UNCLASSIFIED

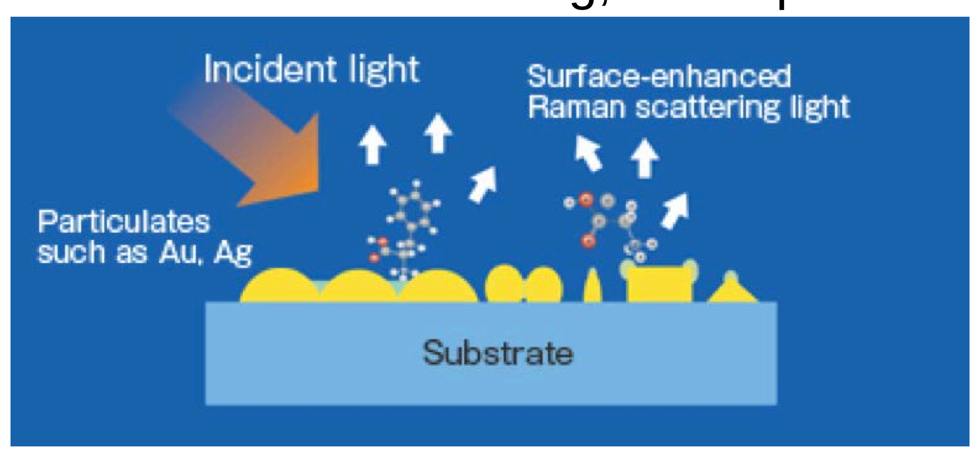
# Robust Design and Optimization of Nanoparticles: Morphology and Arrays

Y. He[1,2], J M. Razi[5], R. Wang[3], C. Forestiere[4], L. Dal Negro[3], R. M. Kirby[5]
1 University of North Texas, 2 New Mexico Tech, 3 Boston University, 4 Universita degli Studi di Napoli Federico II, 5 University of Utah

## Research Area

Nanostructured metal can help to boost the performance of many plasmonic devices (e.g., Surface Enhanced Raman Scattering substrates, novel plasmonic nanosensors, etc.) by enhancing the near-filed quantifies such as local electric field and optimizing the far-field synthetic parameters such as the scattering, absorption or extinction efficiencies.

Uncertainty quantification (UQ) tools and efficient optimization algorithms are applied to the design of metallic nanoparticles.

