COMSOL Conference
Boston 2016

Multiphysics and Multiscale Simulations

Advancing Basic Science and Industrial Applications

Prof. Edward P. Furlani

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Dept. of Chemical & Biological Engineering
Dept. Electrical Engineering
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Computational Research

Dr. Edward Furlani
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Industrial Research: Eastman Kodak Research Labs

Senior Principal Scientist : Computational modeling and simulation for the development of commercial materials and devices.

Academic Research: SUNY at Buffalo

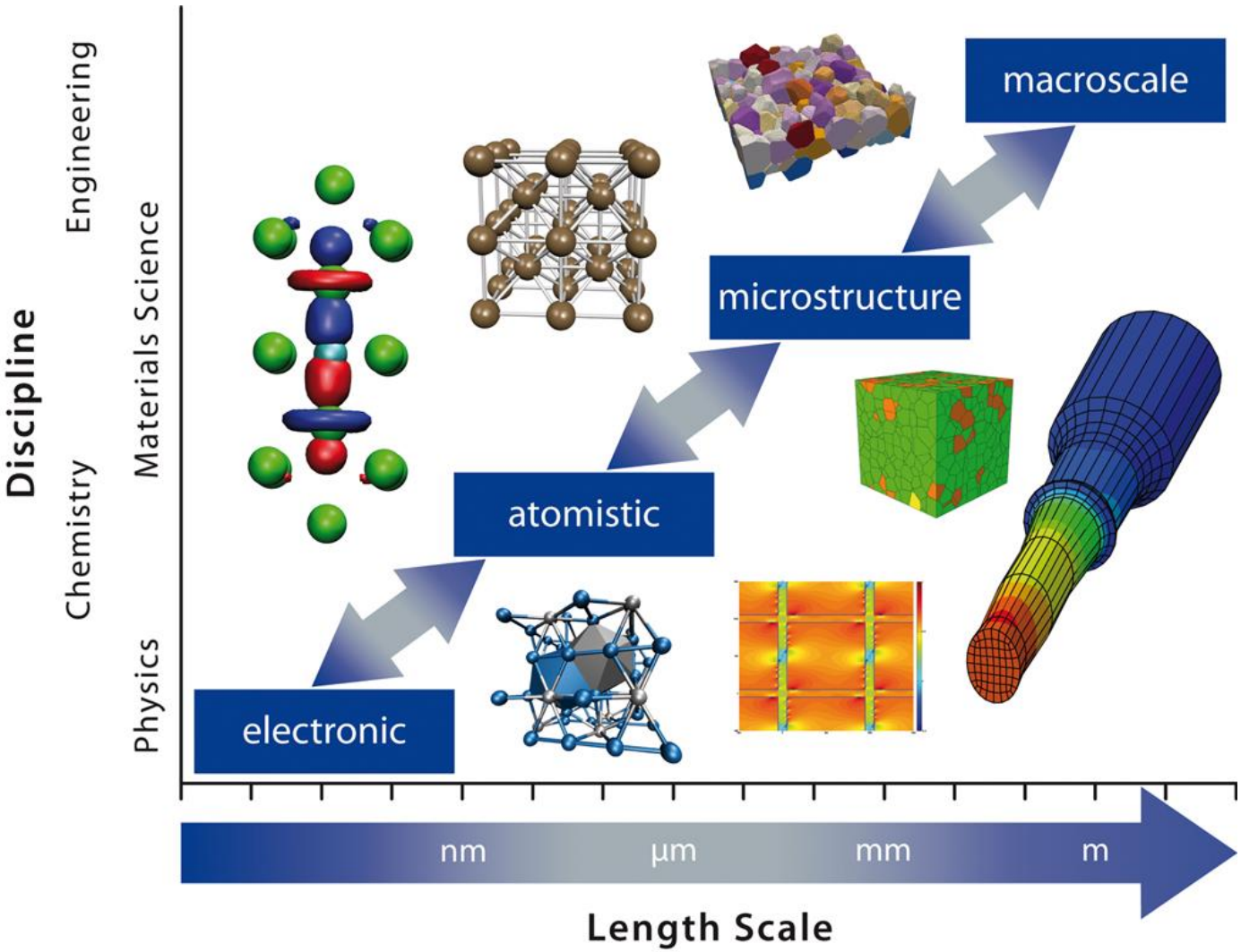
Prof. Chemical and Biological Engineering

Prof. Electrical Engineering

Computational Modeling and Simulation

- **Micro and Nano-structured materials, devices and processes - analysis & design**
- **Photonics - light-matter interactions, nanophotonics, metamaterials, plasmonics**
- **Computational Fluid Dynamics - transport phenomena, multiphase flow, ink-jet systems, nanofluids**
- **Microfluidics/MEMS - design and simulation**
- **Computational Magnetics - field/force analysis, self-assembly, bioseparation**

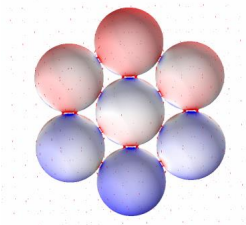
Multiphysics and Multiscale Simulations



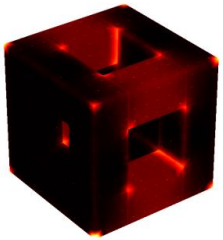
www.icams.de/content/research

Computational Research

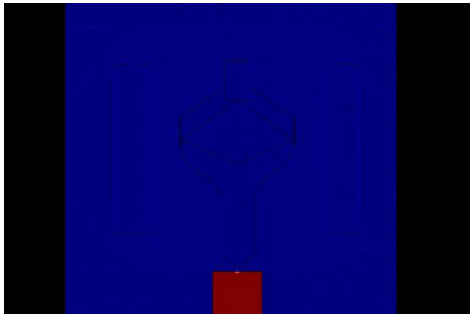
Nanophotonics in Colloidal Cluster



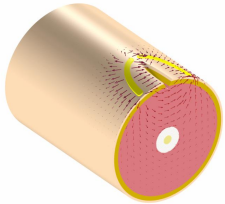
Heating of Colloidal Particle



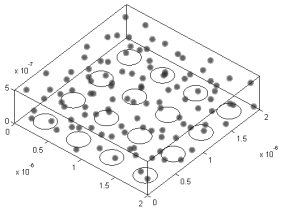
Magnetohydrodynamic Liquid Metal Printing

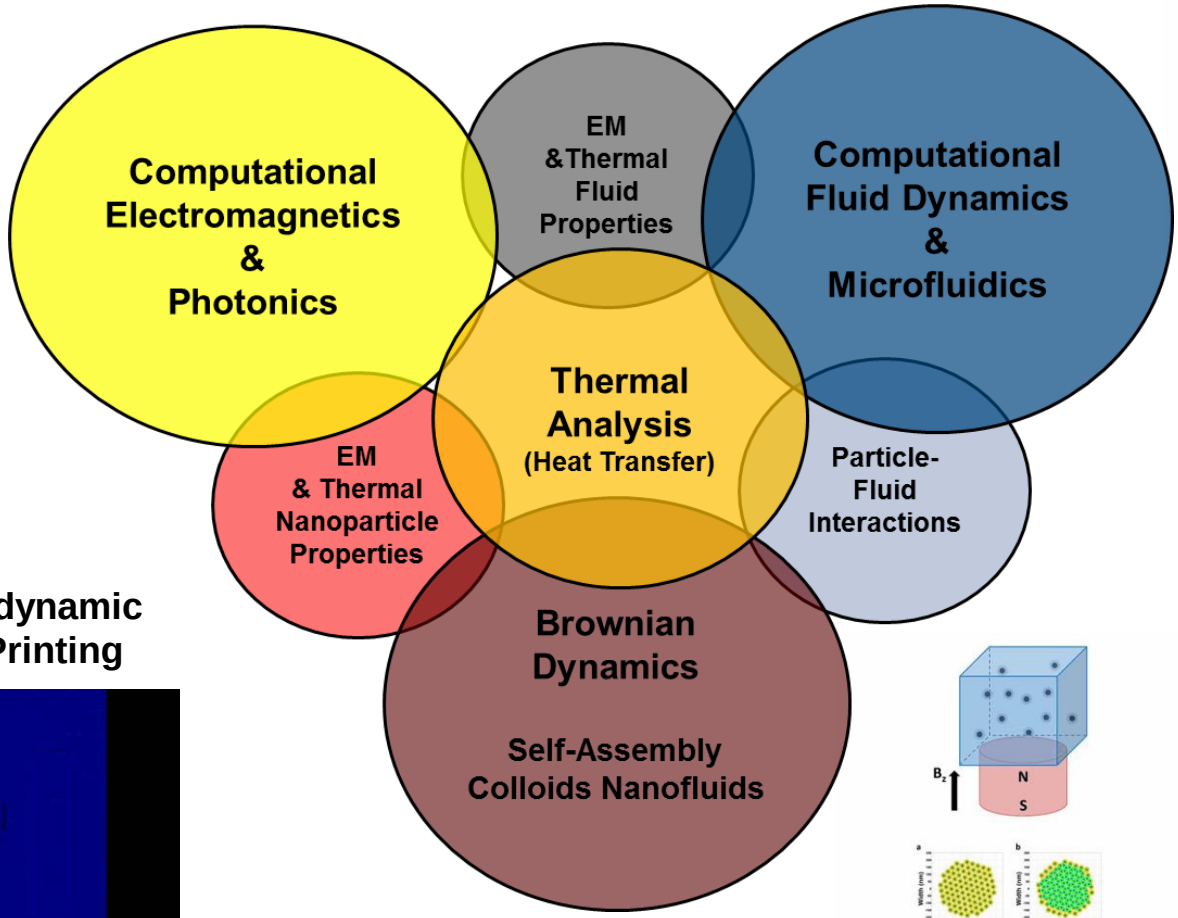


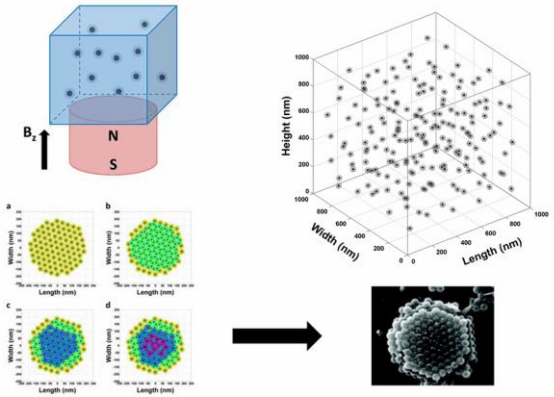
Electrical Stimulation Wound Healing



Field-Directed Self-Assembly







Laboratory for Interdisciplinary Modeling and Simulation

Laboratory Resources:

