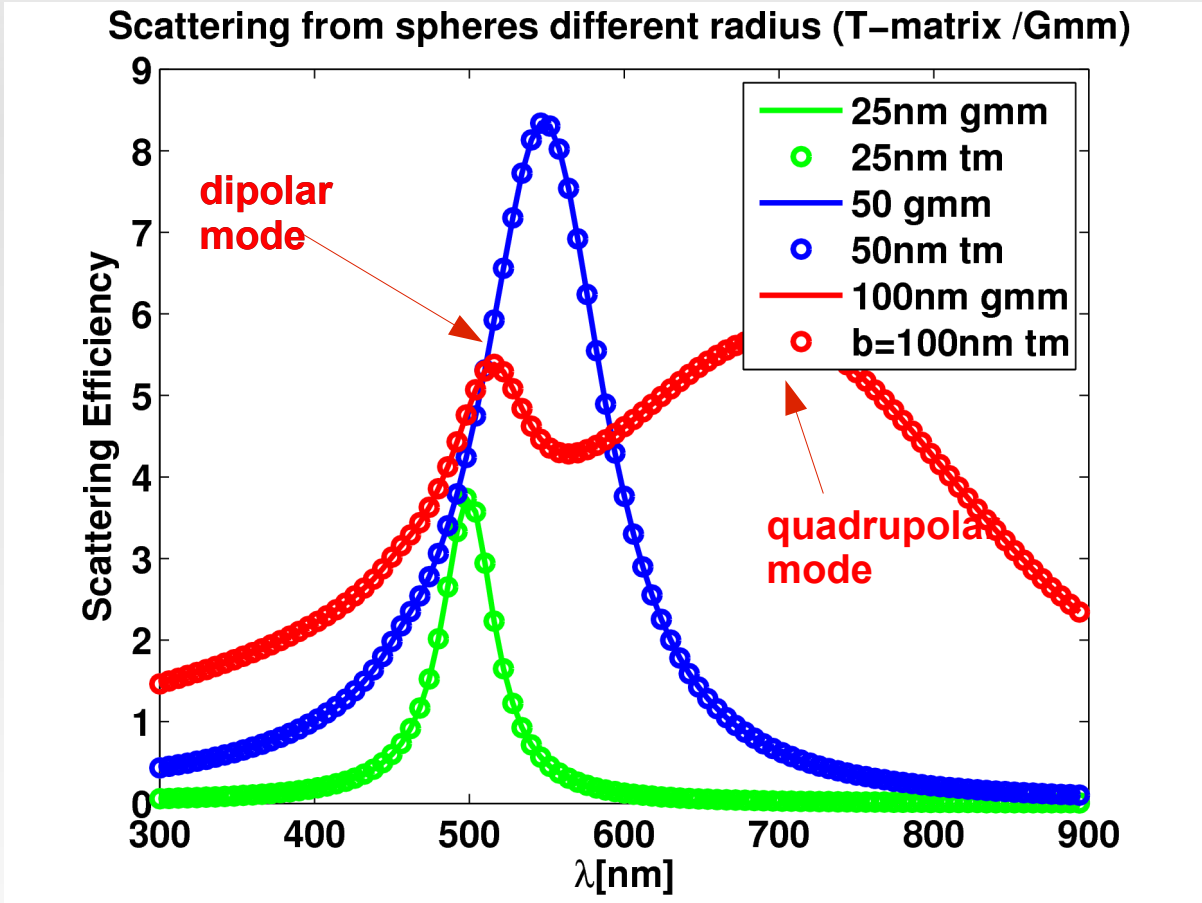
$$C_{scatt} = \frac{2\zeta W_{scat}}{|E_0|^2} \qquad C_{ext} = \frac{2\zeta W_{ext}}{|E_0|^2}$$

Numerical Methods

- **Coupled Dipole Approximation (CDA)**
  each particle is modeled with an electric dipole
- **DDSCAT**
  each particle is modeled with an array of electric dipoles
- **Null field method (T-matrix method)**
  Superficial formulation based on Stratton-Chu equation
- **Generalized Multiple Mie Method (GMM)**
  Semi-analytical solution based on the separation variable method (SVM) applied to Helmholtz equation
- **Finite Element Method**
- **Finite Difference Time Domain method**

