VirtualLab Fusion Technology – Solvers and Functions

FMM / RCWA [S-Matrix]

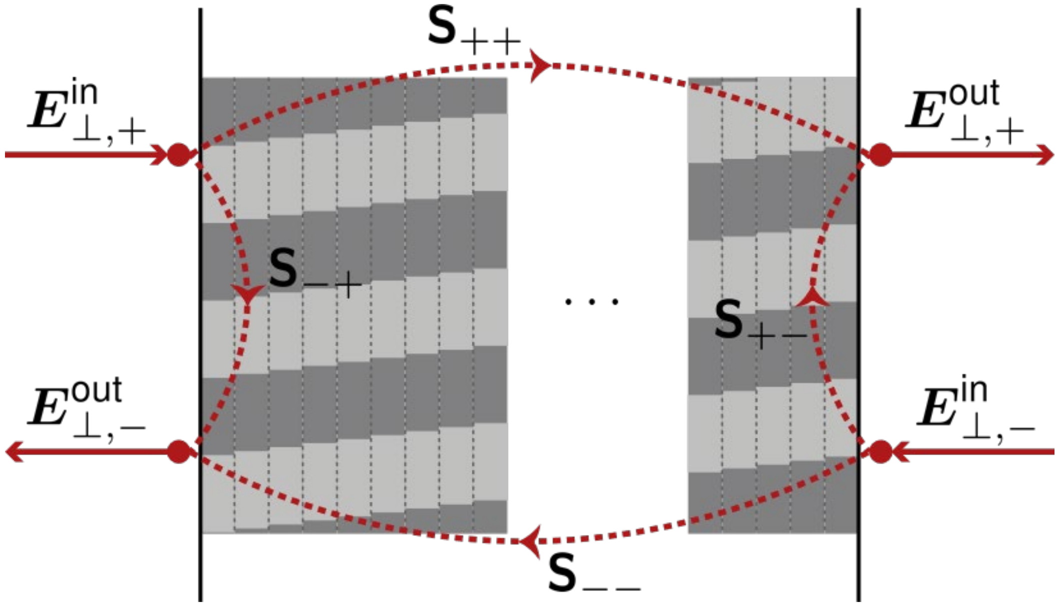
For the **Grating Component**

Abstract

The FMM/RCWA solver works in the spatial frequency domain (**k domain**). It consists of

1. an eigenmode solver for each periodically modulated layer and
2. an S-matrix for matching the boundary conditions between the layers.

The eigenmode solver computes the field solution in the k domain for the periodically modulated medium in each layer. The S-matrix algorithm calculates the response of the whole layer system by matching the boundary conditions in a recursive manner. It is well-known for its unconditional numerical stability since, unlike the traditional transfer matrix, it avoids the exponentially growing functions in the calculation steps.



Solver Algorithm – Eigenmode Solver

- The FMM/RCWA solves the following two Maxwell equations

$$\nabla \times \boldsymbol{E}(\boldsymbol{r}) = \mathrm{i}k_0 \boldsymbol{H}(\boldsymbol{r}) \,,$$
$$\nabla \times \boldsymbol{H}(\boldsymbol{r}) = -\mathrm{i}k_0 \epsilon(\boldsymbol{\rho}, z) \boldsymbol{E}(\boldsymbol{r})$$

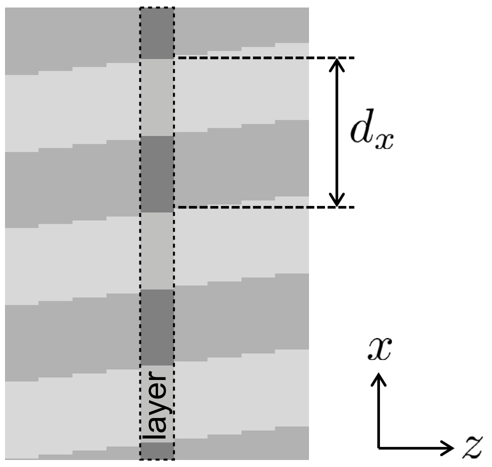
  for the modal fields (i.e., the eigen solutions), which are computed for the periodically modulated medium in each layer.

- The periodicity of the medium can be seen in the **permittivity distribution**, given by

$$\epsilon(\boldsymbol{\rho}, z) = \epsilon(\boldsymbol{\rho} + \boldsymbol{d}, z) \,,$$

  where $\boldsymbol{d} = (d_x, d_y)$, d_x and d_y being the **period** along x and y respectively.

