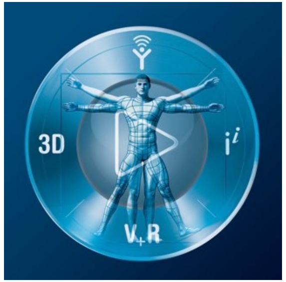
Simulations for Optical, Photonic, and Plasmonic Applications using Dassault Systemes SIMULIA CST Studio Suite®

3DEXPERIENCE®

Agenda

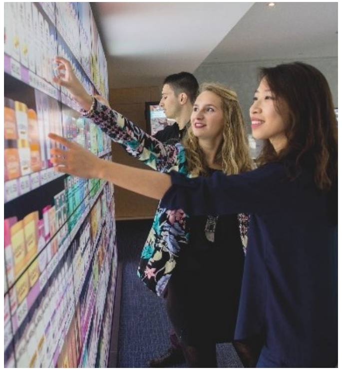
- Introduction
  - About Dassault Systemes
  - Technology offering for optical and photonics simulations
    - Solver options and selection
    - Materials
    - Boundaries
    - Meshing
    - Results postprocessing
- Examples
  - BxDF Calculation
  - Photonic Crystal Microcavity
  - Metal-Insulator-Metal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

Dassault Systèmes | The **3D**EXPERIENCE 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 **3D**EXPERIENCE solutions

12,600 partners

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

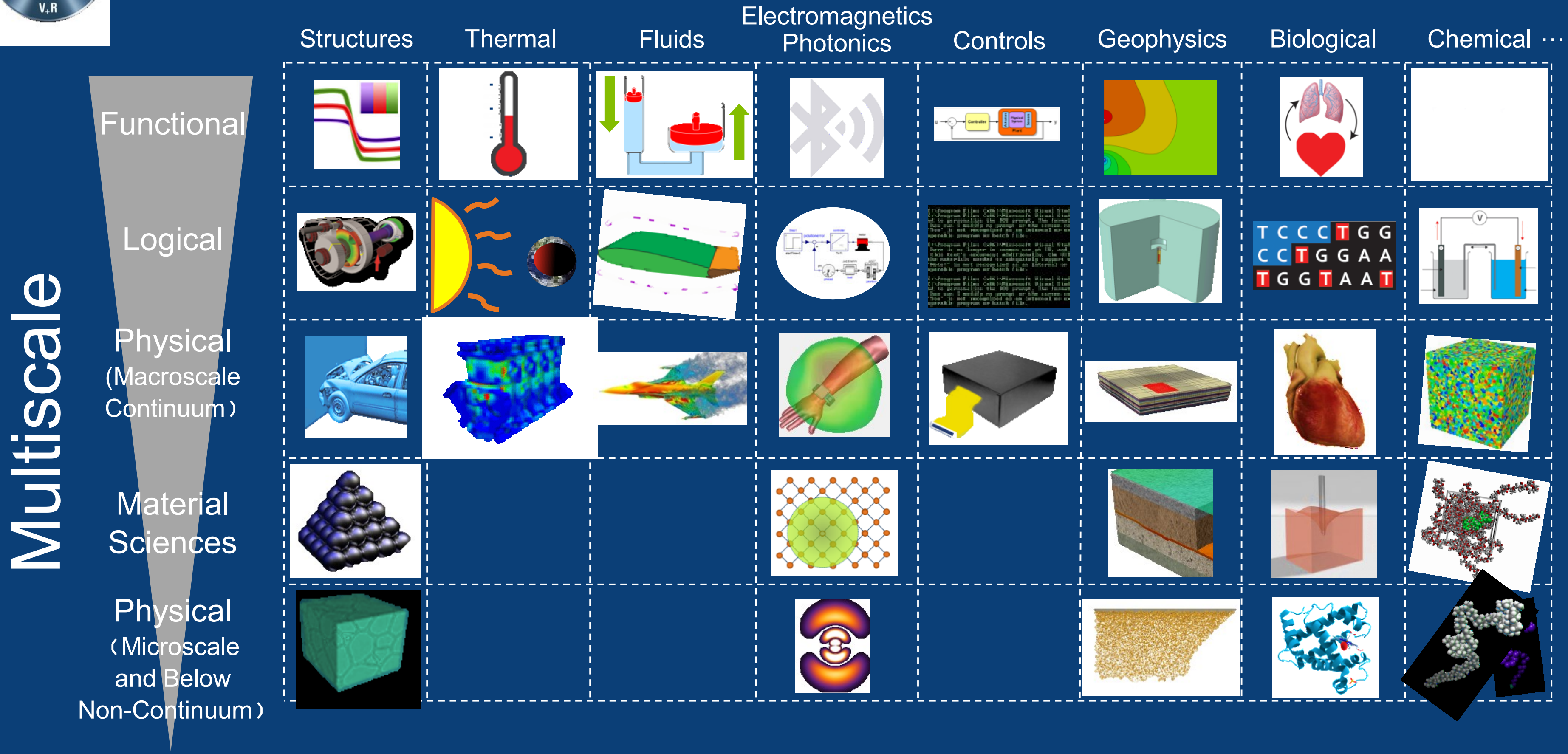
Long-term driven

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

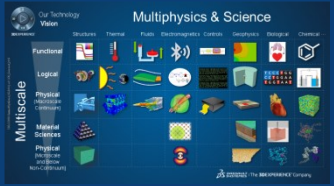
** Figures as of FY 2018 / Non-IFRS*

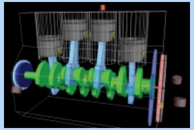
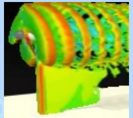
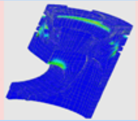
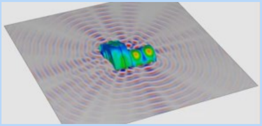
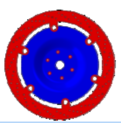
Our Technology
Vision

Multiphysics & Science



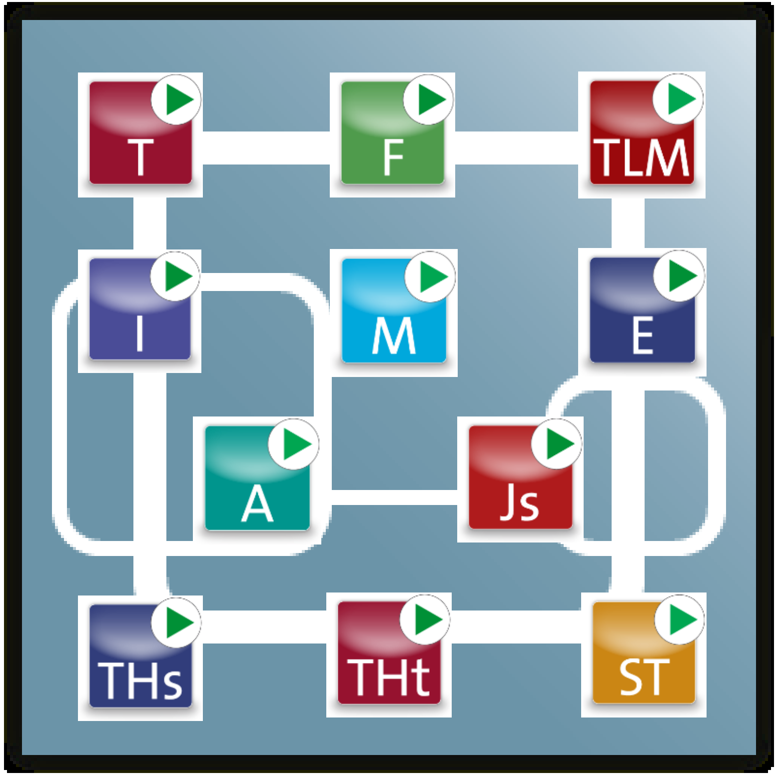
Building blocks of Multiphysics & Multiscale vision



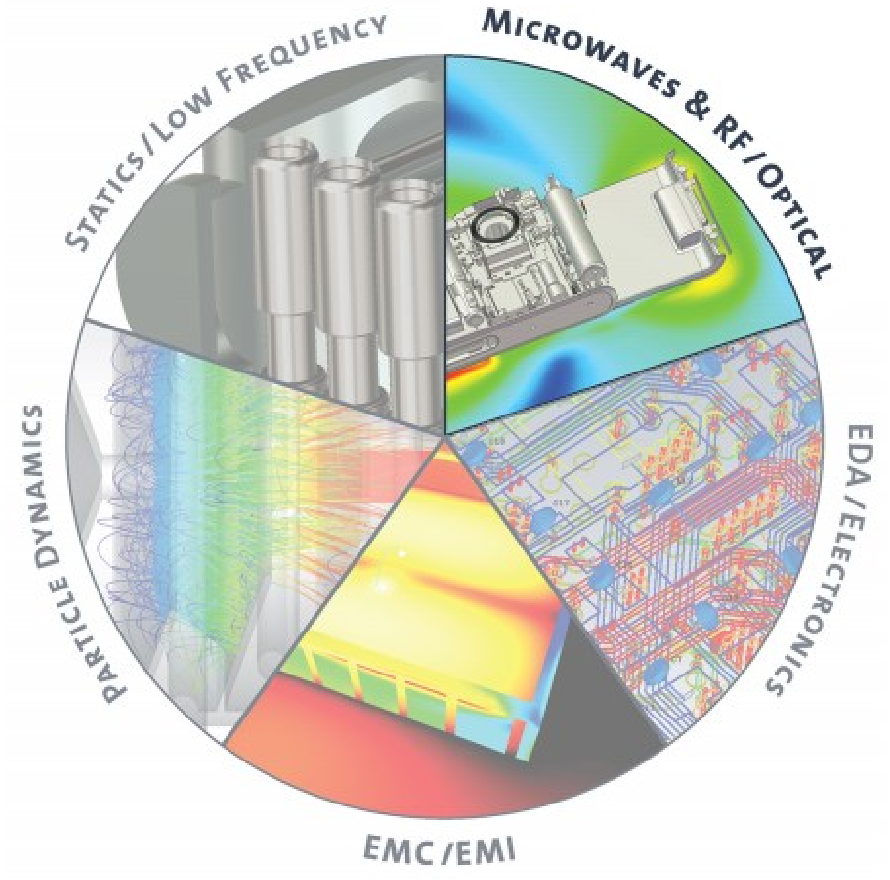
Structures	Abaqus 	**Electromagnetics Photonics**	CST Studio Suite Opera 
Multibody	Simpack 	**Fluids**	PowerFLOW XFlow 3DEXPERIENCE Flo 
Durability	fe-safe 	**Automation**	Isight 
Vibro-acoustics	Wave6 	**Optimization**	Tosca Isight  

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)

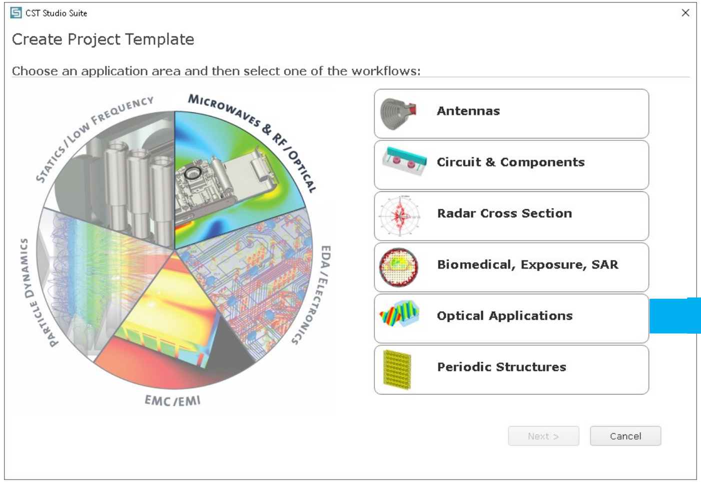


Optical Applications in CST Studio Suite



Optical Applications in CST Studio Suite

Optical Waveguides, Couplers and Fibers | Solar Cells | Photonic Bandgap Structures | Filters and Resonators



