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► **To cite this version:**

Antoine Lejay. Simulation of a stochastic process in a discontinuous, layered media. 2011. inria-00583127v1

HAL Id: inria-00583127

<https://inria.hal.science/inria-00583127v1>

Preprint submitted on 4 Apr 2011 (v1), last revised 30 Nov 2011 (v4)

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Simulation of a stochastic process in a discontinuous, layered media

Antoine Lejay^{*†}

April 4, 2011

Abstract: In this note, we provide a simulation algorithm for a diffusion process in a layered media. Our main tools are the properties of the Skew Brownian motion and a path decomposition technique for simulating occupation times.

Keywords: Skew Brownian motion, discontinuous media, occupation time, local time, last passage time, path decomposition, Brownian bridge, first hitting time, geophysics, Monte Carlo simulation

1. Introduction

(1) Simulation of diffusion processes in multi-dimensional discontinuous media is still a challenging problem, while recent progresses have been done for one-dimensional media (See Parag. 5). The object of this note is to deal with the simulation of the stochastic process generated by the divergence form operator

$$\mathcal{L} = \frac{1}{2}\nabla(D\nabla\cdot) + U\nabla,$$

in a multi-dimensional layered media. By this, we mean that there is a direction \mathbf{n} orthogonal to the discontinuities of a diffusion coefficient D and a convective term U that are constant in each layers.

(2) This could be used for example to model a solute in a vertically layered porous media submitted to a advective flow U and diffusion effects given by D [1, 33–35]. The concentration $C(t, x)$ of the solute is then

$$\frac{\partial C(t, x)}{\partial t} = \frac{1}{2}\nabla(D(x)\nabla C(t, x)) - \nabla(U(x)C(t, x)) \quad (1)$$

with $C(t, x) \xrightarrow[t \rightarrow 0]{} \delta_y$ if the solute is initially at y . Eq. (1) is interpreted as a Fokker-Planck equation, and $C(t, x)$ is then the density of the process Z at time t generated by \mathcal{L} with starting point y .

^{*}Project-team TOSCA, INRIA, IECN, Campus scientifique, BP239, 54506 Vandœuvre-lès-Nancy, France, Antoine.Lejay@iecn.u-nancy.fr

[†]This work has been supported by the ANR SIMUDMRI (Simulation of diffusion MRI signals in biological tissue).

Note also that our method may be locally used for media with such a geometry. In addition to geophysics, many domains faces the problem of the simulation in discontinuous media: magneto-electro-encephalography [26], ecology [30], astrophysics [43], ...

(3) We simplify our analysis by considering that the dimension is equal to 2 and

$$D(x, y) = \begin{bmatrix} D^x(x) & 0 \\ 0 & D^y(x) \end{bmatrix} \text{ and } U(x, y) = \begin{bmatrix} 0 \\ U^y(x) \end{bmatrix}$$

Hence, \mathbf{n} points toward the y -direction. There is no difficulty to generalize our results in any dimension $d \geq 3$. We also assume that there exists a finite or countable set of separated points $\{x_i\}$ such D^x , D^y and U^y are discontinuous at these points and constant elsewhere.

(4) The main idea is the following. If $Z = (X, Y)$, then X does not depend on Y and is generated by the one-dimensional operator

$$\mathcal{L}^x = \frac{1}{2} \nabla (D^x(x) \nabla \cdot),$$

while Y is solution to the equation

$$Y_t = y + \int_0^t \sqrt{D^y(X_s)} dW_s^y + \int_0^t U^y(X_s) ds,$$

where W^y is a Brownian motion independent from X . The discontinuities of D may be seen as interfaces. From the heuristic point of view, these interfaces play the rôle of permeable barriers. However, this can only be said from a “mesoscopic” and not microscopic point of view, due to the irregularity of the paths of X . In particular, claims such that “the particle passes on one side with a given probability” makes no senses unless one says precisely where and when the particle goes.

(5) The simulation of one-dimensional stochastic processes generated by a divergence-form operator with discontinuous coefficients has now been the subject of a large literature and several algorithms have been proposed (See [7–10, 14, 16, 23, 27, 35, 38] for a non-exhaustive list of possible algorithms). Some of these schemes generate random variates with the true distribution of X_t . Other only provide some approximations. Yet the multi-dimensional case remains largely open and challenging (However, see [22] for some possible schemes, in general for locally isotropic coefficients).

