ECE 695
Numerical Simulations
Lecture 20: Transfer Matrices and S^4

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Outline

- Periodic solution strategy
  - Stacked periodicity
  - Transverse periodicity
- S-Matrix Simulations
- S4 RCWA solver
  - Capabilities
  - Live demonstration

S-Matrices

- For S-matrix, connect incoming to outgoing fields from boundaries of region
- Mathematically,

$$\begin{bmatrix} u^{(p+1)} \\ d^{(0)} \end{bmatrix} = \begin{bmatrix} T_{uu}^{(p)} & R_{ud}^{(p)} \\ R_{du}^{(p)} & T_{dd}^{(p)} \end{bmatrix} \begin{bmatrix} u^{(0)} \\ d^{(p+1)} \end{bmatrix}$$

- For input from below:
  - transmission from bottom to top given by $T_{uu}^{(p)}$
  - reflection at bottom given by $R_{du}^{(p)}$

S-Matrices: Periodicity

- What happens if one or more layers are periodic?
- Then there are two types of coupling:
  - Layer-to-layer (refractive)
  - Mode-to-mode (diffractive)
- Can both be treated in a single framework?

S-Matrices: Stacked Periodicity

- Recall that:

$$s^{(p)} = \begin{bmatrix} t_{11}^{(p)} - t_{12}^{(p)} t_{22}^{(p)\,-1} t_{21}^{(p)} & t_{12}^{(p)} t_{22}^{(p)\,-1} \\ -t_{22}^{(p)\,-1} t_{21}^{(p)} & t_{22}^{(p)\,-1} \end{bmatrix}$$

- For quarter wave stack, express in terms of t-matrix elements:

$$\tilde{s}^{(p)} = \begin{bmatrix} 1 & 0 \\ 0 & \exp\left(-j\beta_{m,-}^{(p)} \Delta y_p\right) \end{bmatrix} s^{(p)} \begin{bmatrix} \exp\left(j\beta_{m,+}^{(p)} \Delta y_p\right) & 0 \\ 0 & 1 \end{bmatrix}$$

S-Matrices: Transverse Periodic Solution

- Divide into layers, uniform in z-direction
- Find Bloch states in each layer
- Calculate transfer function for field amplitudes
- Iteratively develop S-matrix
- Choose inputs from both sides
- Calculate resulting outputs (transmission and reflection) and losses (absorption $A=1-T-R$)

Whittaker & Culshaw, *Phys. Rev. B* **60**, 2610 (1999)
Tikhodeev *et al.*, *Phys. Rev. B* **66**, 045102 (2002)

S-Matrices: Periodic Solution Strategy

- Can use a Fourier series expansion in real space of the H-fields:

$$\mathbf{H}(\mathbf{r},z)=\sum_{\mathbf{G}}\left(\phi_x(\mathbf{G})\left[\hat{\mathbf{x}}-\frac{1}{q}(k_x+G_x)\hat{\mathbf{z}}\right]+\phi_y(\mathbf{G})\left[\hat{\mathbf{y}}-\frac{1}{q}(k_y+G_y)\hat{\mathbf{z}}\right]\right)e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}+iqz}$$

- In momentum space, can represent as:

$$h(z)=e^{iqz}\left\{\phi_x\hat{\mathbf{x}}+\phi_y\hat{\mathbf{y}}-\frac{1}{q}(\hat{k}_x\phi_x+\hat{k}_y\phi_y)\hat{\mathbf{z}}\right\}$$

- And then the electric field as:

$$e(z)=\frac{1}{q}e^{iqz}\,\hat{\eta}\{[\hat{k}_y\hat{k}_x\phi_x+(q^2+\hat{k}_y\hat{k}_y)\phi_y]\hat{\mathbf{x}}$$
$$-[\hat{k}_x\hat{k}_y\phi_y+(q^2+\hat{k}_x\hat{k}_x)\phi_x]\hat{\mathbf{y}}+q[\hat{k}_y\phi_x-\hat{k}_x\phi_y]\hat{\mathbf{z}}\}$$

S-Matrices: Periodic Solution Strategy

- Eigenvalue equation becomes

$$\left\{ \begin{pmatrix} \hat{\eta} & 0 \\ 0 & \hat{\eta} \end{pmatrix} \left[q^2 + \begin{pmatrix} \hat{k}_x \hat{k}_x & \hat{k}_x \hat{k}_y \\ \hat{k}_y \hat{k}_x & \hat{k}_y \hat{k}_y \end{pmatrix} \right] + \begin{pmatrix} \hat{k}_y \hat{\eta} \hat{k}_y & -\hat{k}_y \hat{\eta} \hat{k}_x \\ -\hat{k}_x \hat{\eta} \hat{k}_y & \hat{k}_x \hat{\eta} \hat{k}_x \end{pmatrix} \right\} \times \begin{pmatrix} \phi_x \\ \phi_y \end{pmatrix} = \omega^2 \begin{pmatrix} \phi_x \\ \phi_y \end{pmatrix}$$

