

Simulations for Optical, Photonic, and Plasmonic Applications using Dassault Systemes SIMULIA CST Studio Suite®

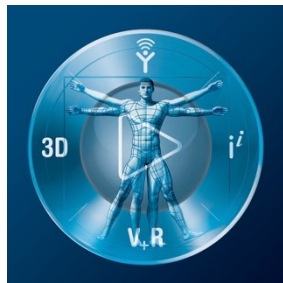


3DEXPERIENCE®

Agenda

- ▶ Introduction
 - ▷ About Dassault Systemes
 - ▷ Technology offering for optical and photonics simulations
 - ▶ Solver options and selection
 - ▶ Materials
 - ▶ Boundaries
 - ▶ Meshing
 - ▶ Results postprocessing
- ▶ Examples
 - ▷ BxDF Calculation
 - ▷ Photonic Crystal Microcavity
 - ▷ Metal-Insulator-Metal Plasmon Coupling Diffraction Gratings
 - ▷ Silicon Waveguide Based TE Mode Converter
 - ▷ Convex Microlens Simulation
- ▶ Conclusion

Dassault Systèmes | The 3DEXPERIENCE Company



a Scientific company

Combining **Science**, **Technology** and **Art** for a sustainable society



17,000 passionate people

- 130 nationalities
- 181 sites
- One global R&D / 64 labs



250,000 customers

- 11 industries in 140 countries
- 25 million users
- Game-changing 3DEXPERIENCE solutions



12,600 partners

- Software, Technology & Architecture
- Content & Online Services
- Sales
- Consulting & System Integrators (C&SI)
- Education
- Research



Long-term driven

- Majority shareholder control
- **Revenue:** €3,488 million*
- Operating margin: 31,8%*



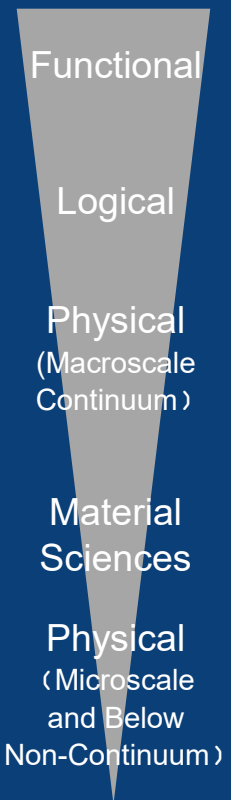
Our Technology
Vision

Multiphysics & Science

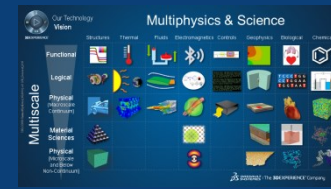
Structures Thermal Fluids Electromagnetics Photonics Controls Geophysics Biological Chemical ...

Functional								
Logical								
Physical (Macroscale Continuum)								
Material Sciences								
Physical (Microscale and Below Non-Continuum)								

Multiscale



Building blocks of Multiphysics & Multiscale vision



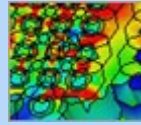
Structures

Abaqus



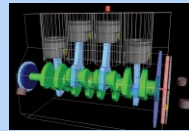
**Electromagnetics
Photonics**

CST Studio Suite
Opera



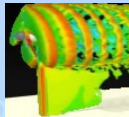
Multibody

Simpack



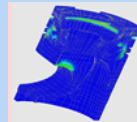
Fluids

PowerFLOW
XFlow
3DEXPERIENCE Flow



Durability

fe-safe



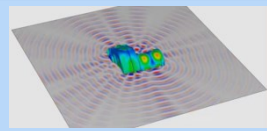
Automation

Isight



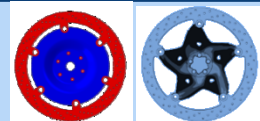
Vibro-acoustics

Wave6



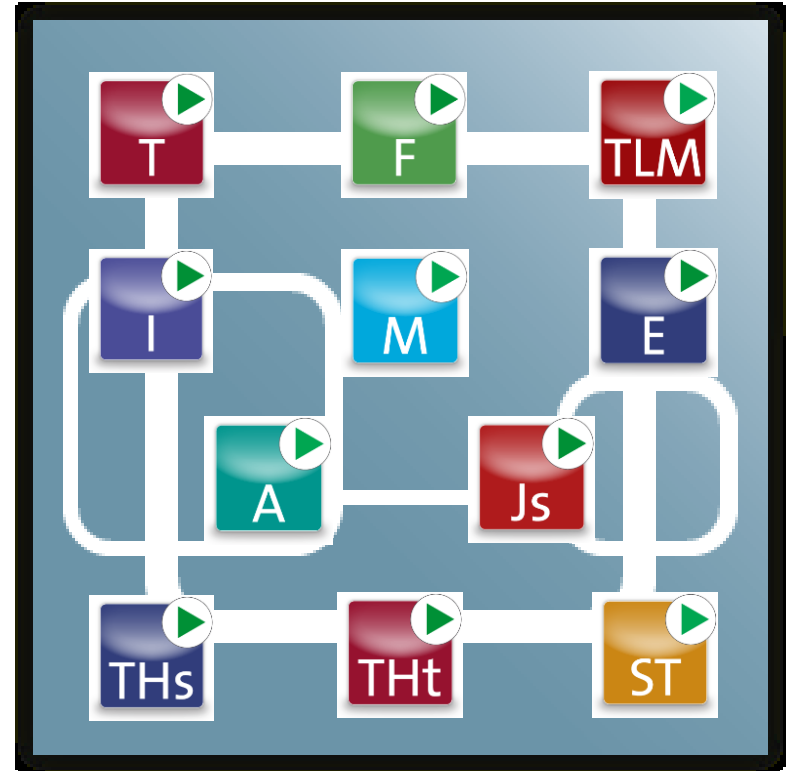
Optimization

Tosca
Isight

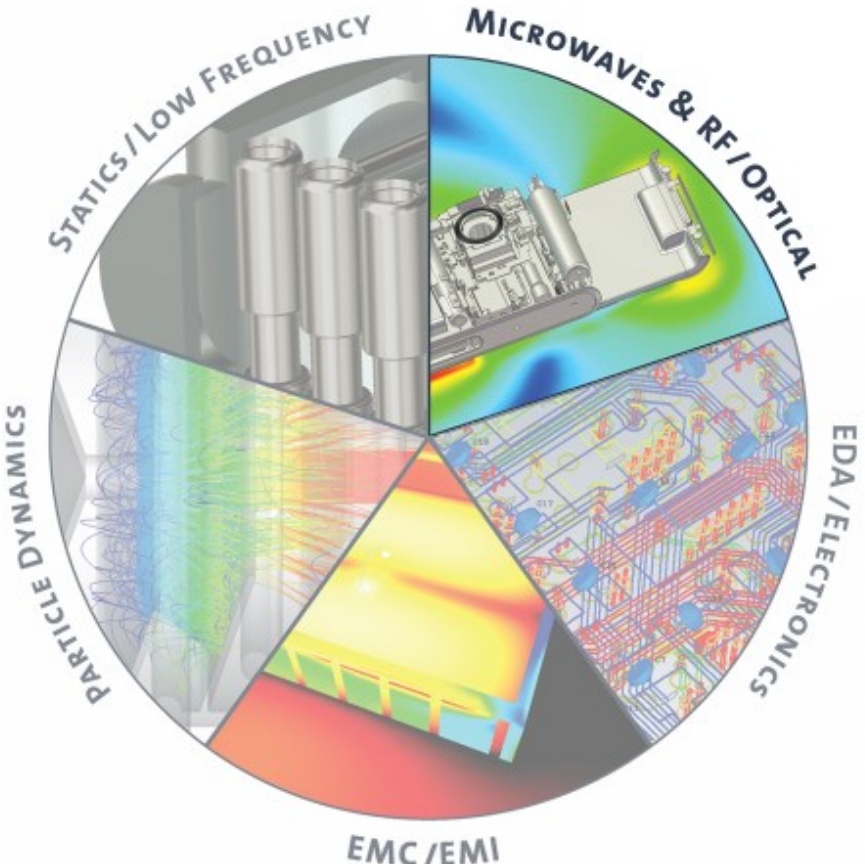


Technology Offering SIMULIA CST Studio Suite

- ▶ The best simulation method depends upon the application
- ▶ Dassault Systemes SIMULIA CST Studio Suite® offers a range of methods in a single package
- ▶ User is guided to the most appropriate method(s)



Optical Applications in CST Studio Suite



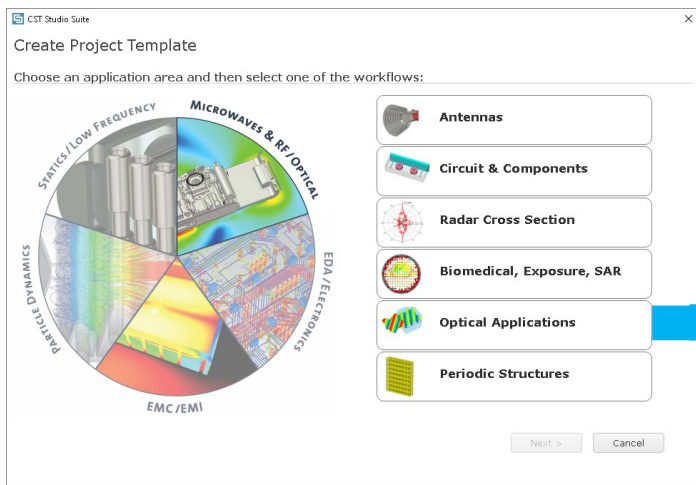
Optical Applications in CST Studio Suite

Optical Waveguides,
Couplers and Fibers

Solar Cells

Photonic Bandgap
Structures

Filters and Resonators



Dielectric/Photonic Structures

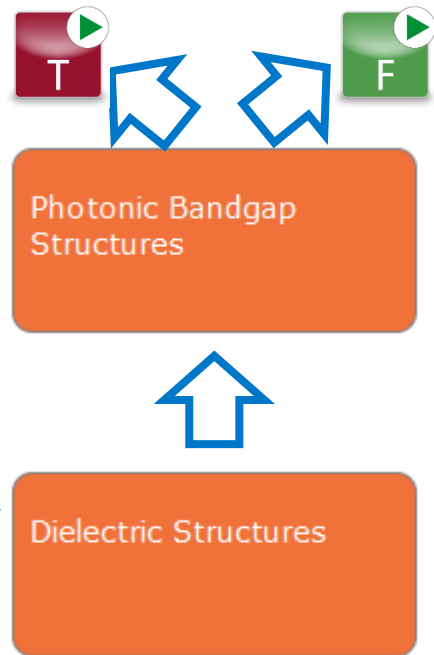
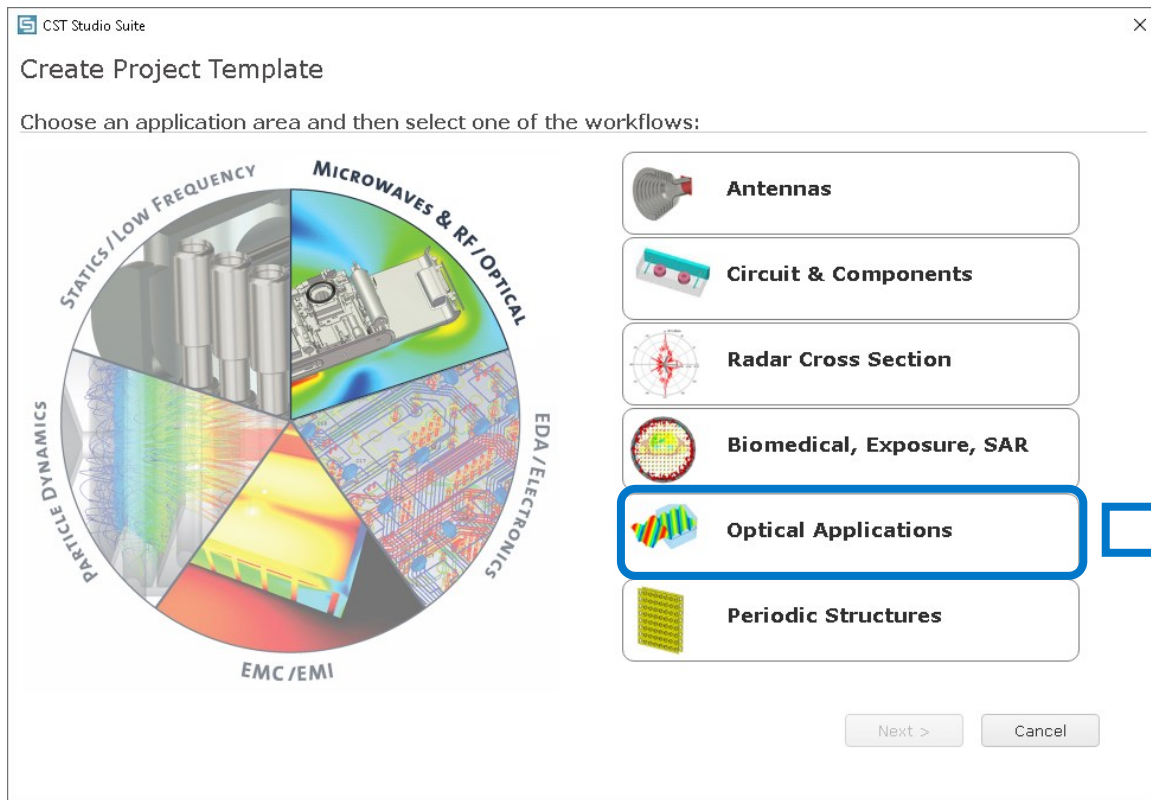
Metallic/Plasmonic Structures

