Probabilistic approaches to divergence form operators with discontinuous coefficients

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Outline

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On PDEs driven by divergence form operators

Consider elliptic or parabolic PDEs driven by the strongly elliptic divergence form operator

$$\mathcal{L} := \frac{1}{2}\mathrm{div}(a(x)\nabla),$$

where

$$0 < \lambda|\xi|^2 \leq (a(x)\xi,\xi) \leq \Lambda|\xi|^2 < +\infty \text{ for all } x,\xi \in \mathbb{R}^d.$$

Analytical techniques:

- Variational formulations: Aronson, Stroock;
- Transmission (or Diffraction) formulations: J–L. Lions, Ladyzenskaya–Solonnikov–Ural'ceva;
- Dirichlet form theory applied to forms of the type

  $$\mathcal{E}(u,u) := \frac{1}{2}\int \nabla u(x)\cdot a(x)\nabla u(x) q(x)\,dx,$$

  where q is a strictly positive density.
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A key point in all these approaches: Aronson's inequalities for the fundamental solution of the parabolic PDE driven by $\mathcal{L}$: there exist $\alpha > 0$, $\beta > 0$ and $C > 0$ depending on λ, Λ and T only, such that

$$\frac{1}{C}\exp(-\tfrac{|y-x|^2}{\alpha t}) \leq p(t,x,y) \leq C\exp(-\tfrac{|y-x|^2}{\beta t}).$$

Examples of probabilistic interpretations:

Using Dirichlet forms,

- Existence of a strong (canonical) Markov process $(X_t, t \leq T)$ with generator $\mathcal{L}$ and a transition density $p(t,x,y)$ which satisfies Aronson's inequalities (Stroock, Fukushima).
- 'Pseudo SDEs' (Lyons–Zheng decompositions: Fukushima, Roskoz, Slominski): For all function ϕ in $W_p^{1,\mathrm{loc}}(\mathbb{R}^d)$, there exists a pair of local martingales (M^ϕ, N^ϕ) respectively adapted with respect to the filtration generated by $(X_t, 0 \leq t \leq T)$ and the filtration generated by $(X_{T-t}, 0 \leq t \leq T)$, such that

$$\phi(X_t) = \phi(X_0) + \frac{1}{2}M_t^\phi + \frac{1}{2}N_t^\phi + \frac{1}{2}\int_0^t \frac{a(X_\theta)\nabla p(\theta,x,X_\theta)}{p(\theta,x,X_\theta)} \cdot \nabla\phi(X_\theta)\,d\theta,$$

and

$$\langle M^\phi\rangle_t = \int_0^t a\nabla\phi\cdot\nabla\phi(X_\theta)\,d\theta \text{ and } \langle N^\phi\rangle_t = \int_0^t a\nabla\phi\cdot\nabla\phi(X_{T-\theta})\,d\theta.$$

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Remark.

- Pardoux–Williams have exhibited a Lyons–Zheng decomposition for Dirichlet forms with degenerate Neumann boundary conditions.
- The Lyons–Zheng decompositions cannot lead to algorithms since one should first compute the transition density $p(t, x, y)$ of the Markov process.

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Outline

We consider the one dimensional parabolic problem

$$(\diamond) \quad \begin{cases} \partial_t u(t,x) - Au(t,x) = 0 \text{ for all } (t,x) \in (0,T] \times \mathbb{R}, \\ u(0,x) = f() \text{ for all } x \in \mathbb{R}, \end{cases}$$

where

$$A := \frac{d}{dx}\left[\frac{1}{2}\sigma^2(x)\frac{d}{dx}\right],$$

and f is a fonction in $L^2(\mathbb{R})$.

A transmission problem

Let σ^+ and σ^- respectively denote the restrictions of the function σ to $\mathbb{R}^+$ and $\mathbb{R}^-$. We set $a^+(x) := (\sigma^+(x))^2$ and $a^-(x) := (\sigma^-(x))^2$. As shown in Ladyzenskaja et al. there exists a unique solution $u(t,x)$ to the PDE $(\diamond)$ belonging to the space $V_2^{1,1/2}([0,T]\times\mathbb{R})$; this solution is continuous, twice continuously differentiable in space and once continuously differentiable in time on $(0,T]\times(\mathbb{R}-\{0\})$, and also solves the transmission problem

$$\begin{cases} \partial_t u(t,x) - \frac{1}{2}\partial_x(a^+(x)\partial_x u(t,x)) = 0, \ (t,x)\in(0,T]\times(0,+\infty), \\ \partial_t u(t,x) - \frac{1}{2}\partial_x(a^-(x)\partial_x u(t,x)) = 0, \ (t,x)\in(0,T]\times(-\infty,0), \\ u(t,0+) = u(t,0-), \\ u(0,x) = f(x), \ x\in\mathbb{R}, \\ a(0+)\partial_x u(t,0+) = a(0-)\partial_x u(t,0-) \quad (\star). \end{cases}$$

