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

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Outline

1. Analytic transparent boundary conditions
2. Artificial boundary conditions
   - Straight artificial boundary
   - General convex artificial boundary
3. Approximations of TBC

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ANALYTIC TRANSPARENT BOUNDARY CONDITIONS

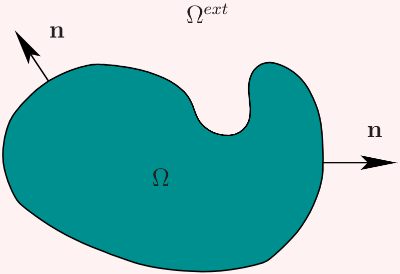
$$\begin{array}{ll} i\partial_t u + \Delta u = 0, & (\mathbf{x}, t) \in \mathbb{R}^2 \times \mathbb{R}^+, \\ u(\mathbf{x}, 0) = u^I(\mathbf{x}), & \mathbf{x} \in \mathbb{R}^2. \end{array} \tag{1}$$

Schädle (02)

➠ similar tools already used in 1D :

- transmission problem
- Laplace transform : $\mathcal{L}(w)(\mathbf{x}, \tau) = \hat{w}(\tau) = \int_0^\infty w(\mathbf{x}, t) e^{-\tau t} dt$, Re$(\tau) > 0$

- Step 1 : split problem (1) as a transmission problem between Ω and Ω^{ext}



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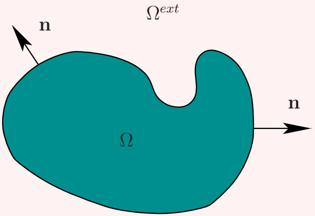

Interior problem

$$
\begin{aligned}
&i\partial_t v + \Delta v = 0, && (\mathbf{x},t) \in \Omega \times \mathbb{R}^+ \\
&v(\mathbf{x},0) = u^I(\mathbf{x}), && \mathbf{x} \in \Omega \\
&v(\mathbf{x},t) = w(\mathbf{x},t), && (\mathbf{x},t) \in \Gamma \times \mathbb{R}^+
\end{aligned}
$$

Exterior problem

$$
\begin{aligned}
&i\partial_t w + \Delta w = 0, && (\mathbf{x},t) \in \Omega^{\mathsf{ext}} \times \mathbb{R}^+, \\
&\partial_{\mathbf{n}} w(\mathbf{x},t) = \partial_{\mathbf{n}} v(\mathbf{x},t), && (\mathbf{x},t) \in \Gamma \times \mathbb{R}^+, \\
&\lim_{|\mathbf{x}|\to+\infty} \sqrt{|\mathbf{x}|}\left(\nabla w \cdot \frac{\mathbf{x}}{|\mathbf{x}|} + \mathrm{e}^{-i\frac{\pi}{4}} \partial_t^{\frac{1}{2}} w\right) = 0. &&
\end{aligned}
$$

Presence of the Sommerfeld-like radiation condition to ensure the uniqueness of the solution in Ω^{ext}.

Analytic transparent boundary conditions

- Step 2 :

Laplace transform in t to the exterior problem

$$\begin{aligned}
&(\Delta + k^2)\hat{w}(\mathbf{x},\tau) = 0, \quad \mathbf{x} \in \Omega^{\text{ext}},\\
&\partial_{\mathbf{n}}\hat{w}(\mathbf{x},\tau) = \partial_{\mathbf{n}}\hat{v}(\mathbf{x},\tau), \quad (\mathbf{x},\tau) \in \Gamma,\\
&\lim_{|\mathbf{x}|\to+\infty} \sqrt{|\mathbf{x}|}\left(\nabla\hat{w}(\mathbf{x},\tau)\cdot\frac{\mathbf{x}}{|\mathbf{x}|} - ik\hat{w}(\mathbf{x},\tau)\right) = 0.
\end{aligned}$$

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

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

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

where

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

setting $G(\mathbf{x},\mathbf{y}) = \frac{i}{4}H_0^{(1)}(k|\mathbf{x}-\mathbf{y}|)$.

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Analytic transparent boundary conditions

Inverse Laplace transform

Dirichlet-to-Neumann map

$$\partial_{\mathbf{n}} v = \mathcal{L}^{-1}\left(L^{-1}\left(\frac{I}{2} - M\right)\hat{v}(\mathbf{x},\cdot)\right)(t), \quad \mathbf{x} \in \Gamma,$$

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.