- Here we use $\boldsymbol{r} = (x, y, z)$ and $\boldsymbol{\rho} = (x, y)$ as the 3D position vector and its 2D projection onto the transversal plane respectively.



Solver Algorithm – Eigenmode Solver

- As a periodic function, the permittivity distribution $\epsilon(\boldsymbol{\rho})$ can be expanded in the form of a Fourier series, as follows:

$$\epsilon(x,y) = \sum_m \sum_m \tilde{\epsilon}_{m,n} \exp(\mathrm{i}k_{xm}x) \exp(\mathrm{i}k_{yn}y) \,,$$

with the spatial frequency components k_{xm} and k_{yn} given by

$$k_{xm} = m2\pi/d_x \,, \quad \text{and} \quad k_{yn} = n2\pi/d_y \,.$$

- Similarly, the electromagnetic field components can also be written in series form:

$$V_\ell(x,y,z) = \sum_m \sum_n \tilde{V}_\ell(k_{xm}, k_{yn}, z) \exp(\mathrm{i}k_{xm}x) \exp(\mathrm{i}k_{yn}y) \,,$$

where V_ℓ ($\tilde{V}_\ell$) represents any of the six field components in the space (spatial frequency) domain.

- The infinite series must, in practice, be truncated:

$$\epsilon(x,y) = \sum_{m=-M}^{M} \sum_{n=-N}^{N} \cdots$$

with $\pm M$ and $\pm N$ the limits for the sum.

- The truncation limits the **number of spatial frequencies** considered in the computation. This magnitude is often referred to as the **number of diffraction orders**.

Solver Algorithm – Eigenmode Solver

- The original Maxwell's equations can be transformed into the k domain, and after some rearranging, the following set of ordinary differential equations is obtained:

$$\frac{\mathrm{d}}{\mathrm{d}z}\begin{pmatrix}[\tilde{E}_x]\\ [\tilde{E}_y]\\ [\tilde{H}_x]\\ [\tilde{H}_y]\end{pmatrix} = \mathrm{i}k_0 \begin{pmatrix}[\![\tilde{\Omega}_{11}]\!] & [\![\tilde{\Omega}_{12}]\!] & [\![\tilde{\Omega}_{13}]\!] & [\![\tilde{\Omega}_{14}]\!]\\ [\![\tilde{\Omega}_{21}]\!] & [\![\tilde{\Omega}_{22}]\!] & [\![\tilde{\Omega}_{23}]\!] & [\![\tilde{\Omega}_{24}]\!]\\ [\![\tilde{\Omega}_{31}]\!] & [\![\tilde{\Omega}_{32}]\!] & [\![\tilde{\Omega}_{33}]\!] & [\![\tilde{\Omega}_{34}]\!]\\ [\![\tilde{\Omega}_{41}]\!] & [\![\tilde{\Omega}_{42}]\!] & [\![\tilde{\Omega}_{43}]\!] & [\![\tilde{\Omega}_{44}]\!]\end{pmatrix} \begin{pmatrix}[\tilde{E}_x]\\ [\tilde{E}_y]\\ [\tilde{H}_x]\\ [\tilde{H}_y]\end{pmatrix} ;$$

  the explicit expressions of $[\![\tilde{\Omega}_{jk}]\!]$ can be found in [1, 2].

- It is worth mentioning that the construction of the matrix elements $[\![\tilde{\Omega}_{jk}]\!]$ requires the Fourier series of the permittivity $\epsilon(\boldsymbol{\rho}, z)$. In VirtualLab Fusion, we have included the correct **Fourier factorization rule** according to [1-3].

- Here we use the following shorthand: $[\tilde{E}_x]$ represents a vector containing all the Fourier coefficients $\tilde{E}_x(k_{xm}, k_{yn})$, and analogously for the matrices $[\![\tilde{\Omega}_{ij}]\!]$.

