Exploring the Application of S4 as a Companion to FDTD in Meta-Surface Transmission Simulations

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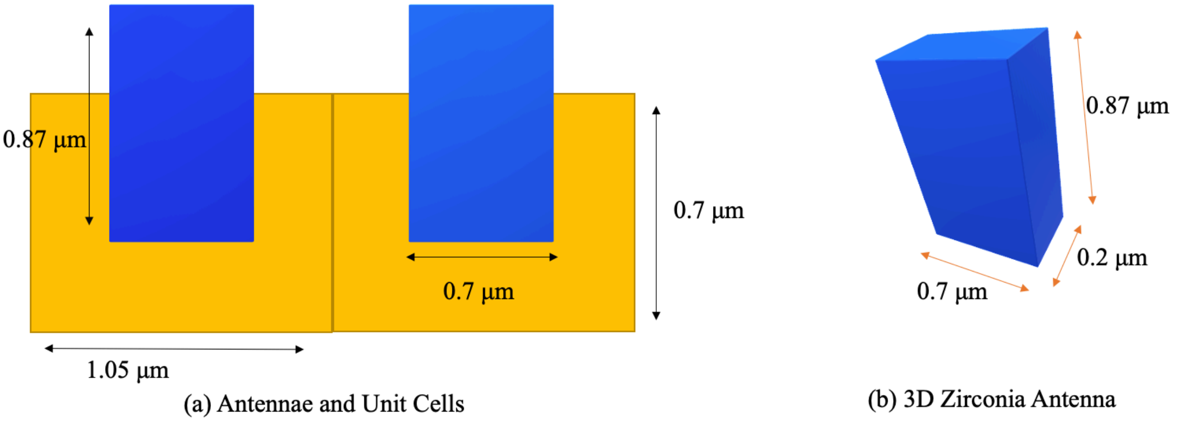
At present, Finite-Difference Time-Domain is the preferred method for simulating electromagnetic transmission through meta-surfaces. However, it is slow. It is therefore of interest to explore whether Stanford Stratified Structure Solver (S4) can be used in conjunction with FDTD to speed up these simulations. When there is a requirement to run large numbers of simulations, FDTD is undesirable. It is hoped, therefore, that S4 will be able to handle the large numbers preliminary simulations, and FDTD would simply repeat the more successful runs with increased accuracy. In order for S4 to be useful in this regard, it must be shown that it provides reasonably accurate results sufficiently swiftly. To do this, S4 simulations will be run on two meta-surfaces and the accuracy of the results assessed against data obtained by FDTD.

The Simulations

Model 1: Glass Slab with ZrO2 Antennas

The first meta-surface modelled with S4 consisted of a thick glass slab with an array of Zirconia (ZrO2) antennas placed upon its top (where light is incident). In the experimental set up, the glass slab was set arbitrarily thick at 10 micrometers (μm), and each ZrO2 antenna was modelled as a rectangle with base dimensions 0.7 x 0.2 μm^2 and a height of 0.87 μm. The simulation region containing each individual antenna, each had dimensions 1.05 x 0.7 μm^2.

Figure 0: Zirconia Antennas



(a) Antennae and Unit Cells

(b) 3D Zirconia Antenna

When examining the following data it is important to note that there are unavoidable differences visible in the graphs due to the input data. The simulation required values for the refractive index of ZrO2 at each wavelength to be loaded into the software, however, values for the refractive index loaded into S4 were different from the ones used in the FDTD runs. Due to the nature of the S4 frontend — the data (used in FDTD) could not be directly inserted into the code. Instead it was required for a polynomial (modelling the index against wavelength) to be fit to the data, but there were such irregularities it was impossible to find a fit with the old data. So alternative data calculated by scientist Wood in 1982 was used with the hope that there would be sufficient similarities between the results to draw a valid conclusion regarding the employability of S4.

