Implementation of a Numerical Model for the Computation of the Electric Field Enhancement of Nanodumbbells

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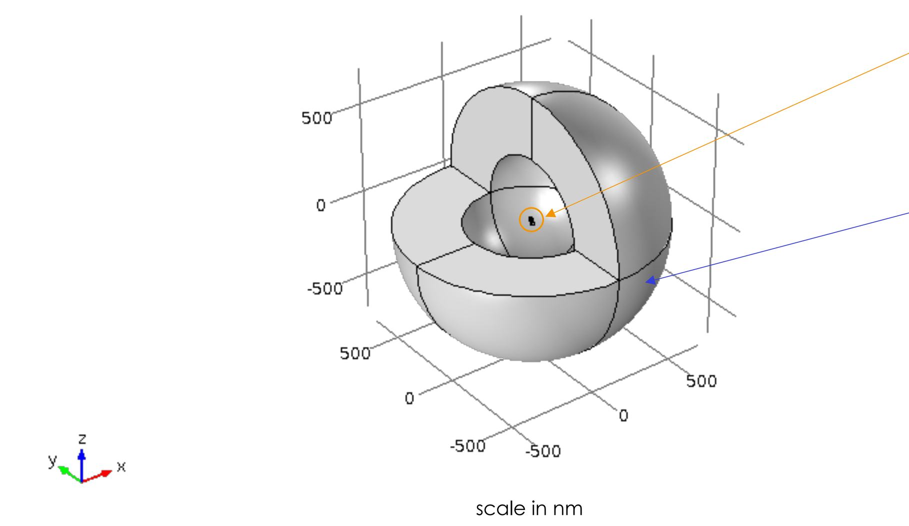
Introduction

In the field of surface-enhanced spectroscopies, there is real need for a **numerical model** to support experimental studies. These results are used to guide the fabrication of the plasmonic substrates based on simulations results. In this work, a finite-element method provided by Grand and Le Ru[1] is implemented in the commercial software COMSOL[2] to compute the enhancement of the electrical field as well as the impact of the size and shape of different gold nanoparticles. This comparison highlights the advantage of using nanodumbbells in the context of Surface-enhanced Raman spectroscopy (**SERS**).

COMSOL model



A gold nanoparticle $\epsilon_{Au} = \left(n_{Au}(\lambda) - jk_{Au}(\lambda)\right)^2$:

- In non-absorbing medium ϵ_1
- Excited by incident field $\mathrm{E_{Inc}}(r) = E_0 e^{-i\frac{2\pi}{\lambda}\sqrt{\epsilon_1}z}\boldsymbol{e_x}$
- Surrounded by perfectly matched layers (PML) to prevent any reflection of the incident or scattered waves.

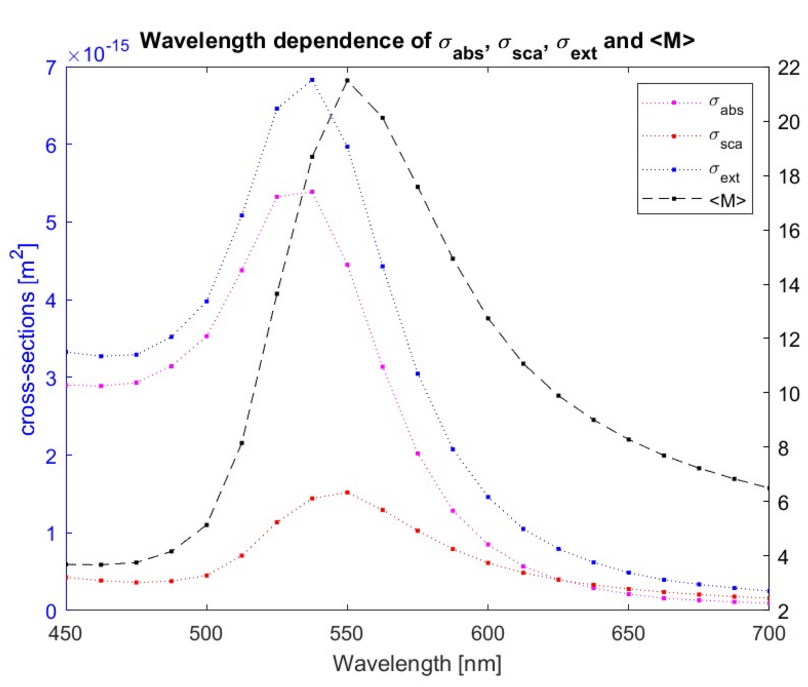
What is calculated:

