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

\[
\left( \frac{\partial^2}{\partial z^2} + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + k_0^2 n^2(\mathbf{r}) \right) E(x, y, z) = 0
\]

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

\[
Y_0 = \frac{1}{k_0^2 n_0^2} \frac{\partial^2}{\partial y^2}
\]

and \( N = \frac{n^2(\mathbf{r})}{n_0^2} - 1 \), we have

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

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

$$\left(\frac{\partial}{\partial z} + i k_0 n_0 \sqrt{1 + H}\right) E(x, y, z) = 0$$

- We then have with $\delta = -i k_0 n_0$

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

• Modal Decomposition

\[ E(x, y, \bar{z}) = \sum_{m} a_m E_m(x, y, \bar{z}) \quad \text{with} \]

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

• Approximate Forward Solution

\[ E(x, y, z + \Delta z) = \sum_{m} e^{-i\beta_m(x, y, \bar{z})\Delta z} E_m(x, y, z) \]
Fresnel Approximation

- Fresnel Approximation

\[ \sqrt{1 + H} \approx 1 + \frac{H}{2} \]

- Slowly-Varying Envelope

\[ E(x, y, z) = E(x, y, z)e^{-\delta z} \]

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

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

\[ = \frac{H}{\sqrt{1 + H} + 1} \]

\[ = \frac{H}{2 + (\sqrt{1 + H} - 1)} \]

• Thus if \( \sqrt{1 + H} - 1 \) we have

\[ f(x) = \frac{x}{2 + f(x)} \]
Continued Fraction Expansion

• Iterating the recursion relation yields

\[
\sqrt{1 + H} - 1 = \frac{H}{2 + \frac{H}{2 + \frac{H}{2 + \cdots}}} = \frac{H}{1 + \frac{H}{2}}
\]

• 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

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

• In a partial fraction representation

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

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

\[ E(z + \Delta z) = e^{\frac{\delta H}{2}} E(z) = e^{\frac{\delta}{2}(X_0Y_0 + N)} E(z) \approx \left( 1 + \frac{\delta H}{4} \right) \left( 1 - \frac{\delta H}{4} \right) E(z) + O(\delta^3) \]
Discrete Representation

- **On a one-dimensional transverse grid** \( \{x_i\} \)

\[
E(x_i, z + \Delta z) = \frac{1 - \frac{i\Delta z}{4k_0 n_0} (k_0^2 (n^2 (x_i) - n_0^2) + D_x^2)}{1 + \frac{i\Delta z}{4k_0 n_0} (k_0^2 (n^2 (x_i) - n_0^2) + D_x^2)} E(x_i, z)
\]

where

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

and for any operator \( O \), \( \frac{1}{O} \) 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

Schematic diagram of modulator

- Ti / Pt / Au p-contact
- 2 μm
- p+ - InGaAs
- 2.0 μm p-InP
- i - MQW
- 2.1 μm n-InP
- n+ - InGaAs
- n+ - InP substrate
- NiGeAu n-contact
Standard Boundary Conditions

Evolution of Unguided Asymmetric Field - Standard Local Transparent Boundary
Improved Boundary Conditions

Evolution of Unguided Asymmetric Field - Hybrid Boundary
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: $E_0, E_{N+1}$ are computed from $E$ at the last propagation step.
  - Nonlocal Boundary Conditions: $E_0, E_{N+1}$ are obtained from previous values of $E$.
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
  \[
  \left( -2ik_0n_0 \frac{\partial}{\partial z} + \frac{d^2}{dx^2} + k_0^2 (n_b^2 - n_0^2) \right) E(x, y, z) = 0
  \]

• 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

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

$Z = \frac{L_a}{\tan \theta}$

$n(\vec{r})$
Approximate and Exact Results

Exact and Approximate Reflection Coefficients - Angle Dependence

Grid Point Reflection
Discretization Error
Absorbing Layer
Impedance-Matched Layer

Reflection Coefficient
Incidence Angle
0 5 10 15 20 25 30
Continuous Nonlocal Boundary

- Assume that \( n^2(x_{N-1}) = n^2(x_N) = n_0^2 \). At the boundary
  \[
  \frac{\partial^2 E}{\partial x^2} = 2i k_0 n_0 \frac{\partial E}{\partial z}
  \]

- Crank-Nicholson method - \( E_j \equiv E(x, z_j) \)
  \[
  \frac{\partial^2}{\partial x^2} \left( \frac{E_{j+1} + E_j}{2} \right) = 2i k_0 n_0 \frac{E_{j+1} - E_j}{\Delta z}
  \]

- Setting \( s \equiv T\{-\Delta z\} = e^{-\Delta z \frac{\partial}{\partial z}} \), we have with \( \nu = \sqrt{4i k_0 n_0 / \Delta z} \),
  \[
  \frac{\partial^2 E_{j+1}}{\partial x^2} = \nu^2 \frac{1 - s}{1 + s} E_{j+1}
  \]
Continuous Nonlocal Boundary

- 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

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

- The electric field is optimally evaluated at \((x_{Nw} + x_{Nw+1})/2\).
Gaussian Beam - Continuous N.L.

