

Open boundary conditions for wave propagation problems on unbounded domains

Anton ARNOLD

TU Vienna
Institute for Analysis and Scientific Computing

Graz, 12. September 2007

Wave propagation in “unbounded domains” – applications:

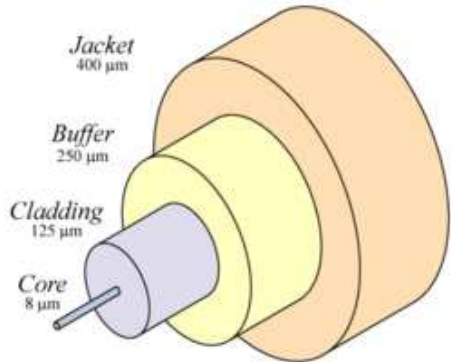
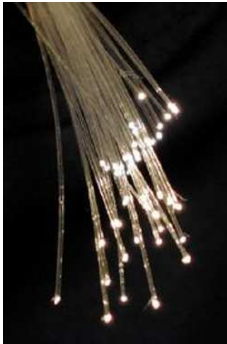
- water waves:



→ shallow water equation, t -dependent wave equation

- open / non-reflecting boundary conditions needed

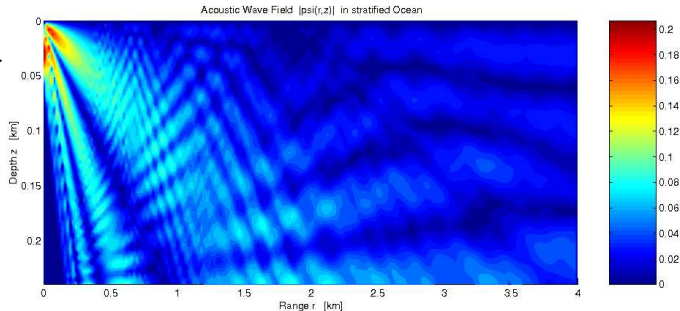
- fiber-optic cables:



- for core diameter $< 10\mu\text{m}$:
Maxwell equations, 1-way wave equation (Schrödinger/parabolic type)
- wave propagation mainly in core \Rightarrow limit the computational domain with open BC

- underwater acoustics:

ocean surface:
sound source →



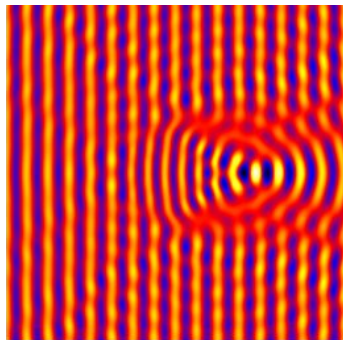
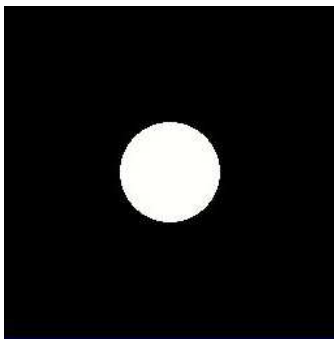
sea bottom:

→ reflection / transmission
→ open BC to artificially
limit computational domain

- original model: 2D-Helmholtz equation (time-harmonic solution)
- simplified model: 1-way wave equation

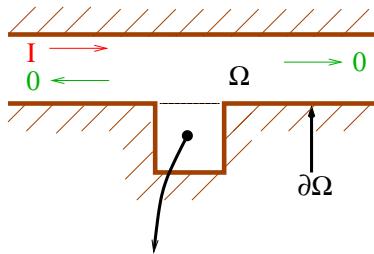
Scattering problems:

- electromagnetic wave scattered by “soft” ball:

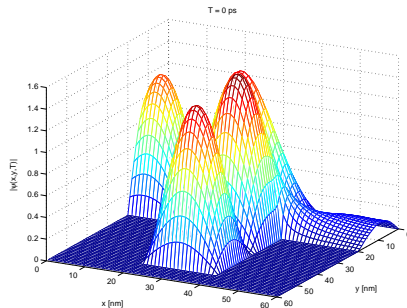


→ Helmholtz equation with incoming plane wave (from left)

- T -shaped quantum waveguide for electron flow:



control potential



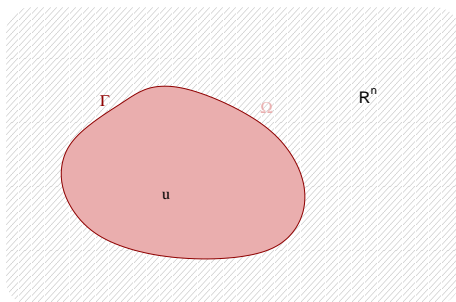
→ Schrödinger equation with incoming plane wave (from left)

- open / non-reflecting boundary condition needed

Outline:

- ❶ non-reflecting boundary conditions
 - ▶ approaches, derivation
- ❷ transparent BCs for Schrödinger equation
 - ▶ rectangular geometry
 - ▶ fast algorithms
 - ▶ circular geometry
- ❸ perfectly matched layer
 - ▶ Klein Gordon equation
- ❹ perspectives

(1) Non-reflecting boundary conditions



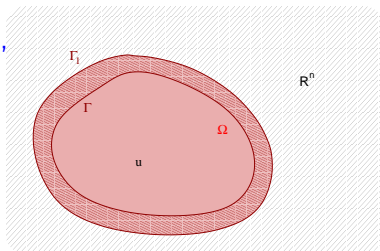
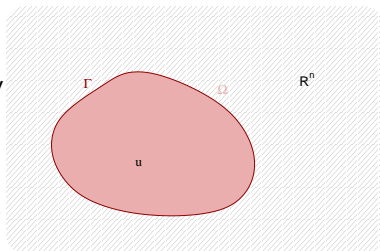
- original PDE for $u(x, t)$ (stationary or transient) on unbounded domain (e.g. \mathbb{R}^n)
- for numerics: introduce **artificial boundary** Γ
→ encloses **finite** domain Ω
- derive **non-reflecting boundary condition** on/around Γ

