Absorbing boundary conditions for Schrödinger equations

by

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Workshop Stochastic Schrödinger Equation
Paris

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Outline

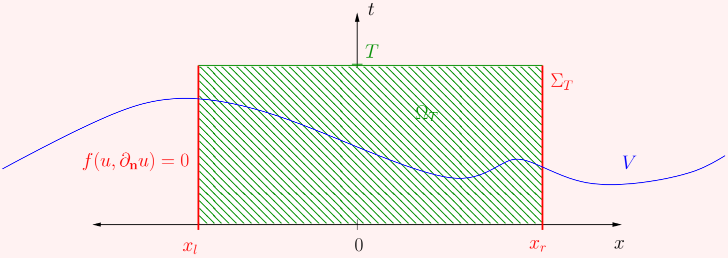
Outline

The Schrödinger Eq. in $\mathbb{R}^d$

$$(S) \quad \begin{cases} i\partial_t u + \Delta u + \mathscr{V}(x,t,u)\,u = 0, & (x,t) \in \mathbb{R}^d \times \mathbb{R}^+ \\ u(x,0) = u_0(x), & x \in \mathbb{R}^d \end{cases}$$

- $u(x,t)$: complex wave function
- $\mathscr{V}$ potential and/or nonlinearity : $\mathscr{V} = V(x,t) + f(|u|)u$
- u_0 compact support in Ω

Problem : Mesh an unbounded domain (here in 1D) $\mathbb{R}^d \times [0;T]$



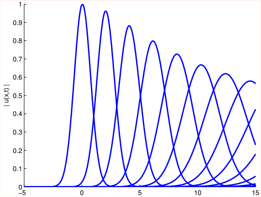
- Truncation $\mathbb{R} \times [0;T] \longrightarrow \Omega_T :=]x_l, x_r[\times [0;T]$
- Introduction of a fictitious boundary $\Sigma := \partial\Omega = \{x_l, x_r\}$
- The boundary condition on x_l must represent the effect of the potential on $]-\infty, x_l]$.

WHAT HAPPENS WHEN ONE DOES NOT TAKE CARE OF BCs ?

Potential $V(x) = x$

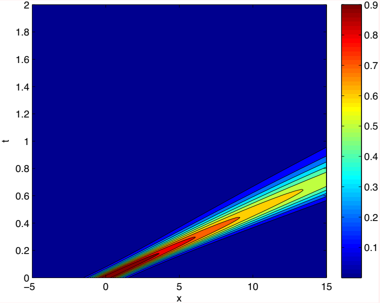
Initial datum : gaussian $u_0(x) = e^{-x^2+10ix}$

Homogeneous Dirichlet BCs : $u|_\Sigma \; = \; 0.$



Evolution of $|u|$

Exact solution



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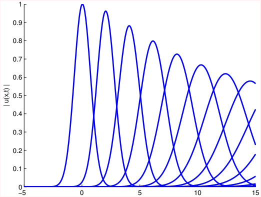
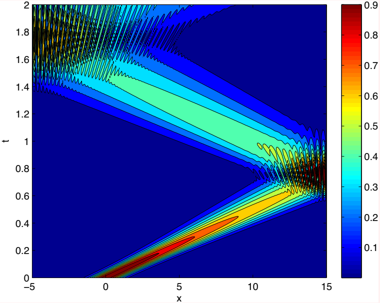


Evolution of $|u|$

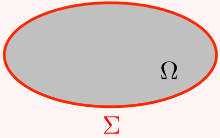


$\Rightarrow$ Parasistic reflexions

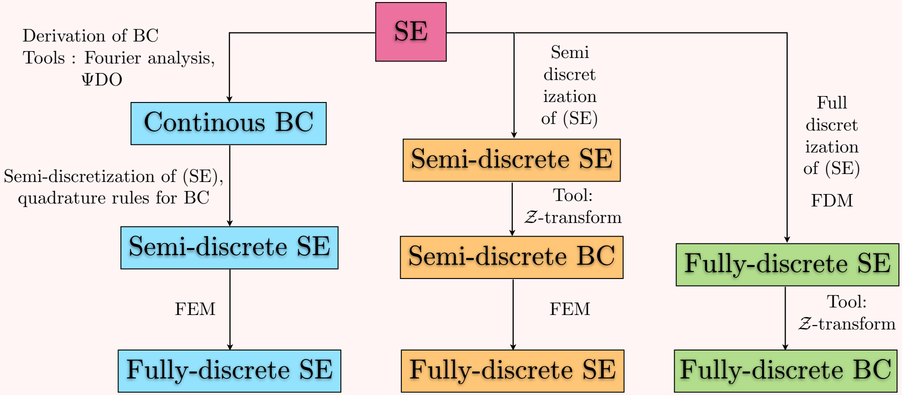
Schrödinger equation (SE)

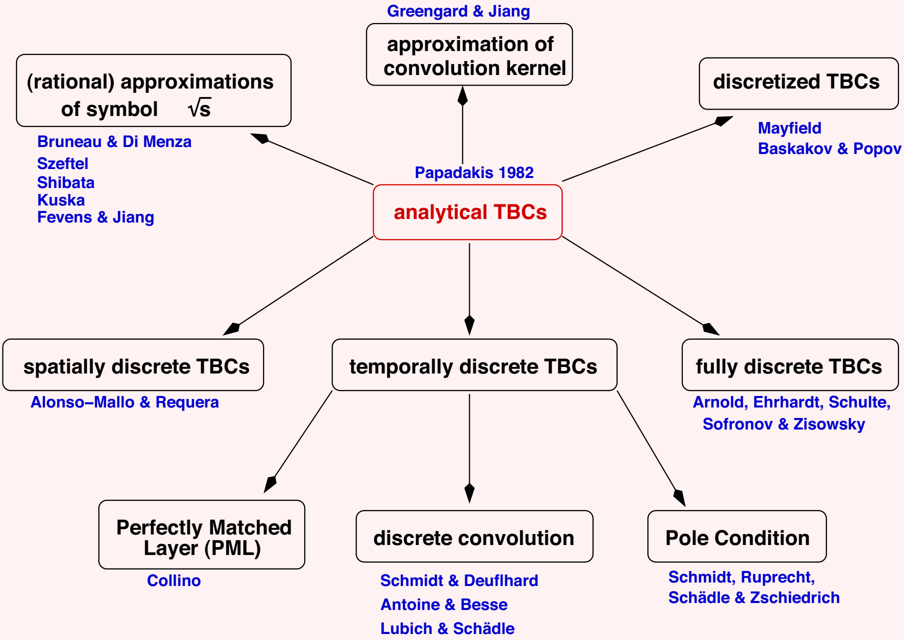
$$\begin{cases} i\partial_t u + \Delta u + V(x,t)u + f(|u|)u = 0, & x \in \mathbb{R}^d, t > 0, \\ u(x,0) = u_0(x), & x \in \mathbb{R}^d. \end{cases}$$

$\mathbb{R}^d \longrightarrow \Omega + \Sigma$



Approximation: 3 ways




Greengard & Jiang
approximation of convolution kernel
(rational) approximations of symbol $\sqrt{s}$
discretized TBCs
Bruneau & Di Menza
Szeftel
Shibata
Kuska
Fevens & Jiang
Papadakis 1982
Mayfield
Baskakov & Popov
analytical TBCs
spatially discrete TBCs
temporally discrete TBCs
fully discrete TBCs
Alonso–Mallo & Requera
Arnold, Ehrhardt, Schulte, Sofronov & Zisowsky
Perfectly Matched Layer (PML)
discrete convolution
Pole Condition
Collino
Schmidt & Deuflhard
Antoine & Besse
Lubich & Schädle
Schmidt, Ruprecht, Schädle & Zschiedrich

GOAL : to derive artificial boundary conditions in order to approximate the exact solution u of (S), restricted to Ω_T.

