Direct Optical Surface Roughness Modelling

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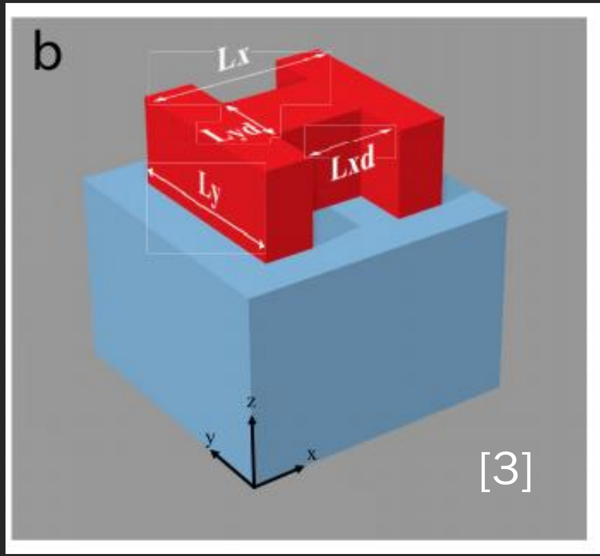
Motivation

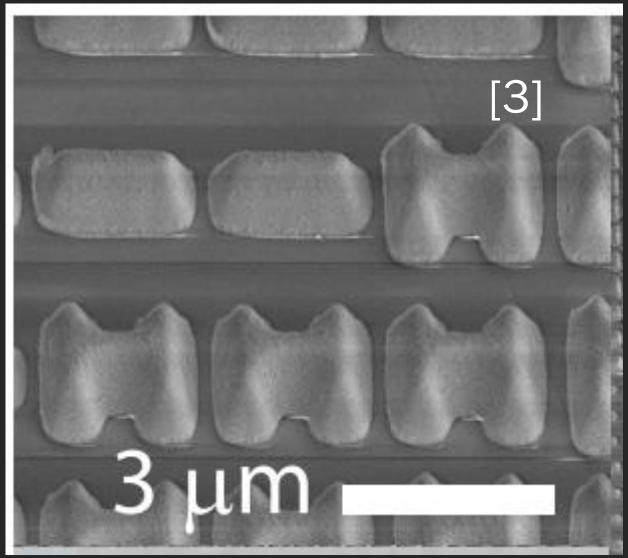
Roughness is implemented either:
- On Structured Meshes [1]
- Or Parameterized Structures
  - Bjorn Sjodin has an excellent blog post on this! [2]

Both approaches relatively limited in scope
- Structured meshes are not valid in many cases
- Parameterized surfaces are limited to very specific geometries
  - Sphere's, Cylinders (even that is tricky).

Autocorrelation based approach on unstructured mesh was recently developed [3]

1. KILDISHEV, ALEXANDER V., ET AL. "NUMERICAL MODELING OF PLASMONIC NANOANTENNAS WITH REALISTIC 3D ROUGHNESS AND DISTORTION." *SENSORS* 11.7 (2011): 7178-7187.
2. HTTPS://WWW.COMSOL.COM/BLOGS/HOW-TO-GENERATE-RANDOM-SURFACES-IN-COMSOL-MULTIPHYSICS/
3. SHALAGINOV, MIKHAIL Y., ET AL. "SINGLE-ELEMENT DIFFRACTION-LIMITED FISHEYE METALENS." *NANO LETTERS* (2020).
4. LOTH, FABIAN, ET AL. "SURFACE ROUGHNESS IN FINITE ELEMENT MESHES." *ARXIV PREPRINT ARXIV:2002.00894* (2020).





