Evolution Operators and Boundary Conditions for Propagation and Reflection Methods

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Outline

- Fundamental Equations
- Non-Local Boundary Conditions
- Improving Accuracy in Fast Reflection Calculations

Part I - Fundamental Equations

Scalar Wave Equation

- Scalar, Monochromatic Electric Field

$$\left(\frac{\partial^2}{\partial z^2}+\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+k_0^2 n^2(\vec{r})\right)\mathrm{E}(x,y,z)=0$$

$$\text{Defining } n_0 = n_{reference},\ X_0 = \frac{1}{k_0{}^2 n_0^2}\frac{\partial^2}{\partial x^2},$$

$$Y_0 = \frac{1}{k_0{}^2 n_0^2}\frac{\partial^2}{\partial y^2} \text{ and } N = \frac{n^2(\vec{r})}{n_0{}^2}-1, \text{ we have}$$

$$\left(\frac{\partial^2}{\partial z^2}+k_0{}^2 n_0^2 (X_0 + Y_0 + N)\right)\mathrm{E}(x,y,z)=0$$

Forward Solution

- Define $H = X_0 + Y_0 + N$. For forward-travelling waves ($e^{i\omega t}$ time-dependence)

$$\left(\frac{\partial}{\partial z} + ik_0 n_0 \sqrt{1+H} \right) \mathrm{E}(x,y,z) = 0$$

- We then have with $\delta = -ik_0 n_0$

$$\mathrm{E}(x,y,z+\Delta z) = e^{\delta \Delta z \sqrt{1+H}}\, \mathrm{E}(x,y,z)$$

Modal Analysis

- Modal Decomposition

$$\mathrm{E}(x,y,\bar{z}) = \sum_m a_m \,\mathrm{E}_m(x,y,\bar{z}) \quad \text{with}$$

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + k_0^2 n^2(x,y,\bar{z})\right]\mathrm{E}_m(x,y,\bar{z}) = \beta_m^2(x,y,\bar{z})\,\mathrm{E}_m(x,y,\bar{z})$$

- Approximate Forward Solution

$$\mathrm{E}(x,y,z+\Delta z) = \sum_m e^{-i\beta_m(x,y,\bar{z})\Delta z}\,\mathrm{E}_m(x,y,z)$$

Fresnel Approximation

- Fresnel Approximation

$$\sqrt{1+H} \approx 1 + \frac{H}{2}$$

- Slowly-Varying Envelope $E(x,y,z) = \mathrm{E}(x,y,z)e^{-\delta z}$

$$\left(\frac{\partial}{\partial z} + \frac{\delta}{2}(X_0 + Y_0 + N)\right)E(x,y,z) = 0$$

Wide-Angle Approximations

- Taylor Series Expansion

$$\sqrt{1+H} \approx 1+\frac{1}{2}H-\frac{1}{8}H^2+\frac{1}{16}H^3-\frac{5}{128}H^4+O(H^5)$$

- Padé [2,0] approximant:

$$\sqrt{1+H} \approx 1+\frac{H}{2}-\frac{H^2}{8}$$

- Padé [1,1] approximant

$$\sqrt{1+H} \approx \frac{1+3H/4}{1+H/4}$$

$$=1+\frac{1}{2}H-\frac{1}{8}H^2+\frac{1}{32}H^3-\frac{1}{128}H^4+O(H^5)$$

Square-Root Operator Recursion

- Recursion Relation

$$\sqrt{1+H}-1=\left(\sqrt{1+H}-1\right)\left(\frac{\sqrt{1+H}+1}{\sqrt{1+H}+1}\right)$$

$$=\frac{H}{\sqrt{1+H}+1}$$

$$=\frac{H}{2+\left(\sqrt{1+H}-1\right)}$$

- Thus if $f(x)=\sqrt{1+H}-1$ we have

$$f(x)=x/(2+f(x))$$

Continued Fraction Expansion

- Iterating the recursion relation yields

$$\sqrt{1+H}-1=\frac{H}{2+\frac{H}{2+\ldots\frac{H}{2+\frac{H}{2}}}}$$

- Note that we have employed $f(x)=0$ to terminate the fraction, yielding a real expression.

Padé Representations

- The Padé approximant can be factored as

$$\sqrt{1+H} \approx \prod_{r=1}^{s}\left[\frac{1+\sin^2\left(\frac{r\pi}{2s+1}\right)H}{1+\cos^2\left(\frac{r\pi}{2s+1}\right)H}\right]$$

- In a partial fraction representation

$$\sqrt{1+H} = 1+\sum_{r=1}^{s}\left[\frac{\frac{2}{2s+1}\sin^2\left(\frac{r\pi}{2s+1}\right)H}{1+\cos^2\left(\frac{r\pi}{2s+1}\right)H}\right]$$

Finite Difference Method

- Applying a [1,1] Padé approximant yields the Crank-Nicholson procedure

$$E(z+\Delta z) = e^{\delta\frac{H}{2}} E(z)$$

$$= e^{\frac{\delta}{2}(X_0+Y_0+N)} E(z)$$

$$\approx \left(\frac{1+\delta H/4}{1-\delta H/4}\right) E(z) + O(\delta^3)$$

Discrete Representation

- On a one-dimensional transverse grid $\{x_i\}$

$$E(x_i, z+\Delta z) = \frac{1 - \dfrac{i\Delta z}{4k_0 n_0}\left(k_0^2\left(n^2(x_i) - n_0^2\right) + D_x^2\right)}{1 + \dfrac{i\Delta z}{4k_0 n_0}\left(k_0^2\left(n^2(x_i) - n_0^2\right) + D_x^2\right)} E(x_i, z)$$

where

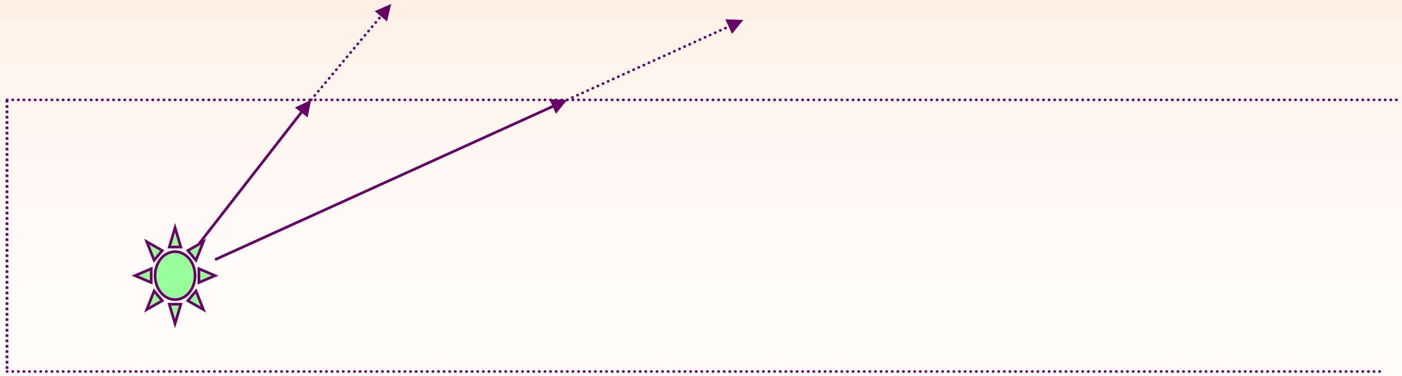
$$D_x^2 E_i = \frac{E_{i+1} - 2E_i + E_{i-1}}{\Delta z^2}$$

and for any operator O, $\dfrac{1}{O}$ represents O^{-1}.