12 High Performance Workstations:

- T7910 (Intel Xeon 20 Logical Core, 128GB)
- T7810 (Intel Xeon 28 Logical Core, 128GB)
- T5810 (Intel Xeon 20 Logical Core, 96GB)

Research Group

- 10 graduate students
- 3 undergraduates

Center for Computational Research (CCR)

- State-of-the-art high performance computing (HPC) environment
- 270 Tflops of compute capacity and 4 PBytes of storage

Dedicated Industrial Modeling Cluster *

- **144 "parallel" nodes (16 core, 64GB ea.)**
- **FDR Infiniband Network Connection**
- **COMSOL Server (4 seats)**

***Funded by Empire State Development and NYSTAR, HPC^{NY}. a partnership between NYSERNet and supercomputing centers at RPI, UB, and Stony Brook. "The program provides NY businesses with advanced computing to accelerate product development."**

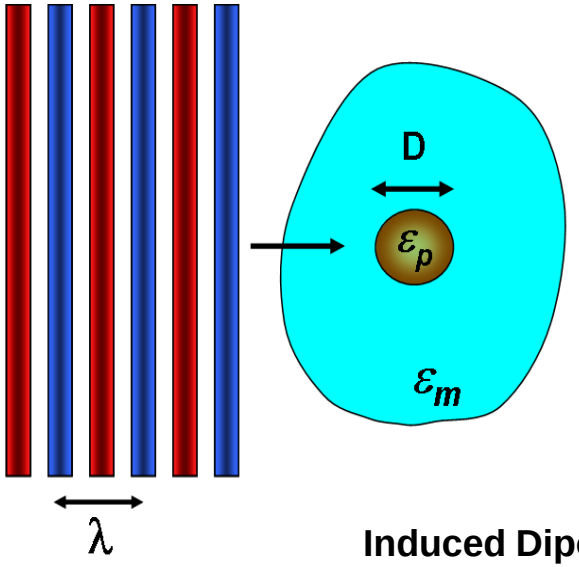
https://www.buffalo.edu/ccr.html

Colloidal Plasmonics

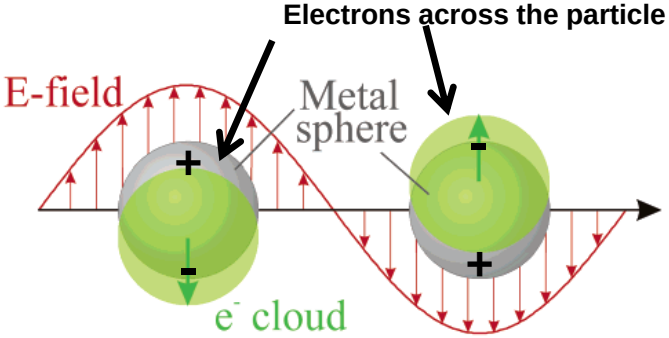
EM field induces Coherent Oscillation of Electrons In Nanoparticle

(Quasi-static limit D << λ)

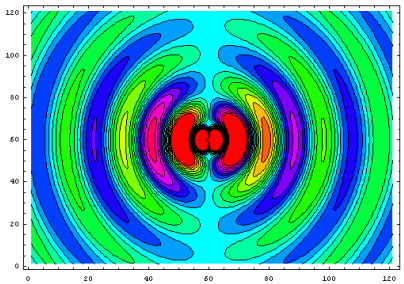
EM Wave



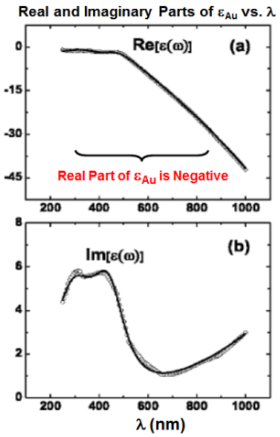
Variation in the Density of Electrons across the particle



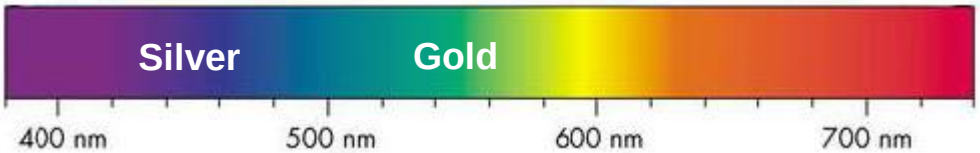
Particle acts as Oscillating Dipole



Induced Dipole Moment: $$P = \left[4\pi\varepsilon_0\varepsilon_m R_p^3 \underbrace{\frac{\varepsilon_p(\omega) - \varepsilon_m}{\varepsilon_p(\omega) + 2\varepsilon_m}} \right] E_0$$

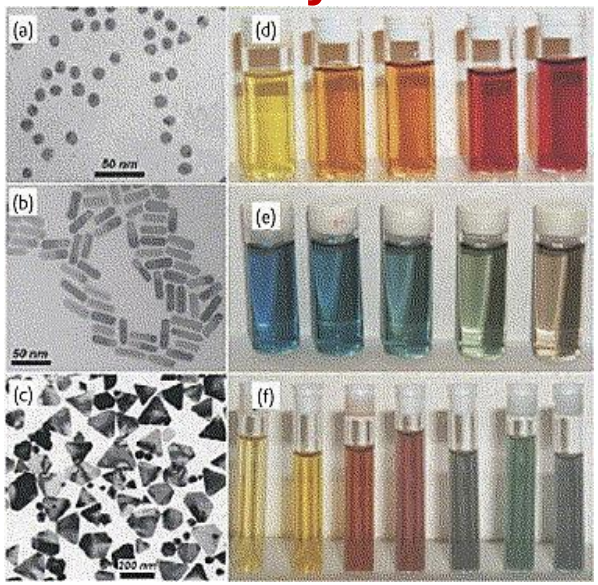


Resonance Frequency ω ➡ $\mathrm{Re}\left[\varepsilon_p(\omega)\right] = -2\varepsilon_m$ ➡ **Optical Absorption & Local Field Enhancement**



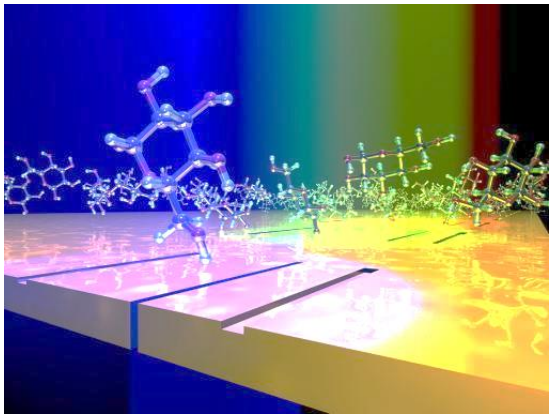
Plasmonics in Chemistry & Biotechnology

Particle Synthesis



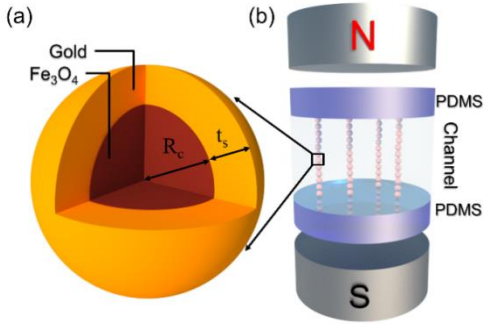
Jain et al, Nano Today, 2(1) 2007, 18–29

Biochemical Sensing



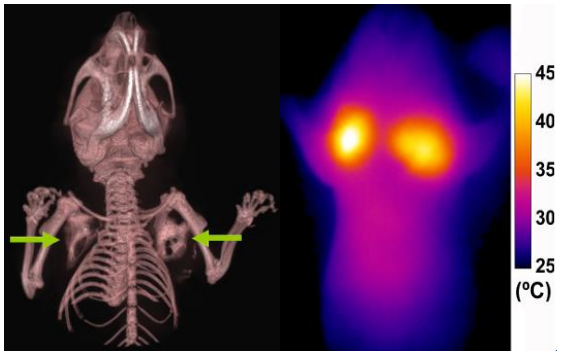
D. Pacifici, Brown University

Self-Assembly Nanofabrication



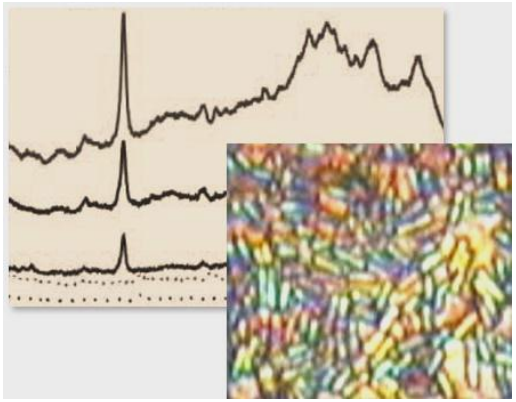
Theranostics

Therapy + Diagnostics



Nanopartz Inc

Spectroscopy



Reinhard group, Boston University

Computational Research

Laboratory for Interdisciplinary Modeling and Simulation

Advisor: Dr. Edward Furlani

Kai Liu
Ph.D. EE Candidate

Advancing Basic Science Light-Matter Interactions

- Plasmonics in Colloidal Nanoparticles
- Bottom-up Nanofabrication/Self-Assembly
- Nanoscale Photothermal Physics and Cancer Therapy

