Uncertain Darcy's problem and the stochastic particle transport

Semester Project - Master in CSE

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Problem statement

Underground flow $\rightarrow$ Uncertain Darcy's problem

$$\begin{cases} u = -A\nabla p, & \text{in } D, \\ \nabla \cdot u = f, & \text{in } D, \\ p = p_0, & \text{on } \Gamma_{in}, \\ p = 0, & \text{on } \Gamma_{out}, \\ \nabla p \cdot n = 0, & \text{on } \Gamma_N. \end{cases}$$

Stochastic particle transport $\rightarrow$ SDE

$$\begin{cases} dX(t) = u(X(t))dt + \sigma dW(t), \quad 0 \leq t \leq T, \\ X(0) = X_0 \in D, \end{cases}$$

Outline of the presentation

- Expected exit time from a domain
  - Setting
  - Numerical methods
  - Numerical experiments
- Theoretical investigation: perturbed SDE's
- The uncertain Darcy's problem

Mean exit time. Setting

Given a domain $D \subset \mathbb{R}^d$, $f\colon D \to \mathbb{R}^d, g\colon D \to \mathbb{R}^{d\times m}$ and an m-dimensional standard Wiener process $W(t)$, consider

$$\begin{cases} dX(t) = f(X(t))dt + g(X(t))dW(t), & 0 < t \leq T, \\ X(0) = X_0, & X_0 \in D. \end{cases}$$

The equation is defined in a domain $D \to$ boundary conditions

- *killing boundaries*: $X(t)$ is stopped,
- *reflecting boundaries*: $X(t)$ is reflected normally inside D.

Mean exit time. Problem statement

Problem. Estimate the exit time of the trajectories

$$\tau = \min\{\tau_e, T\}, \text{ where } \tau_e = \min\{t \colon X(t) \notin D\}.$$

Another quantity of interest, given $F \colon D \to \mathbb{R}$

$$\varphi = \varphi(T, X_0, F) = \mathbb{1}_{\{T<\tau_e\}} F(X(T)).$$

If $F \equiv 1$, exit probability

$$\Phi(T, X_0) := \Pr(\tau < T | X(0) = X_0) = 1 - \mathbb{E}(\varphi(T, X_0, 1)).$$

Goal. Estimate numerically τ and φ.

Discrete Euler-Maruyama (DEM)

Method:

$$\begin{cases} X^d_{h,i+1} = f(X^d_{h,i})h + g(X^d_{h,i})(W(t_{i+1}) - W(t_i)), \\ \quad X^d_{h,0} = X_0. \end{cases}$$

Parameters of interest computed naively

$$\tau^d_h = \min\{\tau^d_{h,e}, T\}, \text{ where } \tau^d_{h,e} = h \min\{i \colon X^d_{h,i} \notin D\}.$$
$$\varphi^d_h = \mathbb{1}_{\{T < \tau^d_{h,e}\}} F(X^d_{h,N}).$$

Missed exits $\to$ $1/2$ loss in weak order:

$$|\mathbb{E}(\tau^d_h) - \mathbb{E}(\tau)| = O(\sqrt{h}),$$
$$|\mathbb{E}(\varphi^d_h) - \mathbb{E}(\varphi)| = O(\sqrt{h}).$$

DEM - Missed exits

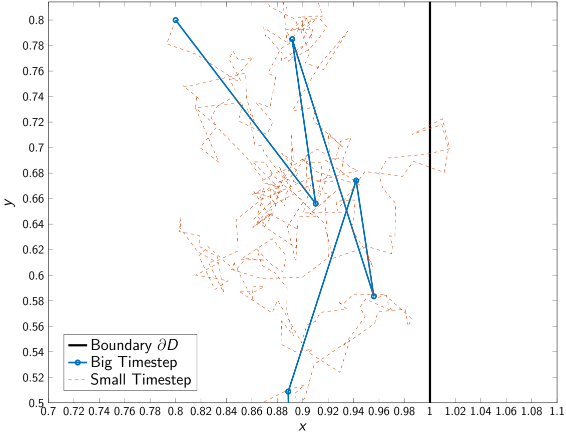


Figure : A missed exit. Running DEM with a big step size h the exit of a trajectory is not detected.