- More compactly represented as:

$$[\mathcal{H}(q^2 + K) + \mathcal{K}]\phi = \omega^2 \phi$$

- Where the eigenvectors ϕ have a unique orthonormality condition:

$$\phi_n^T (\omega^2 - \mathcal{K}) \phi_{n'} = \delta_{nn'}$$

S-Matrices: Periodic Solution Strategy

- Can rephrase:

$$[(\omega^2-\mathcal{K})\mathcal{E}(\omega^2-\mathcal{K})-\omega^2 K]\phi=q^2(\omega^2-\mathcal{K})\phi$$

- Where *H*-fields are written as:

$$\begin{pmatrix} h_x(z) \\ h_y(z) \end{pmatrix}=\sum_n \begin{pmatrix} \phi_{x_n} \\ \phi_{y_n} \end{pmatrix}(e^{iq_n z}a_n+e^{iq_n(d-z)}b_n)$$

$$h_{\parallel}(z)=\Phi[\hat{\mathrm{f}}(z)a+\hat{\mathrm{f}}(d-z)b]$$

- And where *E*-fields are given by:

$$\begin{pmatrix} -e_y(z) \\ e_x(z) \end{pmatrix}=\sum_n \begin{pmatrix} \hat{\eta} & 0 \\ 0 & \hat{\eta} \end{pmatrix}\left[q_n^2+\begin{pmatrix} \hat{k}_x\hat{k}_x & \hat{k}_x\hat{k}_y \\ \hat{k}_y\hat{k}_x & \hat{k}_y\hat{k}_y \end{pmatrix}\right]\times\begin{pmatrix} \phi_{x_n} \\ \phi_{y_n} \end{pmatrix}\frac{1}{q_n}(e^{iq_n z}a_n-e^{iq_n(d-z)}b_n)$$

$$e_{\parallel}(z)=(\omega^2-\mathcal{K})\Phi\hat{q}^{-1}[\hat{\mathrm{f}}(z)a-\hat{\mathrm{f}}(d-z)b]$$

S-Matrices: Periodic Solution Strategy

- Interface matrix in WC notation:

$$\begin{pmatrix} \hat{f}_l a_l \\ b_l \end{pmatrix} = I(l,l+1) \begin{pmatrix} a_{l+1} \\ \hat{f}_{l+1} b_{l+1} \end{pmatrix} = \begin{pmatrix} I_{11} & I_{12} \\ I_{21} & I_{22} \end{pmatrix} \begin{pmatrix} a_{l+1} \\ \hat{f}_{l+1} b_{l+1} \end{pmatrix}$$

- Where:

$$\begin{aligned} I(l,l+1) &= M_l^{-1} M_{l+1} \\ &= \tfrac{1}{2} \hat{q}_l \Phi_l^T (\omega^2 - \mathcal{K}_{l+1}) \Phi_{l+1} \hat{q}_{l+1}^{-1} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \\ &\quad + \tfrac{1}{2} \Phi_l^T (\omega^2 - \mathcal{K}_l) \Phi_{l+1} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \end{aligned}$$

S-Matrix Construction: Recap

- We can relate the *s*-interface matrix to the *t*-interface matrix from before:

$$s^{(p)} = \begin{bmatrix} t^{(p)}_{11} - t^{(p)}_{12}\, t^{(p)\,-1}_{22}\, t^{(p)}_{21} & t^{(p)}_{12}\, t^{(p)\,-1}_{22} \\ -t^{(p)\,-1}_{22}\, t^{(p)}_{21} & t^{(p)\,-1}_{22} \end{bmatrix}$$

- Then iteratively construct next S-matrix via:

$$\begin{bmatrix} T^{(p)}_{uu} & R^{(p)}_{ud} \\ R^{(p)}_{du} & T^{(p)}_{dd} \end{bmatrix} = \begin{bmatrix} \tilde{t}^{(p)}_{uu}\left[1 - R^{(p-1)}_{ud}\,\tilde{r}^{(p)}_{du}\right]^{-1} T^{(p-1)}_{uu} & \tilde{r}^{(p)}_{ud} + \tilde{t}^{(p)}_{uu}\, R^{(p-1)}_{ud}\left[1 - \tilde{r}^{(p)}_{du}\, R^{(p-1)}_{ud}\right]^{-1} \tilde{t}^{(p)}_{dd} \\ R^{(p-1)}_{ud} + T^{(p-1)}_{dd}\,\tilde{r}^{(p)}_{du}\left[1 - R^{(p-1)}_{ud}\,\tilde{r}^{(p)}_{du}\right]^{-1} T^{(p-1)}_{uu} & T^{(p-1)}_{dd}\left[1 - \tilde{r}^{(p)}_{du}\, R^{(p-1)}_{ud}\right]^{-1} \tilde{t}^{(p)}_{dd} \end{bmatrix}$$