- absorbing boundary conditions (ABC) : well posed problem + "energy functional " absorbed at the boundary
- transparent boundary conditions (TBC) : approximate solution coincides with u on Ω_T.

- ABC : local in space and/or in time
- TBC : non local in space and time

Which formulation for the BC ?

- The boundary condition is formulated with the Dirichlet-to-Neumann map :

$$\partial_{\mathbf{n}} u + i\Lambda^{+} u = 0, \quad \text{on } \Sigma_T$$

- Interesting in a variational formulation for a finite element method.

$$\int_{\Omega} \Delta u \psi \, d\omega \longrightarrow -\int_{\Omega} \nabla u \cdot \nabla \psi \, d\omega + \int_{\Sigma} \partial_{\mathbf{n}} u \psi \, d\sigma.$$

- Λ^{+} brings into play fractional operators

Fractional operators

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

$$I_t^{\alpha/2} f(t) = \frac{1}{\Gamma(\alpha/2)} \int_0^t (t-s)^{\alpha/2} f(s) \, ds,$$

Outline

TBCs are non local w.r to t and connect $\partial_x u(x_{l,r},t)$ with $u(x_{l,r},t)$.

Dirichlet-to-Neumann (DtN) map

$$\partial_{\mathbf{n}} u(x,t) = -\frac{e^{-i\frac{\pi}{4}}}{\sqrt{\pi}}\, e^{-iV_{l,r}t}\, \frac{\partial}{\partial t} \int_0^t \frac{u(x,\tau)e^{iV_{l,r}\tau}}{\sqrt{t-\tau}}\, d\tau \quad \text{in } x = x_l, x_r,$$

where $\mathbf{n}$ denotes the outwardly unitary normal vector in x_l, x_r.

Notations and hypothesis :

- $\Omega =]x_l, x_r[$, $\Omega_l =]-\infty, x_l]$, $\Omega_r = [x_r, \infty[$, $\Gamma = \{x_l, x_r\}$
- Continuity of u and $\partial_x u$ through Γ

Interior problem

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

Exterior problem

$$\begin{cases} (i\partial_t + \partial_x^2)w = 0, \ x \in \overline{\Omega}, t > 0, \\ w(x,t) = v(x,t), \ x = x_{l,r}, \ t > 0, \\ \lim\limits_{|x|\to\infty} w(x,t) = 0, \ t > 0, \\ w(x,0) = 0, \ x \in \overline{\Omega}. \end{cases}$$

Laplace in Ω_r $\quad i\partial_t w + \partial_x^2 w = 0 \quad \longrightarrow \quad i\omega\hat{w} + \partial_x^2 \hat{w} = 0$

Solution : $\quad \hat{w}(x,\omega) = A^+(\omega) e^{\sqrt[+]{-i\omega}\, x} + A^-(\omega) e^{-\sqrt[+]{-i\omega}\, x}$
with the determination of the square root s.t. $Re(\sqrt[+]{\cdot}) > 0$.
$w \in L^2(\Omega_r) \Rightarrow A^+ = 0$

$$\hat{w}(x,\omega) = e^{-\sqrt[+]{-i\omega}\,(x - x_r)} \mathcal{L}(w(x_r,\cdot))(\omega),$$

then, taking derivative and thanks to continuity

$$\begin{aligned} \partial_x \hat{w}(x,\omega)|_{x=x_r} &= -\sqrt[+]{-i\omega}\, \hat{w}(x,\omega)|_{x=x_r} \\ &= -e^{-i\pi/4} \omega \frac{\hat{w}(x,\omega)|_{x=x_r}}{\sqrt{\omega}} \end{aligned}$$

Inversee Laplace transform

$$\partial_x w(x,t)|_{x=x_r} = -e^{-i\pi/4}\partial_t \left(\frac{1}{\sqrt{\pi}} \int_0^t \frac{w(x,s)|_{x=x_r}}{\sqrt{t-s}} ds \right) = -e^{-i\pi/4}\partial_t^{1/2} w(x_r,t)$$

Similar condition in x_l

$$-\partial_x w(x,t)|_{x=x_l} = -e^{-i\pi/4}\partial_t \left(\frac{1}{\sqrt{\pi}} \int_0^t \frac{w(x,s)|_{x=x_l}}{\sqrt{t-s}} ds \right) = -e^{-i\pi/4}\partial_t^{1/2} w(x_l,t)$$

Boundary condition :

$$(\partial_{\mathbf{n}} + e^{-i\pi/4}\partial_t^{1/2})v = 0 \text{ on } \Gamma \times [0,T[.$$

Remark

$$i\partial_t + \partial_x^2 = (\partial_x + \sqrt{-i\partial_t})(\partial_x - \sqrt{-i\partial_t}).$$

Linear equations with time dependent potentials

- $\mathscr{V} = 0$: Dirichlet-to-Neumann map

$$\partial_{\mathbf{n}} u + e^{-i\pi/4} \partial_t^{1/2} u = 0, \quad \text{on } \Sigma_T$$

  Tool : Fourier analysis
  Factorization : $i\partial_t + \partial_x^2 = \left(\partial_x + i\sqrt{i\partial_t}\right)\left(\partial_x - i\sqrt{i\partial_t}\right)$

- Variant : $\mathscr{V} = V_{l,r}$ constant outside of Ω

- $\mathscr{V} = V(t)$: Gauge change

$$v(x,t) = u(x,t) e^{i\mathcal{V}(t)} \quad \text{with} \quad \mathcal{V}(t) = \int_0^t V(s)\, ds$$

  v is solution to the free Schrödinger equation. We have access to the exact BC (see above). Therefore, the TBC is for u :

$$\partial_{\mathbf{n}} u + e^{-i\pi/4}\, e^{i\mathcal{V}(t)} \partial_t^{1/2} \left(e^{-i\mathcal{V}(t)} u\right) = 0 \quad \text{on } \Sigma_T$$

Summary : derivation of the analytic TBCs

1. To separate the original problem as a system of two coupled equations : interior and exterior problems
2. To apply the Laplace transform in time t
3. To solve the ODE in x
4. To authorize only the outgoing waves by selecting the decaying solution when $x \to \pm\infty$
5. To identify the values of Dirichlet and Neumann in $x_{l,r}$
6. Inverse Laplace transform

