# Blackbody Simulations Usage Guide

Updated 8/12/2025 Jason Wang

\* For more details, see <u>here</u>

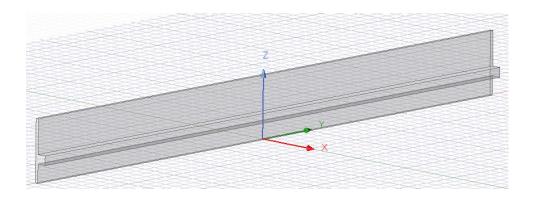
#### Big Picture

- Simulate the response of a waveguide to an incoming photon, modeled as a plane wave
  - What is the probability the photon makes it to the other side of the waveguide without being absorbed?
  - Where on the outgoing face will the photon be emitted?
  - Toward which direction will the outgoing photon be emitted?
- Frequency dependent, polarization dependent, incoming angle dependent...
- Run Ansys HFSS simulations!

## Initial Setup

#### Importing the Geometry

- On the HFSS main menu, open a new project, go to Modeler / Import and choose the .STL file to import
  - Alternatively, build your own model geometry
  - The ingoing and outgoing face should be planar, and the ingoing and outgoing faces are preferably aligned with one of the XY, XZ, or YZ planes. This makes specifying the ingoing and outgoing angles much easier (to be explained later)



#### Opening the Code

- Create an Anaconda environment with the following packages: pyaedt, scipy, pandas, numpy, seaborn
- On Github, make a copy of the latest version of the bbsim.py <u>code</u>.
- Following the import statements, there is a list of parameters to be filled. We'll go through them one at a time

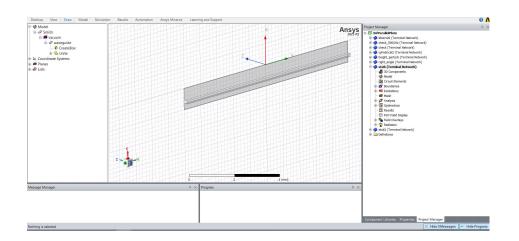
### Variables in the Code

#### Frequency

- Frequency: the frequency at which the simulation is run (GHz)
  - Specified via the command-line argument in terminal, e.g. python bbsim1freq.py 500
    - Runs the simulation at 500GHz
- The simulation creates a COPY of the existing design in HFSS, where the new design name is {old\_design\_name}\_{frequency}GHz

#### Project, Design, Feature Name

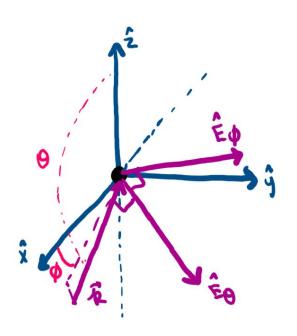
- project\_name, design name, feature name: Name of the project and design (project manager) and the feature to model (layout manager)
  - In the example
    - project\_name = InfParallelPlate
    - design\_name = stub
    - feature\_name = waveguide



#### import\_from\_existing\_csv

- import\_from\_existing\_csv: Whether to import the data file from an existing.csv.
  - If import\_from\_existing\_csv = True, then rather than running the simulation from the start, the code runs a refined simulation from the imported csv file
    - Need to specify the waveguide csv (giving |S21| and the electric field at the outgoing face as a fxn of ingoing angles) and the far-field csv (giving the far-field electric field as a fxn of ingoing angles)
    - The code automatically infers the frequency and polarization from the name of the file, so it should be of the form {project\_name}\_{design\_name}\_{frequency}GHz\_Ephi={0 or 1}/{waveguide or far\_field}.csv"
      - Ephi = 0 corresponds to polarization in the  $\theta$  direction; Ephi = 1 corresponds to polarization in the  $\phi$  direction (see conventions on next slide)
- Most of this time, we can safely set import\_from\_existing\_csv to be False