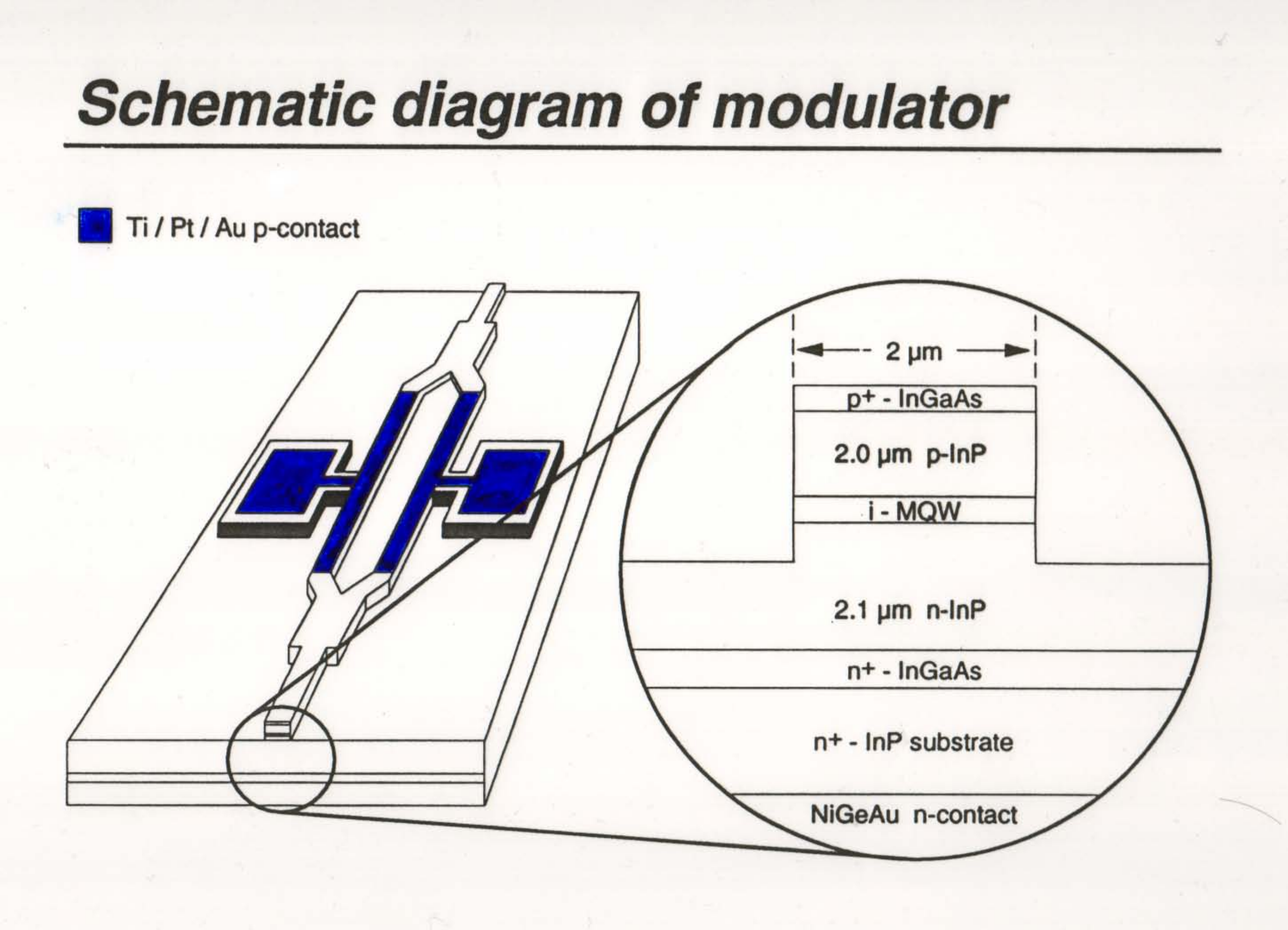
Part II - Nonlocal Boundary Conditions

Objective

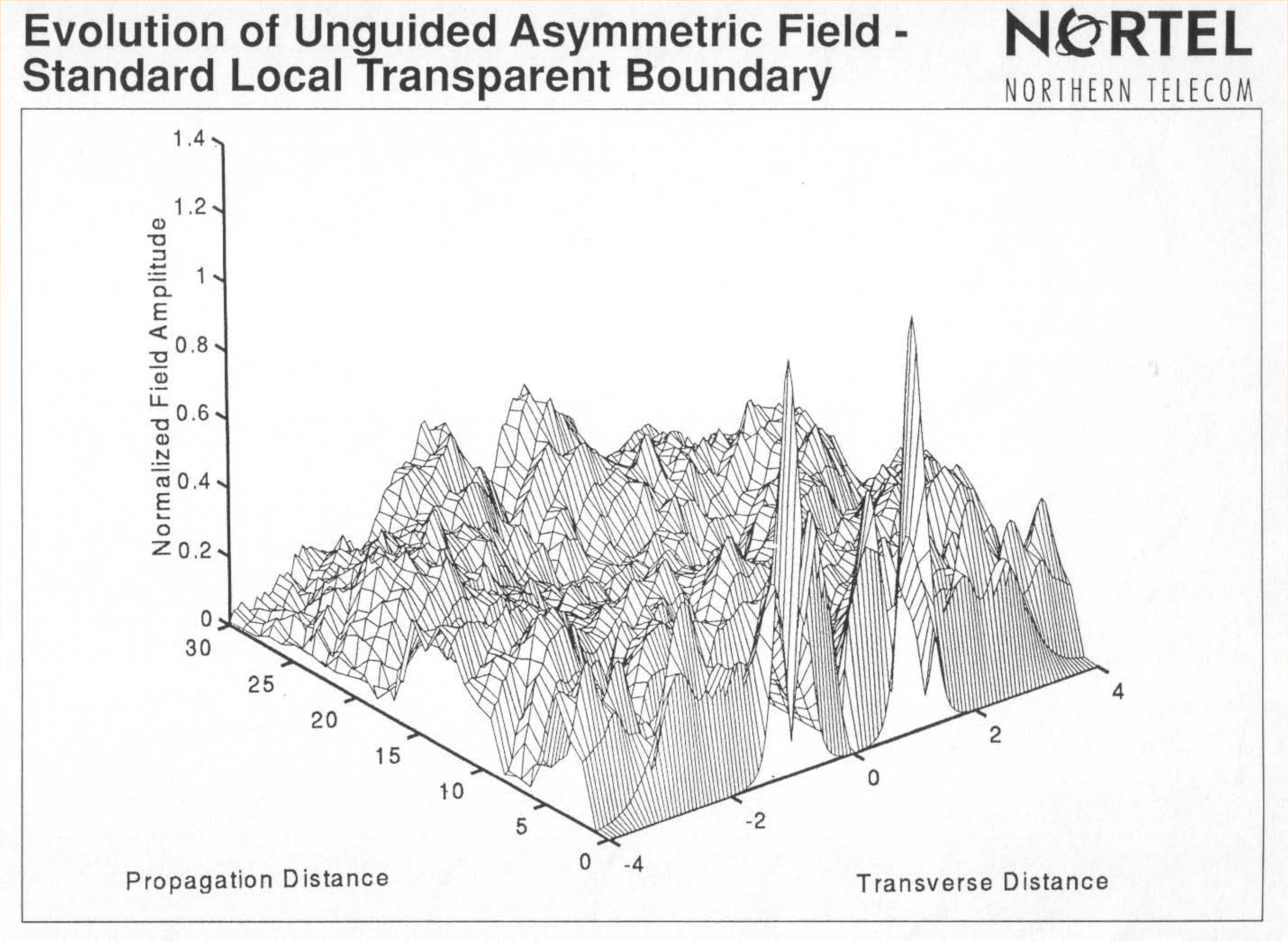
- To simulate on a finite, discrete computational grid the field radiated from a local source into a homogeneous semi-infinite medium.