Necessary features of non-reflecting BCs:

- 1 yield a well-posed BVP or IBVP on Ω
- 2 no (or little) spurious wave reflections due to BC — compared to whole space problem
- 3 allow for efficient numerical implementation

3 basic approaches for non-reflecting BCs:

- 1 PDE-based: exact **transparent BC**
(DtN map: non-local operator in x, t)
→ tricky implementation, high accuracy
- 2 PDE-based: local **absorbing BC**
(low order differential operator)
→ simple implementation, low accuracy
[Engquist-Majda, 1977] for wave equ.
- 3 material-based: '**perfectly matched layer**'
(PML)
→ add dissipative media around Ω
⇒ damp outgoing waves
[Bérenger, 1994] for Maxwell



Derivation of exact / transparent BCs:

- simple idea:

- ▶ factorize wave-like PDE into incoming/outgoing modes
- ▶ add BC \Rightarrow outgoing waves cross Γ freely

- difficult realization:

- ▶ exact factorization only for linear PDEs on Ω with 'regular shape' — else: approximate factorization
- ▶ BC is pseudo-differential (non-local in x, t)
- ▶ tricky & expensive discretization

Transparent boundary condition for 1D wave equation:

- computational domain $\Omega = (0, L)$
- assume: constant coefficients on left/right exterior domains Ω^c
- assume: initial condition supported in Ω
- factorization:

$$0 = u_{tt} - u_{xx} = \underbrace{(\partial_t - \partial_x)}_{\leftarrow} \underbrace{(\partial_t + \partial_x)}_{\rightarrow} u$$

$$\left. \begin{array}{l} u_t = u_x \quad , \quad x = 0 \\ u_t = -u_x \quad , \quad x = L \end{array} \right\} \text{“perfect”} = \text{transparent BCs}$$

\Rightarrow Waves leave the domain Ω without being reflected back.

Transparent boundary conditions for 2D wave equation:

- computational domain $\Omega = \{(x, y), x > 0\}$
- factorization:

$$u_{xx} - (u_{tt} - u_{yy}) = \underbrace{\left(\partial_x - \sqrt{\partial_t^2 - \partial_y^2} \right)}_{\leftarrow} \underbrace{\left(\partial_x + \sqrt{\partial_t^2 - \partial_y^2} \right)}_{\rightarrow} u = 0$$

TBC at $x = 0$:

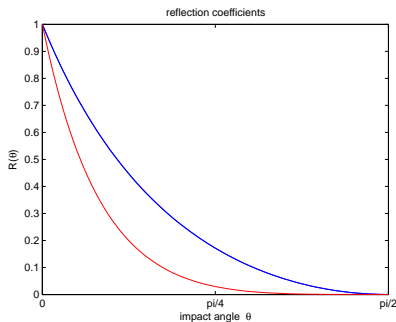
$$u_x - \underbrace{\sqrt{\partial_t^2 - \partial_y^2}}_{\Psi\text{DO; nonlocal in } y, t} u = 0 \quad \text{or} \quad \hat{u}_x - i \underbrace{\sqrt{\omega^2 - \eta^2}}_{y-t\text{-Fouriertransform}} \hat{u} = 0$$

Absorbing boundary conditions for 2D wave equation:

- rational approximation of Ψ DO-symbol $\sqrt{\omega^2 - \eta^2}$ (Taylor, Padé) :
- high frequency approximation, i.e. $|\frac{\eta}{\omega}| \ll 1$
 \Rightarrow hierarchy of local ABCs at $x = 0$ [Engquist-Majda 1977] :

$$u_x - u_t = 0, \quad u_{xt} - u_{tt} + \frac{1}{2}u_{yy} = 0 \rightarrow \text{well-posed IBVP}$$

- ▶ reflection coefficient depends on impact angle at $\partial\Omega$
- ▶ $|R(\theta)| < 1 \Rightarrow$ “absorbing BC”



2nd order Taylor approximation \rightarrow strongly ill-posed IBVP

(2) Transparent boundary cond. for Schrödinger equation:

- Example: 1D-Schrödinger equation:

wavefunction: $\psi(x, t) \in \mathbb{C}$

$$\left\{ \begin{array}{l} i\psi_t = -\psi_{xx} + V(x, t)\psi; \quad x \in \mathbb{R}, t > 0 \\ \text{supp}\psi^0 \subset (0, L) \quad \dots \quad \text{computational domain} \\ V(x, t) = V_l(t), x \leq 0; \quad V(x, t) = V_r(t), x \geq L \end{array} \right.$$

Goal: reproduce $\psi_{[0,L]}$ with artificial BCs at $x = 0, L$

① exterior potential $V_I = \text{const} = 0 \rightarrow$ factorization:

$$0 = \psi_{xx} - (-i)\psi_t = \underbrace{(\partial_x - \sqrt{-i}\sqrt{\partial_t})}_{\leftarrow} \underbrace{(\partial_x + \sqrt{-i}\sqrt{\partial_t})}_{\rightarrow} \psi$$

$$\text{TBC at } x = 0: \quad \psi_x(0, t) = \sqrt{-i\partial_t} \psi = \frac{e^{-\frac{\pi}{4}i}}{\sqrt{\pi}} \frac{d}{dt} \int_0^t \frac{\psi(0, \tau)}{\sqrt{t - \tau}} d\tau$$

- ▶ BC non-local in t (memory-type \rightarrow store $\psi(t)|_\Gamma$)
[Papadakis '82, Baskakov-Popov '91, Hellums-Frenslley '94]

