Construction of Stable Discretization Schemes of Non-Reflecting Boundary Conditions for the 1D Schrödinger Equation

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Overview of the talk

Principle :

Under some simplifications, you can meet e.g. the Schrödinger equation in Wave Propagation as a simplified model (approximating the Helmholtz equation) : it is then better known as the Standard Parabolic Equation (SPE) in Electromagnetism, Fresnel Equation in optics,...

An example : the SPE

$$i\partial_x u + \frac{1}{2k}\partial_z^2 u + \frac{k}{2}(n^2 - 1)u = 0 \quad \text{(SPE = LSE)}$$

where u is an approximation of the true wavefield, x is the direction of propagation, z the transverse direction, k the wavenumber and n the index of the medium
Moreover, you must add an initial value of the field at the initial "time" $x = 0$

$$u(0, z) = u_0(z)$$

1.2. The linear Schrödinger equation

The Linear Schrödinger Equation (LSE) is defined more generally by $(x,t) \in \mathbb{R}_x^N \times \mathbb{R}_t^{*+}$, $N = 1, 2$

$$\begin{cases} (i\partial_t + \Delta + V(x,t))u(x,t) = 0, \\ u(x,0) = u_0(x). \end{cases}$$

Δ is the Laplace operator, V is a potential

What we guess :

Our goal is to compute an (approximation ?) of u inside a finite computational domain Ω_i. We consider $N = 1$ (and $N \geq 2$ will be treated in other talks) : This is exactly the aim of the so-called Non-Reflecting Boundary Conditions, Artificial or Absorbing BC, PML...

2.1 The beginning of the story

- Baskakov & Popov 89, Arnold 91, DiMenza 95, etc ...
- 1D-LSE

$$\begin{cases} i\partial_t u + \partial_x^2 u + Vu = 0, \ x \in \mathbb{R}, \ t > 0, \\ u(x,0) = u_0(x) \end{cases} \quad (1)$$

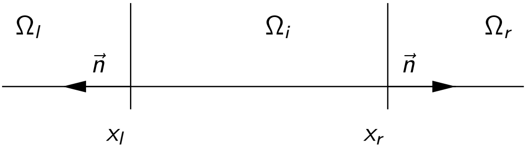
Proposition

If $u_0 \in L^2(\mathbb{R})$, $V \in C(\mathbb{R}_t^+, L^\infty)$, there exists a unique solution $u \in C(\mathbb{R}_t, L^2(\mathbb{R}))$ and

$$\|u(.,t)\|_2 = \|u_0\|_2, \forall t > 0$$

2.2 Building the continuous non-reflecting boundary condition (NRBC)

- Let $\Omega_i =]x_l, x_r[$, $\Gamma = \{x_l, x_r\}$,



- Assumptions : $supp(u_0) \subset \Omega_i$ and $V = 0$. Continuity of u and $\partial_x u$ across the fictitious boundary Γ

Splitting the problem : introduction of the DN operator

- Interior problem

$$\begin{cases} i\partial_t u + \partial_x^2 u = 0, x \in \Omega_i, t > 0, \\ u(x,0) = u_0(x), x \in \Omega_i, \\ \partial_x u = \partial_x v,\ \ x \in \Gamma, t > 0, \end{cases}$$

and exterior problem

$$\begin{cases} i\partial_t v + \partial_x^2 v = 0, x \in \Omega_{l,r}, t > 0, \\ v(x,0) = 0, x \in \Omega_{l,r}, \\ v(x,t) = u(x,t),\ \ x \in \Gamma,\ \ t > 0, \\ \lim_{|x|\to\infty} v(x,t) = 0, t > 0. \end{cases}$$

- In other words, we want to compute the exterior Dirichlet-Neumann (DN) operator $\Lambda_{l,r}$ such that : $\partial_x u = \Lambda_{l,r} u$

Some basic properties of the Laplace transform

A few classical properties

$$\mathcal{L}(v)(x,\tau) = \hat{v}(\tau) = \int_0^{\infty} v(x,t)e^{-\tau t}dt$$

setting $\tau = \eta + i\zeta$, $\eta > 0$

$$\mathcal{L}(\partial_t v)(x,\tau) = \tau\hat{v}(x,\tau) - v(0)$$
$$\mathcal{L}(f \star g) = \hat{f}\hat{g}$$
$$\mathcal{L}^{-1}(\hat{f}\hat{g}) = \int_0^t f(s)g(t-s)ds$$
$$\mathcal{L}^{-1}(\frac{1}{\sqrt{\tau}}) = \frac{1}{\sqrt{\pi}}t^{-1/2}$$