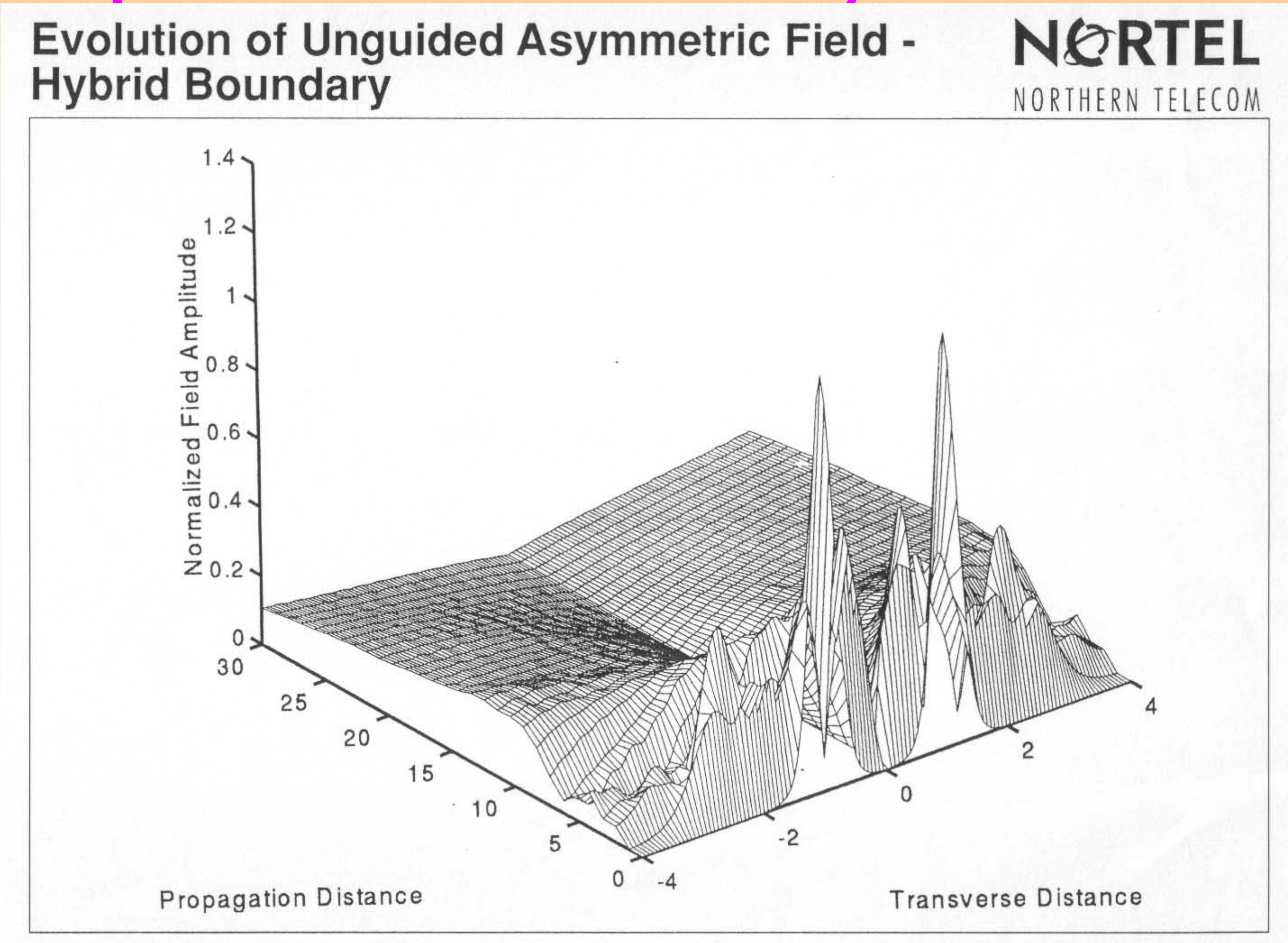
Electrorefraction Modulator



Standard Boundary Conditions

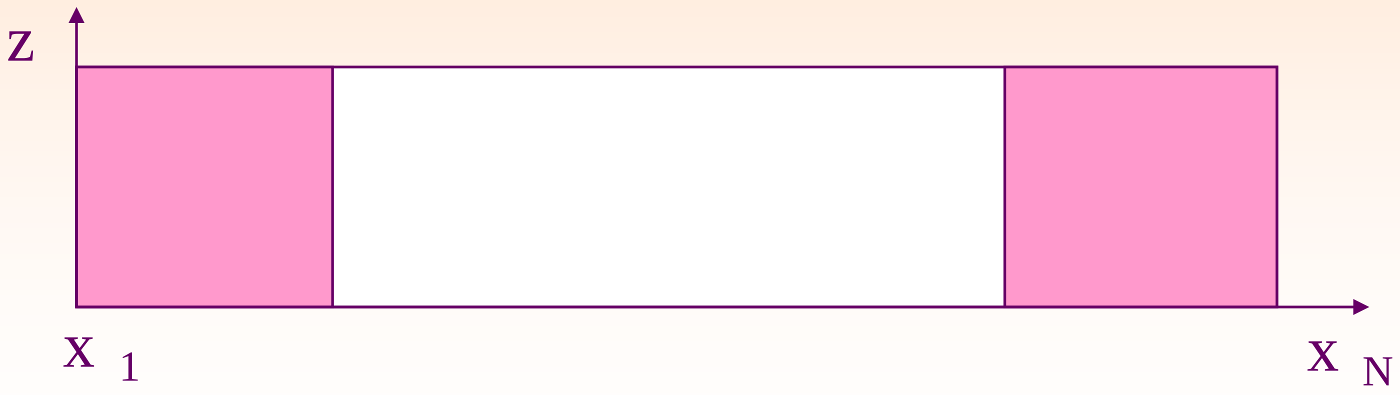


Improved Boundary Conditions



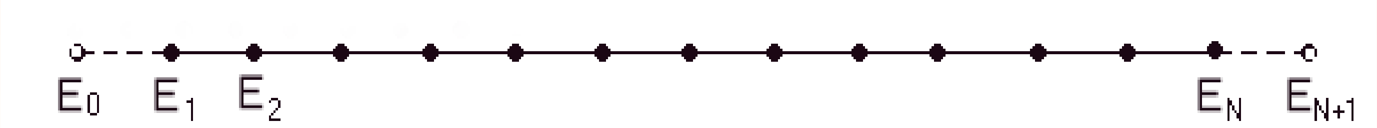
Boundary Layers

– The approximate propagation operators introduced above are unitary. To remove the outward propagating electric field at the boundary we can introduce absorbing or impedance-matched boundary layers.



Transparent Boundaries

- Set E_0 and E_{N+1} to be consistent with purely outgoing waves at the boundary.
  - Local Boundary Conditions: $\boldsymbol{E}_0,\ \boldsymbol{E}_{N+1}$ are computed from $\boldsymbol{E}$ at the last propagation step.
  - Nonlocal Boundary Conditions: $E_0,\ E_{N+1}$ are obtained from previous values of Ǝ .



Impedance-Matched Layer

- For a non-equidistant grid, $\Delta X_i = (1 - b_i)\Delta X$ the governing equation in a homogeneous refractive index layer near the boundary is

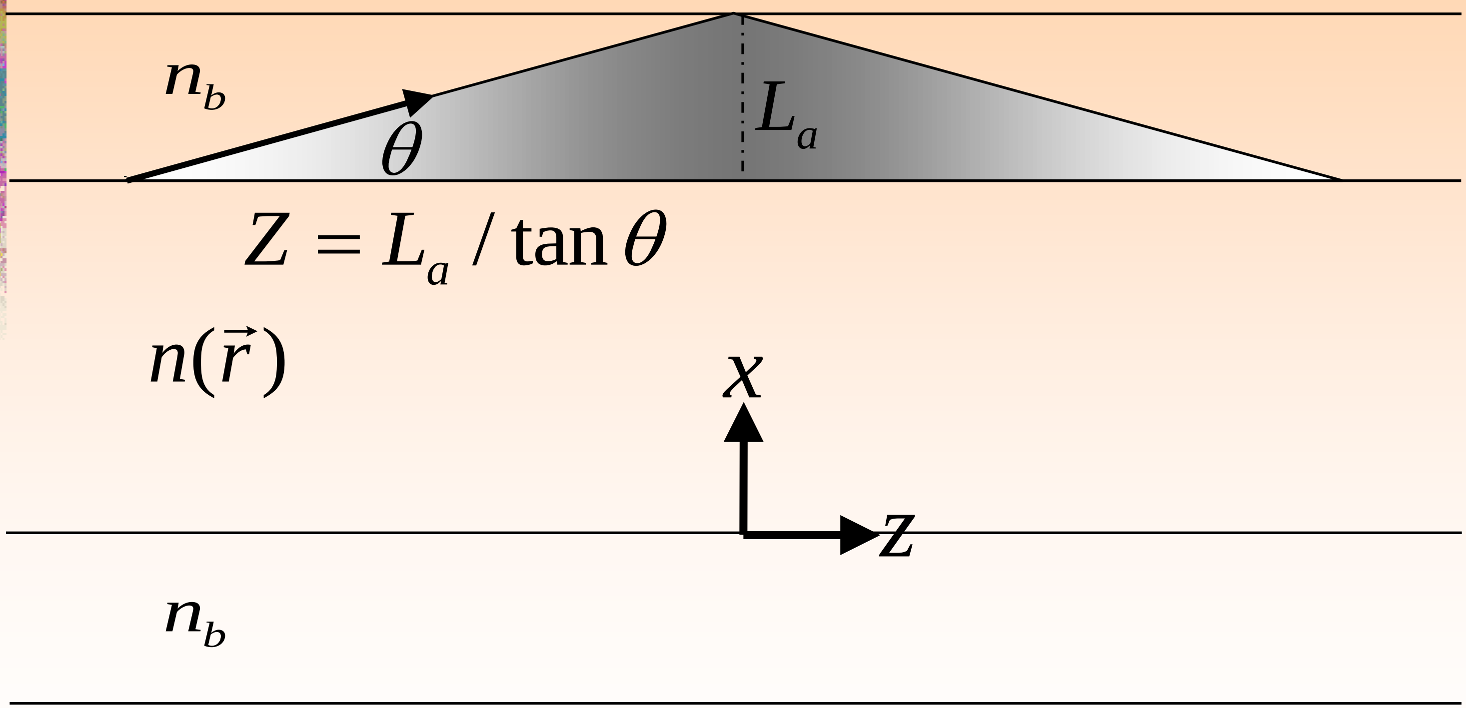
$$\left(-2ik_0 n_0 \frac{\partial}{\partial z} + \frac{d^2}{dx^2} + k_0^{\,2}(n_b^{\,2} - n_0^{\,2}) \right) E(x, y, z) = 0$$

- For continuous $x, \; z$, no spurious effects.
- Thus, if $b_i \rightarrow ia_i$, we have

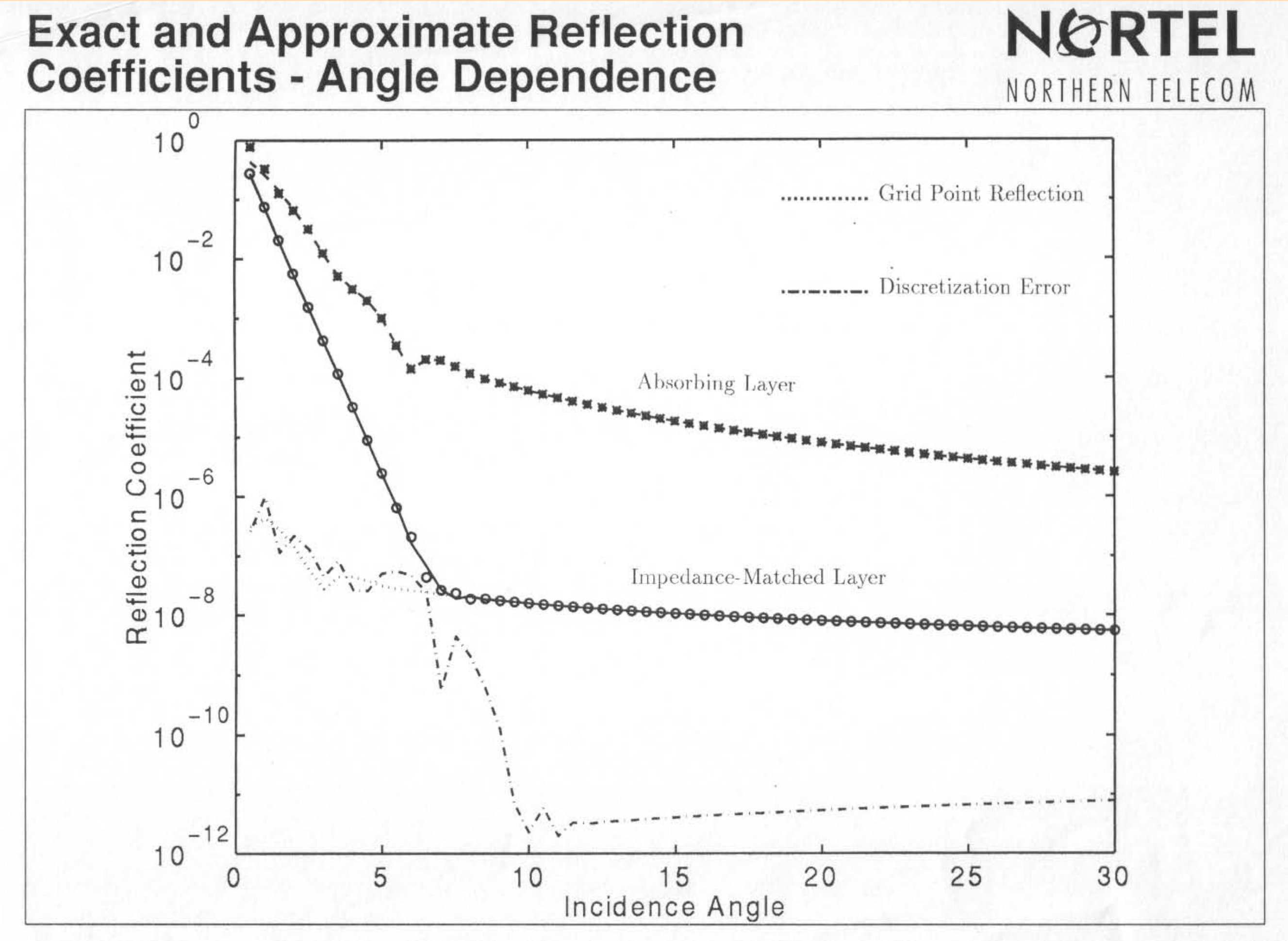
$$E_{k_x, k_z}(x, z) \propto e^{ik_x(1+ia_i)x + ik_z z}$$