① exterior potential $V_I = \text{const} = 0 \rightarrow$ factorization:

$$0 = \psi_{xx} - (-i)\psi_t = \underbrace{(\partial_x - \sqrt{-i}\sqrt{\partial_t})}_{\leftarrow} \underbrace{(\partial_x + \sqrt{-i}\sqrt{\partial_t})}_{\rightarrow} \psi$$

TBC at $x = 0$: $\psi_x(0, t) = \sqrt{-i\partial_t}\psi = \frac{e^{-\frac{\pi}{4}i}}{\sqrt{\pi}} \frac{d}{dt} \int_0^t \frac{\psi(0, \tau)}{\sqrt{t-\tau}} d\tau$

► BC non-local in t (memory-type \rightarrow store $\psi(t)|_\Gamma$)
[Papadakis '82, Baskakov-Popov '91, Hellums-Frenslley '94]

② exterior potential $V_I = V_I(t) \neq 0 \Rightarrow$ TBC at $x = 0$:

$$\psi_x(0, t) e^{i \int_0^t V_I(\tau) d\tau} = \frac{e^{-\frac{\pi}{4}i}}{\sqrt{\pi}} \frac{d}{dt} \int_0^t \frac{\psi(0, \tau)}{\sqrt{t-\tau}} e^{i \int_0^\tau V_I(s) ds} d\tau$$

① exterior potential $V_I = \text{const} = 0 \rightarrow$ factorization:

$$0 = \psi_{xx} - (-i)\psi_t = \underbrace{(\partial_x - \sqrt{-i}\sqrt{\partial_t})}_{\leftarrow} \underbrace{(\partial_x + \sqrt{-i}\sqrt{\partial_t})}_{\rightarrow} \psi$$

TBC at $x = 0$: $\psi_x(0, t) = \sqrt{-i\partial_t}\psi = \frac{e^{-\frac{\pi}{4}i}}{\sqrt{\pi}} \frac{d}{dt} \int_0^t \frac{\psi(0, \tau)}{\sqrt{t-\tau}} d\tau$

► BC non-local in t (memory-type \rightarrow store $\psi(t)|_\Gamma$)
 [Papadakis '82, Baskakov-Popov '91, Hellums-Frenslley '94]

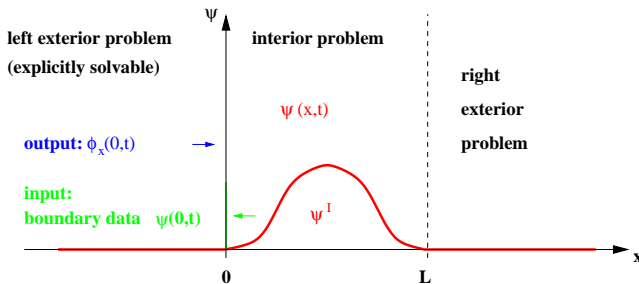
② exterior potential $V_I = V_I(t) \neq 0 \Rightarrow$ TBC at $x = 0$:

$$\psi_x(0, t) e^{i \int_0^t V_I(\tau) d\tau} = \frac{e^{-\frac{\pi}{4}i}}{\sqrt{\pi}} \frac{d}{dt} \int_0^t \frac{\psi(0, \tau)}{\sqrt{t-\tau}} e^{i \int_0^\tau V_I(s) ds} d\tau$$

③ scattering problem with incoming wave $\psi^{in}(0, t)$:

inhomogeneous TBC: $(\partial_x - \sqrt{-i\partial_t})(\psi(0, t) - \psi^{in}(0, t)) = 0$

rigorous derivation of transparent boundary conditions



- **elimination of left exterior problem** —
analytically (via Fourier/Laplace transforms) or numerically
⇒ **left TBC** $\psi_x(0, t) = (T \psi)(0, t)$ from :

$$\begin{cases} i\phi_t &= -\phi_{xx}, & x < 0 \\ \phi^0(x) &= 0 \\ \phi(0, t) &= \psi(0, t), & \phi(-\infty, t) = 0 \end{cases}$$

$$\Rightarrow (T \psi)(t) = \phi_x(0, t), \quad T \dots \text{Dirichlet-to-Neumann (DtN) operator}$$

Schrödinger boundary value problem

$$\left\{ \begin{array}{l} i\psi_t = -\psi_{xx} + V(x, t)\psi; \quad x \in (0, L), \quad t > 0 \\ \text{supp}\psi^0 \subset (0, L) \\ \left(V(x, t) = V_l(t), x \leq 0; \quad V(x, t) = V_r(t), x \geq L \right) \\ \text{TBC at } x = 0, L \end{array} \right. \quad (1)$$

Theorem (DiMenza, 1995)

Let $\psi^0 \in H^1(0, L) \Rightarrow$ unique solution of (1) is whole-space solution.

- [Ben Abdallah-Méhats-Pinaud '04] : extension to 2D, 3D + scattering problem for $\psi^0 \in H^2(\Omega)$

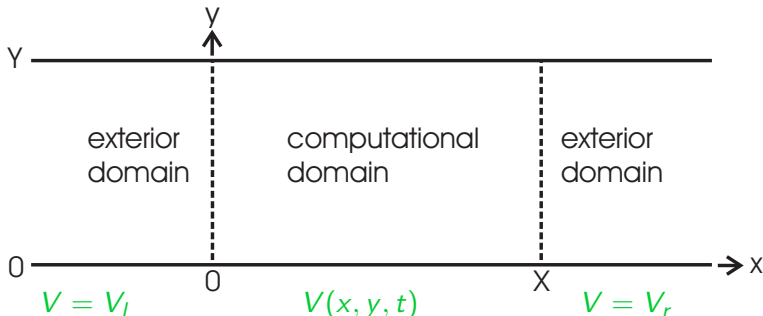
2D Schrödinger equation – waveguide geometry