Arbitrary Surface Roughness Modelling

D is a vector consisting of normal displacements, d_i is normal displacement at ith vertex

$$\langle DD^T \rangle = R, R_{ij} = \exp\left(-\frac{|t_i - t_j|}{2l^2}\right)$$

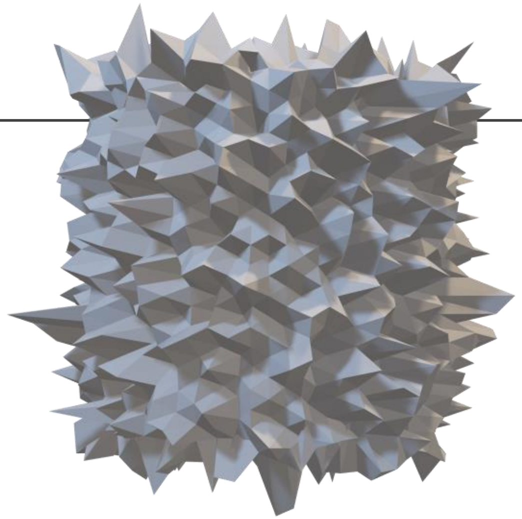
W is a vector consisting of random numbers.
Each w_i has a gaussian distribution and it satisfies:

$$\langle WW^T \rangle = I, \mathrm{I}_{ij} = \delta_{ij}$$

Notice, D may be constructed from white noise

$$D = LW$$

$$R = \langle DD^T \rangle = \langle (LW)(LW)^T \rangle = \langle LWW^T L^T \rangle = L\langle WW^T \rangle L^T = LL^T$$



Practical Implementation

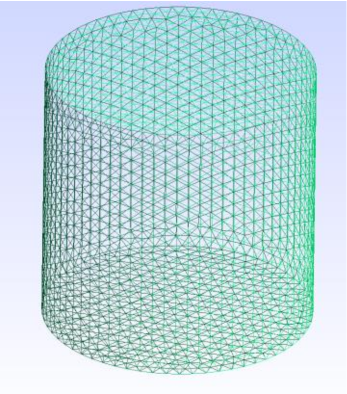
1. Generate a mesh of the nominal surface in GMSH (Python)

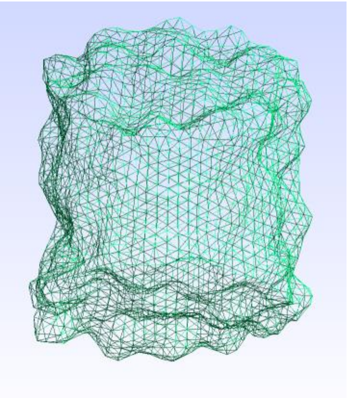
2. Generate the correlated roughness mesh
   - Using excellent package by Fabian Loth et al.
   - Using method outlined previously
   - Generate a whole family of related meshes

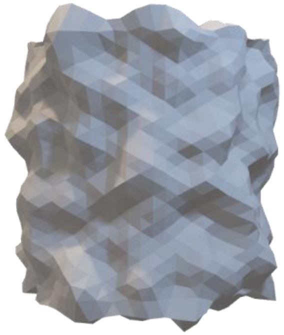
3. Reimport mesh to GMSH and export to STL

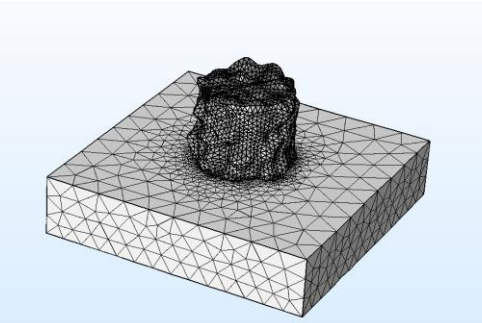
4. Using Matlab-Comsol Livelink
   - Automatic Import
   - Geometry Creation
   - Meshing
   - Multi-node 60 core supercomputer simulations
   - CSV File output for dataprocessing