Impedance-Matched Layer

$$\text{Attenuation} = e^{-2k_x \Delta x \sum_l a_l} = e^{-2k_0 n_b \Delta x \sin\theta \sum_l a_l}$$



Approximate and Exact Results



Continuous Nonlocal Boundary

- Assume that $n^2(x_{N-1}) = n^2(x_N) = n_0^2$. At the boundary

$$\frac{\partial^2 E}{\partial x^2} = 2ik_0 n_0 \frac{\partial E}{\partial z}$$

- Crank-Nicholson method - $E_j \equiv E(x, z_j)$

$$\frac{\partial^2}{\partial x^2}\left(\frac{E_{j+1} + E_j}{2}\right) = 2ik_0 n_0 \frac{E_{j+1} - E_j}{\Delta z}$$

- Setting $s \equiv T_{\{-\Delta z\}} = e^{-\Delta z \frac{\partial}{\partial z}}$, we have with $\nu = \sqrt{4ik_0 n_0/\Delta z}$,

$$\frac{\partial^2 E_{j+1}}{\partial x^2} = \nu^2 \frac{1-s}{1+s} E_{j+1}$$

Continuous Nonlocal Boundary

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- Outgoing condition (right boundary)

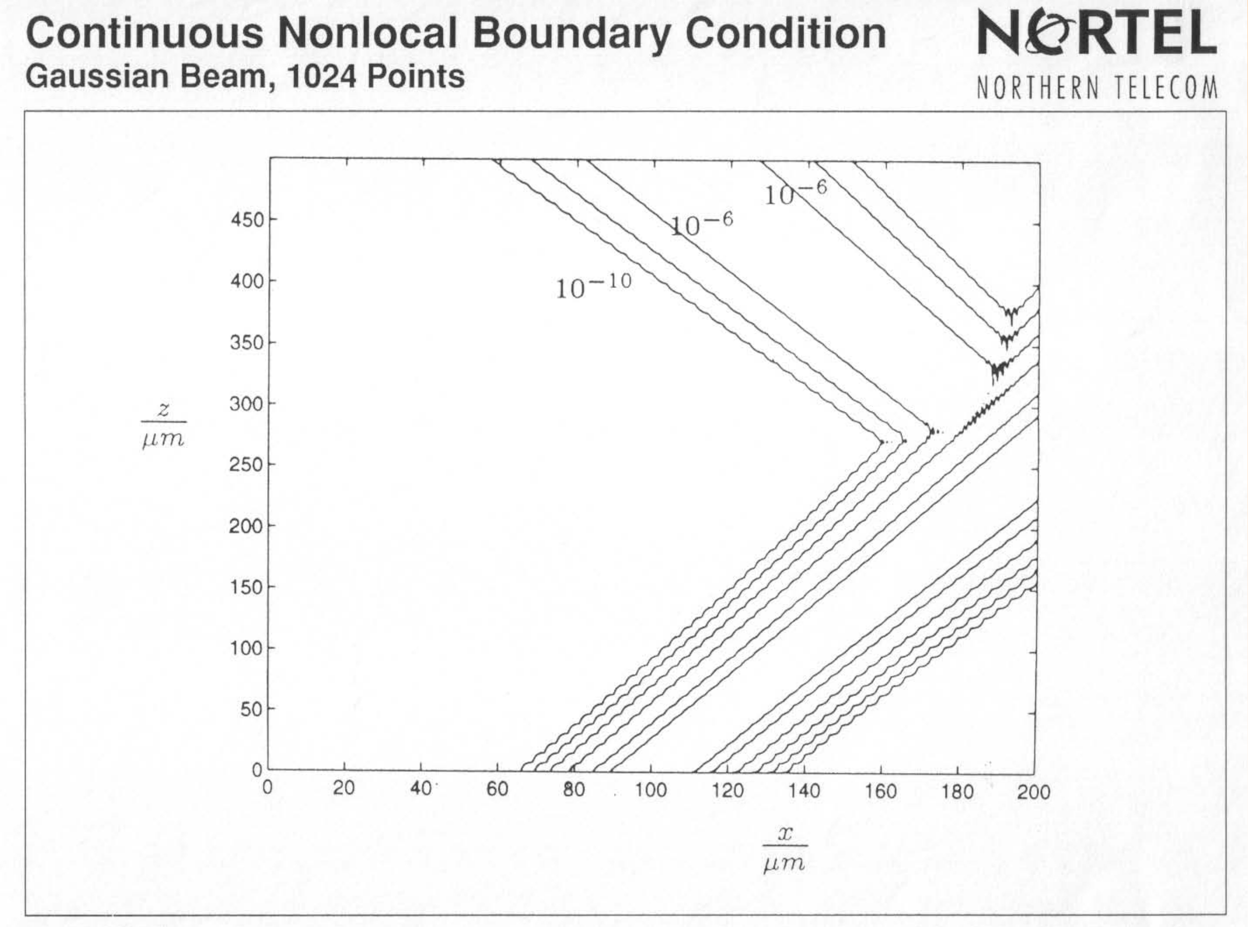
$$\frac{\partial E_{j+1}}{\partial x} = -\nu \sqrt{\frac{1-s}{1+s}} E_{j+1}$$

With $s^l E(x,z) = E(x, z - l\Delta z)$, we have

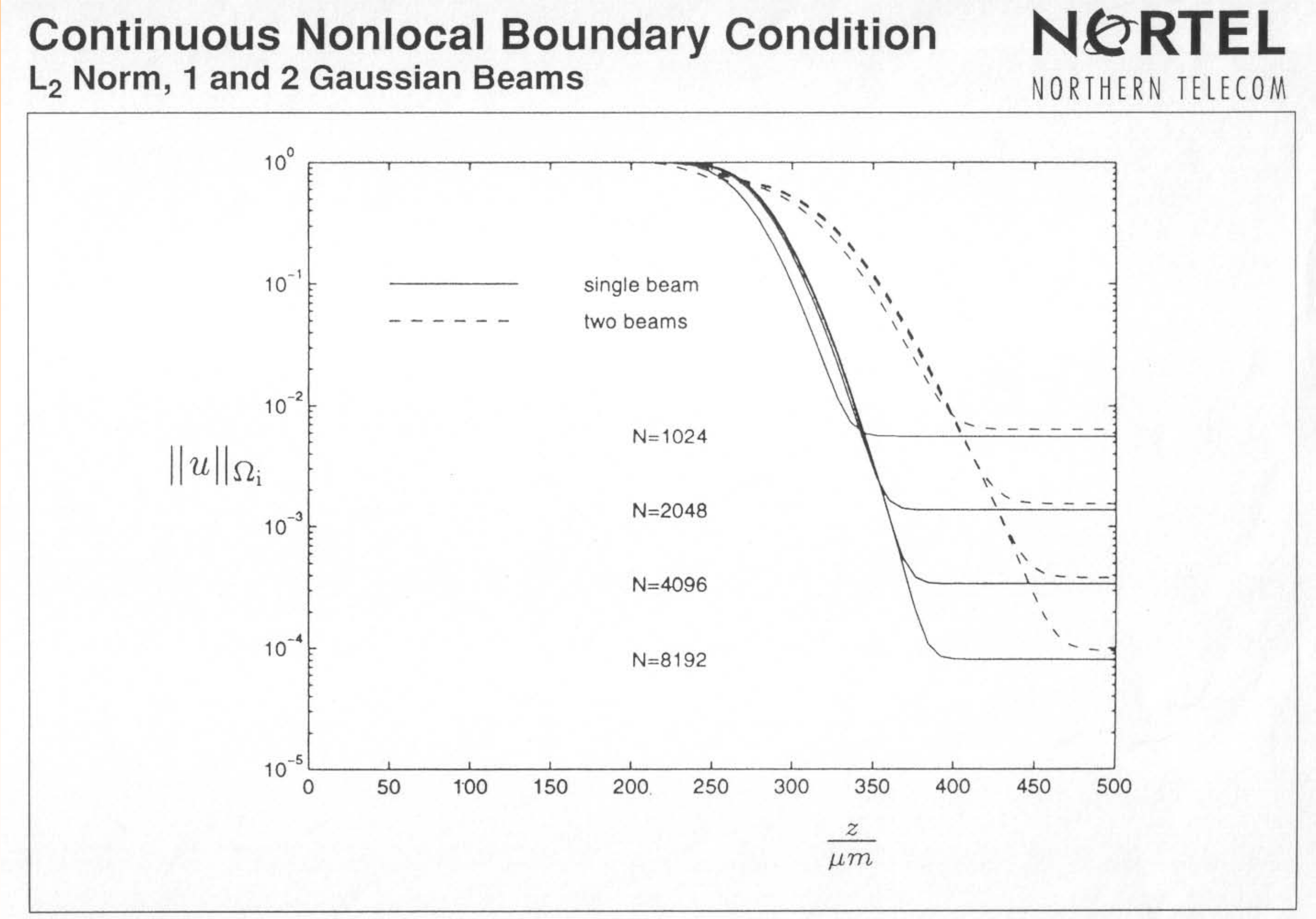
$$\frac{\partial E(x, z_{j+1})}{\partial x} + \nu E(x, z_{j+1}) =$$
$$\nu \left[E(x, z_j) - \frac{1}{2} E(x, z_{j-1}) + \right.$$
$$\left. \frac{1}{2} E(x, z_{j-2}) - \frac{3}{8} E(x, z_{j-3}) + \ldots \right].$$

- The electric field is optimally evaluated at $(x_{N_w} + x_{N_w+1})/2$.