- factorization of $\psi_{xx} = -\psi_{yy} - i\psi_t + V\psi$

\Rightarrow TBC at $x = 0$ is **non-local** (pseudo-differential) **in t and y** :

$$\psi_x(0, y, t) = \sqrt{-\partial_{yy} - i\partial_t + V} \psi$$

- BC for waveguides: $\psi(x, 0, t) = \psi(x, Y, t) = 0$:



2D Schrödinger equation – waveguide geometry

- Fourier series in y : $\psi(x, y, t) = \sum_{m \in \mathbb{N}} \hat{\psi}^m(x, t) \sin \frac{m\pi y}{Y}$
- $V = \text{const} = V_l$ in left exterior domain \Rightarrow y -modes are decoupled
- TBC is **local in y for each sine-mode** [AA-Ehrhardt-Sofronov '03] :

$$\begin{aligned}\hat{\psi}_x^m(0, t) &= \sqrt{-i\partial_t + V^m} \hat{\psi}^m \\ &= \sqrt{\frac{-i}{\pi}} e^{-iV^m t} \frac{d}{dt} \int_0^t \frac{\hat{\psi}^m(0, \tau) e^{iV^m \tau}}{\sqrt{t - \tau}} d\tau \\ V^m &= V_l + \left(\frac{m\pi}{Y}\right)^2, \quad m \in \mathbb{N}\end{aligned}$$

Discretization of analytic TBC

- Dangers :

- ▶ may destroy the (unconditional) stability of the whole-space scheme
- ▶ may introduce numerical reflections at the boundary

Discretization of analytic TBC

- Dangers :

- ▶ may destroy the (unconditional) stability of the whole-space scheme
- ▶ may introduce numerical reflections at the boundary

- one option: “discrete transparent boundary conditions”

STRATEGY :

- ▶ discretize left exterior problem ($j \leq 0$)
- ▶ derivation of the discrete TBC (for discrete scheme)
instead of: discretization of the analytic TBC
- ▶ for many linear equ, many discretization schemes

Discretization of analytic TBC

- Dangers :

- ▶ may destroy the (unconditional) stability of the whole-space scheme
- ▶ may introduce numerical reflections at the boundary

- one option: “discrete transparent boundary conditions”

STRATEGY :

- ▶ discretize left exterior problem ($j \leq 0$)
- ▶ derivation of the discrete TBC (for discrete scheme)
instead of: discretization of the analytic TBC
- ▶ for many linear equ, many discretization schemes

- alternatives :

- ▶ semidiscrete TBCs [Alonso-Mallo-Reguera '03], [Lubich-Schädle '02]
- ▶ TBCs from ‘pole condition’ [Ruprecht-Schädle-Schmidt-Zschiedrich '07]
- ▶ ...

discrete transparent boundary conditions (DTBCs)

- Ex: Crank-Nicolson finite difference-scheme for free Schrödinger equ:
 $\psi_j^n \approx \psi(j\Delta x, n\Delta t)$, unconditionally stable: $\|\psi^n\|_2 = \|\psi^0\|_2$

$$i \frac{\psi_j^{n+1} - \psi_j^n}{\Delta t} = -\frac{1}{2} \frac{\psi_{j-1}^{n+1} - 2\psi_j^{n+1} + \psi_{j+1}^{n+1}}{\Delta x^2} - \frac{1}{2} \frac{\psi_{j-1}^n - 2\psi_j^n + \psi_{j+1}^n}{\Delta x^2}$$

- **Z-transformed exterior problem** ($\psi_j^0 = 0, j \leq 0$)
with $\mathcal{Z}\{\psi_j^n\} = \hat{\psi}_j(z) = \sum_{n=0}^{\infty} \psi_j^n z^{-n}, z \in \mathbb{C}$:

$$\hat{\psi}_{j-1} - 2\left(1 - i \frac{\Delta x^2}{\Delta t} \frac{z-1}{z+1}\right) \hat{\psi}_j + \hat{\psi}_{j+1} = 0, \quad j \leq 1$$

- choose decaying solution as $j \rightarrow -\infty$: $\hat{\psi}_j(z) = \alpha(z)^j$
 \Rightarrow **transformed DTBC** :

$$\hat{\psi}_1(z) = \alpha(z) \hat{\psi}_0(z), \quad |\alpha(z)| > 1$$

discrete transparent boundary conditions

transformed DTBC : $\hat{\psi}_1(z) = \alpha(z)\hat{\psi}_0(z)$

- inverse Z-transform (explicit or numerical): $(s_n) := \mathcal{Z}^{-1}\{\frac{z+1}{z}\alpha(z)\}$
- discrete TBC: $\psi_1^n = \sum_{k=1}^n \psi_0^k s_{n-k} - \psi_1^{n-1}$... discrete convolution
- 3-point recursion for (s_n)
- $s_n = O(n^{-3/2})$

Theorem (AA '98)

CN - FD scheme for Schrödinger equation with discrete TBC is unconditionally stable:

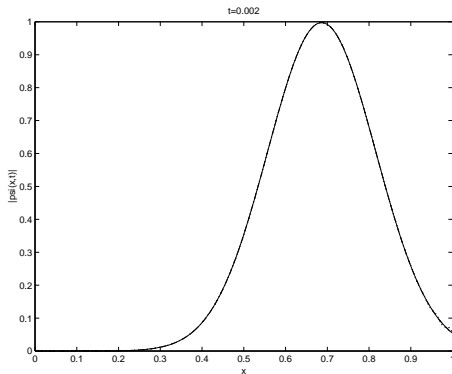
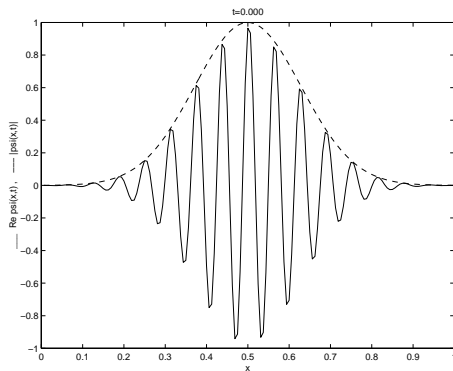
$$\|\psi^n\|_2^2 := \Delta x \sum_{j=1}^J |\psi_j^n|^2 \leq \|\psi^0\|_2^2, \quad n \geq 1$$