The key SDE with weighted local time

The one dimensional case allows specific analytical and numerical tools: Portenko (1979), Le Gall (1985), Lejay-Martinez (2003)...
Consider the one-dimensional stochastic differential equation with local time

$$dX_t = \sigma(X_t)\,dB_t + \sigma(X_t)\sigma'_-(X_t)\,dt + \frac{\sigma^2(0+) - \sigma^2(0-)}{2\sigma^2(0+)}\,dL_t^0(X).$$

Here $L_t^0(X)$ is the right-sided local time corresponding to the sign function defined as $\mathrm{sgn}(x) := 1$ for $x > 0$ and $\mathrm{sgn}(x) := -1$ for $x \leq 0$ and σ'_- is the left derivative of σ.
Under mild hypotheses on σ this SDE has a unique weak solution which is a strong Markov process : see, e.g., Le Gall (1984). Notice that (X_t) is a semi–martingale .

Probabilistic interpretation

Theorem 1 *Suppose that there exists $\lambda > 0$ and $\Lambda > 0$ such that*

$$0 < \lambda \leq \sigma^2(x) \leq \Lambda < +\infty \text{ for all } x \in \mathbb{R}.$$

Suppose also that the function σ is of class $\mathcal{C}_b^2(\mathbb{R} - \{0\})$ and right continuous at point 0. Suppose finally that the two first derivatives of function σ have finite left and right limits at 0. Let f be a function bounded with bounded derivatives in the set

$$\mathcal{H}^0 := \Big\{ g \in \mathcal{C}^3(\mathbb{R}),\ g \text{ is } \mathcal{C}^4(\mathbb{R}), \\ g^{(i)} \in L^2(\mathbb{R}) \cap L^1(\mathbb{R}),\ g^{(i)}(0) = 0 \text{ for } i = 1, \dots, 4 \Big\}.$$

Then

$$u(t,x) := \mathbb{E}^x[f(X_t)],\ (t,x) \in [0,T] \times \mathbb{R},$$

is the unique function in $\mathcal{C}^{1,2}([0,T] \times (\mathbb{R} - \{0\}))$ and continuous on $[0,T] \times \mathbb{R}$ solution to the transmission problem. If, in addition, the function f belongs to $L^2(\mathbb{R})$, then $u(t,x)$ is the unique solution to $(\star)$ in $L^2([0,T]; H^1(\mathbb{R}))$.

We develop a probabilistic technique to prove this result.
Difficulties:

- One cannot apply Itô-Tanaka's formula to $u(t, X_t)$.
- Astonishingly, exhibiting the transmission condition is not simple.

Easy part: The function $u(t,x)$ solves the PDE in $\mathbb{R} - \{0\}$. This relies on Itô's formula and (see Lunardi) : The function $u^-(t,x)$ belongs to the Hölder space $\mathcal{C}^{1+\alpha,2+\alpha}([0,T]\times\mathbb{R}_-)$ for all $0<\alpha<1$ and

$$\|u^-\|_\infty + \sup_{0\le t\le T}\left\|\frac{\partial u^-}{\partial t}\right\|_\infty + \sup_{0\le t\le T}\left\|\frac{\partial u^-}{\partial x}\right\|_\infty + \sup_{0\le t\le T}\left\|\frac{\partial^2 u^-}{\partial x^2}\right\|_\infty \le C\|f\|_{\mathcal{C}^{2+\alpha}(\mathbb{R}_-)} + C\|\Phi\|_{\mathcal{C}^{1+\alpha}([0,T])},$$

where

$$\|\phi\|_{\mathcal{C}^{\ell+\alpha}(D)} := \sum_{i=0}^{\ell} |\phi|_{L^\infty(D)} + \sup_{\xi,\xi'\in D\xi<\xi'} \frac{|\phi(\xi)-\phi(\xi')|}{|\xi-\xi'|}.$$

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A SDE with discontinuous coefficients without local time