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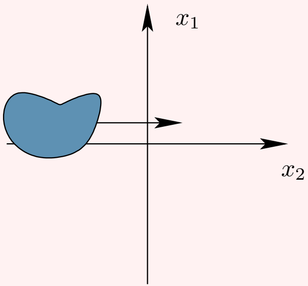
Straight artificial boundary

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

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



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

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

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

Differential equation in the normal variable x_2 for the solution w in Ω^{ext}

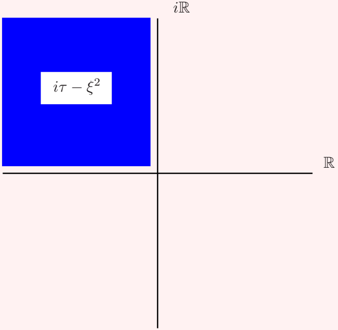
$$\left(\partial_{x_2}^2 + i\tau - \xi^2\right) \mathcal{F}\hat{w}(x_2, \xi, \tau) = 0, \quad x_2 > 0,$$

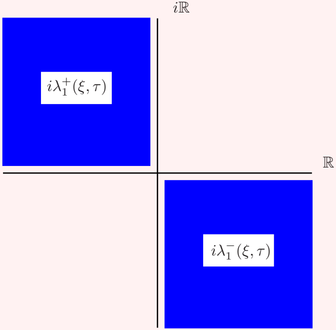
Solution given as the superposition of two waves

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

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

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





Straight artificial boundary

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

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

Remarks

- The part of the wave $\hat{w}$ at point (x_1,t,ξ,ρ) 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 τ and ξ in the symbols $\lambda_1^\pm$
- The points (x_1,t,ξ,ρ) in the cone $\mathcal{H} = \left\{(x_1,t,\xi,\rho),\ \rho + \xi^2 < 0\right\}$ represent the propagative part of the wave. This zone is referred to as the *M-quasi hyperbolic part*.
- The complementary zone $\mathcal{G} = \left\{(x_1,t,\xi,\rho),\ \rho + \xi^2 = 0\right\}$ 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 Γ.

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Straight artificial boundary

Apply the normal derivative operator ∂_{x_2} to $\mathcal{F}\hat{w}(x_2,\xi,\tau) = A^+(\xi,\tau)e^{i\lambda_1^+(\xi,\tau)x_2}$ and choose $x_2 = 0$, $\mathbf{n} = (1,0)$ as the outwardly unitary normal vector to the computational domain.

Inverse Laplace-Fourier transform

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

with

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

Formally,

Artificial boundary condition

$$\partial_{\mathbf{n}} u - i\sqrt{i\partial_t + \Delta_\Gamma}\,u = 0 \qquad \text{on } \Gamma \times \mathbb{R}^+$$

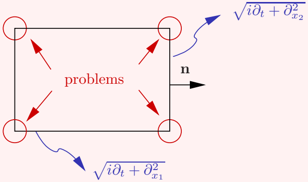
where Δ_Γ denotes the *surface Laplace-Beltrami operator* $\partial_{x_1}^2$.

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

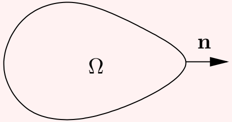
Straight artificial boundary

Remarks :

- This derivation leads inevitably to junction problems located in corners



One must work on a convex open set



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

Transparent Boundary Condition

$$\partial_{\mathbf{n}} u - iOp_{|\mathcal{H}}(\sqrt{i\tau - \xi^2})u = 0 \quad \text{on } \Gamma \times \mathbb{R}^+$$

- 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

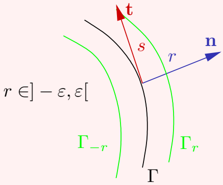
General convex open set $\Omega \subset \mathbb{R}^2$: factorization of the operator $i\partial_t + \Delta$

Methodology

- Generalized coordinates system of the boundary :

variable r	normal variable along the unit normal vector $\mathbf{n}$
variable s	curvilinear abscissa along Γ

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



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

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

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

$$r \leftrightsquigarrow x_2 \qquad s \leftrightsquigarrow x_1 \qquad t \leftrightsquigarrow t$$

General convex artificial boundary

- Define ψdo 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–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 $\mathcal{G}$.