Gaussian Beam - Continuous N.L.



Remaining Power - Continuous



Exact Nonlocal Boundary

- With $E_m \equiv E(x_m, z_j + \Delta z)$ the Crank-Nicholson method yields on a discrete grid

$$(1+s)(E_{m+1} - (2 - k_0^2 \Delta n^2)E_m + E_{m-1}) = \nu^2 (1-s) E_m$$

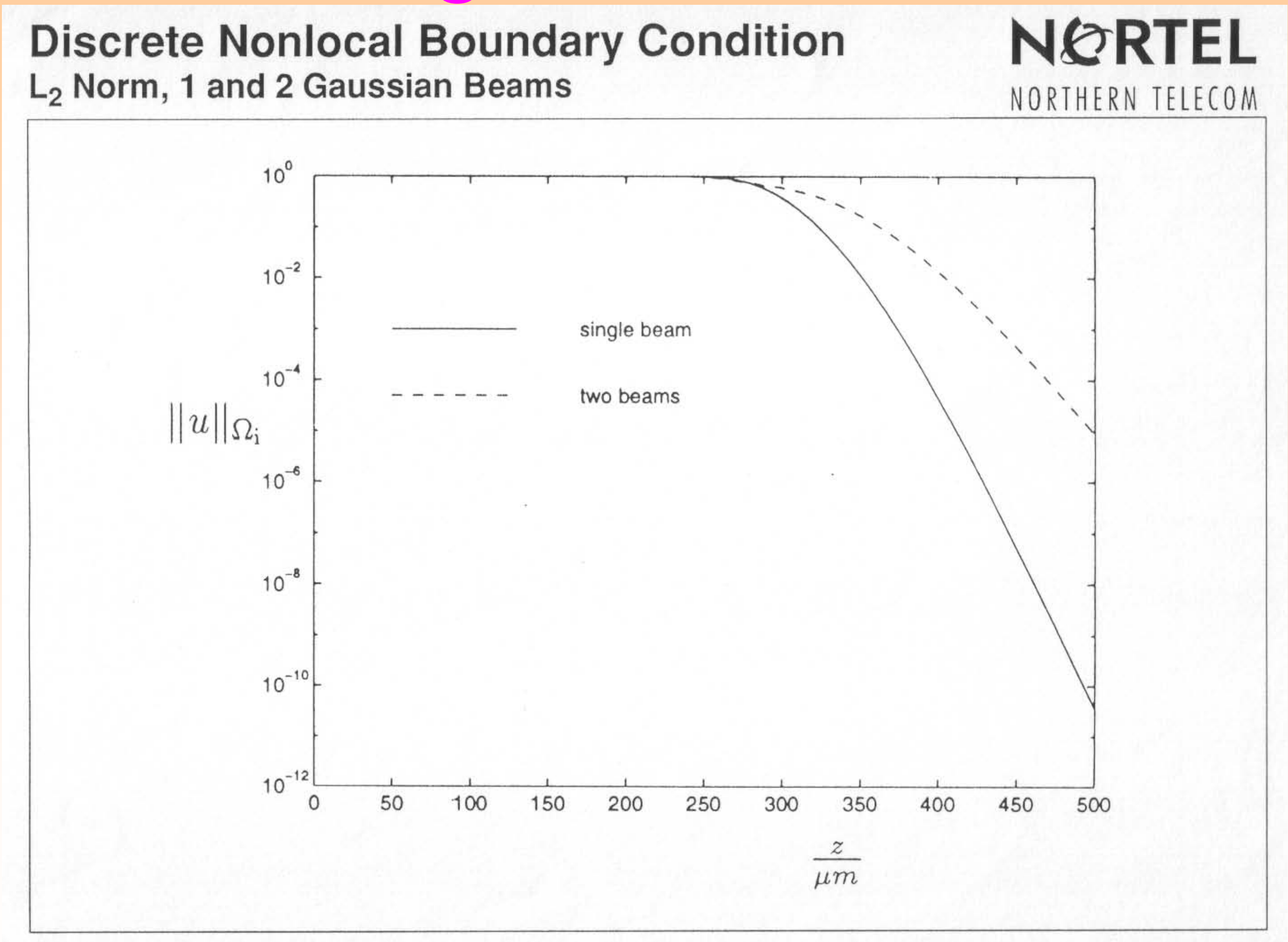
- Applying the x-translation operator $r \equiv T_{\{-\Delta x\}} = e^{-\Delta x \frac{\partial}{\partial x}}$

$$r^2 - (2 - k_0^2 \Delta n^2) r + 1 = \nu^2 \frac{1-s}{1+s} r$$

- If the root with $|r| < 1$ is denoted by r_-, the discrete transparent boundary condition is

$$E_{N+1} = r_- \cdot E_N$$

Remaining Power - Discrete



Padé [1,1] Boundary Conditions

- [1,1] Padé Approximation

$$-1+\sqrt{1+H} \approx \frac{H/2}{1+H/4}$$

- Claerbout's Equation

$$\left[\left(1+\frac{H}{4}\right)\frac{\partial}{\partial z}+\delta\frac{H}{2}\right]E(x,y,z)=0$$

- Boundary Condition Equation ($n_b = n_0$)

$$\left(1+\frac{X_0}{4}\right)\left[\frac{1-s}{\Delta z}\right]E(z+\Delta z) = -\delta\frac{X_0}{4}(1+s)E(z+\Delta z)$$

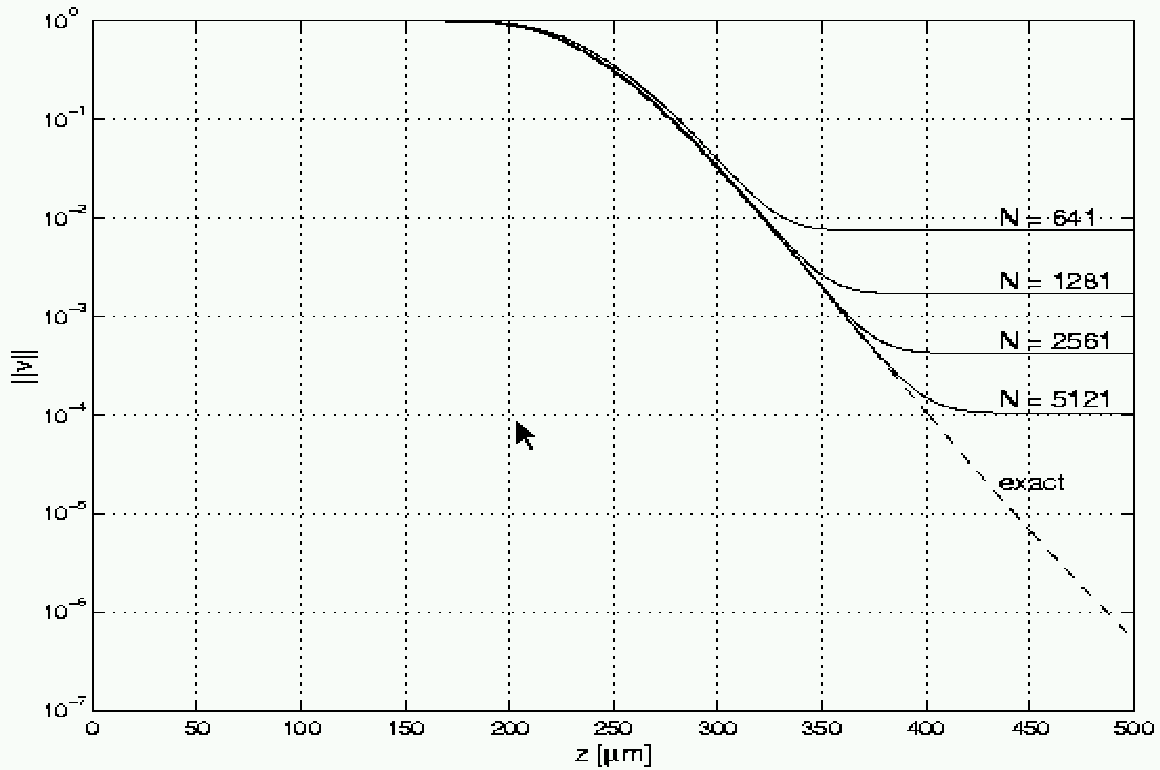
Padé [2,0] Boundary Conditions

- [2,2] Padé Equation

$$\left(\frac{1-s}{\Delta z}\right)E_{j+1}(x) = -\delta\left(1+\frac{X_0}{2}-\frac{{X_0}^2}{8}\right)\left(\frac{1+s}{2}\right)E_{j+1}(x)$$

- Laplace transform this equation with respect to x in the exterior region.
- Requiring that no poles are present in the right-hand plane of the transform yields the desired boundary condition.