→ no numerical reflections

→ same numerical effort as 'conventional' discretizations of

$$\psi_x(0, t) = C \frac{d}{dt} \int_0^t \frac{\psi(0, \tau)}{\sqrt{t-\tau}} d\tau$$

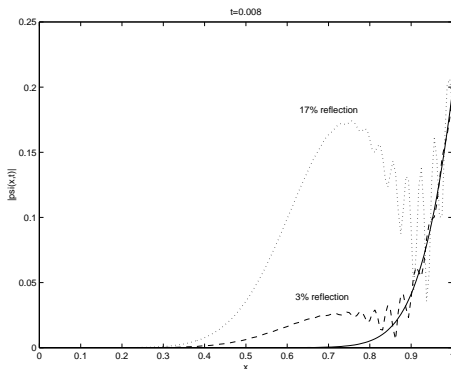
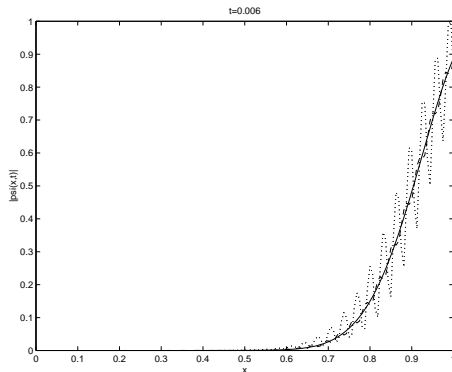
free Schrödinger equation ($V = 0$) with TBC



Gaussian beam $|\psi(x, t)|$, $x \in \mathbb{R}$; right-traveling

$\Delta x = \frac{1}{160}$, $\Delta t = 2 \cdot 10^{-5}$ (rather coarse discretization)

free Schrödinger equation ($V = 0$) with TBC



... [B. Mayfield 1989]

- - - [Baskakov & Popov 1991]

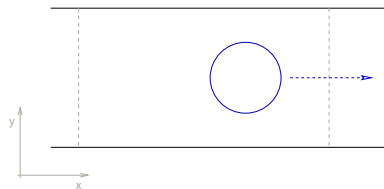
— [AA 1998]



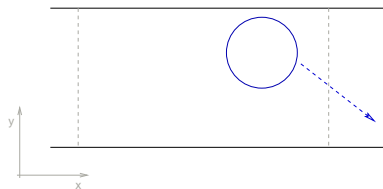
discretization of
the analytic TBC

discrete TBC

Gaussian beam in 2D waveguide:



right traveling Gaussian beam on $\Omega = (0, 1)^2$
aligned with waveguide



at 45° with waveguide

- $\Delta x = \Delta y = 1/120$, $\Delta t = 5 \cdot 10^{-5}$
- TBC local in y for each sine-mode
 \Rightarrow implementation of TBC in y -Fourier space faster [Schulte-AA '07]

Gaussian wave aligned with waveguide:

Gaussian wave at 45° with waveguide:

- advantage of discrete TBCs:
 - ▶ absolutely reflection-free
 - ▶ unconditionally stable

- advantage of discrete TBCs:
 - ▶ absolutely reflection-free
 - ▶ unconditionally stable
- disadvantage (for long-time calculations):
 - ▶ compute boundary-convolutions: $O(N^2)$ -effort;
 $N \dots \#$ of time steps
 - ▶ memory requirement for boundary data: $O(N)$

- advantage of discrete TBCs:
 - ▶ absolutely reflection-free
 - ▶ unconditionally stable
- disadvantage (for long-time calculations):
 - ▶ compute boundary-convolutions: $O(N^2)$ -effort;
 $N \dots \#$ of time steps
 - ▶ memory requirement for boundary data: $O(N)$
- goal:
approximate convolution kernel $(s_n) \rightarrow O(N)$ -effort

approximate TBCs – fast evaluation of convolutions

- if $s_k = q^{-k}$: trivial update of convolutions:

$$\sum_{k=0}^n u_k s_{n-k} = \frac{1}{q} \left(\sum_{k=0}^{n-1} u_k s_{n-1-k} \right) + u_n s_0$$

approximate TBCs – fast evaluation of convolutions

- if $s_k = q^{-k}$: trivial update of convolutions:

$$\sum_{k=0}^n u_k s_{n-k} = \frac{1}{q} \left(\sum_{k=0}^{n-1} u_k s_{n-1-k} \right) + u_n s_0$$

- **Idea**: approximation of s_n by sum of exponentials; $s_n = O(n^{-3/2})$ — **discrete** analogue of [Grote-Keller '95]:

$$s_n \approx \tilde{s}_n = \sum_{l=1}^L b_l q_l^{-n}, \quad n \in \mathbb{N}, \quad |q_l| > 1, \quad L \sim 10 - 20$$
$$\mathcal{Z}\{\tilde{s}_n\} = s_0 + \sum_{l=1}^L \frac{b_l}{q_l z - 1}, \quad |z| \geq 1.$$

approximate TBCs – fast evaluation of convolutions

- if $s_k = q^{-k}$: trivial update of convolutions:

$$\sum_{k=0}^n u_k s_{n-k} = \frac{1}{q} \left(\sum_{k=0}^{n-1} u_k s_{n-1-k} \right) + u_n s_0$$