Nano Antennas

Plasmonic Waveguides

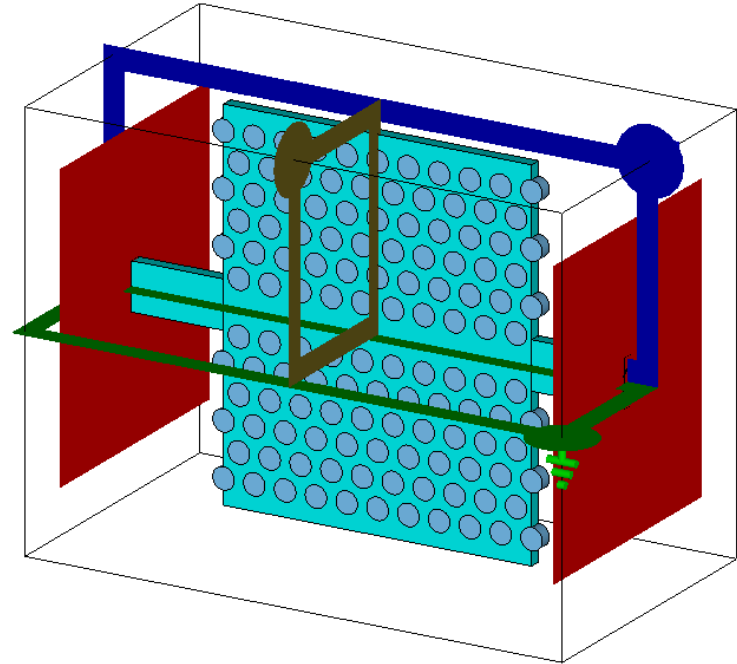
Plasmonic Solar Cells

Configuration Wizard



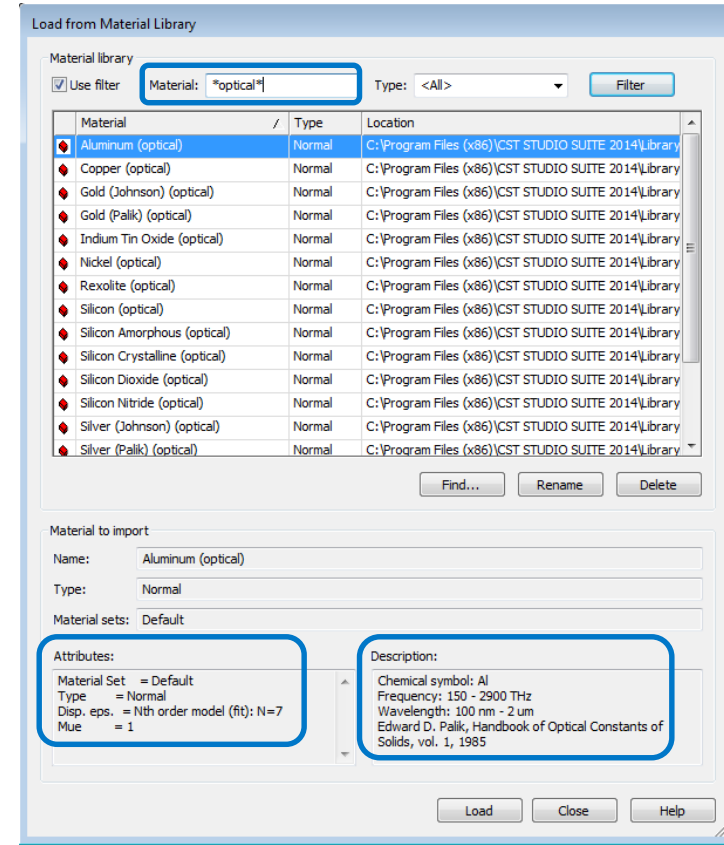
Creating the Geometry

- ▶ Built-in CAD/scripting environment
- ▶ Import CAD or EDA data:
 - ▷ CATIA
 - ▷ GDSII
 - ▷ DXF
 - ▷ STEP
 - ▷ ... and many more
- ▶ Direct links:
 - ▷ 3DEXPERIENCE Power'By
 - ▷ SOLIDWORKS
 - ▷ Luceda IPKISS
 - ▷ CREO



Material Assignment

- ▶ CST Studio Suite comes with a number of predefined materials for photonic and plasmonic applications
- ▶ Typically, these are higher order dispersive materials based on standard text books



Material Data: Causal Fit

- ▶ Dispersive data need to satisfy Kramers-Kronig to ensure causality
- ▶ CST Studio Suite offers a number of causal dispersion models (Drude, Lorentz, etc.)
- ▶ Generalized nth order model to automatically fit tabulated data:

$$\varepsilon(\omega) = \varepsilon_{\infty} + \sum_{n=1}^N \frac{\beta_{0,n}}{\alpha_{0,n} + j\omega} + \sum_{n=1}^M \frac{\gamma_{0,n} + j\omega\gamma_{1,n}}{\delta_{0,n} + j\omega\delta_{1,n} - \omega^2}$$

Material Data Resource: www.refractiveindex.info

The image shows a software interface with a macro menu on the left and a web browser on the right. The macro menu includes options like 'Create Cole-Cole Model Material', 'Create Drude Material for Optical Applications', and 'Import CSV Data from refractiveindex.info'. The web browser displays the 'Optical constants of Si (Silicon)' page from refractiveindex.info, showing a refractive index of $n = 3.4407$ at a wavelength of 2.4373 μm . A graph plots the refractive index against wavelength from 2.5 to 10 μm . A blue box highlights the text '[CSV - comma separated]' in the browser window.

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Mesh View Global Properties Mesh Properties History List Parametric Update Calculator Parameters Parametric Update Edit

Macros

Run Macro

- Calculate
- Construct
- File
- Matching
- Materials
- Parameter
- Report and
- Results
- Solver
- Wizard

Edit Macro

- Open VBA
- Make VBA
- Import VBA
- Edit / Mov

Optical constants of Si (Silicon)
Salzberg and Villa 1957 - n 1.36-11 μm ; 26 °C

Wavelength: 2.4373 μm (1.357 – 11.04) [line select](#) [unit converter](#)

Refractive index [i]

$n = 3.4407$

Other optical constants

Chromatic dispersion [i]
 $dn/d\lambda = -0.020208 \mu\text{m}^{-1}$

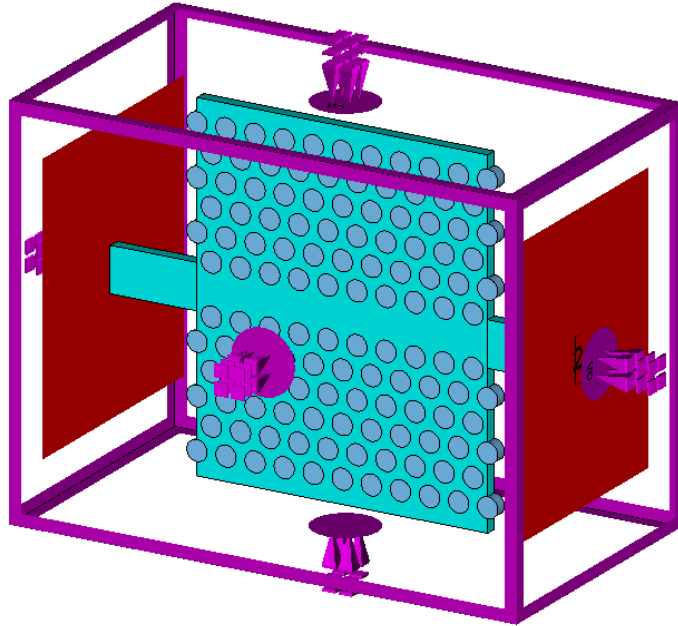
Group velocity dispersion [i] [i] [i]
 $GVD = 649.31 \text{ fs}^2/\text{mm}$
 $D = -205.89 \text{ ps}/(\text{nm km})$

RefractiveIndex.INFO
Si (Silicon)
Salzberg and Villa 1957 - n 1.36-11 μm ; 26 °C

Wavelength, μm

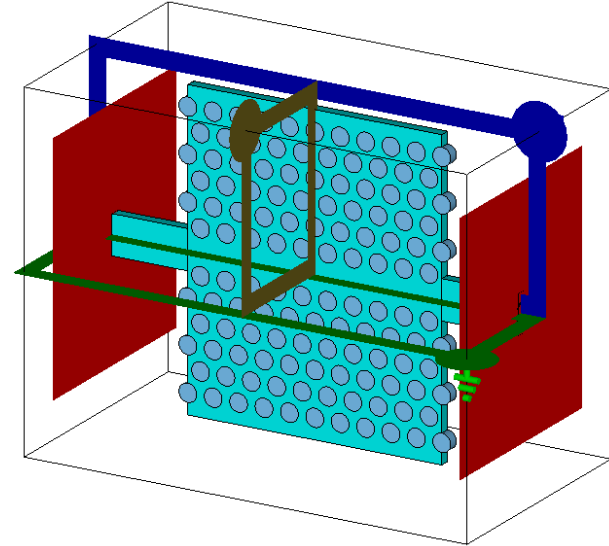
[CSV - comma separated]

PML Boundaries and Symmetry Planes



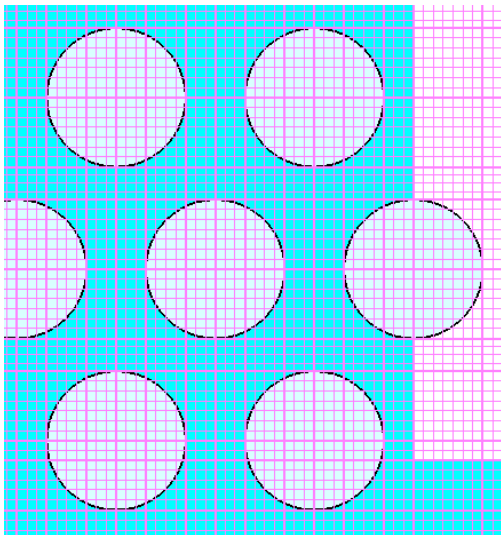
State-of-the-art PML technology
with extremely low reflection

Reduce simulated model down to 1/2, 1/4, or 1/8.
Results will be automatically mapped to full
model for visualization and post processing.

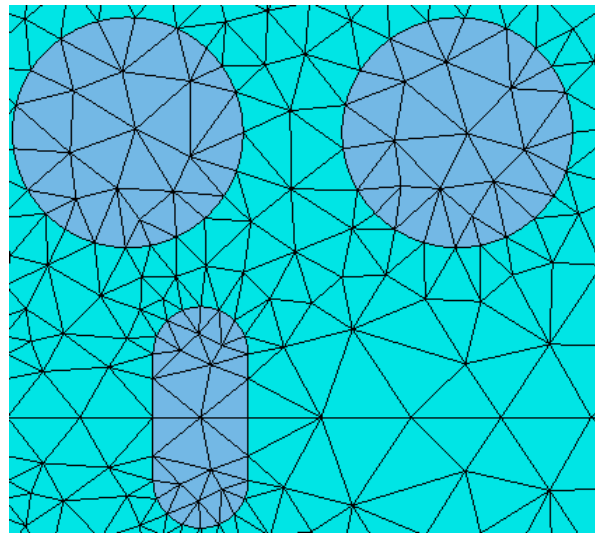


Meshing

► Automatic hexahedral and tetrahedral mesh generation




4th generation conformal mesh PBA
(1st generation in 1998)

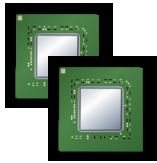


Higher order curved
tetrahedral mesh

Time or Frequency Domain?

- ▶ T and F represent the most commonly used solvers
- ▶ Both will provide highly accurate full-wave results for any structure
- ▶ Depending upon the application, one might be faster than the other:
 - ▷ TD provides broadband results in a single solver run
 - ▷ FD favorable for high Q values
- ▶ Memory requirements scale differently
 - ▷ Linear memory scaling of TD (based on FIT/FDTD/TLM) makes it suitable for models that are large compared to the wavelength
- ▶  asymptotic solver for extremely large models (e.g., free space and lenses)

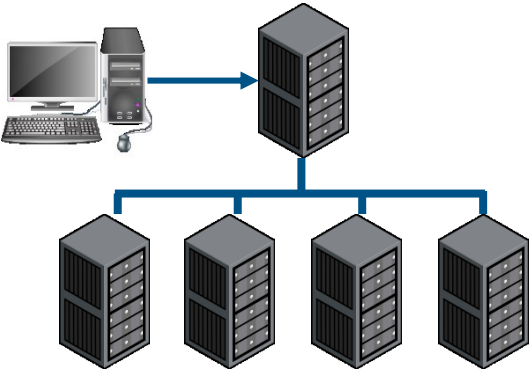
SIMULIA CST Studio Suite® Acceleration Techniques



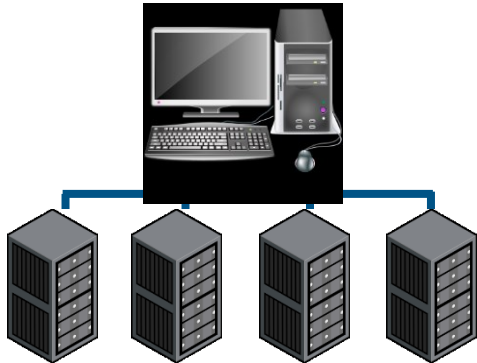
CPU Multithreading



GPU Computing



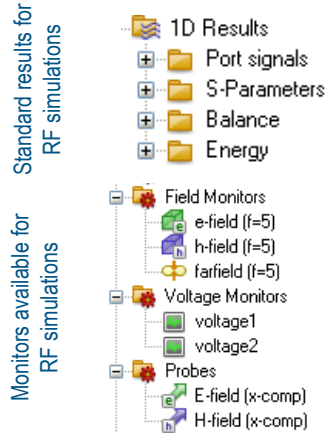
Distributed Computing



MPI Computing

Result Handling

There are different types of results in CST Studio Suite:



1. Standard results: Computed automatically for every simulation.

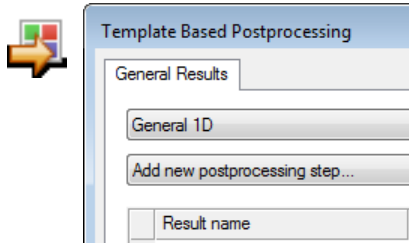
Typically not resource intensive (e.g. S-parameters)

2. Result monitors: User can preserve other results using monitors.

Typically resource intensive results
(e.g. field distribution in 3D space)

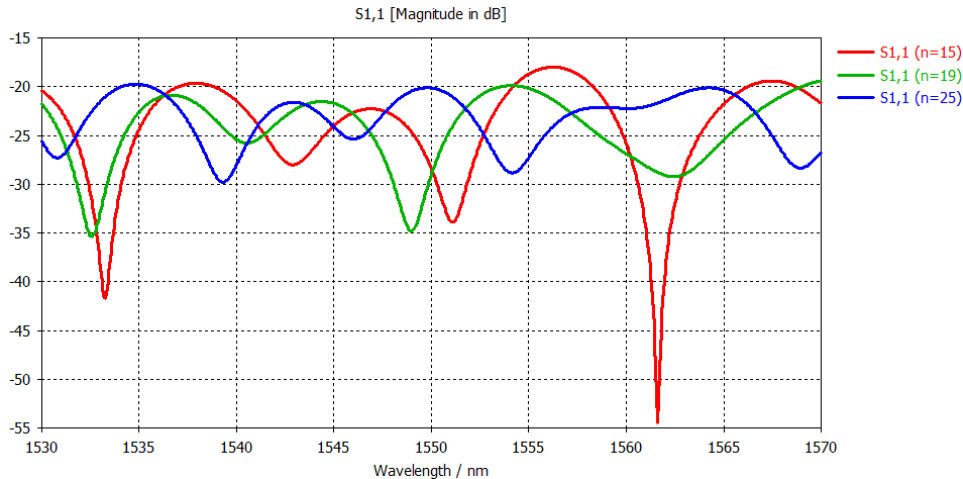
3. Result templates: Highly configurable mechanism to extract special values from either standard results or result monitors.