Here, we consider a Euler type scheme which computes $X_{t+\delta t}$ from X_t for small values of δt . The probability that the particle leaves a ball of radius $R\sqrt{\delta t}$ centered on X_t during $[t, t + \delta t]$ is exponentially small as R increases.

Hence, if $\sqrt{\delta t}$ is much smaller than the distance between two discontinuities, then the behavior of the particle is mostly influence by the closest interface.

(6) Following the previous discussion and for the sake of simplicity, we also assume that there is only one interface at $x_1 = 0$. At time $t + \delta t$, the y -component given $(X_s)_{s \in [t, t + \delta t]}$ is then

$$Y_{t+\delta t} = Y_t + G + \bar{U}$$

where G is a Gaussian random variable independent from $(X_s)_{s \in [t, t + \delta t]}$ with mean 0 and variance

$$\text{Var}(G | (X_s)_{s \in [t, t + \delta t]}) = \int_t^{t+\delta t} D^y(X_s) ds$$

and $\bar{U} = \int_t^{t+\delta t} U^y(X_s) ds$. The possible values of $D^y(X_s)$ (resp. $V^y(X_s)$) are D_+^y and D_-^y (resp. U_+^y and U_-^y) according to the sign of X_s . Hence

$$\sigma^2 = D_+^y A^+(t, t + \delta t) + D_-^y A^-(t, t + \delta t) \text{ and } \bar{U} = U_+^y A^+(t, t + \delta t) + U_-^y A^-(t, t + \delta t)$$

where $A^+(t, t + \delta t)$ and $A^-(t, t + \delta t)$ are the *occupation times*:

$$A^+(t, t + \delta t) = \int_t^{t+\delta t} \mathbf{1}_{\{X_s \geq 0\}} ds \text{ and } A^-(t, t + \delta t) = \int_t^{t+\delta t} \mathbf{1}_{\{X_s < 0\}} ds.$$

Hence, the problem of simulating $Y_{t+\delta t}$ from Y_t reduces to the problem of simulating the occupation times A^+ and A^- .

(7) Following the seminal work of P. Lévy on the occupation time for the Brownian motion and the Arc-Sine distribution, the characterization of the occupation time distribution for general Markov processes has been the subject to a large literature since [17] (See e.g. [39–41]). A special branch of these researches concerns Brownian motions, Skew Brownian motions, Walsh Brownian motions (a generalization of the Skew Brownian motion by considering a Brownian diffusion on rays) and Skew Bessel processes. For this, the whole technology of excursions theory, scaling property, ... can be used (See e.g. [2, 31, 32]).

(8) The occupation time of the Skew Brownian motion has already been used in relation with modelling in geophysics [1] or in population ecology [30]. In particular, the trivariate density of the position of the Skew Brownian motion, its occupation time and its local time is given in [1]. However, it does not give rise to straightforward simulation algorithms.

(9) Hence, we combine techniques that consists in transforming X into a Skew Brownian motion as in [8, 23], in using the Brownian bridge properties

to determine the first hitting time of zero, and then use some known densities for the last passage of zero and the occupation time for the Skew Brownian motion.

This technique may also be seen as a refinement of the one proposed in [19], which was a variant of [13] for the simulation of Reflected Stochastic Differential Equations.

(10) Since our key point is the reduction to the Skew Brownian motion, all that is said in this article could also be applied to the process generated by a non-divergence form operator

$$\frac{1}{2} \sum_{i,j=1}^d D_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} + \sum_{i,j=1}^d U_i \frac{\partial}{\partial x_i}$$

under the same assumptions on D and U as above. In this case, the value of θ given in Eq. (3) shall be changed into $-\theta$ (See [23]).

2. The Stochastic Differential Equation the process solves

The existence of a diffusion (Feller process) associated to the divergence-form operator \mathcal{L} under our conditions of Parag. 3 and 6 follows from Gaussian estimates on the semi-group [37]. Proposition 1 gives some insight about the process. See [5] for a closely related representation of a diffusion process generated by a divergence-form operator. For an alternative construction, see [33, 34].