S-Matrices: Periodic Solution Strategy

- In WC's notation:

$$S_{11}(l',l+1) = (I_{11} - \hat{f}_l S_{12}(l',l) I_{21})^{-1} \hat{f}_l S_{11}(l',l)$$

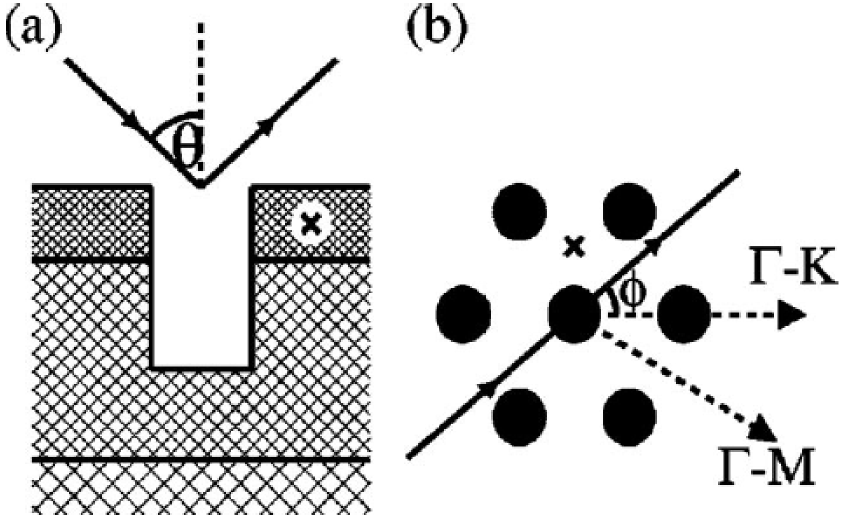
$$S_{12}(l',l+1) = (I_{11} - \hat{f}_l S_{12}(l',l) I_{21})^{-1} \times (\hat{f}_l S_{12}(l',l) I_{22} - I_{12}) \hat{f}_{l+1}$$

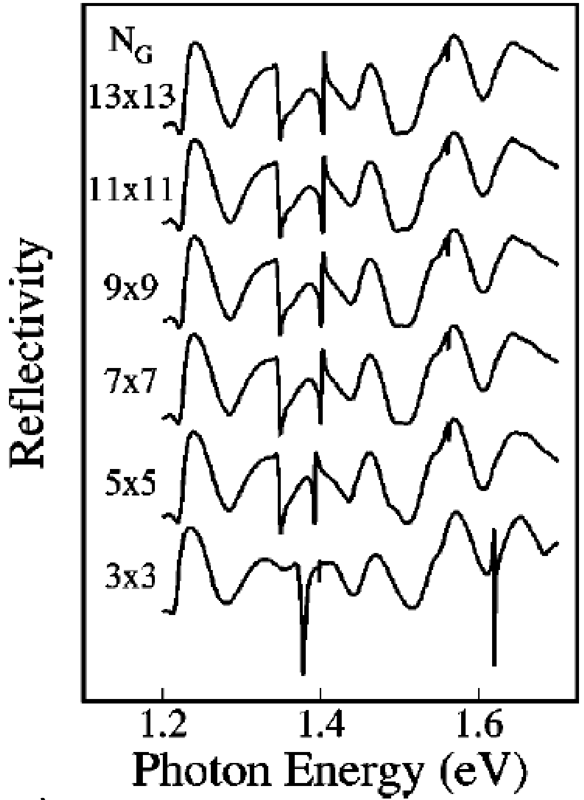
$$S_{21}(l',l+1) = S_{22}(l',l) I_{21} S_{11}(l',l+1) + S_{21}(l',l)$$

$$S_{22}(l',l+1) = S_{22}(l',l) I_{21} S_{12}(l',l+1) + S_{22}(l',l) I_{22} \hat{f}_{l+1}$$

S-Matrix Simulations

- Transmission through triangular lattice converges as number of plane waves N_G increases

