Construction of 2D artificial boundary conditions for the linear Schrödinger equation via fractional pseudo-differential operators

by

Christophe Besse

joint work with X. Antoine

Univ Lille 1/ Paul Painlevé Lab./ Inria Project Team Simpaf

6th International Congress on Industrial and Applied Mathematics
16 - 20 July 2007
Outline

1. Analytic transparent boundary conditions

2. Artificial boundary conditions
   - Straight artificial boundary
   - General convex artificial boundary

3. Approximations of TBC
Outline

1. Analytic transparent boundary conditions

2. Artificial boundary conditions
   - Straight artificial boundary
   - General convex artificial boundary

3. Approximations of TBC
Analytic transparent boundary conditions

\[ i\partial_t u + \Delta u = 0, \quad (x, t) \in \mathbb{R}^2 \times \mathbb{R}^+, \]
\[ u(x, 0) = u^I(x), \quad x \in \mathbb{R}^2. \]  

Schädle (02)

- similar tools already used in 1D:
  - transmission problem
  - Laplace transform: \( \mathcal{L}(w)(x, \tau) = \hat{w}(\tau) = \int_0^\infty w(x, t)e^{-\tau t} dt, \quad \text{Re}(\tau) > 0 \)

Step 1: split problem (1) as a transmission problem between \( \Omega \) and \( \Omega^{\text{ext}} \)
Analytic transparent boundary conditions

Interior problem

\[ i \partial_t v + \Delta v = 0, \quad (x, t) \in \Omega \times \mathbb{R}^+ \]
\[ v(x, 0) = u^I(x), \quad x \in \Omega \]
\[ v(x, t) = w(x, t), \quad (x, t) \in \Gamma \times \mathbb{R}^+ \]

Exterior problem

\[ i \partial_t w + \Delta w = 0, \quad (x, t) \in \Omega^{\text{ext}} \times \mathbb{R}^+ \]
\[ \partial_n w(x, t) = \partial_n v(x, t), \quad (x, t) \in \Gamma \times \mathbb{R}^+ \]
\[ \lim_{|x| \to +\infty} \sqrt{|x|} \left( \nabla w \cdot \frac{x}{|x|} + e^{-i \frac{\pi}{4}} \partial_{\tau}^{\frac{1}{2}} w \right) = 0. \]

**Presence of the Sommerfeld-like radiation condition** to ensure the uniqueness of the solution in \( \Omega^{\text{ext}} \).
Step 2:

**Laplace transform in $t$ to the exterior problem**

$$(\Delta + k^2) \hat{w}(x, \tau) = 0, \quad x \in \Omega^{ext},$$

$$\partial_n \hat{w}(x, \tau) = \partial_n \hat{v}(x, \tau), \quad (x, \tau) \in \Gamma,$$

$$\lim_{|x| \to +\infty} \sqrt{|x|} \left( \nabla \hat{w}(x, \tau) \cdot \frac{x}{|x|} - ik \hat{w}(x, \tau) \right) = 0.$$

Helmholtz–like equation: wave number $k = \sqrt{i \tau}$, with $\text{Re}(k) > 0$.

Theory of potential for the 2D Helmholtz equation: representation formula of the exterior field by a superposition of the single- and double–layer potentials

$$\left( \frac{I}{2} - M \right) \hat{w}(x, \tau) = L \partial_n \hat{w}, \quad x \in \Gamma.$$
Step 2:

**Laplace transform in** \( t \) **to the exterior problem**

\[
(\Delta + k^2) \hat{w}(x, \tau) = 0, \quad x \in \Omega^{\text{ext}},
\]

\[
\partial_n \hat{w}(x, \tau) = \partial_n \hat{v}(x, \tau), \quad (x, \tau) \in \Gamma,
\]

\[
\lim_{|x| \to +\infty} \sqrt{|x|} \left( \nabla \hat{w}(x, \tau) \cdot \frac{x}{|x|} - ik \hat{w}(x, \tau) \right) = 0.
\]

Helmholtz–like equation : wave number \( k = \sqrt{i\tau} \), with \( \text{Re}(k) > 0 \).