Proposition 1. *Given a two-dimensional Brownian motion (W^x, W^y) , the process (X, Y) with $(X_0, Y_0) = (x, y)$ is the unique solution to the Stochastic Differential Equation (SDE) with local time*

$$\begin{cases} X_t = x + \int_0^t \sqrt{D^x(X_s)} dW_s^x + \frac{D_+^x - D_-^x}{D_+^x + D_-^x} L_t^0(X), \\ Y_t = y + \int_0^t \sqrt{D^y(X_s)} dW_s^y + \int_0^t U^y(X_s) ds, \end{cases} \quad (2)$$

where $L_t^0(X)$ is the symmetric local time of X .

Proof. The problem of existence and uniqueness of (2) reduces to the problem of existence of the SDE solved by X . The x -component of the SDE may be interpreted as a particular case of SDE with local time whose theory is developed in [18]. In particular, strong existence and uniqueness hold.

If one takes a regularization of the coefficients, the corresponding stochastic processes (X^n, Y^n) is solution to a system of SDEs

$$\begin{cases} X_t^n = x + \int_0^t \sqrt{D_n^x(X_s^n)} dW_s^x + \frac{1}{2} \int_0^t \frac{dD_n^x}{dx}(X_s^n) ds, \\ Y_t^n = y + \int_0^t \sqrt{D_n^y(X_s^n)} dW_s^y + \int_0^t U_n^y(X_s^n) ds, \end{cases}$$

where D_n^x , D_n^y and U_n^y are smooth approximations of D^x , D^y and U^y . In particular, X^n is generated by the one-dimensional divergence form operator $\frac{1}{2} \left(\frac{d}{dx} D_n^x \frac{d}{dx} \right)$. As n goes to infinity, (X^n, Y^n) converges to (X, Y) under $\mathbb{P}_{(x,y)}$ [20, 37].

It is also known that X^n converges to X given by the first component of (2) [18, 23]. The convergence of Y^n to the second component of (2) follows from standard convergence results in this case (See for example [20]). \square

3. The x -component and the Skew Brownian motion

(11) Let us set

$$\begin{aligned} \Psi(x) &= \frac{1}{\sqrt{D_+^x}} \mathbf{1}_{x \geq 0} + \frac{1}{\sqrt{D_-^x}} \mathbf{1}_{x < 0} \\ \text{and } \theta &= \frac{\sqrt{D_+^x} - \sqrt{D_-^x}}{\sqrt{D_+^x} + \sqrt{D_-^x}}. \end{aligned} \quad (3)$$

The main point of our analysis is the following result, found for example in [8, 23, 29, 33, 34]. This is a direct consequence of the Itô-Tanaka formula and some manipulations on the local time $L_t^0(X)$ to the local time $L_t^0(V)$.

Proposition 2. *The process $V_t = \Psi(X_t)$ is a Skew Brownian motion of parameter θ , which means the unique strong solution to the SDE with local time*

$$V_t = \Psi(x) + W_t^x + \theta L_t^0(V). \quad (4)$$

(12) The Skew Brownian motion (SBM) was introduced by K. Itô and H.P. McKean [15] by the following way: a SBM is constructed by choosing the sign of each excursion of a Reflected Brownian motion independently with a Bernoulli random variable of parameter $\alpha = (1 + \theta)/2 \in (0, 1)$. That is, with probability α , the excursion has a positive sign. Otherwise, it has a negative sign. Its relationship with the solution of (4) was proved by J. Harrison and L. Shepp [12]. For a summary of the possible constructions of the SBM and its main property, see [21].

In the case of multiple discontinuities, the same kind of transforms may be applied but it gives rise to a SDE with local time at different points.

(13) Let us note that the occupation time for the SBM V is the same as for the process X . Hence, we still denote by $A^\pm(s, t)$ the occupation time of V .

4. The occupation time

Using the strong Markov property, simulating $A^\pm(s, t)$ when $X_s = 0$ reduces to the simulation of the occupation time $A^+(0, t)$ when $X_0 = 0$. Besides, using the scaling property for the SBM, $A^+(0, t)$ is equal in distribution to $tA^+(0, 1)$ for any $t > 0$.

Let us also note the trivial relation: $A^+(0, 1) + A^-(0, 1) = 1$.