Continuous Nonlocal Boundary Condition
Gaussian Beam, 1024 Points

\[ \frac{z}{\mu m} \]

\[ \frac{x}{\mu m} \]

10^{-6}
10^{-10}

0 20 40 60 80 100 120 140 160 180 200

0 50 100 150 200 250 300 350 400 450
Remaining Power - Continuous

Continuous Nonlocal Boundary Condition
\[ L_2 \text{ Norm, 1 and 2 Gaussian Beams} \]

\[ \| u \|_{\Omega_i} \]

\[ N = 1024, \quad N = 2048, \quad N = 4096, \quad N = 8192 \]

\[ z \mu m \]
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

Discrete Nonlocal Boundary Condition
$L_2$ Norm, 1 and 2 Gaussian Beams

\[ \| u \|_{\Omega_i} \]

- single beam
- two beams

\[ \frac{z}{\mu m} \]

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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 (\(n_b = n_0\))**

\[
\left(1 + \frac{X_0}{4}\right)\left[1 - \frac{s}{\Delta z}\right]E(z + \Delta z) = -\delta\frac{X_0}{4}(1 + s)E(z + \Delta z)
\]
Padé [2,0] Boundary Conditions

• [2,2] Padé Equation

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

• Laplace transform this equation with respect to \( \chi \) in the exterior region.

• Requiring that no poles are present in the right-hand plane of the transform yields the desired boundary condition.
\[ (2,2) \text{ Boundary Condition Results} \]
Padé [N,N] Boundary Conditions

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

\[
\begin{align*}
\text{Padé } [N,N] \text{ Boundary Conditions} \\
\text{For the } [N,N] \text{ case, } sE_i(x) &= E_{i-1}(x), \text{ where} \\

\begin{align*}
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)
\end{align*}
\]
General Boundary Conditions (2)

- Introducing a vector \( g_i(x) \) with

\[
g_{i,j}(x) = g_i^{(j)}(x), \quad j = 1 \ldots k - 1, \quad g_{i,k}(x) = E_i(x)
\]

yields

\[
(E + A \partial_x^2)g_i(x) = 0
\]

with boundary conditions

\[
\dot{g}_{i,+} = B + g_{i,+}, \quad \dot{g}_{i,-} = B + g_{i,-}
\]
General Boundary Conditions (3)

- After Laplace transforming, this yields

\[(E + p^2 A) \hat{g}_i(p) = A(p g_{i,0} + \dot{g}_{i,0})\]

or, defining \[C^2 = -A^{-1} E,\]

\[(p^2 I - C^2) \hat{g}_i(p) = p g_{i,0} + \dot{g}_{i,0}\]

- Problem: Construct \(C\) such that all poles of \((p I + C)^{-1}\) have \(\Re p_j > 0\).
[N,N] Boundary Condition Results

![Graph showing [N,N] Boundary Condition Results]

- $\Delta x = 0.2 \mu m$
- $\Delta x = 0.1 \mu m$
- $\Delta x = 0.05 \mu m$
- $\Delta x = 0.025 \mu m$
- $\Delta x = 0.01 \mu m$
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

$$\Psi_y = \Psi^+_o e^{-i k_o n_o L_IT \frac{z}{L}} + \Psi^-_o e^{i k_o n_o L_IT \frac{z}{L}}$$

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

<table>
<thead>
<tr>
<th>Air</th>
</tr>
</thead>
<tbody>
<tr>
<td>n_2</td>
</tr>
<tr>
<td>n_1</td>
</tr>
<tr>
<td>2d</td>
</tr>
<tr>
<td>n_{co}</td>
</tr>
<tr>
<td>n_{cl}</td>
</tr>
</tbody>
</table>
Standard Operator Results

![Graph showing comparison between different methods using Padé operator orders.](image)

- Bidirectional PE
- Mode-matching
- Split-operator

Power Reflectivity vs. Order of Padé Operator
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

![Complex Padé Reflection Graph](image)

- **Complex Padé**
- **Real Padé**
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

![Graph showing Rotated Padé Reflection](image)

- Red line: Rotation Angle 0
- Blue line: Rotation Angle 30
- Yellow line: Rotation Angle 60
- Orange line: Rotation Angle 90

Reflection Power vs. Pade Order chart.
Refractive Index Discretization

\[
\begin{align*}
\begin{pmatrix}
\Psi^+_\text{out} \\
\Psi^-\text{out}
\end{pmatrix}
&= G
\begin{pmatrix}
\Psi^+_\text{in} \\
\Psi^-\text{in}
\end{pmatrix} \\
G &= \begin{pmatrix}
g_{11} & g_{12} \\
g_{21} & g_{22}
\end{pmatrix} = T_n P_n T_{n-1} P_{n-1} \ldots T_2 P_2 T_1 P_1
\end{align*}
\]

**Reflected field**
\[
\Psi^-\text{in} = -g_{22}^{-1} g_{21} \Psi^+_\text{in}
\]

**Transmitted field**
\[
\Psi^+_\text{out} = \left(g_{11} - g_{12} g_{22}^{-1} g_{21}\right) \Psi^+_\text{in}
\]
Transition, Propagation Operator

\[ T_j = \frac{1}{2} \begin{pmatrix} 1 + \frac{n_{o_j}}{n_{o_{j+1}}} L_{j+1}^{-1} L_j & 1 - \frac{n_{o_j}}{n_{o_{j+1}}} L_{j+1}^{-1} L_j \\ 1 - \frac{n_{o_j}}{n_{o_{j+1}}} L_{j+1}^{-1} L_j & 1 + \frac{n_{o_j}}{n_{o_{j+1}}} L_{j+1}^{-1} L_j \end{pmatrix} \]

\[ P_m = \begin{pmatrix} e^{-jk_o n_{om} L_m z} & 0 \\ 0 & e^{jk_o n_{om} L_m z} \end{pmatrix} \]
Distributed Feedback

Input waveguide

$n_{co}$

$n_{cl}$

Output waveguide

One period

Normalized power

Reflectivity using rotated $[1/1]$ Padé
Reflectivity using rotated $[3/3]$ Padé
Reflectivity using rotated $[5/5]$ Padé
Coupled wave theory [14]
Total power using $[1/1]$ Padé
Total power using $[3/3]$ Padé
Total power using $[5/5]$ Padé
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.