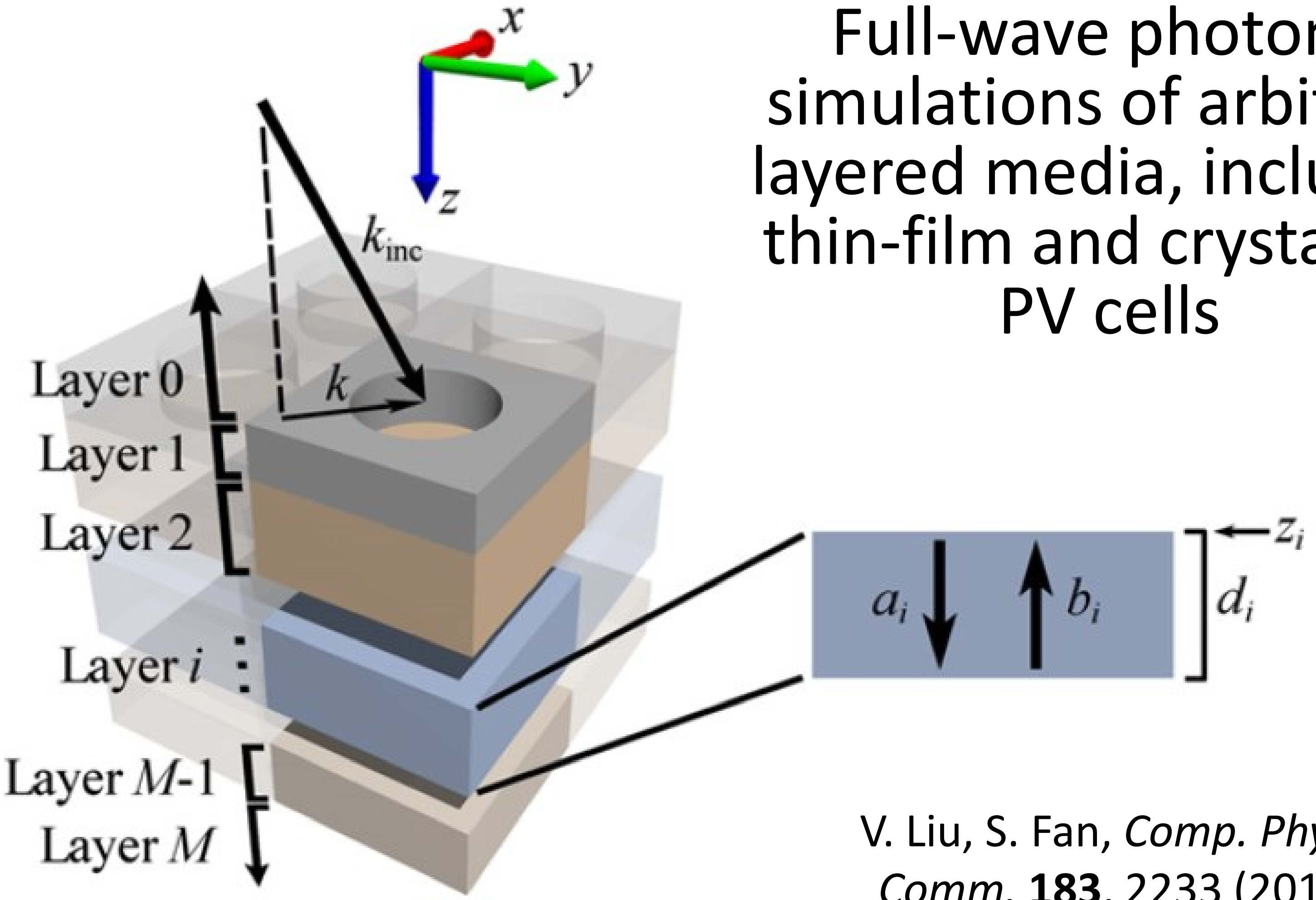




$$\varepsilon(\mathbf{G})=\begin{cases} 2(\varepsilon_a-\varepsilon_b)\beta J_1(G\rho)/(G\rho) & \mathbf{G}\neq 0 \\ \varepsilon_a\beta+\varepsilon_b(1-\beta) & \mathbf{G}=0, \end{cases}$$

Whittaker & Culshaw, *Phys. Rev. B* **60**, 2610 (1999)