The density and the distribution of the occupation time for the Skew Brownian motion of parameter α is explicitly known. We will not use Theorem 1 below under its full form, yet we recall it for it contains the density of the Arc-Sine distribution that will be used for simulating the last-passage time.

Theorem 1 ([17, Theorem 1]). *The density $f^{(\alpha)}(x)$ of $A^+(0, 1)$ is*

$$f^{(\alpha)}(x) = \frac{\alpha(1-\alpha)}{\pi} \frac{(x(1-x))^{-1/2}}{\alpha^2(1-x) + (1-\alpha)^2x}, \quad x \in (0, 1)$$

and its distribution function is

$$F^{(\alpha)}(x) = \frac{2}{\pi} \arcsin \sqrt{\frac{(1-\alpha)^2x}{(1-\alpha)^2x + \alpha^2(1-x)}}, \quad x \in [0, 1].$$

Note also that the triple $(A^+(0, 1), A^-(0, 1), L_1^0(V)^2)$ may also be represented in term of independent stable positive random variables of indice $1/2$ (See [2, Theorem 1]).

(14) Hence, it is possible to simulate $A^+(0, 1)$ easily but inverting its distribution function: If $U \sim \mathcal{U}(0, 1)$, where $\mathcal{U}(0, 1)$ is the uniform distribution on $[0, 1)$, then

$$A^+(0, 1) \stackrel{\text{law}}{=} (F^{(\alpha)})^{-1}(U),$$

which means that

$$A^+(0, 1) \stackrel{\text{law}}{=} \frac{\alpha^2\Gamma}{\alpha^2\Gamma + (1-\alpha)^2(1-\Gamma)}, \quad \Gamma = \sin^2\left(\frac{\pi U}{2}\right).$$

(15) When $\alpha = 1/2$, then V is a Brownian motion. In this case, $f^{(1/2)}$ is the density of the Arc-Sine distribution and Theorem 1 yields the famous result of P. Lévy [25] that the occupation time of the Brownian motion follows the Arc-Sine distribution.

5. Decomposition of the path

We have seen that the distribution of $(X_{t+\delta t}, Y_{t+\delta t})$ when (X_t, Y_t) is known is deduced from the one of $(X_{t+\delta t}, A^+(t, t + \delta t))$ when (X_t, Y_t) is known. Up to a simple transform, one may equivalently consider the couple $(V_{t+\delta t}, A^+(t, t + \delta t))$ when (V_t, Y_t) is known.

(16) Let us start with the simulation of $V_{t+\delta t}$ when V_t is known. For this, we apply an idea already used to simulated a Brownian motion which is killed at a boundary (See *e.g.* [11, 24]). Regarding the hitting time of zero, see *e.g.* [3].

For this, let us simulate a guess $V_{t+\delta t}$ as if there is no interface, that is $V_{t+\delta t} = V_t + \xi$ with $\xi \sim \mathcal{N}(0, \delta t)$.

If $V_{t+\delta t}V_t < 0$, then the path $(V_s)_{s \in [t, t+\delta t]}$ crosses zero at a stopping time \mathbf{g} . Using the properties of the Brownian bridge, $\mathbf{g} = t + \delta t \zeta / (1 + \zeta)$ where ζ follows an inverse Gaussian distribution $\mathcal{IG}(-x/y, x^2/\delta t)$ with $x = V_t$ and $y = V_{t+\delta t}$.

The inverse Gaussian distribution $\mathcal{IG}(\mu, \lambda)$ has density

$$r(\mu, \lambda, x) = \sqrt{\frac{\lambda}{2\pi x^3}} \exp\left(\frac{-\lambda(x - \mu)^2}{2\mu^2 x}\right).$$

Random variates following the inverse Gaussian distribution are easily simulated using the algorithm of [28] (See also [6, p. 148]).

If $V_{t+\delta t}V_t > 0$, then the path $(V_s)_{s \in [t, t+\delta t]}$ may cross zero. This happens with probability $\exp(-2xy/\delta t)$. If this happens, then the first hitting time of 0 is $\mathbf{g} = t + \delta t \zeta / (1 + \zeta)$ with $\zeta \sim \mathcal{IG}(x/y, x^2/\delta t)$.