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$$\downarrow r \to 0$$
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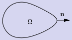

Identification of the different terms

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

Therefore, one has

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

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.
- Retriction to the boundary $r = 0$ and $\widetilde{\lambda} = \lim_{r\to 0}\lambda$.

$$\widetilde{\lambda_1^+} = \sqrt{i\tau - \xi^2},\ \widetilde{\lambda_0^+} = \frac{1}{2\widetilde{\lambda_1^+}}\left(-i\kappa\widetilde{\lambda_1^+} - i\frac{\kappa\xi^2}{\widetilde{\lambda_1^+}}\right),\ \ldots$$

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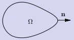

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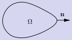

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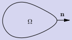

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- $(\partial_r + i\Lambda^-)(\partial_r + i\Lambda^+) = \partial_r^2 + i(\Lambda^+ + \Lambda^-)\partial_r + iOp(\partial_r \lambda^+) - \Lambda^-\Lambda^+$

Therefore, one has

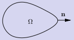
$$\begin{cases} i(\lambda^+ + \lambda^-) = \kappa_r, \\ i\partial_r \lambda^+ - \sigma(\Lambda^-\Lambda^+) = i\xi(h^{-1}\partial_s h^{-1}) - \xi^2 h^{-2} + i\tau, \end{cases}$$

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.
- Retriction to the boundary $r = 0$ and $\widetilde{\lambda} = \lim_{r\to 0} \lambda$.

$$\widetilde{\lambda_1^+} = \sqrt{i\tau - \xi^2},\ \widetilde{\lambda_0^+} = \frac{1}{2\widetilde{\lambda_1^+}}\left(-i\kappa\widetilde{\lambda_1^+} - i\frac{\kappa\xi^2}{\widetilde{\lambda_1^+}}\right), \ldots$$

General convex artificial boundary



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General convex artificial boundary

Approximate TBC

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

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 :

- 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 $\leftrightsquigarrow$ $\mathcal{Z}$–transform   Fourier $\leftrightsquigarrow$ discrete Fourier transform in θ–direction.

- Dimenza (95), Szeftel (04) : since TBCs are $\partial_{\mathbf{n}} u - iOp(\sqrt{i\tau - \xi^2})u = 0$, 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 φ_j satisfying the surface Schrödinger equations

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

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Approximations of TBC

- Third way :

Transparent Boundary Condition

$$\partial_{\mathbf{n}} u - iOp_{|\mathcal{H}}(\sqrt{i\tau - \xi^2})u = 0 \quad \text{on } \Gamma \times \mathbb{R}^+, \ \tau = \sigma + i\rho$$

Since we restrict symbol to $\mathcal{H}$ region, $-\rho > \xi^2 \Rightarrow |\tau| > \xi^2$.
high frequency assumption : $|\tau| \gg \xi^2$
Example for λ_1^+ :

$$\underbrace{\sqrt{i\tau - \xi^2}}_{\text{non local in x and t}} = \sqrt{i\tau}\underbrace{\sqrt{1 - \frac{\xi^2}{i\tau}}}_{|i\tau| \gg \xi^2 \text{ Taylor exp.}} \approx \sqrt{i\tau} - \underbrace{\frac{\xi^2}{2\sqrt{i\tau}}}_{\text{local in space}} + \underbrace{\cdots}_{\text{local in space}}$$

The ABC of order $(m+2)/2$ is $(\partial_{\mathbf{n}} + i\mathrm{Op}(\sum_{j=-1}^{m} (\widetilde{\lambda_{-j}})_{(m+2)}))v = 0$ on $\Gamma \times [0, T]$ where $(\widetilde{\lambda_{-j}})_{(m+2)}$ are Taylor expansions with respect to the small parameter τ^{-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 λ_1^+.

$$(\partial_{\mathbf{n}} + e^{-i\pi/4}\partial_t^{\frac{1}{2}})u = 0, \quad \text{on } \Gamma \times \mathbb{R}^+,$$

and

$$(\partial_{\mathbf{n}} + e^{-i\pi/4}\partial_t^{\frac{1}{2}} - e^{i\pi/4}\frac{1}{2}\Delta_\Gamma I_t^{\frac{1}{2}})u = 0, \quad \text{on } \Gamma \times \mathbb{R}^+.$$