Theory of potential for the 2D Helmholtz equation : representation formula of the exterior field by a superposition of the single- and double–layer potentials

\[
\begin{pmatrix}
I_2 - M
\end{pmatrix} \hat{w}(x, \tau) = L \partial_n \hat{w}, \quad x \in \Gamma.
\]

where

- Single-layer potential \( L \varphi(x) = - \int_{\Gamma} G(x, y) \varphi(y) d\Gamma(y), \quad x \in \Gamma, \)
- Double-layer potential \( M \varphi(x) = \int_{\Gamma} \partial_n G(x, y) \varphi(y) d\Gamma(y), \quad x \in \Gamma, \)

setting \( G(x, y) = \frac{i}{4} H_0^{(1)}(k|x - y|) \).
Analytic transparent boundary conditions

Inverse Laplace transform

**Dirichlet-to-Neumann map**

\[
\partial_n v = \mathcal{L}^{-1} \left( \mathcal{L}^{-1} \left( \frac{I}{2} - M \right) \hat{v}(x, \cdot) \right)(t), \quad x \in \Gamma,
\]

Composition of an inverse Laplace transform and spatial integral operators: numerical evaluation would be difficult and costly (nonlocality).

**Artificial boundary conditions**

- Mimic the pioneering work of Engquist and Majda (77,79): leads to families of approximate (non–local and local) artificial boundary conditions.
- Main defect: conditions are not exact.
Analytic transparent boundary conditions

Inverse Laplace transform

**Dirichlet-to-Neumann map**

\[
\partial_n v = \mathcal{L}^{-1} \left( L^{-1} \left( \frac{I}{2} - M \right) \hat{v}(x, \cdot) \right)(t), \quad x \in \Gamma,
\]

Composition of an inverse Laplace transform and spatial integral operators: numerical evaluation would be difficult and costly (nonlocality).

**Artificial boundary conditions**

- Mimic the pioneering work of Engquist and Majda (77,79): leads to families of approximate (non–local and local) artificial boundary conditions.
- Main defect: conditions are not exact.
Outline

1. Analytic transparent boundary conditions

2. Artificial boundary conditions
   - Straight artificial boundary
   - General convex artificial boundary

3. Approximations of TBC
Straight artificial boundary

Straight boundary: Dimenza (95), Arnold (98)

\[
\Omega = \{ \mathbf{x} = (x_1, x_2); x_2 < 0 \} \\
\Omega^{\text{ext}} = \{ \mathbf{x} = (x_1, x_2); x_2 > 0 \} \\
\Gamma = \{ \mathbf{x} \in \mathbb{R}^2 | x_2 = 0 \}
\]

\[
\begin{cases}
(i\partial_t + \Delta)u = 0, & (\mathbf{x}, t) \in \Omega \times \mathbb{R}^+, \\
u(\mathbf{x}, 0) = u^I(\mathbf{x}), & \forall \mathbf{x} \in \Omega, \\
supp(u^I) \subset \Omega
\end{cases}
\]

- Step 1: transmission problem
- Step 2: Laplace transform in time (with dual variable \(\tau\)) and tangential Fourier transform \(\mathcal{F}\) in the \(x_1\)-direction (with dual variable \(\xi\))

\[
\mathcal{F}\hat{u}(x_2, \tau, \xi) = \int_0^{+\infty} \int_{\mathbb{R}_{x_1}} e^{-i\xi x_1 - \tau t} u(t, x_1, x_2) dx_1 dt, \quad \tau = \sigma + i\rho
\]
Straight artificial boundary

Differential equation in the normal variable $x_2$ for the solution $w$ in $\Omega^{\text{ext}}$

$$
(\partial_{x_2}^2 + i\tau - \xi^2) \mathcal{F}\hat{w}(x_2, \xi, \tau) = 0, \quad x_2 > 0,
$$

Solution given as the superposition of two waves

$$
\mathcal{F}\hat{w}(x_2, \xi, \tau) = A^+(\xi, \tau)e^{i\lambda_1^+(\xi, \tau)x_2} + A^-\lambda_1^-\xi, \tau)e^{i\lambda_1^-(\xi, \tau)x_2},
$$

with $\lambda_1^\pm(\xi, \tau) = \pm \sqrt{i\tau - \xi^2}$.