- Develop Multiphysics Comsol Models
- Run Parametric Analysis on HPC Cluster

Viktor Sukhotskiy
Ph.D. EE Candidate

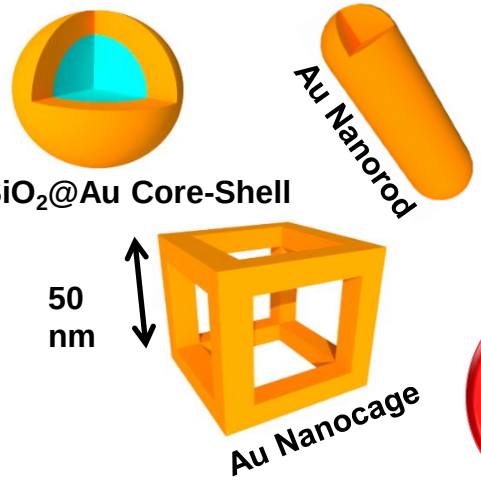
Industrial Applications Quasi-Static Field Theory

- Inductive Loop Traffic Sensing
- Electrical Stimulation Therapy
- 3D Liquid Metal Printing

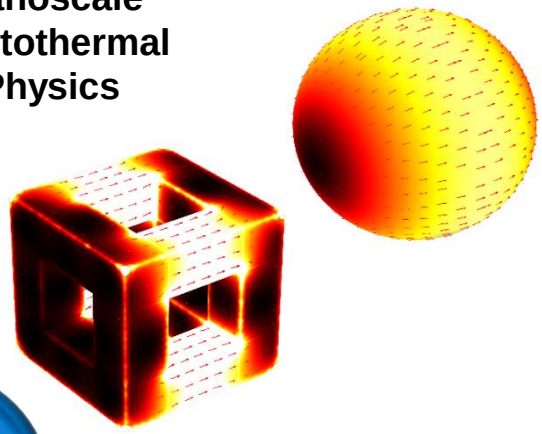
- Use Comsol Applications Builder
- Run COMSOL Solver on HPC Cluster for Parametric Analysis

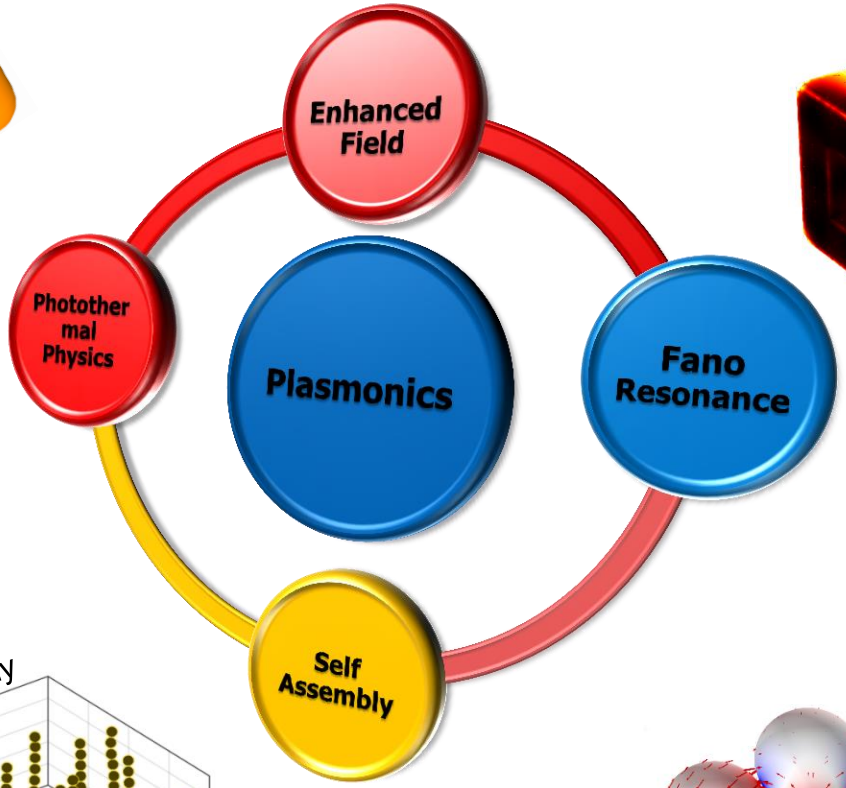
Understanding Nanoscale Light-Matter Interactions

Colloidal Plasmonic (Au) Nanostructures

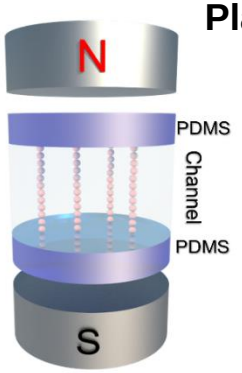


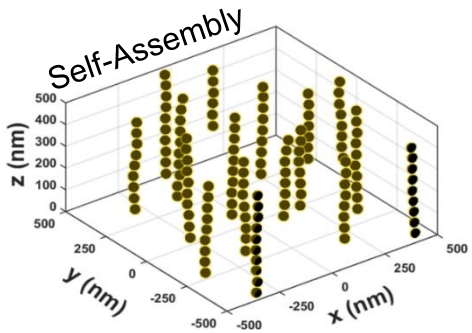
Nanoscale Photothermal Physics



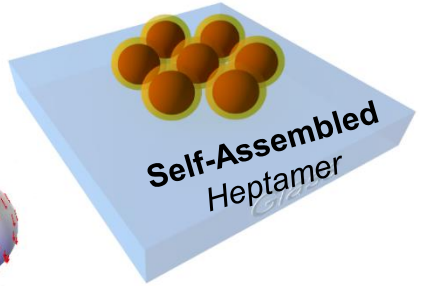


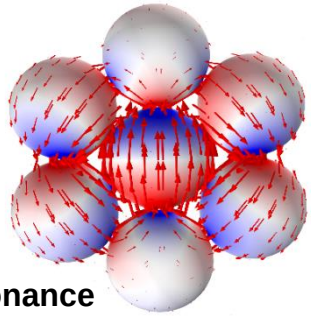
Magneto-Plasmonics





Self-Assembled Metamaterials

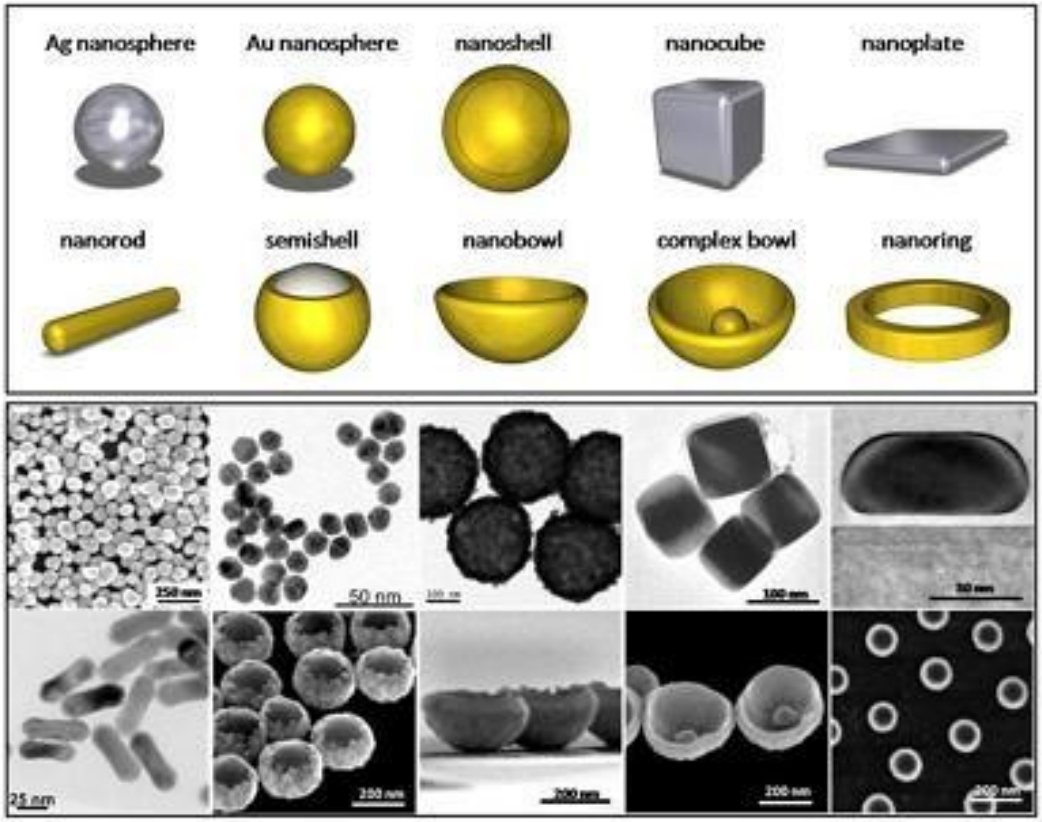




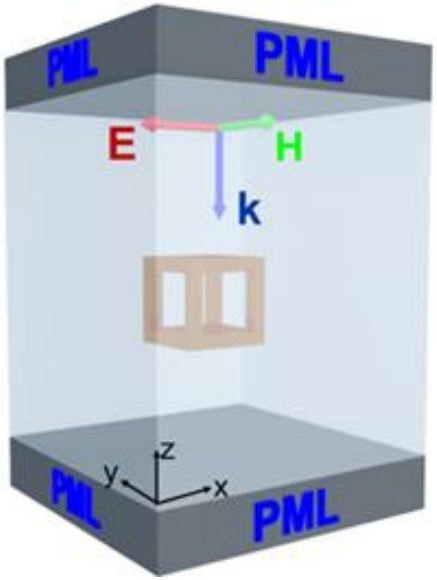
Fano Resonance

Colloidal Plasmonics
Field Enhancement & Photothermal Physics

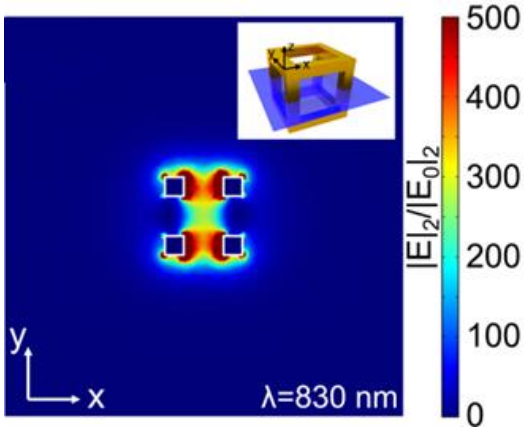
Synthesized Plasmonic (Ag, Au) Nanoparticles