[2,2] Boundary Condition Results



Padé [N,N] Boundary Conditions

- For the [N,N] case, $sE_i(x) = E_{i-1}(x)$, where

$$g_i^{(1)}(x) = \left(\frac{1 - a_1{}' \partial_x^2}{1 - a_1 \partial_x^2}\right) E_{i-1}(x)$$

$$g_i^{(2)}(x) = \left(\frac{1 - a_2{}' \partial_x^2}{1 - a_2 \partial_x^2}\right) g_i^{(1)}(x)$$

$$\vdots$$

$$g_i^{(k-1)}(x) = \left(\frac{1 - a_{k-1}{}' \partial_x^2}{1 - a_{k-1} \partial_x^2}\right) g_i^{(k-2)}(x)$$

$$E_i(x) = \left(\frac{1 - a_k{}' \partial_x^2}{1 - a_k \partial_x^2}\right) g_i^{(k-1)}(x)$$

General Boundary Conditions (2)

- Introducing a vector $\mathbf{g}_i(x)$ with

$\mathbf{g}_{i,j}(x) = g_i^{(j)}(x),\ j = 1\ldots k-1,\ \mathbf{g}_{i,k}(x) = E_i(x)$ yields

$$(\mathbf{E} + \mathbf{A}\partial_x^2)\mathbf{g}_i(x) = 0$$

with boundary conditions

$$\dot{\mathbf{g}}_{i,+} = \mathbf{B}_+\mathbf{g}_{i,+},\ \dot{\mathbf{g}}_{i,-} = \mathbf{B}_+\mathbf{g}_{i,-}$$

General Boundary Conditions (3)

- After Laplace transforming, this yields

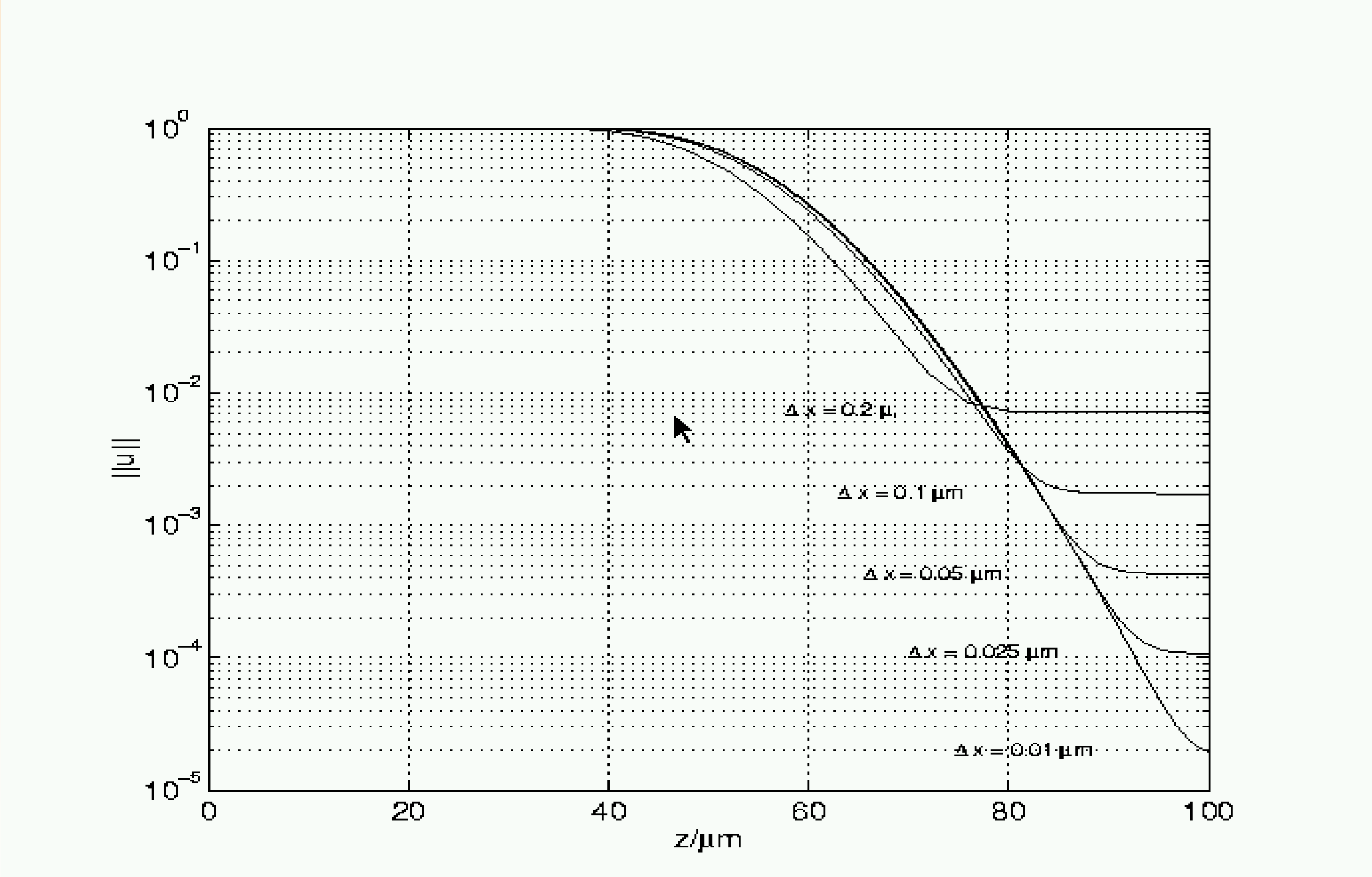
$$\left(\mathbf{E} + p^2\mathbf{A}\right)\hat{\mathbf{g}}_i(p) = \mathbf{A}(p\mathbf{g}_{i,0} + \dot{\mathbf{g}}_{i,0})$$

or, defining $\mathbf{C}^2 = -\mathbf{A}^{-1}\mathbf{E}$,

$$\left(p^2\mathbf{I} - \mathbf{C}^2\right)\hat{\mathbf{g}}_i(p) = p\mathbf{g}_{i,0} + \dot{\mathbf{g}}_{i,0}$$

- Problem: Construct $\mathbf{C}$ such that all poles of $\left(p\mathbf{I} + \mathbf{C}\right)^{-1}$ have $\Re p_j > 0$

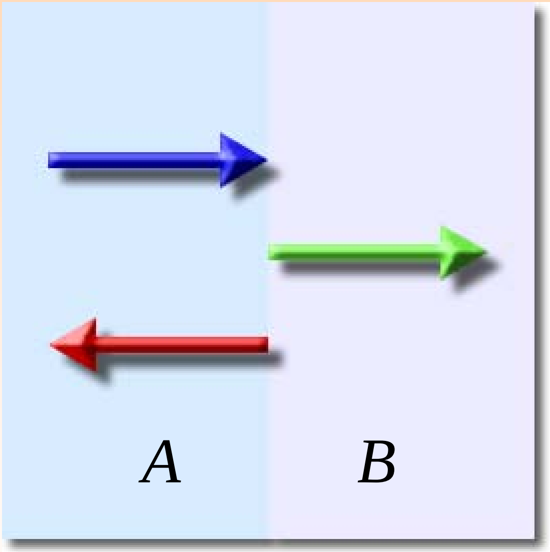
[N,N] Boundary Condition Results



Part III - Improving Accuracy in Fast Reflection Calculations

Facet Reflection Coefficient

- Matching E_y and $\frac{\partial E_y}{\partial z}$ at the boundary gives

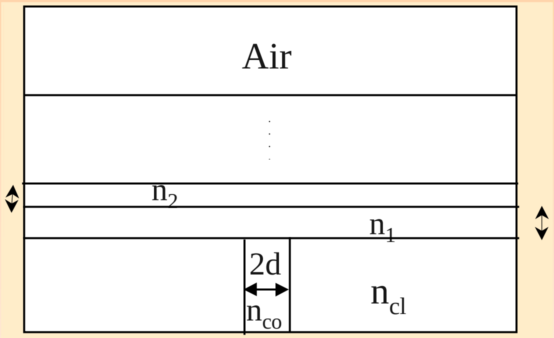


$$\Psi_y = \Psi_o^+ e^{-ik_o n_{ol} L_l z} + \Psi_o^- e^{ik_o n_{ol} L_l z}$$

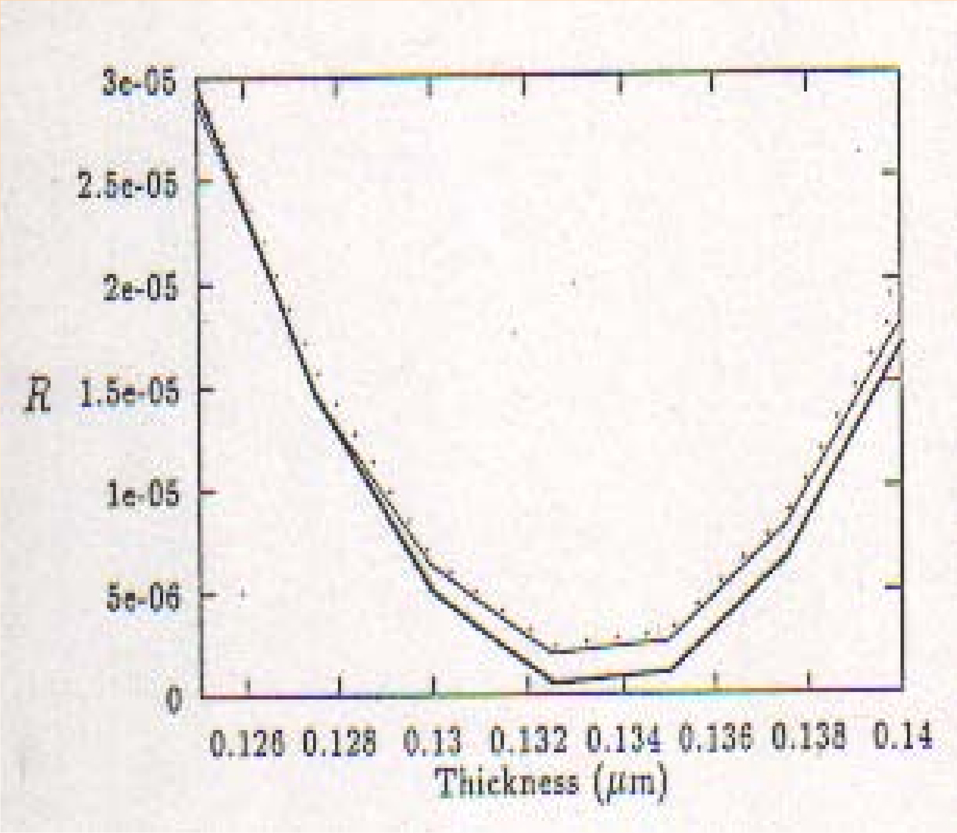
$$E_{yr}^{(k+1)} = \frac{1}{2}(1 - L_B L_A)(E_{yr}^{(k)} - E_{yi})\text{ , or}$$

$$[R]_{TE} = \frac{E_{yr}}{E_{yi}} = \frac{n_{oA} L_A - n_{oB} L_B}{n_{oA} L_A + n_{oB} L_B}$$