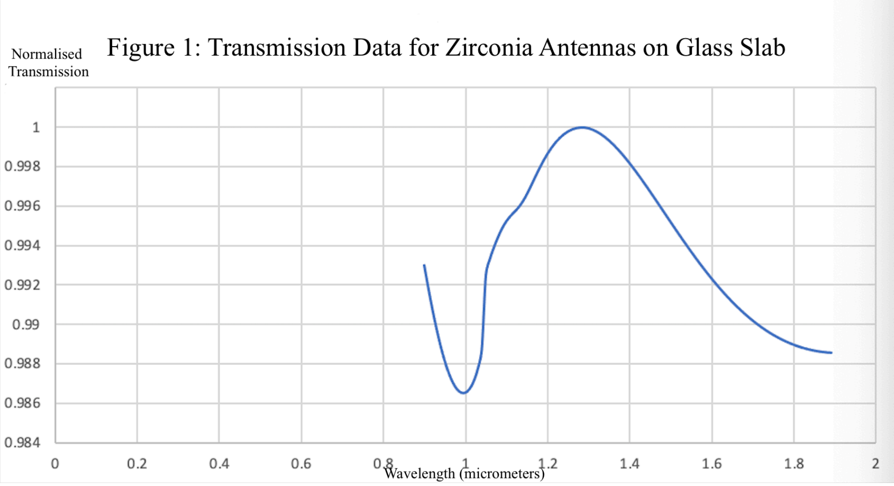


Figure 1: Transmission Data for Zirconia Antennas on Glass Slab

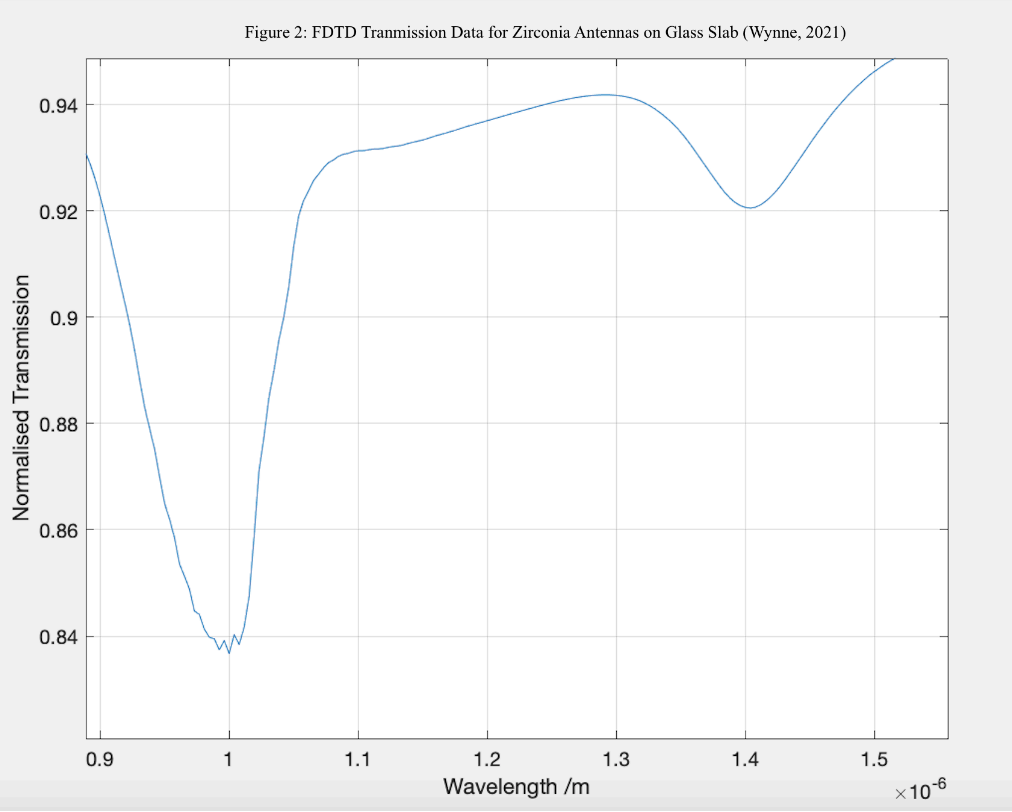


Figure 2: FDTD Tranmission Data for Zirconia Antennas on Glass Slab (Wynne, 2021)

Above are the S4 and FDTD graphs for the electromagnetic transmission through the surface, Figure 1 and Figure 2 (Wynne, 2021) respectably, for the surface. Note the general form of Figure 2 (Wynne, 2021): the negative gradient between 0.9-1µm, the global minimum at approximately 1µm, the positive gradient until approximately 1.3µm, the negative gradient until the second minima at 1.4 µm, and finally the positive gradient until 1.5µm. In figure 1, we see the same negative gradient between 0.9-1µm and the global minima at 1µm. From this point forward we see the same pattern shown in figure 2 (positive gradient, slight plateau followed by a minima, and a positive gradient) but it appears confined between 1-1.3µm. We further note that the the S4 transmission spectrum falls between 0.984-0.999 compared to 0.84-0.95 as seen in the FDTD results.