If no crossing occurs, then we keep $V_{t+\delta t}$ as the next position of the Skew Brownian motion. In this case, $A^+(t, t + \delta t) = \delta t$ (resp. $A^+(t, t + \delta t) = 0$) if $V_t > 0$ (resp. $V_{t+\delta t} < 0$).

(17) Let us consider now the case where a crossing occurs at time $\mathbf{g} < \delta t$. Using the strong Markov property of the Skew Brownian motion and up to changing δt to $\delta t - \mathbf{g}$, one may assume that $\mathbf{g} = 0$ and consider that $V_t = 0$.

Hence, let us set $\mathfrak{d} = \inf \{ t \leq \delta t \mid V_t = 0 \}$ be the last passage time to 0. This is not a stopping time. Basically, this time relies on the lengths of the excursions of the Skew Brownian motion [32]. Hence, the distribution of \mathfrak{d} is the same as the one of the Brownian motion, and the ratio $\mathfrak{d}/\delta t$ is known to be Arc-Sine distributed on $[0, 1]$ (See [2, 25]). This means that $\mathfrak{d}/\delta t$ has a density $f^{(1/2)}$ introduced in Theorem 1. If U is a uniform random variable on $[0, 1)$, $\mathfrak{d} = \delta t \cos^2(2\pi U)$, so that \mathfrak{d} is easily simulated.

(18) We are now in a situation similar to the Williams' decomposition of the Brownian path [4, 36, 42].

As a Skew Brownian motion may be constructed from a Brownian motion by choosing the sign of the excursions independently, $(\mathfrak{d}^{-1/2}V_{\mathfrak{d}t})_{t \in [0, 1]}$ is inde-

pendent from the σ -algebra generated by $(V_t)_{t \geq \mathfrak{d}}$ and by \mathfrak{d} under \mathbb{P}_0 [2]. The process $(\mathfrak{d}^{-1/2}V_{\mathfrak{d}t})_{t \in [0,1]}$ has the distribution of a Skew Brownian bridge.

The part $(V_t)_{t \in [\mathfrak{d}, \delta t]}$ is called a *meander* and is a part of an excursion straddling t . Again from the construction of the Skew Brownian motion, $\mathbb{P}[V_{\delta t} > 0 | \mathfrak{d}] = \alpha$ and $\text{sgn}(V_{\delta t})$ and $|V_{\delta t}|$ are independent when \mathfrak{d} is given. In addition, $(|V_t|)_{t \in [\mathfrak{d}, \delta t]}$ is equal in distribution to $(|W_t|)_{t \in [\mathfrak{d}, \delta t]}$ for a Brownian motion W . The distribution $|W_{\delta t}|$ given \mathfrak{d} is the same as the distribution of e_κ with $\kappa = t + \delta t - \mathfrak{d}$, where e is an excursion whose length is greater than κ . It is also the distribution of a 3-dimensional Bessel process at time κ and is known to have the density [4, 13]

$$\frac{x}{\kappa} \exp\left(-\frac{x^2}{2\kappa}\right).$$

This density is called the *entrance law* for the excursion. Using the corresponding distribution function, $V_{t+\delta t}$ given \mathfrak{d} is distributed as

$$\varepsilon \sqrt{-2(t + \delta t - \mathfrak{d}) \log(U)},$$

where $U \sim \mathcal{U}(0, 1)$ and ε is an independent Bernoulli random variable with $\mathbb{P}[\varepsilon = 1] = 1 - \mathbb{P}[\varepsilon = -1] = \alpha$. Once the sign $\varepsilon = \text{sgn}(V_{t+\delta t})$ is known, $A^+(\mathfrak{d}, t + \delta t) = t + \delta t - \mathfrak{d}$ if $\varepsilon = 1$ and $A^+(\mathfrak{d}, t + \delta t) = 0$ if $\varepsilon = -1$.

(19) To conclude, it remains to simulate $A^+(0, \mathfrak{d})$ under \mathbb{P}_0 . As already noted, this random variable is independent from $V_{t+\delta t}$ given \mathfrak{d} . Under \mathbb{P}_0 , $A^+(0, \mathfrak{d})$ is equal in distribution to $\mathfrak{d}A^{\text{br}}$ [32, Eq. (84)], where A^{br} is the occupation time above 0 of the Skew Brownian bridge over $[0, 1]$ (which means the path $(V_t)_{t \in [0,1]}$ conditioned to $V_0 = V_1 = 0$).