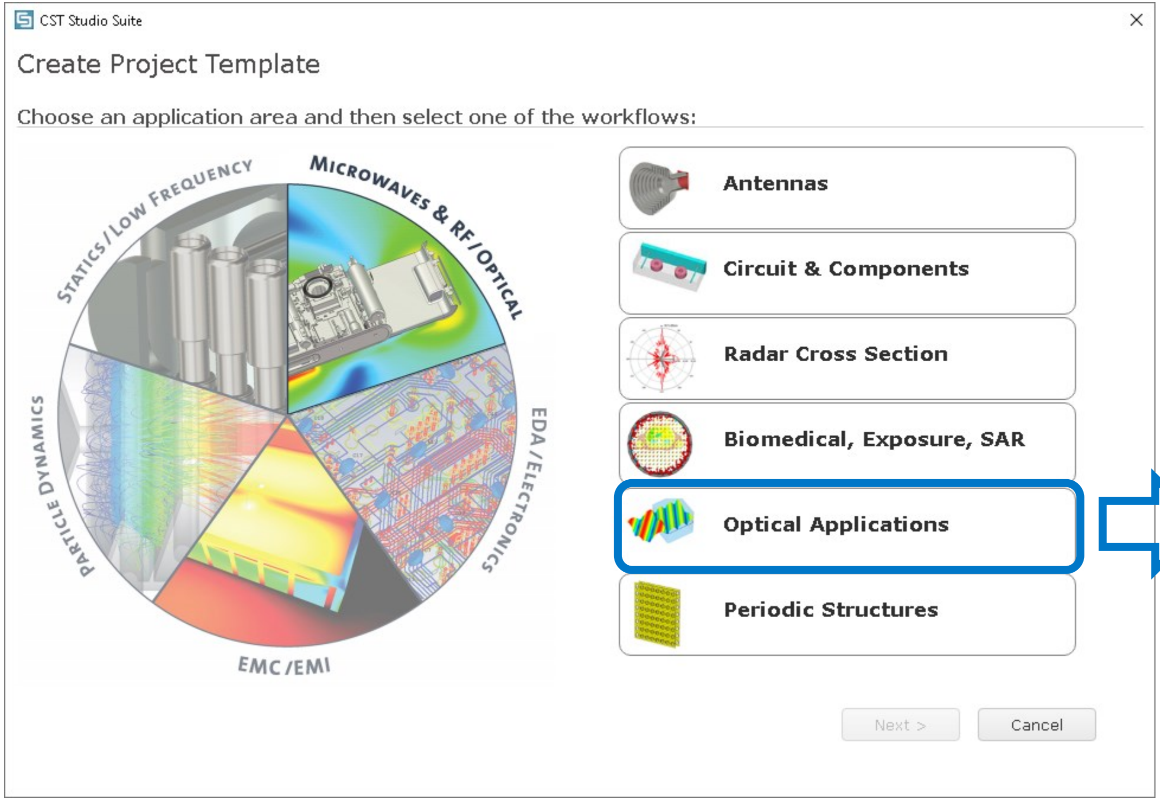
Dielectric/Photonic Structures

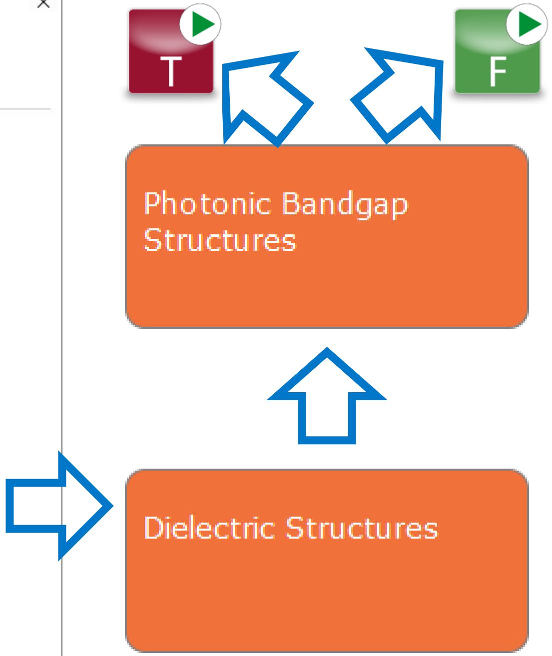
Metallic/Plasmonic Structures

Nano Antennas | Plasmonic Waveguides | Plasmonic Solar Cells

DASSAULT SYSTEMES

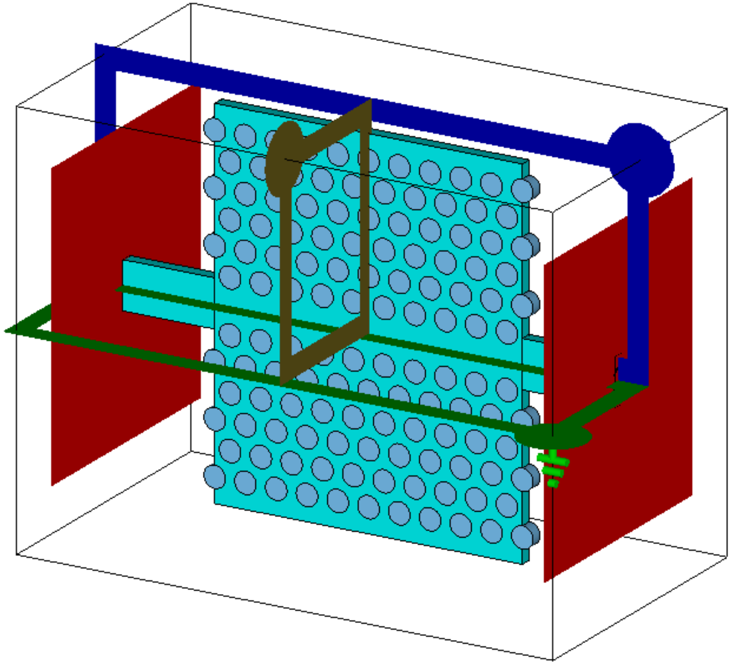
Configuration Wizard





Creating the Geometry

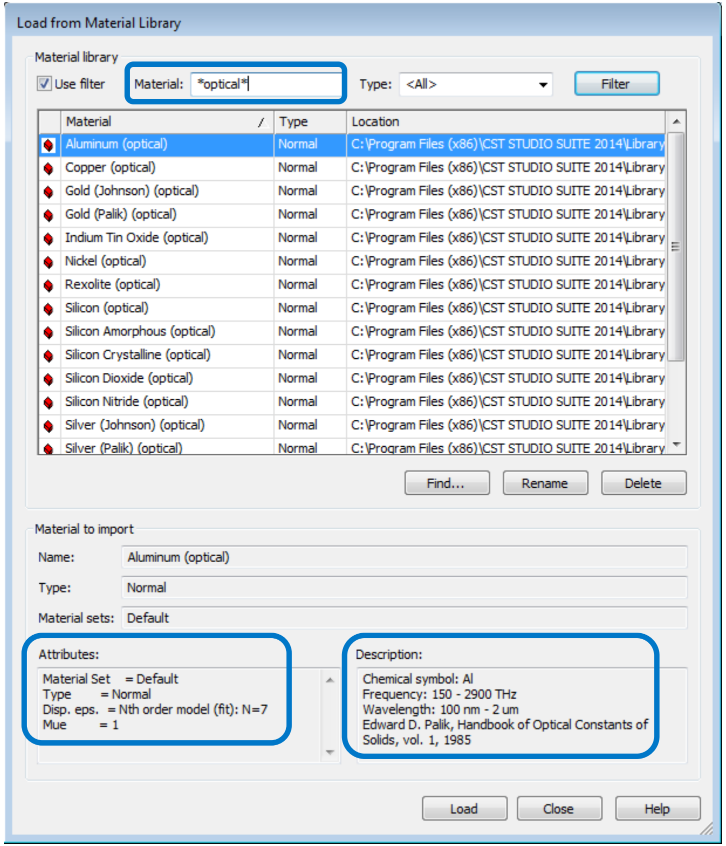
- Built-in CAD/scripting environment
- Import CAD or EDA data:
  - CATIA
  - GDSII
  - DXF
  - STEP
  - ... and many more
- Direct links:
  - 3DEXPERIENCE Power'By
  - SOLIDWORKS
  - Luceda IPKISS
  - CREO



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

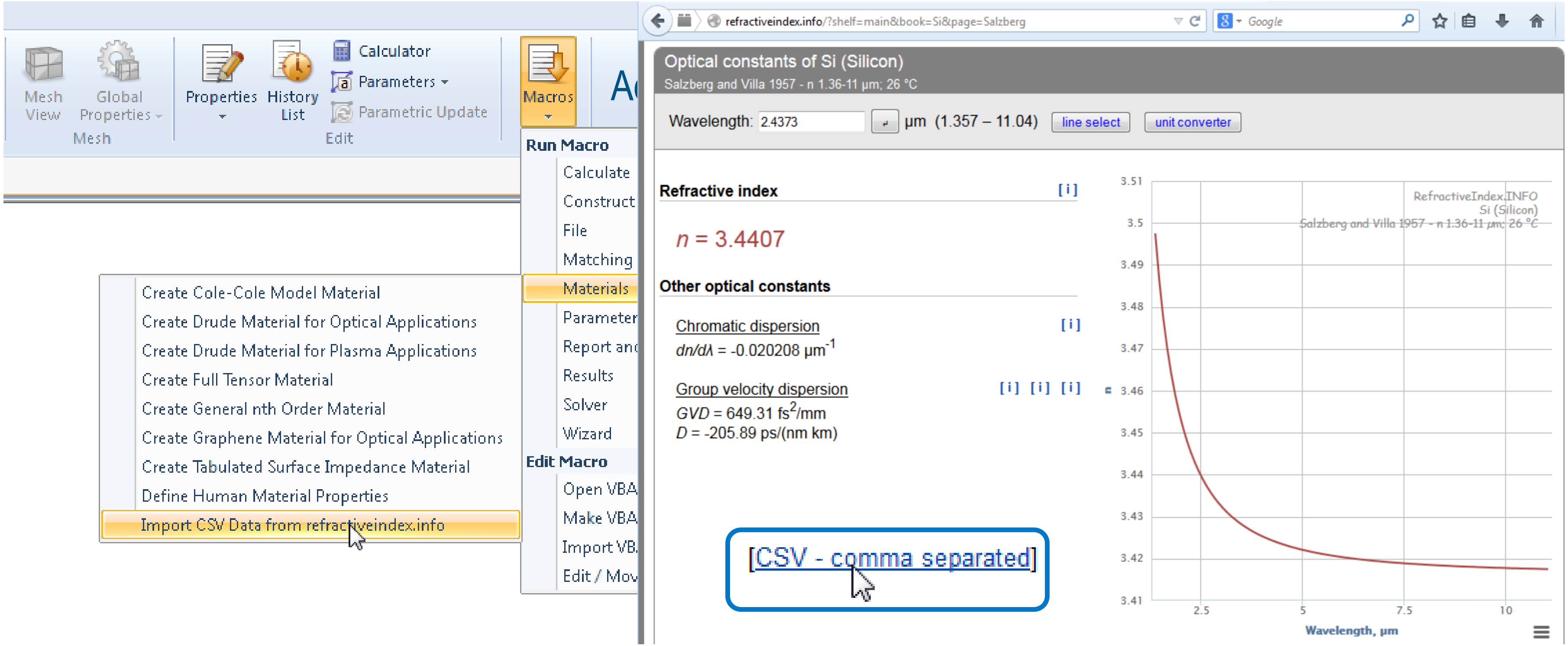
- Dispersive data need to satisfy Kramers-Kronig to ensure causality

- CST Studio Suite offers a number of causal dispersion models (Drude, Lorentz, etc.)

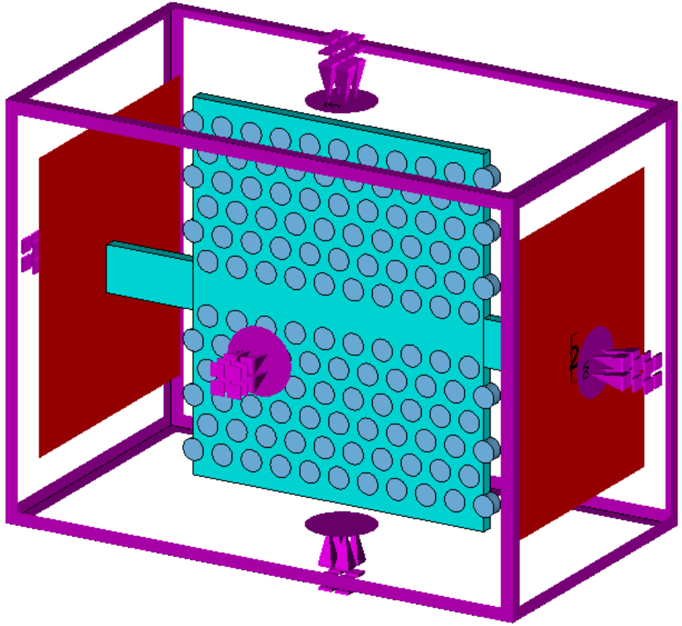
- Generalized nth order model to automatically fit tabulated data:

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

Material Data Resource: www.refractiveindex.info

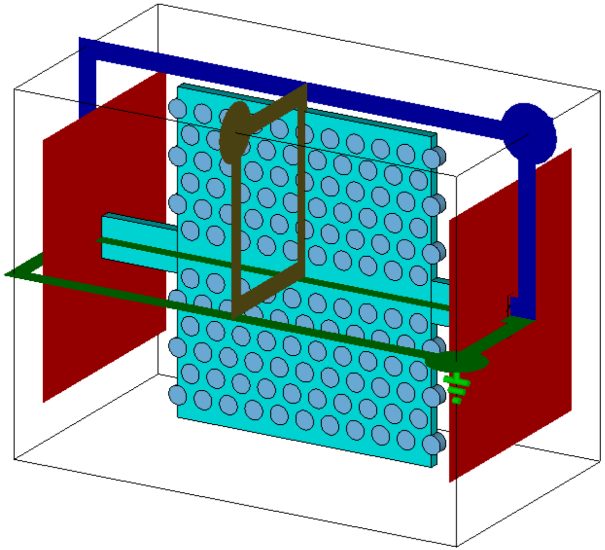


PML Boundaries and Symmetry Planes



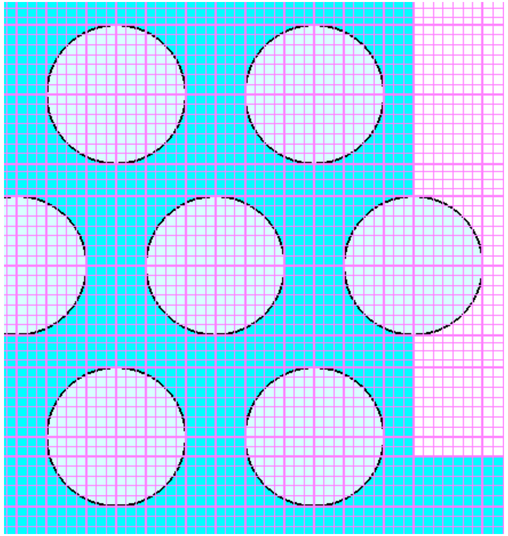
State-of-the-art PML technology
with extremely low reflection

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.

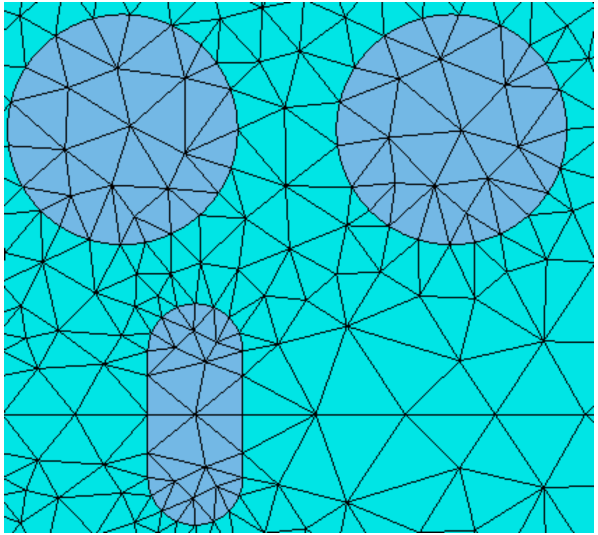


Meshing

- Automatic hexahedral and tetrahedral mesh generation



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



Higher order curved
tetrahedral mesh

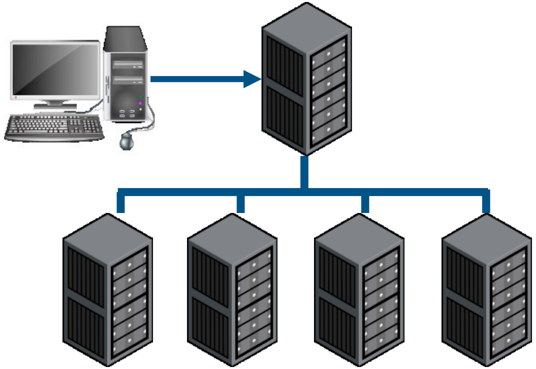
Time or Frequency Domain?

- 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)

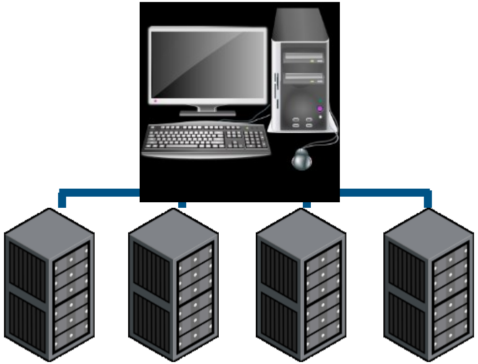
SIMULIA CST Studio Suite® Acceleration Techniques

CPU Multithreading

GPU Computing



Distributed Computing



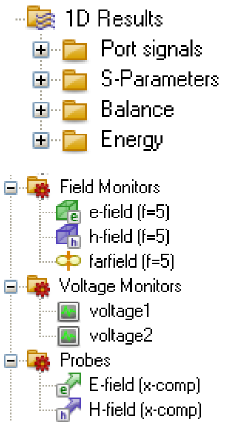
MPI Computing

Result Handling

There are different types of results in CST Studio Suite:

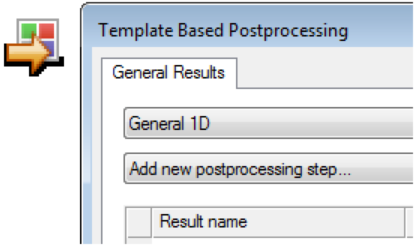
Standard results for RF simulations

Monitors available for RF simulations



1. **Standard results:** Computed automatically for every simulation.
   Typically not resource intensive (e.g. S-parameters)

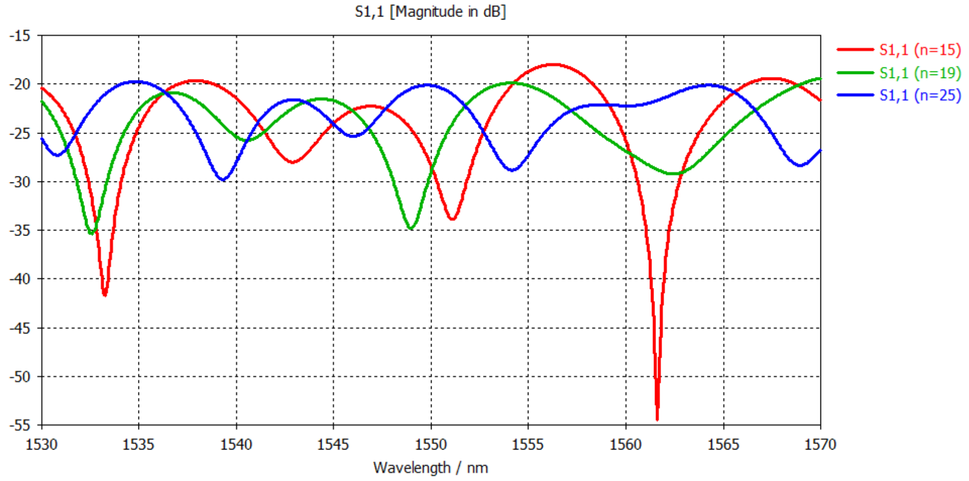
2. **Result monitors:** User can preserve other results using monitors.
   Typically resource intensive results (e.g. field distribution in 3D space)

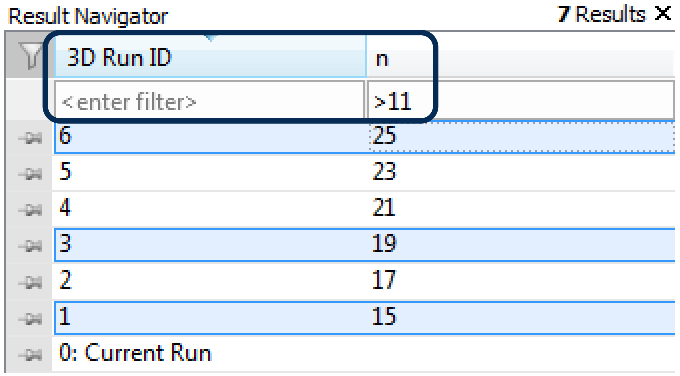


3. **Result templates:** Highly configurable mechanism to extract special values from either standard results or result monitors.
   The power and flexibility of the VBA programming language is available.