Let $(x_1, t, \xi, \rho) \in \mathcal{E} := \{(x_1, t, \xi, \rho) \in \mathbb{R}^4, \rho + \xi^2 > 0\}$.
Straight artificial boundary

In order to $\mathcal{F}\hat{w}(., \xi, \tau) \in L^2(\mathbb{R}^+)$, we require $A^- = 0$

$$\mathcal{F}\hat{w}(x_2, \xi, \tau) = A^+(\xi, \tau)e^{i\lambda_1^+(\xi, \tau)x_2}, \quad \lambda_1^+(\xi, \tau) = \sqrt{i\tau - \xi^2}$$

Remarks

- The part of the wave $\hat{w}$ at point $(x_1, t, \xi, \rho)$ in $\mathcal{E}$ is exponentially decaying (as $x_2 \to \infty$) and usually called evanescent.
- $\mathcal{E}$ is called the $M$-quasi elliptic region setting $M = (1, 2)$.
- The pair $M$ is introduced to recall the different homogeneities of the dual variables $\tau$ and $\xi$ in the symbols $\lambda_1^\pm$.
- The points $(x_1, t, \xi, \rho)$ in the cone $\mathcal{H} = \{(x_1, t, \xi, \rho), \rho + \xi^2 < 0\}$ represent the propagative part of the wave. This zone is referred to as the $M$-quasi hyperbolic part.
- The complementary zone $\mathcal{G} = \{(x_1, t, \xi, \rho), \rho + \xi^2 = 0\}$ corresponds to the rays propagating along the boundary (grazing waves). This region is called the $M$-quasi glancing zone. It is reduced to $\{(0, 0, 0, 0)\}$ if the wave $u$ is not tangentially incident to $\Gamma$. 
In order to $\mathcal{F}\hat{w}(., \xi, \tau) \in L^2(\mathbb{R}^+)$, we require $A^- = 0$

$$\mathcal{F}\hat{w}(x_2, \xi, \tau) = A^+(\xi, \tau)e^{i\lambda_1^+(\xi, \tau)x_2}, \quad \lambda_1^+(\xi, \tau) = \sqrt{i\tau - \xi^2}$$

**Remarks**

- The part of the wave $\hat{w}$ at point $(x_1, t, \xi, \rho)$ in $\mathcal{E}$ is exponentially decaying (as $x_2 \to \infty$) and usually called evanescent.

- $\mathcal{E}$ is called the *M-quasi elliptic region* setting $M = (1, 2)$.

- The pair $M$ is introduced to recall the different homogeneities of the dual variables $\tau$ and $\xi$ in the symbols $\lambda_1^\pm$.

- The points $(x_1, t, \xi, \rho)$ in the cone $\mathcal{H} = \{(x_1, t, \xi, \rho), \rho + \xi^2 < 0\}$ represent the propagative part of the wave. This zone is referred to as the *M-quasi hyperbolic part*.

- The complementary zone $\mathcal{G} = \{(x_1, t, \xi, \rho), \rho + \xi^2 = 0\}$ corresponds to the rays propagating along the boundary (grazing waves). This region is called the *M-quasi glancing zone*. It is reduced to $\{(0, 0, 0, 0)\}$ if the wave $u$ is not tangentially incident to $\Gamma$. 
In order to $\mathcal{F}\hat{w}(.,\xi,\tau) \in L^2(\mathbb{R}^+)$, we require $A^- = 0$

$$
\mathcal{F}\hat{w}(x_2,\xi,\tau) = A^+(\xi,\tau)e^{i\lambda_1^+(\xi,\tau)x_2}, \quad \lambda_1^+(\xi,\tau) = \sqrt{i\tau - \xi^2}
$$

**Remarks**

- The part of the wave $\hat{w}$ at point $(x_1,t,\xi,\rho)$ in $\mathcal{E}$ is exponentially decaying (as $x_2 \to \infty$) and usually called *evanescent*.
- $\mathcal{E}$ is called the *$M$-quasi elliptic region* setting $M = (1,2)$.
- The pair $M$ is introduced to recall the different homogeneities of the dual variables $\tau$ and $\xi$ in the symbols $\lambda_1^\pm$.
- The points $(x_1,t,\xi,\rho)$ in the cone $\mathcal{H} = \{(x_1,t,\xi,\rho), \rho + \xi^2 < 0\}$ represent the propagative part of the wave. This zone is referred to as the *$M$-quasi hyperbolic part*.
- The complementary zone $\mathcal{G} = \{(x_1,t,\xi,\rho), \rho + \xi^2 = 0\}$ corresponds to the rays propagating along the boundary (grazing waves). This region is called the *$M$-quasi glancing zone*. It is reduced to $\{(0,0,0,0)\}$ if the wave $u$ is not tangentially incident to $\Gamma$. 
In order to $\mathcal{F}\hat{w}(., \xi, \tau) \in L^2(\mathbb{R}^+)$, we require $A^- = 0$

$$\mathcal{F}\hat{w}(x_2, \xi, \tau) = A^+(\xi, \tau)e^{i\lambda_1^+(\xi, \tau)x_2}, \quad \lambda_1^+(\xi, \tau) = \sqrt{i\tau - \xi^2}$$