Set

$$\begin{aligned}
\beta^+ &:= \frac{2\,a(0-)}{a(0+)+a(0-)},\\
\beta^- &:= \frac{2\,a(0+)}{a(0+)+a(0-)},\\
\beta(x) &:= x\left(\beta^-\mathbb{I}_{x<0} + \beta^+\mathbb{I}_{x>0}\right),\\
\beta^{-1}(x) &= \tfrac{x}{\beta^-}\mathbb{I}_{x<0} + \tfrac{x}{\beta^+}\mathbb{I}_{x>0}.
\end{aligned}$$

Set also

$$\begin{aligned}
\tilde{\sigma}(x) &:= \sigma\circ\beta^{-1}(x)\left(\beta^-\mathbb{I}_{x\le 0} + \beta^+\mathbb{I}_{x>0}\right),\\
\tilde{b}(x) &:= \sigma\circ\beta^{-1}(x)\sigma'_-\circ\beta^{-1}(x)\left(\beta^-\mathbb{I}_{x\le 0} + \beta^+\mathbb{I}_{x>0}\right).
\end{aligned}$$

Adapt a calculation in Le Gall and apply Itô–Tanaka's formula to $\beta(X_t)$. The process $Y := \beta(X)$ satisfies the SDE with discontinuous coefficients :

$$Y_t = \beta(X_0) + \int_0^t \tilde{\sigma}(Y_s)\,dB_s + \int_0^t \tilde{b}(Y_s)\,ds.$$

Construction of a discretization scheme

We now present a Euler type scheme. For other methds: see A. Lejay. Let

$$h_n := \frac{T}{n} \text{ and } t_k^n := k\ h_n.$$

Approximate (Y_t) by

$$\overline{Y}_t^n = \overline{Y}_{t_k^n}^n + \tilde{\sigma}(\overline{Y}_{t_k^n}^n)\mathbb{I}_{\overline{Y}_{t_k^n}^n \neq 0}(B_t - B_{t_k^n}) + \tilde{b}(\overline{Y}_{t_k^n}^n)\mathbb{I}_{\overline{Y}_{t_k^n}^n \neq 0}(t - t_k^n).$$

Then set

$$\overline{X}_t^n = \beta^{-1}(\overline{Y}_t^n),\ 0 \leq t \leq T.$$

Remark.

The Euler scheme $(\overline{X}_t)$ converges weakly to (X_t) since $(\overline{Y}_t)$ converges weakly to (Y_t) (see Yan). However, as the coefficients $\tilde{b}$ and $\tilde{\sigma}$ are discontinuous, no classical convergence rate estimate applies.

Convergence rate estimates

Theorem 2 *There exists a positive number C such that, for all exponent $0 < \rho < \frac{1}{2}$, for all n large enough, all x_0 in $\mathbb{R}$, and all function f in $\mathcal{H}^0$,*

$$\left|\mathbb{E}^{x_0} f(X_T) - \mathbb{E}^{x_0} f(\overline{X}^n_T)\right| \\ \leq h_n^{3\rho-1} \|f'\|_{1,1} + h_n^{1/2+\rho} \|f'\|_{3,1} + C\sqrt{h_n} \|f''\|_{L^1(\mathbb{R})}.$$

Theorem 3 *Let $f : \mathbb{R} \mapsto \mathbb{R}$ be in the space*

$$\mathcal{H} := \left\{ g \in \mathcal{C}^3(\mathbb{R}),\ g \text{ is } \mathcal{C}^4(\mathbb{R}),\ g^{(i)} \in L^2(\mathbb{R}) \cap L^1(\mathbb{R}) \right\}.$$

There exists a positive number C (depending on f) such that, for all exponent $0 < \rho < \frac{1}{2}$, all n large enough, and all x_0 in $\mathbb{R}$,

$$\left|\mathbb{E}^{x_0} f(X_T) - \mathbb{E}^{x_0} f(\overline{X}^n_T)\right| \leq C h_n^{\frac{1+2\rho}{6}}.$$