NONLINEARITIES AND GENERAL REPULSIVE POTENTIALS $x\partial_x V > 0$ FOR $x \in \overline{\Omega}$

J. Szeftel (04), X. Antoine - C.B. - S. Descombes (06), X. Antoine - C. B. - P. Klein (09)

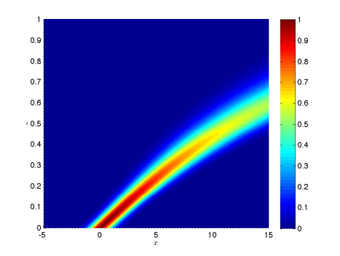
$\mathscr{V} = f(x,u)$

- $\mathscr{V} = f(x,u)$ and $\mathcal{V}(x,t) = \int_0^t f(x,u(x,s))ds$
- Absorbing boundary conditions (ABC), tool : ΨDO

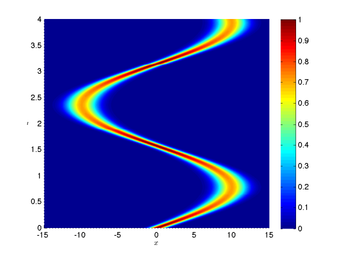
$$ABC_1^4: \quad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2}\left(e^{-i\mathcal{V}}u\right) - i\frac{\partial_{\mathbf{n}}\mathscr{V}}{4} e^{i\mathcal{V}} I_t\left(e^{-i\mathcal{V}}u\right) = 0$$

$$ABC_2^4: \quad \partial_{\mathbf{n}} u - i\sqrt{i\partial_t + \mathscr{V}}\,u + \frac{1}{4}\partial_{\mathbf{n}}\mathscr{V}(i\partial_t + \mathscr{V})^{-1}u = 0$$

Examples : $\mathscr{V} = q|u|^2$, $\mathscr{V} = \alpha x^2 + \beta|u|^2$, $\alpha \geq 0$, $\ldots$.



$|u|$ in the (x,t)-plane $V(x) = x^2$



$|u|$ in the (x,t)-plane $V(x) = -x^2$

Semi-discrete discretization in time of

SCHRÖDINGER EQUATION IN 1D

$$i\partial_t u = -\partial_x^2 u\,, \quad (x,t) \in \mathbb{R}_x \times \mathbb{R}_t^{*+}$$

A-stable method : time step Δt, u^n approx. of $u(x, n\Delta t)$.

$$\frac{i}{\Delta t}\sum_{j=0}^{K} \alpha_j u^{n-j} = \sum_{j=0}^{K} \beta_j \left(-\partial_x^2\right) u^{n-j}, \quad n \geq K.$$

Example : Crank-Nicolson $K = 1$, $\alpha_0 = 1$, $\alpha_1 = -1$, $\beta_{0,1} = 1/2$.

$$i\frac{u^{n+1} - u^n}{\Delta t} = -\partial_x^2 \frac{u^{n+1} + u^n}{2}, \quad x \in \mathbb{R}, \forall n \in \mathbb{N},$$

One proceed like for analytic TBCs : splitting in interior and exterior problems.

Instead of Laplace :

$\mathcal{Z}$-transform

$$\mathcal{Z}(u^n) = \hat{u}(z) := \sum_{n=0}^{\infty} u^n \, z^{-n}, \quad z \in \mathbb{C}, \quad |z| > R(\mathcal{Z}(u^n)),$$

where $R(\mathcal{Z}(u^n))$ is the radius of convergence of the Laurent series. $\mathcal{Z}(u^n)$.

Interesting property :

$$\mathcal{L}(u')(\tau) = s\hat{u}(\tau) - u(0^+)$$

$$\mathcal{Z}(u_{n+1}) = z\hat{u}(z) - zu_0$$

$$\mathcal{Z}(u_{n+1} \pm u_n) = (z \pm 1)\hat{u}(z) - zu_0$$

Application of the $\mathcal{Z}$-transform to the numerical scheme with the hypothesis $\mathrm{supp}(u^j) \subset [x_l, x_r],\ 0 \leq j \leq K-1$:

$$\left(\partial_x^2 + i\frac{\delta(z)}{\Delta t}\right)\hat{w}(z) = 0, \quad x > x_r,$$

where

$$\delta(z) = \frac{\displaystyle\sum_{j=0}^{K} \alpha_j z^{K-j}}{\displaystyle\sum_{j=0}^{K} \beta_j z^{K-j}}$$

is the generating function of the time integration scheme.

Examples :

- Crank Nicolson : $\delta(z) = 2\dfrac{z-1}{z+1}$
- Implicit Euler : $\delta(z) = \dfrac{z-1}{z}$

Solution of the ODE $\left(\partial_x^2 + i\dfrac{\delta(z)}{\Delta t}\right)\hat{w}(z) = 0$ in x

$$\hat{w}(x,z) = A^+ e^{i \sqrt[+]{i\frac{\delta(z)}{\Delta t}}\, x} + A^- e^{-i \sqrt[+]{i\frac{\delta(z)}{\Delta t}}\, x}, \quad x > x_r.$$

One has $w^n \in L^2(]x_r,\infty[)$. But, A-stable method $\Rightarrow \delta$ sends $\{|z|>1\}$ into $\{\mathrm{Re}(z)>0\}$

$$\mathrm{Re}\left(-i \sqrt[+]{i\frac{\delta(z)}{\Delta t}}\right) > 0 \quad \forall |z|>1 \quad A^- = 0$$

Derivation of $\hat{w}(x,z)$ w.r.t x

$$\mathcal{Z}(\partial_x w^n)(z) = -e^{-i\pi/4} \sqrt[+]{\frac{\delta(z)}{\Delta t}}\, \mathcal{Z}(w^n)(z),$$

in $x = x_r$, then inverse $\mathcal{Z}$ transform.

Example for Crank-Nicolson (Schmidt-Deuflhard 95, Antoine-Besse 03, ...)