**Remarks**

- The part of the wave $\hat{w}$ at point $(x_1, t, \xi, \rho)$ in $\mathcal{E}$ is exponentially decaying (as $x_2 \to \infty$) and usually called *evanescent*.
- $\mathcal{E}$ is called the **M-quasi elliptic region** setting $M = (1, 2)$.
- The pair $M$ is introduced to recall the different homogeneities of the dual variables $\tau$ and $\xi$ in the symbols $\lambda_1^\pm$.
- The points $(x_1, t, \xi, \rho)$ in the cone $\mathcal{H} = \{(x_1, t, \xi, \rho), \rho + \xi^2 < 0\}$ represent the propagative part of the wave. This zone is referred to as the **M-quasi hyperbolic part**.
- The complementary zone $\mathcal{G} = \{(x_1, t, \xi, \rho), \rho + \xi^2 = 0\}$ corresponds to the rays propagating along the boundary (grazing waves). This region is called the **M-quasi glancing zone**. It is reduced to $\{(0, 0, 0, 0)\}$ if the wave $u$ is not tangentially incident to $\Gamma$. 
Apply the normal derivative operator $\partial_{x_2}$ to $\mathcal{F}\hat{w}(x_2, \xi, \tau) = A^+(\xi, \tau)e^{i\lambda_1^+(\xi, \tau)x_2}$ and choose $x_2 = 0$, $n = (1, 0)$ as the outwardly unitary normal vector to the computational domain.

Inverse Laplace-Fourier transform

$$\partial_n u + i\Lambda^+(\partial_{x_1}, \partial_t)u = 0, \quad \text{on } \Gamma \times \mathbb{R}^+,$$

with

$$\Lambda^+(\partial_{x_1}, \partial_t)w(x_1, 0, t) = \frac{1}{(2\pi)^2i} \int_{\gamma-i\infty}^{\gamma+i\infty} \int_{\mathbb{R}} \lambda_1^+(\xi, \tau)\mathcal{F}\hat{w}(0, \xi, \tau)e^{i\xi x_1 + st} \, d\xi \, d\tau,$$

Formally,

Artificial boundary condition

$$\partial_n u - i\sqrt{i}\partial_t + \Delta_{\Gamma}u = 0 \quad \text{on } \Gamma \times \mathbb{R}^+$$

where $\Delta_{\Gamma}$ denotes the surface Laplace-Beltrami operator $\partial_{x_1}^2$.

The exact DtN operator is therefore non-local both in space and time.
Remarks:

- This derivation leads inevitably to junction problems located in corners.

One must work on a convex open set.

- One can restrict $\Lambda^+$ to $\mathcal{H}$: filtering of the propagative part of the wave field $\Rightarrow$

**Transparent Boundary Condition**

$$\partial_n u - i Op_{|H}(\sqrt{i\tau - \xi^2})u = 0 \quad \text{on} \quad \Gamma \times \mathbb{R}^+$$

- Factorization: $(i\partial_t + \Delta)u = (\partial_{x_2} - i\sqrt{i\partial_t + \partial_{x_1}^2})(\partial_{x_2} + i\sqrt{i\partial_t + \partial_{x_1}^2})$
**General convex artificial boundary**

**General convex open set** $\Omega \subset \mathbb{R}^2$ : factorization of the operator $i\partial_t + \Delta$

**Methodology**

- Generalized coordinates system of the boundary :
  - variable $r$ normal variable along the unit normal vector $\mathbf{n}$
  - variable $s$ curvilinear abscissa along $\Gamma$

\[
\Delta = \partial_r^2 + \kappa_r \partial_r + h^{-1} \partial_s (h^{-1} \partial_s)
\]

$\kappa_r = h^{-1} \kappa$ : curvature on the parallel surface $\Gamma_r$ to $\Gamma$

\[h(r, s) = 1 + r\kappa.\]

$\Rightarrow$ $L := i\partial_t + \Delta = \partial_r^2 + \kappa_r \partial_r$

+ $i\partial_t + h^{-1} \partial_s (h^{-1} \partial_s)$

$r \leftrightarrow x_2 \quad s \leftrightarrow x_1 \quad t \leftrightarrow t$
Define $\psi$ do classes