There are both similarities and dissimilarities between the datasets. Most notably, the overarching trends observed in the FDTD graph are maintained in the S4 data. Secondly, the primary differences between the graphs are the shift in period after the global minima and the compression of the transmission range. However, this does not necessarily pose a problem. The transformations are sufficiently simple to allow the data to be shifted into phase with the FDTD data, which would enable the relevant information to be extracted. The primary concern here is that these differences might be particular to this simulation, for then it would be impossible to account for them when translating data from S4 to FDTD. This point will be considered throughout further simulations.

Sweeps

S4 has potential as a companion for FDTD, therefore considering its applications is of interest. S4 is particularly useful for running sweeps: where the simulation is run many times with sets of parameters changing against one another. To conduct a sweep, the range of values each parameter is varied over is set. Then a series of simulations is run, with the input parameters corresponding to some possible combination of the values within the given ranges. Two main sweeps were run, one examining alterations of the antenna in one dimension and the other in three.

In the first sweep height was varied and the transmission results were plotted against wavelength and height. On this graph it is important to note that the pigmentation indicates the transmission, where black is the maximal normalised transmission (~0.99) and white indicates transmission =0.98

Figure 3: Height Sweep (Grayscale Gradient Indic Transmission)

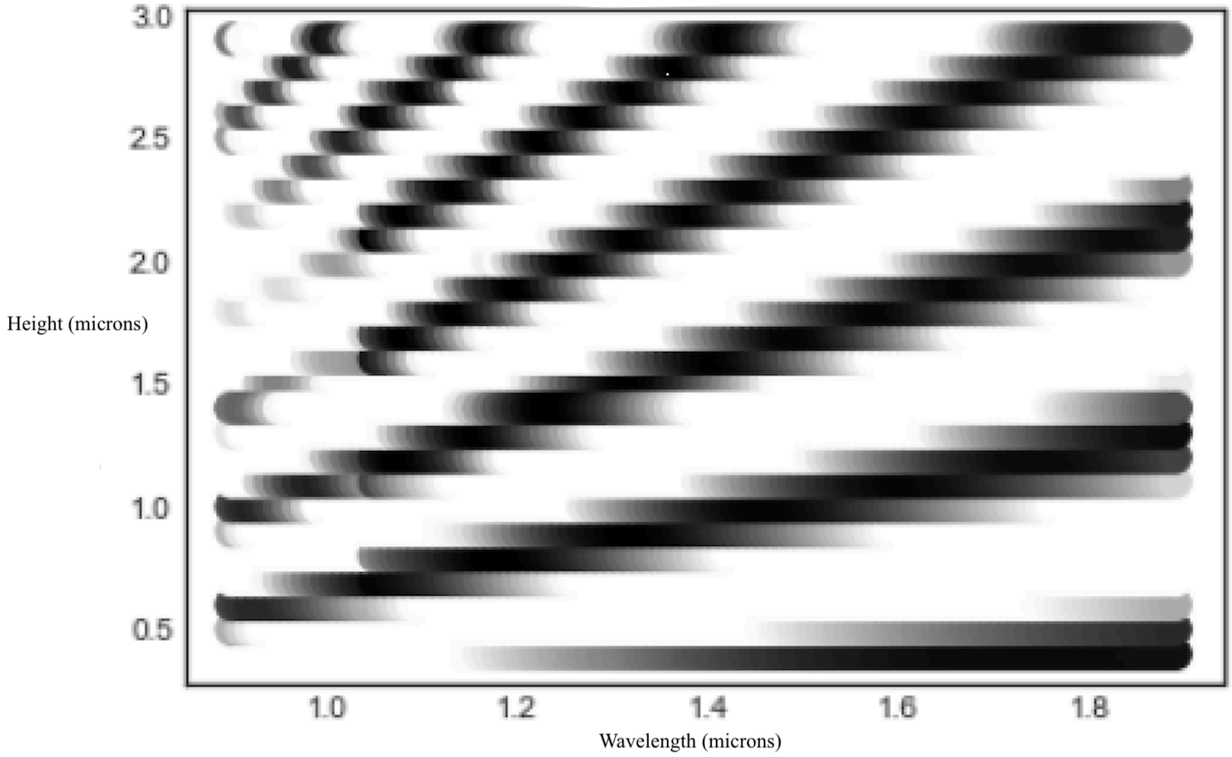
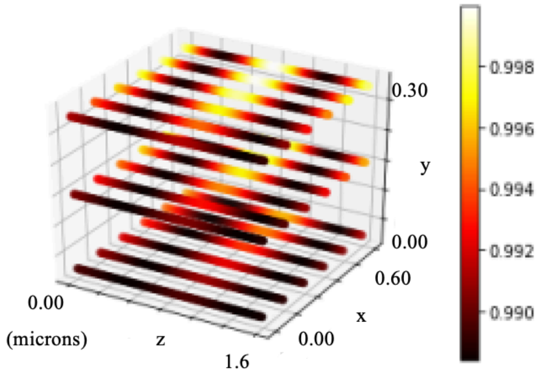