Solver Algorithm – Eigenmode Solver

- The set of ordinary differential equations can be solved numerically as an eigenvalue-eigenvector problem, which shows the modal field solution to be given by

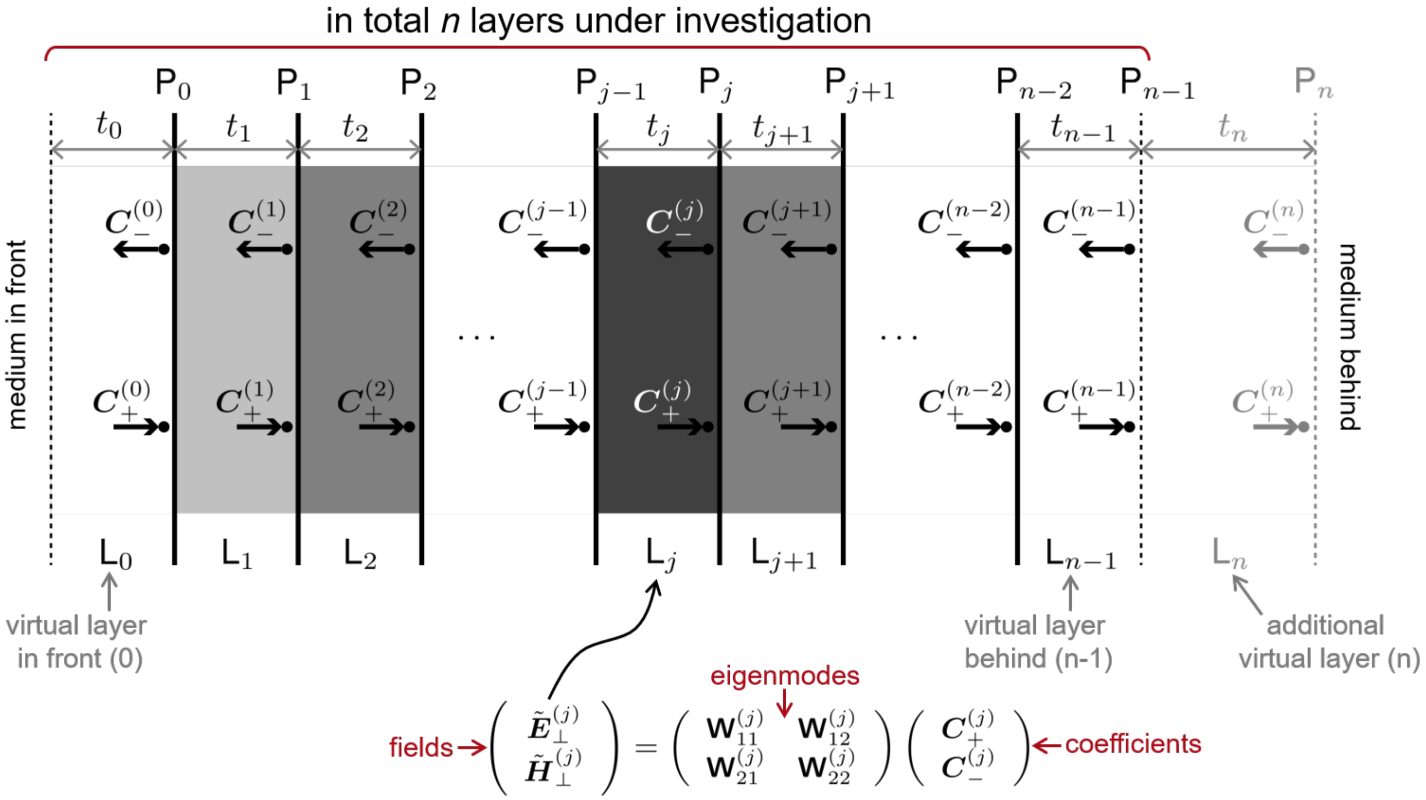
$$\begin{pmatrix}[\tilde{E}_x]\\[\tilde{E}_y]\\[\tilde{H}_x]\\[\tilde{H}_y]\end{pmatrix} = \begin{pmatrix} [\![\tilde{W}_+^{\mathsf{I},\mathsf{Ex}}]\!] & [\![\tilde{W}_+^{\mathsf{II},\mathsf{Ex}}]\!] & [\![\tilde{W}_-^{\mathsf{I},\mathsf{Ex}}]\!] & [\![\tilde{W}_-^{\mathsf{II},\mathsf{Ex}}]\!] \\ [\![\tilde{W}_+^{\mathsf{I},\mathsf{Ey}}]\!] & [\![\tilde{W}_+^{\mathsf{II},\mathsf{Ey}}]\!] & [\![\tilde{W}_-^{\mathsf{I},\mathsf{Ey}}]\!] & [\![\tilde{W}_-^{\mathsf{II},\mathsf{Ey}}]\!] \\ [\![\tilde{W}_+^{\mathsf{I},\mathsf{Hx}}]\!] & [\![\tilde{W}_+^{\mathsf{II},\mathsf{Hx}}]\!] & [\![\tilde{W}_-^{\mathsf{I},\mathsf{Hx}}]\!] & [\![\tilde{W}_-^{\mathsf{II},\mathsf{Hx}}]\!] \\ [\![\tilde{W}_+^{\mathsf{I},\mathsf{Hy}}]\!] & [\![\tilde{W}_+^{\mathsf{II},\mathsf{Hy}}]\!] & [\![\tilde{W}_-^{\mathsf{I},\mathsf{Hy}}]\!] & [\![\tilde{W}_-^{\mathsf{II},\mathsf{Hy}}]\!] \end{pmatrix} \begin{pmatrix} [\tilde{C}_+^{\mathsf{I}}][\![\exp(\gamma_+^{\mathsf{I}} z)]\!] \\ [\tilde{C}_+^{\mathsf{II}}][\![\exp(\gamma_+^{\mathsf{II}} z)]\!] \\ [\tilde{C}_-^{\mathsf{I}}][\![\exp(\gamma_-^{\mathsf{I}} z)]\!] \\ [\tilde{C}_-^{\mathsf{II}}][\![\exp(\gamma_-^{\mathsf{II}} z)]\!] \end{pmatrix}.$$