**Définition**

1. $a \in S^m$ symbol, said to be quasi homogeneous of degree $m$ if
   \[
   a(r, s, \mu \xi, \mu^2 \omega) = \mu^m a(r, s, \mu, \omega)
   \]

2. $A \in OPS^m$ if $a = \sigma(A)$ admits an asymptotic expansion of the form
   \[
   a \sim \sum_{j=-m}^{+\infty} a_{-j}, \quad a_{-j} \in S^{-j} \quad \text{and} \quad \forall p \geq -m, \quad a - \sum_{j=-m}^{p} a_{-j} \in S^{-(p+1)}
   \]

- Nirenberg–like factorization theorem
  \[\exists \Lambda^\pm \in OPS^1, \ r–\text{regular function}\]
  \[
  L = (\partial_r + i\Lambda^-(r, s, \partial_s, \partial_t)) \ (\partial_r + i\Lambda^+(r, s, \partial_s, \partial_t)) + R
  \]

  with $R \in OPS^{-\infty}$. The factorization theorem holds in $\mathcal{H}$, $\mathcal{E}$ but not $\mathcal{G}$. 
Define $\psi$ do classes

Définition

1. $a \in S^m$ symbol, said to be quasi homogeneous of degree $m$ if
   \[ a(r, s, \mu \xi, \mu^2 \omega) = \mu^m a(r, s, \mu, \omega) \]

2. $A \in OPS^m$ if $a = \sigma(A)$ admits an asymptotic expansion of the form
   \[ a \sim \sum_{j=-m}^{+\infty} a_{-j}, \quad a_{-j} \in S^{-j} \text{ and } \forall p \geq -m, \quad a - \sum_{j=-m}^{p} a_{-j} \in S^{-(p+1)} \]

Nirenberg–like factorization theorem

$\exists \Lambda^\pm \in OPS^1$, $r$–regular function

\[ L = (\partial_r + i \Lambda^- (r, s, \partial_s, \partial_t)) (\partial_r + i \Lambda^+ (r, s, \partial_s, \partial_t)) + R \]

\[ \downarrow r \to 0 \]

\[ (\partial_n + i \Lambda^+ (s, \partial_s, \partial_t)) \]

with $R \in OPS^{-\infty}$. The factorization theorem holds in $\mathcal{H}$, $\mathcal{E}$ but not $\mathcal{G}$.
IDENTIFICATION OF THE DIFFERENT TERMS

- \( L = \partial_r^2 + \kappa_r \partial_r + i \partial_t + h^{-1} \partial_s (h^{-1} \partial_s) \)
- \( (\partial_r + i \Lambda^-) (\partial_r + i \Lambda^+) = \partial_r^2 + i (\Lambda^+ + \Lambda^-) \partial_r + i Op (\partial_r \lambda^+) - \Lambda^- \Lambda^+ \)

Therefore, one has

\[
\begin{align*}
    i(\lambda^+ + \lambda^-) &= \kappa_r, \\
    i \partial_r \lambda^+ - \sigma (\Lambda^- \Lambda^+) &= i \xi (h^{-1} \partial_s h^{-1}) - \xi^2 h^{-2} + i \tau,
\end{align*}
\]

with \( \lambda^\pm \sim \sum_{j=-1}^{+\infty} \lambda^\pm_j, \lambda^\pm_j \in S^{-j} \).

- Consider the asymptotic expansions of the symbols, the rules of symbolic calculus of \( \sigma (\Lambda^- \Lambda^+) \) and identification of the symbols by homogeneity.
- Restriction to the boundary \( r = 0 \) and \( \tilde{\lambda} = \lim_{r \to 0} \lambda \).

\[
\tilde{\lambda}^+_1 = \sqrt{i \tau - \xi^2}, \quad \tilde{\lambda}^+_0 = \frac{1}{2 \lambda^+_1} (-i \kappa \tilde{\lambda}^+_1 - i \frac{\kappa \xi^2}{\lambda^+_1}), \ldots
\]
Identify the different terms

1. \( L = \partial^2_r + \kappa r \partial_r + i \partial_t + h^{-1} \partial_s (h^{-1} \partial_s) \)
2. \((\partial_r + i \Lambda^-)(\partial_r + i \Lambda^+) = \partial^2_r + i(\Lambda^+ + \Lambda^-)\partial_r + iOp(\partial_r \lambda^+) - \Lambda^- \Lambda^+\)

Therefore, one has

\[ \begin{cases} 
  i(\lambda^+ + \lambda^-) = \kappa_r, \\
  i\partial_r \lambda^+ - \sigma(\Lambda^- \Lambda^+) = i\xi(h^{-1} \partial_s h^{-1}) - \xi^2 h^{-2} + i\tau,
\end{cases} \]

with \( \lambda^\pm \sim \sum_{j=-1}^{+\infty} \lambda^\pm_j, \lambda^\pm_j \in S^{-j} \).