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

Approximated IBVP

$$(DN^{m/2}) \quad \begin{cases} (i\partial_t + \Delta)v = 0, & (x,t) \in \Omega \times [0,T], \\ \partial_{\mathbf{n}} v + T_{m/2} v = 0, & (x,t) \in \Gamma \times [0,T], \\ v(x,0) = v_0(x), & x \in \Omega. \end{cases}$$

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

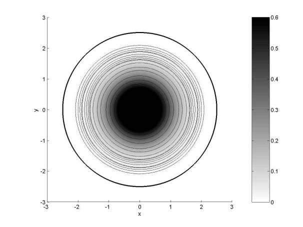
$$\begin{aligned} T_{1/2}v &= e^{-i\pi/4}\partial_t^{1/2} v, \\ T_1 v &= T_{1/2}v + \frac{\kappa}{2} v, \\ T_{3/2}v &= T_1 v - e^{i\pi/4}\left(\frac{\kappa^2}{8} + \frac{1}{2}\Delta_\Gamma\right) I_t^{1/2} v, \\ T_2 v &= T_{3/2}v + i\left(\frac{\kappa^3}{8} + \frac{1}{2}\partial_s(\kappa\partial_s) + \frac{\Delta_\Gamma \kappa}{8}\right) I_t v, \end{aligned}$$

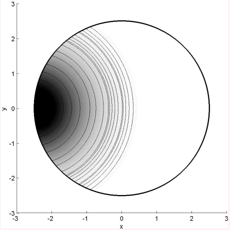
with $I_t^{1/2} = I_t \partial_t^{1/2}$.

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





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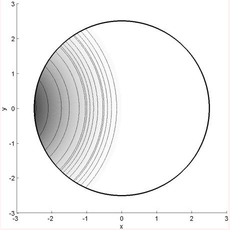

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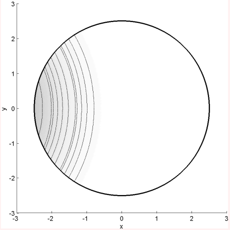

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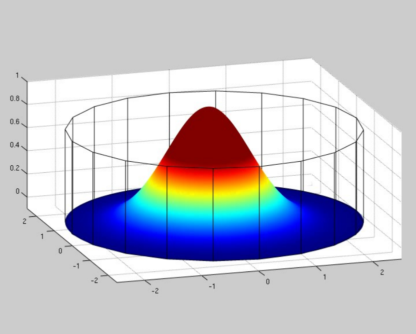
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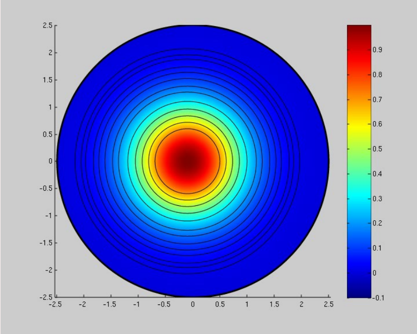
0.8
0.6
0.4
0.2
0
2 1 0 -1 -2
-2 -1 0 1 2


2.5 2 1.5 1 0.5 0 -0.5 -1 -1.5 -2 -2.5
-2.5 -2 -1.5 -1 -0.5 0 0.5 1 1.5 2 2.5
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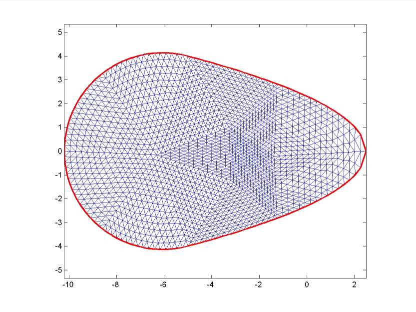
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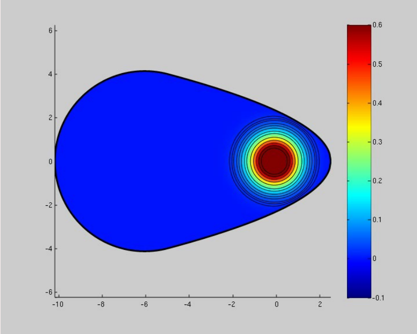
-10 -8 -6 -4 -2 0 2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-10 -8 -6 -4 -2 0 2
0.6 0.5 0.4 0.3 0.2 0.1 0 -0.1