Figure 3 shows a clear trend in the transmission pattern, with the number of nodes and anti-nodes gradually increasing with height. The transmission domain remains in 0.98-0.999, which provides evidence that the condensation of the transmission range by S4 is a systemic consistent over all relevant values.

In the second sweep all three dimensions of the antennae — the height (z), and the base dimensions (x and y) — were varied, enabling a graph to be drawn up to examine transmission trends across further variations. Figure 4 considers only transmission at the wavelength 1.5μm.

Figure 4: 3D Transmission – Zirconia Antennae on Glass



There are some clear trends in the transmission as the dimensions vary. For example, we see higher peaks of transmission as the base components (x & y) approach 0.6μm and 0.30 μm. Further we note that the transmission values remain condensed as in Figure 4, which indicates that the previous trends are systemic.

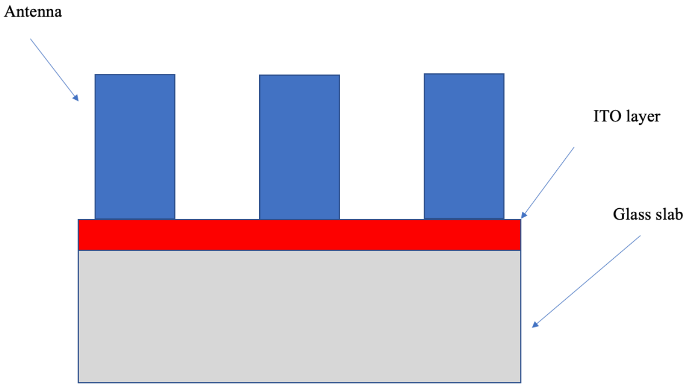
Example of Use

There is a particular interest in having meta-surfaces with their global transmission minimum occurring at a wavelength of approximately 1.6μm. Figure 3 shows that for the present configuration antennas (with base 0.2x0.7μm^2), heights in ranges 0.9-1.3μm, 1.7-2.0μm, and 2.3-2.9μm have high transmission at 1.6μm and therefore would be undesirable in a meta-surface with a minima there. Similarly in Figure 4 we can easily read off the undesirable combinations of values. Therefore, within mere hours we have been able to eliminate entire groups of antennae, leaving a far more compact group of values to examine closer in the more in-depth FDTD simulations.

Model 2: Introducing the ITO - Can S4 Handle A Highly Dispersive Layer?

The previous discussion demonstrated that S4 is capable of providing adequate simulations for simple surfaces involving Zirconia antennae upon a glass slab. This however is a particularly simple surface, and consequently has a more simple dispersion relation. Therefore it is of interest to explore the accuracy with which S4 manages more complex dispersions. The previous surface will be modified by inserting an Iridium Tin Oxide (ITO) layer (a highly dispersive material) into the previous glass-antenna structure.