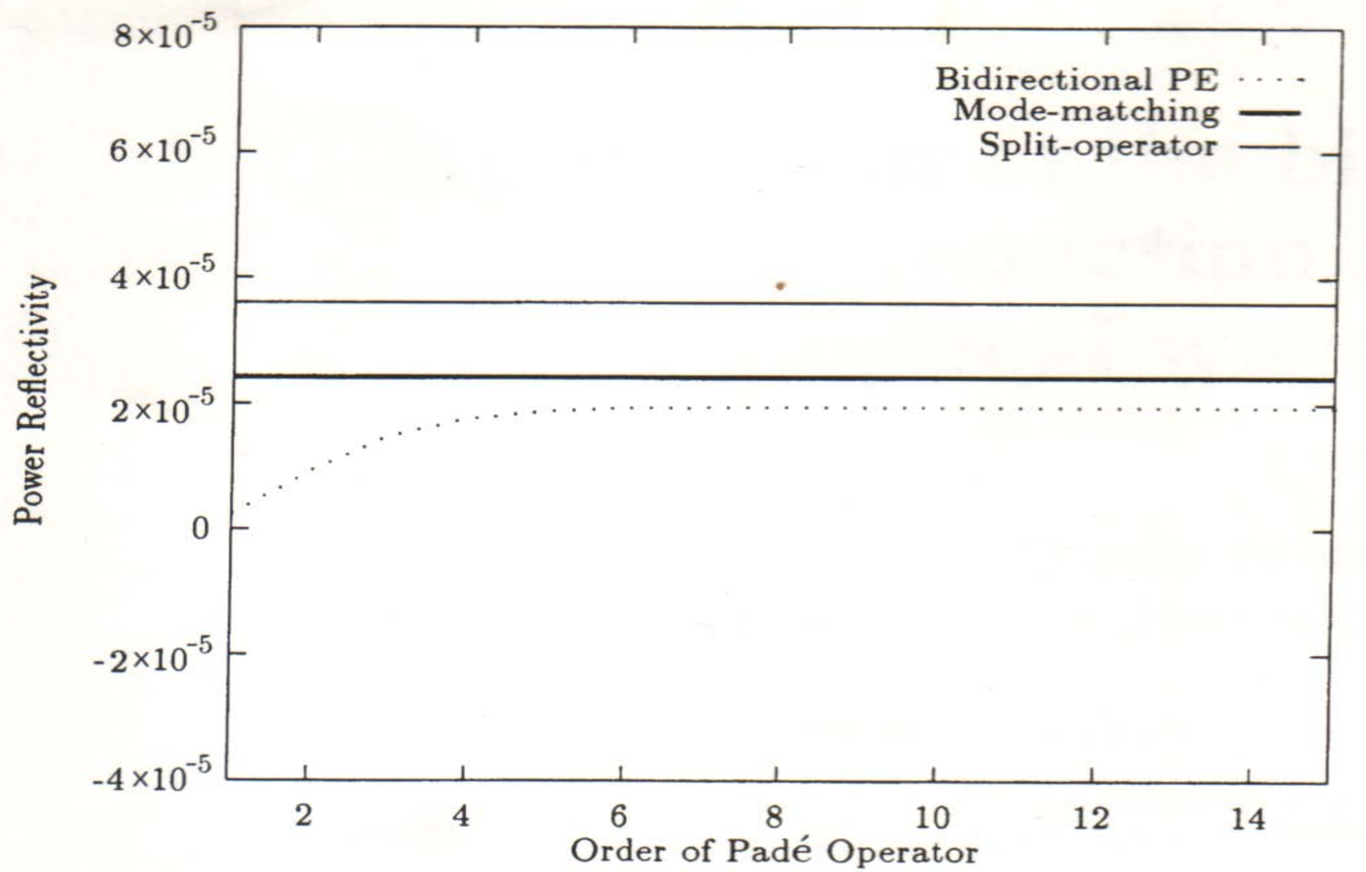
Reflection Coefficients



Waveguide Geometry



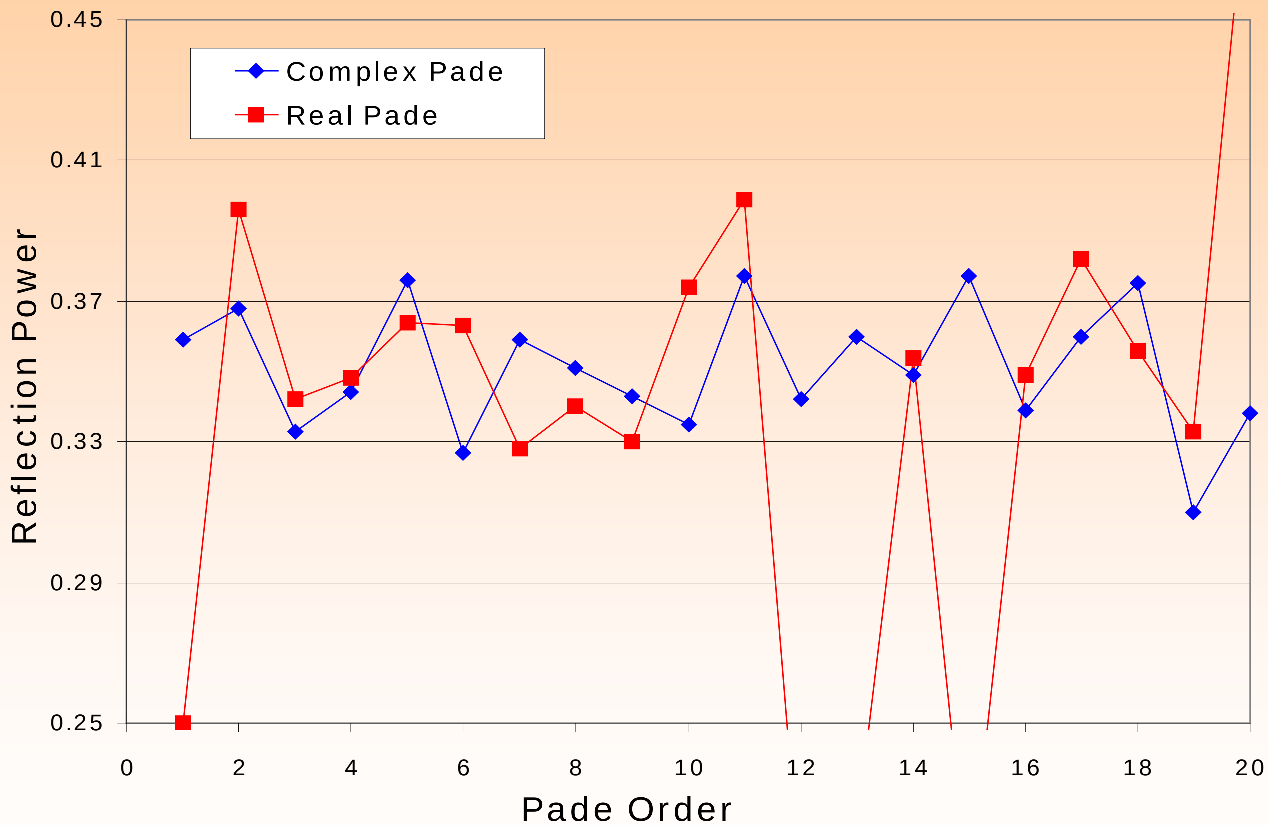
Standard Operator Results



Calculated Reflection Error

- Since the Padé approximation for L has poles in the evanescent spectral region, uncontrollable errors can develop.
- One method to resolve this - Generate an approximant with complex coefficients by selecting an imaginary termination condition for the continued fraction representation of $\sqrt{1+H}$.