Continuous Euler-Maruyama (CEM)

Goal. Restore the weak order of convergence 1 of Euler-Maruyama
$\rightarrow$ Brownian bridge approach.
Method:

$$\begin{cases} X_h^c(t) = f(X_h^c(t_i))(t - t_i) + g(X_h^c(t_i))(W(t) - W(t_i)), \ t_i < t \leq t_{i+1}, \\ X_h^c(0) = X_0. \end{cases}$$

Estimate at each time step the probability of exit. If D is an half-space

$$\begin{aligned} &\Pr(\exists t \in [t_i, t_{i+1}] \quad X_h^c(t) \notin D | X_h^c(t_i) = x_i, X_h^c(t_{i+1}) = x_{i+1})) \\ &\quad = p(x_i, x_{i+1}, h) \\ &\quad = \exp\Big(-2 \frac{[n \cdot (x_i - z_i)][n \cdot (x_{i+1} - z_i)]}{hn \cdot (gg^T(x_i)n)} \Big). \end{aligned}$$

Continuous Euler-Maruyama (CEM)

Parameters of interest. Given $\tilde{U}$ a realization of U uniform random variable in $(0, 1)$

$$
\begin{aligned}
\tau_h^c &= \min\{T, \tau_{h,e}^c\}, \\
\text{where } \tau_{h,e}^c &= \min\{\tau_{h,e1}^c, \tau_{h,e2}^c\}, \\
\tau_{h,e1}^c &= \min\{h \min\{i \colon X_h^c(t_i) \notin D\}, \\
\tau_{h,e2}^c &= h \min\{i \colon \tilde{U} < p(X_h^c(t_{i-1}), X_h^c(t_i), h)\}, \\
\varphi_h^c &= \mathbb{1}_{\{T < \tau_{h,e}^c\}} F(X_h^c(T)).
\end{aligned}
$$

Weak order 1 is restored:

$$
\begin{aligned}
|\mathbb{E}(\tau_h^c) - \mathbb{E}(\tau)| &= O(h), \\
|\mathbb{E}(\varphi_h^c) - \mathbb{E}(\varphi)| &= O(h).
\end{aligned}
$$

Adaptivity

Goal. Restore the weak order of convergence 1 of Euler-Maruyama
$\to$ Adaptivity in space.
Setting. Consider $\sigma \in \mathbb{R}$ and

$$\begin{cases} dX(t) = f(X(t))dt + \sigma dW(t), & 0 < t \leq T, \\ X(0) = X_0, & X_0 \in D. \end{cases}$$

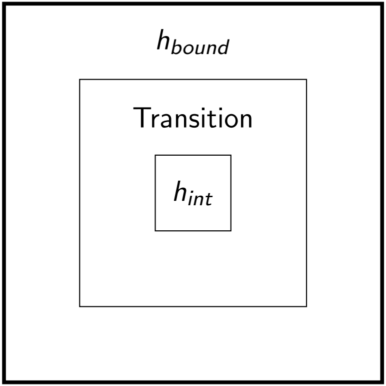
Idea. Given $l \in \mathbb{N}$, $h_0 > 0$, adapt step size h in DEM as follows

$$h = \max\left\{h_{bound}, \min\left\{h_{int}, \left(\frac{d}{(l+3)\sigma}\right)^2\right\}\right\}.$$

where

$$h_{bound} = 2^{-2l} h_0,$$
$$h_{int} = 2^{-l} h_0.$$

Adaptivity



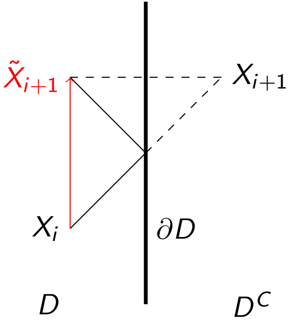
Domain divided in three parts

- Interior zone
  $\rightarrow h = h_{int} = 2^{-l} h_0,$
- Boundary zone
  $\rightarrow h = h_{bound} = 2^{-2l} h_0,$
- Intermediate zone
  $\rightarrow h = \left(\frac{d}{(l+3)\sigma}\right)^2.$

<u>Aim</u>. Order of convergence $O(\sqrt{h_{bound}}) = O(h_{int})$ saving computational time.