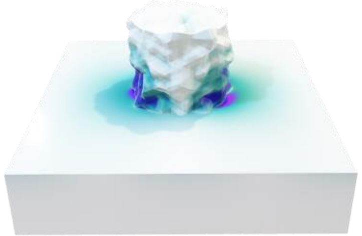
Postprocessing & Analysis

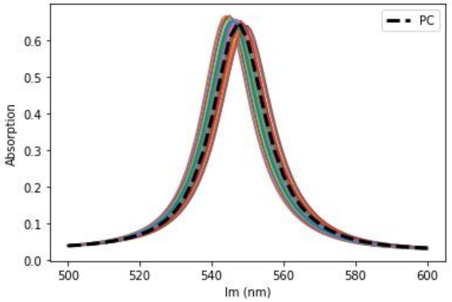












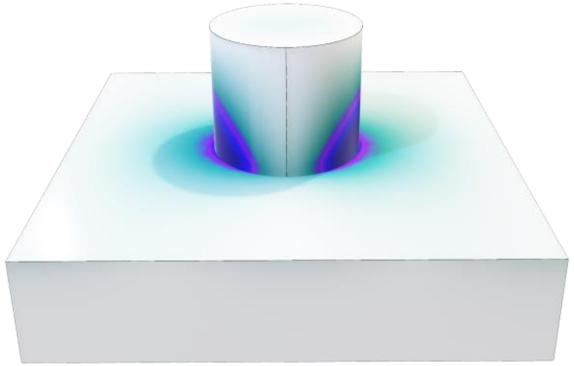
Ideal Nano-antenna Model

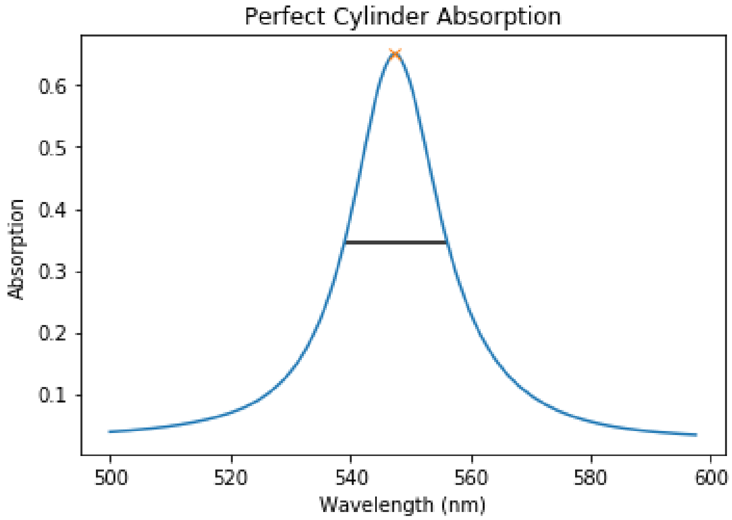
Perfect Cylinder

- Height=130nm
- Width=150nm
- Uses built in material models
  - Cylinder is SiN (Luke et al. 2015)
  - Substrate is Ag (J&C 1972)
- Antenna based on work by F Callewaert et al, 2016.[1]

Absorption Peak Properties

- Resonance Wavelength: 547.4nm
- FWHM: 17.2nm
- Peak Absorption: 65%
- Quality Factor: 31.82