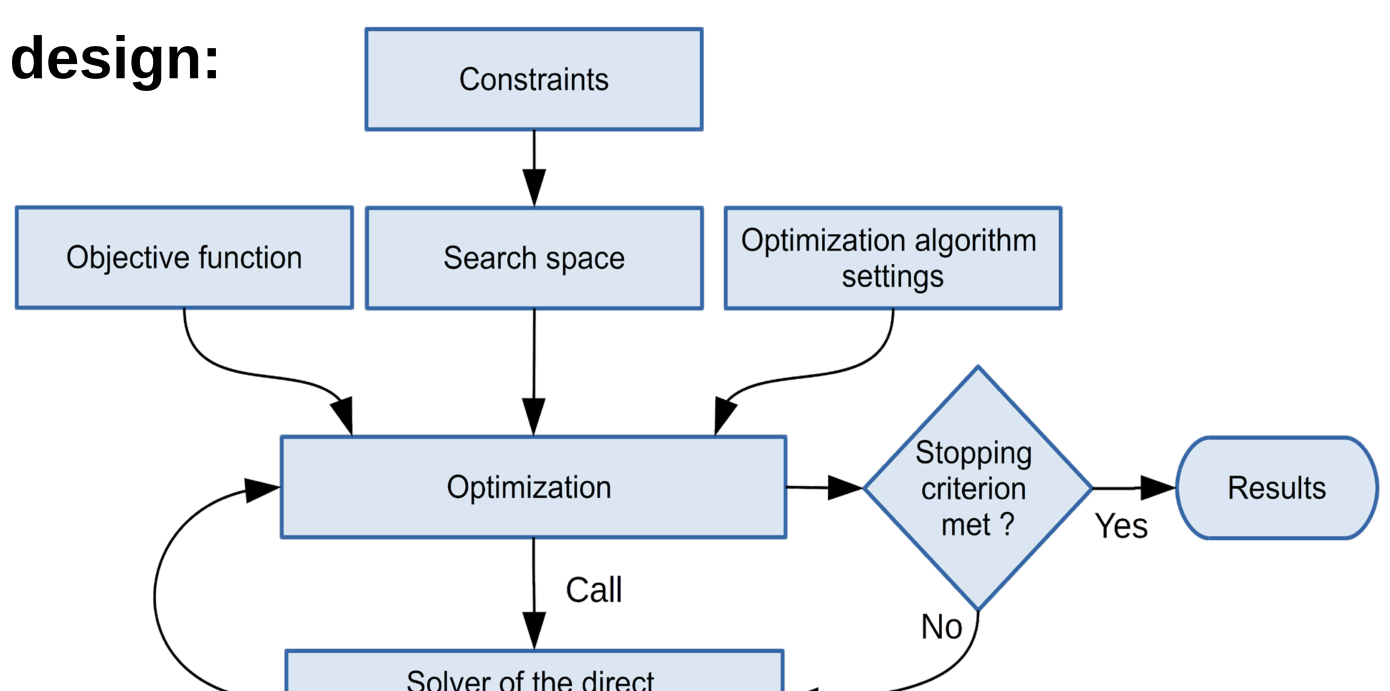



## Goals

- UQ-guided robust design of individual nanoparticles for the optimization of near-field property (e.g., local field enhancement).
- Design of large-scale nanoparticle (Vogel Spiral) arrays for the optimization of far-field properties (e.g., absorption and scattering).

## Current State and Challenges

**Inverse design:**




**Challenges:**

- Direct inverse design may fail due to the uncertainty in the nanofabrication process. However, consideration of uncertainty in design process could be computationally expensive.
- Design of large-scale nanoparticle arrays requires an efficient optimization algorithm to deal with the large number of degrees of freedom.

## Strategy

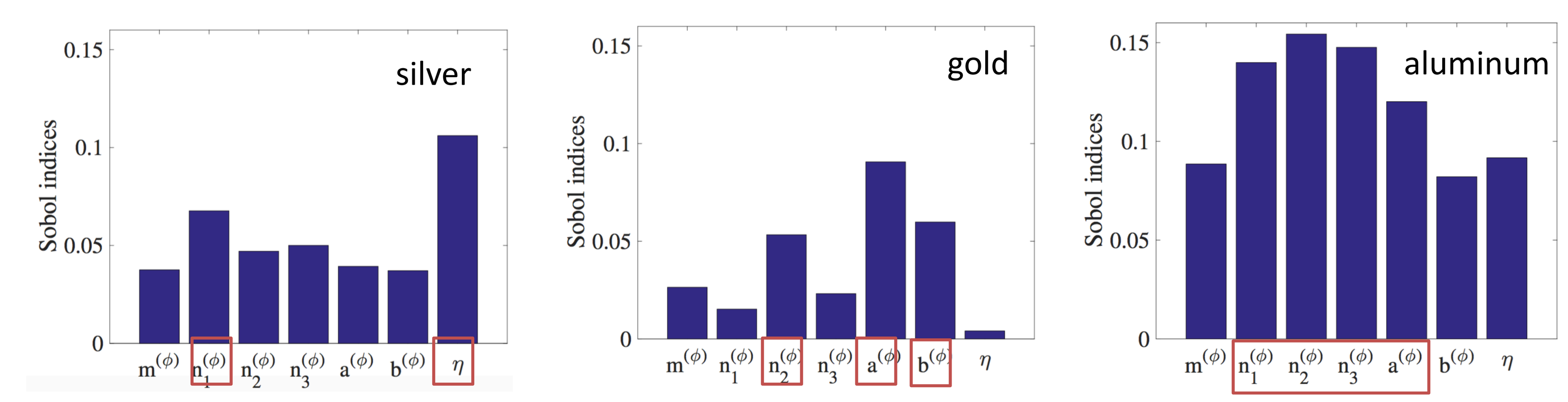
**UQ guided robust design:**

Uncertain inputs : $\Gamma$ shape parameters (distributions) → electromagnetic solver (3D SIE) → Uncertain output : $g$ local field enhancement (mean, variance)

