Multiphysics and Multiscale Simulations
Advancing Basic Science and Industrial Applications

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Computational Research

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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
Computational Research

Nanophotonics in Colloidal Cluster

Heating of Colloidal Particle

Magnetohydrodynamic Liquid Metal Printing

Electrical Stimulation Wound Healing

Field-Directed Self-Assembly

Computational Electromagnetics & Photonics

Computational Fluid Dynamics & Microfluidics

EM & Thermal Fluid Properties

Particle-Fluid Interactions

Thermal Analysis (Heat Transfer)

Brownian Dynamics

Self-Assembly Colloids Nanofluids
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)

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

Research Group
- 10 graduate students
- 3 undergraduates

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, HPCNY, 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 $D \ll \lambda$)

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

Resonance Frequency $\omega$ $\rightarrow$ $\text{Re}\left[\varepsilon_p(\omega)\right] = -2\varepsilon_m$

Optical Absorption & Local Field Enhancement

Silver
Gold

400 nm 500 nm 600 nm 700 nm
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

Spectroscopy

Nanopartz Inc

Reinhard group, Boston University
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

Viktor Sukhotskiy
Ph.D. EE Candidate

Industrial Applications
Quasi-Static Field Theory

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

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

- Use Comsol Applications Builder
- Run COMSOL Solver on HPC Cluster for Parametric Analysis
Understanding Nanoscale Light-Matter Interactions

Colloidal Plasmonic (Au) Nanostructures

SiO$_2$@Au Core-Shell

Au Nanorod

Au Nanocage

50 nm

Enhanced Field

Photothermal Physics

Self-Assembly

Magnetoplasmonics

Nanoscale Photothermal Physics

Fano Resonance

Self-Assembled Metamaterials

Self-Assembled Heptamer

Fano Resonance

Understanding Nanoscale Light-Matter Interactions
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!

Field Enhancement

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

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

The absorbed optical power (or the generated heat) \( Q_{\text{plasmon}} \) in the Photonics model acts as a heat source in the heat transfer model.
Plasmon-Enhanced Nanomedicine
Photothermal Cancer Therapy and Imaging

Plasmon-Enhanced Photothermal Therapy

Gold Nanocage

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*

Pulsed Laser Intensity

\[ \lambda = 780 \text{ nm} \]

Self-Assembled Magnetic-Plasmonic Metamaterials

Brownian Dynamics (Monte Carlo Analysis)

Self-Assembled Magnetic-Plasmonic Metamaterials

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)

COMSOL RF Optical Model of 1D Chain Structures

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

Assembled Plasmonic Chains Provide Unique Spectral Signature Useful for Biosensing

Absorption Spectrum vs. # Particles in Chain
Industrial Applications

- Inductive Loop Traffic Sensing
- Electrical Stimulation Wound Healing
- COMSOL Application Builder & COMSOL Server
- 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**

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

Inductance vs. Wheel Position With Respect to Coil

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

COMSOL AC/DC, CFD, Heat Transfer and COMSOL Server
Predict Droplet Generation Modeling Magnetohydrodynamics
Time Dependent Flux Density

Simplified Ejection Chamber
Solid Metal Wire Feed
Reservoir
Molten Metal Flow
Coil Windings
Orifice
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