COMSOL RF Model
Colloidal Nanocage



Field Enhancement
Nanocage Interior



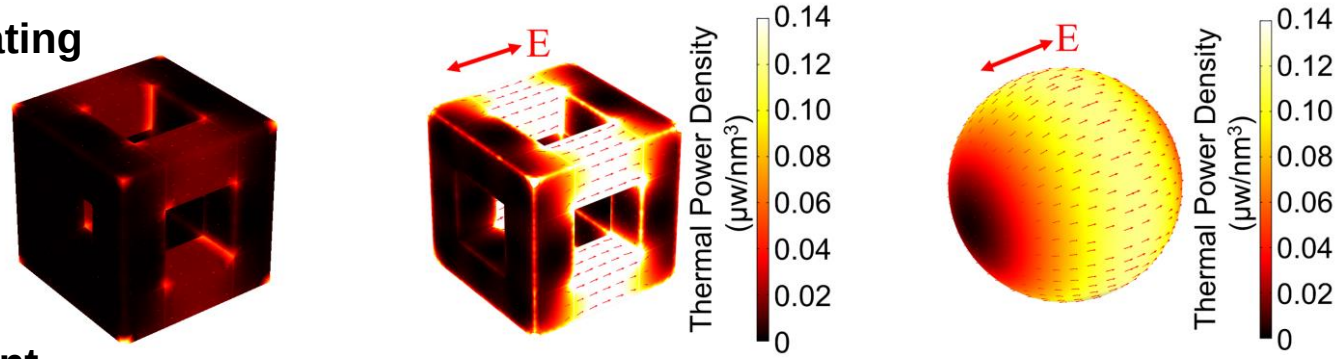
Nanoscale Photothermal Physics

Comparison of Electric Field Enhancement and Photothermal Heating
SiO_2@Au Core-Shell vs. Au Nanocage

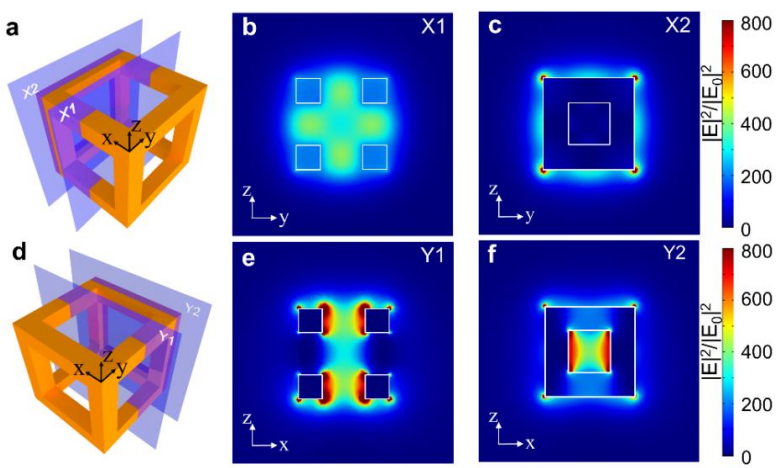
COMSOL RF and Heat Transfer Modules

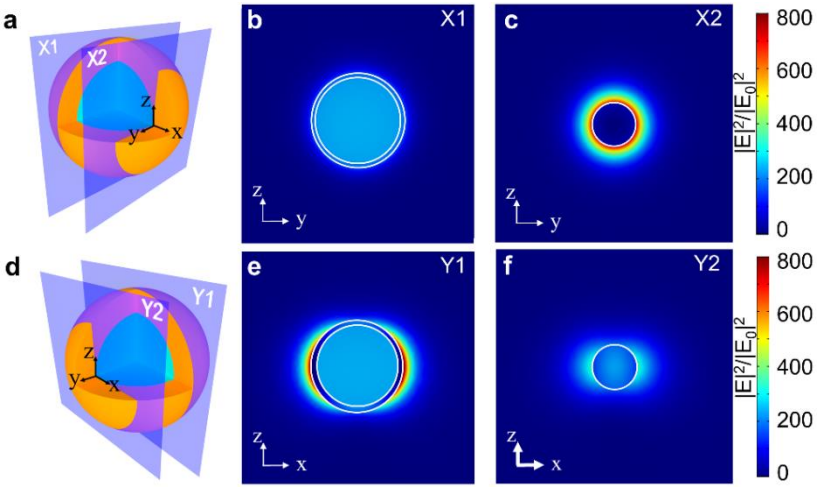
Nanocage Provides Superior Field Enhancement and Comparable Heating!

Photothermal Heating



Field Enhancement





K. Liu, X. Xue, E. P. Furlani, Sci. Rep. 6, 34189 (2016)

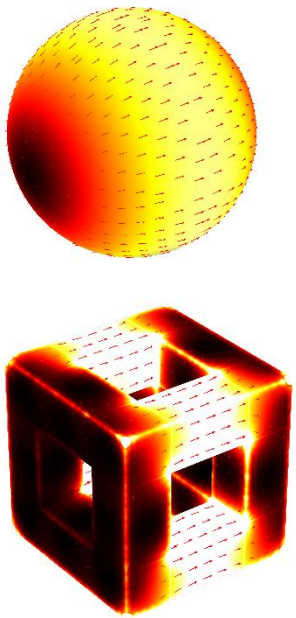
Nanoscale Photothermal Physics

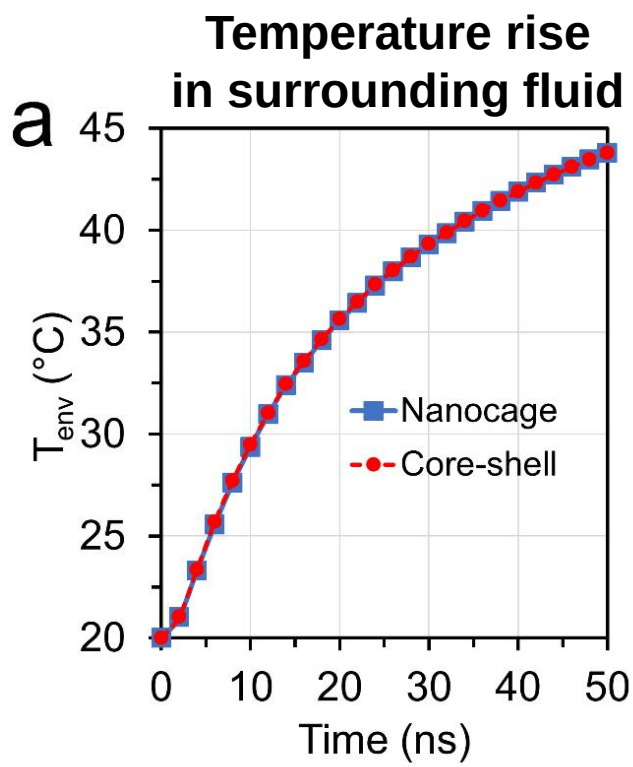
COMSOL RF and Heat Transfer Modules

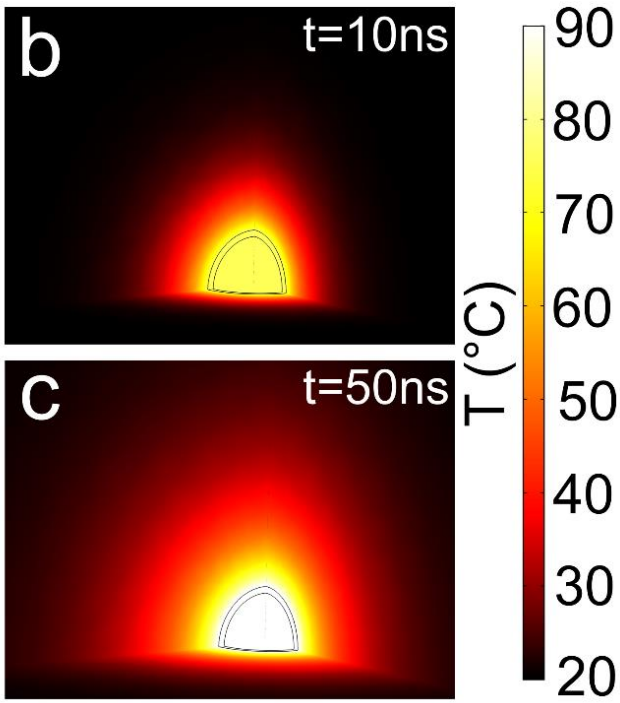
Heat Transfer is Coupled to Photonic Analysis through Absorbed Power at Plasmon Resonance

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = Q_{plasmon}$$

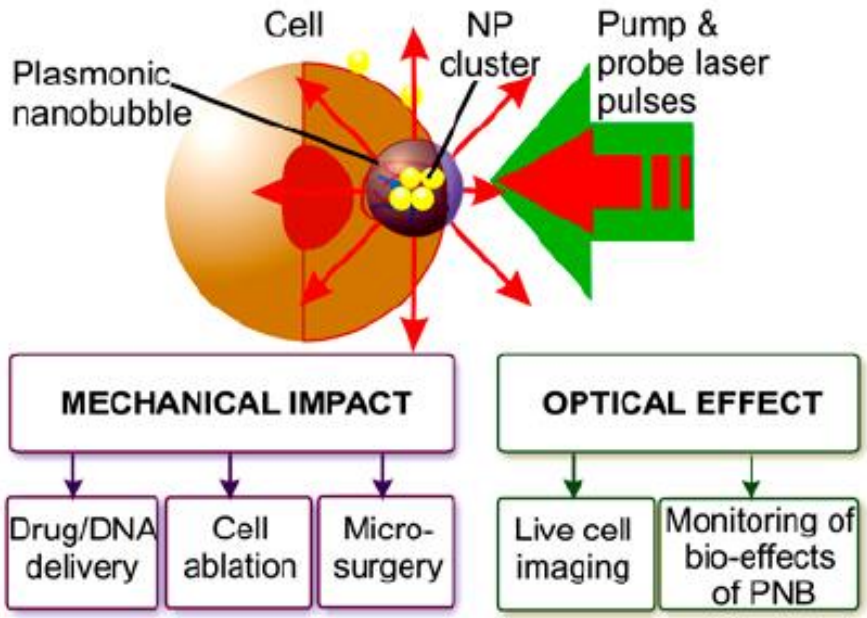
The absorbed optical power (or the generated heat) $Q_{plasmon}$ in the Photonics model acts as a heat source in the heat transfer model.