Isolated Sphere Gmm/T matrix simulations

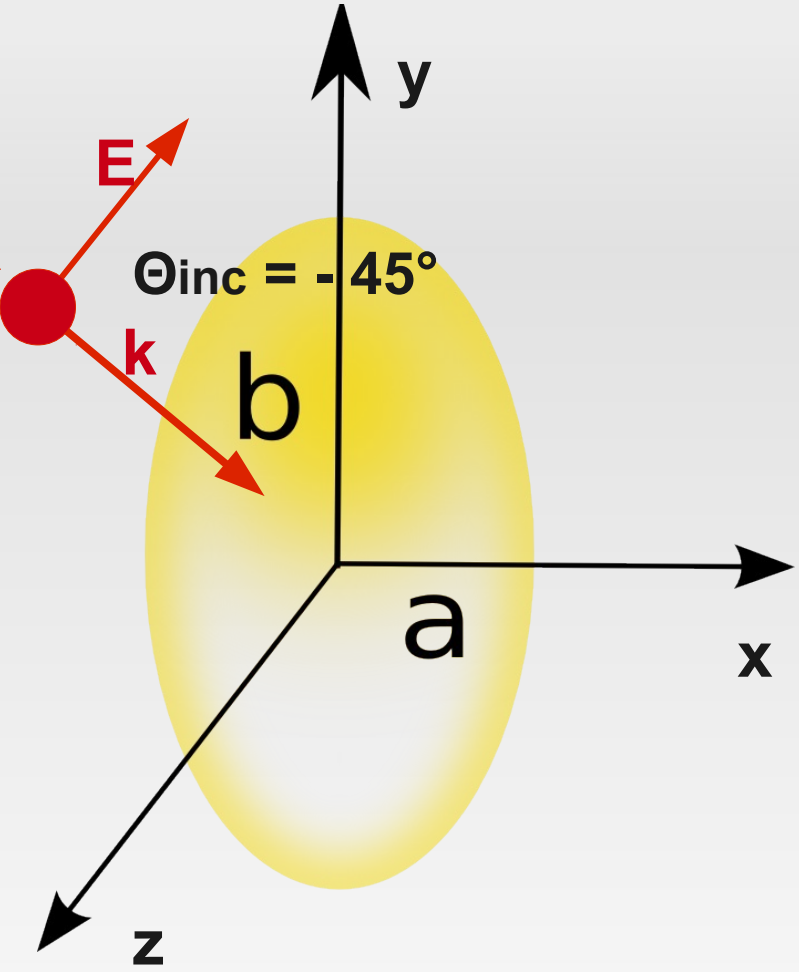


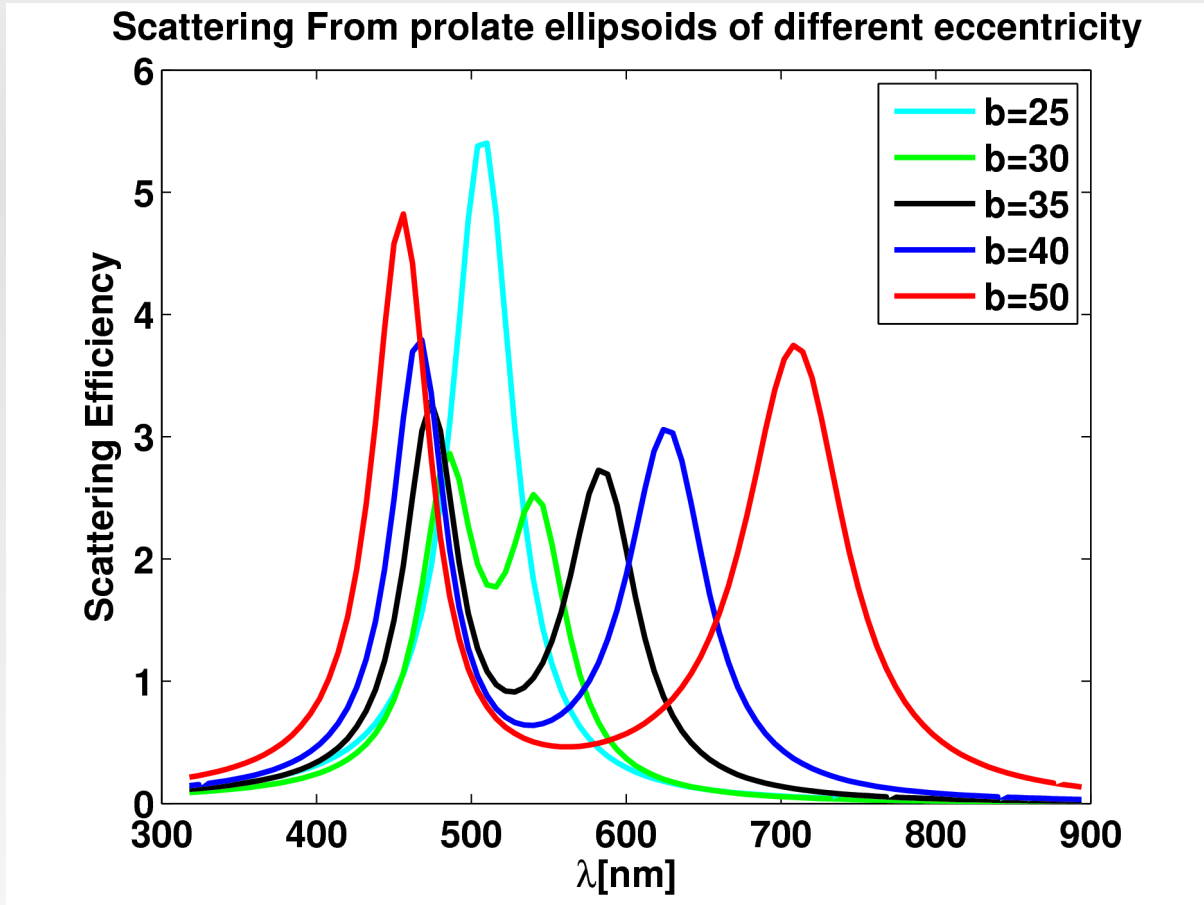


This figure shows how the color of a single metallic nanoparticle can be changed via alterations in particle **size**.

The splitting visible in the case of radius $\mathbf{r_c}$**=100nm** is due to the quadrupolar mode.

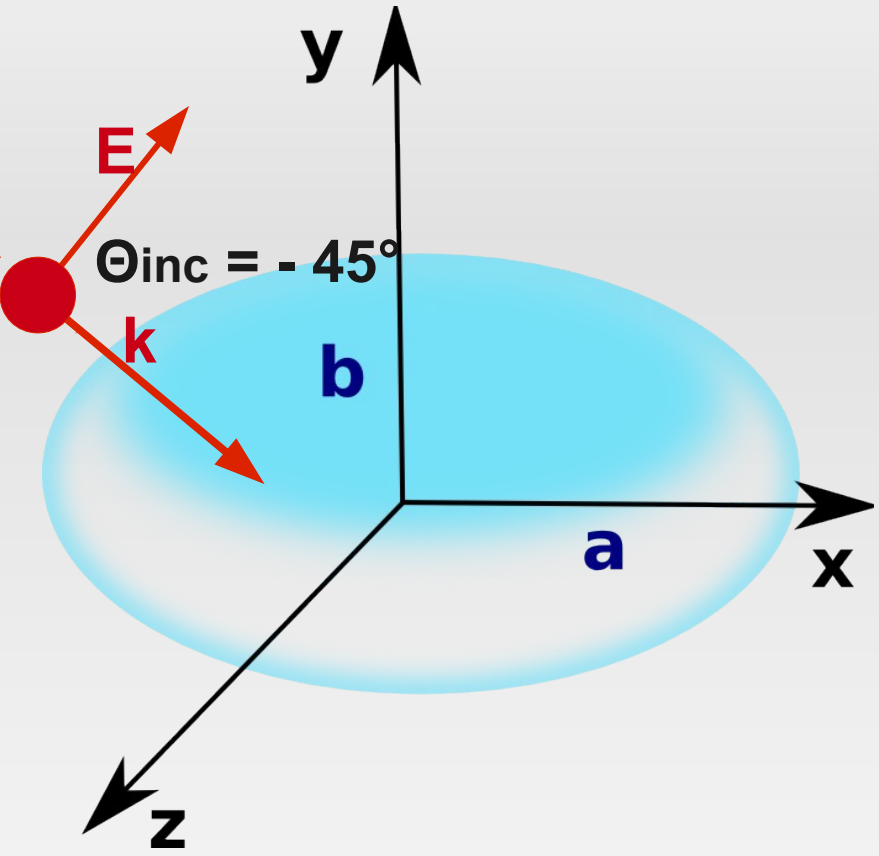
Prolate Spheroid T matrix simulations

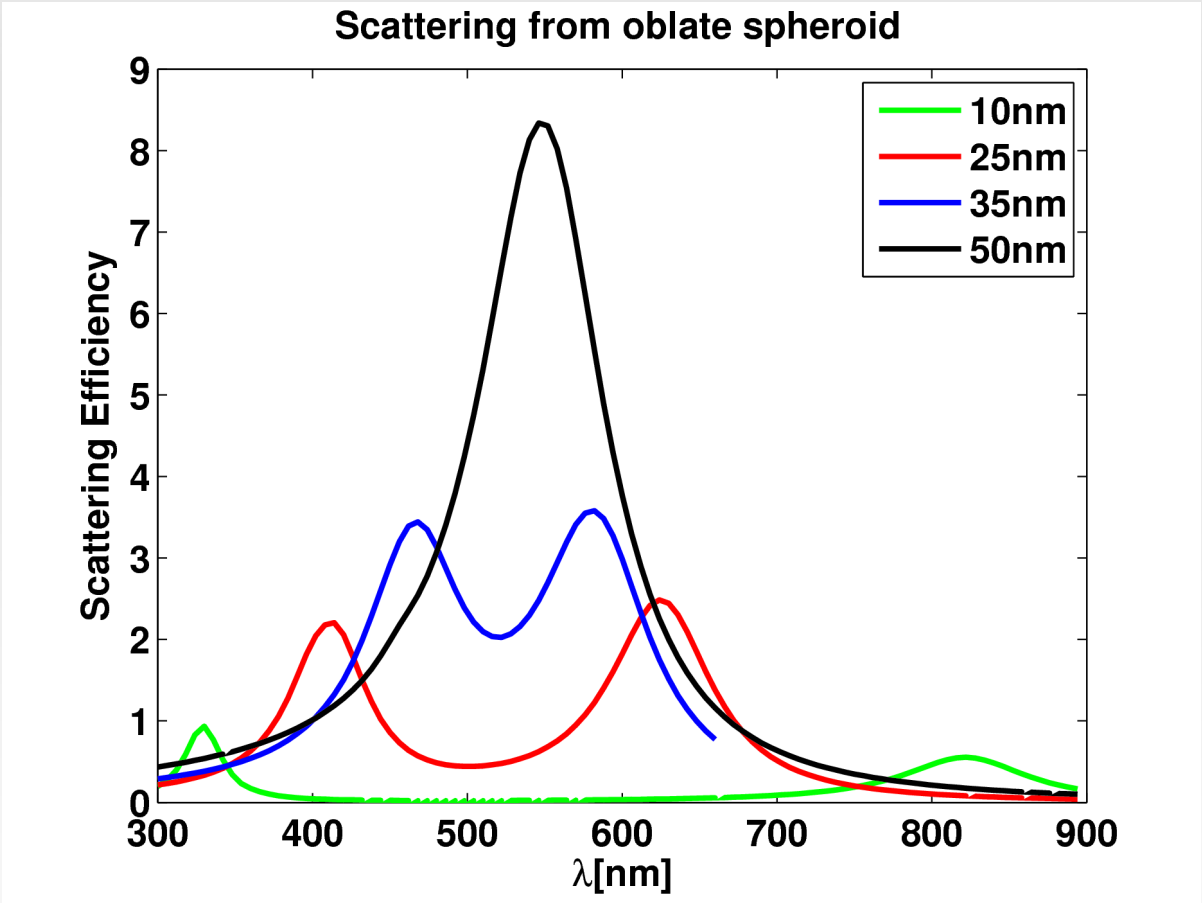




LP resonance of a single metallic nanoparticle can be also shifted in frequency via alterations in particle **shape** as for example by changing the **eccentricity** a prolate spheroid. In the figure the two resonances are associated to each ellipsoid axis.