Figure 0 (b) : Graph Illustrating Insertion of ITO



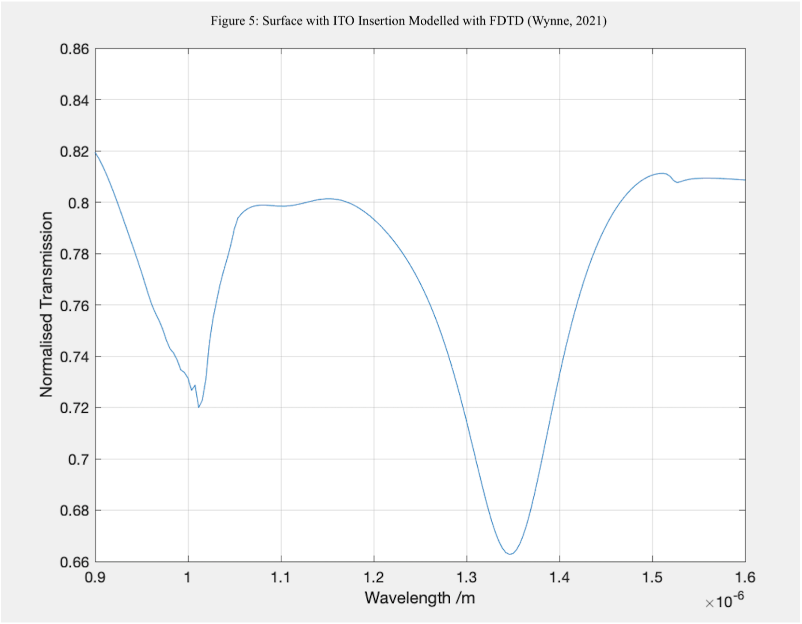
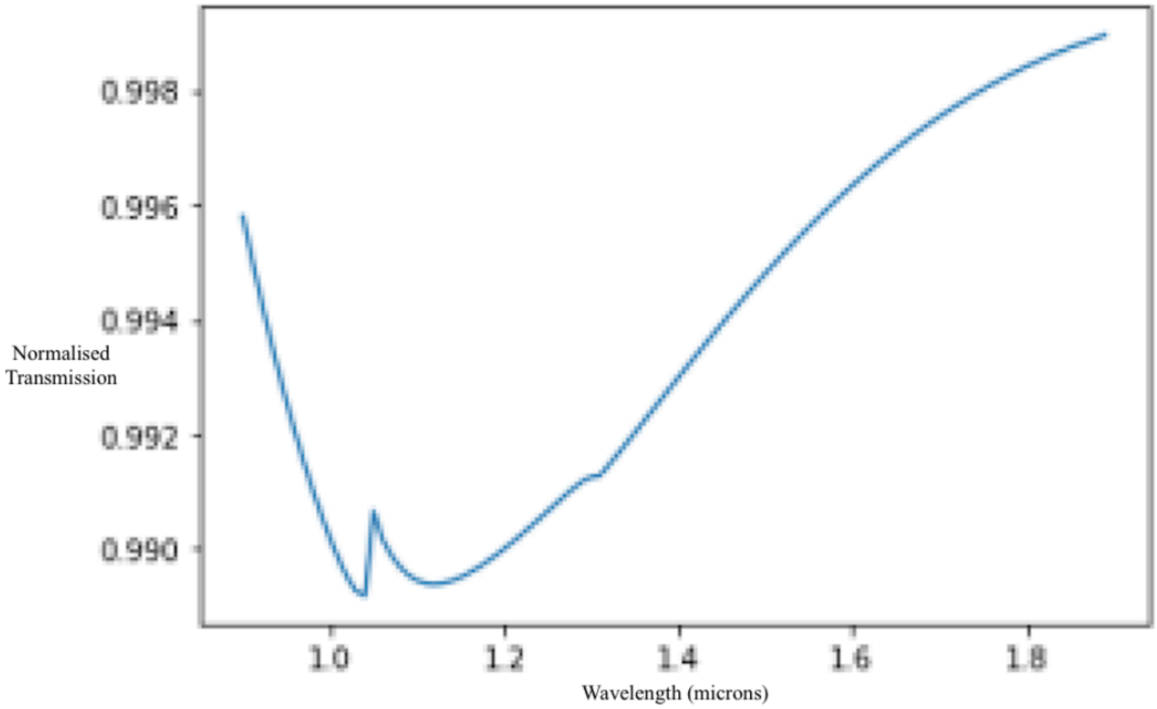


Figure 5: Surface with ITO Insertion Modelled with FDTD (Wynne, 2021)

In Figure 5 (Wynne, 2021) the Transmission for a surface with an ITO layer inserted, as modelled by FDTD, is presented. There are some clear characteristics to pay attention to in this graph: the minima ~1µm and at ~1.35µm, the plateau between the minima, and the kink in the curve at ~1.55µm. Below in Figure 6 we note that the main trends of the graph (minima, plateau, minima and kink) are maintained by S4, however we also see the graph squished after the first minimum (as we saw previously).