Building the NRBC

- In the exterior domain, one gets

$$i\tau\hat{v} + \partial_x^2 \hat{v} = 0,$$

with trivial solution

$$\hat{v}(x,\tau) = Ae^{\sqrt{-i\tau}x} + Be^{-\sqrt{-i\tau}x}$$

- But $v \in L^2$, $v(\infty,\tau) = 0$, $A = 0$ and we have e.g. at x_r

$$\hat{v}(x,\tau) = e^{-\sqrt{-i\tau}(x-x_r)}\hat{u}(x_r,\tau)$$

- Derivation and continuity yield

$$\partial_x \hat{u}(x_r,\tau) = -\sqrt{-i\tau}\hat{u}(x_r,\tau) = -e^{-i\pi/4}\tau(\frac{\widehat{u}(x_r,\tau)}{\sqrt{\tau}})$$

Building the NRBC

- Finally, using the inverse Laplace transform leads to the DN-type exact NRBC

$$\partial_{\mathbf{n}} u + e^{-i\pi/4} \partial_t^{1/2} u = 0, \ \ x \in \Gamma, \tag{2}$$

with the 1/2 fractional derivative

$$\partial_t^{1/2} u(x,t) = \frac{1}{\sqrt{\pi}} \frac{d}{dt} \int_0^t \frac{u(x,s)}{\sqrt{t-s}} ds \tag{3}$$

- In a similar way, one gets the Neumann-Dirichlet NRBC

$$u(x,t) + e^{i\pi/4} I_t^{1/2} \partial_{\mathbf{n}} u(x,t) = 0, \ \ x \in \Gamma, \tag{4}$$

with fractional integral

$$I_t^{1/2} v(x,t) = \frac{1}{\sqrt{\pi}} \int_0^t \frac{v(x,s)}{\sqrt{t-s}} ds$$

- Consider for example the ND problem (same for DN)

$$\begin{cases} (i\partial_t + \partial_x^2)u(x,t) = 0, & \text{in } \Omega_i,\ t > 0, \\ u_{l,r} + e^{i\pi/4} I_t^{1/2}(\partial_{\mathbf{n}} u_{l,r}) = 0, & \text{on } \Gamma,\ t > 0, \\ u(x,0) = u_0, \text{in } \Omega_i. \end{cases} \tag{5}$$

Proposition

If $u_0 \in H^1(\Omega_i)$, there exists one and only one solution $u \in C(\mathbb{R}_t, H^1(\Omega_i))$. Moreover, u satisfies

$$\|u(t)\|_{L^2(\Omega_i)} \leq \|u_0\|_{L^2(\Omega_i)},\ \forall t > 0.$$

3.1 Semi-discrete time scheme : what about stability ?

Question : Being given an interior semi-discrete scheme (Crank-Nicolson here), are we able to build a globally stable scheme including the discretization of the NRBC ?

Our strategy

Starting from the Crank-Nicolson scheme

$$i\frac{u^{n+1}-u^n}{\delta t}+\partial_x^2\left(\frac{u^{n+1}+u^n}{2}\right)=0,$$

we mimic the different steps of the continuous case using the $\mathcal{Z}$-transform instead of the Laplace transform

$$\mathcal{Z}(f_n)(z)=\hat{f}(z):=\sum_{n=0}^{\infty} f_n\, z^{-n}, \quad z\in\mathbb{C}, \quad |z|>R_{\hat{f}}, \tag{6}$$

with $R_{\hat{f}}\geq 0$ the radius of convergence

Discretization

for the DN NRBC, one gets

$$\partial_{\mathbf{n}} u^n = -e^{-i\pi/4} \frac{2}{\sqrt{2\delta t}} \sum_{k=0}^{n} \beta_k u^{n-k}$$

and for the ND NRBC

$$u^n = -e^{i\pi/4} \frac{\sqrt{2\delta t}}{2} \sum_{k=0}^{n} \alpha_k \partial_{\mathbf{n}} u^{n-k},$$

at Γ, with

$$(\alpha_0, \alpha_1, \ldots) = (1, 1, \frac{1}{2}, \frac{1}{2}, \frac{1 \times 3}{2 \times 4}, \frac{1 \times 3}{2 \times 4}, \ldots)$$

and

$$\beta_k = (-1)^k \alpha_k.$$

Conclusion

Proposition

If $t_n = n\delta t$ *and* $\{f^n\}_{n\in\mathbb{N}} \simeq \{f(t_n)\}_{n\in\mathbb{N}}$*, then*

$$I_t^{1/2} f(t_n) \approx \frac{\sqrt{2\delta t}}{2} \sum_{k=0}^{n} \alpha_k f^{n-k}$$

$$\partial_t^{1/2} f(t_n) \approx \frac{2}{\sqrt{2\delta t}} \sum_{k=0}^{n} \beta_k f^{n-k}.$$