1. Scattering, absorption and extinction cross section, where: $\sigma_{ext} = \sigma_{sca} + \sigma_{abs}$
2. Local field intensity enhancement factor (**LFIEF**): $M(r) = \left|\frac{E(r)}{E_0}\right|^2$ and $\boxed{\langle M\rangle = \frac{1}{A}\iint_{NP}\left|\frac{E(r)}{E_0}\right|^2 dS}$

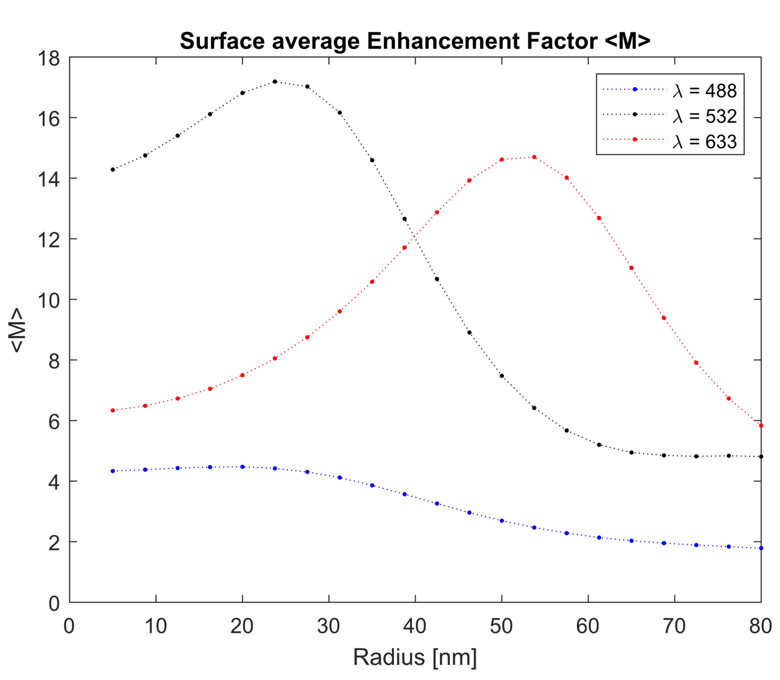
Nanosphere

The maximum enhancement depends on multiple factors:

- Wavelength λ of the exciting wave
- Permittivity of the surrounding medium ϵ_1
- **Size (radius)**



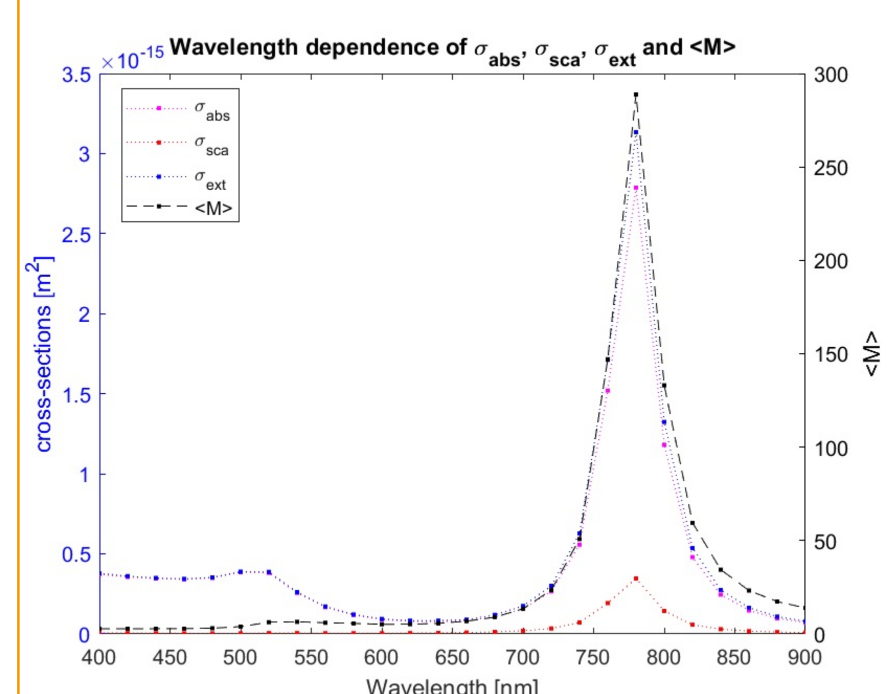
Wavelength dependence of σ_{abs}, σ_{sca}, σ_{ext} and $\langle M\rangle$ of a Au nanosphere with a 30 nm radius in water $\epsilon = 1.33$