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

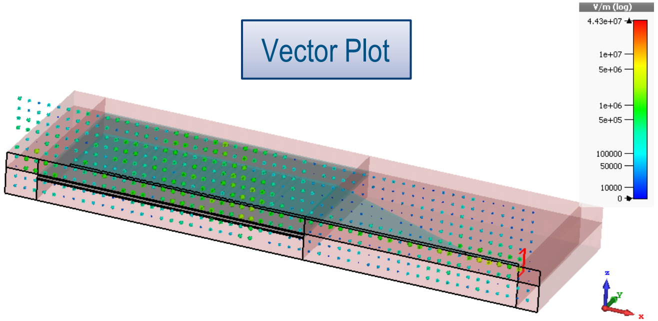




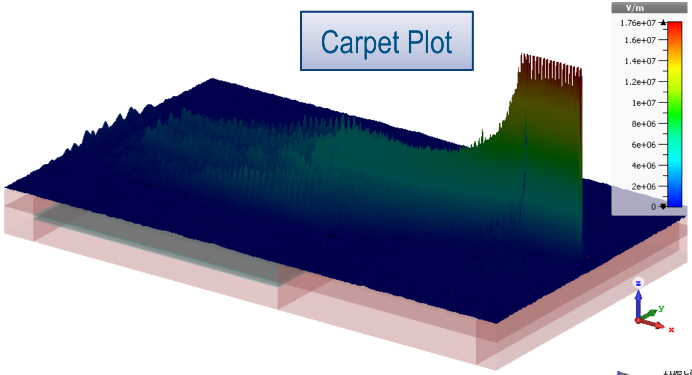
3D Plot Options

Some examples for field plot types:

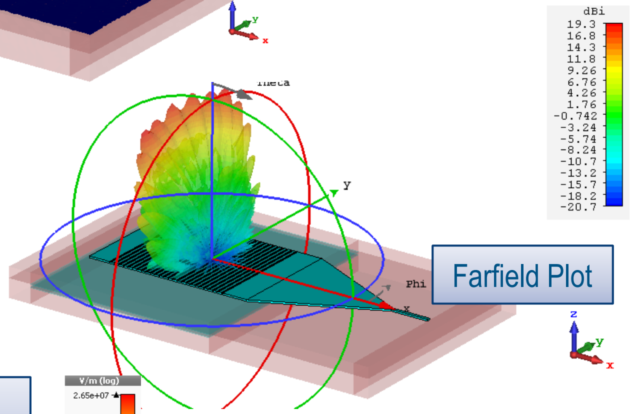
Vector Plot



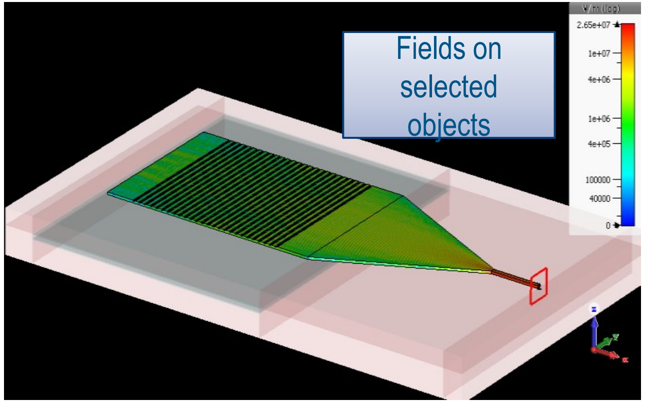
Carpet Plot



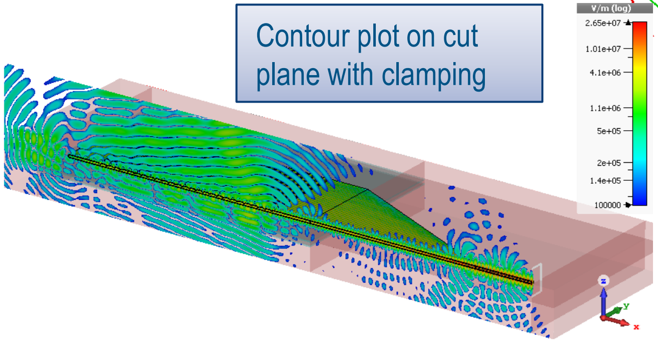
Farfield Plot



Fields on selected objects

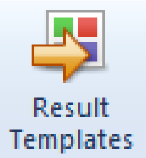


Contour plot on cut plane with clamping



Post Processing Templates

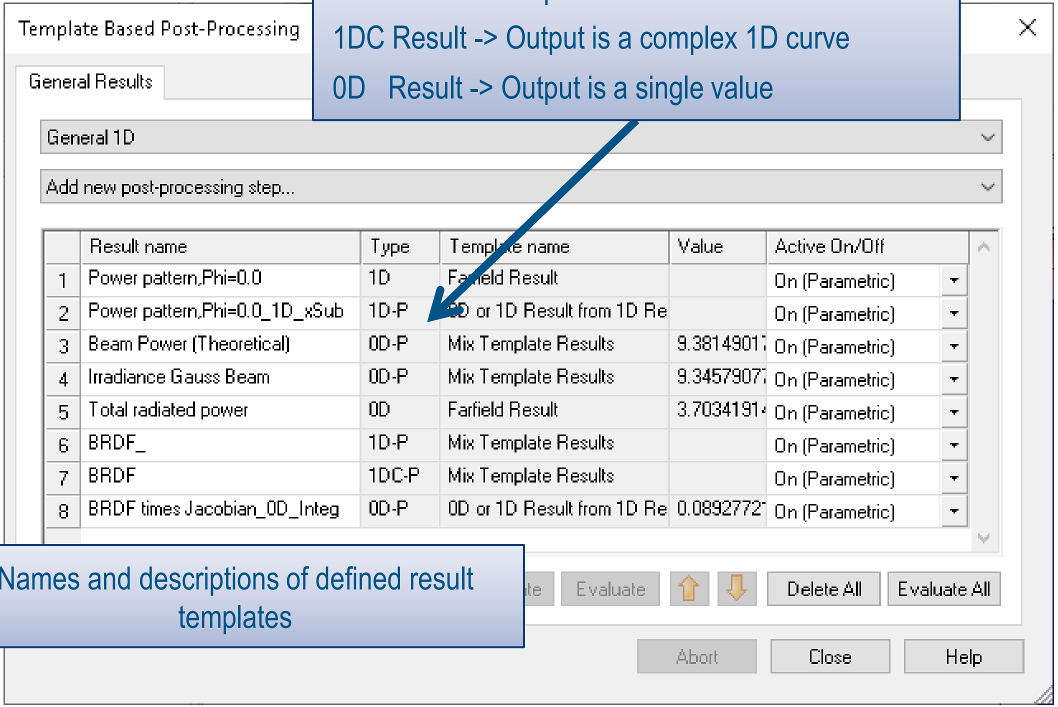
Post processing templates provide a convenient way to derive values from the standard results and 3D field results:



1D Result -> Output is a 1D curve

1DC Result -> Output is a complex 1D curve

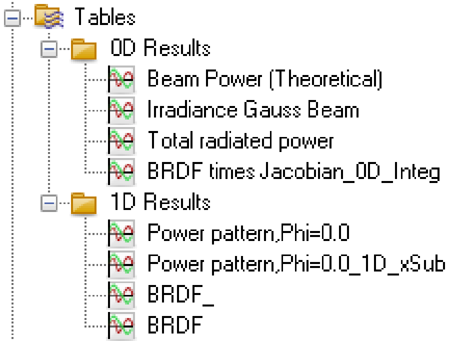
0D Result -> Output is a single value



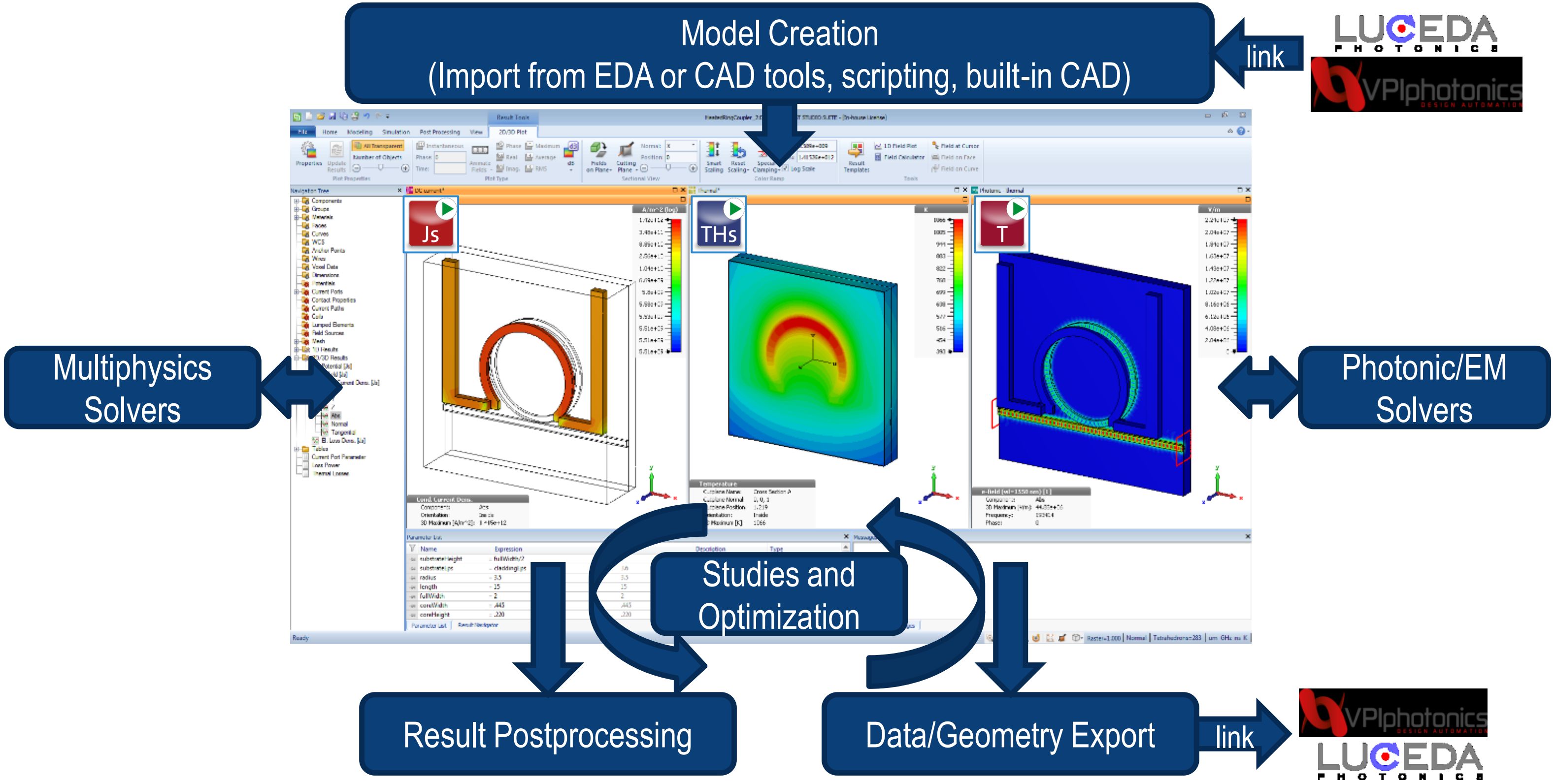
	Result name	Type	Template name	Value	Active On/Off
1	Power pattern,Phi=0.0	1D	Farfield Result		On (Parametric)
2	Power pattern,Phi=0.0_1D_xSub	1D-P	0D or 1D Result from 1D Re		On (Parametric)
3	Beam Power (Theoretical)	0D-P	Mix Template Results	9.3814901	On (Parametric)
4	Irradiance Gauss Beam	0D-P	Mix 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

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



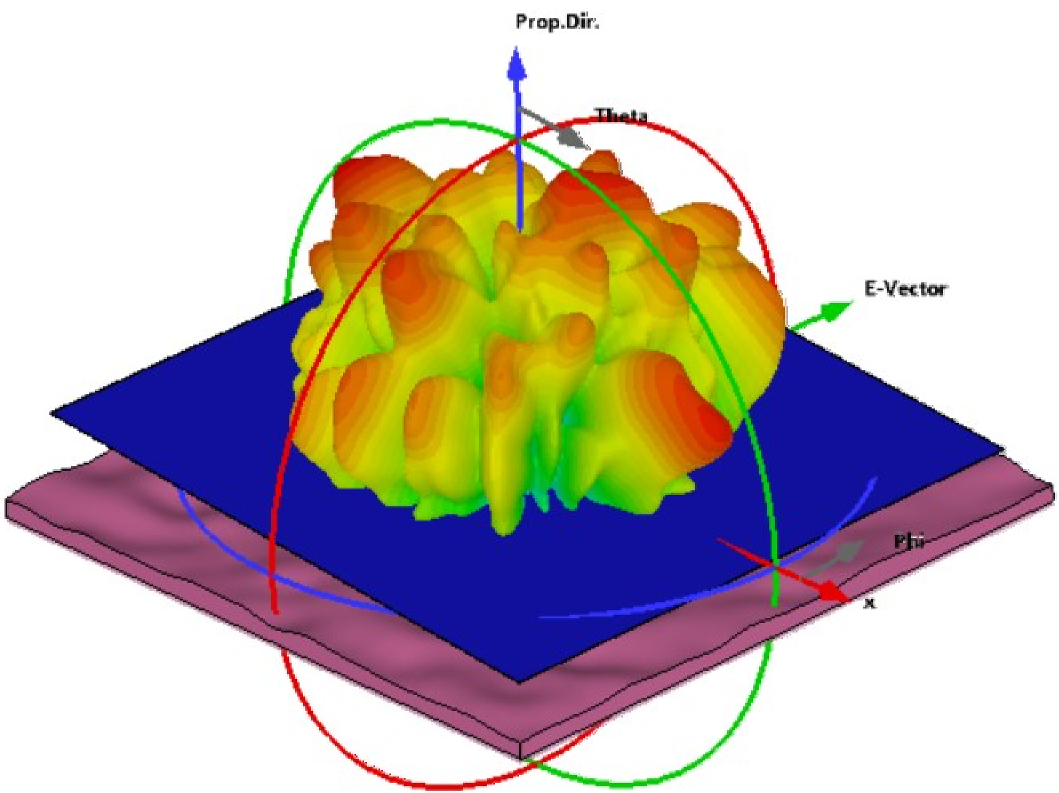
CST Studio Suite for Accurate Component-Level Simulation