- Here, the modes are sorted into positive and negative directions, as preparation for later use in the S-matrix. We write the expression above in the following, more compact, form:

$$\begin{pmatrix}\tilde{\boldsymbol{E}}_\perp\\ \tilde{\boldsymbol{H}}_\perp\end{pmatrix} = \begin{pmatrix}\mathbf{W}_{11} & \mathbf{W}_{12}\\ \mathbf{W}_{21} & \mathbf{W}_{22}\end{pmatrix}\begin{pmatrix}\boldsymbol{C}_+\\ \boldsymbol{C}_-\end{pmatrix}.$$

- The convergence of the solution to the eigenvalue-eigenvector problem depends on the truncation **number of spatial frequencies** in the computation.

Solver Algorithm – S-Matrix



The task of the S-matrix is to compute the coefficients that connect the field in front of and behind the layered slab:

$$\begin{pmatrix} C_+^{(n)} \\ C_-^{(0)} \end{pmatrix} = \begin{pmatrix} \mathbf{S}_{11}^{(0,n)} & \mathbf{S}_{12}^{(0,n)} \\ \mathbf{S}_{21}^{(0,n)} & \mathbf{S}_{22}^{(0,n)} \end{pmatrix} \begin{pmatrix} C_+^{(0)} \\ C_-^{(n)} \end{pmatrix} .$$

Solver Algorithm – S-Matrix

- At the surface with index (j), based on the boundary conditions, it is not hard to write down the following relation

$$\begin{pmatrix} \mathbf{W}_{11}^{(j)} & \mathbf{W}_{12}^{(j)} \\ \mathbf{W}_{21}^{(j)} & \mathbf{W}_{22}^{(j)} \end{pmatrix} \begin{pmatrix} \boldsymbol{C}_{+}^{(j)} \\ \boldsymbol{C}_{-}^{(j)} \end{pmatrix} = \begin{pmatrix} \mathbf{W}_{11}^{(j+1)} & \mathbf{W}_{12}^{(j+1)} \\ \mathbf{W}_{21}^{(j+1)} & \mathbf{W}_{22}^{(j+1)} \end{pmatrix} \begin{pmatrix} [\boldsymbol{\Phi}_{+}^{(j+1)}]^{-1} & 0 \\ 0 & [\boldsymbol{\Phi}_{-}^{(j+1)}]^{-1} \end{pmatrix} \begin{pmatrix} \boldsymbol{C}_{+}^{(j+1)} \\ \boldsymbol{C}_{-}^{(j+1)} \end{pmatrix}.$$

- By applying the boundary conditions at each surface, a recursive relation can be found to relate the field in front of and behind the layered slab in the form below

$$\begin{pmatrix} \boldsymbol{C}_{+}^{(n)} \\ \boldsymbol{C}_{-}^{(0)} \end{pmatrix} = \begin{pmatrix} \mathbf{S}_{11}^{(0,n)} & \mathbf{S}_{12}^{(0,n)} \\ \mathbf{S}_{21}^{(0,n)} & \mathbf{S}_{22}^{(0,n)} \end{pmatrix} \begin{pmatrix} \boldsymbol{C}_{+}^{(0)} \\ \boldsymbol{C}_{-}^{(n)} \end{pmatrix}.$$

- There are different variations to derive the recursive relation. In VirtualLab Fusion, we follow the **W→t→S variation**, according to [4, 5].