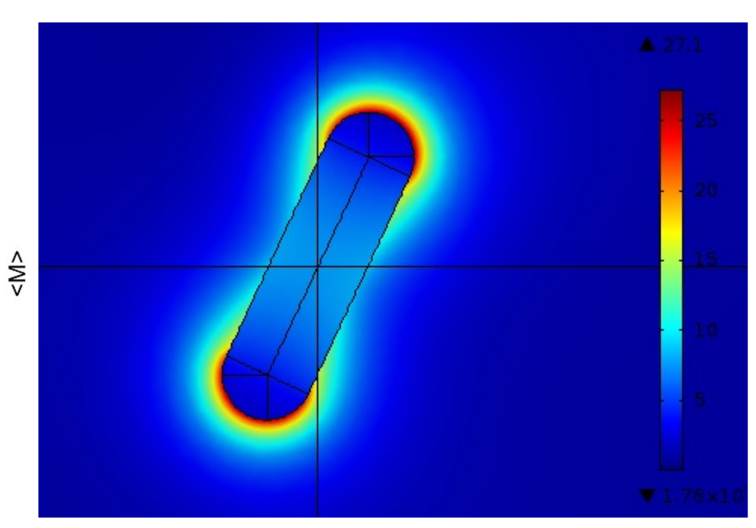
Dependence of $\langle M\rangle$ of a Au nanosphere in water at different excitation wavelengths

Nanorod

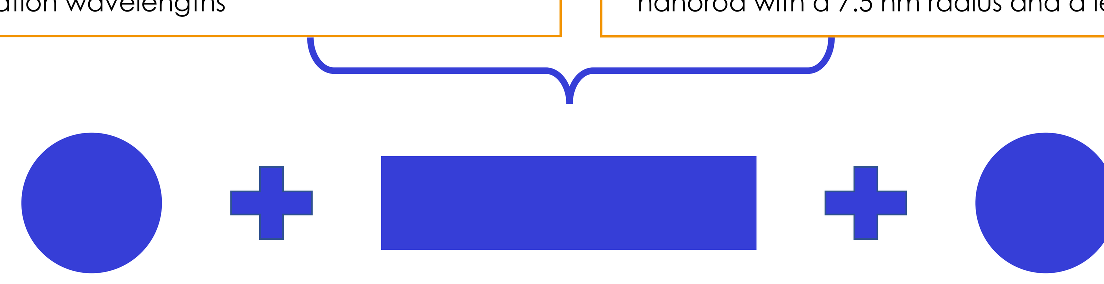
The **shape** of the particles also impacts the enhancement factor. Lower symmetry increases the field enhancements, particularly at the tips of the nanoparticle.



Wavelength dependence of σ_{abs}, σ_{sca}, σ_{ext} and $\langle M\rangle$ of a Au nanorod with a 7.5 nm radius and a length of 55 nm in water

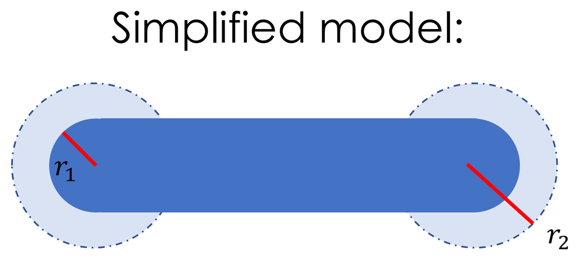


Electric field [V/m] of a Au nanorod with a 7.5 nm radius and a length of 55 nm in water $\epsilon = 1.33$ and $\lambda = 780\ nm$