Reflecting boundaries

For all methods, equal treatment of reflecting boundaries. Consider $\partial D = \Gamma_r \cup \Gamma_k$ reflecting and killing boundaries.



1. Compute X_{i+1};
2. If the segment connecting X_i and X_{i+1} crosses Γ_r:
   $X_{i+1} \leftarrow \tilde{X}_{i+1}$ reflection of X_{i+1};
3. If $\tilde{X}_{i+1} \notin D$:
   Check the segment connecting X_i and $\tilde{X}_{i+1}$;

This method does not spoil the order of convergence.

A PDE approach

Consider the differential operator

$$\mathcal{L}u = f \cdot \nabla u + \frac{1}{2} g g^T : \nabla\nabla u,$$

Mean exit time. The mean exit time

$$\bar{\tau}(x) = \mathbb{E}(\tau | X(0) = x)$$

is solution of the following PDE

$$\begin{cases} \mathcal{L}\bar{\tau}(x) = -1, & \text{in } D, \\ \bar{\tau}(x) = 0, & \text{on } \Gamma_k, \\ \nabla\bar{\tau}(x) \cdot n = 0, & \text{on } \Gamma_r, \end{cases}$$

A PDE approach

Exit probability. The exit probability

$$\Phi(x, s, T) = \Pr(\tau < T | X(s) = x)$$

is solution of the following PDE

$$\begin{cases} \dfrac{\partial}{\partial t}\Phi(x,t,T) + \mathcal{L}\Phi(x,t,T) = 0, & \text{in } D, s \leq t < T, \\ \Phi(x,t,T) = 1, & \text{on } \Gamma_k, s \leq t \leq T, \\ \nabla\Phi(x,t,T) \cdot n = 0, & \text{on } \Gamma_r, s \leq t \leq T, \\ \Phi(x,T,T) = 0, & \text{in } D, \end{cases}$$

Solution of PDE's $\rightarrow$ reference solution for computation of weak error of CEM and DEM.

One-dimensional case - Setup

Consider $D = [-1, 1]$ and the SDE

$$\begin{cases} dX(t) = f(X(t))dt + g(X(t))dW(t), & 0 < t \leq T, \\ X(0) = X_0, & X_0 \in D. \end{cases}$$

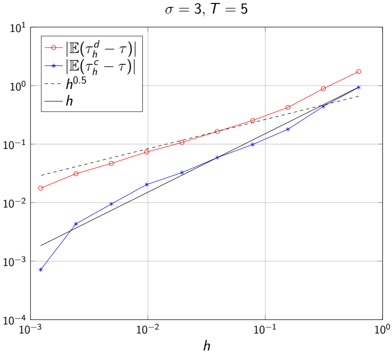
Set mixed boundary conditions and

$$f(x) = -V'(x), \text{ where } V(x) = 0.1(8x^4 - 8x^2 + x + 2),$$
$$g(x) = \sigma \in \mathbb{R}.$$

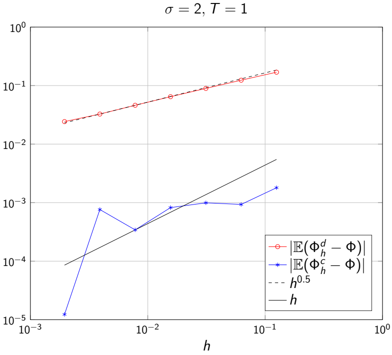
<u>Goal</u>. Verify the weak order of convergence of DEM and CEM.
<u>Reference solution</u>. Solution of PDE's

- Analytic solution in one-dimensional case for $\bar{\tau}$,
- Finite Differences for Φ.

One-dimensional case - Results

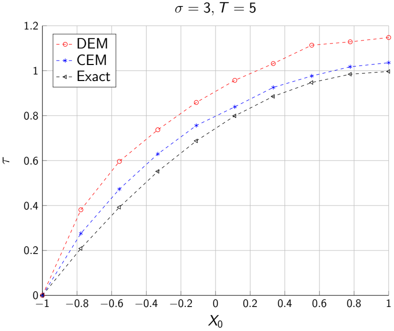


(a) Approximation of τ

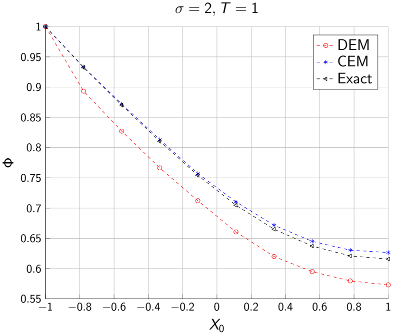


(b) Approximation of Φ

Figure : Results for the one-dimensional case.