The power and flexibility of the VBA programming language is available.



Result Navigator

- ▶ A unique “Run ID” identifies each solver run.
 - ▷ The corresponding parameter sets are shown.
- ▶ The Result Navigator allows to show only some of the curves.
- ▶ Filter options are available, too



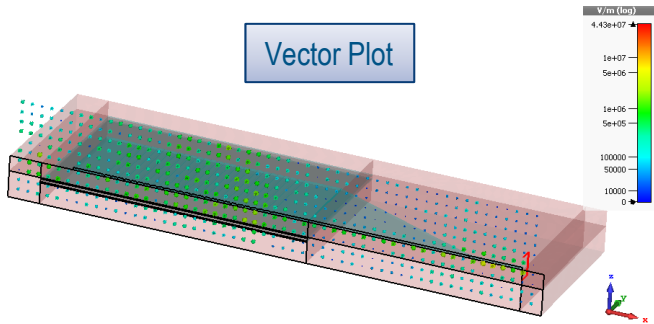
Result Navigator 7 Results ×

3D Run ID	n
< enter filter >	>11
6	25
5	23
4	21
3	19
2	17
1	15
0: Current Run	

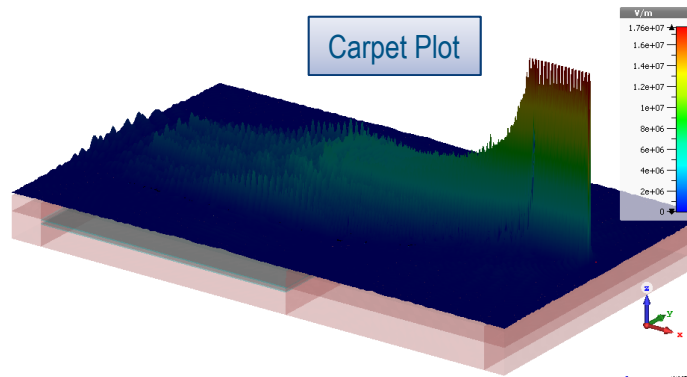
3D Plot Options

Some examples for field plot types:

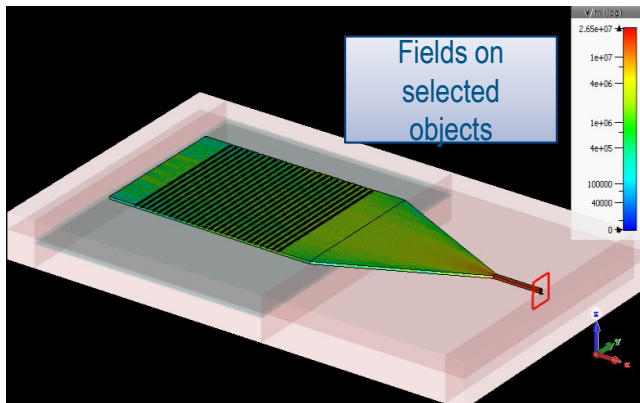
Vector Plot



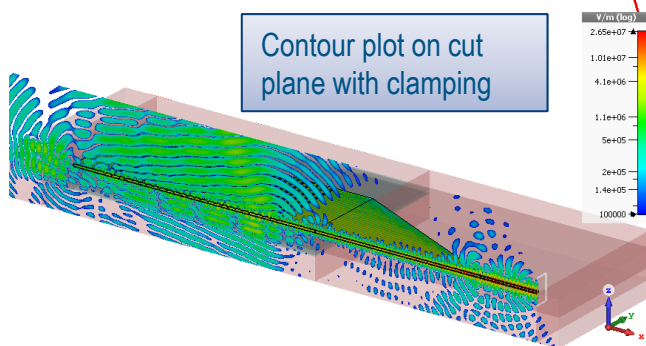
Carpet Plot



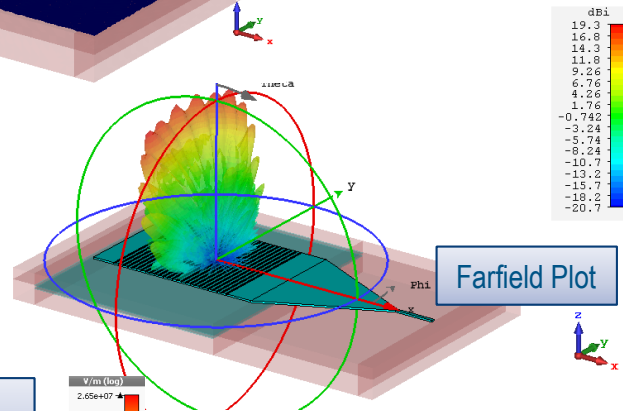
Fields on selected objects



Contour plot on cut plane with clamping



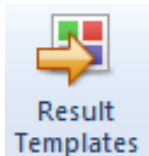
Farfield Plot



Post Processing Templates

Post processing templates provide a convenient way to derive values from the standard results and 3D field results:

1D Result -> Output is a 1D curve
1DC Result -> Output is a complex 1D curve
0D Result -> Output is a single value



Template Based Post-Processing

General Results

General 1D

Add new post-processing step...

Result name	Type	Template name	Value	Active On/Off
1 Power pattern,Phi=0.0	1D	Farfield Result		On (Parametric)
2 Power pattern,Phi=0.0_1D_xSub	1D-P	0D or 1D Result from 1D Re		On (Parametric)
3 Beam Power (Theoretical)	0D-P	Mix Template Results	9.3814901	On (Parametric)
4 Irradiance Gauss Beam	0D-P	Mix Template Results	9.3457907	On (Parametric)
5 Total radiated power	0D	Farfield Result	3.7034191	On (Parametric)
6 BRDF_	1D-P	Mix Template Results		On (Parametric)
7 BRDF	1DC-P	Mix Template Results		On (Parametric)
8 BRDF times Jacobian_0D_Integ	0D-P	0D or 1D Result from 1D Re	0.0892772	On (Parametric)

Names and descriptions of defined result templates

Evaluate Evaluate All Delete All Evaluate All

Abort Close Help



Template results are stored under "Tables" in the navigation tree.

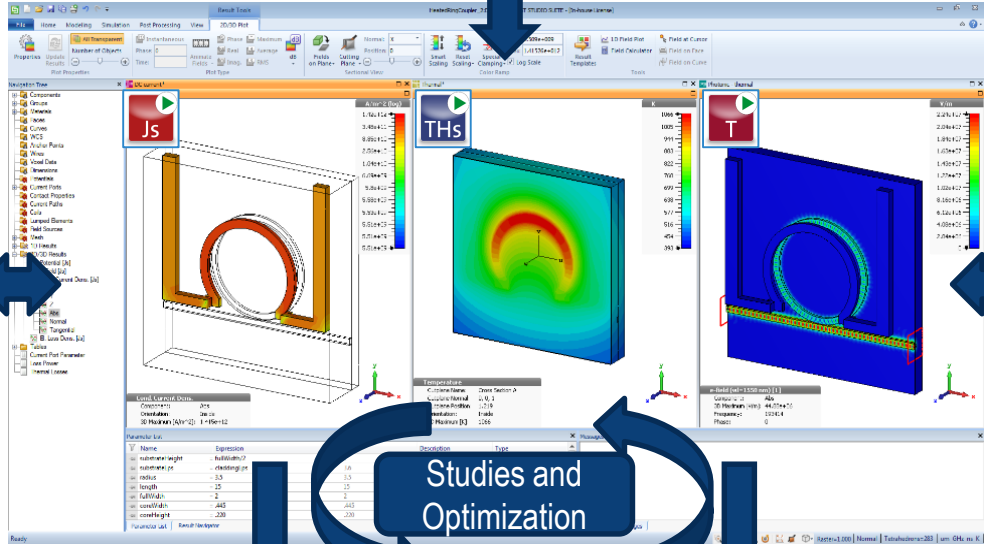
Tables

- 0D Results
 - Beam Power (Theoretical)
 - Irradiance Gauss Beam
 - Total radiated power
 - BRDF times Jacobian_0D_Integ
- 1D Results
 - Power pattern,Phi=0.0
 - Power pattern,Phi=0.0_1D_xSub
 - BRDF_
 - BRDF

CST Studio Suite for Accurate Component-Level Simulation

Model Creation
(Import from EDA or CAD tools, scripting, built-in CAD)

link



Multiphysics Solvers

Photonic/EM Solvers

Studies and Optimization

Result Postprocessing

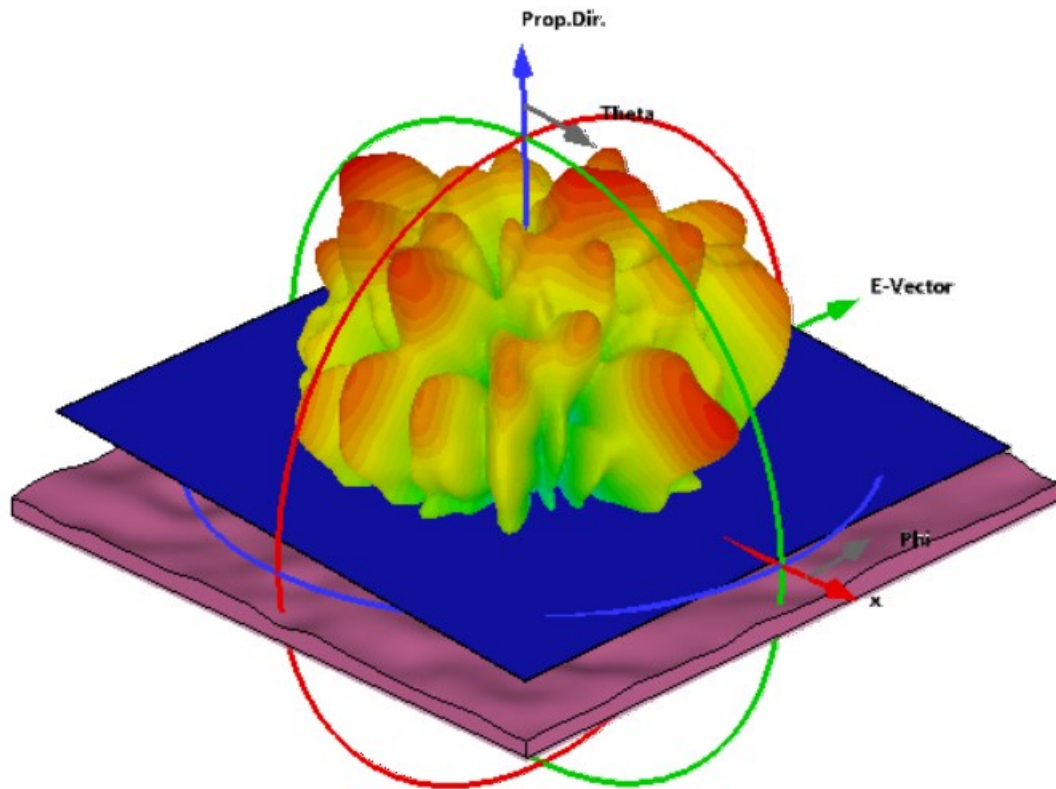
Data/Geometry Export

link

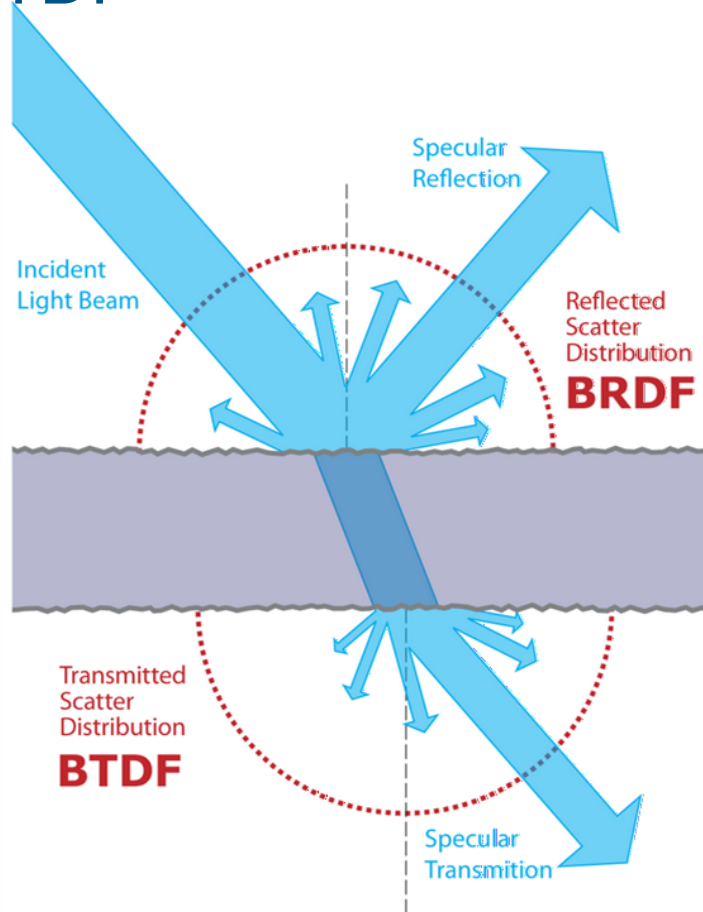


Examples

Example: BxDF Calculation



$$\text{BSDF} = \text{BRDF} + \text{BTDF}$$



Bidirectional Reflectance Distribution Function

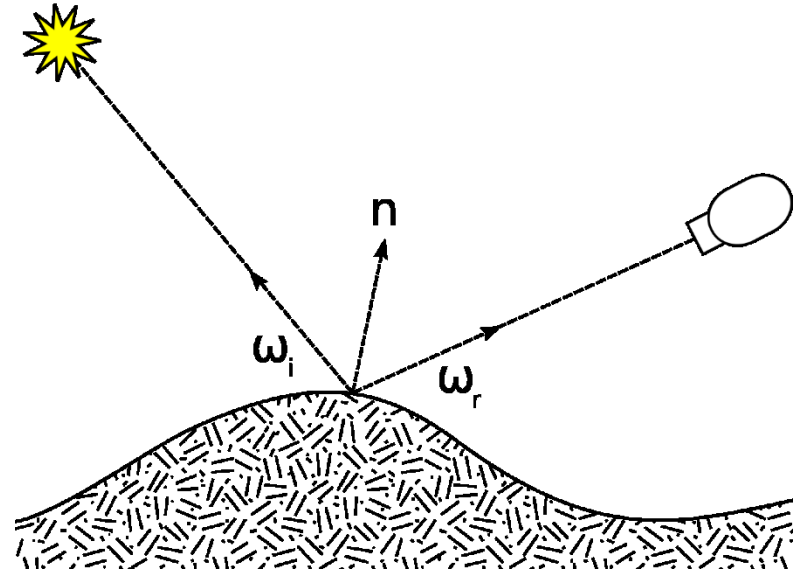
$$f_r(\omega_i, \omega_r) = \frac{dL_r(\omega_r)}{dE_i(\omega_i)} = \frac{dL_r(\omega_r)}{L_i(\omega_i) \cos \theta_i d\omega_i}$$