#### Conventions for $E_{\phi}$ and $E_{\theta}$



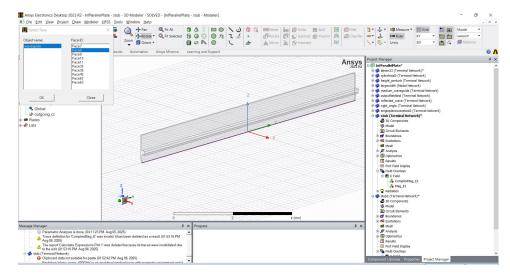
- $\theta$ -direction is  $(\cos \theta \cos \phi, \cos \theta \sin \phi, -\sin \theta)$
- $\varphi$ -direction is  $(-\sin \varphi, \cos \varphi, 0)$

#### HFSS Analysis Parameters

- Ei: Strength of ingoing electric field, used to calculate the ingoing power. For the purposes of the simulation, there is no reason to change it, since probability distributions are agnostic to the absolute strength of the electric field
- max\_delta\_E, max\_passes, num\_cores: HFSS parameters
  - max\_delta\_E: Criterion for HFSS simulation convergence. 0.02 is a good balance between speed and accuracy
  - max\_passes: Maximum number of adaptive passes the HFSS simulation runs before termination
  - num\_cores: Number of cores used in the HFSS simulation

#### Ingoing and Outgoing Face ID's

- ingoing\_face\_id, outgoing\_face\_id: the numerical IDs of the faces where the plane wave should enter and exit
  - Where it says "Select" on the HFSS home screen, change "Object" to "Face"
  - Under "Object Name", click on your model object
  - Identify which faces correspond to the ingoing and outgoing faces.
    - In the image, we see that in this geometry ingoing\_face\_id = 8



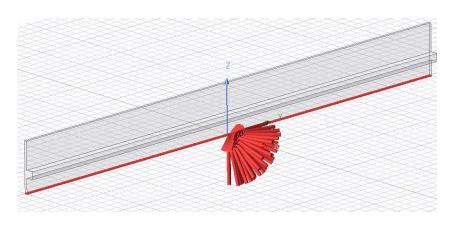
#### Electric Field at Outgoing Face

- manual\_field, outgoing\_face\_boundary, outgoing\_face\_field\_resolution:
  - o If manual\_field is set to False, HFSS will infer the appropriate sampling resolution, but it is coarse. If manual\_field is set to True and outgoing\_face\_boundary is set to None, the bounding region for the outgoing face is inferred, but it only works for rectilinear faces aligned with the coordinate axis. outgoing\_face\_boundary can also be manually specified for non-rectilinear geometries (coordinates relative to global CS)

```
manual_field = True
outgoing_face_boundary = None # Or specify ([x1, y1, z1], [x2, y2, z2]), e.g.([0, -5, 1], [0.05, 5, 1]) Boundary of the outgoing face (relative to global CS)
outgoing_face_field_resolution = ["0.001mm", "0.1mm", "0.mm"] # Resolution in outputting the electric field at the outgoing face
```

#### Frequency and Ingoing Angle Sweeps

- i\_theta\_lower, i\_theta\_upper, i\_phi\_lower, i\_phi\_upper
  - The code will scan the ingoing angles for  $\theta$  from [i\_theta\_lower, i\_theta\_upper] and  $\varphi$  from [i\_phi\_lower, i\_phi\_upper]. These angles are defined relative to the global coordinate system, and the angle is defined relative to the tail of the ingoing wavevector
- i\_theta\_step, i\_phi\_step: the coarseness of the initial sweep, in degrees. 0.8 degrees is a good starting point.