A discretization error decomposition

The discretization error satisfies

$$\epsilon_T := \left|\mathbb{E}(f\circ\beta^{-1}(Y_T)) - \mathbb{E}(f\circ\beta^{-1}(\overline{Y}^n_T))\right|$$
$$= \left|\sum_{k=0}^{n-1}(\mathbb{E}(u(T-t^n_k,\beta^{-1}(\overline{Y}^n_{t^n_k}))) - \mathbb{E}u(T-t^n_{k+1},\beta^{-1}(\overline{Y}^n_{t^n_{k+1}})))\right|,$$

from which

$$\epsilon_T \leq \left|\sum_{k=0}^{n-2}\mathbb{E}\left\{u(\theta^n_k,\beta^{-1}(\overline{Y}^n_{t^n_k})) - u(\theta^n_{k+1},\beta^{-1}(\overline{Y}^n_{t^n_k}))\right.\right.$$
$$\left.\left. + u(\theta^n_{k+1},\beta^{-1}(\overline{Y}^n_{t^n_k})) - u(\theta^n_{k+1},\beta^{-1}(\overline{Y}^n_{t^n_{k+1}}))\right\}\right|$$
$$+\left|\mathbb{E}u(\theta^n_1,\beta^{-1}(\overline{Y}^n_{t^n_{n-1}})) - \mathbb{E}u(0,\beta^{-1}(\overline{Y}^n_T))\right|$$
$$=: \left|\sum_{k=0}^{n-2}\mathbb{E}\{T_k - S_k\}\right| + |\mathbb{E}R_{n-1}|.$$

Methodology

We distinguish several cases.

- When $\overline{Y}^n_{t^n_k}$ and $\overline{Y}^n_{t^n_{k+1}}$ are simultaneously positive or negative, we use a Taylor expansion of $u(t^n_{k+1}, \cdot)$ around $(t^n_k, \overline{Y}^n_{t^n_k})$ and then apply accurate estimates of the derivatives of $u(t, x)$ for t in $(0, T]$ and x in $\mathbb{R} - \{0\}$.
- We prove that $\overline{Y}^n_{t^n_k}$ and $\overline{Y}^n_{t^n_{k+1}}$ have opposite signs with small probability when $|\overline{Y}^n_{t^n_k}|$ is large enough.
- When $|\overline{Y}^n_{t^n_k}|$ is small, we explicit the expansion of $u(t^n_{k+1}, \cdot)$ around 0 and use the fact that $u(t, x)$ solves the transmission problem, which allows us to cancel the lower order term in the expansion.

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Two key estimates:

A discrete version of Krylov's inequality: There exists $C > 0$ such that, for all $\xi \in \mathbb{R}^d$ and $0 < \varepsilon < 1/2$, there exists $h_0 > 0$ satisfying

$$\forall\, h \leq h_0,\ \ h \sum_{k=0}^{N_h} f(kh) \mathbb{P}(\|X_{ph} - \xi\| \leq h^{1/2-\varepsilon}) \leq C h^{1/2-\varepsilon},$$

where $N_h := \lfloor T/h \rfloor - 1$.

Estimates on the derivatives of $u(t,x)$: For all $j = 0, 1, 2$ and $i = 1, \dots, 4$ such that $2j + i \leq 4$, there exists $C > 0$ such that, for all f in $\mathcal{H}^0$ and all t in $(0, T]$,

$$\|\partial_t^j \partial_x^i u(t, \cdot, f)\|_\infty \leq \frac{C}{\sqrt{t}} \|f'\|_{\gamma,1},$$

where $\gamma = 1$ if $2j + i = 1$ or 2, and $\gamma = 3$ if $2j + i = 3$ or 4, and

$$\|g\|_{\ell,p} := \sum_{i=0}^{\ell} \|g^{(i)}\|_{L^p(\mathbb{R})}.$$

Here we use:

$$u^-(t,x) = \mathbb{E}^x[f(X_t)\mathbb{I}_{t \leq \tau_0}] + \mathbb{E}^x[\Phi(t - \tau_0)\mathbb{I}_{\tau_0 < t}],$$

where $\Phi(t) := \mathbb{E}^0 f(X_t)$, and Pauwels' representation of the density of $\tau_0 := \inf\{s > 0;\ X_s = 0\}$ in terms of the probability laws of Bessel(3) processes and Brownian bridges.

Outline

The Poisson-Boltzmann PDE

The Poisson-Boltzmann (PB) PDE in Molecular Dynamics describes the electrostatic potential around a biomolecular assembly, and is used to compute global characteristics of the system such as

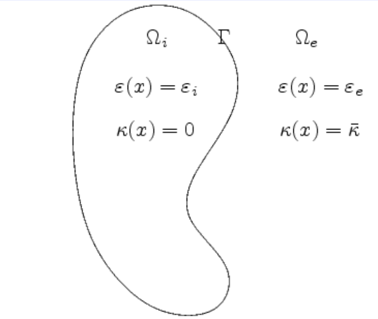
- the solvatation free energy,
- the electrostatic forces exerted by the solvent on the molecule.