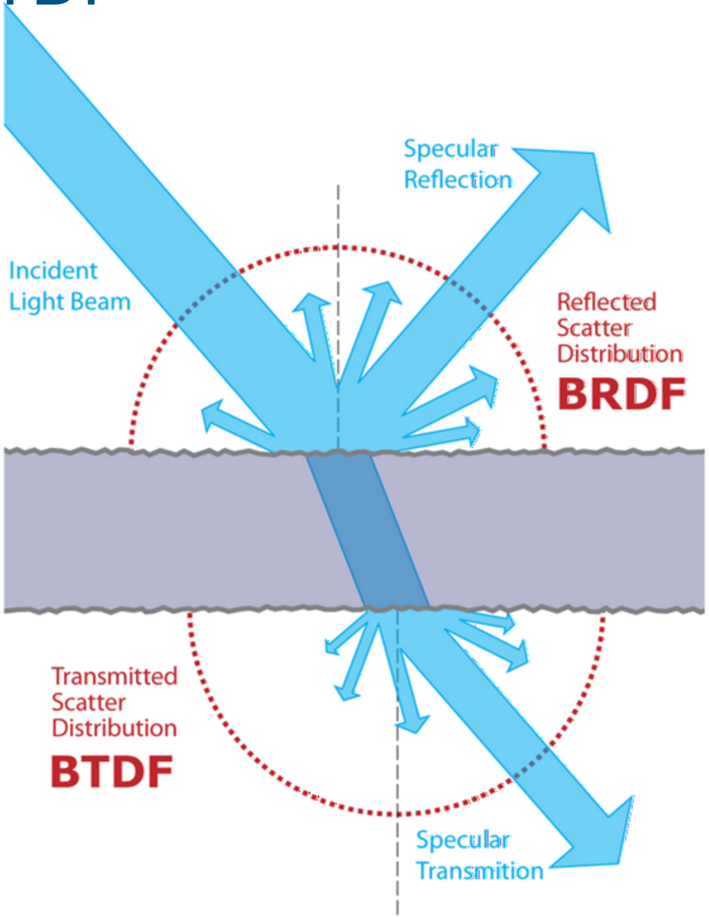
DASSAULT SYSTEMES

Examples

Example: BxDF Calculation



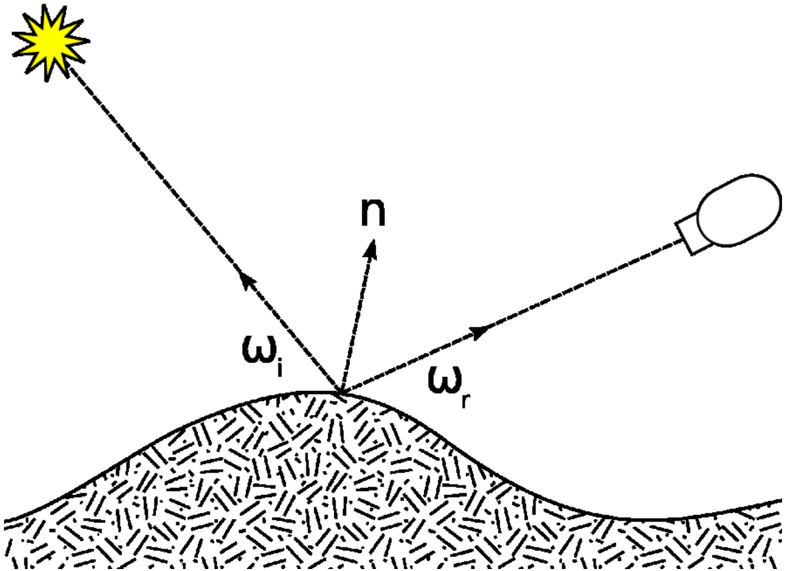
BSDF = BRDF + BTDF



Bidirectional Reflectance Distribution Function

$$f_r(\omega_i, \omega_r) = \frac{\mathrm{d}L_r(\omega_r)}{\mathrm{d}E_i(\omega_i)} = \frac{\mathrm{d}L_r(\omega_r)}{L_i(\omega_i)\cos\theta_i \mathrm{d}\omega_i}$$

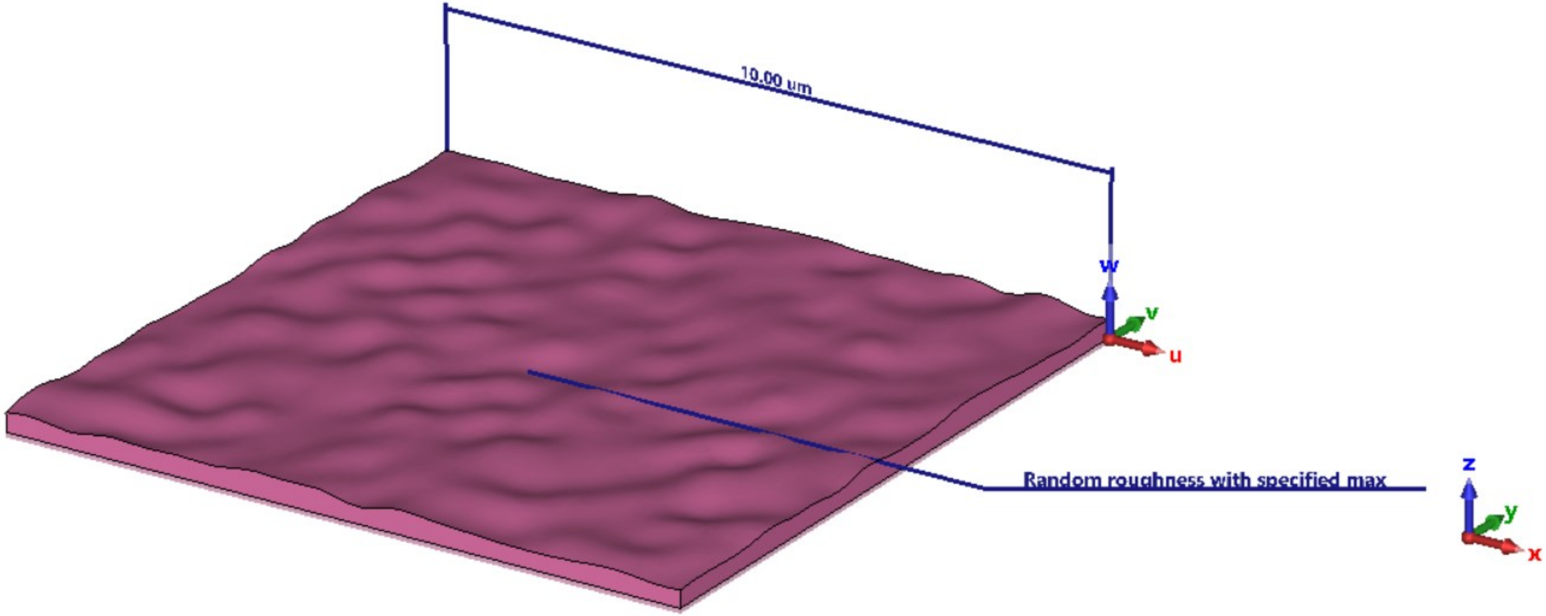
L = Radiance
E = Irradiance
Θ = Angle between incident light and surface normal
ω = Solid angle for incident/reflected light



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

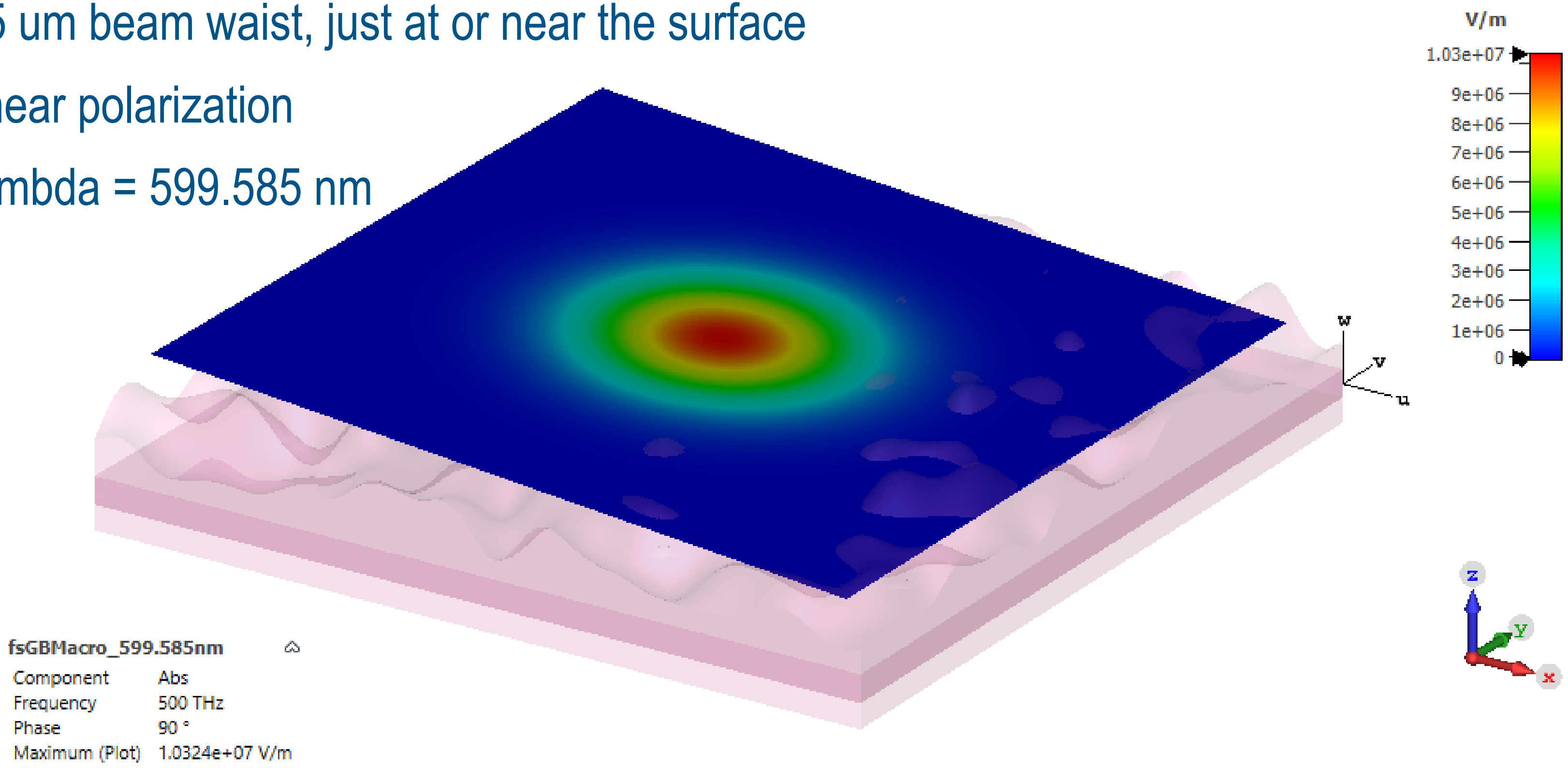
Example Geometry

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



Illumination Source: Gaussian Beam

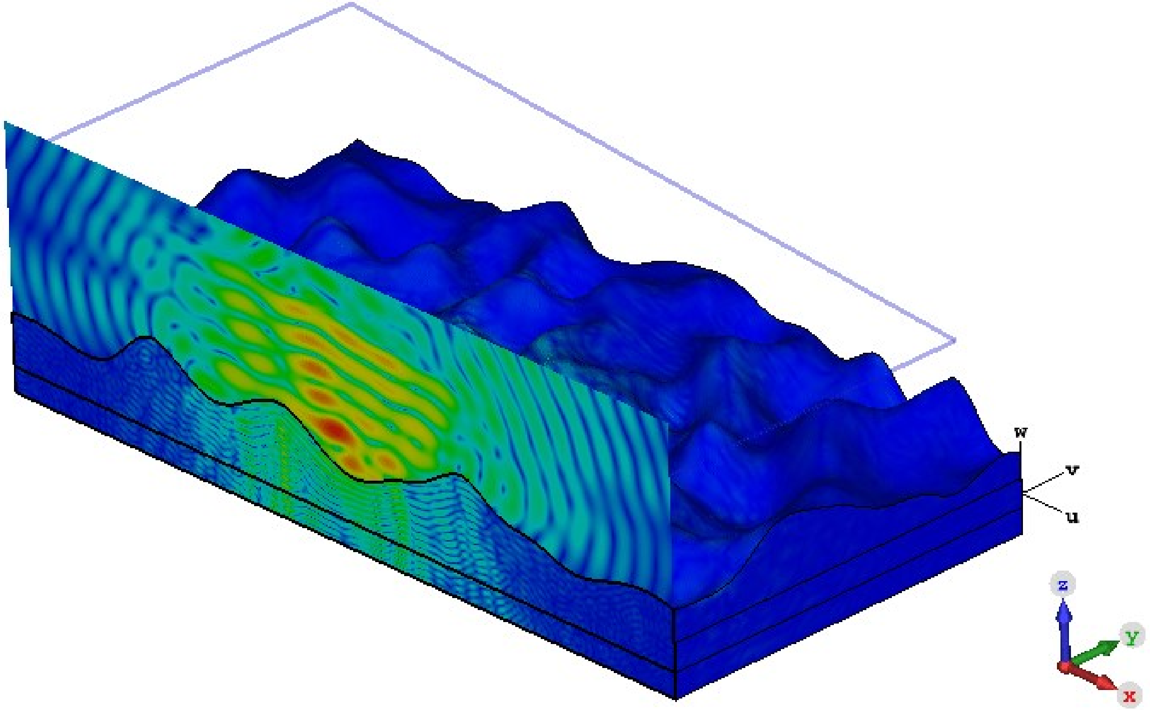
- 1.5 um beam waist, just at or near the surface
- Linear polarization
- Lambda = 599.585 nm