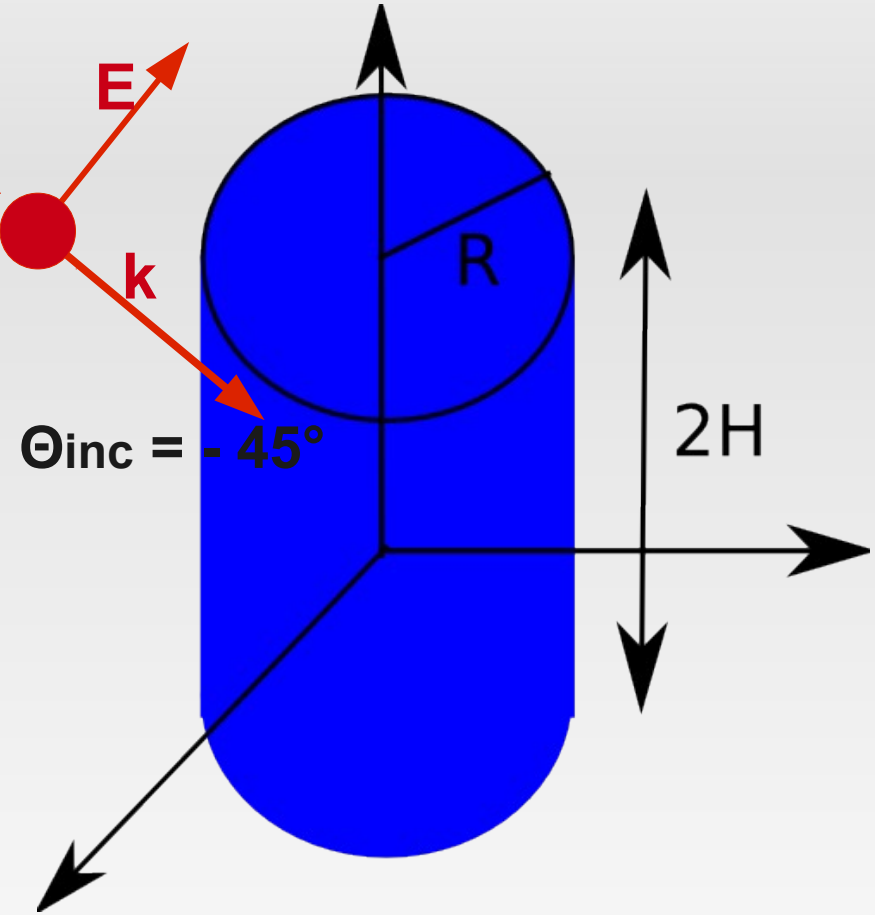
Oblate Spheroid T matrix simulations

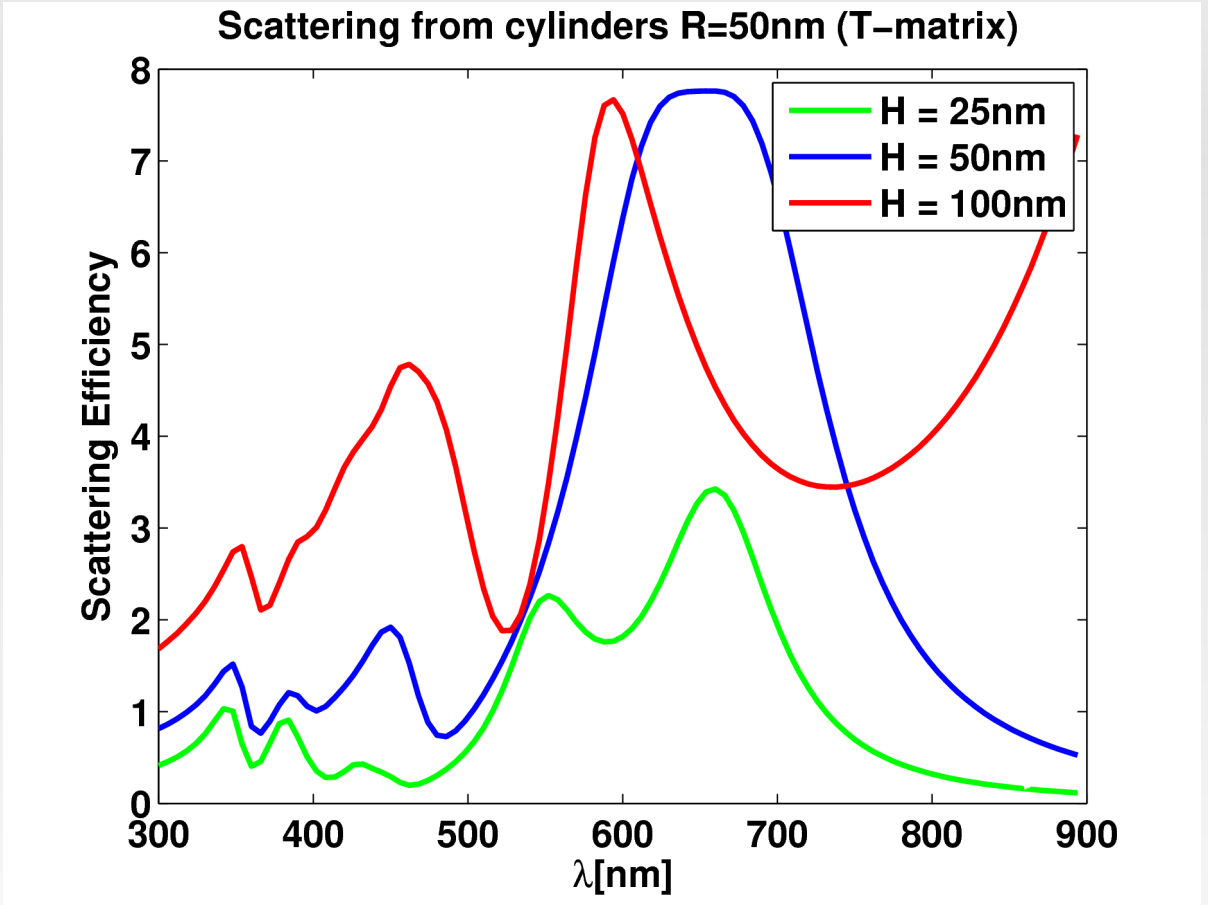




LP resonance of a single metallic nanoparticle can be also shifted in frequency via alterations in particle shape as for example by changing the **eccentricity** a prolate spheroid.