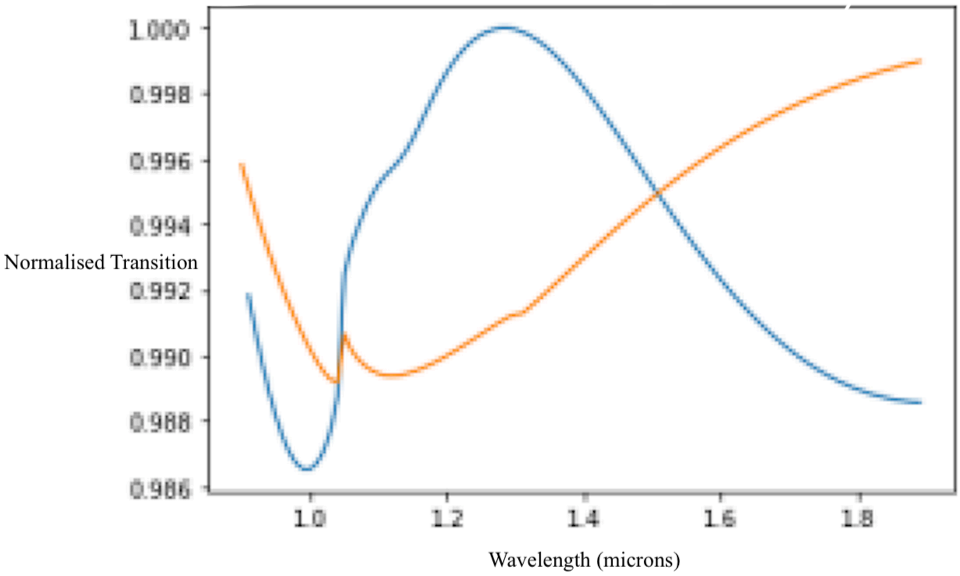
The way that the ITO and non-ITO graphs relate to one another (See Figure 7 and Figure 8 (Wynne, 2021)) is the same irregardless of whether the simulations were run in FDTD or in S4. The following trends are present in both the S4 and the FDTD results. Comparing the ITO and Non-ITO graphs of each simulation

Figure 6: S4 Modelled Transmission with ITO



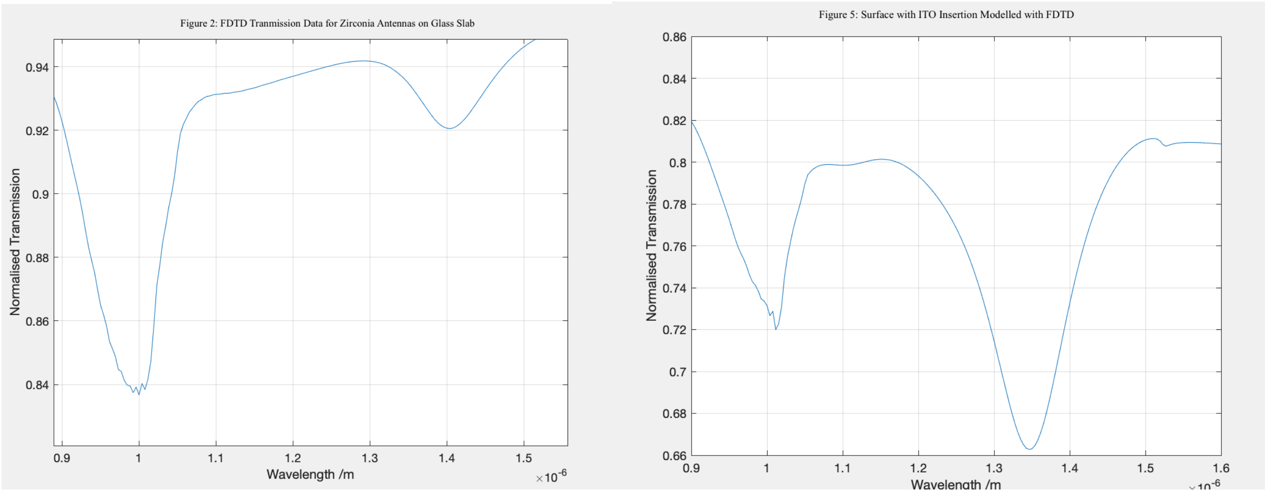
method against each other we see: the first minima corresponding to one another, the “plateau” in both graphs occurring at the same wavelength, the kink in the ITO graph appearing after the maxima in the non-ITO graph. Thus we can see that the relation between the two graphs seen observed in FDTD simulations likewise are maintained in S4. For all simulations S4 compressed the total normalised transmission range, and condensed the data after the first minima. This indicates that the translations and condensations of the data are systemic and therefore can be easily accounted for, allowing for no threat to be posed to the

Figure 7 :
Surface Without ITO (blue) vs With ITO (orange)



usefulness of the data. Therefore, it is clear that S4 is capable of producing results comparable to those produced by FDTD.