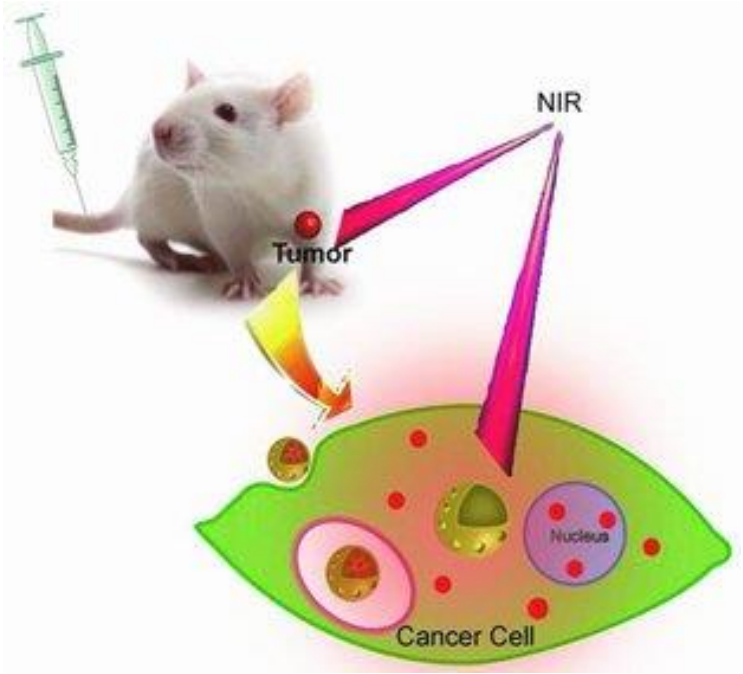


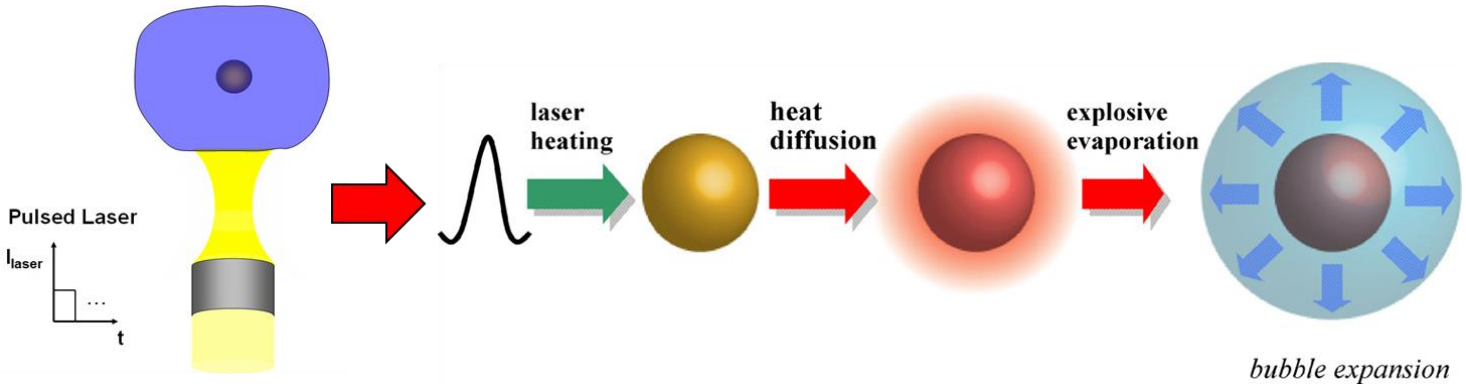




Plasmon-Enhanced Nanomedicine Photothermal Cancer Therapy and Imaging



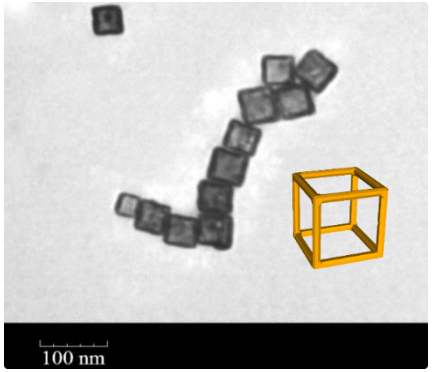




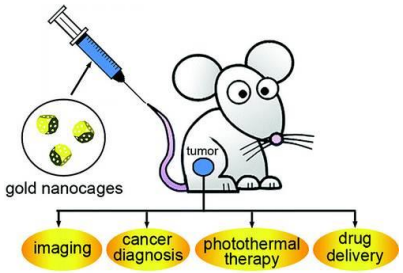
Lukianova-Hleb et al. Nanotechnology 21 (2010)

Plasmon-Enhanced Photothermal Therapy

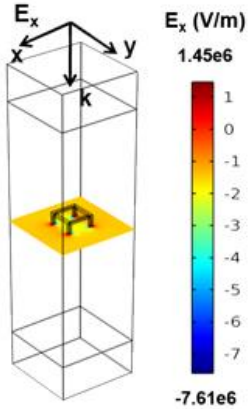
Gold Nanocage



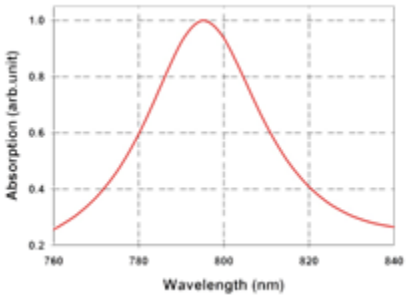
Therapy



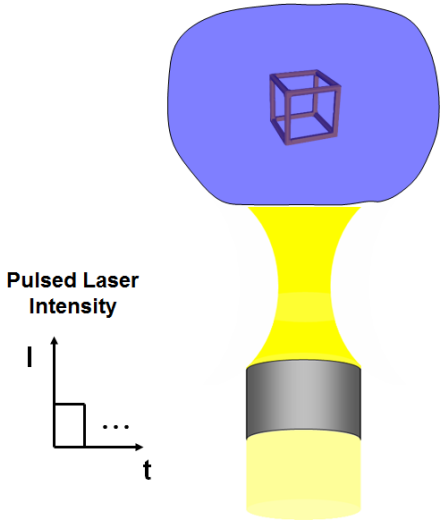
Photonic Analysis



Absorption Spectra

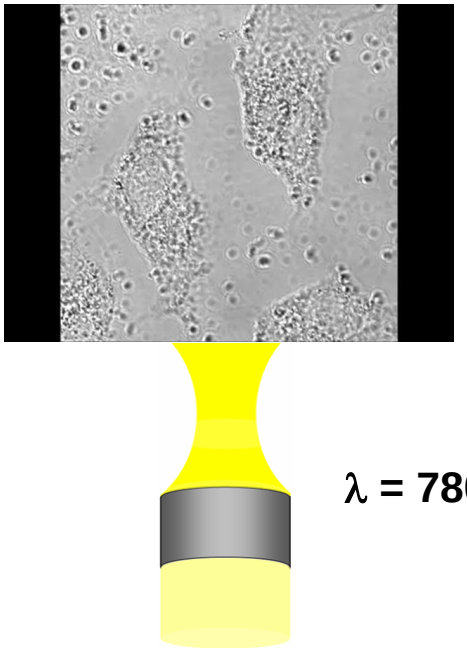


Nanosecond-Pulsed Heating leading to Nanobubble Generation and Cell Destruction



Plasmonic nanoparticles uptaken into Hela Cells

Cell destruction via Bubble Generation*



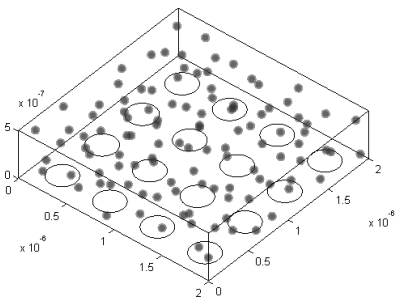
λ = 780 nm

*Ohulchanskyy, Furlani et al. Nanomed.-Nanotechnol. Biol. Med. 9, (2013)

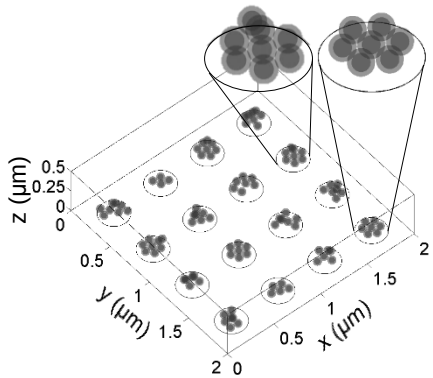
Self-Assembled Magnetic-Plasmonic Metamaterials

Brownian Dynamics (Monte Carlo Analysis)

Brownian Dynamics Self-Assembly

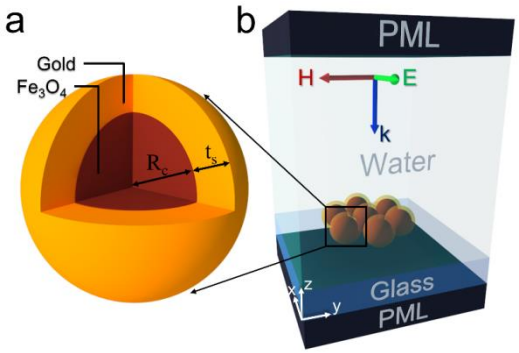


Final Equilibrium Particle Distribution

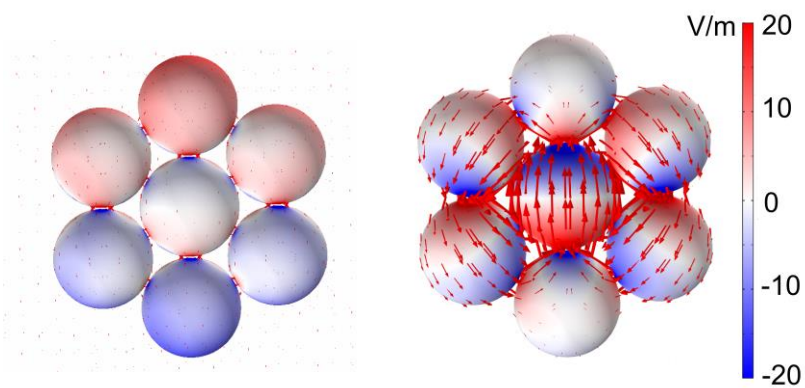


Self-Assembled Particle Positions (x_i,y_i,z_i)