L = Radiance

E = Irradiance

θ = Angle between incident light and surface normal

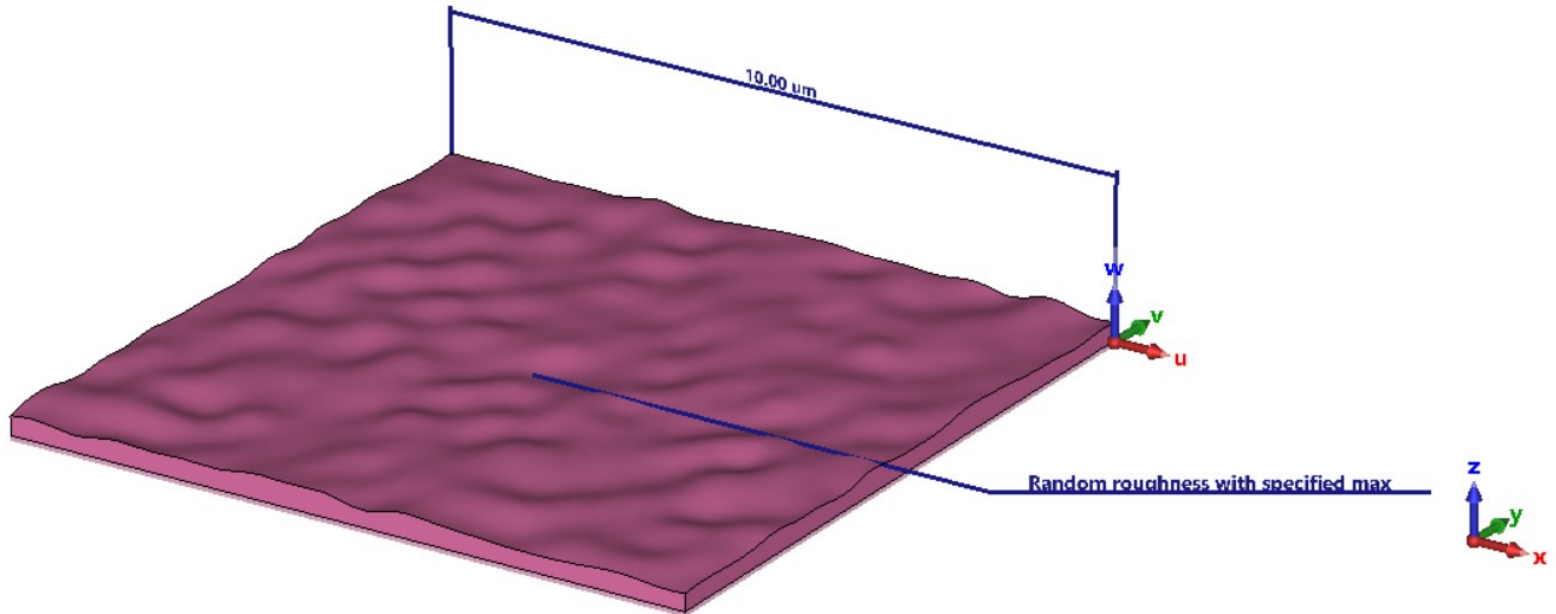
ω = Solid angle for incident/reflected light



By BRDF_Diagram.png: Meekohiderivative work: tiZom(2ϕ) - BRDF_Diagram.png, CC BY-SA 3.0, <https://commons.wikimedia.org/w/index.php?curid=6404479>

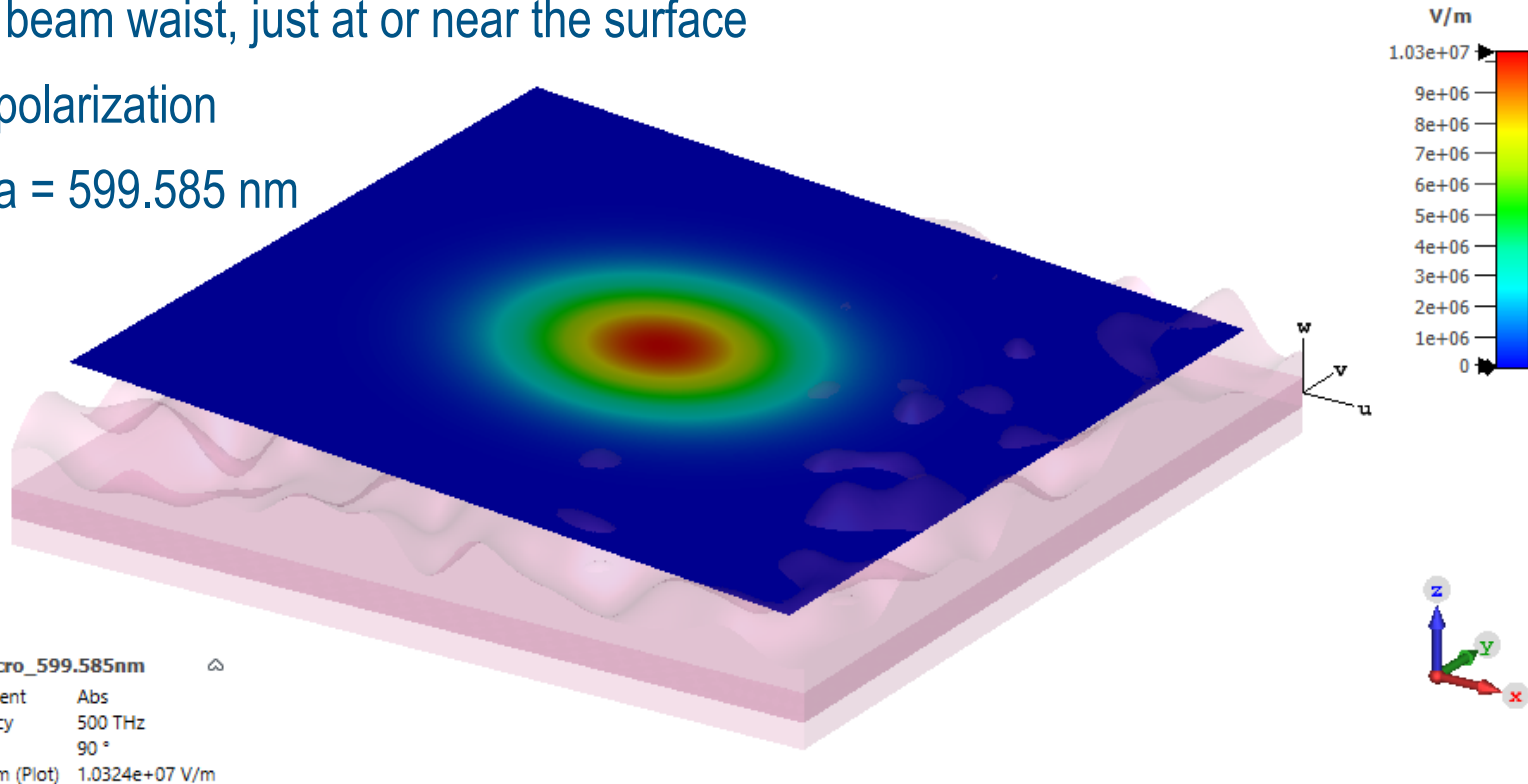
Example Geometry

- ▶ The model under investigation is a 10 μm x 10 μm silicon substrate
- ▶ Random surface roughness with max distortion height as parameter



Illumination Source: Gaussian Beam

- ▶ 1.5 μm beam waist, just at or near the surface
- ▶ Linear polarization
- ▶ $\lambda = 599.585 \text{ nm}$



fsGBMacro_599.585nm
Component Abs
Frequency 500 THz
Phase 90 °
Maximum (Plot) 1.0324e+07 V/m

Solver Setup and GPU Acceleration



	Peak memory used (kB)	Free physical memory (kB)	
		At begin	Minimum
CAD preparation	16920	258982268	258982268
Matrices calc.	26301757	258962890	232424804
Solver run total	33538548	259006976	228098060

Solver Statistics:

Hardware:

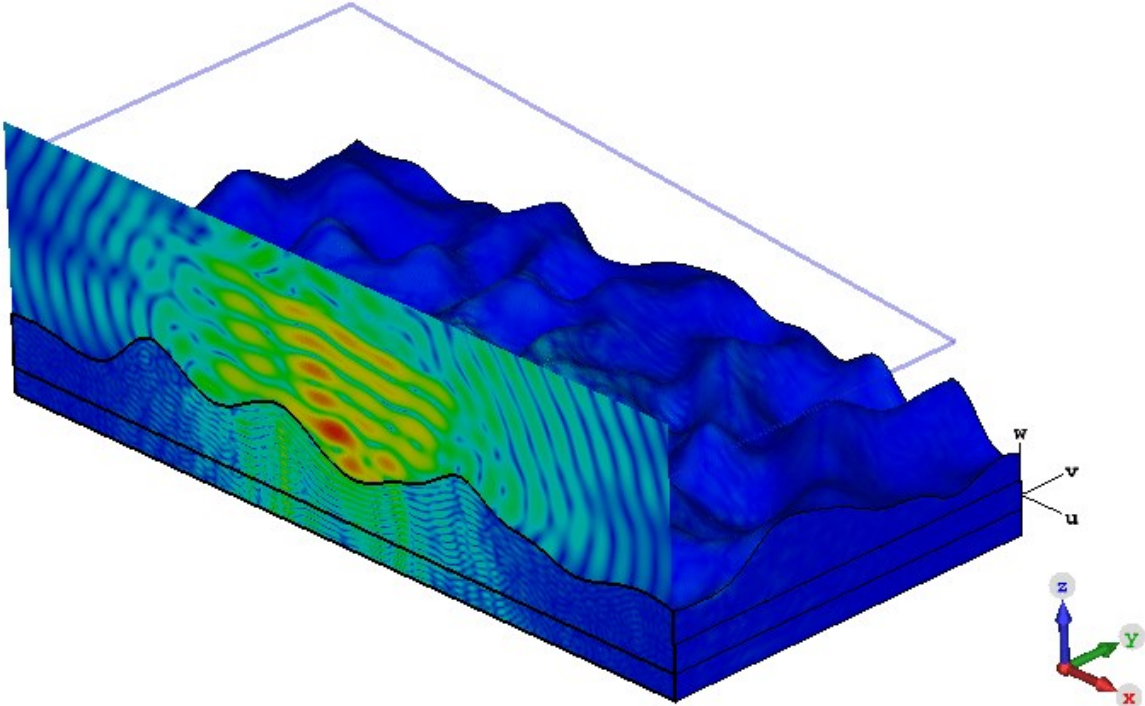
Computer name: [REDACTED]

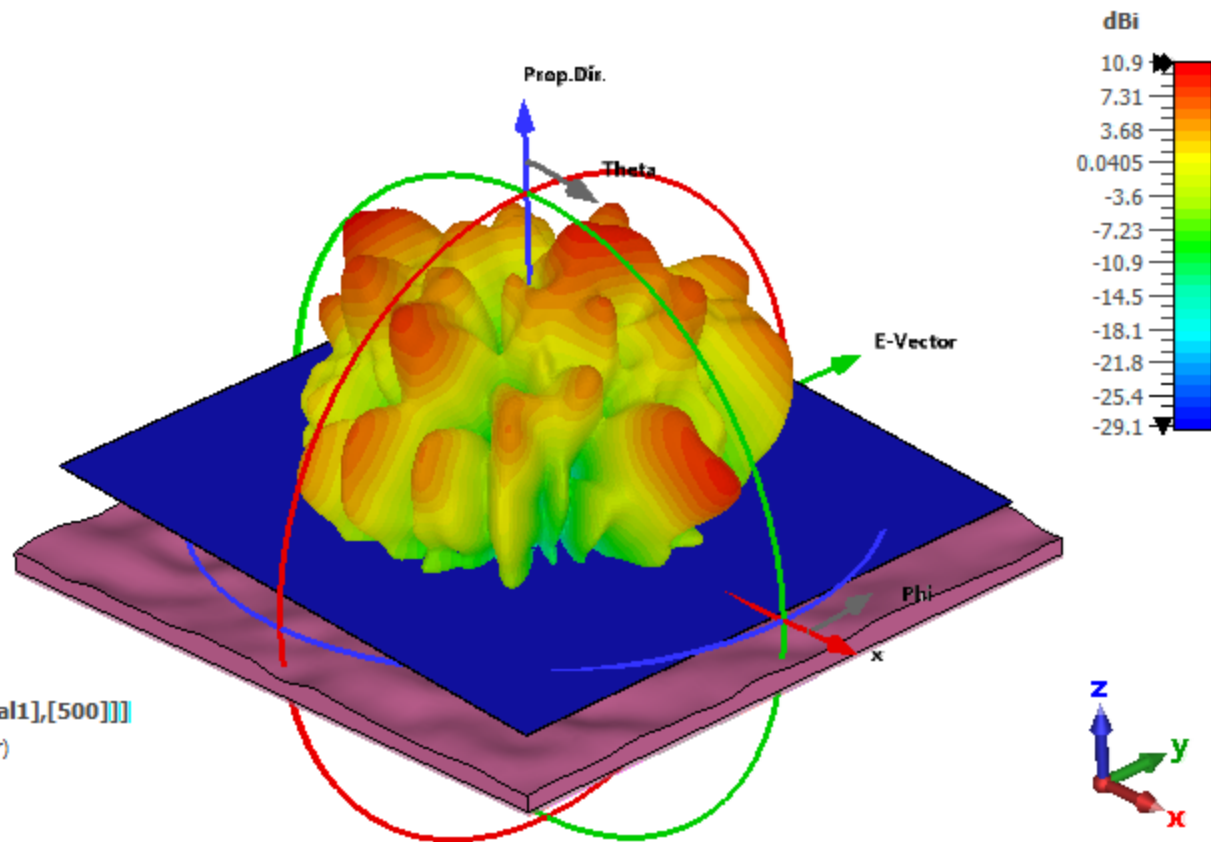
Number of GPU threads:	16
hardware type:	2 CUDA GPU solvers, Kepler/Maxwell
GPU memory usage:	approx. 30 %