The density $f^{(\alpha), \text{br}}$ of A^{br} with respect to the Lebesgue measure is known to be (See [40, Example 3.2] or [41])

$$f^{(\alpha), \text{br}}(x) = \frac{1}{2} \frac{\alpha(1-\alpha)}{(\alpha^2(1-x) + (1-\alpha)^2x)^{3/2}}, \quad x \in (0, 1).$$

For $\alpha = 1/2$, $f^{(\alpha), \text{br}}$ is the identity and A^{br} is uniformly distributed on $[0, 1]$. If $\alpha \neq 1/2$, the distribution function is

$$F^{(\alpha), \text{br}}(x) = \frac{\alpha(1-\alpha)}{1-2\alpha} \left(\frac{1}{\alpha} - \frac{1}{\sqrt{\alpha^2(1-x) + (1-\alpha)^2x}} \right).$$

and A^{br} is easily simulated by

$$A^{\text{br}} \stackrel{\text{law}}{=} \frac{\alpha^2}{1-2\alpha} \left(\frac{1}{\left(1 - \frac{1-2\alpha}{1-\alpha}U\right)^2} - 1 \right)$$

where $U \sim \mathcal{U}(0, 1)$.

(20) The simulation method presented in Algorithm 1 relies then on a combination of all the previous facts. This scheme was tested using the method given in [22] and gave good results.

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```

Input: The position  $X_t$  of the particle at time  $t$  and a time step  $\delta t$ .
Output: The couple  $(X_{t+\delta t}, A^+(t, t + \delta t))$  of the position  $X_{t+\delta t}$  of the
particle at time  $t + \delta t$  and its occupation time above 0.
/* Initialization */
Set  $x \leftarrow X_t / \sqrt{D^x(X_t)}$ ;
/* First guess of the position */
Set  $y \leftarrow x + \xi$  for a random variate  $\xi \sim \mathcal{N}(0, \delta t)$ ;
if  $xy > 0$  then Generate  $U_1 \sim \mathcal{U}(0, 1)$ ;
/* Check for a crossing */
if  $xy < 0$  or  $U_1 < \exp(-2xy/\delta t)$  then
| /* A crossing occurs */
| /* Compute the crossing time */
| Set  $\mathfrak{g} \leftarrow \delta t \zeta / (1 + \zeta)$  for a random variate  $\zeta \sim \mathcal{IG}(|x|/|y|, x^2/\delta t)$ ;
| /* Compute the last passage time */
| Set  $\mathfrak{d} \leftarrow \mathfrak{g} + (\delta t - \mathfrak{g})(F^{(1/2)})^{-1}(U_2)$  for a random variate  $U_2 \sim \mathcal{U}(0, 1)$ ;
| /* Set the position at time  $\delta t$  */
| Generate  $U_3 \sim \mathcal{U}(0, 1)$ ;
| if  $U_3 < \alpha$  then Set  $\varepsilon \leftarrow 1$  else Set  $\varepsilon \leftarrow -1$ ;
| Set  $y \leftarrow \varepsilon \sqrt{-2(\delta t - \mathfrak{d}) \log(U_4)}$  for a random variate  $U_4 \sim \mathcal{U}(0, 1)$ ;
| /* Compute the occupation time */
| if  $x > 0$  then Set  $A^1 \leftarrow \mathfrak{g}$  else Set  $A^1 \leftarrow 0$ ;
| Set  $A^2 \leftarrow (\mathfrak{d} - \mathfrak{g})(F^{\alpha, \text{br}})^{-1}(U_5)$  for a random variate  $U_5 \sim \mathcal{U}(0, 1)$ ;
| if  $y > 0$  then Set  $A^3 \leftarrow \delta t - \mathfrak{d}$  else Set  $A^3 \leftarrow 0$ ;
| return  $(y\sqrt{D^x(y)}, A^1 + A^2 + A^3)$ ;
else
| /* No crossing occurs */
| return  $(y\sqrt{D^x(y)}, \delta t)$ 
end

```

Algorithm 1: Simulation of the couple $(X_{t+\delta t}, A^+(t, t + \delta t))$ when X_t is given, under the hypotheses of Parag. 3 and 6.