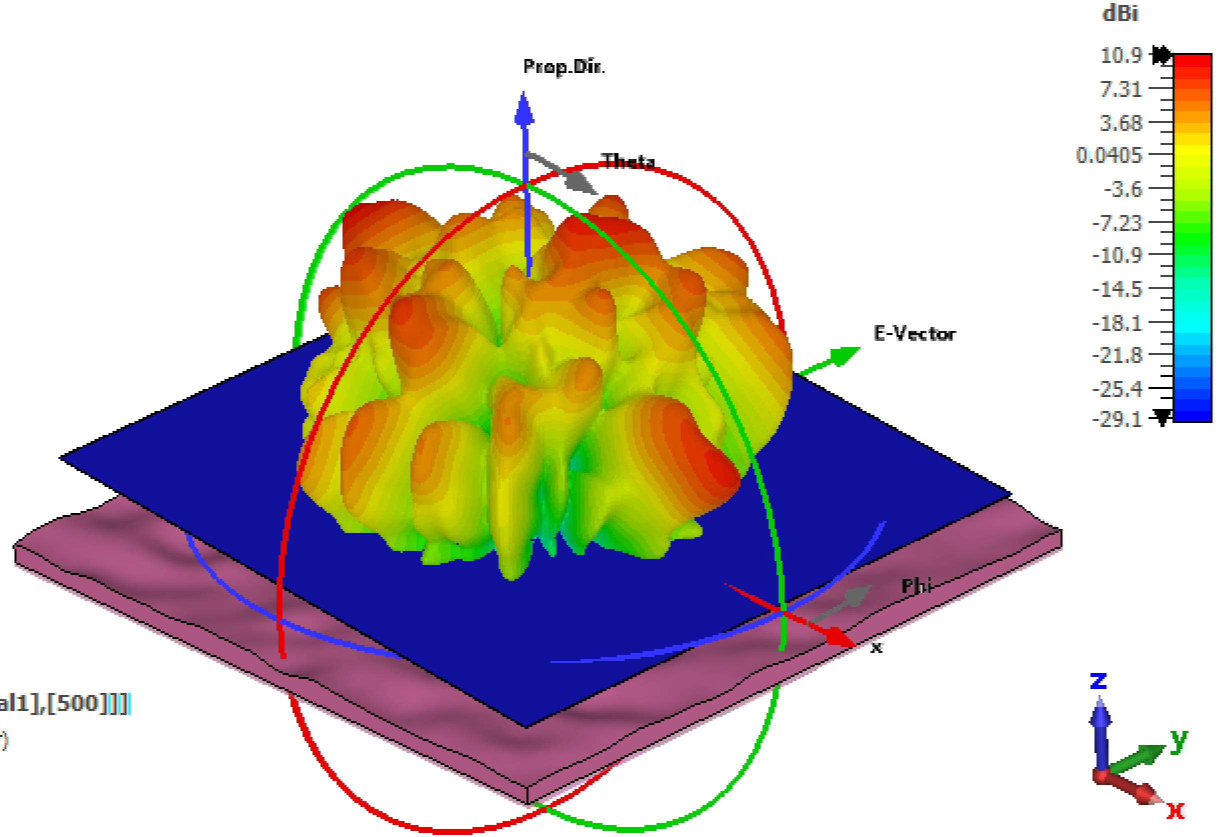


Solver Setup and GPU Acceleration

```
                    Peak memory used (kB)        Free physical memory (kB)
                                                  At begin      Minimum
  ---------------------------------------------------------------------
  CAD preparation   16820                         258982268     258982268
  Matrices calc.    26301757                      258962890     232424804
  Solver run total  33538548                      259006976     228098060
  ---------------------------------------------------------------------

-------------------------------------------------------------------------
Solver Statistics:

  Hardware:
     Computer name:

     Number of CPU 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 )
```

Nearfield Results



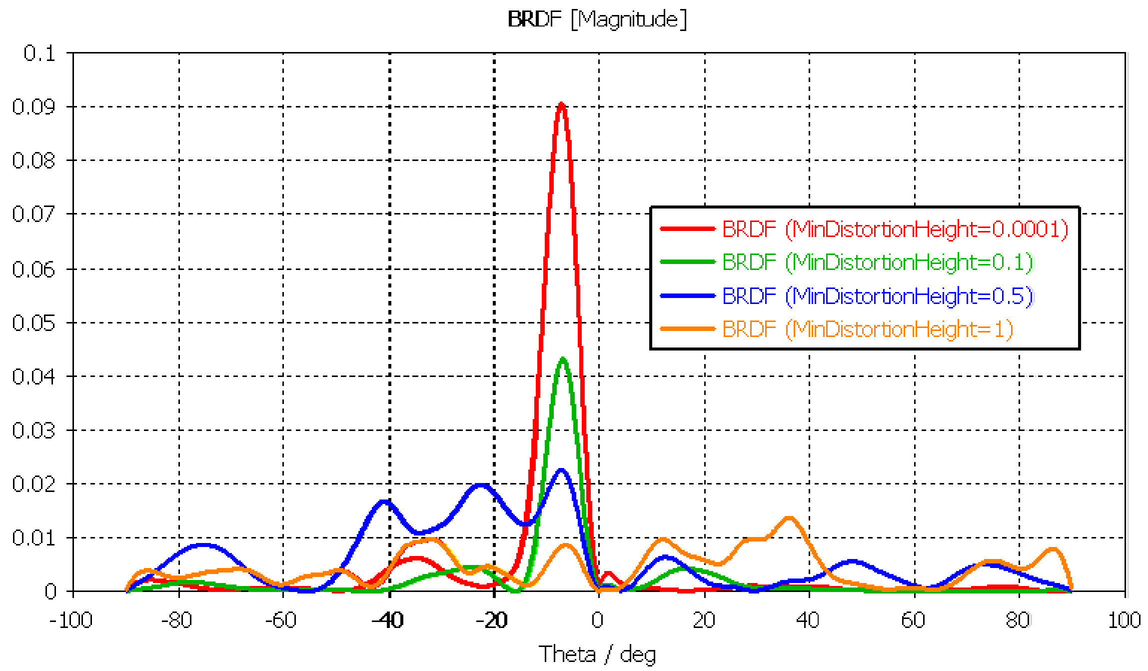


farfield (f=500) [fsG...,0.0,signal1],[500]]]

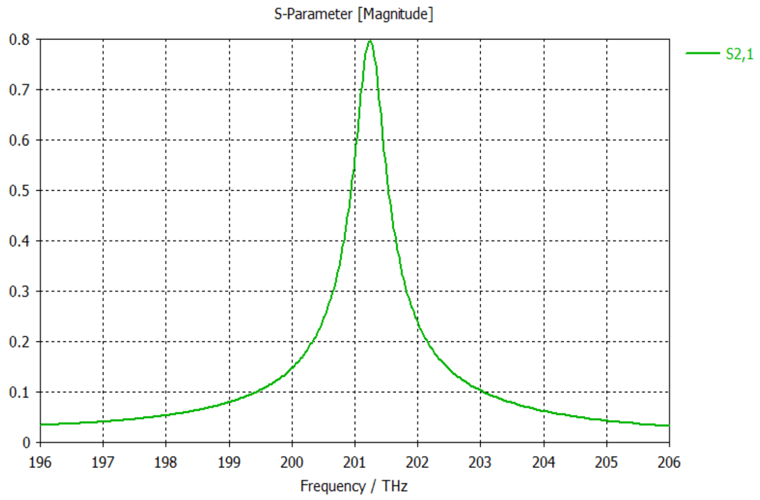
Type	Farfield (Multilayer)
Approximation	enabled (kR >> 1)
Component	Abs
Output	Directivity
Frequency	500 THz
Dir.	10.95 dBi

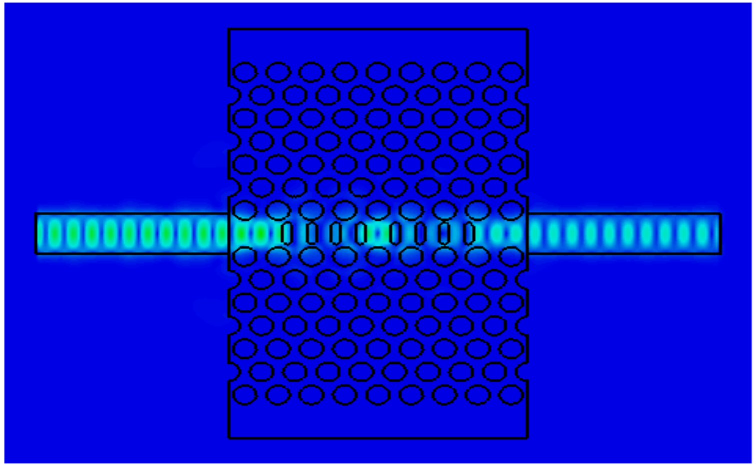
BRDF Result

- 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

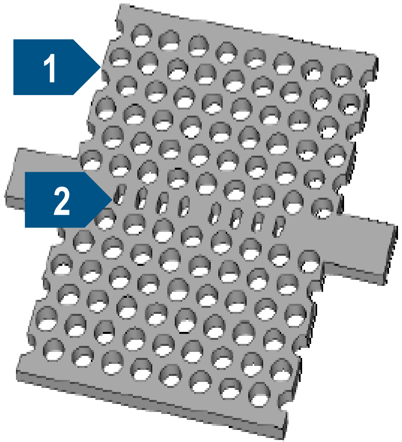




Ref: Tuning the resonance of a photonic crystal microcavity with an AFM probe *Iwan Märki, Martin Salt and Hans Peter Herzig*, OPTICS EXPRESS 2969 *Vol. 14, No.* 3 April 2006

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

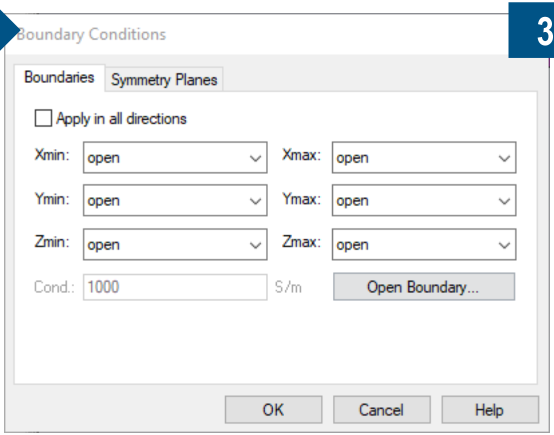


Define Boundary and Symmetry

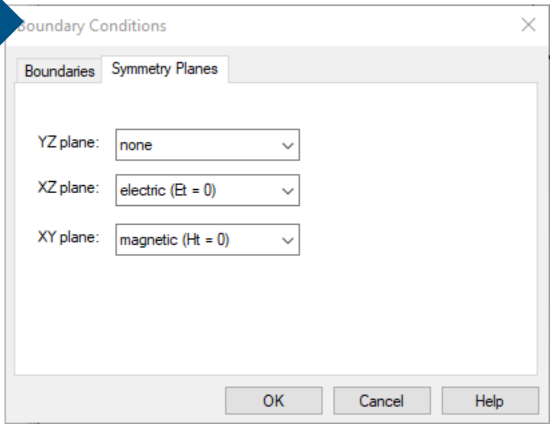
- Under the Simulation ribbon set up the boundaries
- Boundaries open in all directions
- Symmetry Planes as shown

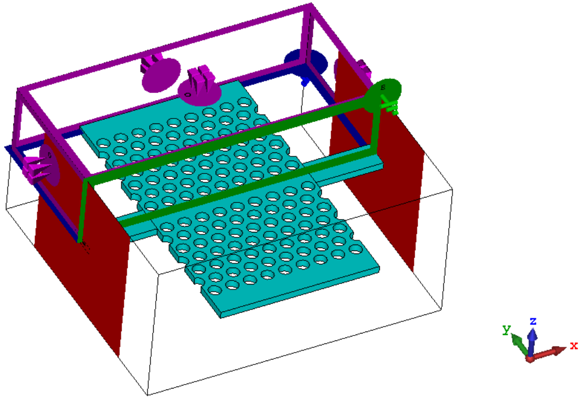
1

2



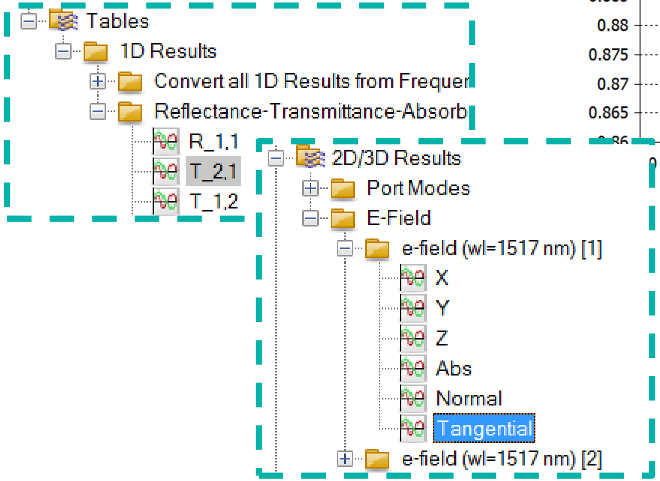
3

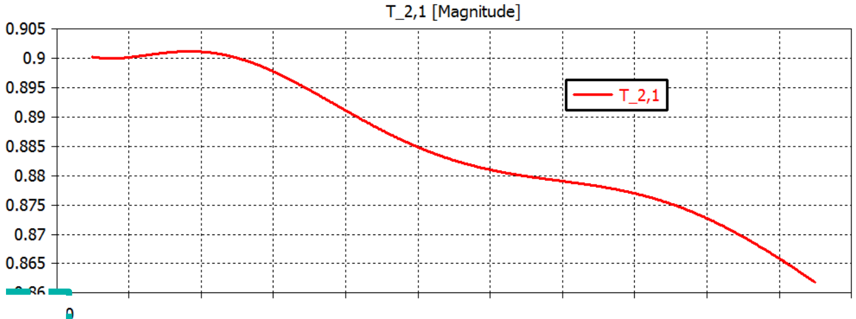


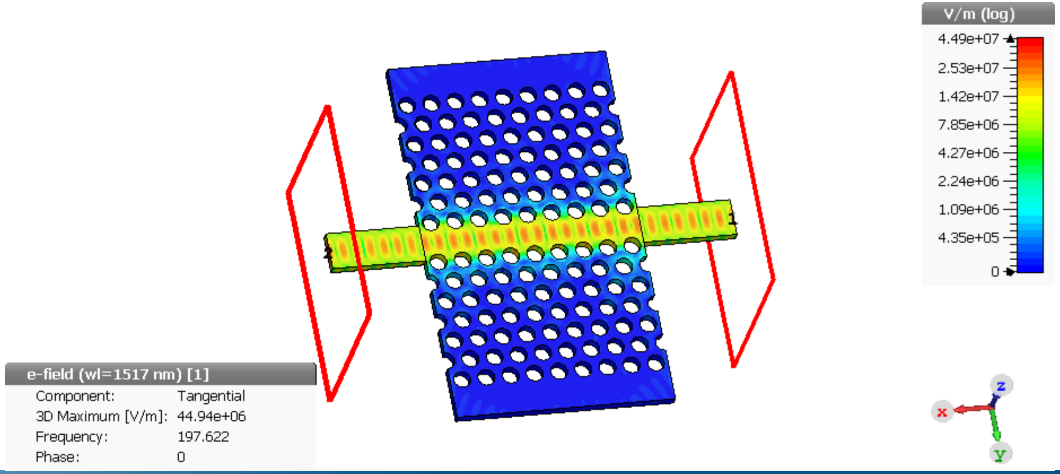


Simulation Results

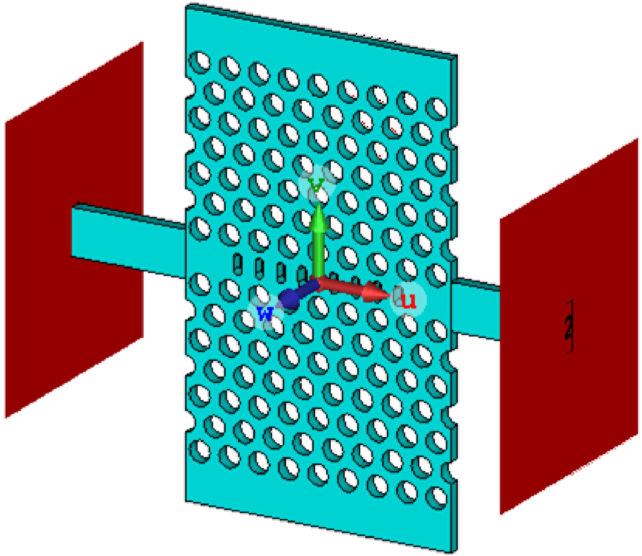
Dielectric waveguide (launch) is operated at the bandgap of photonic crystal, where wave can propagate without much interaction.