The implicit solvent equation, which means that the solvent is considered as a continuum, reads

$$-\nabla \cdot (\varepsilon(x)\nabla u(x)) + \kappa^2(x)u(x) = f(x), \qquad x \in \mathbb{R}^3,$$

where

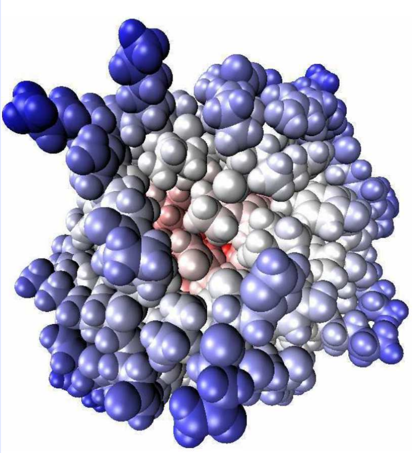
- $\varepsilon(x)$ is the permittivity of the medium,
- $\kappa^2(x)$ is called the ion accessibility parameter .


Ω_i
Γ
Ω_e
$\varepsilon(x) = \varepsilon_i$
$\kappa(x) = 0$
$\varepsilon(x) = \varepsilon_e$
$\kappa(x) = \bar{\kappa}$

The geometry of the problem

The atomic structure of the molecule modelled as

- N atoms at positions $x_1, \ldots, x_N$ in Ω_i with radii $r_1, \ldots, r_N$ and charge q_i,
- $\Omega_i = \cup_{i=1}^{N} B(x_i, r_i)$.



Other difficulties

- The source term is singular

$$f := \sum_{i=1}^{N} q_i \delta_{x_i}.$$

This difficulty can be removed by considering the solution u_0 of $\varepsilon_i \Delta u = f$, that is,

$$u_0(x) = \frac{1}{4\pi\varepsilon_{\text{int}}} \sum_{l=1}^{N} \frac{q_j}{|x - x_l|} \qquad \forall x \in \Omega_{\text{int}}.$$

Then $v := u - \chi u_0$ solves PB equation with a smooth source term if χ has compact support in Ω_i and $\chi \equiv 1$ in the neighborhood of $\{x_1, \dots, x_N\}$.

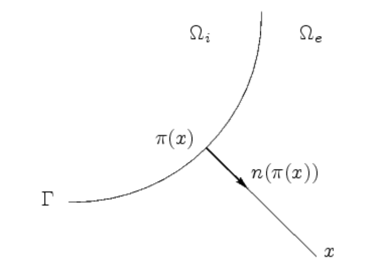
- κ is discontinuous
- The operator has divergence form with discontinuous coefficient ε.

The general case

Assume that Γ is a smooth (C^3) manifold in $\mathbb{R}^d$.
Notation:

- $\pi(x)$ for the orthogonal projection of x on Γ,
- $n(y)$ as the outward normal to Γ for $y \in \Gamma$,
- $\rho(x)$ as the signed distance between x and Γ.

$$\rho(x) := (x - \pi(x)) \cdot n(\pi(x)).$$



A martingale problem

We say that $(\mathbb{P}_x)_{x\in\mathbb{R}^d}$ on $(\mathcal{C},\mathcal{B})$ solves the martingale problem (MP) for $\mathcal{L}$ if, for all $x\in\mathbb{R}^d$, one has

$$\mathbb{P}_x\{w\in\mathcal{C} : w(0)=x\}=1,$$

and, for all φ satisfying

$$\varphi\in C_b^0(\mathbb{R}^d)\cap C_b^2(\mathbb{R}^d\setminus\Gamma),$$
$$\varepsilon\nabla\varphi\cdot(n\circ\pi)\in C_b^0(\mathcal{N}),$$

one has

$$M_t^\varphi(w):=\varphi(w(t))-\varphi(w(0))-\int_0^t\mathcal{L}\varphi(w(s))ds \quad \text{is a } \mathbb{P}_x \text{ martingale.}$$

Remark: the test functions satisfy the transmission property

$$\varepsilon_{\text{int}}\nabla^{\text{int}}\varphi(x)\cdot n(x)=\varepsilon_{\text{ext}}\nabla^{\text{ext}}\varphi(x)\cdot n(x).$$

Our main result

Theorem

The martingale problem for $\mathcal{L}$ is well-posed.
In addition, there is weak existence and uniqueness in law for the SDE

$$\begin{cases} dX_t = \sqrt{2\varepsilon(X_t)}dB_t + \dfrac{\varepsilon_{ext} - \varepsilon_{int}}{2\varepsilon_{ext}} n(X_t)\,dL_t^0(Y), \\ Y_t = \rho(X_t), \end{cases}$$

and the probability law of X solves the MP for $\mathcal{L}$.