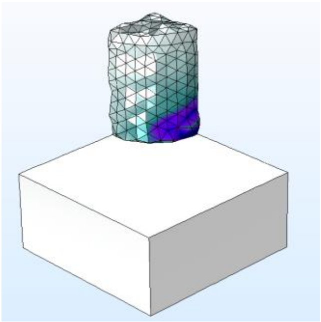


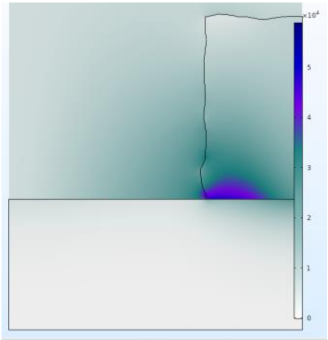


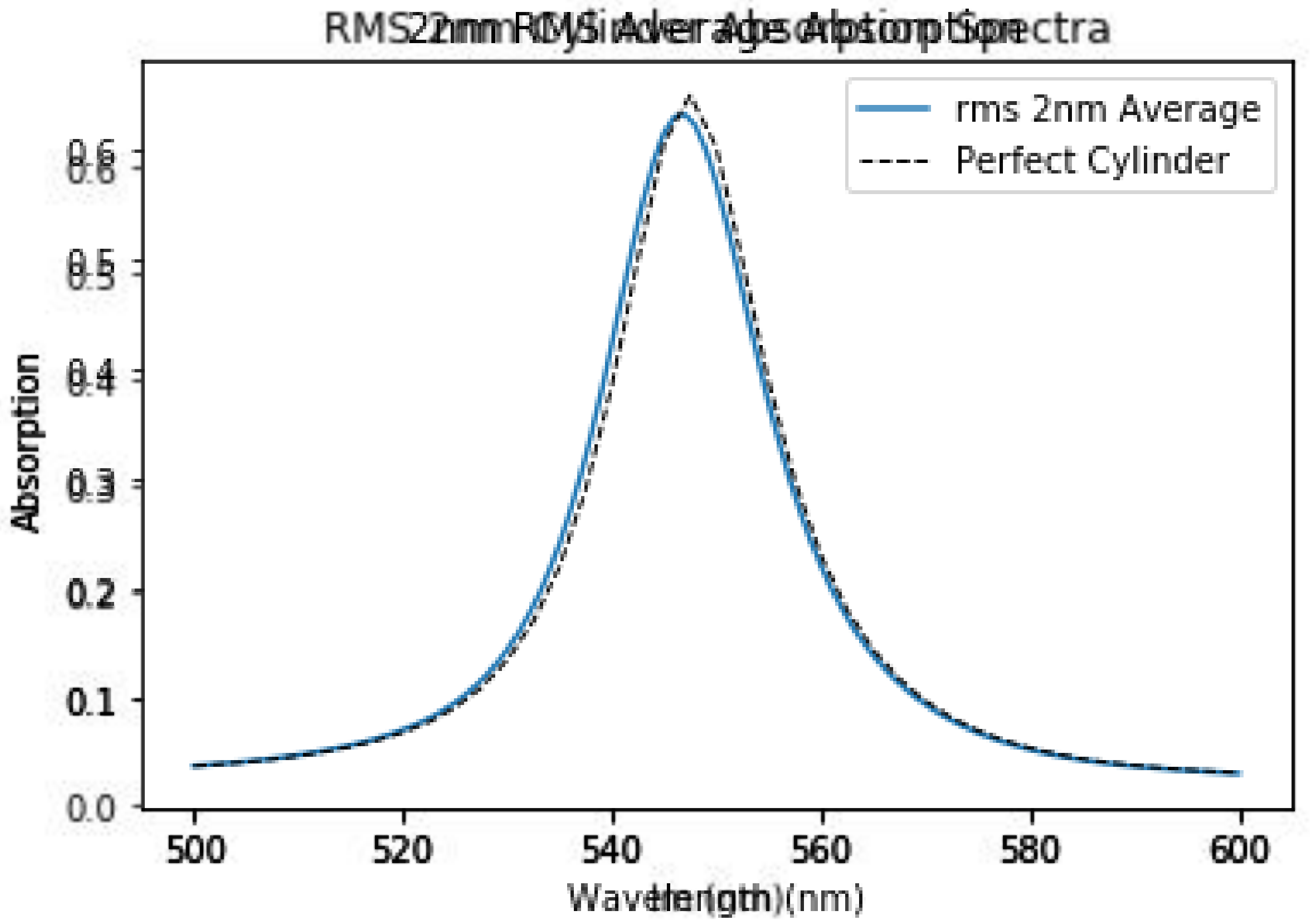
[1] F CALLEWAERT ET AL 2016 J. OPT. 18 075006

Statistics on 2nm Roughness Models

Simulation was run many times
- 26 Antenna Dataset
- Spectra were averaged together:
  - Resonance Wavelength: 546.7nm
  - FWHM: 18.0nm
  - Peak Absorption: 63.37%
  - Quality Factor: 30.37