Photonic Simulations with S^4

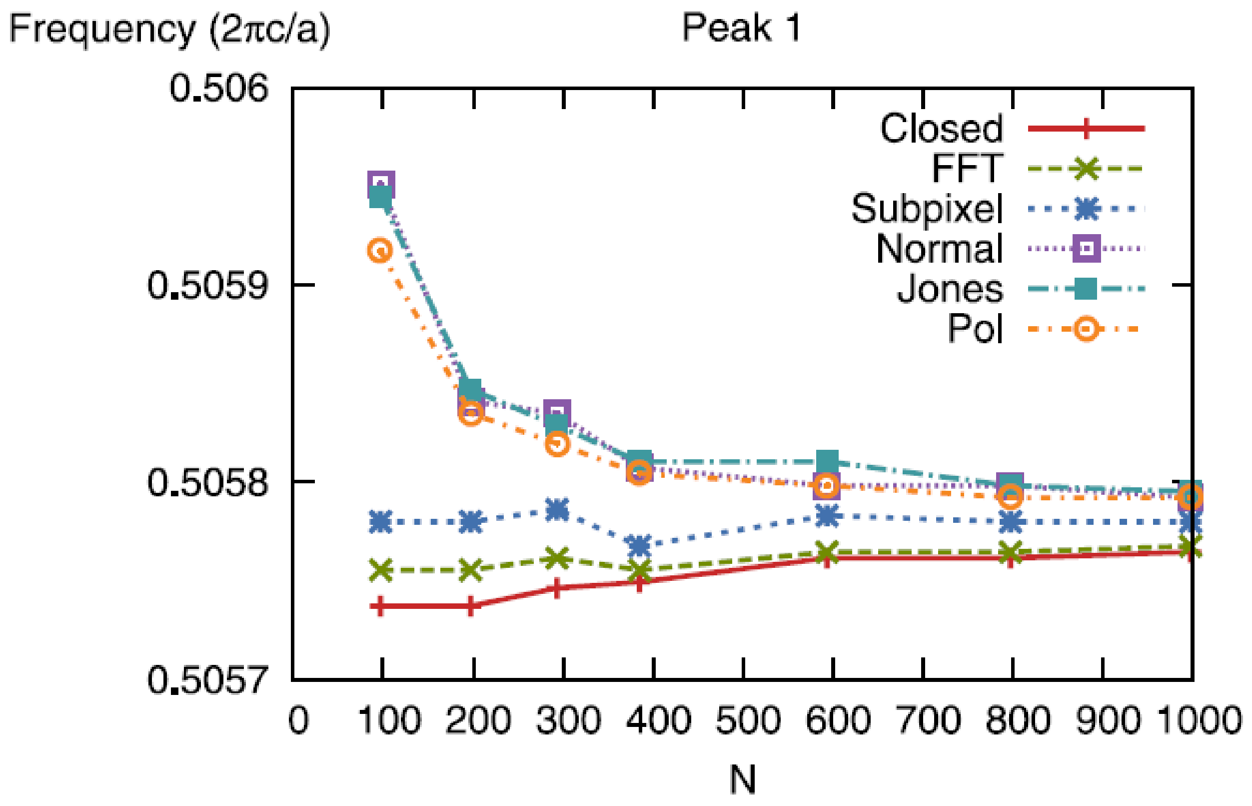


Full-wave photonic simulations of arbitrary layered media, including thin-film and crystalline PV cells

V. Liu, S. Fan, *Comp. Phys. Comm.* **183**, 2233 (2012)

Photonic Simulations with S^4

Accuracy improves systematically with computing power



V. Liu, S. Fan, *Comp. Phys. Comm.* **183**, 2233 (2012)

S^4: Lua Control Files

- Obtain a new, blank simulation object with no solutions:

```
S = S4.NewSimulation()
```

- Define all materials:

```
S:AddMaterial('name', {eps_real, eps_imag})
```

- Add all layers:

```
S:AddLayer('name', thickness, 'material_name')
```

- Add patterning to layers:

```
S:SetLayerPatternCircle('layer_name', 'inside_material', {center_x,
center_y}, radius)
```

S^4: FMM Formulations

- Specify the excitation mechanism:

```
S:SetExcitationPlanewave(
        {angle_phi, angle_theta}, -- phi in [0,180), theta in [0,360)
        {s_pol_amp, s_pol_phase}, -- phase in degrees
        {p_pol_amp, p_pol_phase})
```