(a) Approximation of τ



(b) Approximation of Φ

Figure : Approximation of τ and Φ with respect to initial value X_0.

Two-dimensional case - Setup

Consider $D = [-1, 1]^2$ and the SDE

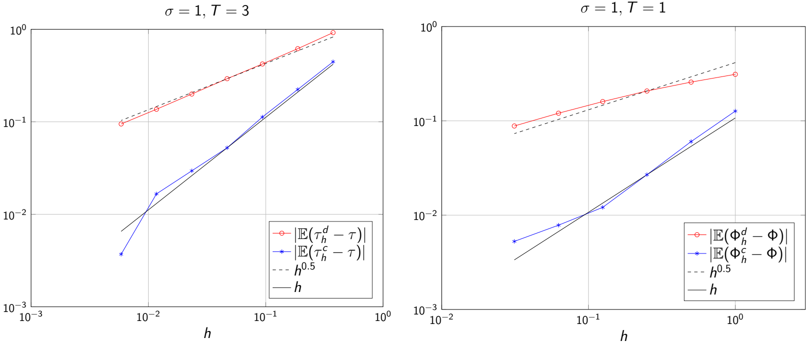
$$\begin{cases} dX(t) = f(X(t))dt + g(X(t))dW(t), & 0 < t \leq T, \\ X(0) = X_0, & X_0 \in D. \end{cases}$$

Setting:

- Mixed boundary conditions,
- $f = 0 \rightarrow$ pure Brownian motion.

Goal. Verify the weak order of convergence of DEM and CEM.
Reference solution. Solution of PDE's with FEM.

Two-dimensional case - Results



(a) Approximation of τ (b) Approximation of Φ

Figure : Results for the two-dimensional case.

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Theoretical investigation - Motivation

Consider the velocity field u solution of the Darcy's problem and an approximation $\tilde{u}$ of u. Consider then the SDE

$$\begin{cases} dX(t) = u(X(t))dt + \sigma dW(t), \quad 0 \leq t \leq T, \\ X(0) = X_0 \in D, \end{cases}$$

and the SDE

$$\begin{cases} d\tilde{X}(t) = \tilde{u}(\tilde{X}(t))dt + \sigma dW(t), \quad 0 \leq t \leq T, \\ \tilde{X}(0) = X_0 \in D, \end{cases}$$

<u>Problem</u>. If $\tilde{u}$ converges to u, does $\tilde{X}(t)$ converge to $X(t)$? What is the effect on the order of convergence of numerical methods?

In an abstract form, consider $f : \mathbb{R} \to \mathbb{R}$ and the SDE

$$\begin{cases} dX(t) = f(X(t))dt + \sigma dW(t), \quad 0 < t \leq T, \\ X(0) = X_0, \end{cases}$$

Consider a perturbation of the transport field $f^\varepsilon : \mathbb{R} \to \mathbb{R}$ and

$$\begin{cases} dX^\varepsilon(t) = f^\varepsilon(X^\varepsilon(t))dt + \sigma dW(t), \quad 0 < t \leq T, \\ X^\varepsilon(0) = X_0. \end{cases}$$

Proposition

If the following assumptions are verified for a constant $K > 0$

1. $|f(x) - f(y)| \leq K|x - y|, \; \forall x, y \in \mathbb{R}$,
2. $|f(x)| \leq K(1 + |x|), \; \forall x \in \mathbb{R}$,

and if the solution $X^\varepsilon(t)$ *of the perturbed SDE exists, then*

$$\mathbb{E} \sup_{0 \leq t \leq T} |X^\varepsilon(t) - X(t)|^2 \leq 2T^2 \|f - f^\varepsilon\|_\infty^2 e^{2K^2 T^2}.$$

Remark. We proved similar results for two independent Brownian motions W_1, W_2 and in the d-dimensional case.