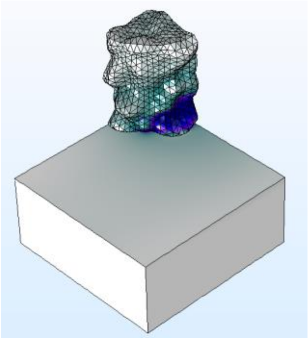


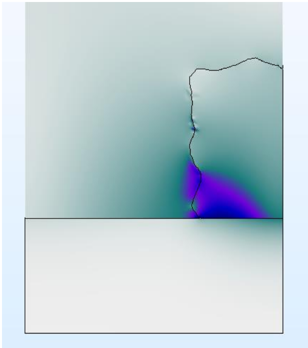


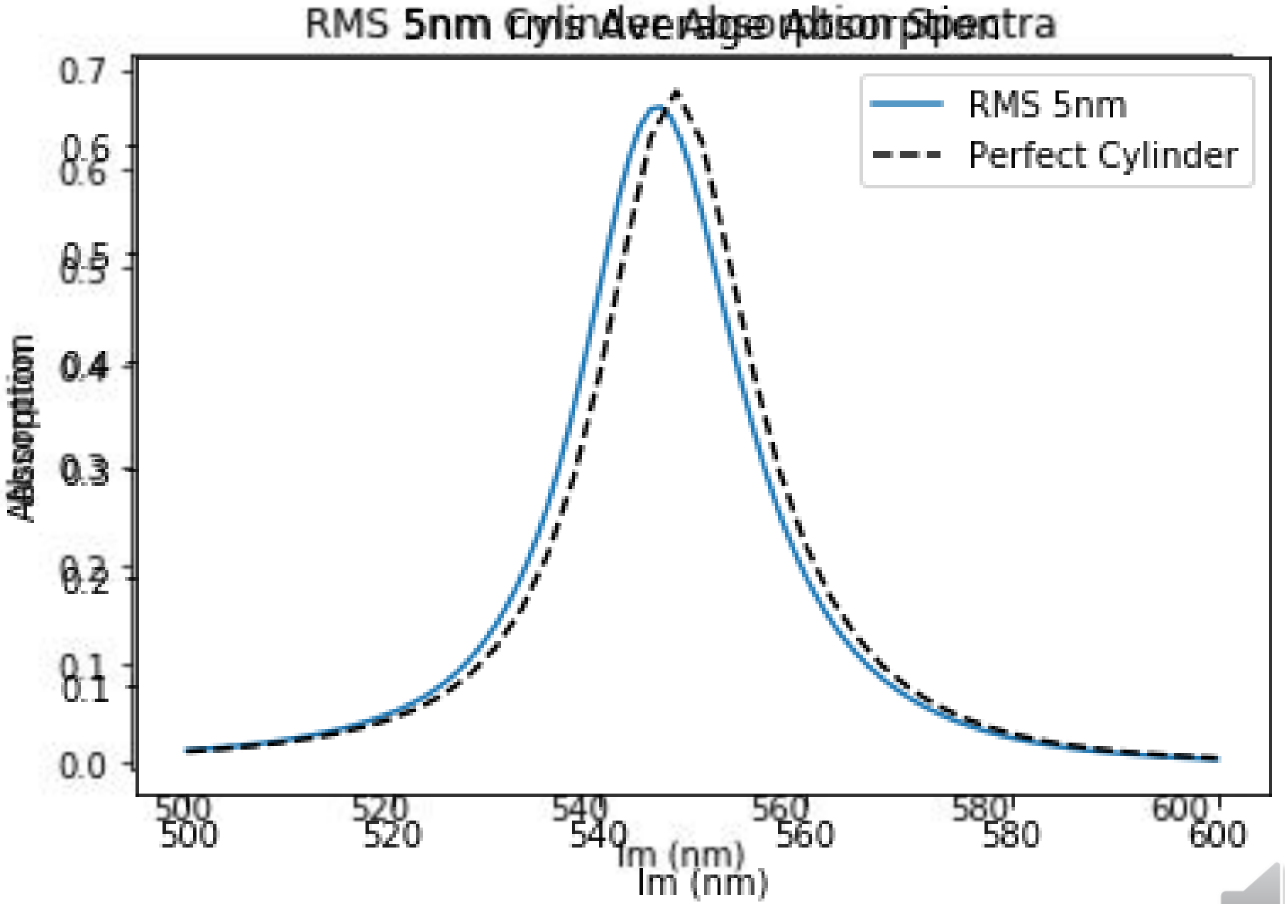
Statistics on 5nm Roughness Models

Simulation was run many times