Crank-Nicolson

$$
\begin{aligned}
& i\frac{v^{n+1}-v^n}{\Delta t} = -\partial_x^2 \frac{v^{n+1}+v^n}{2}, \quad x \in \Omega, \forall n \in \mathbb{N}_0, \\
& v^0(x) = u^0(x), \quad x \in \Omega, \\
& \partial_{\mathbf{n}} v^{n+1} = \sum_{k=0}^{n+1} \omega_k^{(l,r)} v^{n+1-k}, \quad \text{in } x = x_l, x_r, \\
& \omega_k = -e^{-\frac{i\pi}{4}} \frac{2}{\sqrt{2\Delta t}} (-1)^k \tilde{\omega}_k, \quad k \in \mathbb{N}, \\
& (\tilde{\omega}_0, \tilde{\omega}_1, \tilde{\omega}_2, \tilde{\omega}_3, \tilde{\omega}_4, \tilde{\omega}_5, \dots) = (1, 1, \frac{1}{2}, \frac{1}{2}, \frac{1\cdot 3}{2\cdot 4}, \frac{1\cdot 3}{2\cdot 4}, \dots).
\end{aligned}
$$

Consistant quadrature rule with semi-discrete numerical scheme for $\partial_t^{1/2}$

stability

Othe possibilities :

- Quadrature rule : Mayfield (89), Baskakov & Popov (91)

$$\begin{aligned}\frac{d}{dt}\int_0^t \frac{u(x_r,\tau)}{\sqrt{t-\tau}}\,d\tau\Big|_{t=t_{n+1}} &= \int_0^{t_{n+1}} \frac{u_\tau(x_r,\tau)}{\sqrt{t_{n+1}-\tau}}\,d\tau \\ &\approx \frac{1}{\Delta t}\sum_{k=0}^{n}(u_J^{k+1}-u_J^k)\int_{t_k}^{t_{k+1}}\frac{d\tau}{\sqrt{t_{n+1}-\tau}}.\end{aligned}$$

Still non local in time

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$$\approx \frac{1}{\Delta t}\sum_{k=0}^{n}(u_J^{k+1}-u_J^k)\int_{t_k}^{t_{k+1}} \frac{d\tau}{\sqrt{t_{n+1}-\tau}}.$$

  Still non local in time

- Rational approximation of the symbol Bruneau & DiMenza (95), Szeftel (04) To solve

$$\partial_x \hat{u}(x_r,\tau) = -e^{-i\pi/4}\sqrt[+]{i\tau}\,\hat{u}(x_r,\tau).$$

  Approximation of $\sqrt[+]{i\tau}$ by

$$R_m(i\tau) = a_0^m + \sum_{k=1}^{m}\frac{a_k^m i\tau}{i\tau+d_k^m} = \sum_{k=0}^{m} a_k^m - \sum_{k=1}^{m}\frac{a_k^m d_k^m}{i\tau+d_k^m},$$
$$a_k^m > 0, \quad k\in\{0,\cdots,m\}, \quad d_k^m > 0, \quad k\in\{1,\cdots,m\}.$$

The equation becomes

$$\partial_x \hat{u}(x_r,\tau) = -e^{i\pi/4}\left[\left(\sum_{k=0}^{m} a_k^m\right)\hat{u}(x_r,\tau) - \sum_{k=1}^{m}\frac{a_k^m d_k^m}{i\tau + d_k^m}\hat{u}(x_r,\tau)\right].$$

Lindmann trick (85) ; auxiliary functions $\varphi_k = \varphi_k(t)_{k=1,\cdots,m}$ which satisfy

$$\frac{1}{i\tau + d_k^m}\hat{u}(x_r) = \hat{\varphi}_k, \quad k = 1,\cdots,m\,.$$

Inverse Laplace transform : ODE for φ_k

$$i\frac{d\varphi_k}{dt} + d_k^m\varphi_k = u(x_r,t), \quad \varphi_k(0) = 0, \quad k = 1,\cdots,m.$$

so, the BC is

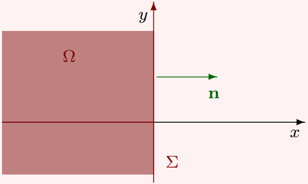
$$\begin{cases} \partial_{\mathbf{n}} u = -e^{-\frac{i\pi}{4}}\left[\left(\sum_{k=0}^{m} a_k^m\right)u - \sum_{k=1}^{m} a_k^m d_k^m \varphi_k\right], & \text{in } x = x_r,\ t>0, \\ i\dfrac{d\varphi_k}{dt} + d_k^m\varphi_k = u(x_r,t), & t>0, k=1,\cdots,m, \\ \varphi_k(0) = 0, & t>0, k=1,\cdots,m. \end{cases}$$

- STRAIGHT BOUNDARY : EXTENSION OF THE 1D STUDY

Domain $\Omega = \{x < 0\}$

$i\partial_t + \partial_y^2$ plays the part of $i\partial_t$ in 1D
∂_x^2 plays the part of ∂_x^2

TBC : $\partial_{\mathbf{n}} u - i\sqrt{i\partial_t + \partial_y^2}\, u = 0.$



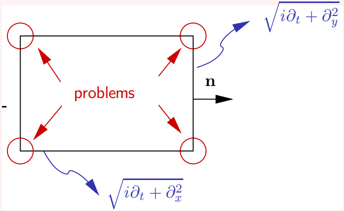
- FACTORIZATION :

$$i\partial_t + \Delta = i\partial_t + \partial_y^2 + \partial_x^2 = \left(\partial_x + i\sqrt{i\partial_t + \partial_y^2}\right)\left(\partial_x - i\sqrt{i\partial_t + \partial_y^2}\right) + R$$

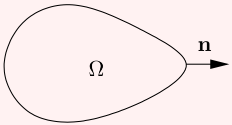
- PROBLEMS :

Junction problems located on the corners

Nonlocal operator both in time and space



- TAKE INTO ACCOUNT THE GEOMETRY : convex set with general boundary, smooth, with curvature κ.



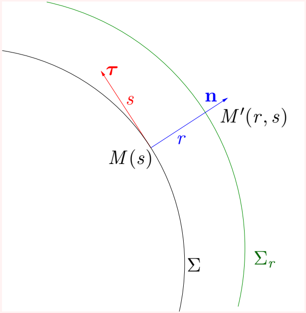
- GENERALIZED COORDINATES SYSTEM of the boundary with respect to normal variable r and curvilinear abscissa s

$$\Delta = \partial_r^2 + \kappa_r \partial_r + h^{-1}\partial_s \left(h^{-1}\partial_s\right)$$

$\kappa_r = h^{-1}\kappa$: curvature of a parallel surface Σ_r to Σ
$h(r,s) = 1 + r\kappa$

$$\Rightarrow \quad L = \partial_r^2 + \kappa_r \partial_r + i\partial_t + h^{-1}\partial_s \left(h^{-1}\partial_s\right) + V$$

Schrödinger equation with variable coefficients : pseudo-differential calculus



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$$\begin{array}{cccll} t & \leftrightsquigarrow & t & \text{dual variable} & \tau \\ x & \leftrightsquigarrow & r & & \\ y & \leftrightsquigarrow & s & \text{dual variable} & \xi \end{array}$$

Strategy 1 : Gauge change

- Change of unknown (which solves the case $\mathscr{V} = V(t)$)

$$v = e^{-i\mathcal{V}} u \quad \text{with} \quad \mathcal{V}(r,s,t) = \int_0^t V(r,s,\sigma)\,d\sigma$$

- We work on the equation with unknown v :

$$i\partial_t v + \partial_r^2 v + (\kappa_r + F)\partial_r v + h^{-1}\partial_s(h^{-1}\partial_s v) + G\,v = 0$$

Strategy 2 : Direct method

- Equation sets in generalized coordinates

$$i\partial_t u + \partial_r^2 u + \kappa_r \partial_r u + h^{-1}\partial_s(h^{-1}\partial_s u) + V\,u = 0$$