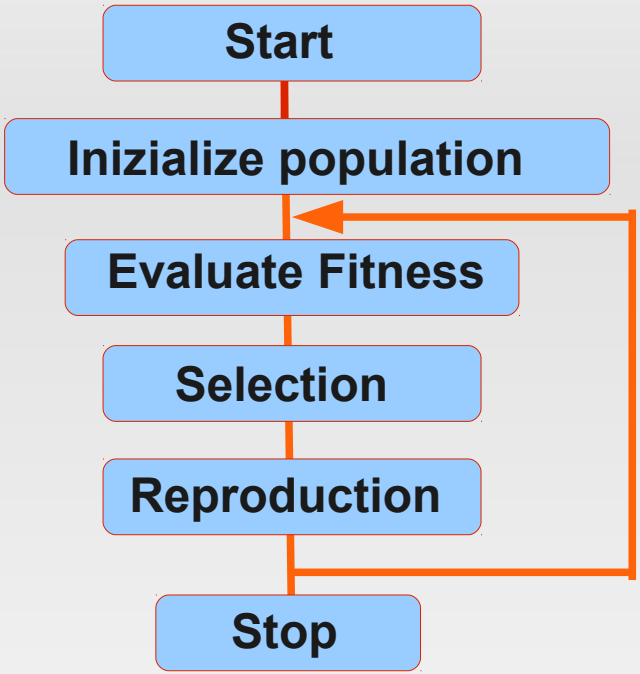
Cylinder T matrix simulations

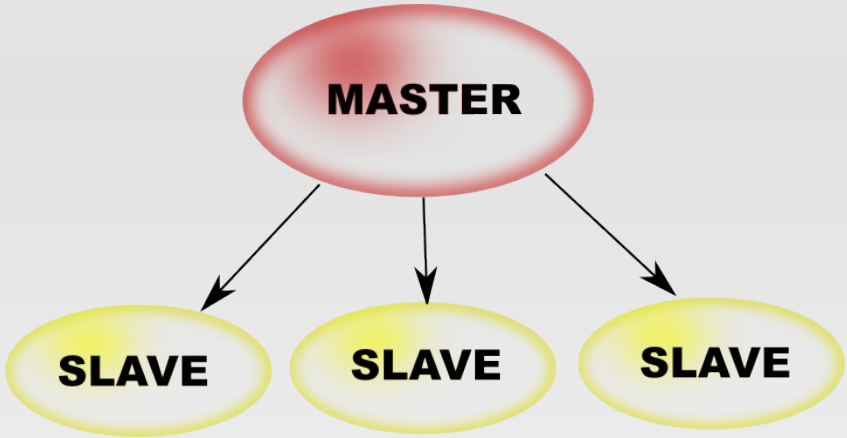




The cylinder is the shape which can more easily fabricated through lithographic techniques. Due to the more irregular shape more resonances will arise.

Genetic Algorithm Grid implementation





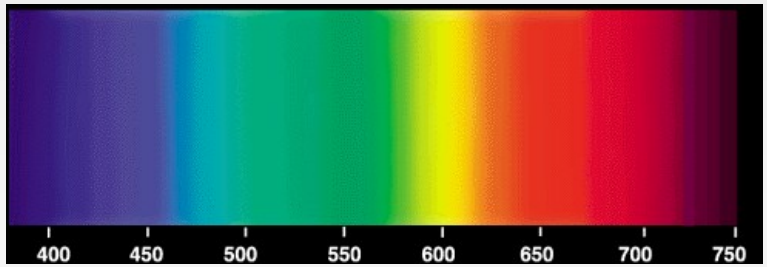
The **Master** process stores the population and does the selection, while the **slave** processes evaluate the fitness.

The simulations have been runned on the **S.C.O.P.E.** Server of Università degli Studi di Napoli ”Federico II”

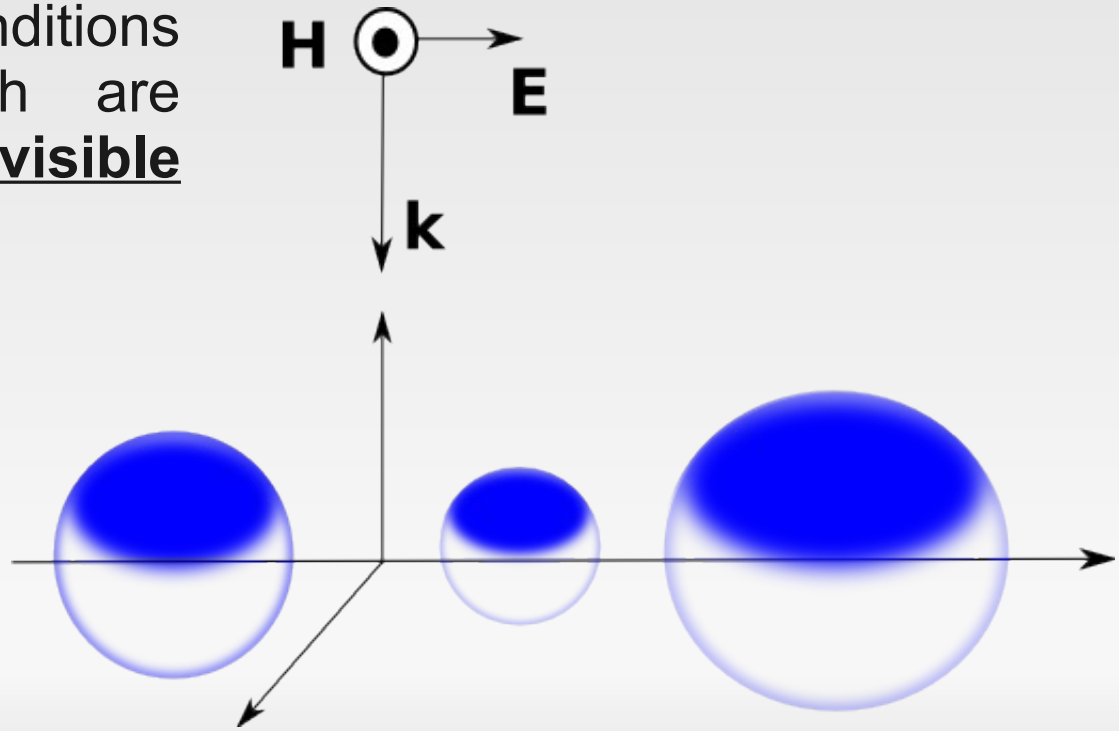
Genetic Algorithm Implementation

We optimized a **one-dimensional array** of gold nanoparticles in order to get the maximum enhancement **(fitness)** in a given point.
The spheres are free to move on a 1D box, provided that they are not compenetrating and the distance between two of them is larger then the minimum distance imposed by the lithography (25nm).
Their radius can assume any value in the range [25, 100]nm.

Three different excitation conditions have been analyzed which are representative of the **whole visible spectrum**.