## Strategy (contd.)

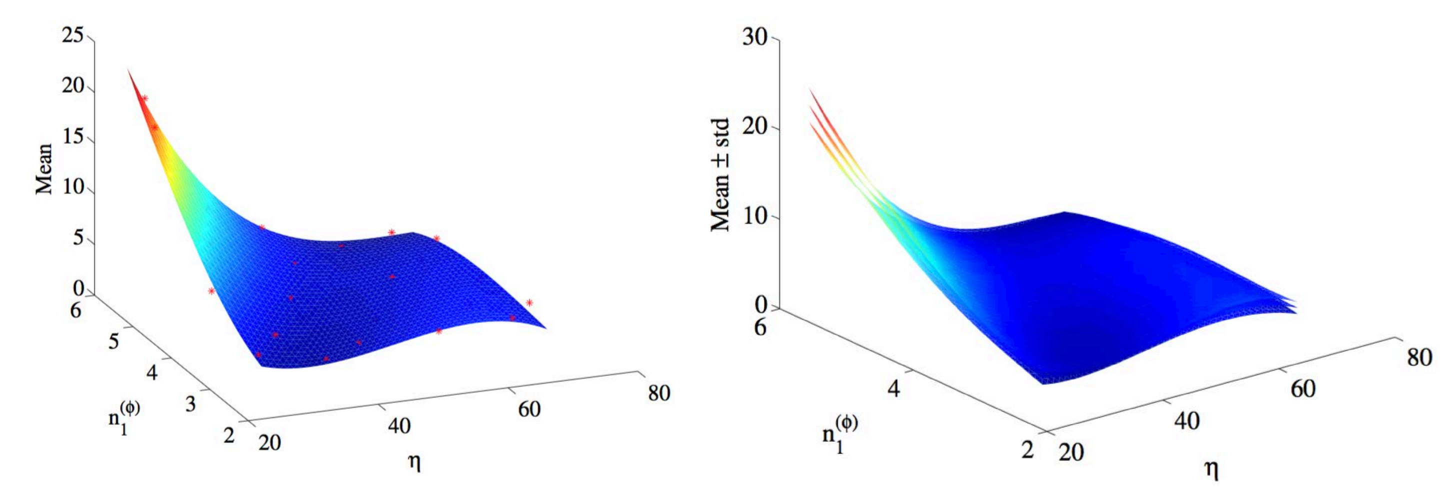
Robust design: $\bar{\Gamma}^* = \underset{\bar{\Gamma}}{\operatorname{argmax}}\, E(g(\Gamma)) - \beta\sigma(g(\Gamma)) \qquad \beta > 0$

➢ Global sensitivity analysis (identify "important" uncertain parameters)




➢ Generalized polynomial chaos expansion

- Constructed over stochastic space of "important" parameters
- Used to approximate true mean and standard deviation




### Design of Vogel Spiral Arrays:

Design parameters: scaling factor, divergence angle, wavelength → electromagnetic solver (CDA) → Outputs: absorption efficien$Q_{abs}$, scattering efficien$Q_{sc}$

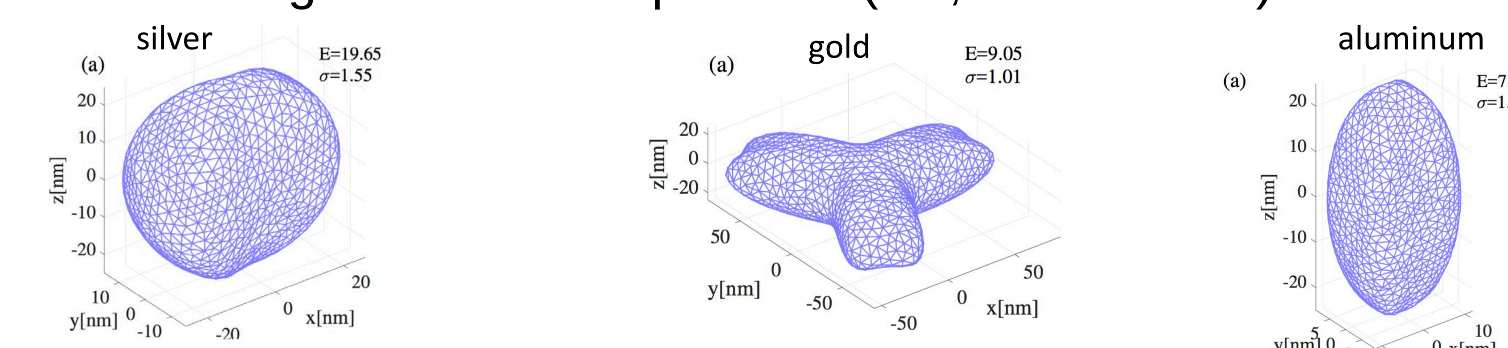
➢ Optimization algorithm (cyclic coordinate optimization)