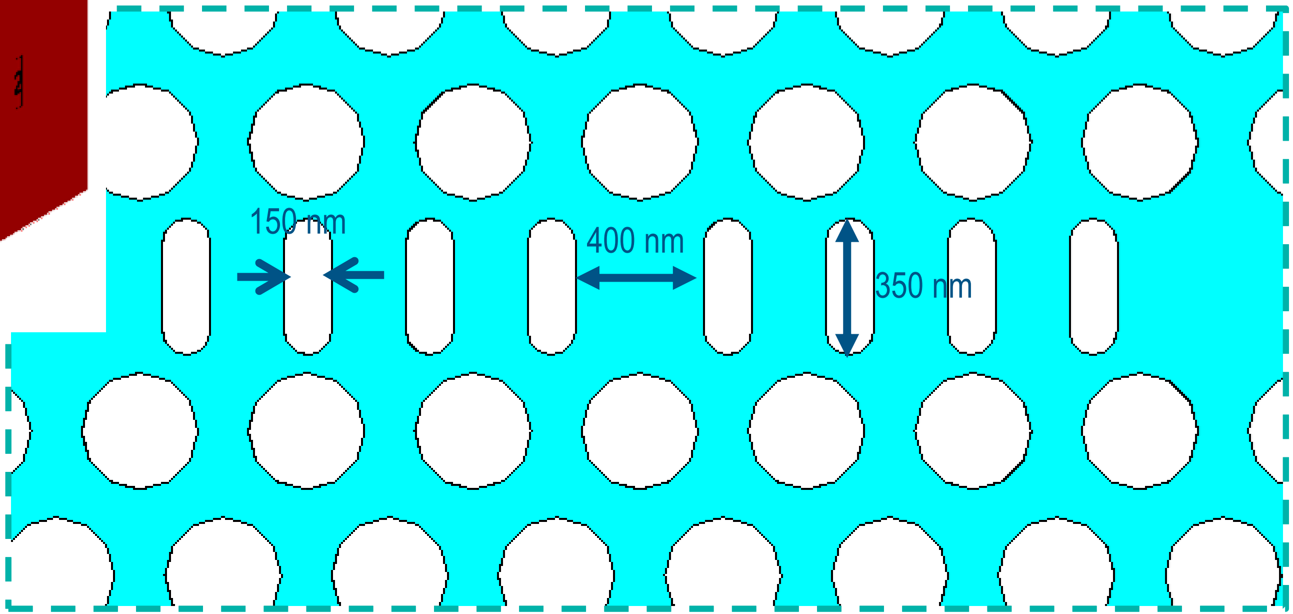






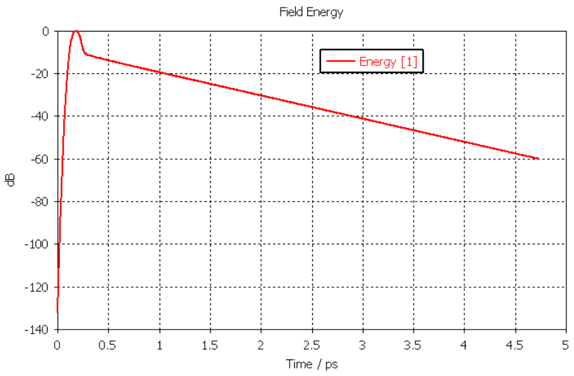
Final Geometry with Bragg Reflector Cavity

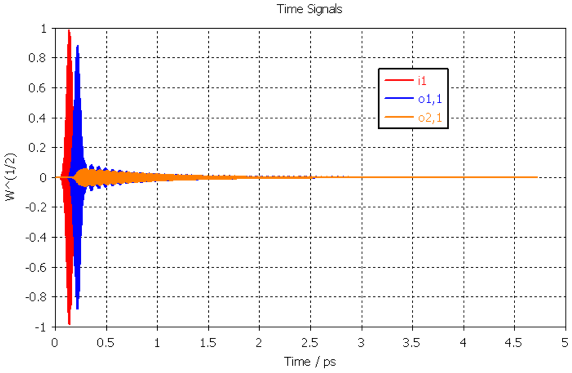


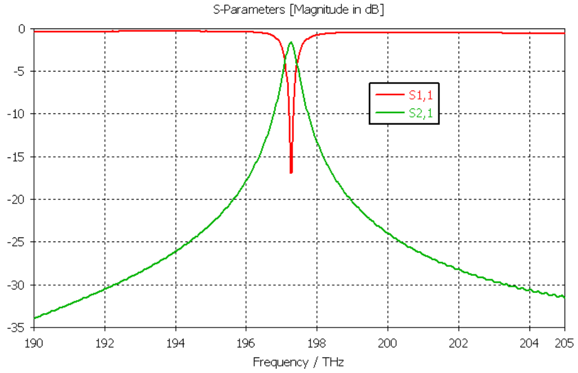


Time Domain Results

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





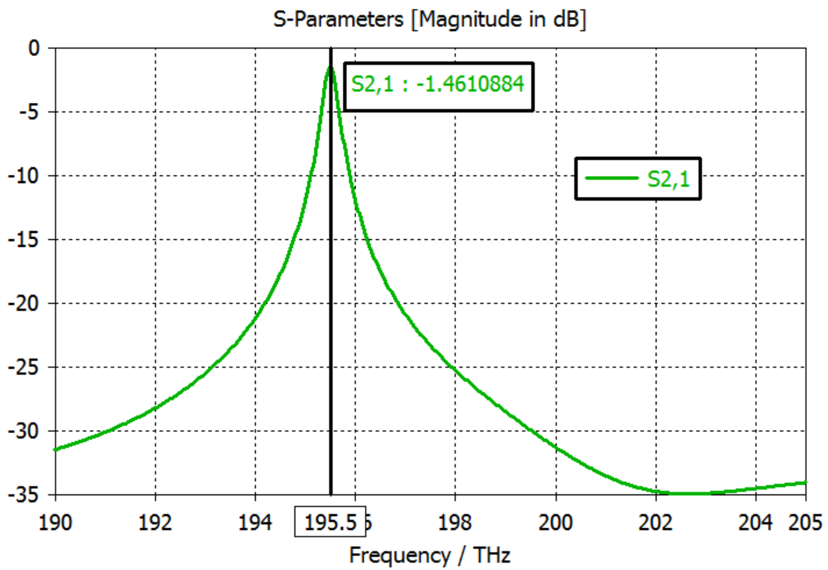


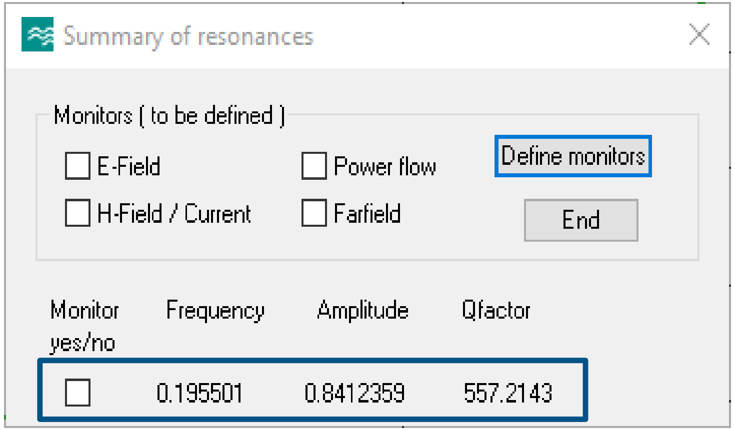
- ▶ Alternative approach: Frequency Domain solver
  - ▷ Increased memory usage but faster results

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

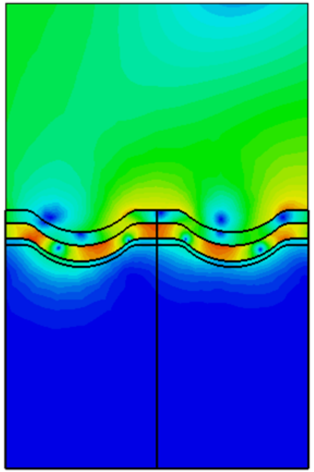
- Execute **Measure Resonances and Q-values from freq-data** macro to calculate Q factor from S2,1

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



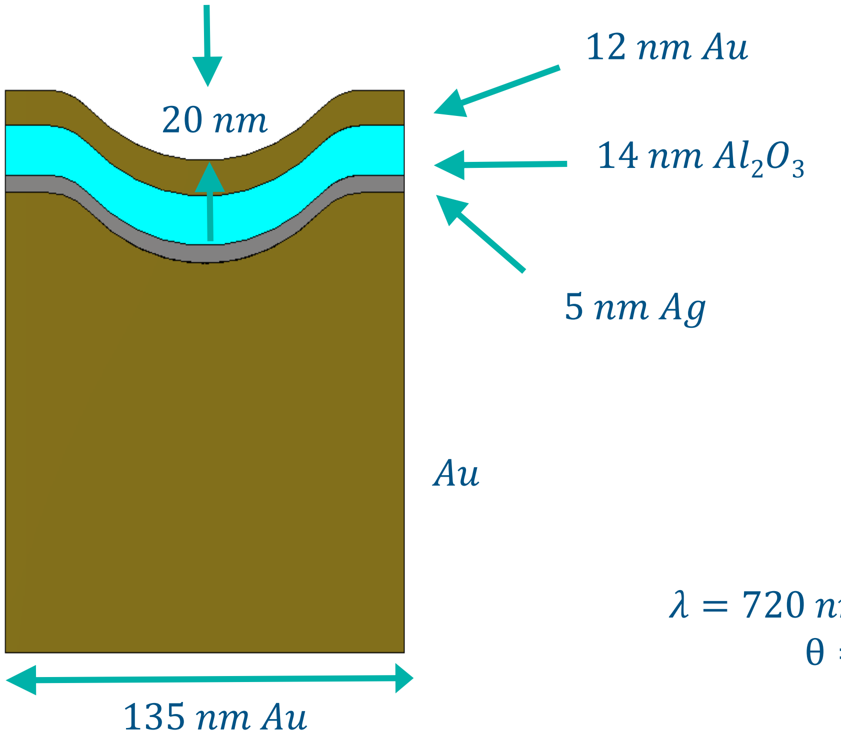


Example: Metal-Insulator-Metal Plasmon Coupling Diffraction Gratings



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

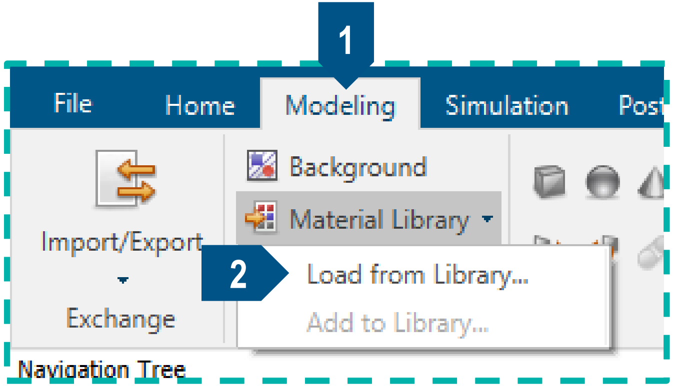
Geometry/Unit Cell Details

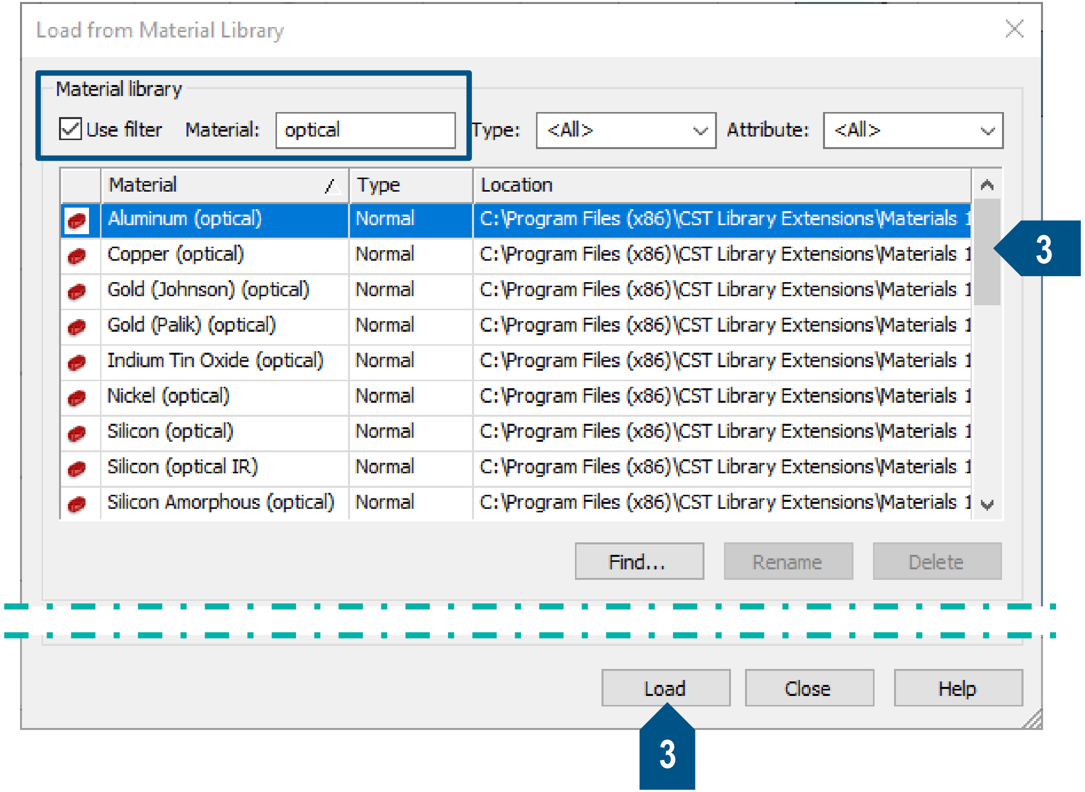


$$\lambda = 720\, nm \rightarrow 416\, THz$$
$$\theta = 53°$$

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



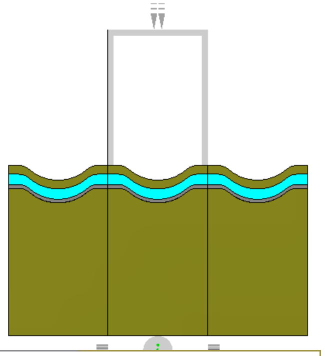


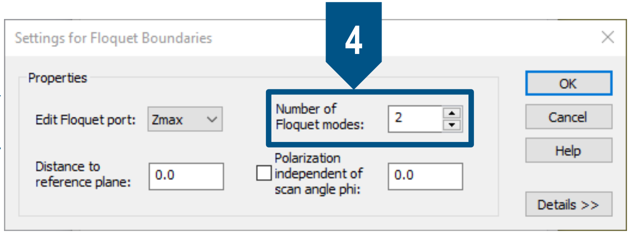
Hint: Use the filter “optical” to only display the materials for the optical frequency range.