Number of mesh cells:	62624364
Excitation duration:	7.10909750e-004 ns
Calculation time for excitation:	0 s
Number of calculated pulse widths:	1.00192
Steady state accuracy limit:	-40 dB
Simulated number of time steps:	32248
Maximum number of time steps:	643725
Time step width:	
without subcycles:	2.208736650e-008 ns
used:	2.208736650e-008 ns
CAD preparation time:	1 s
Matrix calculation time:	434 s
Solver setup time:	252 s
Solver loop time:	1727 s
Solver post-processing time:	259 s

Total solver time:	2673 s (= 0 h, 44 m, 33 s)
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Nearfield Results



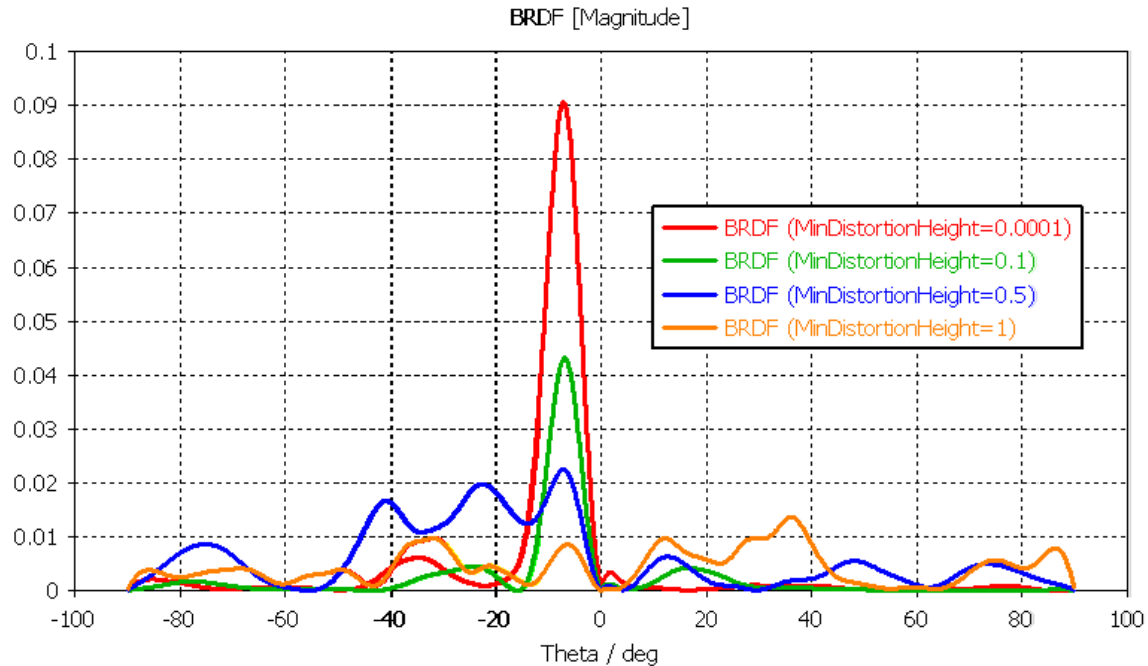


farfield (f=500) [fsG...,0.0,signal1],[500]]]

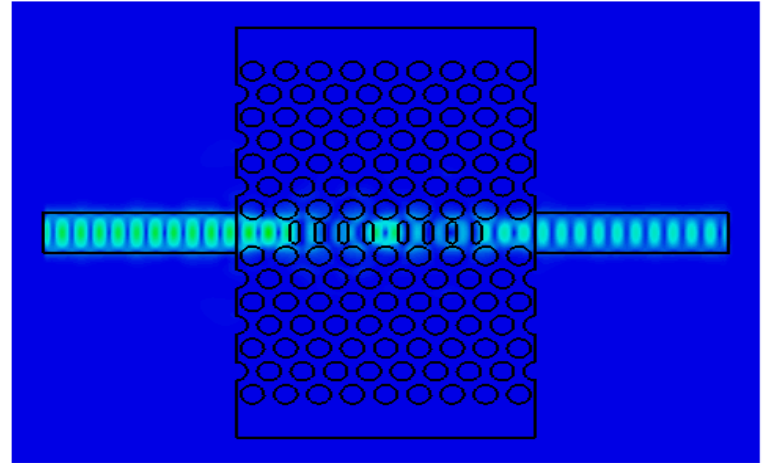
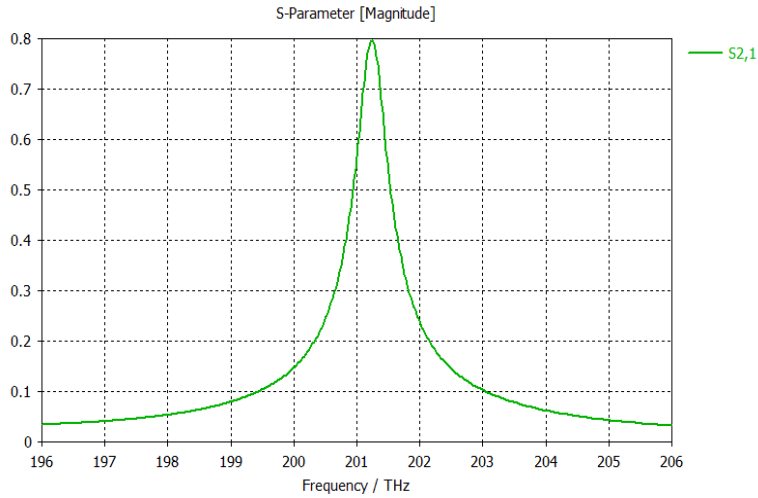
Type	Farfield (Multilayer)
Approximation	enabled ($kR \gg 1$)
Component	Abs
Output	Directivity
Frequency	500 THz
Dir.	10.95 dBi

BRDF Result

- ▶ The BRDF can be extracted from the farfield data
- ▶ Comparison for various surface roughness levels shows expected transition from specular to diffuse reflection



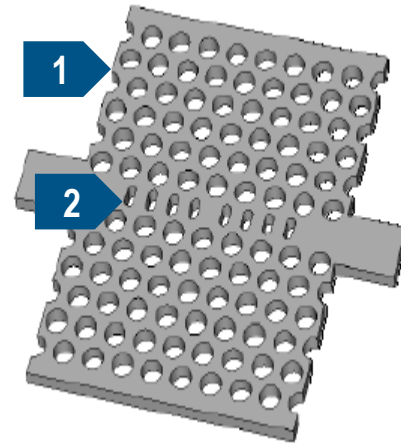
Example: Photonic Crystal Microcavity



Ref: Tuning the resonance of a photonic crystal microcavity with an AFM probe *Iwan Märki, Martin Salt and Hans Peter Herzig, OPTICS EXPRESS 2969 Vol. 14, No. 3 April 2006*

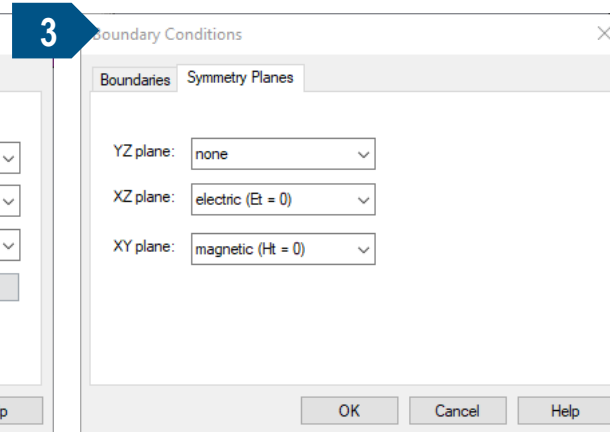
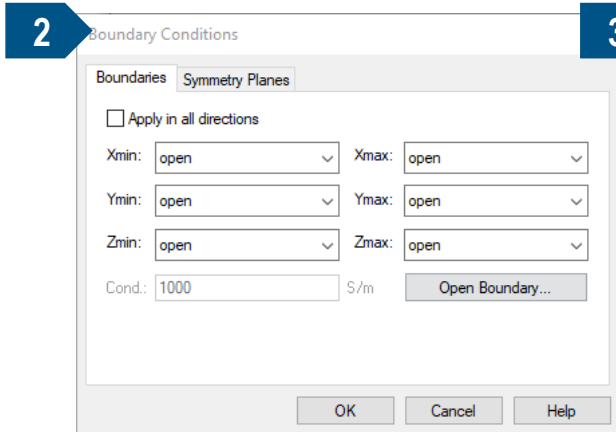
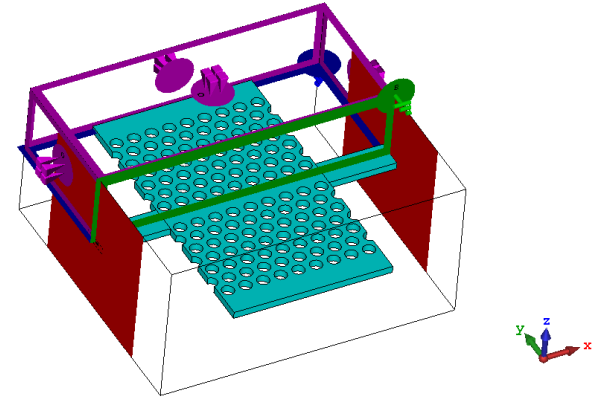
Geometry Details

- ▶ Triangular photonic crystal of cylindrical holes in a thin Si membrane
 - ▷ layer thickness = 205 nm
 - ▷ period = 520 nm
 - ▷ hole radius = 182 nm
- ▶ The Bragg reflectors embedded in the photonic crystal waveguide and has a length of 400 nm (distance between the two Bragg reflectors). The design parameters of the Bragg reflectors:
 - ▷ hole width = 350 nm,
 - ▷ hole length = 150 nm,
 - ▷ Bragg period = 380 nm



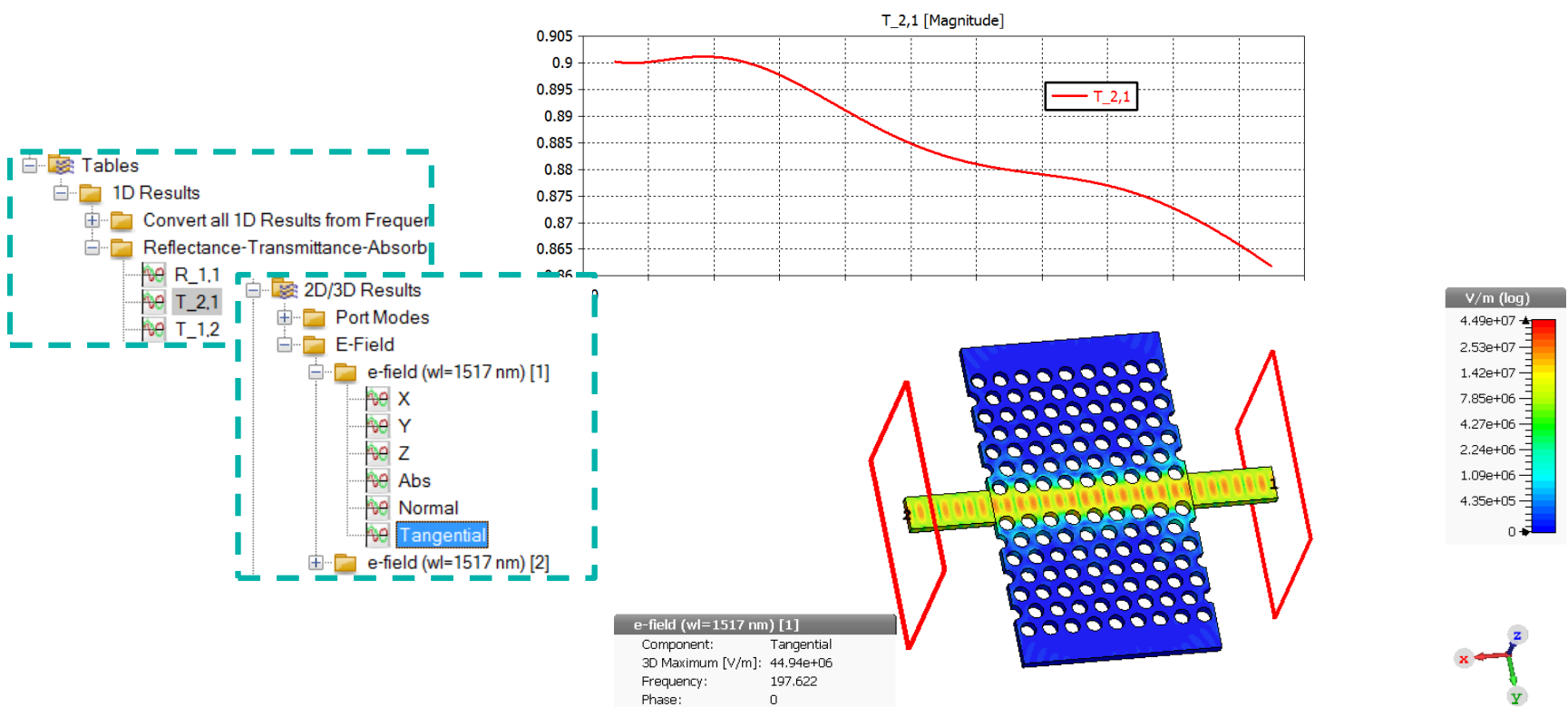
Define Boundary and Symmetry

- ▶ Under the Simulation ribbon set up the boundaries
- ▶ Boundaries open in all directions
- ▶ Symmetry Planes as shown