Figure 8 : Figure 2 & 5 Together for Comparative Point.



Sweeps

The first sweep conducted was a one dimensional sweep in the direction the antennas protruded from the surface (height) — data seen in Figure 9. We see the same fanning effect seen previously in the non-ITO

Figure 9: Height Sweep - Surface Including ITO Insertion

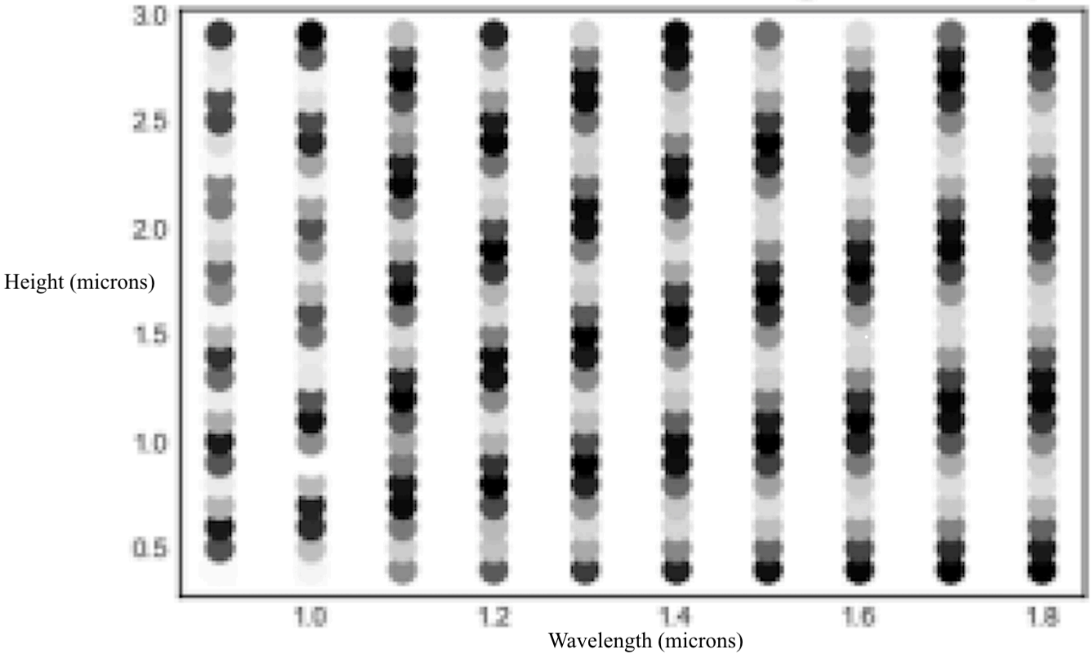
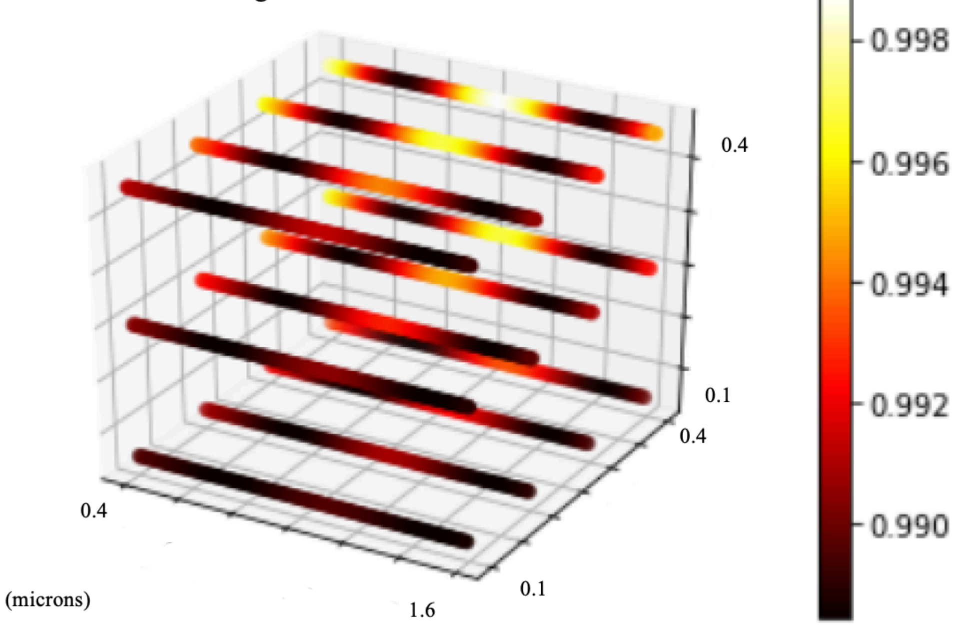