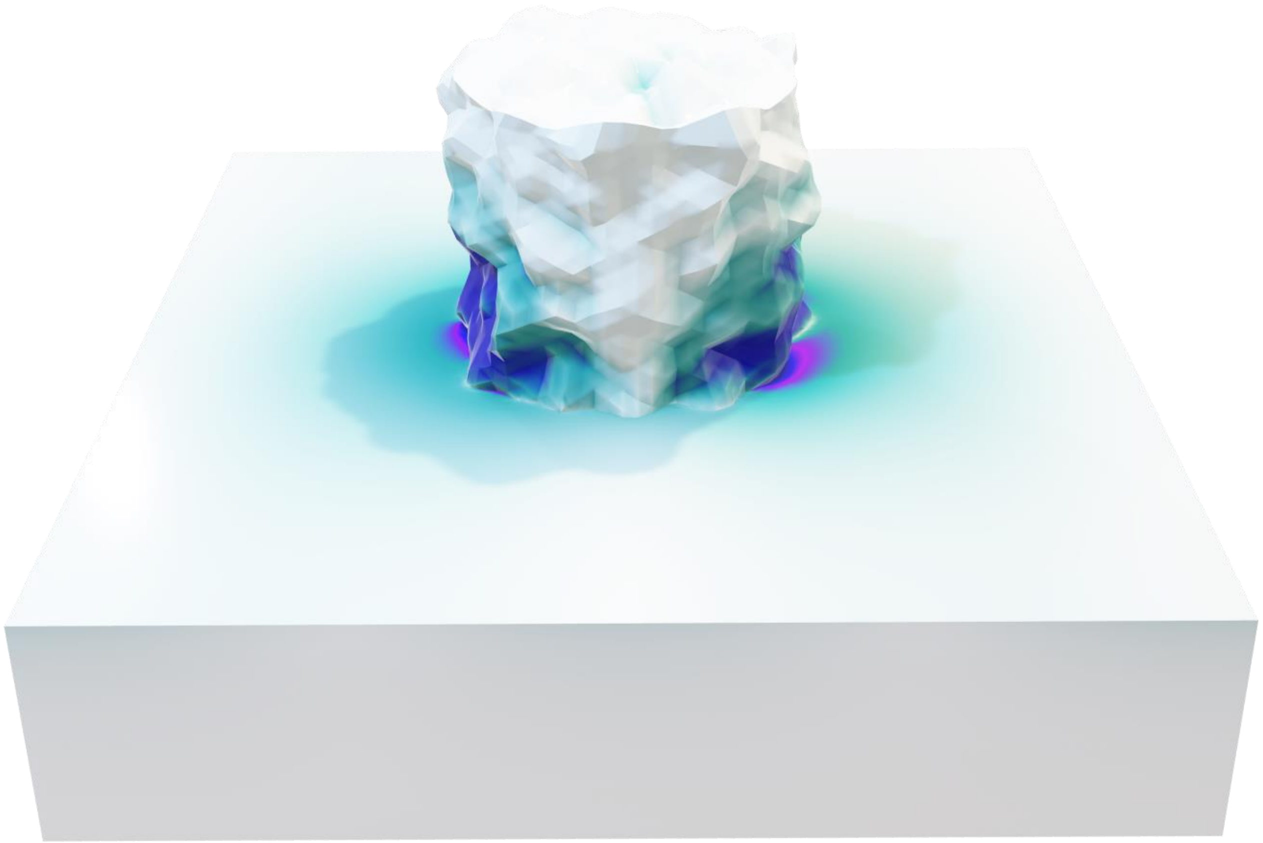
- 31 Antenna Dataset
- All Spectra were averaged together:
  - Resonance Wavelength: 545.7nm
  - FWHM: 19.30nm
  - Peak Absorption: 61.35%
  - Quality Factor: 28.47