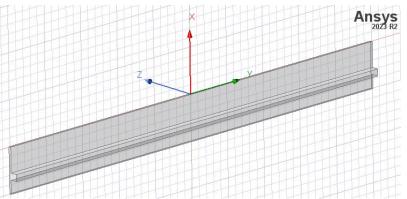
\*Corresponds to i\_theta\_lower = 90, i\_theta\_upper = 180, i\_phi\_lower = 0, i\_phi\_upper = 90, i\_theta\_step = 15, i\_phi\_step = 15

#### Outgoing Angle Sweeps

- outgoing\_face\_cs\_x, outgoing\_face\_cs\_y
  - Allows the user to redefine a coordinate system at the outgoing face
  - outgoing\_face\_cs\_x is the direction of the x-axis in the new coordinate system, and is specified with coordinate with respect to the old coordinate system
    - Example: outgoing\_face\_cs\_x = [0, 0, 1] means that the x-axis of the new coordinate system is the old z-axis. outgoing\_face\_cs\_y = [0, 1, 0] means that the y-axis is left unchanged; see image
- rad\_theta\_lower, rad\_theta\_upper, rad\_phi\_lower, rad\_phi\_upper
  - $\circ$  The code will scan the outgoing angles for  $\theta$  from [rad\_theta\_lower, rad\_theta\_upper] and  $\phi$  from [rad\_phi\_lower, rad\_phi\_upper]. These angles are defined relative to the new coordinate system

#### Outgoing Angle Sweeps (cont.)

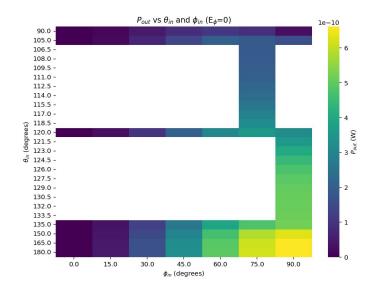
- a, b
  - a is the length scale [mm] of the dimension coinciding with the sweep over outgoing φ (outgoing angles defined with respect to newly defined coordinate system)
  - $\circ$  b is the length scale [mm] of the dimension coinciding with the sweep over outgoing θ
  - The wider the slit in the φ/θ direction, the narrower the diffraction pattern
- fineness
  - o  $\lambda$ /(a\*fineness) is the angular resolution (in radians) of the outgoing sampling. This follows from diffraction theory. fineness = 10 is a good start
- minimum\_coarseness, maximum\_coarseness
  - Hard bounds for the minimum and maximum angular resolutions to sample the far-field radiation pattern from



\*Corresponds to a = 10 mm (the sweep over phi, i.e. a sweep over outgoing angles in the XY plane) and b = 0.05 mm (a sweep over outgoing angles in the XZ plan.

#### Sweep Mode

- sweep = "discrete" or sweep = "adaptive"
  - Discrete sweep has no refinement process, and just runs the simulation and exports the data
  - Adaptive sweep will further look at the data, find the maximum point-to-point outgoing power difference, and find the most important regions to refine based on that
- max\_difference:
  - The maximum point-to-point difference in the outgoing power under which HFSS declares that the simulation has concluded successfully. max\_difference = 0.015 is a good start, and one can interpolate data with this 1.5% difference as a baseline



\*Illustration of adaptive sweep: large jumps between  $(\varphi, \theta) = (75, 120)$  and (75, 105) are patched. Similar, large jumps between  $(\varphi, \theta) = (90, 135)$  and (90, 120) are patched

## Simulation Usage

## No Need to Manually Input Anything Except the Variables

- The code is designed such that there is no need to set up analysis sweeps, parametric radiation boundaries, calculator expressions etc.
  - Simply press the run button (or use the command line) in the Python IDE used
- Additionally, if a mistake is made and the simulation needs to be rerun, there is generally no need to reset the existing simulation (i.e. no need to delete analysis sweeps, etc.)
  - o IMPORTANT: due to a bug in HFSS, you will want to rename the design before running again

#### Run Code Via Terminal

- Changed code to accept one frequency at a time via command line argument
  - E.g. python bbsim1freq.py 500 runs the simulation at 500GHz
- The simulation creates a COPY of the existing design in HFSS, where the new design name is {old\_design\_name}\_{frequency}GHz,
  - Makes it easier to run the different designs in parallel using HPC

```
faith_500GHz (Terminal Network)
faith_600GHz (Terminal Network)
faith_700GHz (Terminal Network)
faith_700GHz (Terminal Network)
```