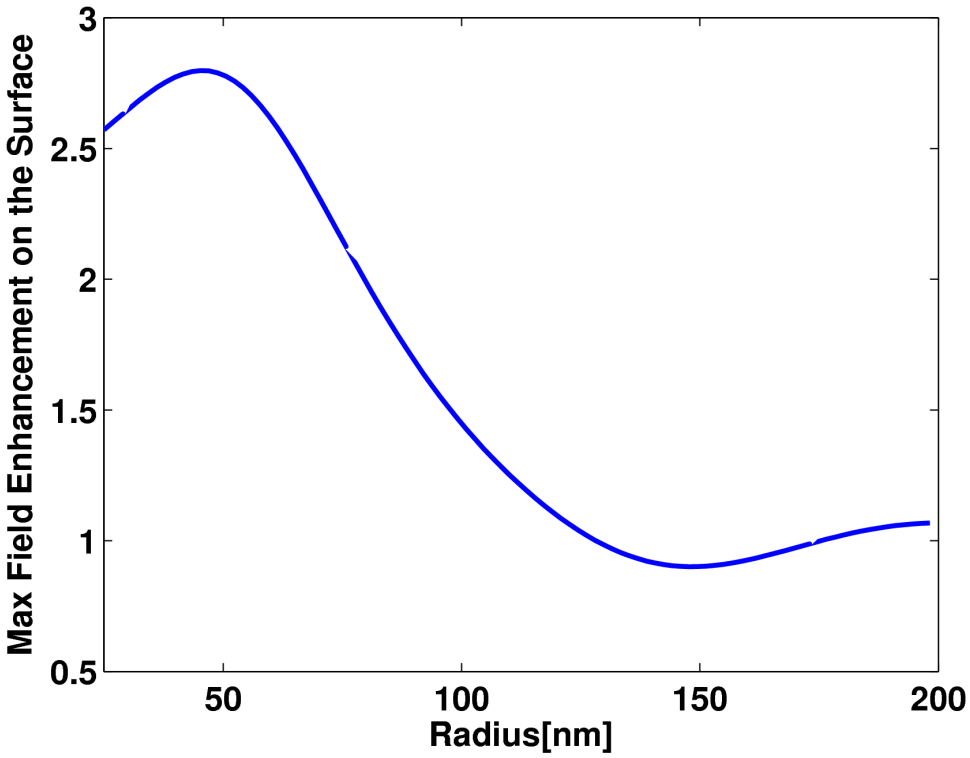
Blue **Green** **Red**



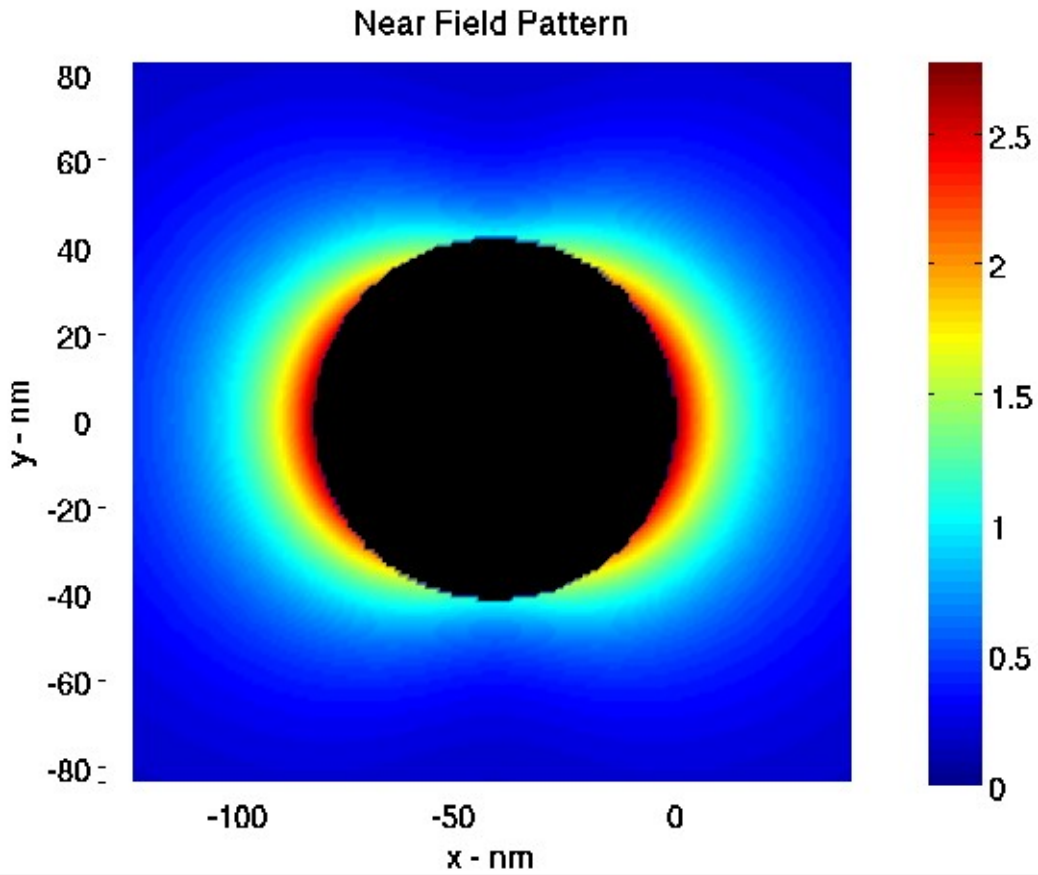
Heuristic Optimization N=1

Goal: *get the maximum enhancement in the origin*

Blue 475nm



Maximum **field enhancement** on the particle surface as a function of its **radius**