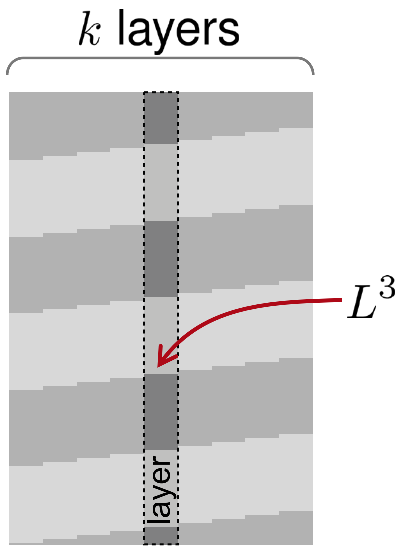
- Other recursion variations will become avaliable in VirtualLab Fusion in future.

Numerical Complexity

- The total number of spatial frequencies for each layer can be calculated as
$$L = (2N+1) \times (2M+1)\,,$$
$(2N+1)$, $(2M+1)$ being the number of spatial frequencies in each of the two dimensions, for general cases.

- Considering the typical numerical operations (e.g., matrix eigenvalue problem, matrix multiplication or inversion), the counts of FLOPs in the FMM/RCWA can be roughly estimated as being proportional to L^3.

- An arbitrary grating structure may consist of several layers. Let us denote the number of layers by k, then the total counts of FLOPs in the FMM/RCWA can be roughly estimated as kL^3.



Numerical Complexity

- Considering a dielectric rectangular grating along x, with varying period d_x, to ensure numerical convergence at least 50 evanescent spatial frequencies must be considered in the computation. Then, we can estimate the FLOPs

d_x/λ	$L = (2N+1)$	L^3 (~FLOP counts)
1	53	148,877
10	71	357,911
50	151	3,442,951

- For a 2D pillar grating, with varying periods d_x and d_y, we always ensure at least 10 evanescent spatial frequencies in both directions are considered, then we can estimate the FLOPs

d_x/λ, d_y/λ	$L = (2N+1) \times (2M+1)$	L^3 (~FLOP counts)
1, 1	13×13	4,826,809
10, 10	31×31	887,503,681
100, 100	211×211	88,245,939,632,761

Usage in VirtualLab Fusion

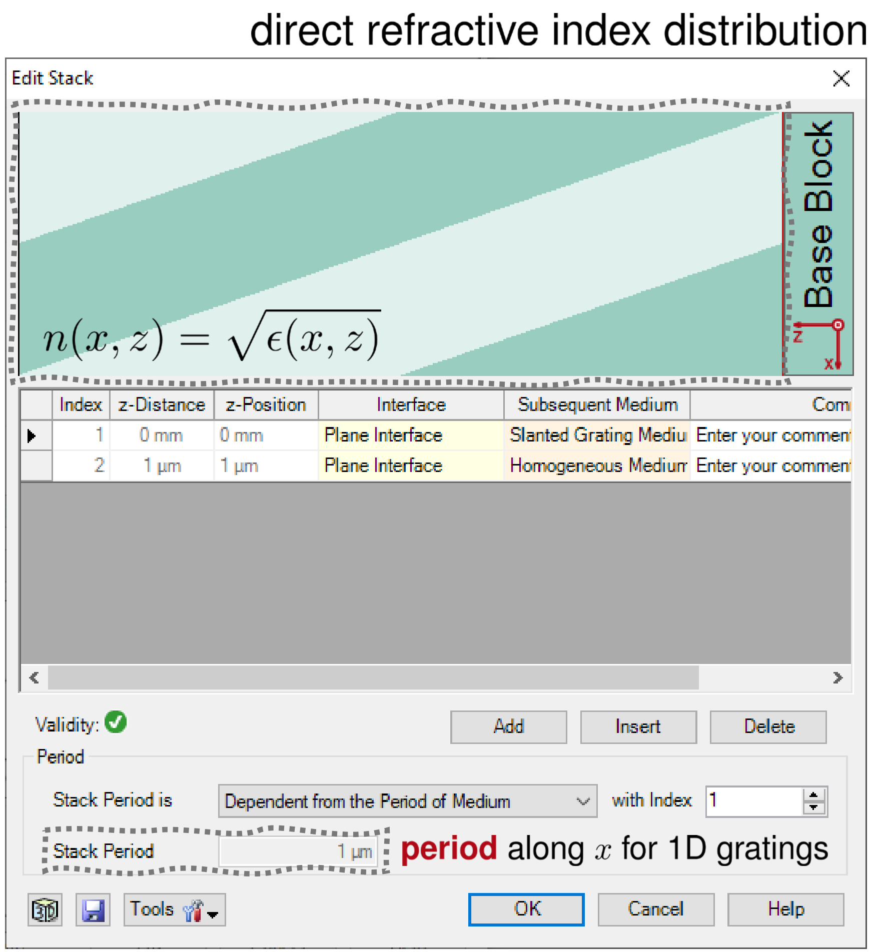
- To apply the FMM/RCWA solver in VirtualLab Fusion, the **permittivity distribution**