**Algorithm 1.** cyclic coordinate optimization

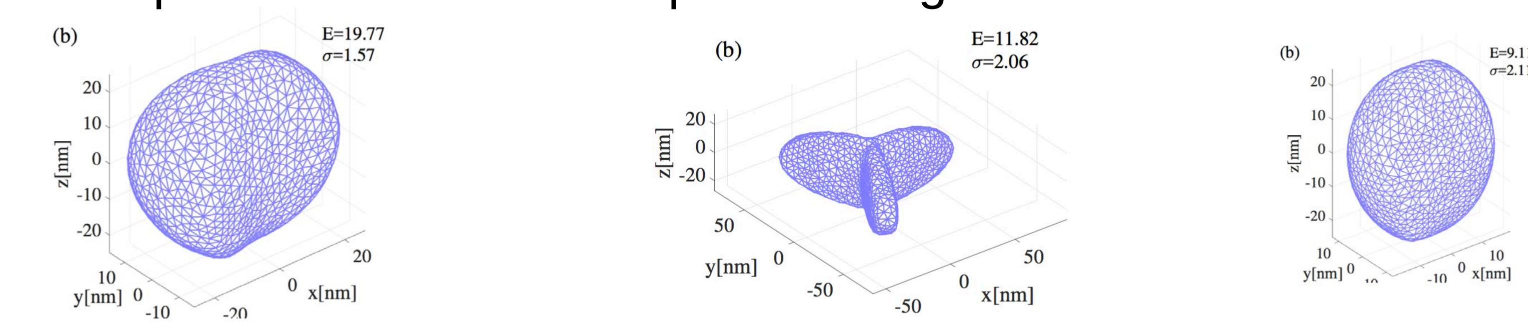
Set the number of particles $N$
Initialization of design variable $X^{(0)}$ s.t. $d \geq 75$
$i \leftarrow 1$
$j \leftarrow 1$
Compute objective function with initialized variables $f^j$
$\epsilon \leftarrow 10^3$
**while** $\epsilon \geq \varepsilon$ and $a \geq \varepsilon$ **do**
  **while** $i \leq 2N+1$ **do**
    $x_i^j \leftarrow \operatorname{argmin}_\alpha f\left(x_1^j, ..., x_{i-1}^j, \alpha, x_{i+1}^{j-1}, ..., x_{2N+1}^{j-1}\right)$
    $i \leftarrow i+1$
  Computing design parameters variation within a cycle: $V \leftarrow X^{new} - X^{old}$
  Pattern search: $a \leftarrow \operatorname{argmin}_a f\left(X^{new} + aV\right)$
  $\epsilon \leftarrow |f^j - f^{j-1}|$
  $j \leftarrow j+1$