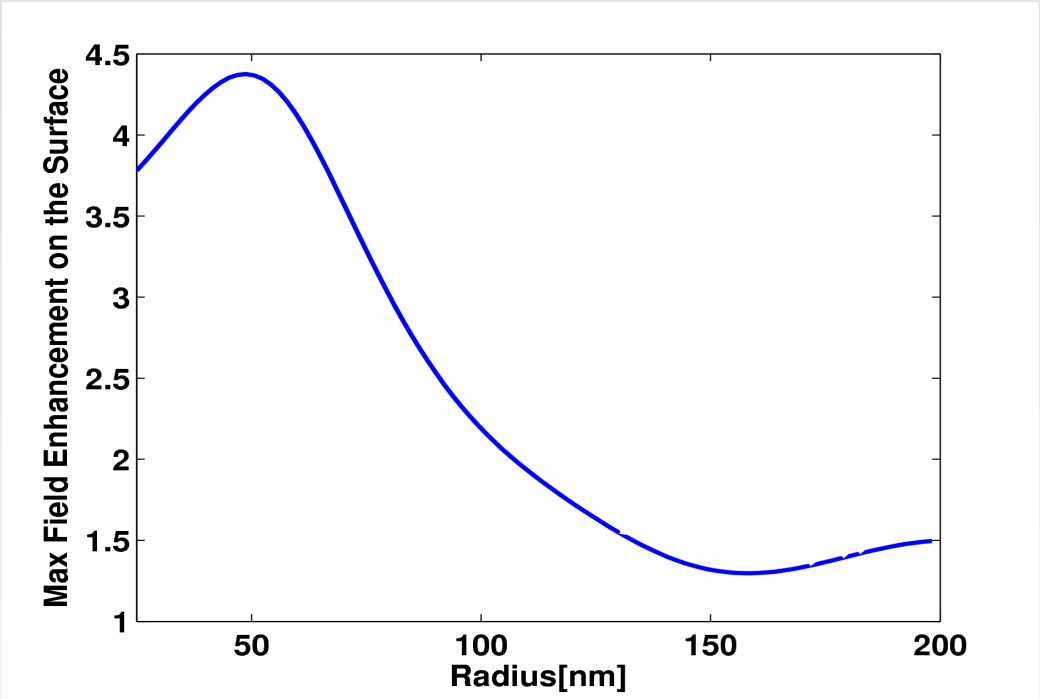
Field Enhancement: **2.8**

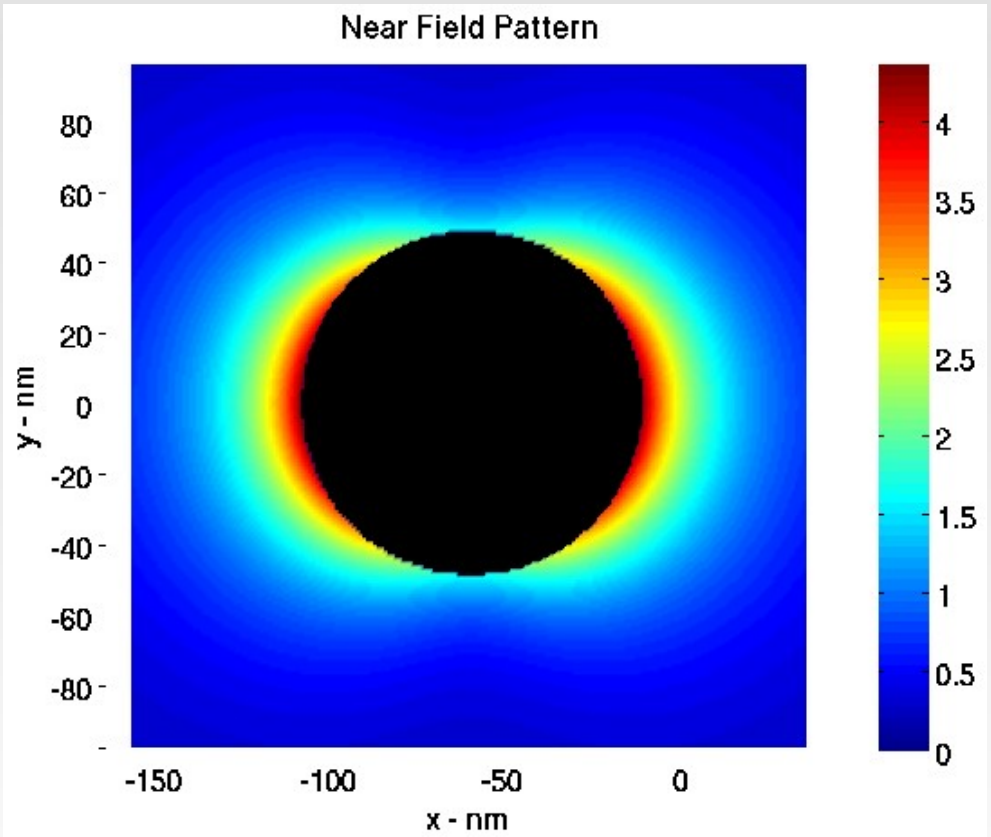
Optimized Radius: **42nm**

Heuristic Optimization N=1

Goal: *get the maximum enhancement in the origin*

Green 520nm





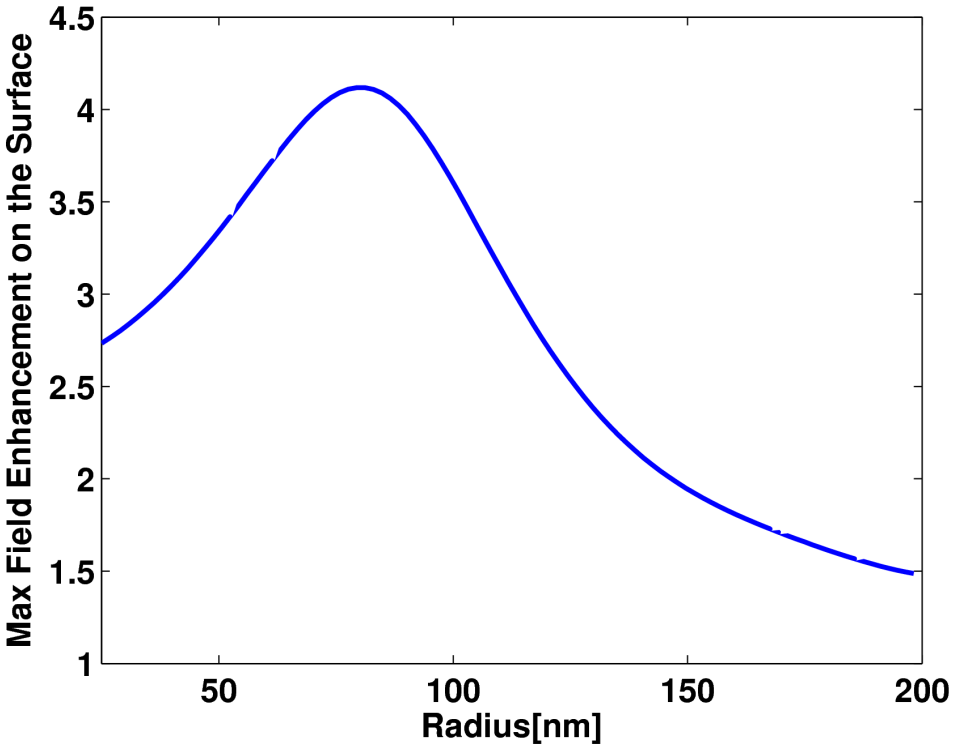
Maximum **field enhancement** on the particle surface as a function of its **radius**

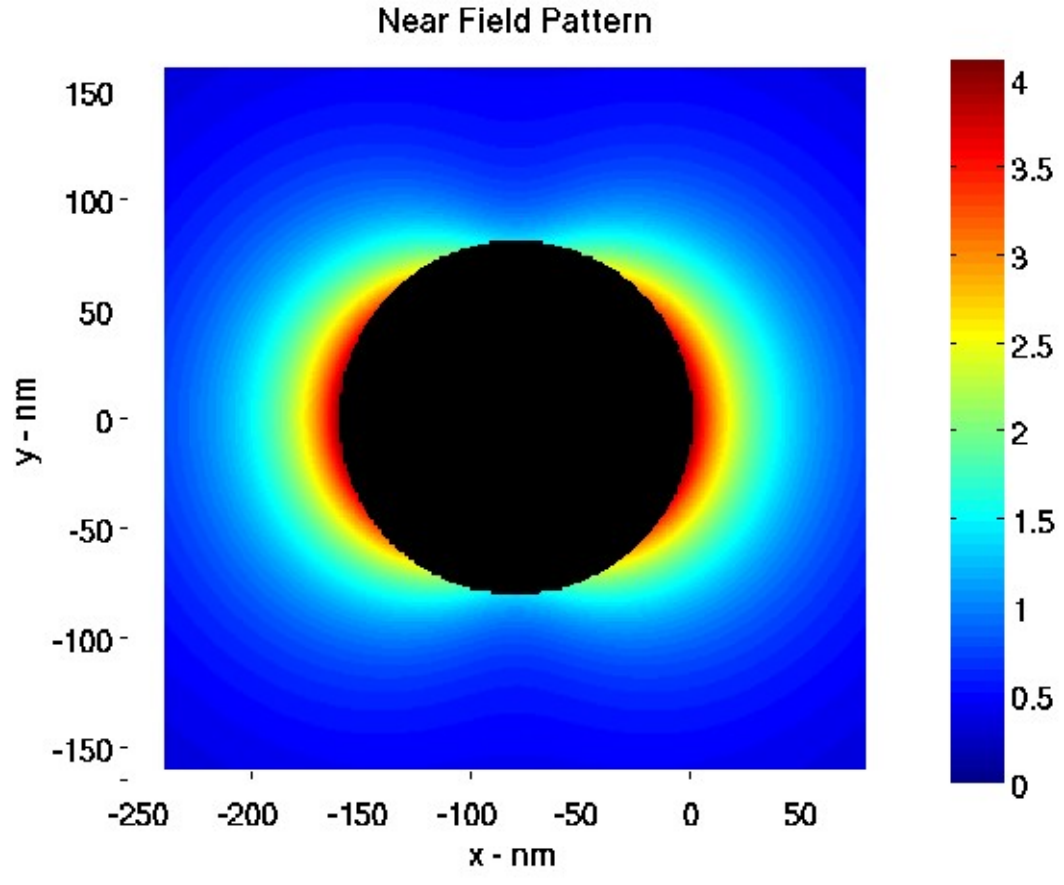
Field Enhancement: **4.35**
Optimized Radius: **49nm**