Generalized Schrödinger equation

$$i\partial_t w + \partial_r^2 w + (\kappa_r + A)\partial_r w + h^{-1}\partial_s(h^{-1}\partial_s w) + Bw = 0$$

S1 $A = F(r,s,t)$ and $B = G(r,s,t)$ if $w = v = e^{-i\mathcal{V}} u$

S2 $A = 0$ and $B = V(r,s,t)$ if $w = u$

Variable coefficients Schrödinger equation

$$Lw := i\partial_t w + \partial_r^2 w + (\kappa_r + A)\partial_r w + h^{-1}\partial_s(h^{-1}\partial_s w) + Bw = 0.$$

- Factorization of L in a neighbourhood of Σ
- Use of ΨDO calculus instead of Fourier
- Symbolic calculus : asymptotic expansion of symbols
- Select outgoing waves : identification of principal symbol
- Come back to the surface Σ
- DtN operator non local both in space and time : localization techniques
  - Taylor approach
  - Padé approach

- $P(r,s,t,\partial_s,\partial_t)$ defined by its total symbol $p(r,s,t,\xi,\tau)$ in Fourier space by $\mathscr{F}_{(s,t)}$ (ξ and τ dual variables of s and t)

$$P(r,s,t,\partial_s,\partial_t)u(r,s,t)=\int_{\mathbb{R}\times\mathbb{R}} p(r,s,t,\xi,\tau)\hat{u}(r,\xi,\tau)e^{is\xi}e^{it\tau}d\xi d\tau$$

  Notations : $P=Op(p)$, $p=\sigma(P)$

- $E=(1,2)$. f is said *E-quasi homogeneous* of order m if

$$f(r,s,t,\mu\xi,\mu^2\tau)=\mu^m f(r,s,t,\xi,\tau)$$

  Example : $\sqrt{-\tau-\xi^2}$ is E-quasi homogeneous of order 1.
- $p\in S_E^m$ (or $P\in OPS_E^m$) if it admits an asymptotic expansion in E-quasi homogeneous symbols

$$p(r,s,t,\xi,\tau)\sim\sum_{j=0}^{+\infty}p_{m-j}(r,s,t,\xi,\tau),$$

  which means

$$\left(p(r,s,t,\xi,\tau)-\sum_{j=0}^{\tilde{m}}p_{m-j}(r,s,t,\xi,\tau)\right)\in S_E^{m-(\tilde{m}+1)},\quad\forall\tilde{m}\in\mathbb{N}.$$

- $p=q \mod S_E^m$ means $p-q\in S_E^m$.
- Composition rule : $\sigma(AB)\sim\sum_{|\alpha|=0}^{+\infty}\frac{(-i)^{|\alpha|}}{\alpha!}\partial^\alpha_{(\xi,\tau)}\sigma(A)\,\partial^\alpha_{(s,t)}\sigma(B)$

$$i\partial_t w + \partial_r^2 w + (\kappa_r + A)\partial_r w + h^{-1}\partial_s(h^{-1}\partial_s w) + Bw = 0.$$

Engquist & Majda method.

There exist two ΨDO Λ^- and Λ^+ of OPS^1_E s.t. we get the following Nirenberg-like factorization

$$i\partial_t + \partial_r^2 + (\kappa_r + A)\partial_r + h^{-1}\partial_s(h^{-1}\partial_s) + B = (\partial_r + i\Lambda^-)(\partial_r + i\Lambda^+) + R$$

where R is a smoothing operator of OPS$^{-\infty}_E$.

Λ^+ (resp. Λ^-) has an asymptotic expansion in E-quasi homogeneous symbols :

$$\sigma(\Lambda^+) = \lambda^+ \sim \sum_{j=0}^{+\infty} \lambda^+_{1-j} = \lambda^+_1 + \lambda^+_0 + \lambda^+_{-1} + \lambda^+_{-2} + \dots$$

with $\lambda^+_{1-j} \in S^{1-j}_E$.

Come back to the surface Σ : $\widetilde{\Lambda^+} = \Lambda^+_{|r=0}$ and $\widetilde{\lambda_j} = \left(\lambda^+_j\right)_{|r=0}$.

TBC : $\partial_{\mathbf{n}} w + i\,\widetilde{\Lambda^+} w = 0$

$$\partial_{\mathbf{n}} w + i\sum_{j=0}^{+\infty} Op\left(\widetilde{\lambda_{1-j}}\right) w = 0\ , \quad \text{on } \Sigma_T.$$

Approximated condition of order M : we only keep the first M terms

$$\partial_{\mathbf{n}} w_M + i \sum_{j=0}^{M} Op\left(\widetilde{\lambda}_{1-j}\right) w_M = 0 \ , \quad \text{on } \Sigma_T$$

- λ_{1-j}^{+}, $j \geq 0$, depends on λ_1^{+}.
- Identification of the principal symbol λ_1^{+} :

$$\text{Outgoing wave} \quad \mathrm{Im}(\lambda_1^{+}(s,t,\xi,\tau)) \leq 0, \quad \text{for } |\tau| \gg 1$$

$$\text{Strategy 1} \quad \lambda_1^{+} = -\sqrt{-\tau - h^{-2}\xi^2}$$

$$\text{Strategy 2} \quad \lambda_1^{+} = -\sqrt{-\tau - h^{-2}\xi^2 + V}$$

Asymptotic expansion : $\widetilde{\lambda}_j$ are functions of parameter $\sqrt{-\tau - \xi^2}$ (resp. $\sqrt{-\tau - \xi^2 + V}$).

$\Longrightarrow$ non local operators both in time AND in space

Two approaches, valid for both strategies :

- "TAYLOR" APPROACH : Taylor expansion of the symbols for $|\tau| \gg \xi^2$

$$-\tau - \xi^2 + V = -\tau \left(1 + \frac{\xi^2}{\tau} - \frac{V}{\tau}\right)$$

Thereby :

$$\sqrt{-\tau - \xi^2 + V} \approx \sqrt{-\tau}\left(1 + \frac{\xi^2}{2\tau} - \frac{V}{2\tau}\right) = \sqrt{-\tau} - \frac{\xi^2}{2}\frac{1}{\sqrt{-\tau}} + \frac{V}{2}\frac{1}{\sqrt{-\tau}}$$

$\Longrightarrow$ Localizing in space only

- PADÉ APPROXIMATION APPROACH :

$$Op\left(\sqrt{-\tau - \xi^2 + V}\right) \sim \sqrt{i\partial_t + \Delta_\Sigma + V} \quad \text{mod } OPS^{-1}$$

formal approximation of $\sqrt{\cdot}$ by Padé approximants $\Longrightarrow$ Localizing both in space AND time

Two possible approaches for each strategy, so 4 families of ABC.