#### Other Useful Things

- Due to the extensive sweeps, the code may take a while to run. Be patient!
- Calculating and exporting the data from HFSS takes a large amount of CPU, so be wary of that
- If, in the middle of the simulation, you need to stop the simulation, you can KeyboardInterrupt, which will then ask you if you want to save the existing data to a csv file
  - O By default, the simulation only saves the initial coarse sweep and the final, completed refined sweep to a .csv file. You can save a .csv file in the middle of a simulation via this method

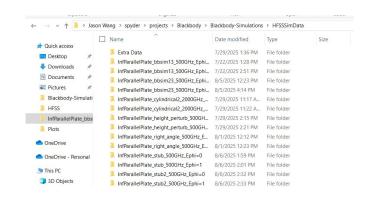
#### Workflow Summary

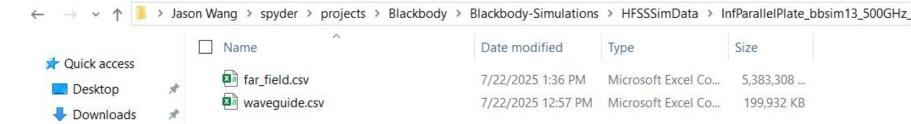
- Import/build new geometry
- Define the variables relevant to the geometry, sweep, etc. desired
- Run simulation via command line
- Process data (next section)

## Processing Data

#### File Structure

- All data files from the simulation will be stored in the same directory where bbsim.py is stored in a folder called HFSSSimData, organized by frequency and polarization
- Inside each folder, there are 2 csv files:
  - (refined)\_far\_field.csv
  - (refined)\_waveguide.csv
  - Whether or not there are files that have "refined" in front depends on whether adaptive or discrete sweep is chosen





#### (refined)\_far\_field.csv

- (refined)\_far\_field.csv: gives the electric field at outgoing angles specified as a function of ingoing angles specified
  - $\circ$  Gives complex-valued (real + i\*imag)  $E_{\phi}$  and  $E_{\theta}$  (with conventions on the polarizations in the  $\phi$  and  $\theta$  direction as given before in a diagram)

	А	В	С	D	E	F	G	Н	1	J
1	Freq	Ephi	<b>IW</b> avePhi	<b>IWaveThet</b>	Phi	Theta	rEphi_real	rEphi_imag	rEtheta_re	rEtheta_imag
2	500GHz	0	0	90	-90	0	0.000136	0.000133	2.26E-08	1.29E-07
3	500GHz	0	0	90	-89.6565	0	0.000136	0.000133	8.39E-07	9.29E-07
4	500GHz	0	0	90	-89.3129	0	0.000136	0.000133	1.65E-06	1.73E-06
5	500GHz	0	0	90	-88.9694	0	0.000136	0.000133	2.47E-06	2.53E-06
6	500GHz	0	0	90	-88.6259	0	0.000136	0.000133	3.29E-06	3.33E-06
7	500GHz	0	0	90	-88.2823	0	0.000136	0.000133	4.10E-06	4.13E-06
8	500GHz	0	0	90	-87.9388	0	0.000136	0.000133	4.92E-06	4.93E-06
9	500GHz	0	0	90	-87.5952	0	0.000136	0.000133	5.73E-06	5.73E-06
10	500GHz	0	0	90	-87.2517	0	0.000136	0.000133	6.55E-06	6.53E-06
11	500GHz	0	0	90	-86.9082	0	0.000136	0.000133	7.36E-06	7.32E-06
12	500GHz	0	0	90	-86.5646	0	0.000136	0.000133	8.18E-06	8.12E-06
13	500GHz	0	0	90	-86.2211	0	0.000136	0.000133	8.99F-06	8.92F-06

#### (refined)\_waveguide.csv

- (refined)\_far\_field.csv: gives the electric field at different (X, Y, Z) locations specified as a function of ingoing angles specified
  - $\circ$  Gives complex-valued (real + i\*imag)  $E_x$ ,  $E_v$ , and  $E_z$
  - Also gives OutgoingPower, and hence |S21|^2 = OutgoingPower/IngoingPower