Sktech of the proof

- We construct a smooth local straightening ψ of Γ defined on a neighborhood $\mathcal{U}$ of x, s.t. $\psi_1 = \rho$ and $Z_t := \psi(X_t)$ satisfies

$$dZ_t^1 = \sqrt{2\varepsilon(X_t)}\,dB_t + \frac{\varepsilon_e - \varepsilon_i}{2\varepsilon_e}\,dL_t^0(Z^1) + (\text{drift})(Z_t)\,dt,$$

  and there is no local time term in the SDE solved by $Z_t^2, \dots, Z_t^d$.
- Girsanov's formula allows one to remove the drift term, so that Z_t^1 solves a one-dimensional SDE.
- Conditionnally to Z^1, $Z^2, \dots, Z^d$ solves a classical SDE with time dependent coefficients.
- $\rightsquigarrow$ Only weak existence.

Lemma (Generalized Itô-Meyer formula)

If X is a continuous semimartingale and if u is a test function for the MP for $\mathcal{L}$, then

$$u(X_t) = u(X_0) + \int_0^t \nabla^{int} u(X_s) \cdot dX_s + \frac{1}{2} \sum_{i,j=1}^{3} \int_0^t \frac{\partial^2 u}{\partial x_i \partial x_j}(X_s)\, d\langle X^i, X^j \rangle_s + \frac{1}{2} \int_0^t f(X_s)\, dL_s^0(Y), \quad \forall t \geq 0 \ a.s.,$$

where $f(x) = \left(\frac{\varepsilon_{int}}{\varepsilon_{ext}} - 1 \right) \nabla^{int} u(\pi(x)) \cdot n(\pi(x))$.

- The formula would be easily obtained from Itô's and Itô-Tanaka's formulas if the functions $u(x) - f(x)[\rho(x)]_+$ and $f(x)$ were C^2.
- If (X_t) solves the preceding SDE, the local time terms cancel.

Feynman-Kac formulas

Proposition (First Feynman-Kac representation)

Let v be the solution of $-\nabla \cdot (\varepsilon \nabla v) + \kappa^2 v = g$, where g is a smooth function. Then, for all $x \in \mathbb{R}^3$,

$$v(x) = \mathbb{E}_x \left[\int_0^{+\infty} g(X_t) \exp\left(- \int_0^t \kappa^2(X_s)\, ds \right) dt \right].$$

This representation does not allow one to develop an efficient numerical scheme because

- One needs to precisely discretize X everywhere where g is nonzero.
- In general, the computation of g is costly.

Since X has (scaled) Brownian paths aaway from Γ, it is better to have formulas only involving informations on the entrance time and position in small neighborhoods of Γ.

A second Feynman-Kac formula

Fix $h > 0$.

- We define the stopping times

$$\begin{aligned} \tau_k &= \inf\{t \geq \tau'_{k-1} : \rho(X_t) = -h\} \\ \tau'_k &= \inf\{t \geq \tau_k : X_t \in \Gamma\} \end{aligned}$$

- Since $\Delta(u - u_0) = 0$ in Ω_i, for all x s.t. $\rho(x) \leq -h$,

$$u(x) = \mathbb{E}_x[u(X_{\tau'_1}) - u_0(X_{\tau'_1})] + u_0(x).$$

- For all $x \in \Omega_e$,

$$u(x) = \mathbb{E}_x\left[u(X_{\tau_1})\exp\left(-\int_0^{\tau_1} \kappa^2(X_t)dt\right)\right].$$

- Applying these two formulas recursively yields:

Application

Proposition

$$u(x) = \mathbb{E}_x \left[\sum_{k=1}^{+\infty} \left(u_0(X_{\tau_k}) - u_0(X_{\tau_k'}) \right) \exp\left(- \int_0^{\tau_k} \kappa^2(X_t)\, dt \right) \right].$$

Application: Analyze the convergence rates of (improved) Walk on Spheres algorithms introduced in this context by Mascagni and Simonov.