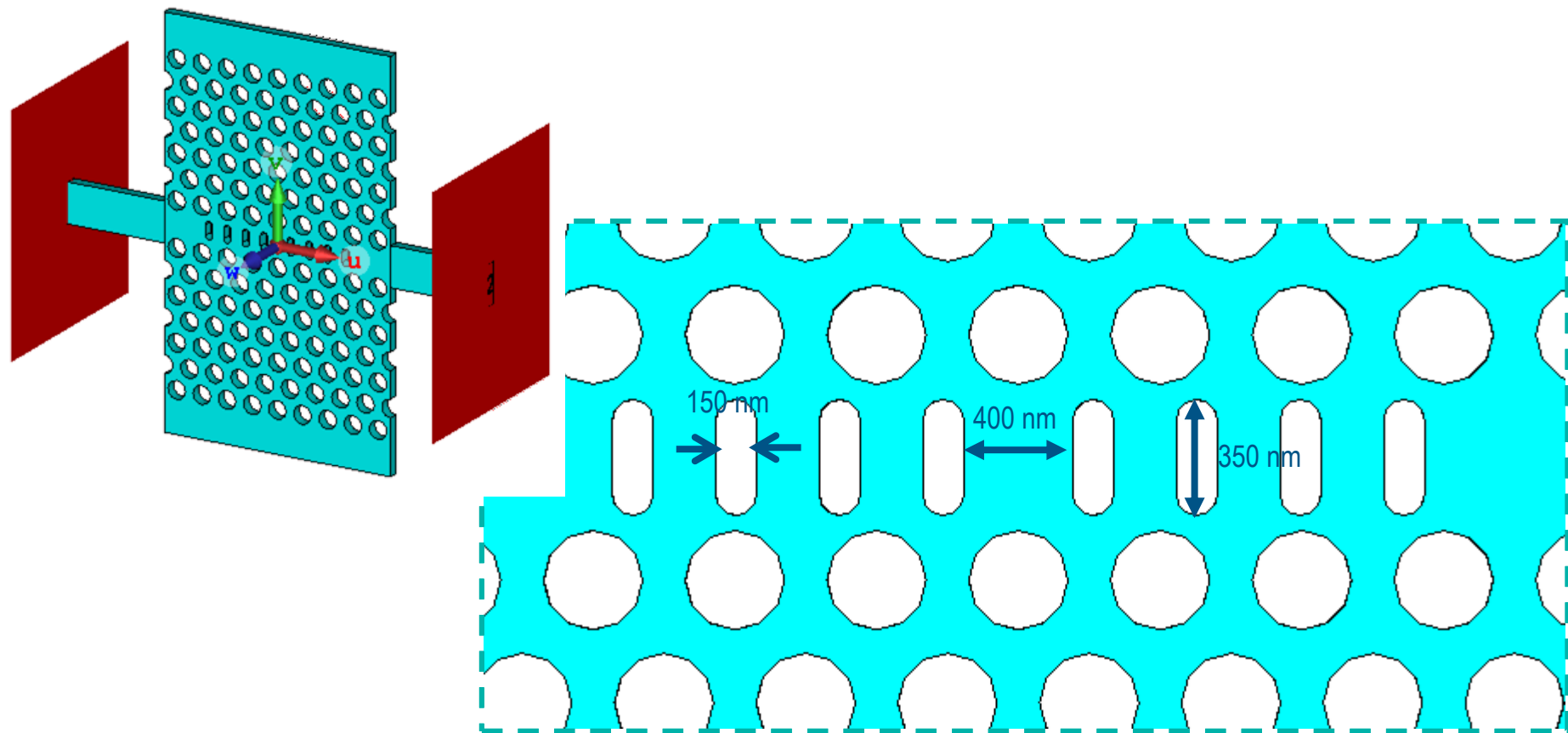


Simulation Results

Dielectric waveguide (launch) is operated at the bandgap of photonic crystal, where wave can propagate without much interaction.

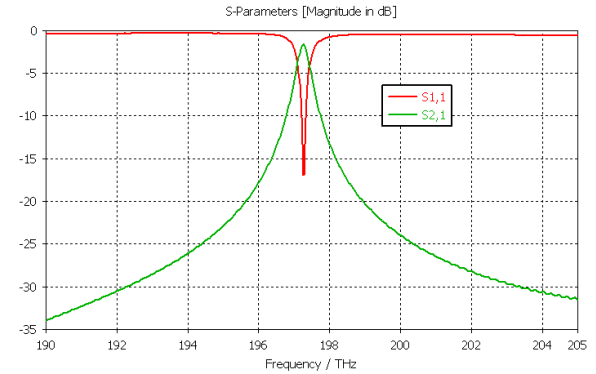
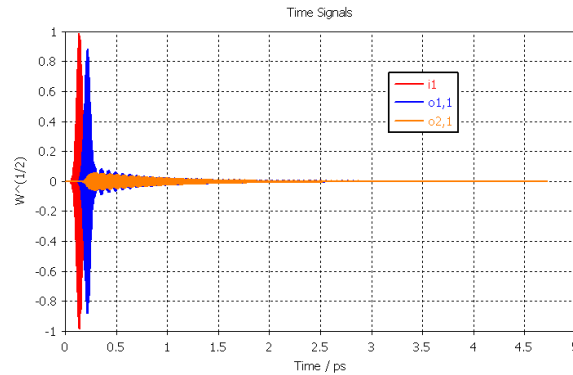
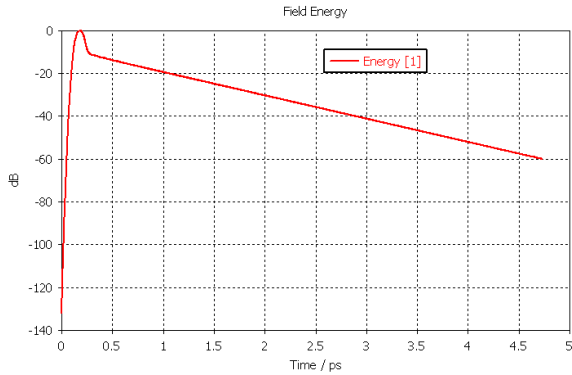


Final Geometry with Bragg Reflector Cavity



Time Domain Results

Time domain approach: slow energy decay due to resonant behavior of the structure

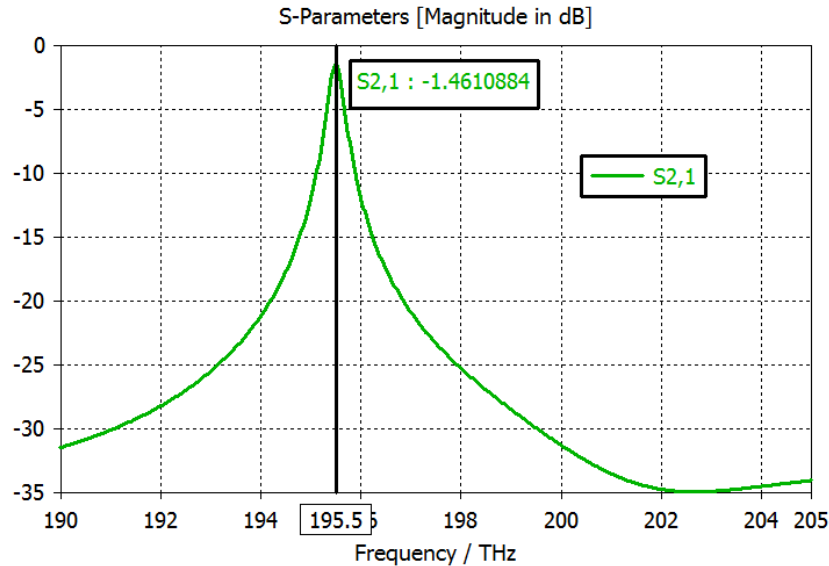


- ▶ Alternative approach: Frequency Domain solver
 - ▷ Increased memory usage but faster results

Q-Factor calculation from S-Parameter (F solver)

- ▶ Execute **Measure Resonances and Q-values** from **freq-data** macro to calculate Q factor from S2,1

$$Q_n = \frac{f_n}{\Delta f_{3dB}}$$



Summary of resonances

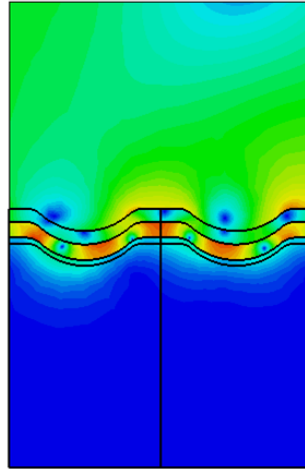
Monitors (to be defined)

E-Field Power flow

H-Field / Current Farfield

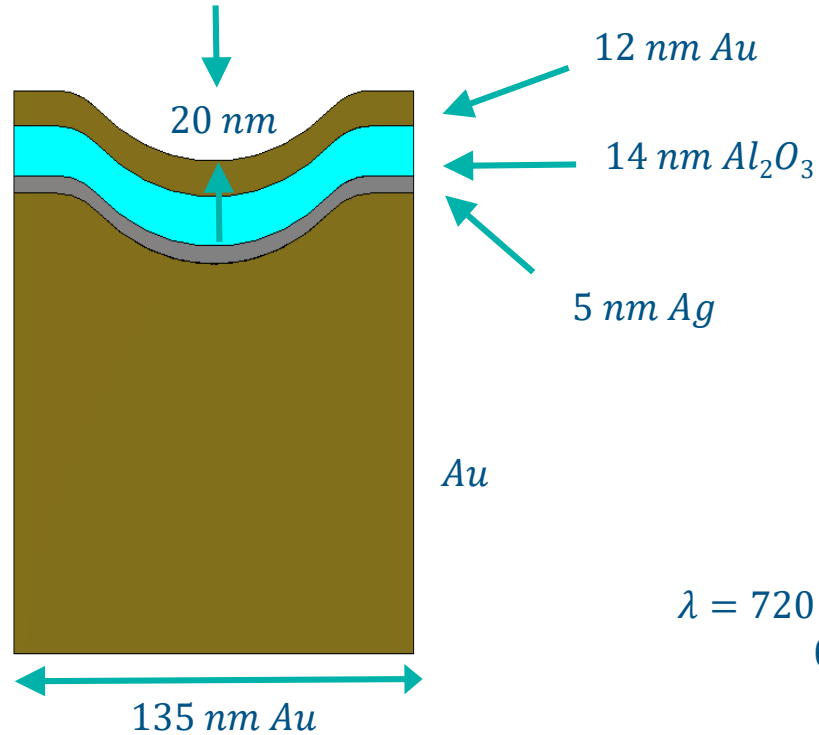
Monitor yes/no	Frequency	Amplitude	Qfactor
<input type="checkbox"/>	0.195501	0.8412359	557.2143

Example: Metal-Insulator-Metal Plasmon Coupling Diffraction Gratings



Ref: *Efficient optical coupling into modes with subwavelength diffraction gratings*, Michael J. Preiner, Ken T. Shimizu, Justin S. White, and Nicholas A. Melosha. APPLIED PHYSICS LETTERS 92, 113109 2008

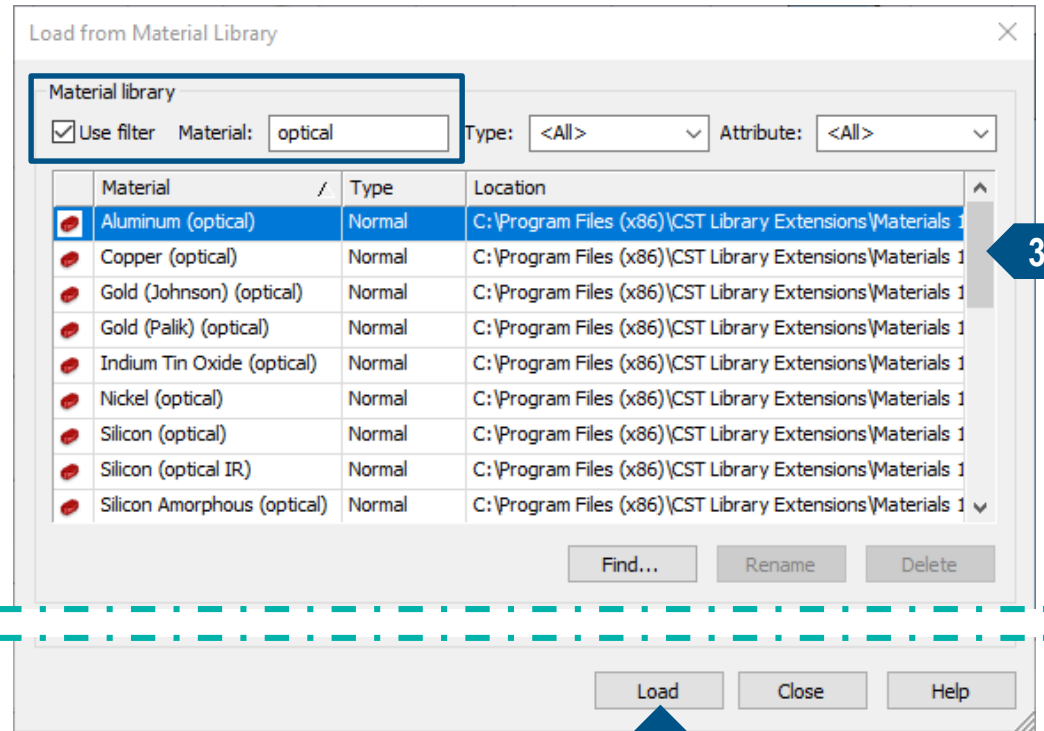
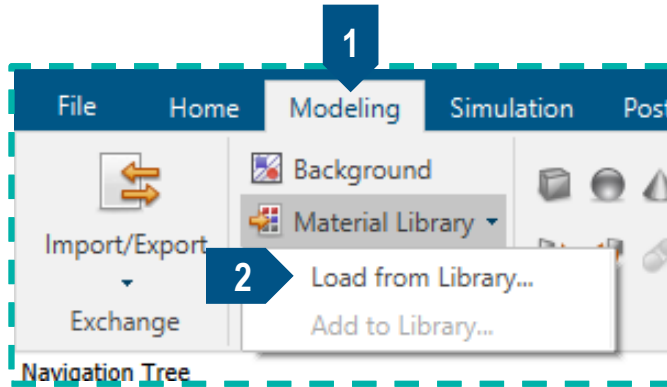
Geometry/Unit Cell Details



$$\lambda = 720 \text{ nm} \rightarrow 416 \text{ THz}$$
$$\theta = 53^\circ$$

Load Materials from Library

- ▶ Switch to the **Modelling** tab
- ▶ Select **Load from Library...**
- ▶ Find and load Silver and Gold in the **Load from Material Library** dialog

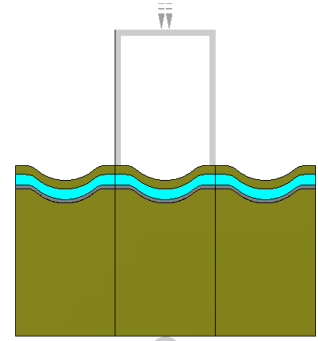


Hint: Use the filter "optical" to only display the materials for the optical frequency range.