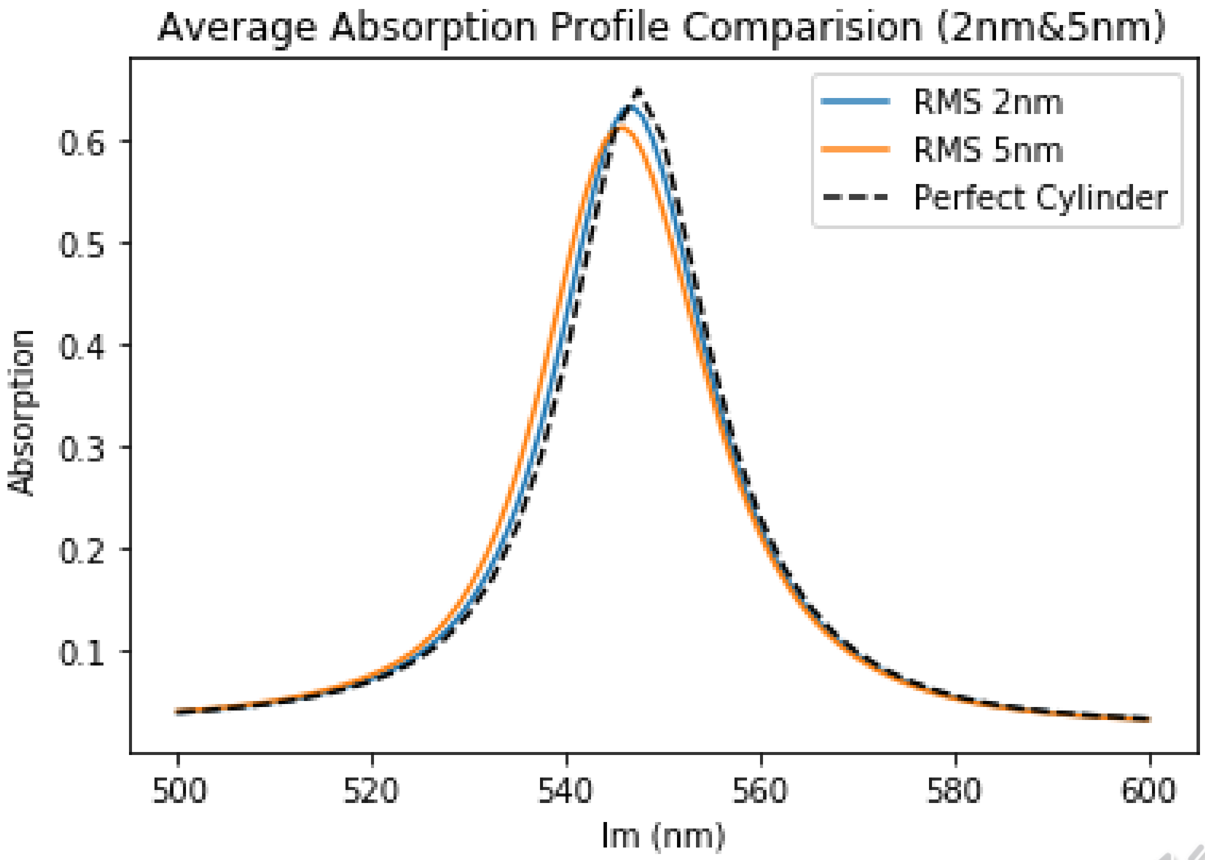


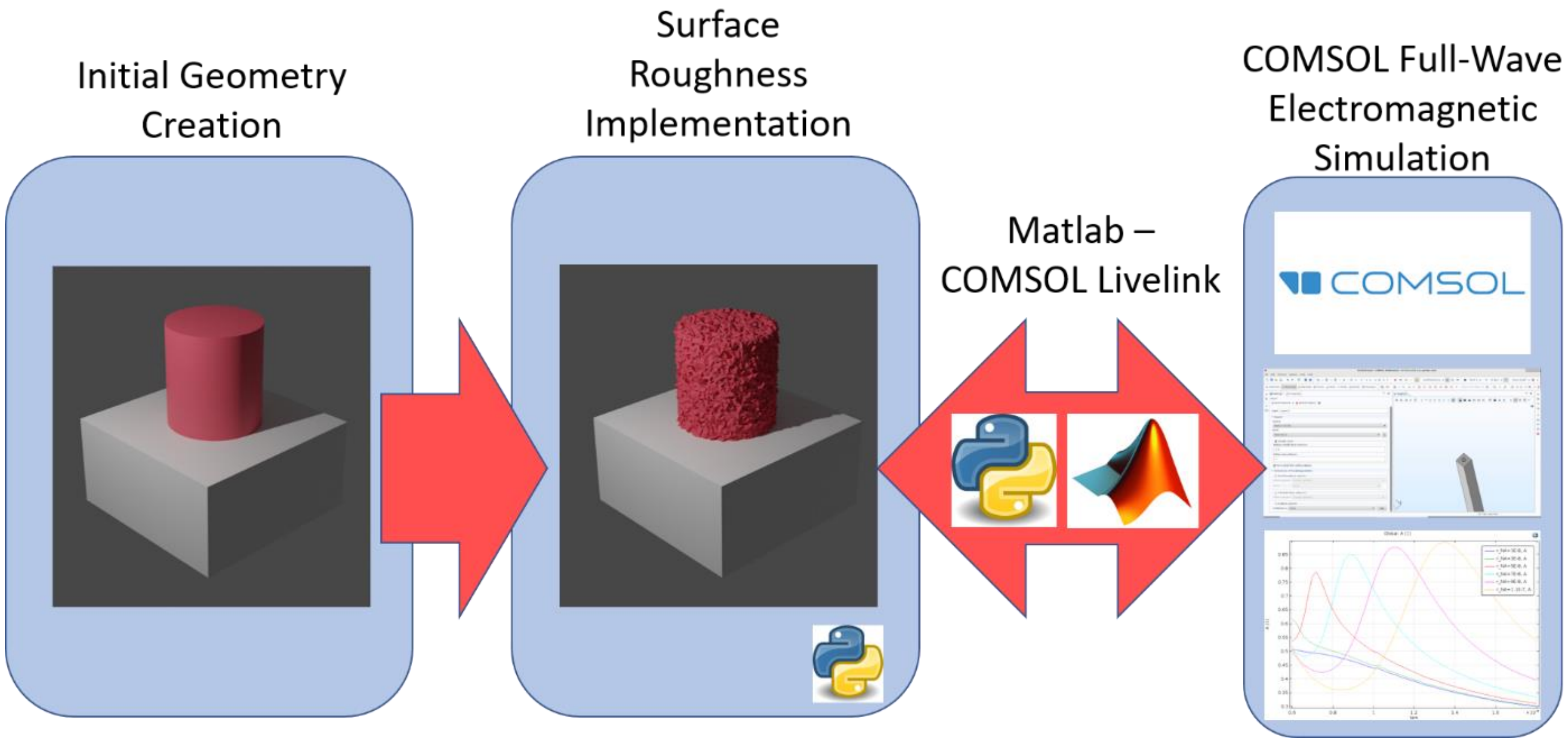
5nm Full Domain Model Simulation



Absorption Spectra Comparison

RMS Roughness	Average Individual Q Factor	“Array” Q	“Array” Resonant Wavelength (nm)	“Array” FWHM
0 nm	31.82	31.82	547.4nm	17.2nm
2 nm	32.11	31.86	546.7nm	18.0nm
5nm	32.33	28.47	545.7nm	19.30nm




Initial Geometry Creation
Surface Roughness Implementation
Matlab – COMSOL Livelink
COMSOL Full-Wave Electromagnetic Simulation
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Summary