Heuristic Optimization N=1

Goal: *get the maximum enhancement in the origin*

Red 650nm



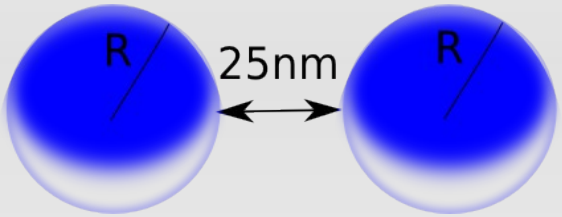


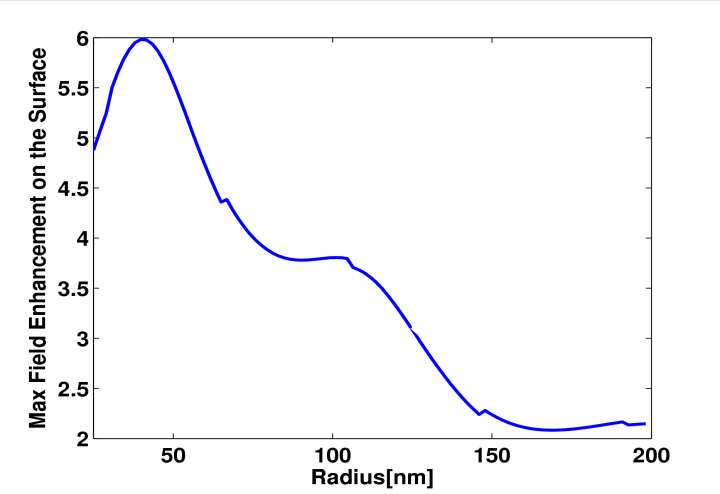
Maximum **field enhancement** on the particle surface as a function of its **radius**

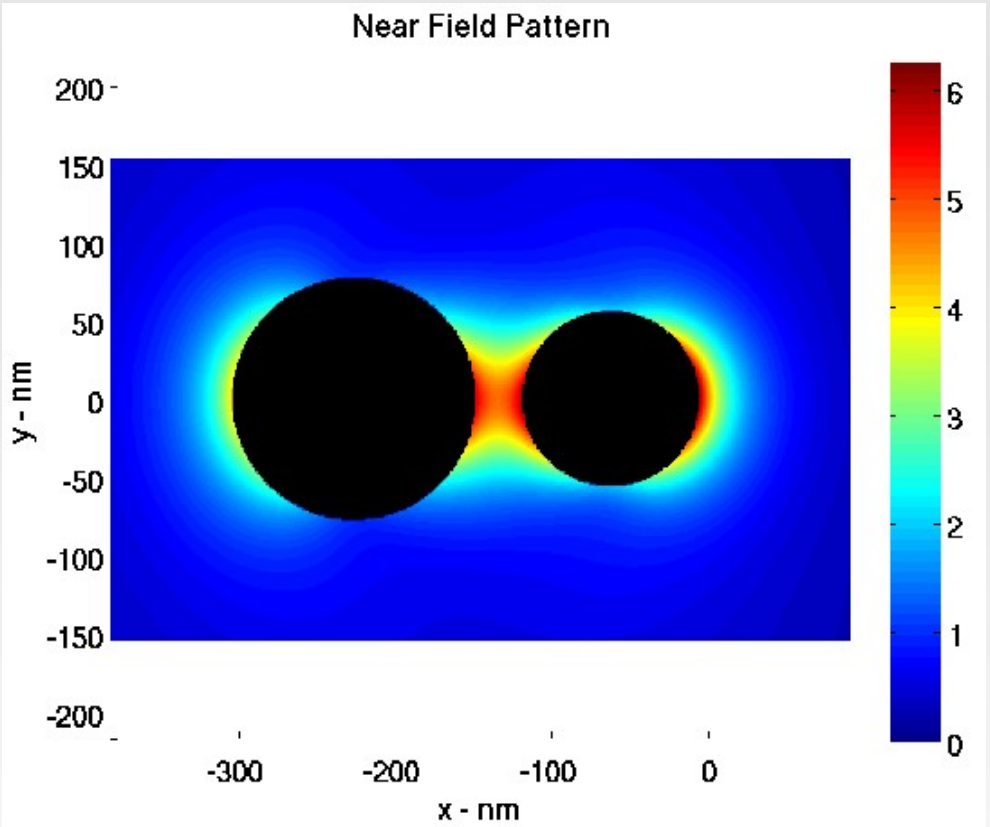
Field Enhancement: **4.1**
Optimized Radius: **80 nm**

Heuristic Optimization N=2

Green 520nm





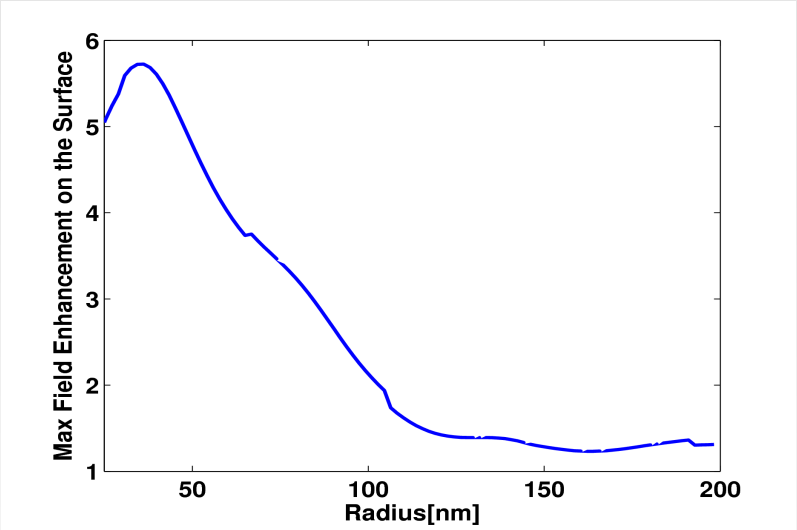


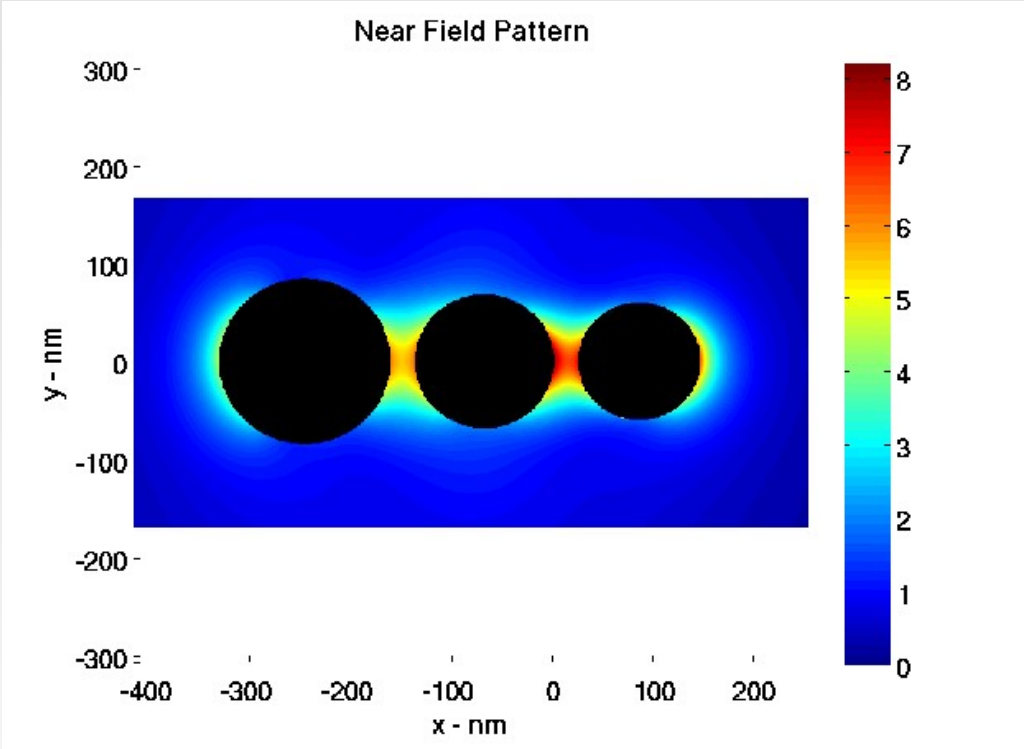
Maximum field enhancement of a dimer made up by **identical particles** at the minimum interparticle distance (**25nm**) as a function of their radius.