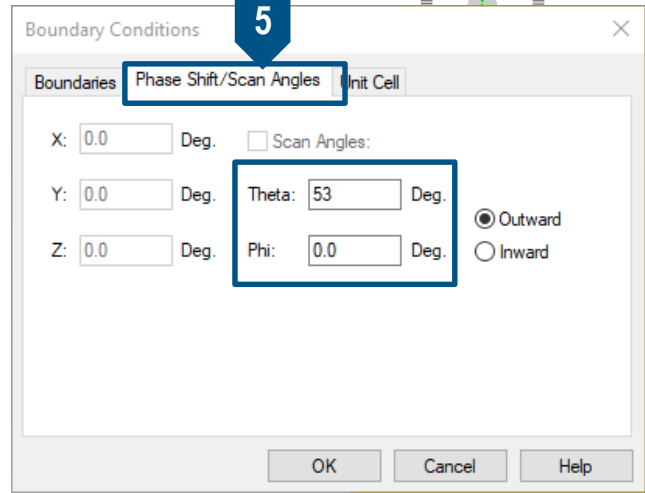
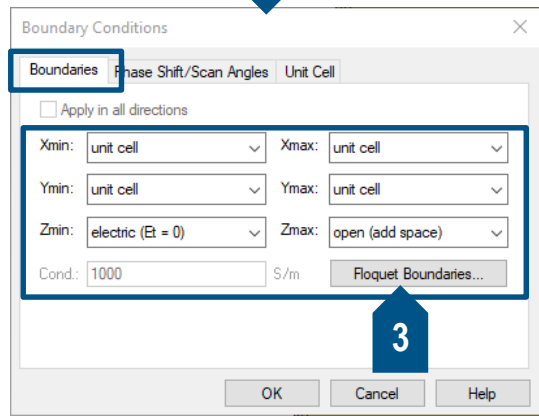
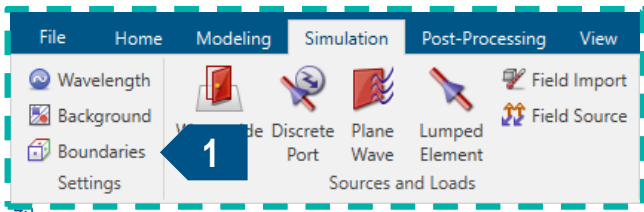
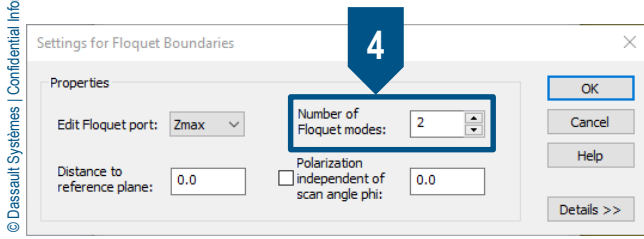
Specify Boundary and Excitation Condition

Specify boundary conditions, scan angle and Floquet port boundaries

- ▶ Select **Boundaries** in the Simulation Tab
- ▶ Set the **Boundaries** settings as shown
- ▶ Switch to the Floquet Boundaries window
- ▶ Change the **Number of Floquet modes**
- ▶ Change the **Phase Shift/Scan Angles** settings



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Start the Frequency Domain Solver



Frequency Domain Solver Parameters

Method

Broadband sweep:
General purpose

Mesh type:
Tetrahedral

Results

Store result data in cache
 Calculate port modes only
 Normalize S-parameter to
50 Ohm

Excitation

Source type: All +Floquet Mode: All

Frequency samples

Active	Type	Adapt.	Samples	From	To	Unit
	Max.Range			400	416	THz
<input checked="" type="checkbox"/>	Monitors		1	416	416	THz
<input checked="" type="checkbox"/>	Automatic	<input checked="" type="checkbox"/>	1			THz
<input type="checkbox"/>	Automatic	<input type="checkbox"/>				THz
<input type="checkbox"/>	Single	<input type="checkbox"/>	1			THz

Adaptive mesh refinement

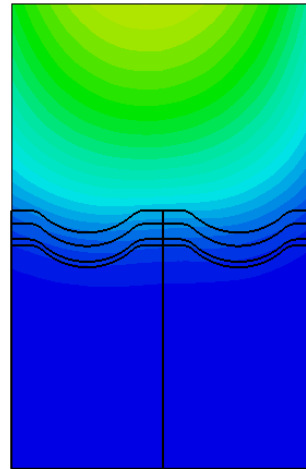
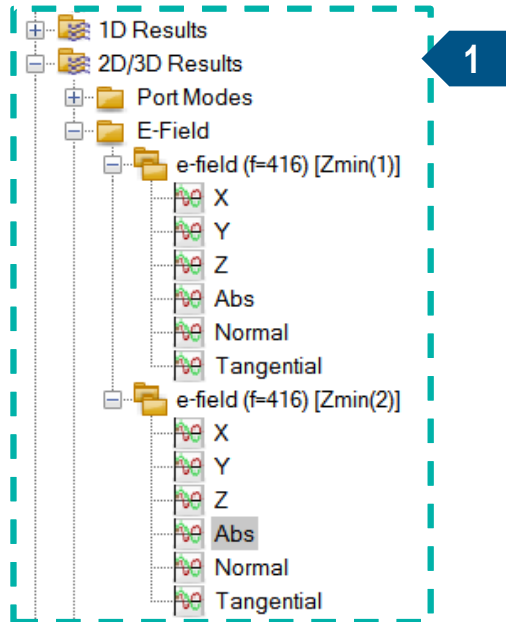
Adaptive tetrahedral mesh refinement

Start
Close
Apply
Optimizer...
Par. Sweep...
Acceleration...
Specials...
Simplify Model...
Domains...
Help

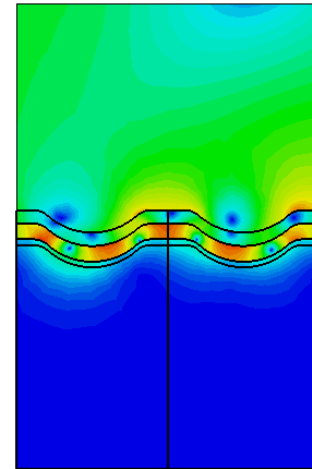
Field Results

Results: Plasmon is generated in dielectric layer when polarization of the field is in parallel to the plane of incident

► View results in the results tree



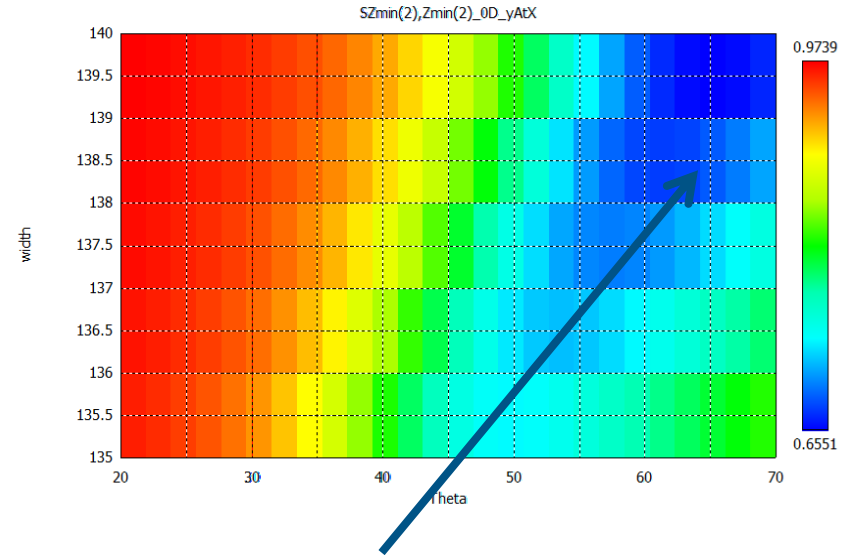
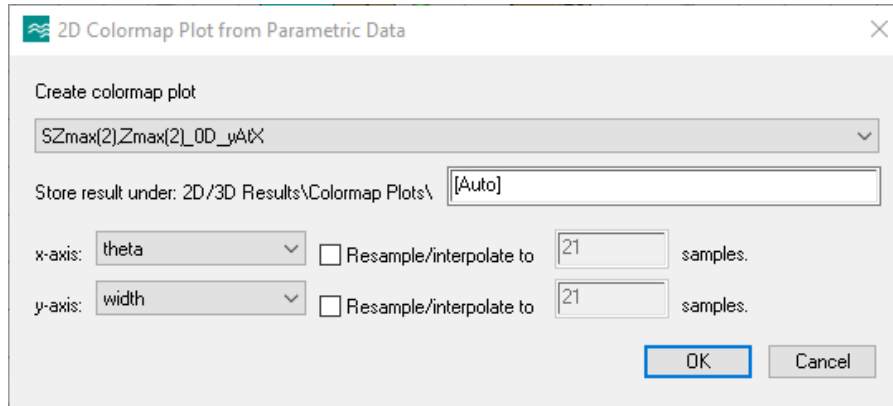
e-field (f=416)	
Cutplane Name:	Cross Section A
Cutplane Normal:	0, 1, 0
Cutplane Position:	-0.2
Component:	Abs
Orientation:	Outside
2D Maximum [V/m]:	1.114e+09
Frequency:	416
Phase:	90



e-field (f=416)	
Cutplane Name:	Cross Section A
Cutplane Normal:	0, 1, 0
Cutplane Position:	-0.2
Component:	Abs
Orientation:	Outside
2D Maximum [V/m]:	2.743e+09
Frequency:	416
Phase:	90

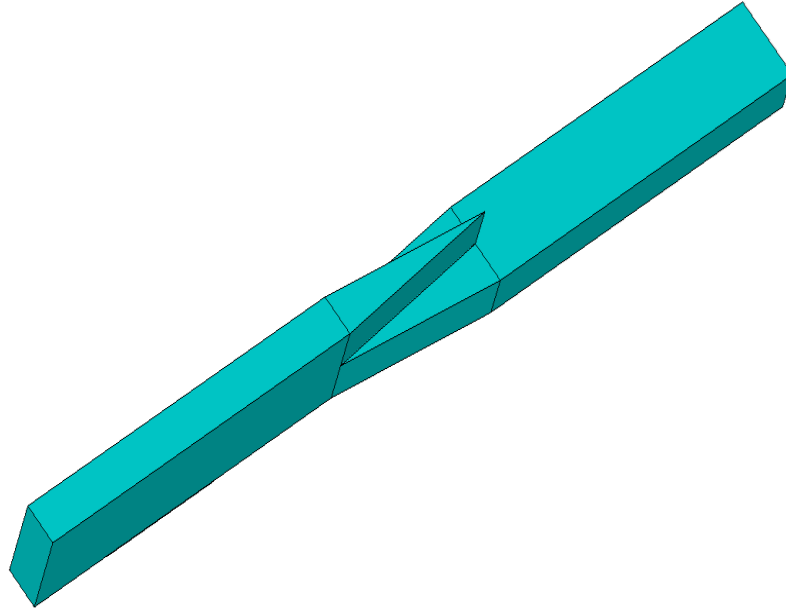
Convert Parametric Data to 2D Colormap

- ▶ Select newly created results
- ▶ Run Macros → Results → Tables → Create 2D Colormap Plot from Parametric Data



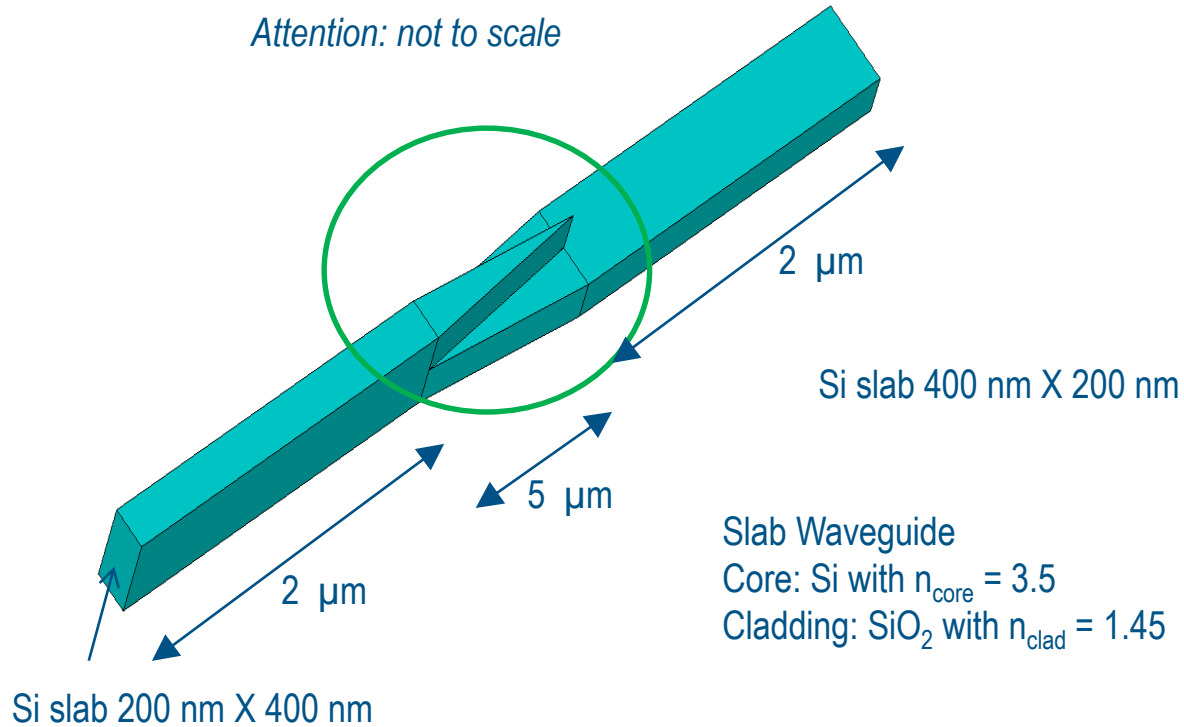
Plasmon coupling efficiency enhances as incident angle of the plane wave and grating width increase.