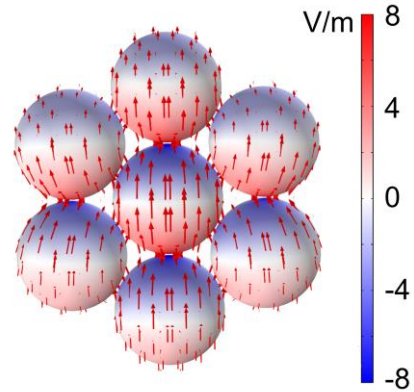
COMSOL RF Optical Model of Self-Assembled Heptamer



Subradiant Mode

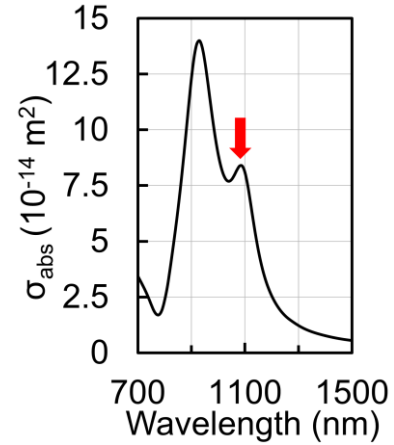


Superradiant Mode



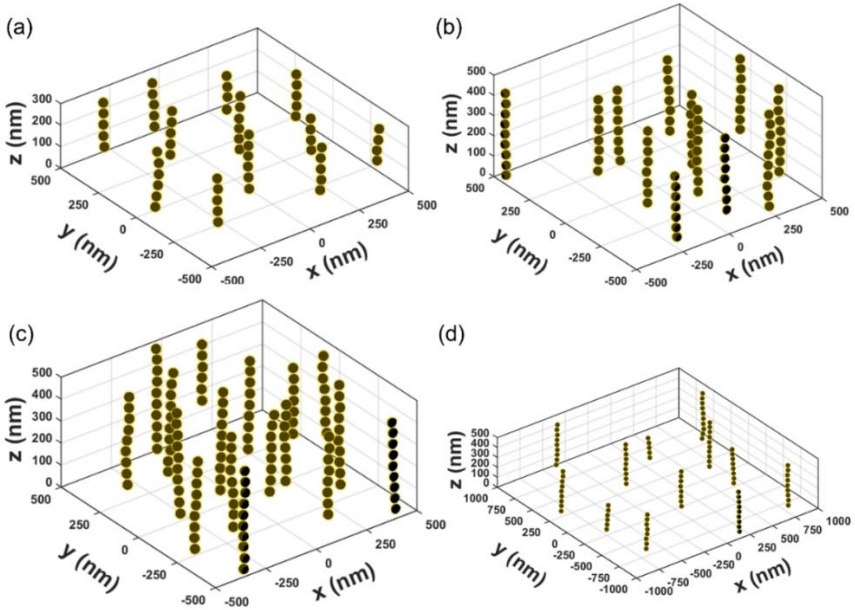
Fano Resonance Absorption Spectrum

Useful for Biosensing



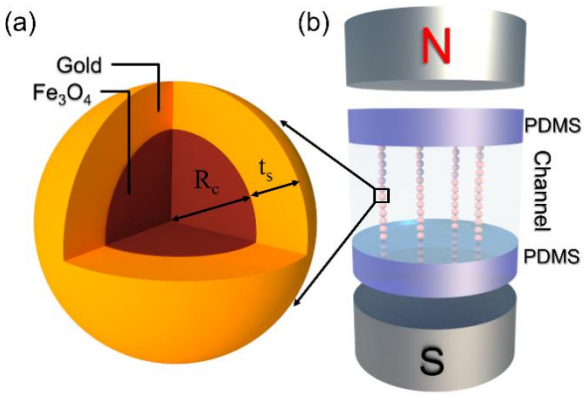
Self-Assembled Magneto-Plasmonic 1D Chains

Brownian Dynamics (Monte Carlo Analysis)

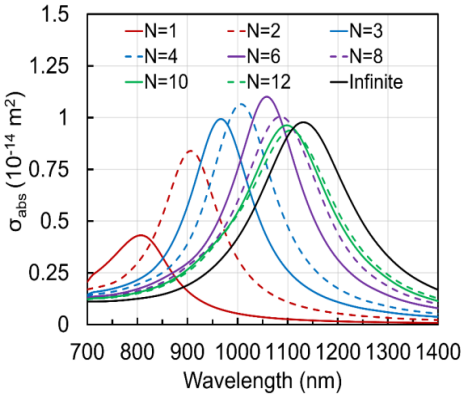


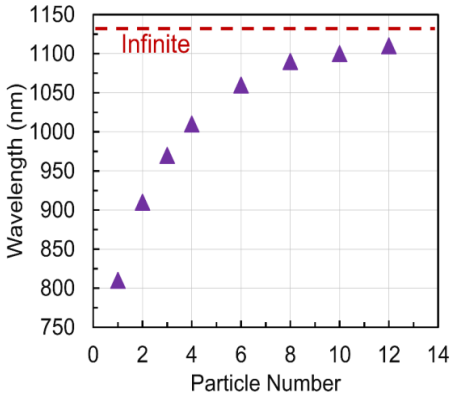
Self-Assembled Particle Positions (x_i,y_i,z_i)

COMSOL RF Optical Model of 1D Chain Structures



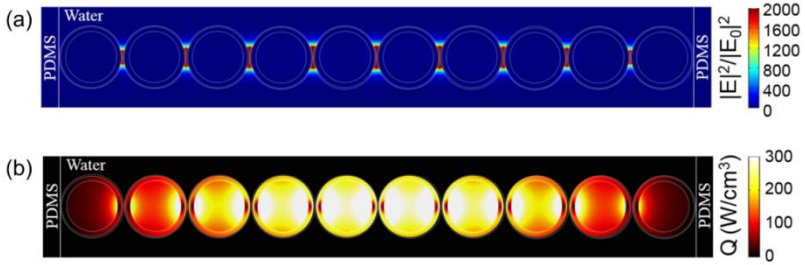
Absorption Spectrum vs. # Particles in Chain





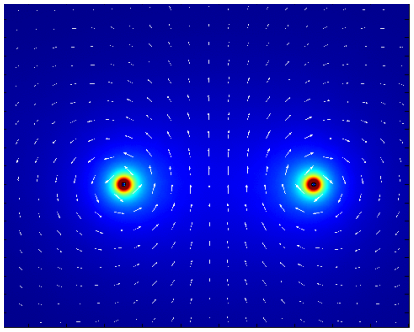
Assembled Plasmonic Chains Provide Unique Spectral Signature