Figure 9 - the greyscale : black high transmission at (0.999) and white, lower at (0.987).

simulation. The regions of low transmission are consistently narrower, which is consistent with Figure 6, and not only does the number of minima and maxima also correspond to the non-ITO figure, but the way they extend over a greater height range is also consistent with the way the non-ITO extension is modelled.

Figure 10: 3D Transmission – ITO Insertion



The second sweep was a three dimensional sweep of the antennae conducted at a wavelength of 1.5 μm. We see clear trends: such as the regular occurrence of transmission minima and maxima throughout the data, with intensity gradients with clear dependance upon the dimensions of the antenna.

Comparison of Results

Comparison between the results run with the ITO and without the ITO can provide a final overview of the covered ability of S4. Beginning with the single simulation non-ITO graph, all the desired qualities were present. However, the transmission range was produced by S4 was 0.9987-0.999 compared to the range

0.84-0.95 produced by FDTD. Further, the curve after the global minima was confined to a 0.1µm range, whereas in FDTD it was over 1.45µm. After the ITO was inserted similar things occurred. The S4 transmission was estimated between 0.990 - 0.996, whilst the FDTD was 0.67 - 0.82; and beyond the global minima, the qualities were condensed into 1.3µm from the FDTD 1.6µm. In the one dimensional sweeps the same trends were exposed in the simulations with and without ITO insertion. There was a regular occurrence of maxima and minima forming a fan pattern. The trend of narrower bands of low transmission as seen in the single run maintained in the ITO build. In the three dimensional sweeps, the fanning effect was extended in the non-ITO build as in the ITO build.

Speeds

Besides the accuracy and usefulness of the S4 data, this project also wished to certify whether it possessed sufficient computational speed in order to be a useful companion to FDTD. Firstly, in the simulations without the ITO, running a simulation requiring 50 Fourier terms to converge took approximately 10 - 20 seconds. The time it takes the software to run is approximately proportional to the number of Fourier terms cubed. Therefore to calculate the running time in seconds the number of Fourier terms used should be cubed and multiplied by 8 x 10^(-5). A simulation of this level of complexity when run on FDTD takes about 4 hours, (14400 seconds). In order for a simulation to take approximately this length on S4 (using the above model) the required number of Fourier terms would be approximately 564. The simulations in this experiment confirm this result, with the ITO insertion layer completing a 600 term Fourier run in ~4.5 hours. Therefore, it is quite obvious to see that the S4 simulations substantially faster than those of FDTD.

Conclusion

In conclusion, the aim of the project was met. Driven by the limitations of FDTD, this project sought to determine whether S4 could be used to supplement FDTD when simulating electromagnetic transmission through meta-surfaces. S4 simulations were run on a simple glass and Zirconia antenna meta-surface, which succeeded in producing not only sufficiently accurate results, but also did so sufficiently quickly. S4 was further shown capable of producing useful results for meta-surfaces with more complex dispersion patterns, by running a series of simulations with a layer of highly dispersive Iridium Tin Oxide inserted into the structure. No drawbacks significant enough to influence the employability of S4 as a companion to FDTD were noted, but there were certain consistent translations and shifts in the simulation data, which would be worth analysing further in order to increase the usefulness of the software.

Bibliography

Wynne, L. (2021). *FDTD Simulation Data.* Unpublished. Permission Granted.

Refractive index of ZrO2 (Zirconium dioxide, Zirconia) - Wood 1982. https://refractiveindex.info/?shelf=main&book=ZrO2&page=Wood Accessed: June 2021.