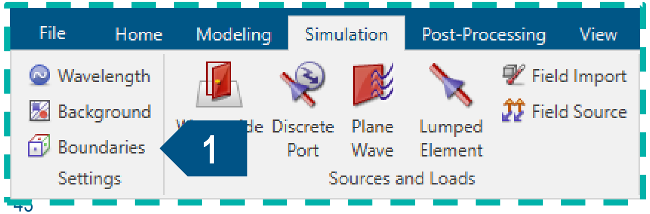
Specify Boundary and Excitation Condition

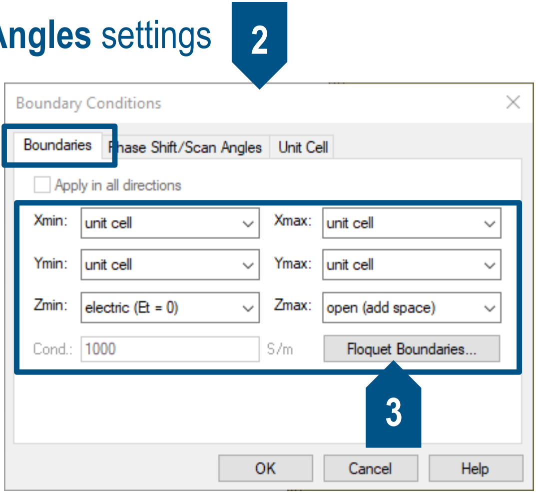
Specify boundary conditions, scan angle and Floquet port boundaries

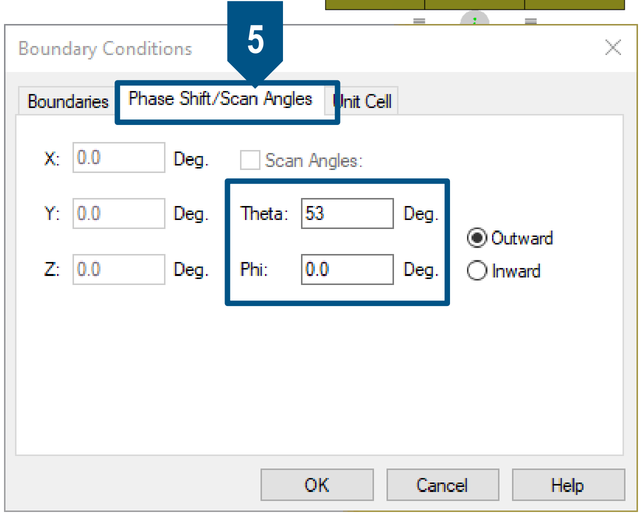
- Select **Boundaries** in the Simulation Tab
- Set the **Boundaries** settings as shown
- Switch to the Floquet Boundaries window
- Change the **Number of Floquet modes**
- Change the **Phase Shift/Scan Angles** settings



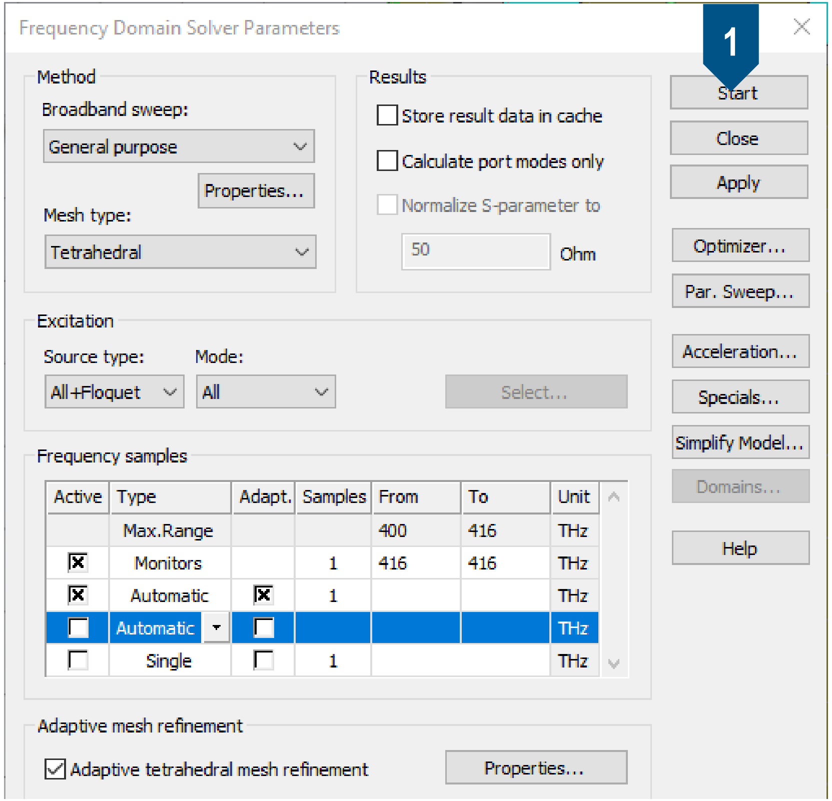








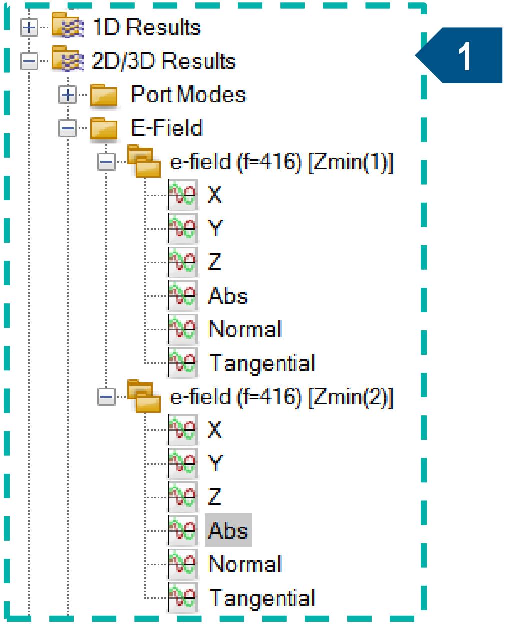
Start the Frequency Domain Solver

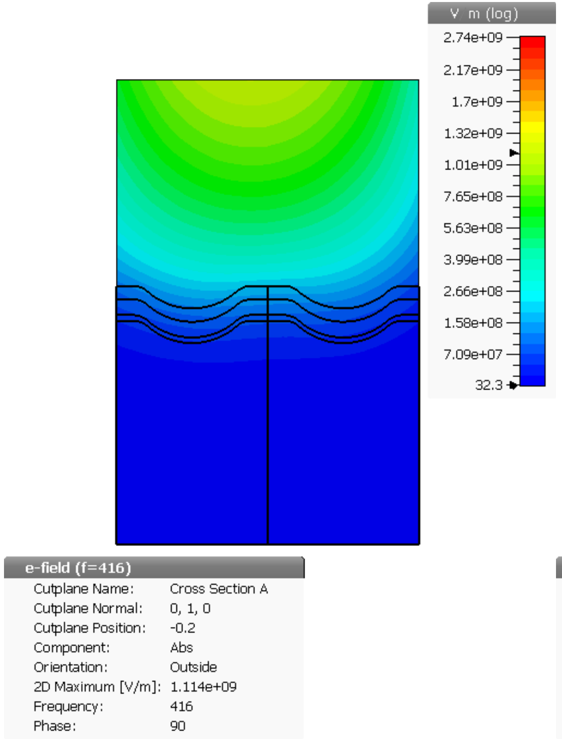


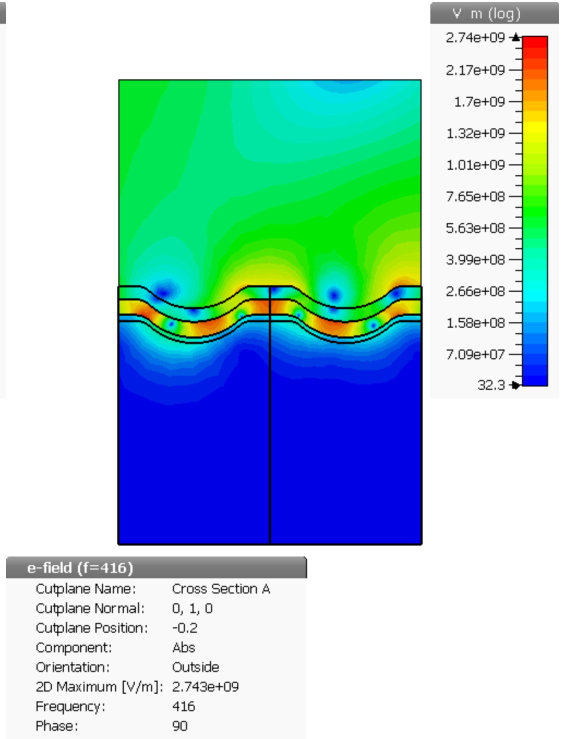
Field Results

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

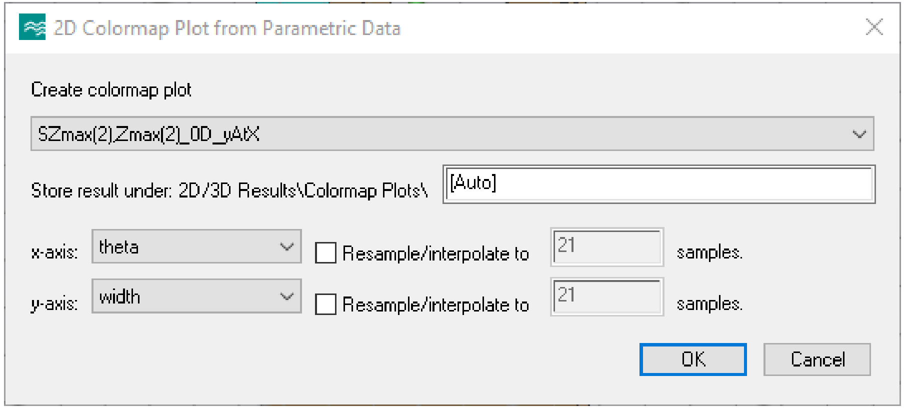


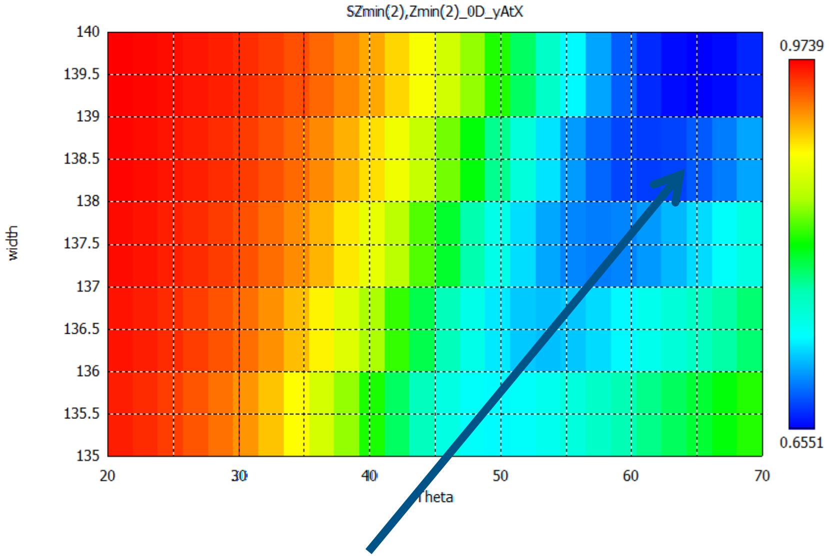




Convert Parametric Data to 2D Colormap

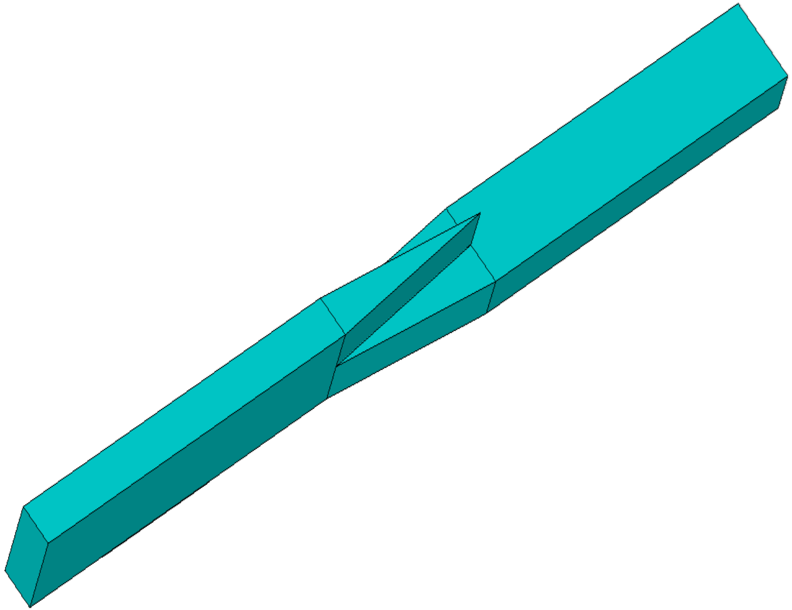
- Select newly created results
- Run Macros → Results → Tables → Create 2D Colormap Plot from Parametric Data





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

Example: Silicon Waveguide Based TE Mode Converter

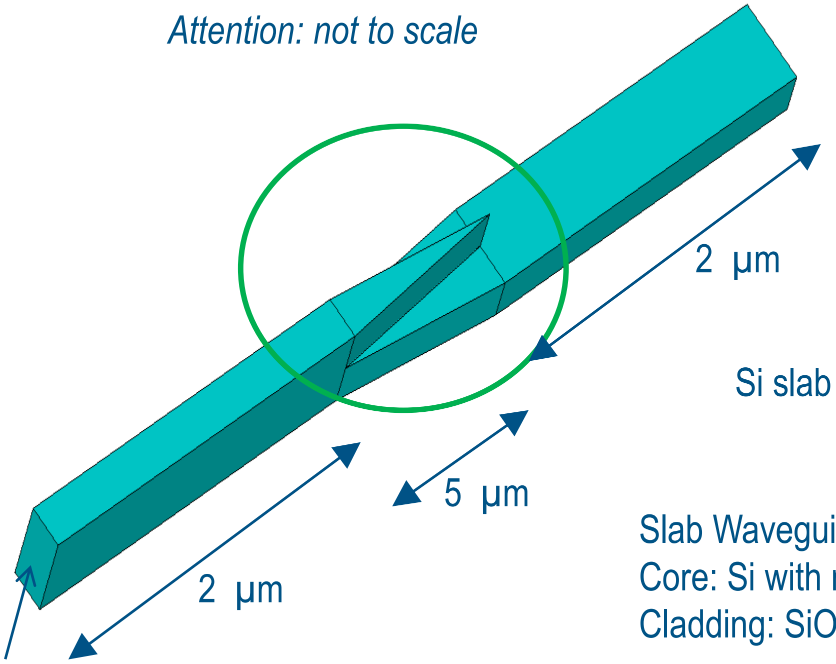


Ref: Silicon waveguide based TE mode converter *Jing Zhang,* Tsung-Yang Liow, Mingbin Yu, Guo-Qiang Lo, and Dim-Lee Kwong*, OPTICS EXPRESS *VOLUME 18, NUMBER 24 18 Nov. 2010*