	А	В	C	D	E	F	G	Н	1	J	K	L	M	N	0	Р	Q
1	Freq	Ephi	<b>IWavePhi</b>	<b>IWaveThet</b>	OutgoingP	IngoingPov X		Υ	Z	Ex_real	Ey_real	Ez_real	Ex_imag	Ey_imag	Ez_imag		
2	500GHz	0	0	90	1.67E-10	6.64E-10	0	-0.00	0.001	. 0	0	0	0	0	0		
3	500GHz	0	0	90	1.67E-10	6.64E-10	0	-0.004	0.001	0.091969	-0.0055	0.000138	3.97E-05	1.42E-05	4.08E-06		
4	500GHz	0	0	90	1.67E-10	6.64E-10	0	-0.004	0.001	0.185312	-0.01488	0.000173	-2.24E-05	1.69E-05	-3.47E-06		
5	500GHz	0	0	90	1.67E-10	6.64E-10	0	-0.004	7 0.001	0.278649	-0.03699	0.000389	0.000566	4.55E-05	6.55E-05		
6	500GHz	0	0	90	1.67E-10	6.64E-10	0	-0.004	0.001	0.360452	-0.07104	8.54E-05	-4.87E-06	-9.66E-05	2.76E-05		
7	500GHz	0	0	90	1.67E-10	6.64E-10	0	-0.004	0.001	0.432306	-0.13332	0.002187	0.000367	-0.00203	0.000645		
8	500GHz	0	0	90	1.67E-10	6.64E-10	0	-0.004	0.001	0.473082	-0.2008	-0.00016	-2.85E-05	0.000153	-4.78E-05		
9	500GHz	0	0	90	1.67E-10	6.64E-10	0	-0.004	0.001	0.494102	-0.27664	-0.00039	-0.00013	0.000694	0.000109		
10	500GHz	0	0	90	1.67E-10	6.64E-10	0	-0.004	0.001	0.493856	-0.35018	0.009855	0.003069	-0.0174	-0.00231		
11	500GHz	0	0	90	1.67E-10	6.64E-10	0	-0.004	0.001	0.478974	-0.40913	-0.0075	-0.0003	-0.04549	-0.00048		
12	500GHz	0	0	90	1.67E-10	6.64E-10	0	-0.00	0.001	0.412717	-0.43842	-0.00296	0.000181	-0.01245	7.66E-05		
13	500GHz	0	_0	90	1.67F-10	6.64F-10	0	-0.003	0.001	0.355649	-0.44797	0.000886	-0.00023	0.004575	0.000105		

## Visualizing Data

#### plot.py

- Also found in <u>Github repo</u>
  - Many useful plots:
    - Heatmap of the outgoing power as a function of ingoing angles (angular sweep)
    - Outgoing power as a function of ingoing angles, with one ingoing angle ( $\varphi$  or  $\theta$ ) held fixed
    - Magnitude of the complex electric field at the outgoing face as a function of ingoing angles
    - Heatmap of the far-field electric field as a function of ingoing angles and outgoing angles (angular sweep)
    - Far-field electric field as a function of ingoing angles and outgoing angles, with one outgoing angle ( $\varphi$  or  $\theta$ ) held fixed

# Connecting Back to Geant4

#### Determining the Probability Distributions

The mechanism for calculating the necessary output probability distributions is modularized over three steps.

(i) Firstly, an incident plane wave is propagated through the waveguide via an incident plane wave excitation in HFSS. The time-averaged power incident on the waveguide can be calculated as

$$P_{in} = \int_{I} |\mathbf{S_{in}}| dA, \tag{52}$$

where  $\int_I$  refers to an integral over the outgoing face and  $\mathbf{S_{in}} = \frac{1}{2} \frac{\mathbf{E} \times \mathbf{B}}{\mu_0}$  indicates the time-averaged Poynting vector of the incoming wave. Notice that in this case, we are not interested in the flux of the Poynting vector  $(\int_I \mathbf{S_{in}} \cdot \mathbf{dA})$  through the input face, because the propagation of the wave is not necessarily aligned with the direction of the waveguide.