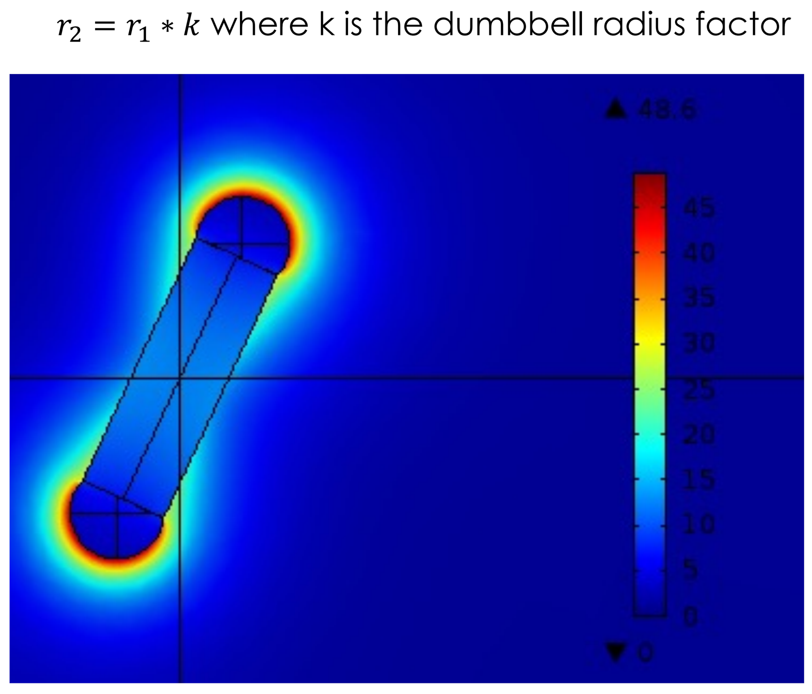


Nanodumbbell

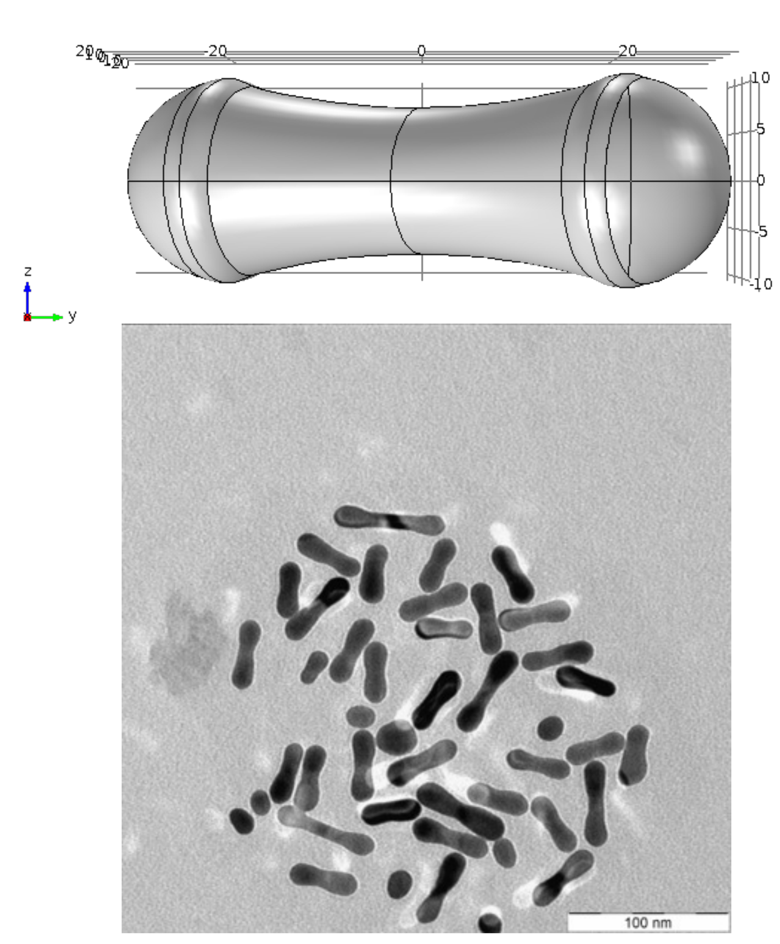
Simplified model:



$r_2 = r_1 * k$ where k is the dumbbell radius factor

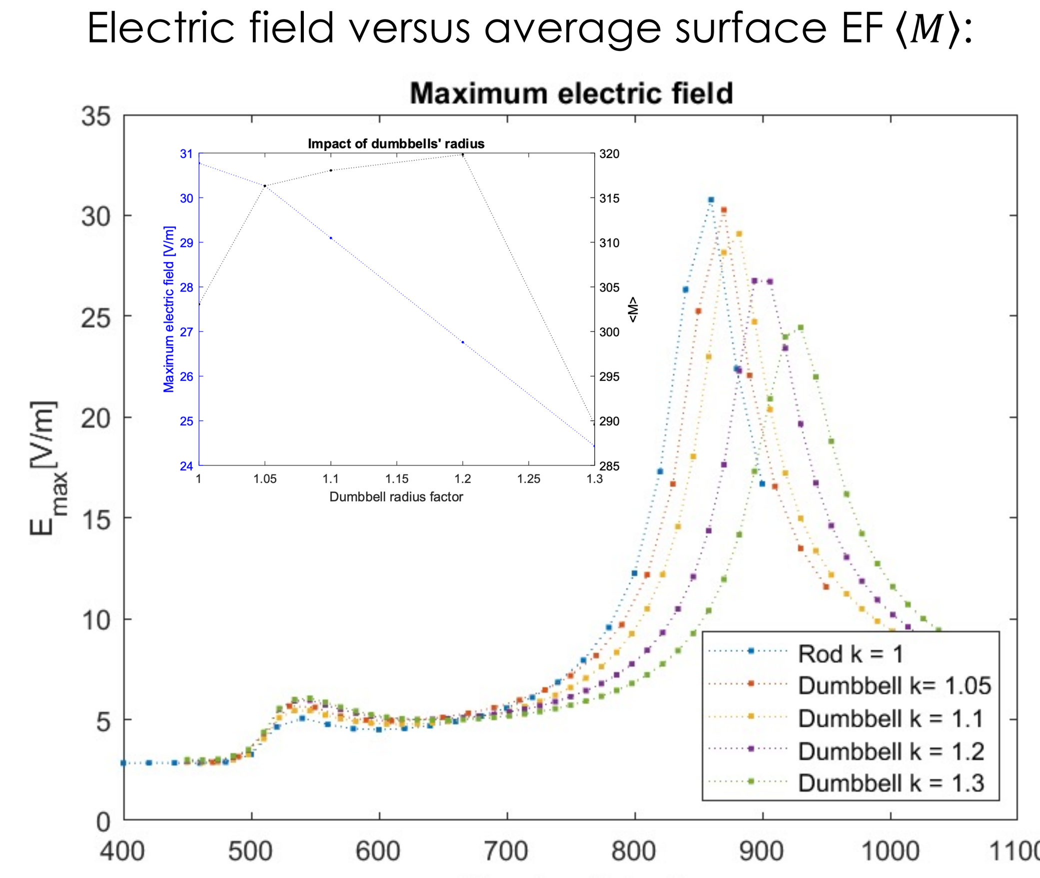


Electric field [V/m] of a Au nanorod with a 7.5 nm radius and a length of 65 nm and k = 1.05 in water $\epsilon = 1.33$ and $\lambda = 866\ nm$



TEM image of synthetized Au nanodumbbells by colleague‡

Electric field versus average surface EF $\langle M\rangle$:



Maximum electric field dependence with the wavelength of a nanorod and nanodumbbells with a 7.5 nm radius and a length of 65 nm in water $\epsilon = 1.33$. Inset: evolution of E_{max} versus $\langle M\rangle$ for different dumbbell radius factors.

Conclusion and Perspectives

In conclusion, the impact of the size and shape of different nanoparticles has been analyzed. This knowledge allowed us to design a nanoparticle that has a higher surface-averaged enhancement factor. This improved shape also showed the difference between the LFIEF and surface average EF $\langle M\rangle$.

We are currently working on the optimization of the average EF $\langle M\rangle$ of the nanodumbbells. Next to this, the simulation of the nanoparticles in different media is also in development, as well as the use of other plasmonic metals. Finally, the SERS measurements of the synthesized nanodumbbells will be compared with SERS spectra of the other shapes, by using methylene blue as analyte.

References

[1] Grand, J., Le Ru, E.C. Practical Implementation of Accurate Finite-Element Calculations for Electromagnetic Scattering by Nanoparticles. *Plasmonics* **15**, 109-121 (2020).

[2] COMSOL Multiphysics® v. 5.0 www.comsol.com COMSOL AB, Stockholm, Sweden.

Acknowledgements

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