	"Taylor" approach	"Padé" approach
Gauge change	$ABC^M_{1,T}$	$ABC^M_{1,P}$
Direct method	$ABC^M_{2,T}$	$ABC^M_{2,P}$

$\downarrow$ $\qquad$ $\downarrow$

$\partial_t^{1/2}$, $I_t^{1/2}$, I_t $\qquad$ $Op\left(\sqrt{-\tau-\xi^2}\right)$

or

$v = e^{-i\mathcal{V}}u$ $\qquad$ $Op\left(\sqrt{-\tau-\xi^2+V}\right)$

- Gauge change

$$\mathrm{ABC}^2_{1,T} \qquad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2}\left(e^{-i\mathcal{V}} u\right) + \frac{\kappa}{2} u$$

$$\mathrm{ABC}^3_{1,T} \qquad - e^{i\pi/4} e^{i\mathcal{V}} \left(\frac{\kappa^2}{8} + \frac{\Delta_\Sigma}{2} + i\partial_s \mathcal{V} \partial_s + \frac{1}{2}(i\partial_s^2 \mathcal{V} - (\partial_s \mathcal{V})^2)\right) I_t^{1/2}\left(e^{-i\mathcal{V}} u\right)$$

$$\mathrm{ABC}^4_{1,T} \qquad + i e^{i\mathcal{V}} \left(\frac{\partial_s(\kappa\partial_s)}{2} + \frac{\kappa^3 + \partial_s^2\kappa}{8} + \frac{i\partial_s\kappa\partial_s\mathcal{V}}{2}\right) I_t\left(e^{-i\mathcal{V}} u\right)$$

$$- i\frac{\mathrm{sg}(\partial_{\mathbf{n}} V)}{4}\sqrt{|\partial_{\mathbf{n}} V|}\, e^{i\mathcal{V}} I_t\left(\sqrt{|\partial_{\mathbf{n}} V|}\, e^{-i\mathcal{V}} u\right) = 0$$

- Direct method

$$\mathrm{ABC}^2_{2,T} \qquad \partial_{\mathbf{n}} u + e^{-i\pi/4} \partial_t^{1/2} u + \frac{\kappa}{2} u$$

$$\mathrm{ABC}^3_{2,T} \qquad - e^{i\pi/4}\left(\frac{\kappa^2}{8} + \frac{\Delta_\Sigma}{2}\right) I_t^{1/2} u - e^{i\pi/4}\frac{\mathrm{sg}(V)}{2}\sqrt{|V|}\, I_t^{1/2}\left(\sqrt{|V|}\, u\right)$$

$$\mathrm{ABC}^4_{2,T} \qquad + i\left(\frac{\partial_s(\kappa\partial_s)}{2} + \frac{\kappa^3 + \partial_s^2\kappa}{8}\right) I_t u - i\frac{\mathrm{sg}(\partial_{\mathbf{n}} V)}{4}\sqrt{|\partial_{\mathbf{n}} V|}\, I_t\left(\sqrt{|\partial_{\mathbf{n}} V|}\, u\right) = 0$$

- Gauge change

$$\mathsf{ABC}^1_{1,P} \qquad \partial_{\mathbf{n}} u - i e^{i\mathcal{V}} \sqrt{i\partial_t + \Delta_\Sigma} \left(e^{-i\mathcal{V}} u \right)$$

$$\mathsf{ABC}^2_{1,P} \qquad + \frac{\kappa}{2} u + \partial_s \mathcal{V} e^{i\mathcal{V}} \partial_s \left(i\partial_t + \Delta_\Sigma \right)^{-1/2} \left(e^{-i\mathcal{V}} u \right)$$

$$- \frac{\kappa}{2} e^{i\mathcal{V}} \left(i\partial_t + \Delta_\Sigma \right)^{-1} \Delta_\Sigma \left(e^{-i\mathcal{V}} u \right) = 0$$

- Direct method

$$\mathsf{ABC}^1_{2,P} \qquad \partial_{\mathbf{n}} u - i \sqrt{i\partial_t + \Delta_\Sigma + V}\, u$$

$$\mathsf{ABC}^2_{2,P} \qquad + \frac{\kappa}{2} u - \frac{\kappa}{2} \left(i\partial_t + \Delta_\Sigma + V \right)^{-1} \Delta_\Sigma u = 0$$

Interior problem :

Semi-discret Crank-Nicolson scheme, symmetrical, unconditionally stable

$$\frac{2i}{\Delta t}u^{n+1/2} + \Delta u^{n+1/2} + V^{n+1/2}u^{n+1/2} = \frac{2i}{\Delta t}u^{n}$$

ABC discretization

- Taylor approach : approximation of the operators $\partial_t^{1/2}$, $I_t^{1/2}$ and I_t by quadrature formulas
- Padé approach : coupled system between $u^{n+1/2}$ and the m auxiliary functions $\varphi_k^{n+1/2}$
  - Rational approximation of the square root by Padé approximants

$$\sqrt{z} \approx R_m(z) = \sum_{k=0}^{m} a_k^m - \sum_{k=1}^{m} \frac{a_k^m d_k^m}{z + d_k^m}$$

  - In the $ABC_{2,P}^{M}$ conditions :

$$\sqrt{i\partial_t + \Delta_\Sigma + V} \quad \underset{R_m}{\rightsquigarrow} \quad R_m\left(i\partial_t + \Delta_\Sigma + V\right)$$

$$\Rightarrow \sqrt{i\partial_t + \Delta_\Sigma + V}u \approx \left(\sum_{k=0}^{m} a_k^m\right)u - \sum_{k=1}^{m} a_k^m d_k^m \underbrace{\left(i\partial_t + \Delta_\Sigma + V + d_k^m\right)^{-1}u}_{\varphi_k}$$

Auxiliary functions φ_k, solutions of a Schrödinger equation on Σ_T.