From the simulation, we obtain a value of the time-averaged transmitted power by integrating the Poynting vector  $S_{out}$  over the outgoing face, i.e.

$$P_{out} = \int_{O} |\mathbf{S_{out}}| dA, \qquad (53)$$

where  $\int_O$  refers to an integral over the input face. As for the input face, we are concerned not about the flux of the Poynting vector through the outgoing face but rather the total power coming out of the output face regardless of directionality. This is because photons leaving the waveguide reenter free space, and we wish to account for the full power carried away, even if it is not perfectly aligned with the waveguide axis.

For the first stage, then, the probability that the photon propagates to the other end of the waveguide without being reflected or absorbed is given as

$$|S_{21}|^2 = \frac{P_{out}}{P_{in}},\tag{54}$$

where  $|S_{21}|^2$  represents the forward transmission coefficient.

#### Determining the Probability Distributions (cont.)

(ii) Secondly, given that the photon arrives at the output face, the probability distribution of output locations on the output face to feed back to Geant4 is given by P(x, y) ∝ |E(x, y)|², i.e. the probability for the photon to be emitted from any given point on the output face is proportional to the electric field squared at that point. We use the complex magnitude squared of the electric field (|E(x, y)|² = |E<sub>x</sub>|² + |E<sub>y</sub>|² + |E<sub>z</sub>|², where E<sub>x</sub>, E<sub>y</sub>, E<sub>z</sub> ∈ C), rather than the magnitude squared of the instantaneous electric field (|Re[E(x, y)]|²) because we are interested in the time-averaged intensity of the electric field over the outgoing face independent of the phase of the wave. Then, the numerical probabilities can be calculated from the discretized electric field positions {(x<sub>i</sub>, y<sub>i</sub>)} as

$$P(x,y) = \frac{|\mathbf{E}(x,y)|^2}{\sum_{(x_i,y_i)} |\mathbf{E}(x_i,y_i)|^2}.$$
 (55)

(iii) Thirdly, given that the photon arrives at the output face, the probability distribution of output wavevectors (parametrized by θ<sub>out</sub> and φ<sub>out</sub>) to feed back to Geant4 can be found by analyzing the far-field radiation pattern, which is calculated in HFSS as the Fourier transform of the electric field at the output face. We can then use the same method as equation 55, i.e. from the discretized output angles {(θ<sub>i</sub>, φ<sub>i</sub>)} as

$$P(\theta, \phi) = \frac{|\mathbf{E}(\theta, \phi)|^2}{\sum_{(\theta_i, \phi_i)} |\mathbf{E}(\theta_i, \phi_i)|^2}.$$
 (56)

where again  $|\mathbf{E}(\theta, \phi)|^2$  denotes the complex magnitude squared of the far-field electric field at outgoing angles  $\theta$  and  $\phi$ . Given an outgoing angle parametrized by  $(\theta, \phi)$ , the polarization of the outgoing photon can be inferred through the far-field radiation pattern as well:

$$\hat{e}_{out} = \frac{\mathbf{E}(\theta, \phi)}{|\mathbf{E}(\theta, \phi)|}.$$
(57)

#### Determining the Probability Distributions (cont.)

The main difficulty in creating these lookup tables lies in the need to evaluate many combinations of input parameters, including frequency, wavevector direction, and input electric field polarization. One simplification is to use symmetry to simulate only a subset of the possible input angles, as shown in figure 3. Another simplification is to simulate only two orthogonal polarization directions. We denote the two orthogonal directions by  $\hat{\mathbf{E}}_{\theta}$  and  $\hat{\mathbf{E}}_{\phi}$ , where the unit vector in the  $\theta$  direction is  $(\cos\theta\cos\phi,\cos\theta\sin\phi, -\sin\theta)$ , and the unit vector in the  $\phi$  direction is  $(-\sin\phi,\cos\phi,0)$ . A depiction of the two polarization states is given in figure 4. Results for any arbitrary polarization can then be reconstructed by linearly combining the outcomes from this basis due to linearity of Maxwell's equations. In particular, if the ingoing electric field polarization is  $\hat{e}_{in} = E_{\theta}\hat{\mathbf{E}}_{\theta} + E_{\phi}\hat{\mathbf{E}}_{\phi}$ , then  $\mathbf{E}(x,y)$  and  $\mathbf{E}(\theta,\phi)$  become