DASSAULT SYSTEMES

Geometry Details

Attention: not to scale



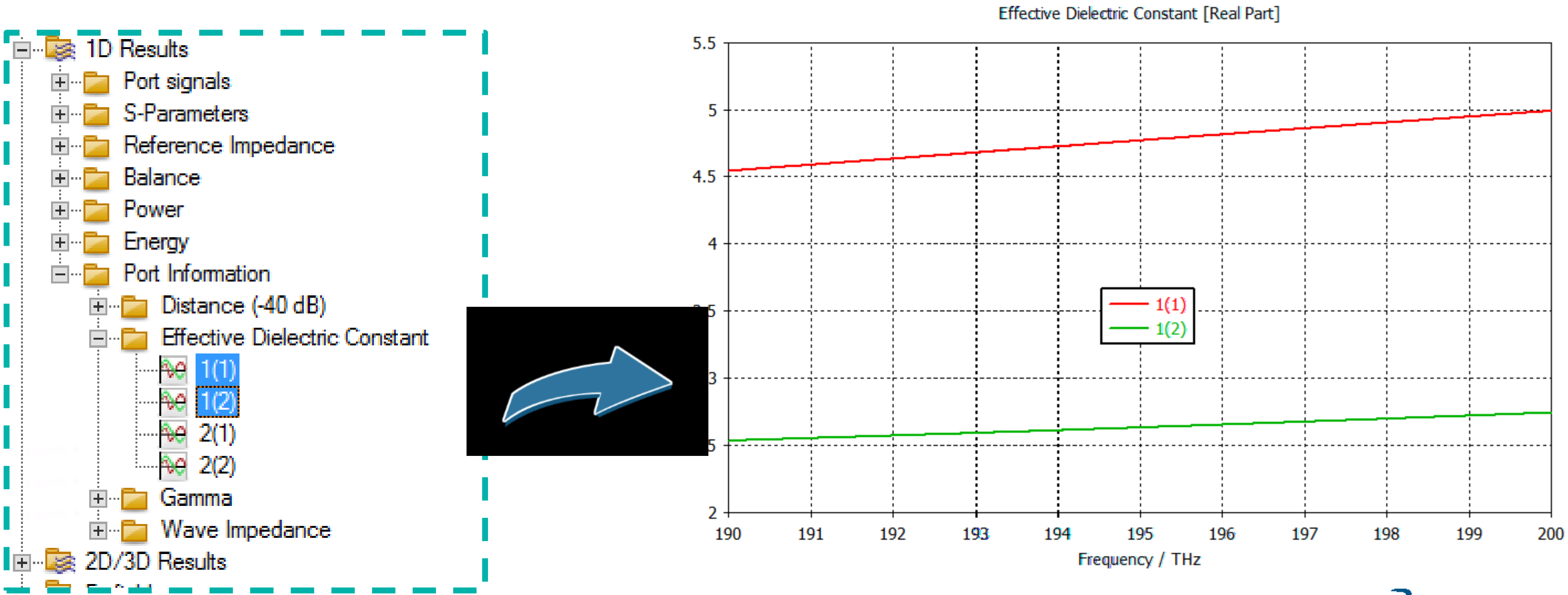
Si slab 400 nm X 200 nm

Si slab 200 nm X 400 nm

Slab Waveguide
Core: Si with n_{core} = 3.5
Cladding: SiO_2 with n_{clad} = 1.45

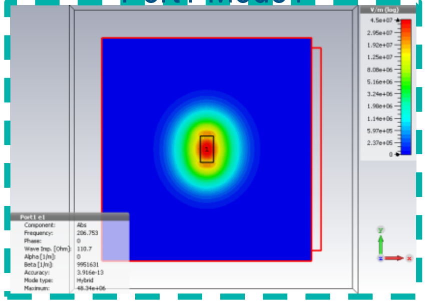
Port Information

- 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

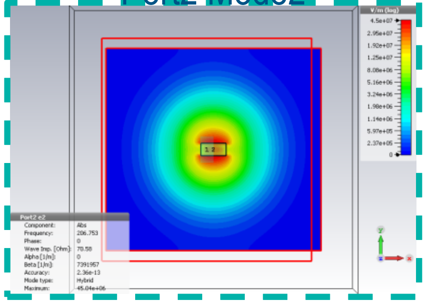


Simulation Results

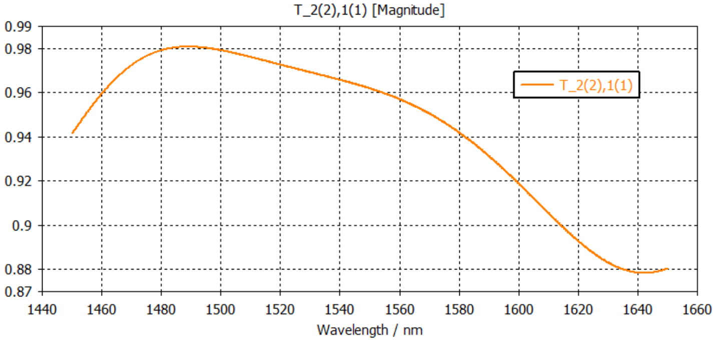
Port1 Mode1

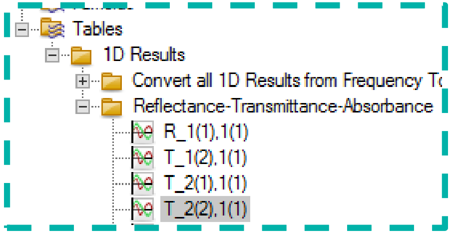


Port2 Mode2

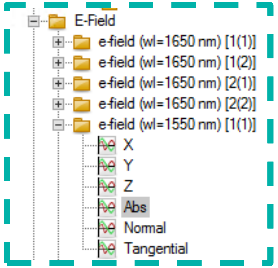


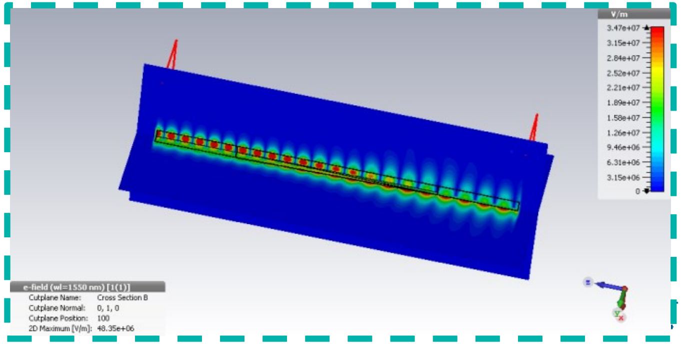
High mode conversion rate (ranging from 88 % to 98 %) over frequencies is observed.



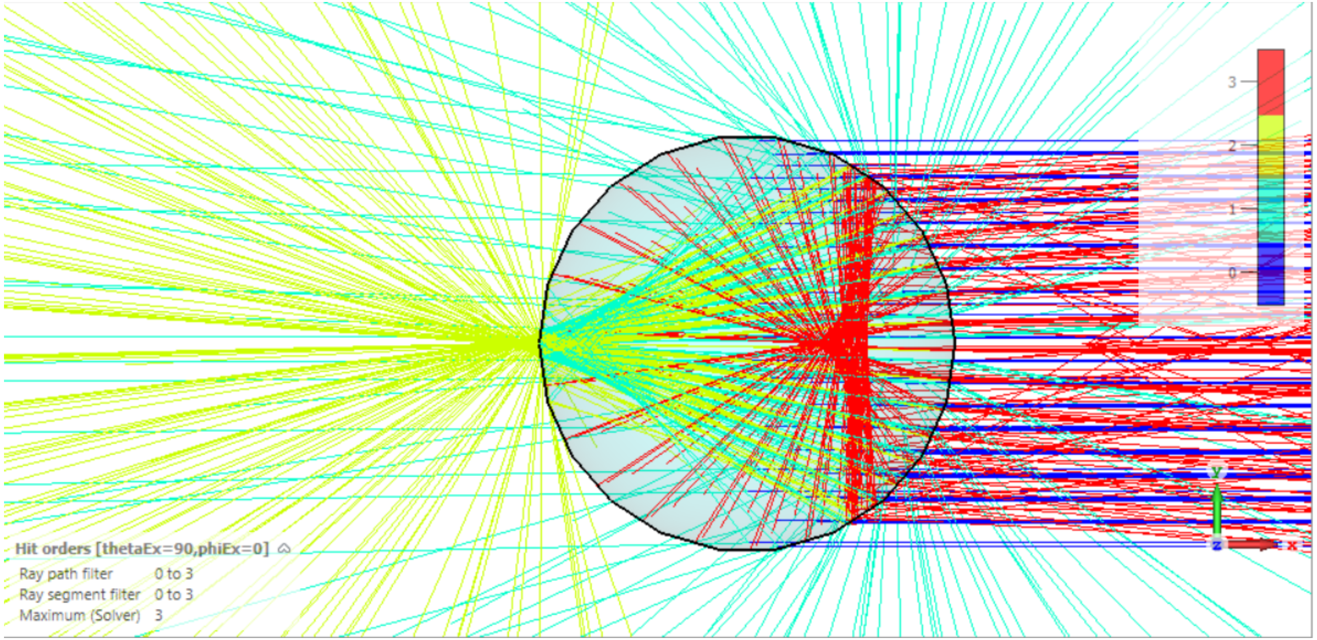


Field monitor results at λ=1550nm



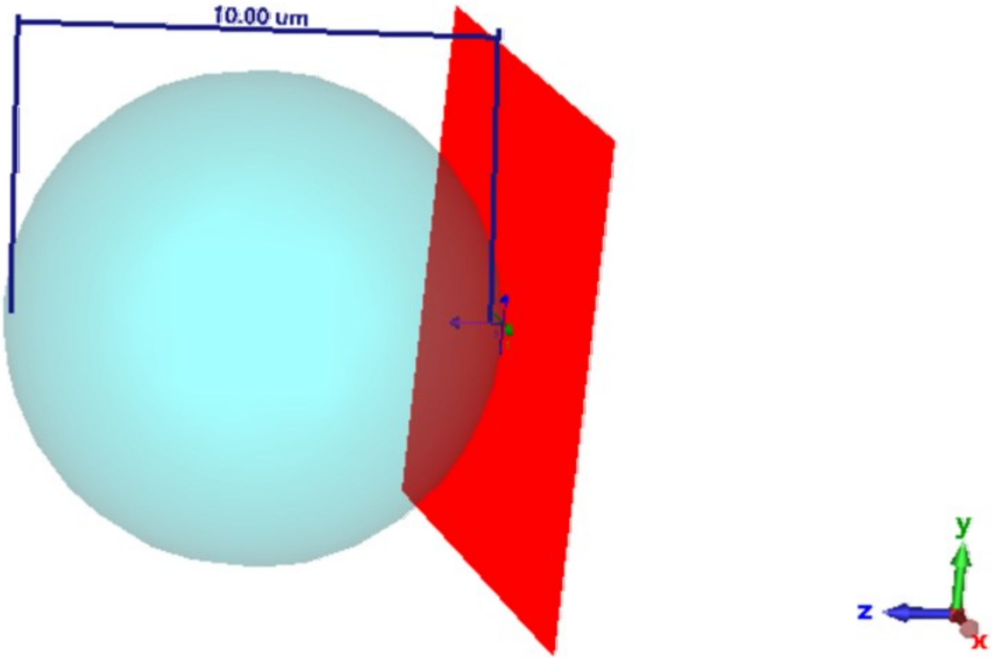


Example: Convex Microlens Simulation



Geometry Details

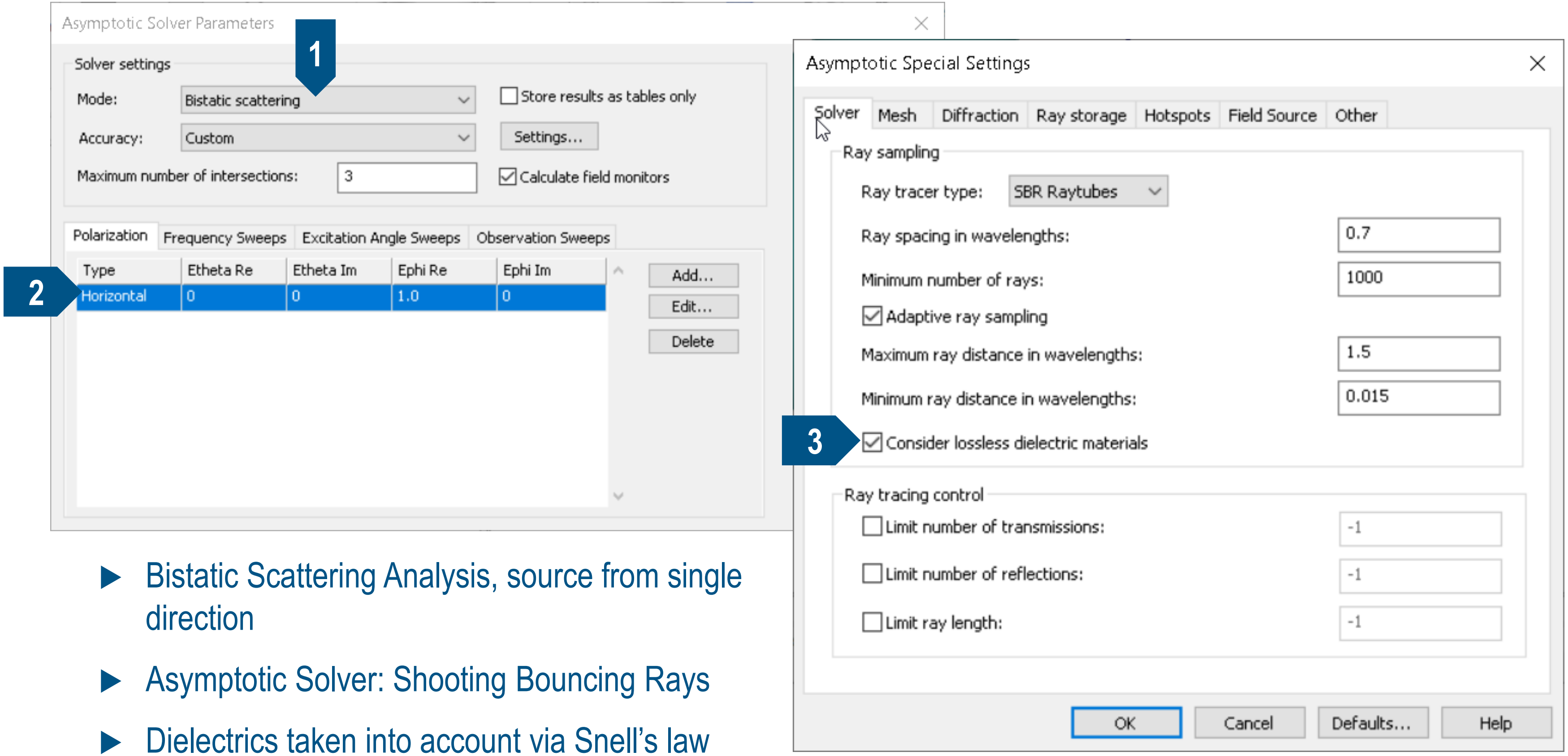
- Simple Geometry: Spherical lens (n=1.7) with plane wave illumination



Planewave

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

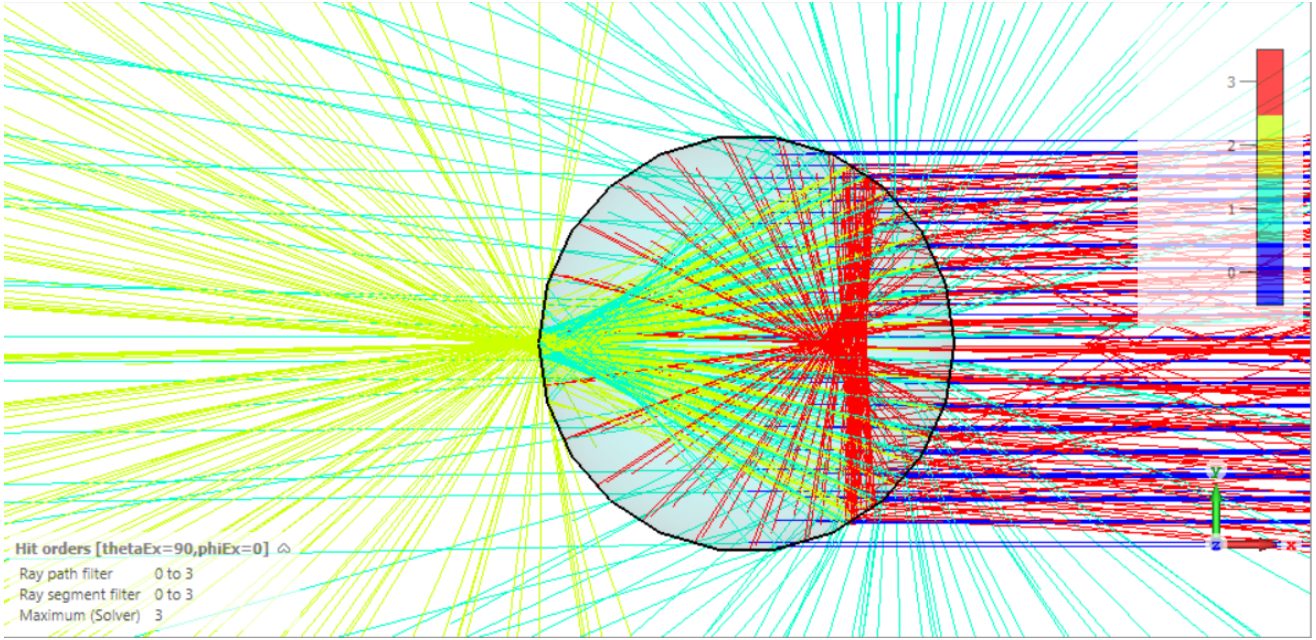
Simulation Details



- 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

DASSAULT SYSTEMES

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?

IF WE™