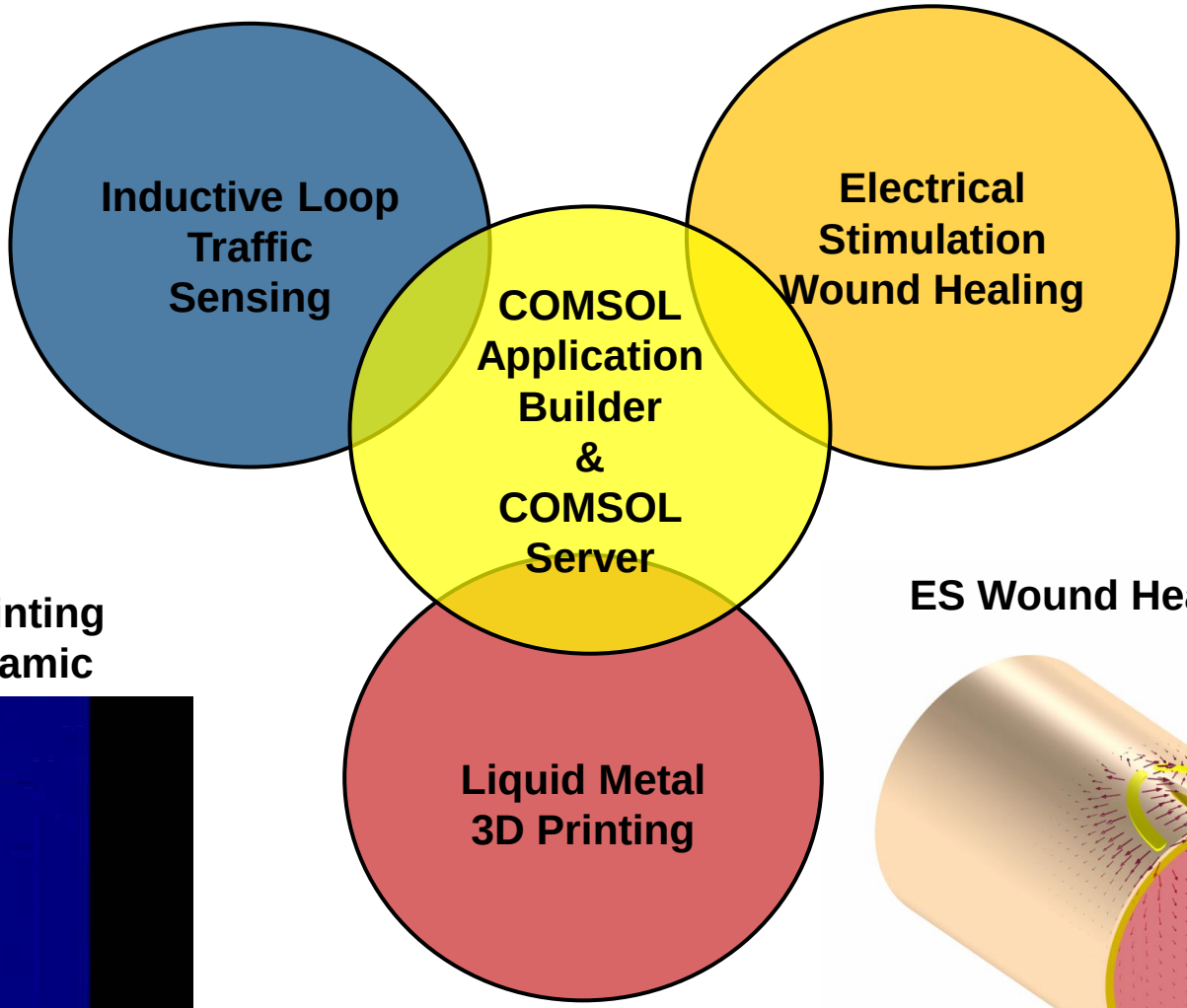
Useful for Biosensing



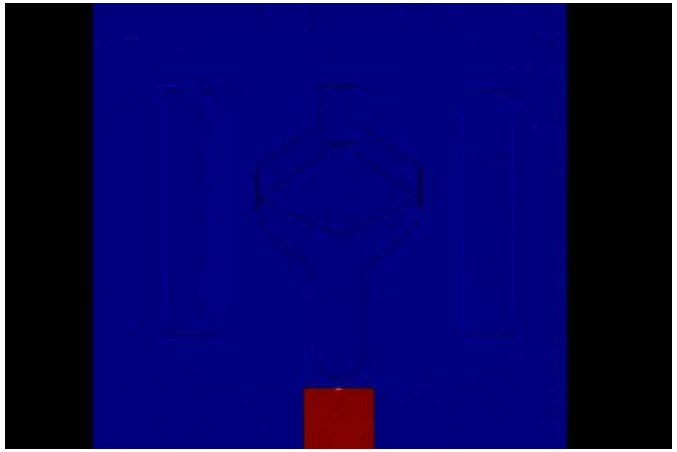
Industrial Applications

Inductive Loop Traffic Sensing

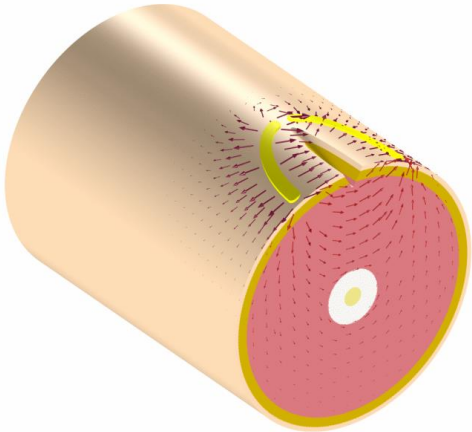




Liquid Metal 3D Printing Magnetohydrodynamic



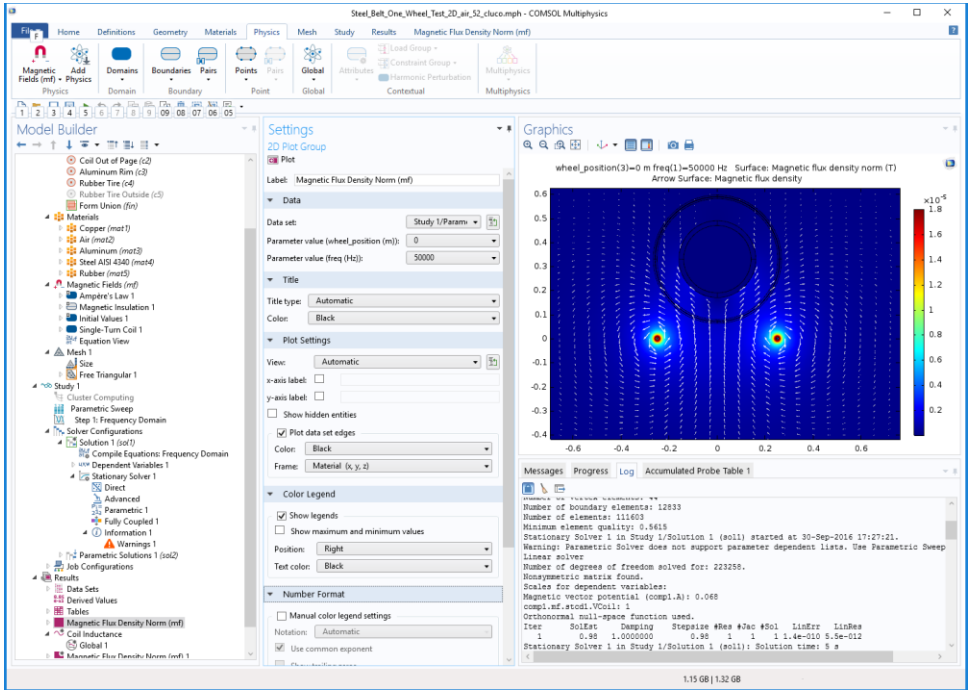
ES Wound Healing



COMSOL Model Builder vs. COMSOL Server

Model and Application Builder

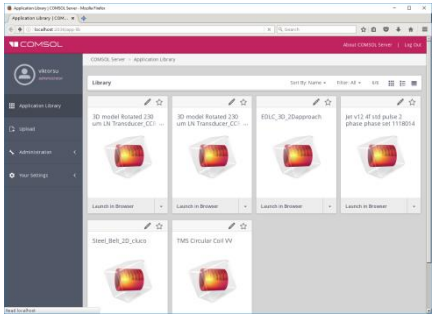
Requires Engineering and Mathematics Expertise and Knowledge of COMSOL Design Process

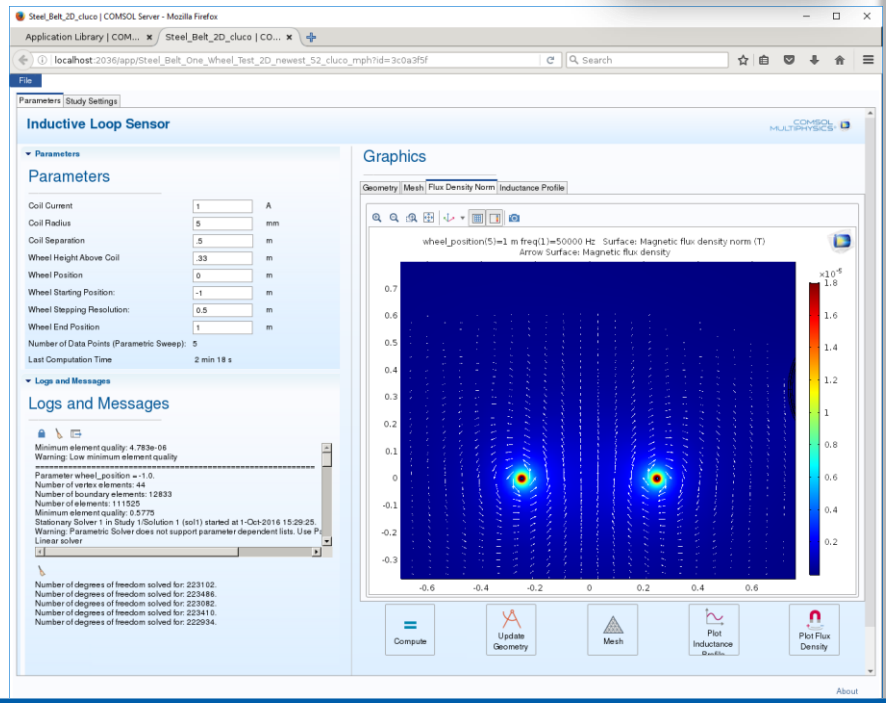


Custom Designed Application GUI

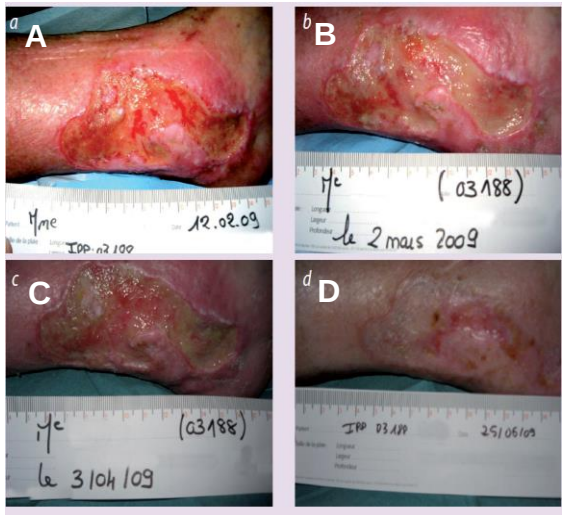
COMSOL Server

Perform Parametric Analysis using Custom GUI
Eliminate Need for Engineering and Mathematics





Electrical Stimulation Therapy

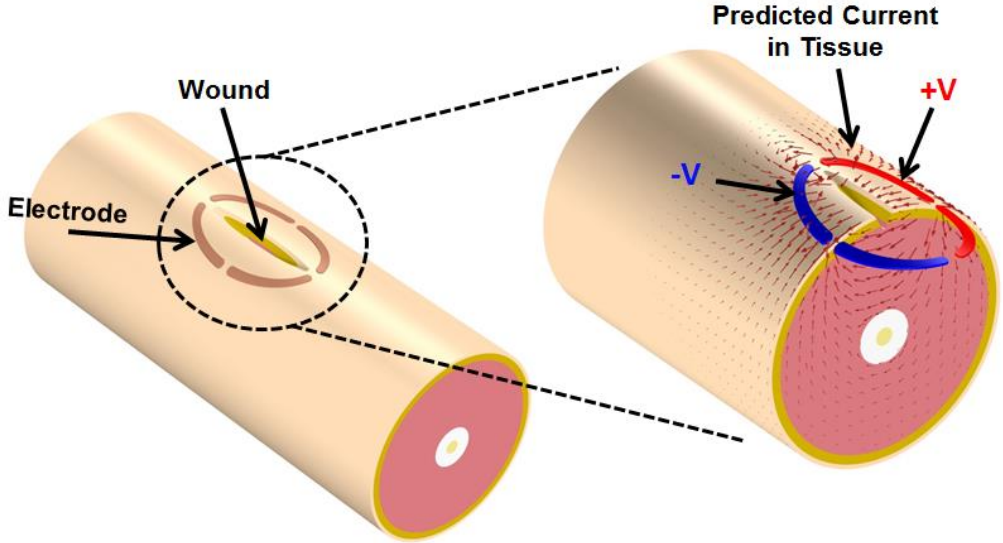


Garwood Medical Devices

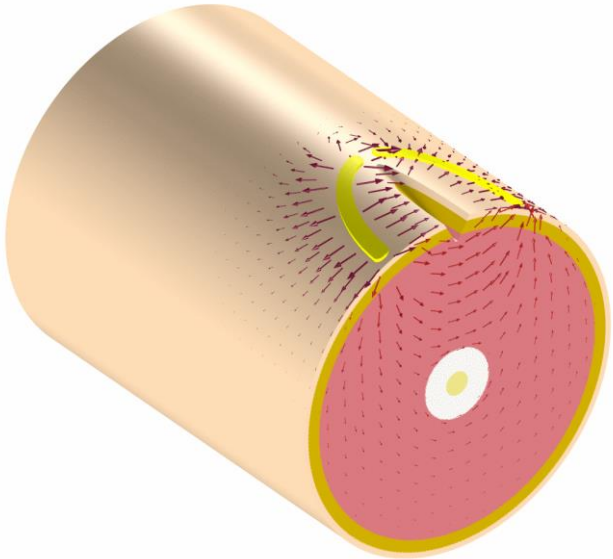
GARWOOD MEDICAL DEVICES, LLC

A) Wound present on patient for 5 years, this image is after 3 months of moist therapy.
B) Wound after 2.5 weeks of ES, 30 min, 2x/day.
C) Wound after 2 months of ES, 30 min, 2x/day.
D) Wound after 3 months of ES, 30 min, 2x/day.