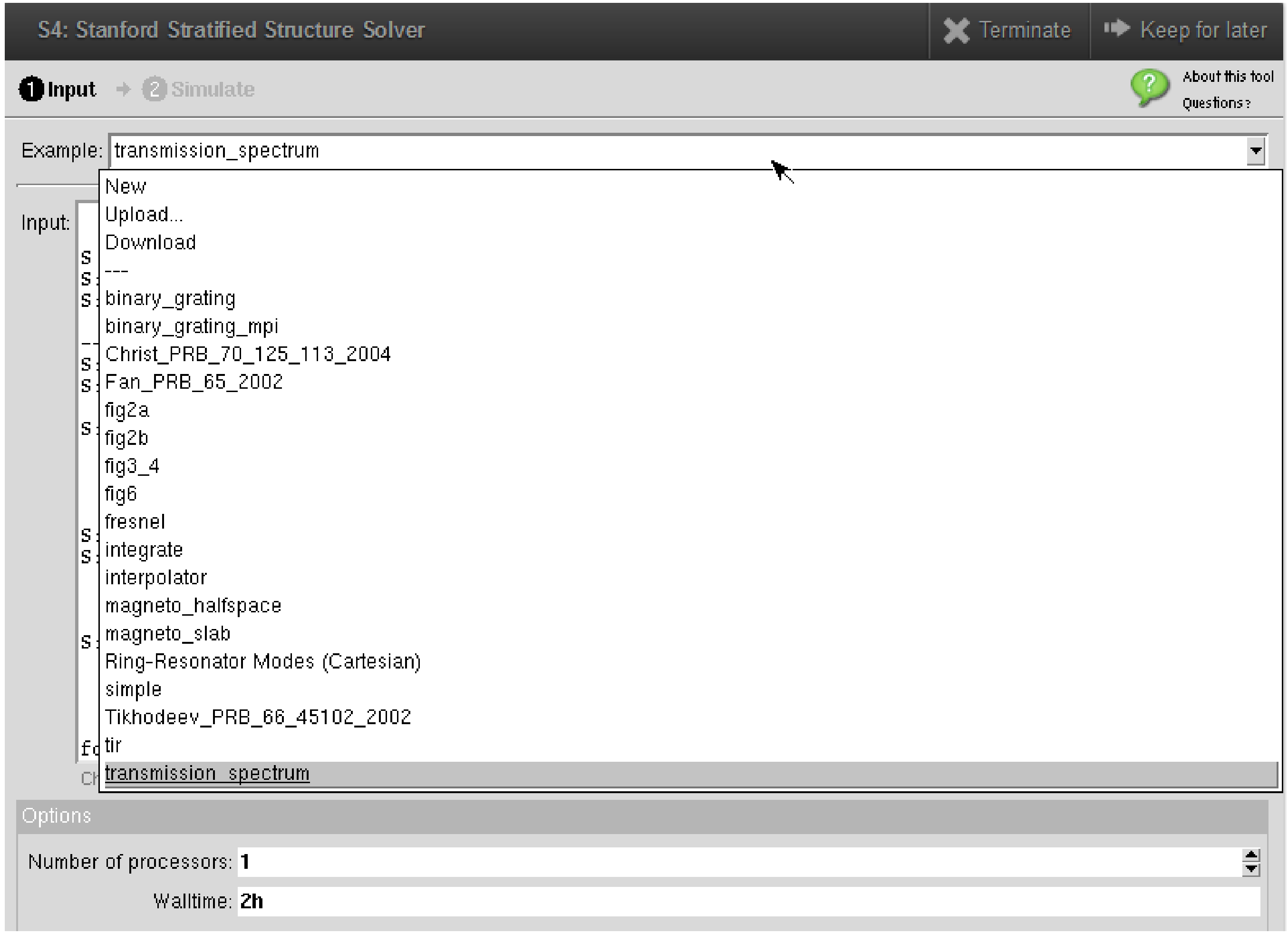
- Specify the operating frequency:

```
S:SetFrequency(0.4)
```

- Obtain desired output:

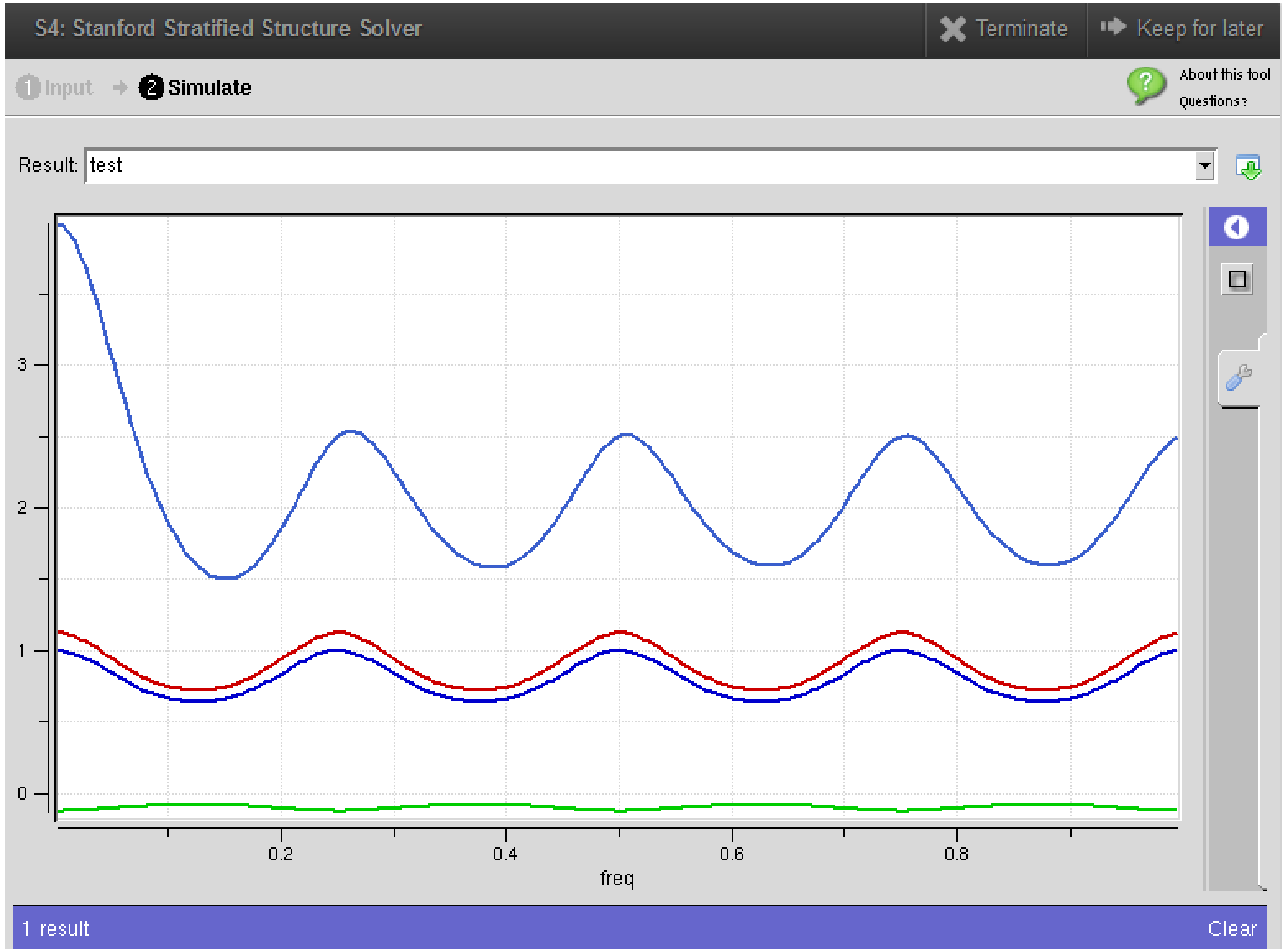
```
forward_power, backward_power = S:GetPoyntingFlux('layer_name', z_offset)
print(forward_power, backward_power)
```