$V(r) = 5r^2$

Domain : disk of radius 5

Initial datum : $u_0(x,y) = e^{-(x^2+y^2)-ik_0x}$, with $k_0 = 10$

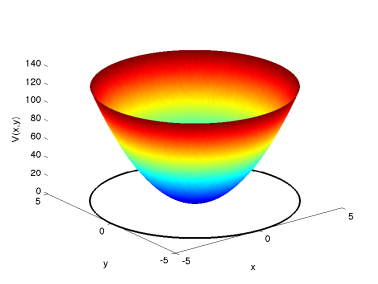
$\Delta t = 10^{-3}, \;\; T = 1$

Mesh : $1\,700\,000$ triangles

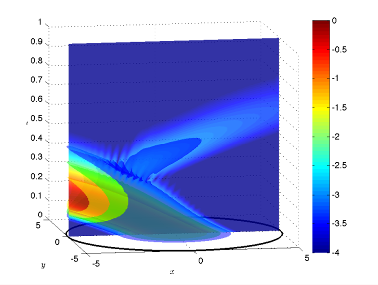
25 Padé functions

Logarithmic levels bounded at 10^{-4}

Movie

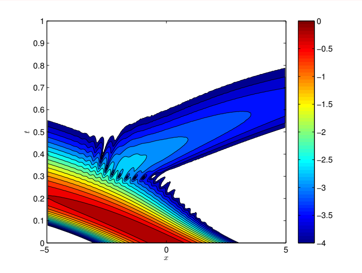
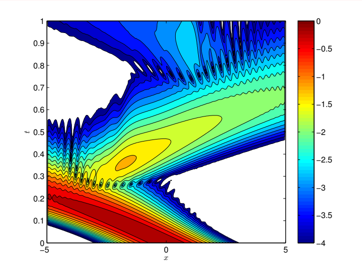
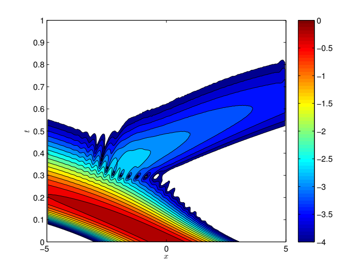
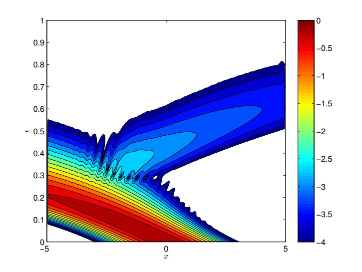


POTENTIAL



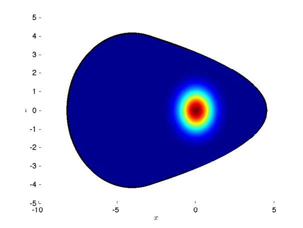
LOG-PROFILE OF AN APPROXIMATED SOLUTION

$V(r) = 5r^2$

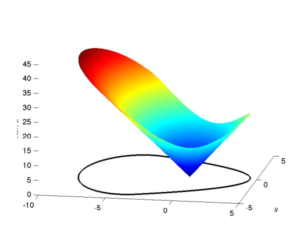
	GAUGE CHANGE	DIRECT METHOD
TAYLOR APPROACH	 $ABC^4_{1,T}$	 $ABC^4_{2,T}$
PADÉ APPROACH	 $ABC^2_{1,P}$	 $ABC^2_{2,P}$

$\Delta t = 2 \times 10^{-3}$

920 000 triangles

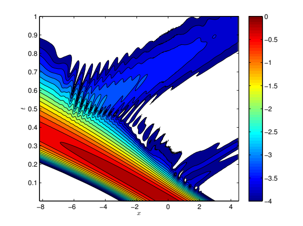


Computational domain

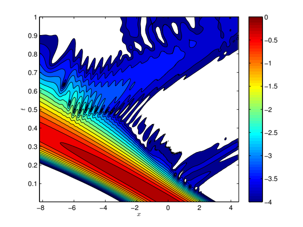


Potential profile

Gauge change

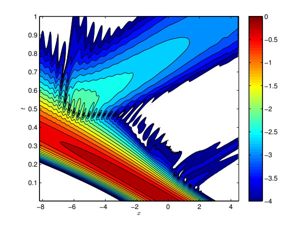


$ABC^4_{1,T}$

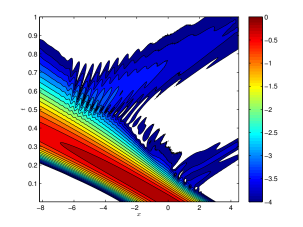


$ABC^2_{1,P}$

Direct method



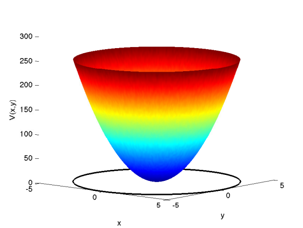
$ABC^4_{2,T}$



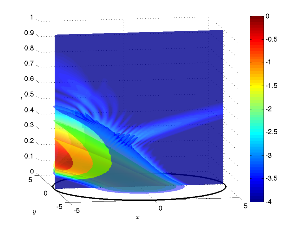
$ABC^2_{2,P}$

$\Delta t = 10^{-3}$

1 700 000 triangles

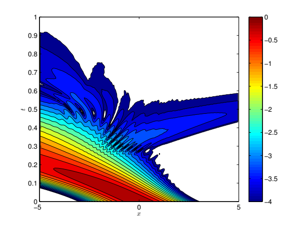


Potential at $t = 0$

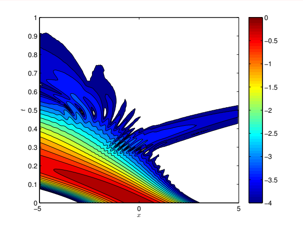


Log-profile of an approximated solution

Gauge change

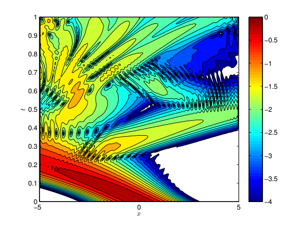


$ABC^4_{1,T}$

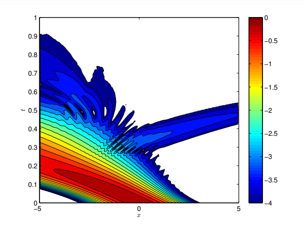


$ABC^2_{1,P}$

Direct method



$ABC^4_{2,T}$



$ABC^2_{2,P}$

Potential $\mathscr{V} = V + f(u)$

- For $k_0 \neq 0$, u is never radially symetrical $\Rightarrow \mathcal{V}$ is never radially symetrical
- Make the implementation of ABC linked to Gauge change more complexe + numerical cost

$\longrightarrow$ limitation to $NLABC_{1,T}^{2}$ ($M = 2$ only)

$\longrightarrow$ Do not use $NLABC_{1,P}^{M}$ (identical precision as $NLABC_{1,T}^{M}$ for a potential)

- We deal with $NLABC_{1,T}^{2}$, $NLABC_{2,T}^{M}$, and $NLABC_{2,P}^{M}$

- Formal substitutions $\mathscr{V} = V + f(u)$ and $\mathcal{V}(x,y,t) = \int_0^t V + \int_0^t f(u)$
- We derive the boundary conditions $\mathrm{NLABC}_{1,T}^{2}$, $\mathrm{NLABC}_{2,T}^{3}$ and $\mathrm{NLABC}_{2,P}^{2}$.