GA optimized gold dimer with resulting field enhancement equal to 6.3

Heuristic Optimization N=3

Green 520nm



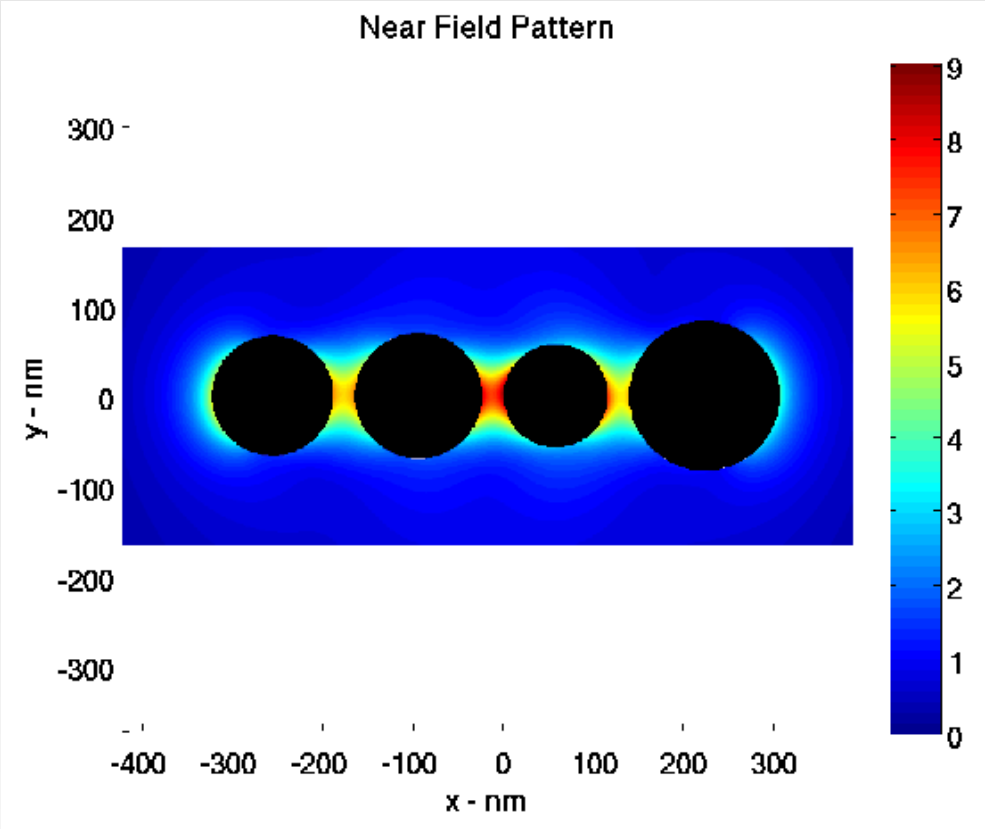


Maximum field enhancement of a trimer made up by identical particles at the minimum interparticle distance (**25nm**) as a function of their radius.

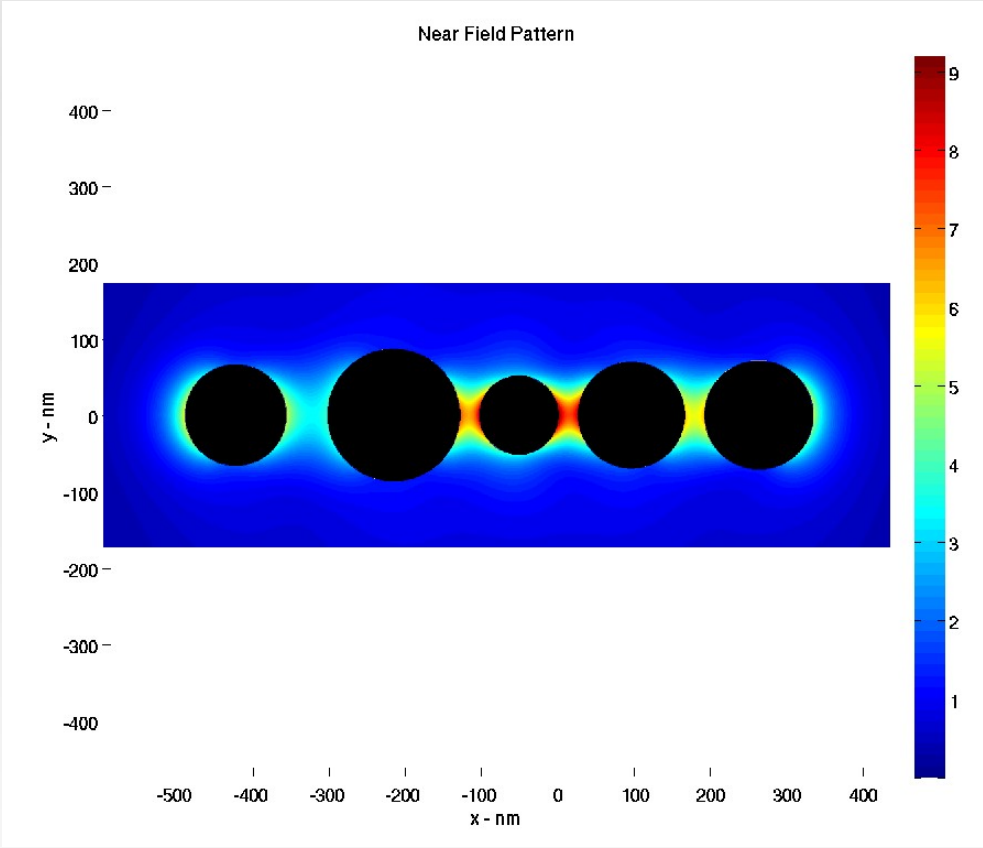
GA optimized gold trimer with field enhancement equal to 8.2

Heuristic Optimization N=4,5

Green 520nm



GA optimized 4-particles structure with field enhancement equal to 9.0



GA optimized 5-particles structure with field enhancement equal to 9.2

Conclusions

- By optimizing the positions and the radii of 5 particles the **maximum field enhancement** we achieve is roughly two times better compared to the single particle enhancement

- We also noticed that by adding further particles the enhancement does not significantly change unless collective effect due to far field coupling play a role.

Future Works

- We aim to use the GA to build optimum clusters to use as elementary **bricks** for the design more complex structures.

- We can arrange those bricks in periodic or aperiodic structures in order to **boost the enhancement due to the far field.**

- We also would like to use this optimization approach in order to design **2D and 3D structures**.

- Moreover due to the larger search space of 2D and 3D problem the genetic code has to be refined in order to avoid incurring in local minima.

More Informations

Published works

[1] **C.Forestiere, G.Miano, S.Boriskina and L. Dal Negro**, ”The role of nanoparticle shapes and deterministic aperiodicity for the design of nanoplasmonic arrays” Optics Express 20, 9649, (2009).

[2] **C.Forestiere, G.Miano, G.Rubinacci, L.Dal Negro**, ”Role of aperiodic order in the spectral, localization, and scaling properties of plasmon modes for the design of nanoparticle arrays”, Physical Review B 79, 85404, (2009).

[3] **C.Forestiere, G.Walsh, G.Miano and L.Dal Negro**, ”Prime numbers plasmonic arrays”, Optic Express 26, 24297, (2009).

[4] **C.Forestiere, G.Miano, M.d'Aquino, C.Serpico, L.Dal Negro**, "Dipolar mode localization and spectral gaps in quasi periodic array of magnetic nanoparticles",Phys. Rev. B, 79, 214419, (2009).

[5] **C.Forestiere, M.Donelli, G.Walsh, E.Zeni, G.Miano, L.Dal Negro,** ”Particle Swarm Optimization of nanoplasmonic arrays”, Optic Letters 35, 133 (2010).

For further informations please mail to:

carlo.forestiere@unina.it