- Consider the asymptotic expansions of the symbols, the rules of symbolic calculus of \( \sigma(\Lambda^- \Lambda^+) \) and identification of the symbols by homogeneity.
- Restriction to the boundary \( r = 0 \) and \( \tilde{\lambda} = \lim_{r \to 0} \lambda. \)

\( \tilde{\lambda}_1^+ = \sqrt{i\tau - \xi^2}, \quad \tilde{\lambda}_0^+ = \frac{1}{2\lambda_1^+}(-i\kappa \tilde{\lambda}_1^+ - i\frac{\kappa \xi^2}{\lambda_1^+}), \ldots \)
General convex artificial boundary

Identification of the different terms

\[ L = \partial_r^2 + \kappa_r \partial_r + i \partial_t + h^{-1} \partial_s (h^{-1} \partial_s) \]
\[ (\partial_r + i \Lambda^-) (\partial_r + i \Lambda^+) = \partial_r^2 + i (\Lambda^+ + \Lambda^-) \partial_r + i Op (\partial_r \lambda^+) - \Lambda^- \Lambda^+ \]

Therefore, one has

\[
\begin{aligned}
    i (\lambda^+ + \lambda^-) &= \kappa_r, \\
    i \partial_r \lambda^+ - \sigma (\Lambda^- \Lambda^+) &= i \xi (h^{-1} \partial_s h^{-1}) - \xi^2 h^{-2} + i \tau,
\end{aligned}
\]

with \( \lambda^\pm \sim \sum_{j=-1}^{+\infty} \lambda^\pm_{-j}, \lambda^\pm_{-j} \in S^{-j} \).

Consider the asymptotic expansions of the symbols, the rules of symbolic calculus of \( \sigma (\Lambda^- \Lambda^+) \) and identification of the symbols by homogeneity.

Restriction to the boundary \( r = 0 \) and \( \tilde{\lambda} = \lim_{r \to 0} \lambda \).

\[
\begin{aligned}
    \tilde{\lambda}^+_1 &= \sqrt{i \tau - \xi^2}, \\
    \tilde{\lambda}^+_0 &= \frac{1}{2 \lambda^+_1} (-i \kappa \tilde{\lambda}^+_1 - i \frac{\kappa \xi^2}{\lambda^+_1}), \\
    \lambda^+_1 &= \sqrt{i \tau - \xi^2}, \\
    \lambda^+_0 &= \frac{1}{2 \lambda^+_1} (-i \kappa \lambda^+_1 - i \frac{\kappa \xi^2}{\lambda^+_1}), \\
    \ldots
\end{aligned}
\]
GENERAL CONVEX ARTIFICIAL BOUNDARY

IDENTIFICATION OF THE DIFFERENT TERMS

- \( L = \partial_r^2 + \kappa_r \partial_r + i \partial_t + h^{-1} \partial_s (h^{-1} \partial_s) \)
- \((\partial_r + i \Lambda^-)(\partial_r + i \Lambda^+) = \partial_r^2 + i(\Lambda^+ + \Lambda^-) \partial_r + i Op(\partial_r \lambda^+) - \Lambda^- \Lambda^+ \)

Therefore, one has

\[
\begin{align*}
i(\lambda^+ + \lambda^-) &= \kappa_r, \\
i \partial_r \lambda^+ - \sigma(\Lambda^- \Lambda^+) &= i \xi (h^{-1} \partial_s h^{-1}) - \xi^2 h^{-2} + i \tau,
\end{align*}
\]

with \( \lambda^{\pm} \sim \sum_{j=-1}^{+\infty} \lambda_{\pm j}, \lambda_{\pm j} \in S^{-j}. \)