- **Idea**: approximation of s_n by sum of exponentials; $s_n = O(n^{-3/2})$ — **discrete** analogue of [Grote-Keller '95]:

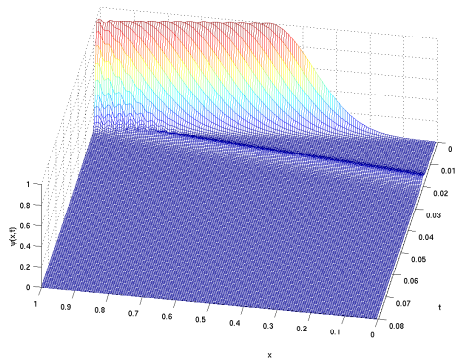
$$s_n \approx \tilde{s}_n = \sum_{l=1}^L b_l q_l^{-n}, \quad n \in \mathbb{N}, \quad |q_l| > 1, \quad L \sim 10 - 20$$
$$\mathcal{Z}\{\tilde{s}_n\} = s_0 + \sum_{l=1}^L \frac{b_l}{q_l z - 1}, \quad |z| \geq 1.$$

- b_l, q_l from Padé approximation of

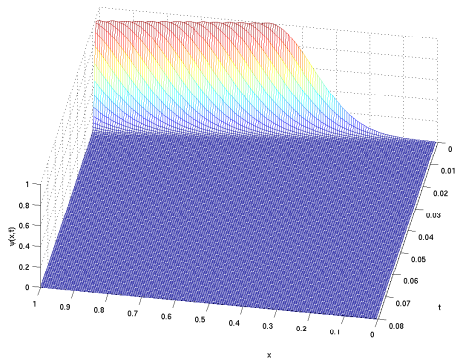
$$f(x) = \sum_{n=0}^{2L-1} s_n x^n, \quad x = \frac{1}{z}$$

- convolution update: **linear effort**, constant memory requirement

approximate TBCs – 1D Schrödinger equation ($V = 0$)



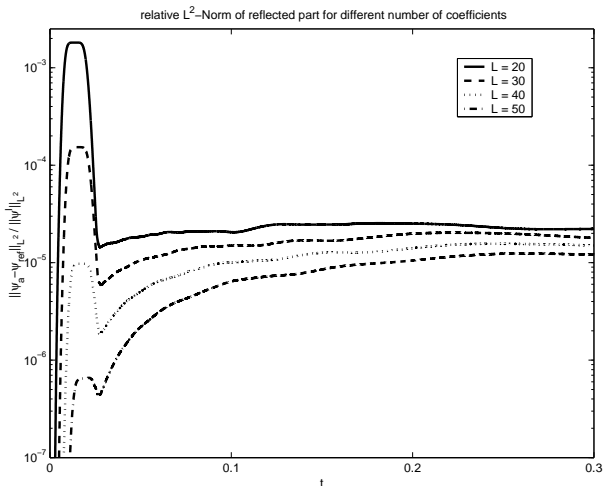
solution with $L = 10$



solution with $L = 20$

[AA-Ehrhardt-Sofronov, 2003]

approximate TBCs: error decreases with L



relative $L^2(0,1)$ -error with approximate TBCs, up to 15.000 time steps
[AA-Ehrhardt-Sofronov, 2003]

approximate TBCs: error estimate

(ψ^n) ... solution with exact TBC

(ψ_L^n) ... solution with approximate TBC

convolution coefficients:

$$(s_n) = \mathcal{Z}^{-1} \left(\frac{z+1}{z} \alpha(z) \right), \quad (s_n^L) = \mathcal{Z}^{-1} \left(\frac{z+1}{z} \alpha_L(z) \right) \quad \dots L \text{ exp. terms}$$

Theorem (AA-Ehrhardt-Sofronov, 2003)

$$\|\psi^n - \psi_L^n\|_{L^2(0,1)} \leq C(n) \|\psi^0\|_{H_{disc}^1} \left\| \frac{1}{\alpha(e^{i\varphi})} - \frac{1}{\alpha_L(e^{i\varphi})} \right\|_{L^\infty(0,2\pi)}, \quad n \in \mathbb{N}_0$$

Example for $\Delta x = 1/160$, $\Delta t = 2 \cdot 10^{-5}$:

$L =$	5	10	15	20
error $\ \frac{1}{\alpha} - \frac{1}{\alpha_L}\ _\infty$	1.8247e-04	1.2808e-07	6.4439e-11	2.962e-14

approximate TBCs: stability

TBC with **approximate** convolution coefficients:

$$(s_n^L) = \mathcal{Z}^{-1} \left(\frac{z+1}{z} \alpha_L(z) \right) \quad \dots L \text{ exp. terms}$$

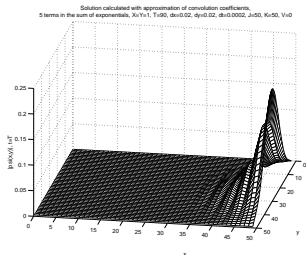
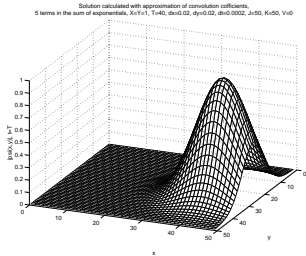
→ stability **not** trivial !