Complex Padé Reflection



Rotated Padé Approximants

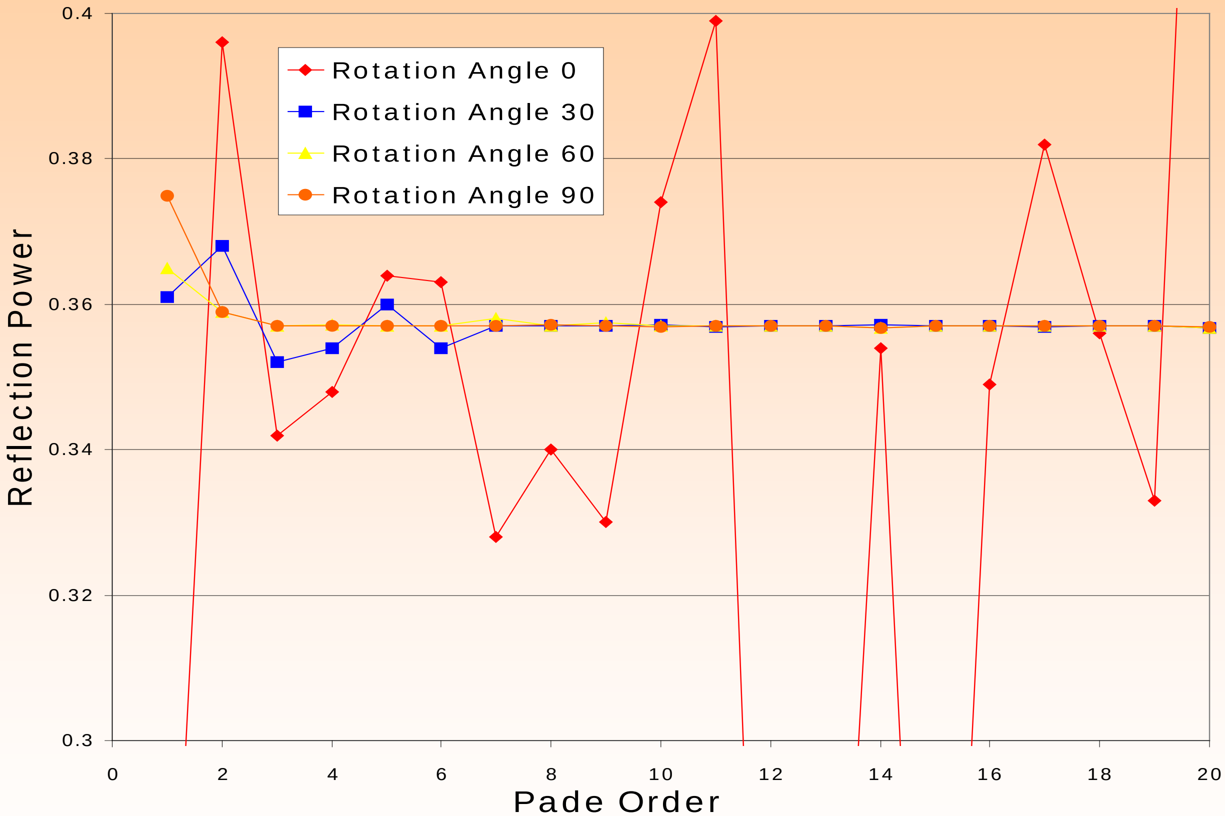
- A second method: Write

$$\sqrt{1+H} = e^{i\alpha/2}\sqrt{1+[(1+x)e^{-i\alpha}-1]}$$

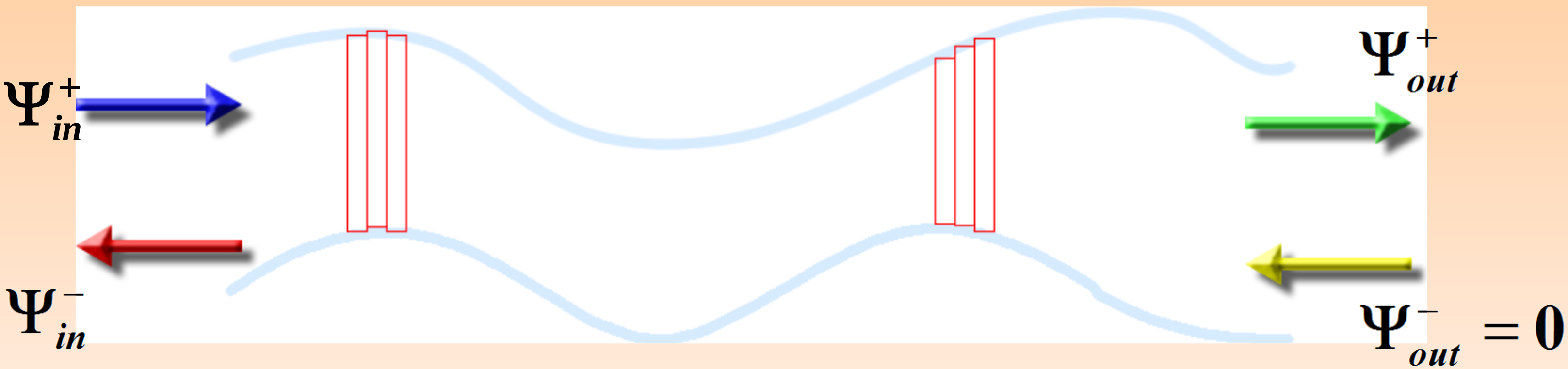
and perform a Padé expansion in the variable

$$y = (1+x)e^{-i\alpha} - 1$$

Rotated Padé Reflection



Refractive Index Discretization



$$\begin{pmatrix} \Psi_{out}^{+} \\ \Psi_{out}^{-} \end{pmatrix} = G \begin{pmatrix} \Psi_{in}^{+} \\ \Psi_{\text{int}}^{-} \end{pmatrix} \qquad G = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} = T_n P_n T_{n-1} P_{n-1} \ldots\ldots T_2 P_2 T_1 P_1$$

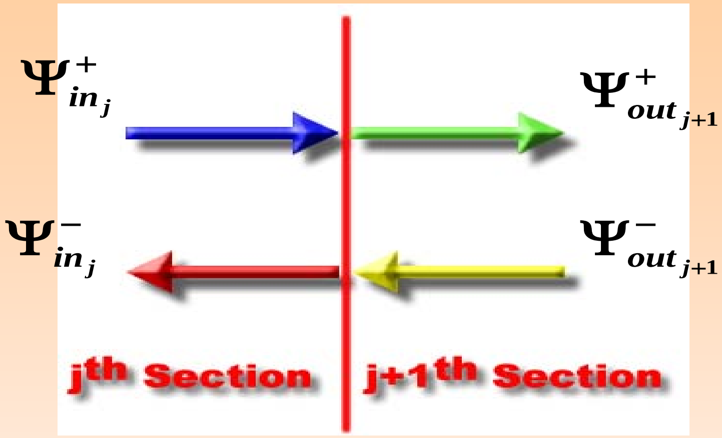
Reflected field

$$\Psi_{in}^{-} = -g_{22}^{-1} g_{21} \Psi_{in}^{+}$$

Transmitted field

$$\Psi_{out}^{+} = \left(g_{11} - g_{12} g_{22}^{-1} g_{21}\right) \Psi_{in}^{+}$$

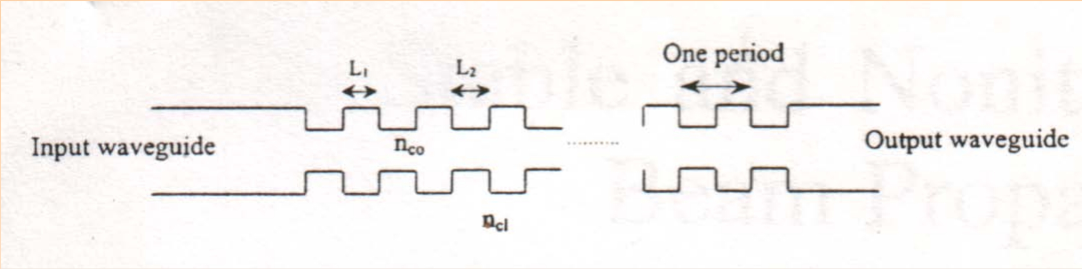
Transition, Propagation Operator

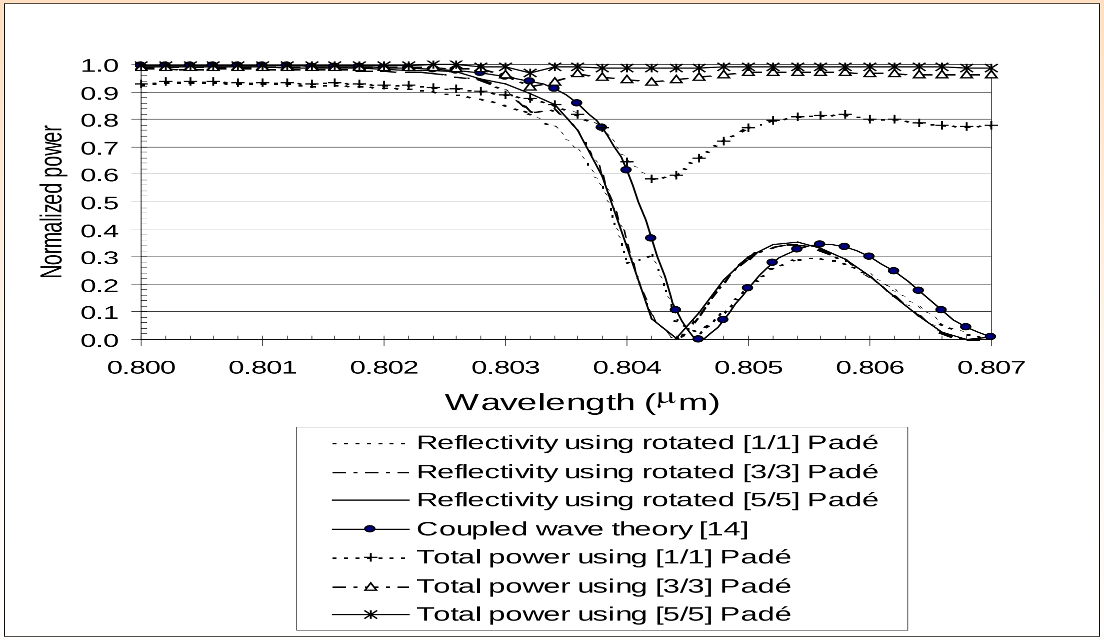


$$P_m = \begin{pmatrix} e^{-jk_o n_{om} L_m z} & 0 \\ 0 & e^{jk_o n_{om} L_m z} \end{pmatrix}$$

$$T_j = \frac{1}{2}\begin{pmatrix} 1+\dfrac{n_{o_j}}{n_{o_{j+1}}} L^{-1}_{j+1} L_j & 1-\dfrac{n_{o_j}}{n_{o_{j+1}}} L^{-1}_{j+1} L_j \\ 1-\dfrac{n_{o_j}}{n_{o_{j+1}}} L^{-1}_{j+1} L_j & 1+\dfrac{n_{o_j}}{n_{o_{j+1}}} L^{-1}_{j+1} L_j \end{pmatrix}$$

Distributed Feedback





Conclusions

- Procedures now exist for constructing exact, nonlocal boundary conditions for wide-classes of two-dimensional parabolic partial differential equations.
- Modified Padé operators can be employed to increase the accuracy of reflection calculations at abrupt interfaces.