## Significant Accomplishments

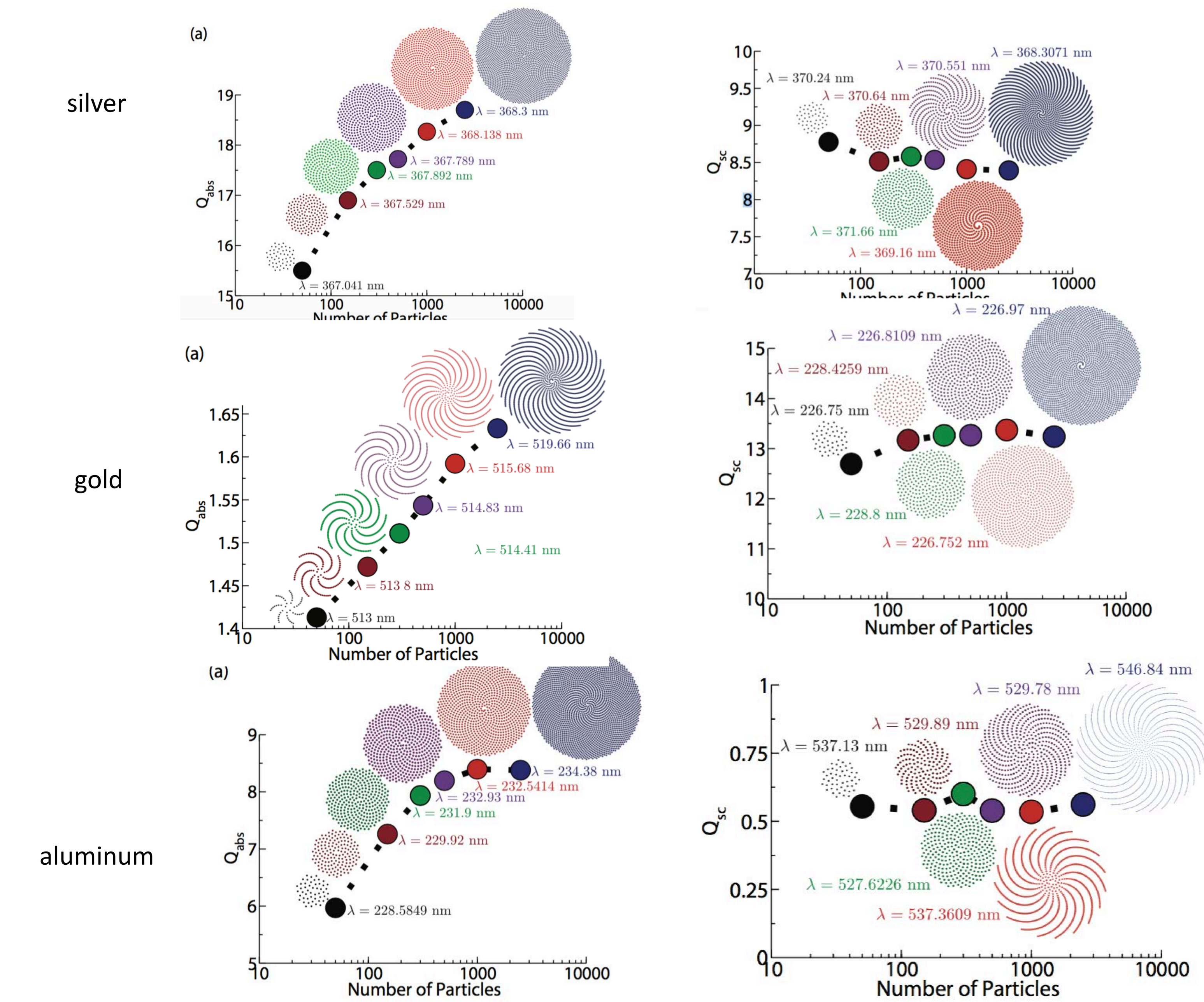
➢ Robust design of individual particles (i.e., more robust)




Compare to deterministic optimal designs



➢ Optimal designs of large-scale particles for absorption/scattering




## Future Directions

- Develop UQ techniques to quantify uncertainty in design process.
- Apply UQ techniques and optimization tools to material designs of interest to the Army.

## Publications

Y. He, M. Razi, C. Forestiere, L. Dal Negro and R.M. Kirby, "Uncertainty Quantification Guided Robust Design for Nanoparticles' Morphology", *Computer Methods in Applied Mechanics and Engineering*, Volume 336, pages 578-593, 2018.
Mani Razi, Ren Wang, Yanyan He, Robert M. Kirby and Luca Dal Negro, "Optimization of Large-Scale Vogel Spiral Arrays of Plasmonic Nanoparticles", *Plasmonics*, Volume 14, Issue 1, pages 253-261, 2019.
Mani Razi, Robert M. Kirby and Akil Narayan, "Fast Predictive Multi-fidelity Prediction with Models of Quantized Fidelity Levels", *Journal of Computational Physics*, Volume 376, pages 992-1008, 2019.

CMSME Center for Multi-Scale Multidisciplinary Modeling of Electronic Materials

UNCLASSIFIED