- Consider the asymptotic expansions of the symbols, the rules of symbolic calculus of \( \sigma(\Lambda^- \Lambda^+) \) and identification of the symbols by homogeneity.
- Restriction to the boundary \( r = 0 \) and \( \tilde{\lambda} = \lim_{r \to 0} \lambda. \)

\[
\begin{align*}
\tilde{\lambda}_1^+ &= \sqrt{i \tau - \xi^2}, \quad \tilde{\lambda}_0^+ = \frac{1}{2 \lambda_1^+} (-i \kappa \tilde{\lambda}_1^+ - i \frac{\kappa \xi^2}{\lambda_1^+}), 
\end{align*}
\]
Identification of the different terms

\[ L = \partial_r^2 + \kappa_r \partial_r + i \partial_t + h^{-1} \partial_s (h^{-1} \partial_s) \]
\[ (\partial_r + i \Lambda^-)(\partial_r + i \Lambda^+) = \partial_r^2 + i(\Lambda^+ + \Lambda^-) \partial_r + iOp(\partial_r \lambda^+) - \Lambda^- \Lambda^+ \]

Therefore, one has

\[
\begin{align*}
  i(\lambda^+ + \lambda^-) &= \kappa_r, \\
  i\partial_r \lambda^+ - \sigma(\Lambda^- \Lambda^+) &= i\xi(h^{-1} \partial_s h^{-1}) - \xi^2 h^{-2} + i\tau,
\end{align*}
\]

with \( \lambda^\pm \sim \sum_{j=-1}^{+\infty} \lambda^\pm_j, \lambda^\pm_j \in S^{-j} \).

Consider the asymptotic expansions of the symbols, the rules of symbolic calculus of \( \sigma(\Lambda^- \Lambda^+) \) and identification of the symbols by homogeneity.

Restriction to the boundary \( r = 0 \) and \( \tilde{\lambda} = \lim_{r \to 0} \lambda \).

\[
\begin{align*}
  \tilde{\lambda}^+_1 &= \sqrt{i\tau - \xi^2}, \\
  \tilde{\lambda}^+_0 &= \frac{1}{2\lambda^+_1} (-i\kappa \tilde{\lambda}^+_1 - i \frac{\kappa \xi^2}{\lambda^+_1}), \\ ... 
\end{align*}
\]
**General convex artificial boundary**

**Approximate TBC**

\[
\partial_n u + i \text{Op} \left( \sum_{j=-1}^{m} \lambda_{-j} \right) u = 0 \text{ on } \Gamma \times [0, T]
\]

Always non local in space-time.
Outline

1 Analytic transparent boundary conditions

2 Artificial boundary conditions
   - Straight artificial boundary
   - General convex artificial boundary

3 Approximations of TBC
Approximations of TBC

Three strategies:

1. Arnold et al. (06) derivation of a Discrete TBCs for the fully discrete time-dependent Schrödinger equation for circular geometry. Crank Nicolson finite difference scheme on Schrödinger eq. in polar coordinates. Laplace ↔ Z–transform Fourier ↔ discrete Fourier transform in θ–direction.

2. Dimenza (95), Szeftel (04) : since TBCs are
\[ \partial_n u - iOp(\sqrt{i\tau - \xi^2})u = 0, \]
use a rational approximation of the square root
\[ \sqrt{z} \approx a_0 + \sum_{j=1}^{m} \frac{a_j z}{z + b_j}, \]
with \( z = i\tau - \xi^2 \), \((a_j, b_j) \in \mathbb{C}^2\).

Lindmann’s trick : auxiliary functions \( \varphi_j \) satisfying the surface Schrödinger equations
\[ (i\partial_t + \Delta_{\Gamma} + b_j)\varphi_j = u, \quad \text{on } \mathbb{R} \times \mathbb{R}^+. \]

Then, ABCs are local and read
\[ \partial_n u = a_0 u + \sum_{j=1}^{m} a_j (i\partial_t + \Delta_{\Gamma})\varphi_j, \]
Approximations of TBC

Three strategies:

- Arnold et al. (06) derivation of a Discrete TBCs for the fully discrete time-dependent Schrödinger equation for circular geometry. Crank Nicolson finite difference scheme on Schrödinger eq. in polar coordinates. Laplace $\leftrightarrow \mathcal{Z}$-transform Fourier $\leftrightarrow$ discrete Fourier transform in $\theta$–direction.