COMSOL AC/DC Module and COMSOL Server

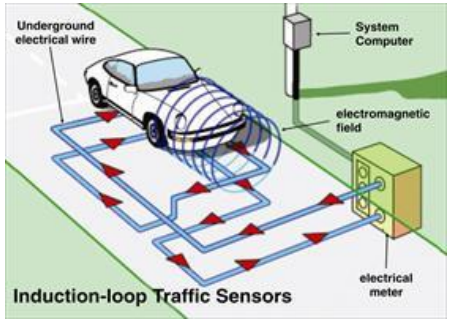


Predict Field Induced Current Density in Tissue



Inductive Loop Traffic Sensing

Intelligent Transportation Systems*

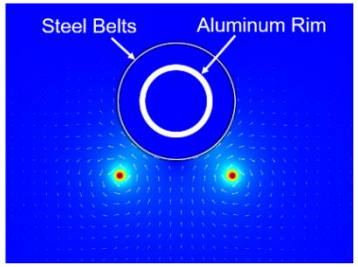


Sponsored by Xerox Corp

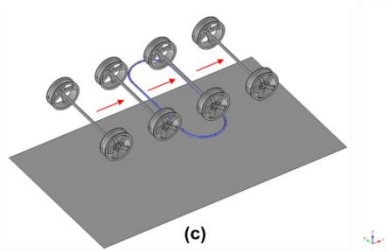
COMSOL AC/DC Module & COMSOL Server

Predict Change in Coil Inductance due to Steel-Belted Tires

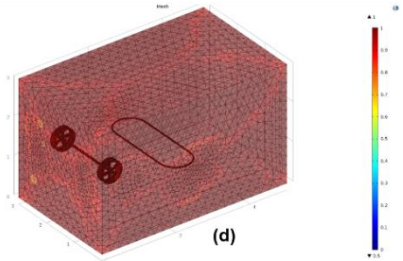
(a)



(b)

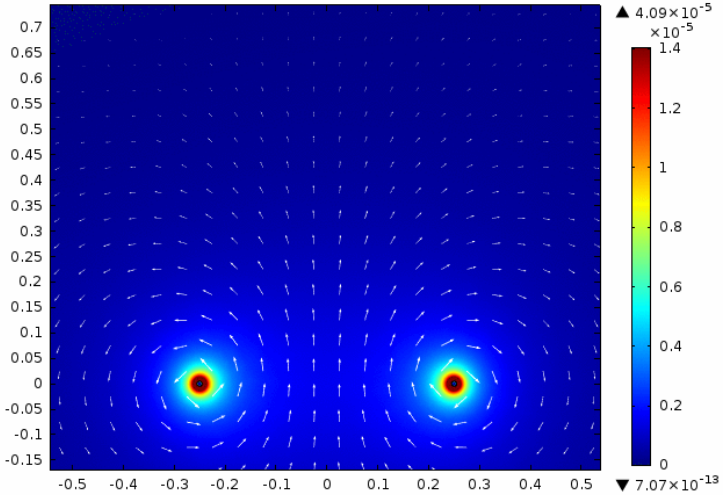


(c)

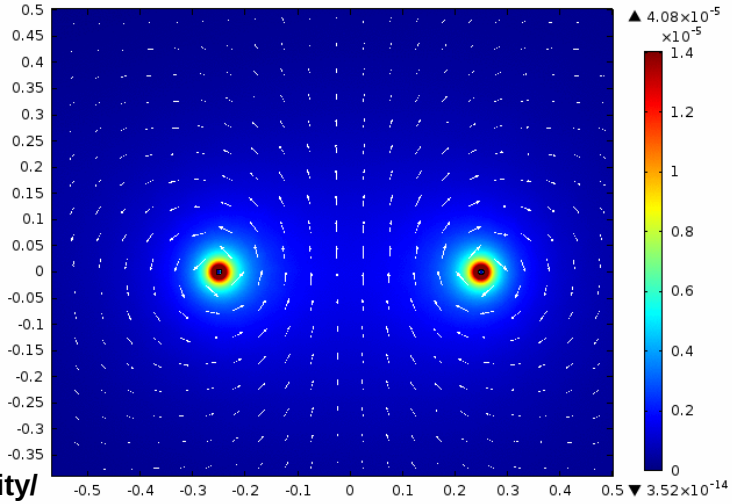


(d)

Without Steel Tire Belts:



With Steel Tire Belts:

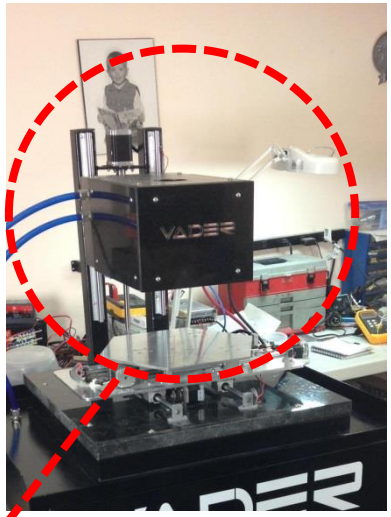


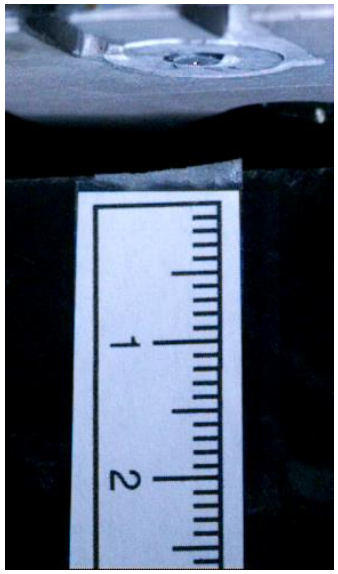
www.masterbuilder.co.in/intelligent-traffic-management-systems-a-growing-necessity/

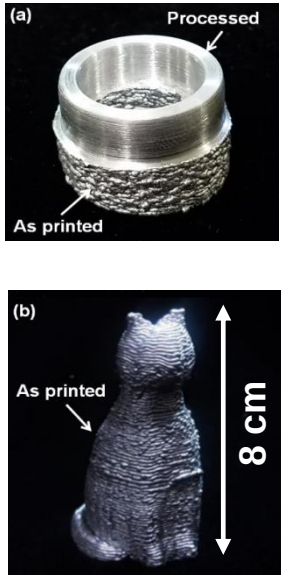
3D Liquid Metal Printing

Vader Systems' Innovative MagnetoJet 3D Metal Printer

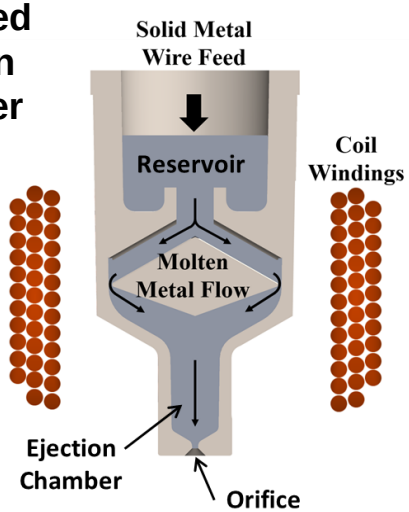
Machine Prototype







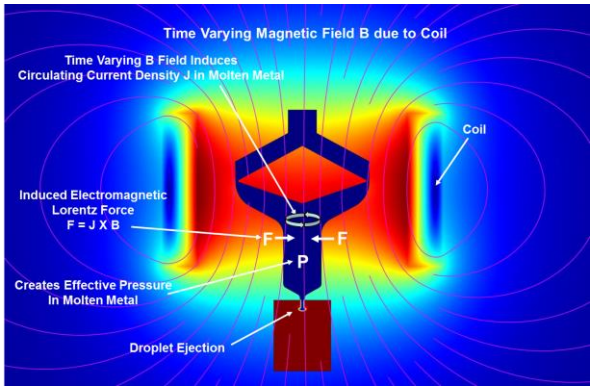
Simplified Ejection Chamber



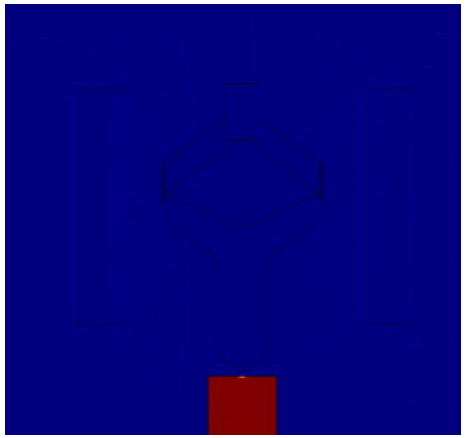
COMSOL AC/DC, CFD, Heat Transfer and COMSOL Server

Predict Droplet Generation

Modeling Magnetohydrodynamics



Time Dependent Flux Density



Acknowledgements

- **Fundamental Analysis**
  - National Science Foundation
- **Industrial Modeling**
  - Vader Systems
  - Xerox Corp
  - Garwood Medical Devices
- **Computational Infrastructure**
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  - UB Center for Materials Informatics
  - Empire State Development and NYSTAR, HPC^{NY}