Lemma (AA-Ehrhardt-Sofronov, 2003)

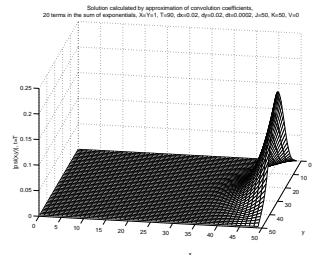
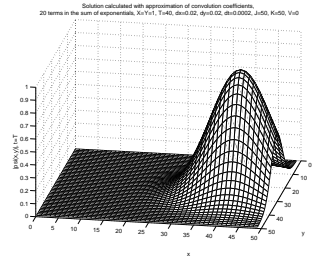
If $\Im \alpha_L(\beta e^{i\varphi}) \leq 0 \quad \forall 0 \leq \varphi \leq 2\pi$ and α_L analytic for $|z| > \beta$

$$\Rightarrow \|\psi^n\|_2 \leq \|\psi^0\|_2 \beta^n, \quad n \in \mathbb{N}$$

approximate TBCs – 2D Schrödinger equation ($V = 0$)



solution with $L = 5$



solution with $L = 20$

TBC at $x = 50$; right-traveling Gaussian beam [Schulte-AA, 2007]

2D Schrödinger equation: discrete TBC for circular domain

in polar coordinates, $V = 0$:

$$i\psi_t = -\frac{1}{2} \left(\frac{1}{r} (r\psi_r)_r + \frac{1}{r^2} \psi_{\theta\theta} \right)$$

- uniform radial off-set grid $r_j = (j + \frac{1}{2})\Delta r$, $j \in \mathbb{N}_0$; uniform angular grid

2D Schrödinger equation: discrete TBC for circular domain

in polar coordinates, $V = 0$:

$$i\psi_t = -\frac{1}{2} \left(\frac{1}{r} (r\psi_r)_r + \frac{1}{r^2} \psi_{\theta\theta} \right)$$

- uniform radial off-set grid $r_j = (j + \frac{1}{2})\Delta r$, $j \in \mathbb{N}_0$; uniform angular grid
- discrete Fourier transform in θ_k , Z-transform in t
 \Rightarrow finite difference equation (**variable coefficients!**) for each mode $\hat{\psi}^m$:

$$a_j \hat{\psi}_{j-1}(z) + b_j^m(z) \hat{\psi}_j(z) + c_j \hat{\psi}_{j+1}(z) = 0, \quad j \geq J-1 \quad (2)$$

- Z-transformed TBC: $\alpha_{J+1}(z) = \frac{\hat{\psi}_{J+1}(z)}{\hat{\psi}_J(z)}$ (for *decaying* solution $\hat{\psi}_j(z)$)

2D Schrödinger equation: discrete TBC for circular domain

in polar coordinates, $V = 0$:

$$i\psi_t = -\frac{1}{2} \left(\frac{1}{r} (r\psi_r)_r + \frac{1}{r^2} \psi_{\theta\theta} \right)$$

- uniform radial off-set grid $r_j = (j + \frac{1}{2})\Delta r$, $j \in \mathbb{N}_0$; uniform angular grid
- discrete Fourier transform in θ_k , Z-transform in t
 \Rightarrow finite difference equation (**variable coefficients!**) for each mode $\hat{\psi}^m$:

$$a_j \hat{\psi}_{j-1}(z) + b_j^m(z) \hat{\psi}_j(z) + c_j \hat{\psi}_{j+1}(z) = 0, \quad j \geq J-1 \quad (2)$$

- Z-transformed TBC: $\alpha_{J+1}(z) = \frac{\hat{\psi}_{J+1}(z)}{\hat{\psi}_J(z)}$ (for *decaying* solution $\hat{\psi}_j(z)$)
- for stability: solve (2) numerically from $j = \infty$ back to $j = J$;
initial condition at $j = \infty$: 1D-TBC
- numerical / discrete inverse Z-transformation of $\frac{z+1}{z} \alpha_{J+1}(z)$, $z \in \mathbb{C}$
 \rightarrow convolution coefficients (s_n) for each mode m

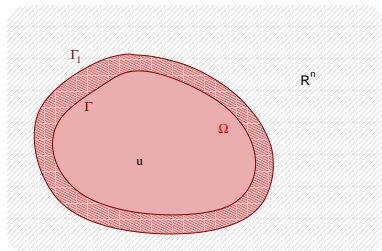
Gaussian wave in circle, traveling south-east

symmetric polar grid: $\Delta r = \frac{1}{128}$, $\Delta \theta = \frac{2\pi}{128}$; $\Delta t = \frac{1}{128}$

[AA-Ehrhardt-Schulte-Sofronov, 2007]

(3) perfectly matched layer (PML)

- surround computational domain Ω with layer of artificial damping medium
- interface Γ : zero reflection (\forall angles)
→ “perfectly matched layer”
- attenuate all outgoing waves
- waves reflected from Γ_1 :
amplitude very small on Γ
- Bérenger-PML for Maxwell :
numerically great;
weakly well-posed [Bécache-Joly, 2001]



PML for 1D stationary equation: derivation

- solution u ; computational domain $\Omega = \mathbb{R}^+$
- define “**modified**” (complex) solution on \mathbb{R} , strong decay as $x \rightarrow -\infty$:

$$u^m(x) := \begin{cases} u(x)e^{f(x)}, & x < 0 \\ u(x), & x \geq 0 \end{cases}$$

damping factor: $\Re f(x) \nearrow$, $f(0) = 0$

- find equation for $u^m(x)$
- truncate layer at $x = -a < 0$
- construction **not unique**

PML for linear 1D Klein-Gordon equation: derivation

Example: $u_{tt} = u_{xx} - u_t, \quad x \in \mathbb{R}, t > 0$

- reformulate as hyperbolic system,
modified solution for each t -Laplace mode
 \Rightarrow **modified** hyperbolic PML-system :