- Dimenza (95), Szeftel (04) : since TBCs are $\partial_n u - iO p(\sqrt{i \tau - \xi^2})u = 0$, use a rational approximation of the square root

$$\sqrt{z} \approx a_0 + \sum_{j=1}^{m} \frac{a_j z}{z + b_j},$$

with $z = i \tau - \xi^2$, $(a_j, b_j) \in \mathbb{C}^2$.

Lindmann’s trick: auxiliary functions $\varphi_j$ satisfying the surface Schrödinger equations

$$(i \partial_t + \Delta_{\Gamma} + b_j) \varphi_j = u, \quad \text{on } \mathbb{R} \times \mathbb{R}^+.$$ 

Then, ABCs are local and read $\partial_n u = a_0 u + \sum_{j=1}^{m} a_j (i \partial_t + \Delta_{\Gamma}) \varphi_j,$
Approximations of TBC

Third way:

**Transparent Boundary Condition**

\[ \partial_n u - iOp|_\mathcal{H}(\sqrt{i\tau - \xi^2})u = 0 \quad \text{on } \Gamma \times \mathbb{R}^+, \quad \tau = \sigma + i\rho \]

Since we restrict symbol to \( \mathcal{H} \) region, \(-\rho > \xi^2 \Rightarrow |\tau| > \xi^2\).

*high frequency assumption*: \( |\tau| \gg \xi^2 \)

Example for \( \lambda_1^+ \):

\[
\sqrt{i\tau - \xi^2} \approx \sqrt{i\tau} - \frac{\xi^2}{2\sqrt{i\tau}} + \cdots
\]

non local in \( x \) and \( t \)

\( |i\tau| \gg \xi^2 \)

Taylor exp.

local in space

The ABC of order \((m + 2)/2\) is \( (\partial_n + iOp(\sum_{j=-1}^{m} \lambda_{-j}(m+2)))v = 0 \) on \( \Gamma \times [0, T] \) where \((\lambda_{-j})_{(m+2)}\) are Taylor expansions with respect to the small parameter \( \tau^{-1} \) truncated to the term \( \tau^{-(m+2)/2} \)
Approximations of TBC

Applications

- Arnold (95), straight line case first and second-order Taylor expansion of the symbol $\lambda_1^+$. 

\[(\partial_n + e^{-i\pi/4} \partial_t^{1/2})u = 0, \quad \text{on } \Gamma \times \mathbb{R}^+,
\]

and 

\[(\partial_n + e^{-i\pi/4} \partial_t^{1/2} - e^{i\pi/4} \frac{1}{2} \Delta \Gamma I_t^{1/2})u = 0, \quad \text{on } \Gamma \times \mathbb{R}^+.
\]

- Antoine–Besse (01), general convex open set, taylor expansion in the hyperbolic zone
Approximations of TBC

**Approximated IBVP**

\[
\begin{aligned}
(DN^{m/2}) \quad & \left\{ \begin{array}{l}
(i\partial_t + \Delta)v = 0, \quad (x,t) \in \Omega \times [0,T], \\
\partial_n v + T_{m/2}v = 0, \quad (x,t) \in \Gamma \times [0,T], \\
v(x,0) = v_0(x), \quad x \in \Omega.
\end{array} \right.
\end{aligned}
\]

The operators \( T_{m/2}, m \in \{1,\ldots,4\} \) are pseudodifferential in time and differential in space, and they are given on \( \Gamma \times \mathbb{R}^+ \) by

\[
\begin{align*}
T_{1/2}v &= e^{-i\pi/4} \partial_t^{1/2} v, \\
T_1v &= T_{1/2}v + \frac{\kappa}{2} v, \\
T_{3/2}v &= T_1v - e^{i\pi/4} \left( \frac{\kappa^2}{8} + \frac{1}{2} \Delta \Gamma \right) I_t^{1/2} v, \\
T_2v &= T_{3/2}v + i \left( \frac{\kappa^3}{8} + \frac{1}{2} \partial_s (\kappa \partial_s) + \frac{\Delta \Gamma \kappa}{8} \right) I_t v,
\end{align*}
\]

with \( I_t^{1/2} = I_t \partial_t^{1/2} \).
Numerical experiments

Explicit solution (2D)

\[ u(x_1, x_2, t) = \frac{i}{i - 4t} \exp \left( -i \frac{x_1^2 + x_2^2 + 5ix_1 + 25it}{i - 4t} \right). \]

Finite elements approximation \((P^1)\): \(\Omega_i = D(0, 10)\), 3278 triangles, \(\delta t = 10^{-2}\).