Example: Silicon Waveguide Based TE Mode Converter



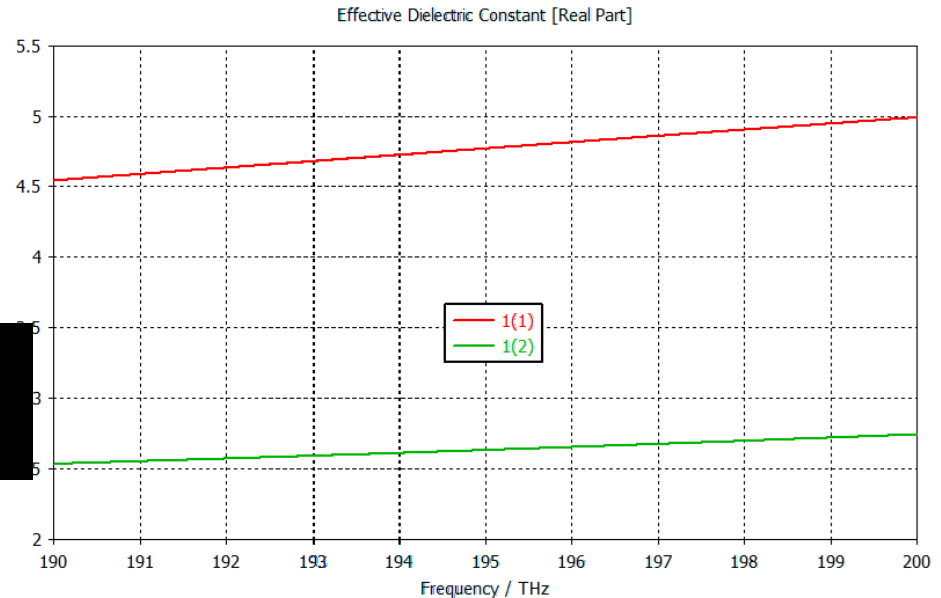
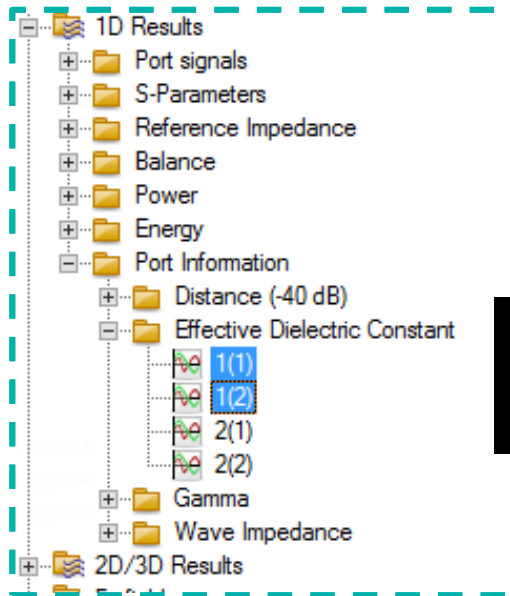
Ref: Silicon waveguide based TE mode converter *Jing Zhang,* Tsung-Yang Liow, Mingbin Yu, Guo-Qiang Lo, and Dim-Lee Kwong, OPTICS EXPRESS VOLUME 18, NUMBER 24 18 Nov. 2010*

Geometry Details



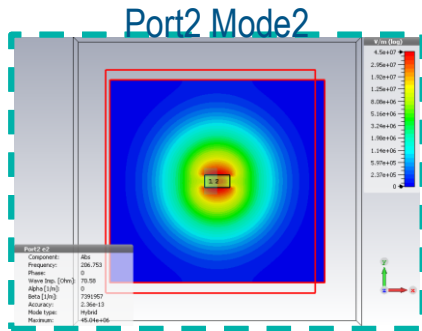
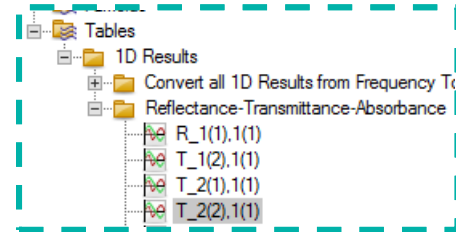
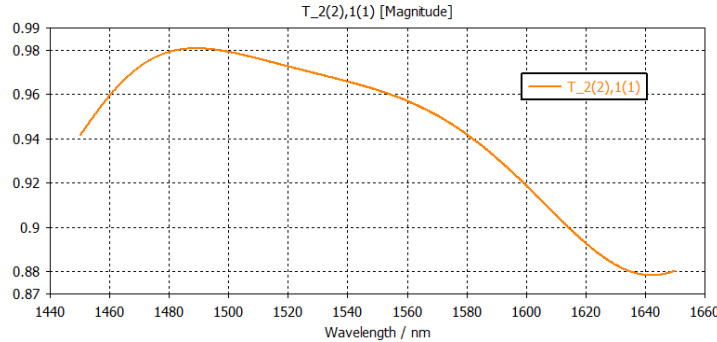
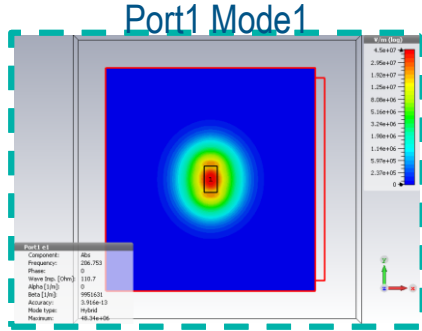
Port Information

- ▶ Dielectric Waveguide Modes are usually dispersive
 - ▷ mode pattern and the effective dielectric constant vary with frequencies.
- ▶ Needs to be taken into account during port mode calculation for accurate results

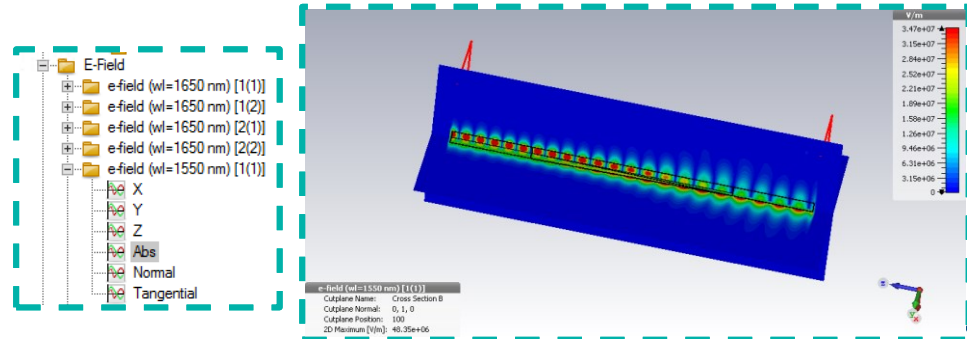


Simulation Results

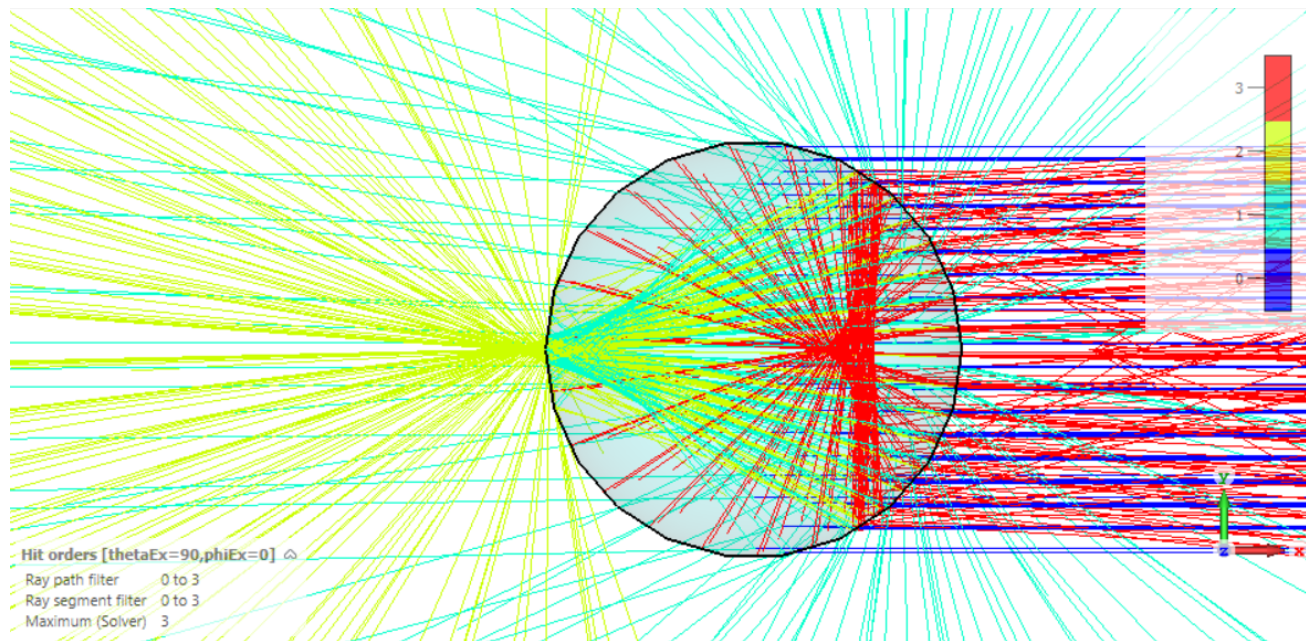
High mode conversion rate (ranging from 88 % to 98 %) over frequencies is observed.



Field monitor results at $\lambda=1550\text{nm}$

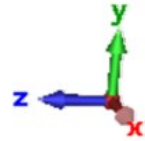
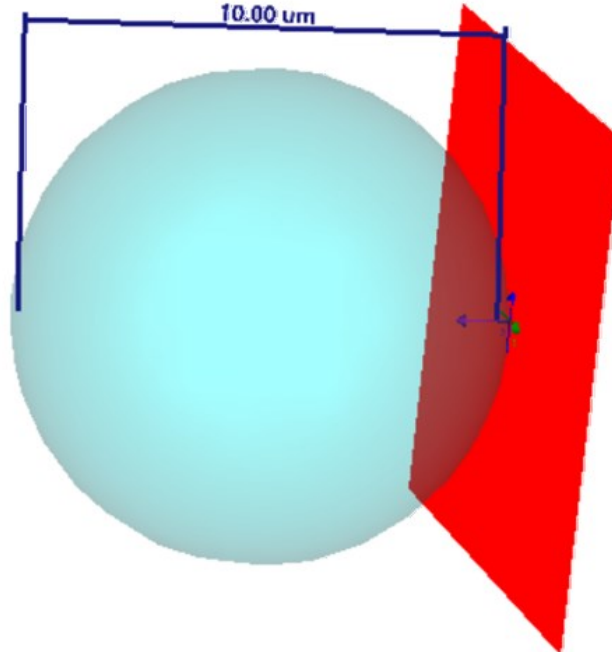


Example: Convex Microlens Simulation



Geometry Details

- ▶ Simple Geometry: Spherical lens ($n=1.7$) with plane wave illumination



Planewave

E-field vector $(x= 1, y= 0, z= 0)$
Plane normal $(x= 0, y= 0, z= 1)$
Plane Wave Linear polarization

Simulation Details

Asymptotic Solver Parameters

1

Solver settings

Mode: Bistatic scattering Store results as tables only

Accuracy: Custom

Maximum number of intersections: 3 Calculate field monitors

Polarization Frequency Sweeps Excitation Angle Sweeps Observation Sweeps

Type	Etheta Re	Etheta Im	Ephi Re	Ephi Im
Horizontal	0	0	1.0	0

Asymptotic Special Settings

Solver Mesh Diffraction Ray storage Hotspots Field Source Other

Ray sampling

Ray tracer type: SBR Raytubes

Ray spacing in wavelengths: 0.7

Minimum number of rays: 1000

Adaptive ray sampling

Maximum ray distance in wavelengths: 1.5

Minimum ray distance in wavelengths: 0.015

3 Consider lossless dielectric materials

Ray tracing control

Limit number of transmissions: -1

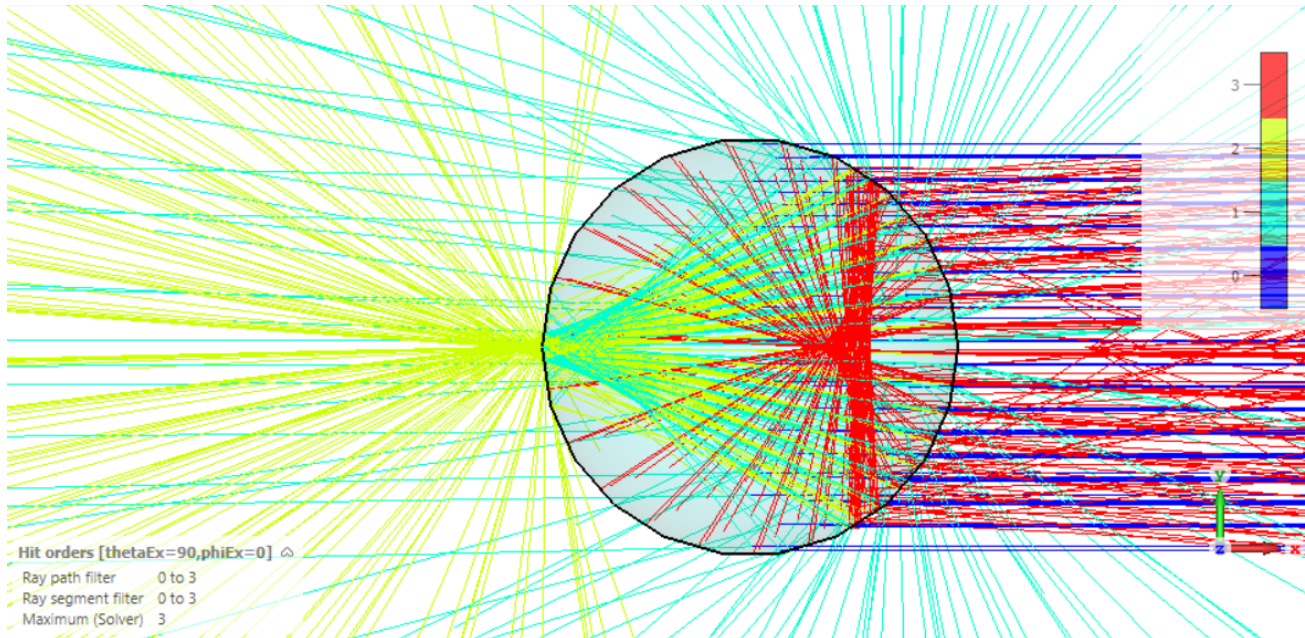
Limit number of reflections: -1

Limit ray length: -1

- ▶ Bistatic Scattering Analysis, source from single direction
- ▶ Asymptotic Solver: Shooting Bouncing Rays
- ▶ Dielectrics taken into account via Snell's law

Results

- ▶ Rays show focusing effect
- ▶ Ray colors indicate number of reflections
- ▶ Focal point position agrees with analytic calculations



Conclusion

Conclusion

- ▶ Optical/photonic problems pose their own challenges due to scale and material properties
- ▶ Metals and Dielectrics often exhibit fundamentally different behaviors
- ▶ A variety of different solver technologies should be employed for efficient simulations

Thank you for your attention! Questions?