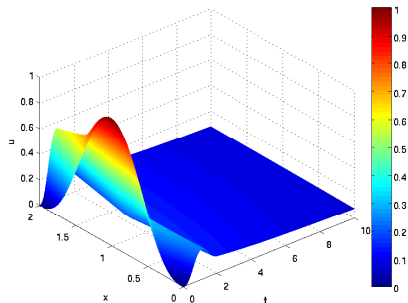
$$\begin{cases} u_t^m = w^m, & x \in \mathbb{R} \\ v_t^m = w_x^m - \sigma(x)p^m \\ w_t^m = v_x^m - u_t^m - \sigma(x)q^m \\ p_t^m = w_x^m - (\alpha(x) + \sigma(x))p^m \\ q_t^m = v_x^m - (\alpha(x) + \sigma(x))q^m \end{cases}$$

- $\alpha, \sigma \dots$ damping parameters on Ω^c (related to f)
 $p, q \dots$ auxiliary PML variables
- well-posed; $u(x) = u^m(x)$ on Ω by construction (for ∞ layer)

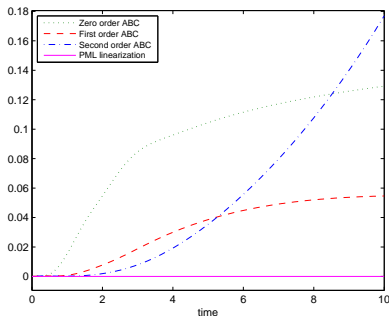
PML for linear 1D Klein-Gordon equation: better than ABC

$$\begin{cases} u_{tt} = u_{xx} - u_t, & x \in \mathbb{R}, t > 0 \\ \text{supp } u^0, u_t^0 \subset \Omega = (0, 2) \end{cases}$$

2 PML-layers; thickness = 0.1



exact solution



relative $L^2(0,2)$ -errors

- local ABC of [Engquist-Majda, 1979]
- max. PML-error on $t \in [0, 10]$: $4 \cdot 10^{-8}$ [AA-Amro-Zheng, 2007]

PML for nonlinear 1D Klein-Gordon equation: derivation

Example: $u_{tt} = u_{xx} - \varphi(u, u_t, u_x)$

- first – linear equation:

$$u_{tt} = u_{xx} - (a u + b u_t + c u_x)$$

- PML-system for linear equation :

$$\begin{cases} u_t = w \\ v_t = w_x - \sigma(x)p \\ w_t = v_x - (a u + b u_t + c u_x) - \sigma(x)q \\ p_t = w_x - (\alpha(x) + \sigma(x))p \\ q_t = v_x - (\alpha(x) + \sigma(x))q \end{cases} \quad (3)$$

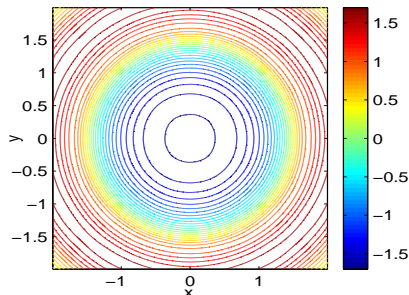
- “PML-linearization”:

replace $(a u + b u_t + c u_x)$ by $\varphi(u, u_t, u_x)$ in (3)

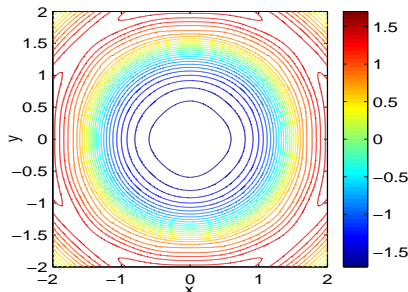
nonlinear Klein-Gordon equation with PML: circular wave

$$u_{tt} = \Delta u - u^3, \quad x, y \in \mathbb{R} \quad (4)$$

PML with layer thickness 0.8:



$u(x, y, t = 3.5)$: “PML linearization”,
(i.e. nonlinear PML-system)



direct linearization of (4)
about $u \equiv 0$ in PML-layer

[AA-Amro-Zheng, 2007], well-posedness ?

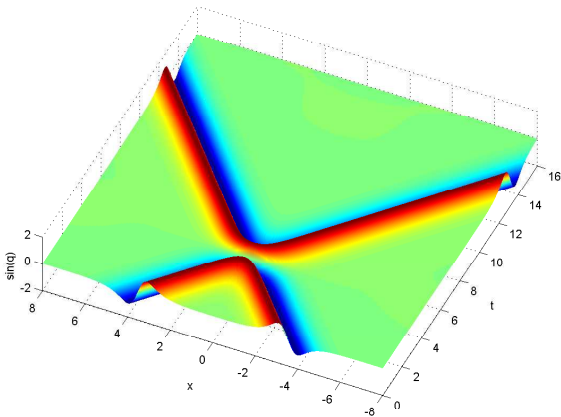
(4) Perspectives / first solution steps:

- inhomogeneous / anisotropic exterior problems :
 - ▶ PML sometimes unstable [Bécache-Fauqueux-Joly, 2003]
 - ▶ [Sofronov-Zaitsev, 2006] : TBC for anisotropic elastic waves, numerical construction of DtN-map in t -Laplace domain
- nonlinear models :
 - ▶ [Szeftel, 2006] : ABCs by pseudo-/paradifferential calculus (special linearization) for many nonlinear wave equations
 - ▶ [Zheng-Amro, 2007] : PML for 2D Euler (compressible) — well-posedness ?

Perspectives / transparent BCs for fully integrable systems

sine-Gordon equation: $u_{tt} - u_{xx} + \sin u = 0$, $x \in \mathbb{R}$, $t > 0$

exact TBC exists (as solution to nonlinear ODE), based on inverse scattering theory [Fokas, 2002]



interaction of 2 solitons, no boundary reflections [Zheng, 2007]
(also for KdV, cubic Schrödinger)

Cooperations / (former) PhD students:

- Ivan Sofronov (Moscow)
- Chunxiong Zheng (Beijing)
- Tareq Amro (Münster)
- Matthias Ehrhardt (Berlin)
- Maike Schulte (Münster)