- Taylor approach, Gauge change

$$NLABC^2_{1,T} \qquad \partial_{\mathbf{n}} u + e^{-i\pi/4} e^{i\mathcal{V}} \partial_t^{1/2} \left(e^{-i\mathcal{V}} u \right) + \frac{\kappa}{2} u = 0$$

- Taylor approach, direct method

$$\begin{aligned}
NLABC^2_{2,T} \quad & \partial_{\mathbf{n}} u + e^{-i\pi/4} \partial_t^{1/2} u + \frac{\kappa}{2} u \\
NLABC^3_{2,T} \quad & - e^{i\pi/4} \left(\frac{\kappa^2}{8} + \frac{\Delta_\Sigma}{2} \right) I_t^{1/2} u - e^{i\pi/4} \frac{\mathrm{sg}(f(u))}{2} \sqrt{|f(u)|}\, I_t^{1/2} \left(\sqrt{|f(u)|}\, u \right) \\
NLABC^4_{2,T} \quad & + i \left(\frac{\partial_s(\kappa \partial_s)}{2} + \frac{\kappa^3 + \partial_s^2 \kappa}{8} \right) I_t u \\
& - i \frac{\mathrm{sg}(\partial_{\mathbf{n}} f(u))}{4} \sqrt{|\partial_{\mathbf{n}} f(u)|}\, I_t \left(\sqrt{|\partial_{\mathbf{n}} f(u)|}\, u \right) = 0
\end{aligned}$$

- Padé approach, direct method

$$\begin{aligned}
NLABC^1_{2,P} \quad & \partial_{\mathbf{n}} u - i \sqrt{i\partial_t + \Delta_\Sigma + f(u)}\, u \\
NLABC^2_{2,P} \quad & + \frac{\kappa}{2} u - \frac{\kappa}{2} \left(i\partial_t + \Delta_\Sigma + f(u) \right)^{-1} \Delta_\Sigma u = 0
\end{aligned}$$

- Interior problem Duràn - Sanz-Serna scheme

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

- Boundary condition : discrte convolutions and Padé approximants

Solution to the nonlinear equation

- Fixed point scheme : Mass inequality valid $\|u^n\|_{L^2(\Omega)} \leq \|u^0\|_{L^2(\Omega)}$
  - for $\text{NLABC}^2_{2,T}$ and $\text{NLABC}^2_{1,T}$
  - for $\text{NLABC}^3_{2,T}$ if $V \geq 0$ and $f(u) \geq 0$.
- Numerical alternative scheme : relaxation method [CB 04] .

- Principle : Solution of the equation $i\partial_t u + \Delta u + f(u)u = 0$ solving the system

$$\begin{cases} i\partial_t u + \Delta u + \Upsilon u = 0, & \text{on } \Omega_T, \\ \Upsilon = f(u), & \text{on } \Omega_T. \end{cases}$$

- Semi-discretization

$$\begin{cases} i\dfrac{u^{n+1} - u^n}{\Delta t} + \Delta u^{n+1/2} + \Upsilon^{n+1/2} u^{n+1/2} = 0, \\ \dfrac{\Upsilon^{n+3/2} + \Upsilon^{n+1/2}}{2} = f(u^{n+1}), \end{cases} \quad \text{for } 0 \leq n \leq N$$

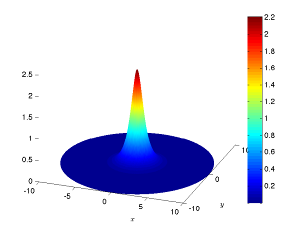
où $\Upsilon^{n+1/2} = \dfrac{\Upsilon^{n+1} + \Upsilon^n}{2}$, $\Upsilon^{-1/2} = f(u^0)$.

- Advantages : Conservation of the invariants (mass, energy), simplicity, speed (no fixed point iteration)

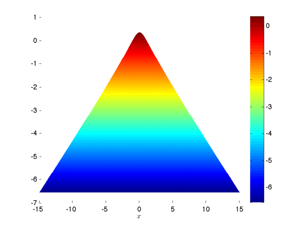
- Cubic equation $i\partial_t + \Delta u + q|u|^2 = 0$
- Numerical fabrication of the soliton : stationary solutions computation leads to

$$\begin{cases} \partial_r^2 \psi + \dfrac{1}{r}\partial_r \psi - \psi + q|\psi|^2\psi = 0, & 0 < r < R, \\ \psi'(0) = 0, \quad \psi(0) = \beta, \end{cases}$$

solved by a shooting method [Di Menza 09]

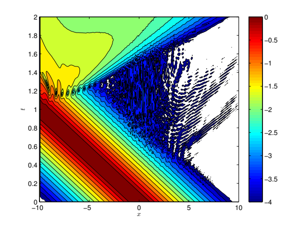


$|u_0|$ for $R = 10$

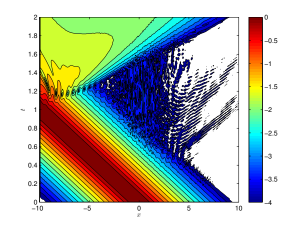


$|u_0|$ in log-scale for $R = 15$

Without potential

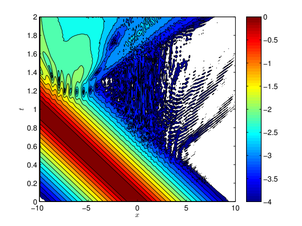


$\mathrm{ABC}^3_{0,T}$



$\mathrm{ABC}^2_{0,P}$

Gauge change



$\mathrm{NLABC}^2_{1,T}$

Initial datum : soliton

Domain : disk of radius 10

$\Delta t = 2 \times 10^{-3}$

1 700 000 triangles

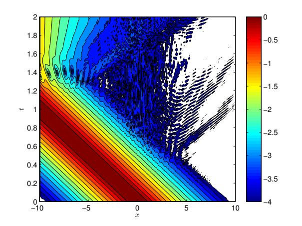
$k_0 = 5$

$T = 2$

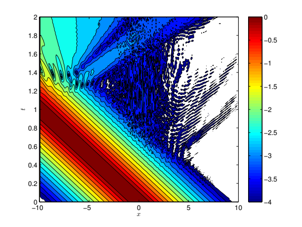
Movie

Movie contour

Direct method

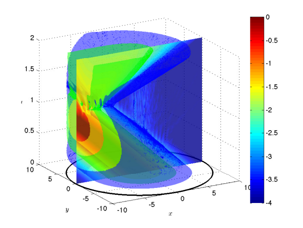


$\mathrm{NLABC}^3_{2,T}$

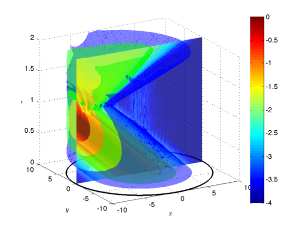


$\mathrm{NLABC}^2_{2,P}$

Without potential

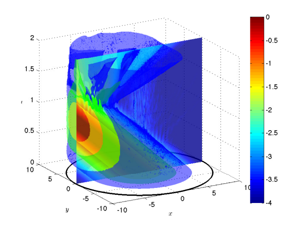


$\mathrm{ABC}^3_{0,T}$



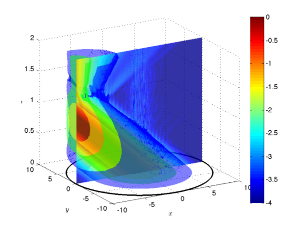
$\mathrm{ABC}^2_{0,P}$

Gauge change

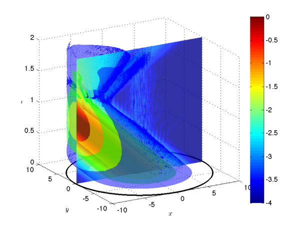


$\mathrm{NLABC}^2_{1,T}$

Direct method



$\mathrm{NLABC}^3_{2,T}$



$\mathrm{NLABC}^2_{2,P}$