S^4: Input



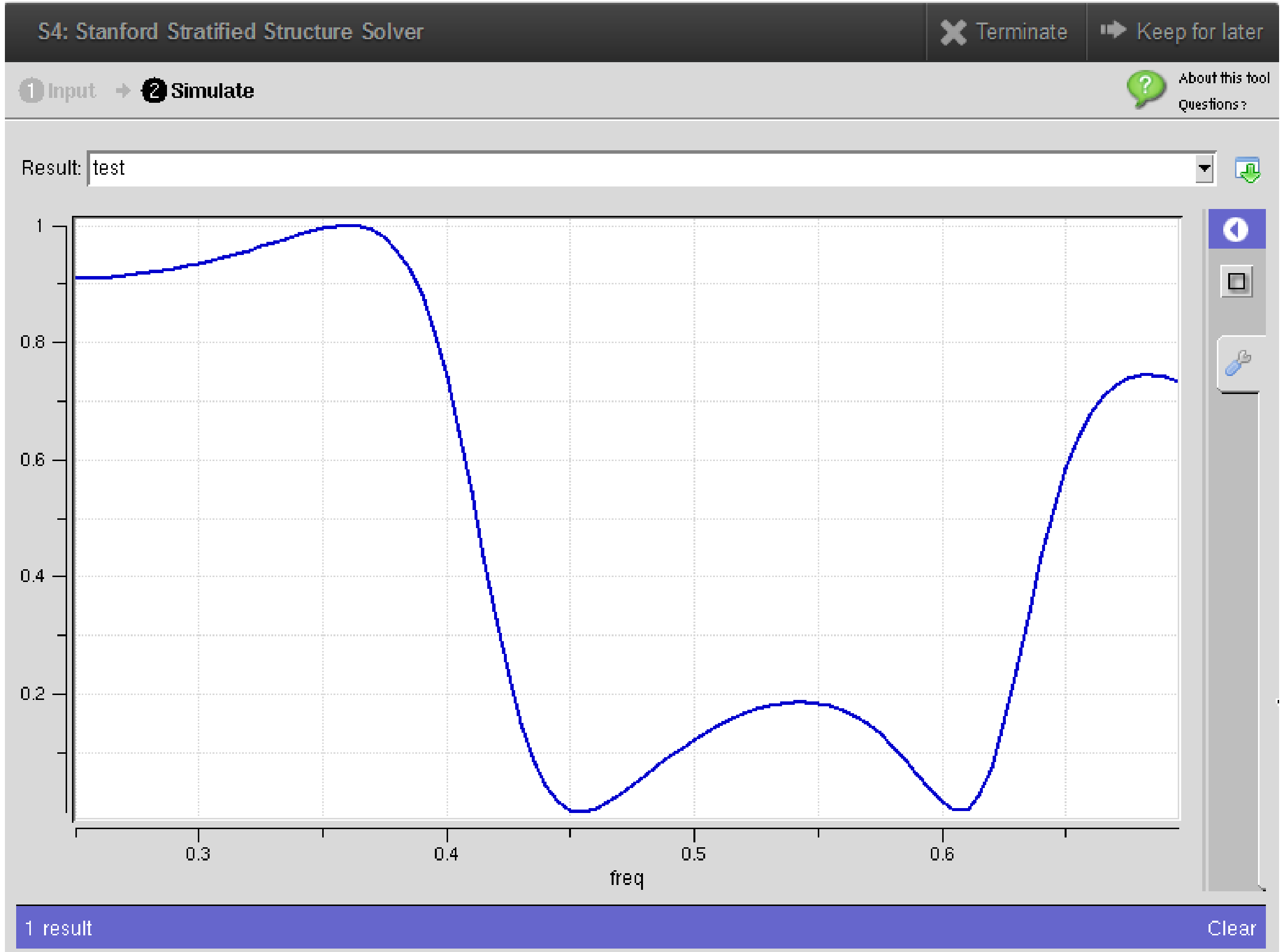
Can choose several examples drawn from the literature