$$\epsilon(\boldsymbol{\rho}, z) = \epsilon(\boldsymbol{\rho} + \boldsymbol{d}, z)$$

must be specified first. Here, $\boldsymbol{d} = (d_x, d_y)$, with d_x and d_y the **period** along x and y respectively.

- There are two ways to define it
  - **direct specification of the refractive index distribution** $n(\boldsymbol{\rho}, z)$, or
  - using surfaces with profiles $h_j(\boldsymbol{\rho})$ and filling materials with constant n_j.

for gratings made of isotropic media.



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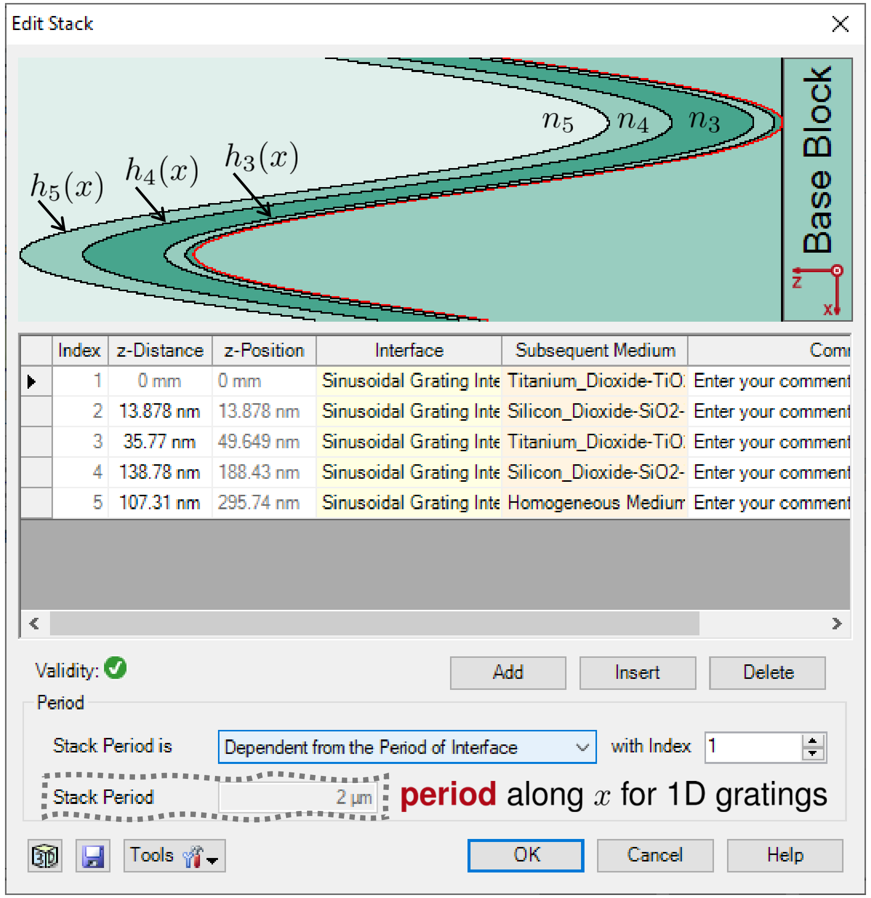
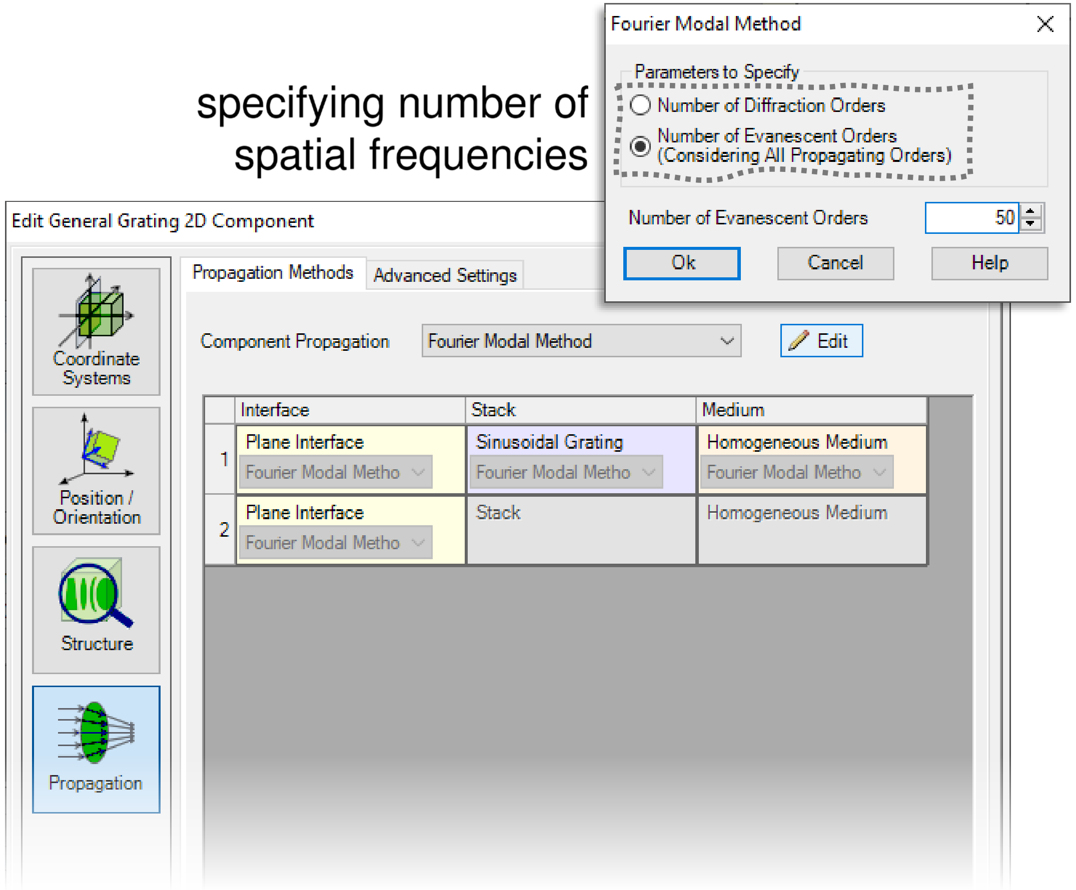
surface profiles with constant refractive indices



Usage in VirtualLab Fusion

- The truncation **number of spatial frequencies** (often referred to as the **number of diffraction orders**), plays a role in the convergence behavior in the computation.
- There are two ways to specify this number
  - directly defininig the total number of spatial frequencies, or
  - including all the propagating orders, plus a certain number of additional evanescent orders.
- The preset number in VirtualLab Fusion gives good convergence for most dielectric gratings; however, for metal gratings, an additional convergence test is recommanded.

specifying number of spatial frequencies



List of References

[1] Lifeng Li, "New formulation of the Fourier modal method for crossed surface-relief gratings," J. Opt. Soc. Am. A 14, 2758-2767 (1997)

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[3] Lifeng Li, "Use of Fourier series in the analysis of discontinuous periodic structures," J. Opt. Soc. Am. A 13, 1870-1876 (1996)

[4] Lifeng Li, "Formulation and comparison of two recursive matrix algorithms for modeling layered diffraction gratings," J. Opt. Soc. Am. A 13, 1024-1035 (1996)

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Document Information

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further reading	- VirtualLab Fusion Technology – Layer Matrix [S-Matrix] - VirtualLab Fusion Technology – Idealized Grating Functions - Thin Element Approximation (TEA) vs. Fourier Modal Method (FMM) for Grating Modeling - Analysis of Slanted Gratings for Lightguide Coupling - Rigorous Analysis of Nanopillar Metasurface Building Block