- In fact it correspond to the non-trivial discretizations with the trapezoidal rule of the fractional operators (Lubich)
- Using the $\mathcal{Z}$-transform, we prove that the semi-discrete scheme are unconditionnally $L^2(\Omega_i)$-stable and we have the energy inequality

$$\left\| u^N \right\|_{L^2(\Omega_i)} < \| u_0 \|_{L^2(\Omega_i)}, \forall N \geq 0.$$

3.2 Fully discrete scheme

We do not give the details but

- It is implemented in a Finite Element solver with weak formulation
- The DN discrete NRBC is naturally implemented into the code
- The ND is rewritten as a mixed (Fourier-Robin) boundary condition

Numerical simulation : the Gaussian solution

- Explicit 1D solution

$$u(x,t) = \sqrt{\frac{i}{-4t+i}} \exp\left(\frac{-ix^2 - k_0 x + k_0^2 t}{-4t+i}\right)$$

- Quadratic FEM on $\Omega_i =]-5,5[$, $k_0 = 8$, 1024 elements, $\delta t = 10^{-3}$.

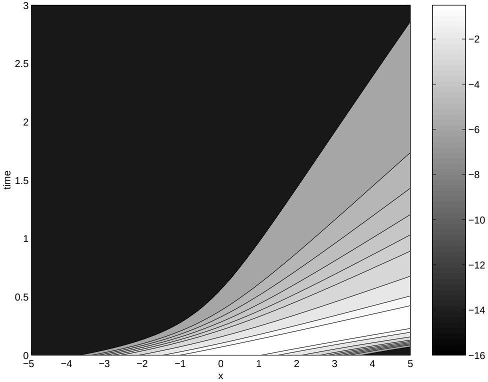


FIG.: Contour plot of $\log_{10}(|u|)$ for the exact solution

Gaussian solution using Baskakov-Popov

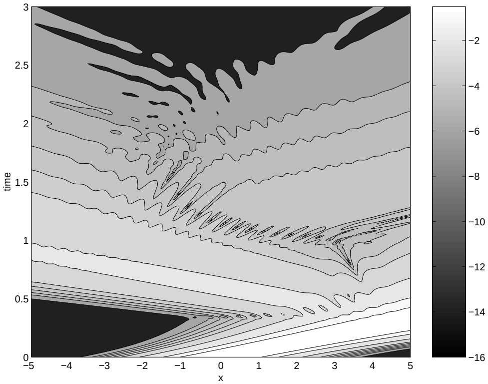


FIG.: Contour plot of $\log_{10}(|u|)$ for the Baskakov-Popov scheme

Gaussian solution using our ND scheme

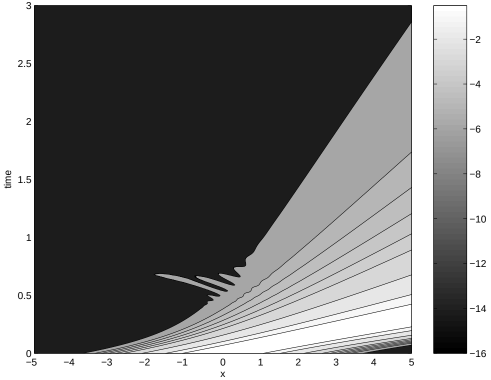


FIG.: Contour plot of $\log_{10}(|u|)$ for the ND scheme

Gaussian solution using our DN scheme

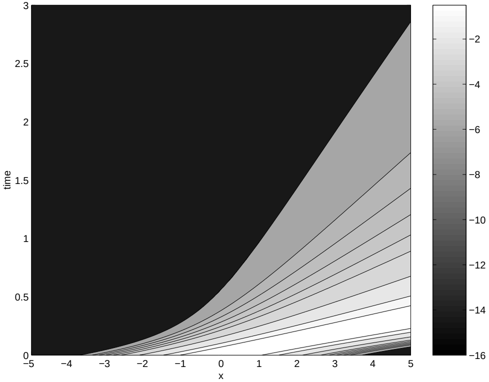


FIG.: Contour plot of $\log_{10}(|u|)$ for the DN scheme

Conclusions for the 1D case

- 1D is solved by a strategy leading to stable schemes for the CN discretization
- You will see other solutions in the next talks
- 2D and nonlinear 1D (see the talks of Besse and Descombes, and others)
- The problem with a global potential or/and with variable coefficients is hard and still open...