$$\mathbf{E}(x,y) \to E_{\theta} \mathbf{E}_{E_{\theta}=1, E_{\phi}=0}(x,y) + E_{\phi} \mathbf{E}_{E_{\theta}=0, E_{\phi}=1}(x,y)$$

$$\mathbf{E}(\theta, \phi) \to E_{\theta} \mathbf{E}_{E_{\theta}=1, E_{\phi}=0}(\theta, \phi) + E_{\phi} \mathbf{E}_{E_{\theta}=0, E_{\phi}=1}(\theta, \phi)$$
(58)

where the subscripts on E indicate one of the two orthogonal polarization directions. Equations 55, 56, and 57 then proceed as before with the replacements given in equation 58.

#### postprocess.py

- Also found in <u>Github repo</u>
- Implements the procedure described on the previous few slides
  - Given photon frequency, polarization vector, incoming angles, determine transmission probability, probability of emission from different points, probability of emission into different outgoing angles
- Can be used after interpolating (see next slide) and evaluating onto a set of discrete points

#### Interpolation

The interpolation procedure proceeds as follows:

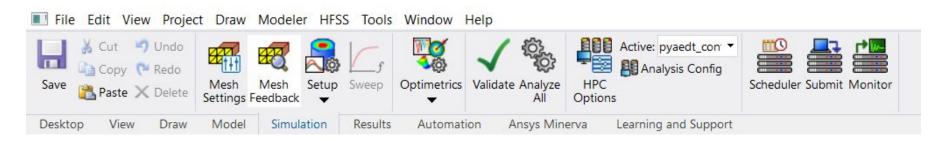
- (i) Interpolation onto a common spatial and angular grid. For each frequency, all output data are interpolated from their native sampling points onto a fixed, common spatial and angular grid that uniformly covers the relevant input and output angular parameters as well as spatial coordinates. The scalar quantity |S<sub>21</sub>|<sup>2</sup> is directly interpolated onto this grid. For the outgoing face and far-field, the complex electric field components ((E<sub>x</sub>, E<sub>y</sub>, E<sub>z</sub>) and (E<sub>θ</sub>, E<sub>φ</sub>), respectively) are represented by their real and imaginary parts, which are interpolated separately.
- (ii) Modal decomposition via principal component analysis. After spatial and angular alignment, principal component analysis (PCA) is performed on the complex electric field data to obtain a modal decomposition. This expresses the fields as a linear combination of orthogonal spatial basis modes weighted by frequencydependent modal coefficients, thereby reducing dimensionality while preserving essential spatial features.
- (iii) Frequency interpolation of scalar values and modal coefficients. Each scalar |S<sub>21</sub>|<sup>2</sup> value at a grid point and each modal coefficient obtained through PCA is treated as a function of frequency. One-dimensional cubic spline interpolation is applied independently to each, enabling smooth and accurate estimation at arbitrary frequencies within the sampled range.
- (iv) Reconstruction at query points. For any desired frequency and spatial/angular coordinate, |S<sub>21</sub>|<sup>2</sup> is obtained by evaluating the frequency-interpolated scalar values on the common grid. The complex electric fields are reconstructed by combining the frequency-interpolated modal coefficients with their corresponding spatial basis modes. This modal decomposition captures the underlying structure of the fields. Finally, evaluating and sampling discretely from the resulting distributions in the style of section 3.1 is then straightforward.

### Future Plans

#### Different Geometries

- Run simulations on actual geometries
  - So far, we've run it on standard rectangular waveguide, cylindrical waveguide, height-perturbed waveguide, right-angle waveguide, stub-filter waveguide
  - Run on SLAC fridge geometries

#### HFSS HPC (High-Performance Computing)



- Parallelize sweep over many frequencies
- Needs to run HFSS at many different frequencies (many different instances of HFSS)