S^4: Output



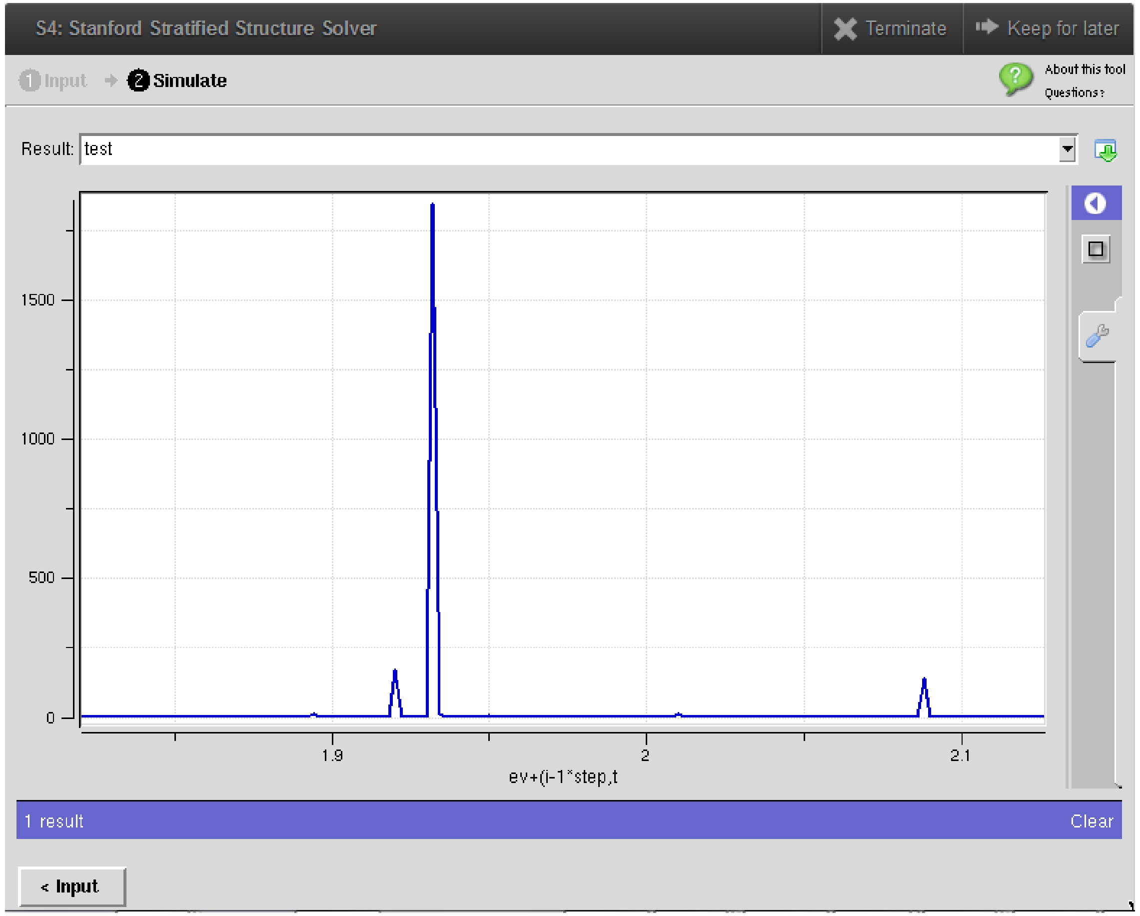
Transmission through multilayer stack matches analytical expression

S^4: Output



Transmission through 1D square grating of silicon and air

S^4: Output



- Transmission from Fig. 4 of Tikhodeev *et al.*, *Phys. Rev. B* **66**, 045102 (2002).

S-Matrix Method: Advantages

- No *ad hoc* assumptions regarding structures
- Applicable to wide variety of problems
- Suitable for eigenmodes or high-Q resonant modes at single frequency
- Can treat layers with large difference in length scales
- Computationally tractable enough on single core machines

S-Matrix Method: Disadvantages

- Accurate solutions obtained more slowly as the following increase:
  - Number of layers
  - Absolute magnitude of Fourier components (especially for metals)
  - Number of plane-wave components ($\sim N^3$)
- Relatively slow for broad-band problems (time-domain is a good alternative)

Next Class

- Is Friday, Mar. 3
- Next time, we will continue with transfer matrix models, focusing on CAMFR