Theoretical investigation - Numerical convergence

Consider the Euler-Maruyama method applied to the perturbed SDE

$$\begin{cases} X_{n+1}^{\varepsilon} = X_n^{\varepsilon} + f^{\varepsilon}(X_n^{\varepsilon})h + \sigma(W(t_{n+1}) - W(t_n)), \quad n = 0, \dots, N-1, \\ X_0^{\varepsilon} = X_0. \end{cases}$$

Problem. Determine the convergence of X_n^{ε} to $X(t)$ with respect to h and ε.

Proposition

If the following assumptions are verified for a constant $K > 0$

1. $|f(x) - f(y)| \leq K|x - y|, \ \forall x, y \in \mathbb{R}$,
2. $|f(x)| \leq K(1 + |x|), \ \forall x \in \mathbb{R}$,

and if the solution $X^\varepsilon(t)$ of the perturbed SDE exists, then

$$\sup_{n=0,\ldots,N} \mathbb{E}\|X(nh) - X_n^\varepsilon\| \leq Ch + \|f^\varepsilon - f\|_\infty \frac{e^{KT} - 1}{K},$$

with C a real constant independent of h and depending only on the final time T and the Lipschitz constant K of f.

Idea of the proof. Use triangular inequality summing and subtracting the variable X_n given by Euler-Maruyama applied to the non-perturbed equation.

Theoretical investigation - Numerical convergence

Remark. If D is a square domain and f^ε is a piece-wise constant interpolation of f on a regular grid of equal size ε in the two directions

$$\sup_{n=0,\dots,N} \mathbb{E}\|X(nh) - X_n^\varepsilon\| = O(h) + O(\varepsilon).$$

Therefore, set $h = O(\varepsilon)$ to avoid extra computational cost.

Numerical experiments confirm this behaviour.

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Darcy's problem - Setting

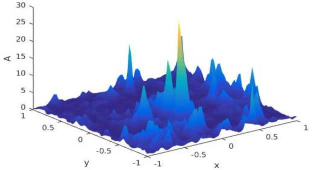
Consider

$$\begin{cases} u = -A\nabla p, & \text{in } D, \\ \nabla \cdot u = 0, & \text{in } D, \\ p = p_0, & \text{on } \Gamma_{in}, \\ p = 0, & \text{on } \Gamma_{out}, \\ \nabla p \cdot n = 0, & \text{on } \Gamma_N, \end{cases}$$

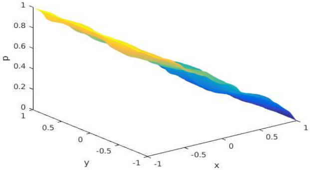
where A is a random field such that $A = e^{\gamma}$, where

$$\mathrm{cov}_{\gamma}(x_1, x_2) = \frac{\sigma_A^2}{\Gamma(\nu) 2^{\nu-1}} \left(\sqrt{2\nu} \frac{|x_1 - x_2|}{L_c} \right)^{\nu} K_{\nu} \left(\sqrt{2\nu} \frac{|x_1 - x_2|}{L_c} \right),$$

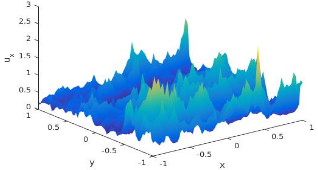
for $\nu \geq 0.5$. For each realization of A, we solve the equation with linear FEM on a regular grid with `FreeFem++`.



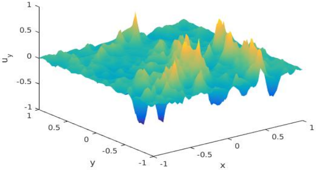
(a) Random field



(b) Pressure



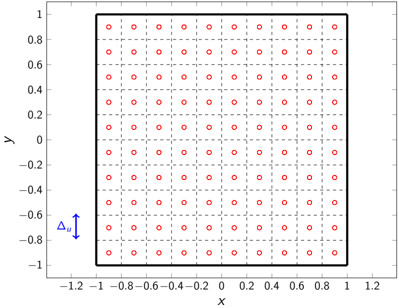
(c) x component of velocity field



(d) y component of velocity field

Darcy's solution in DEM and CEM

Evaluation of the FEM solution at each time step
$\rightarrow$ unaffordable computational cost



1. Define a grid with regular spacing Δ_u in both directions;
2. Evaluate the FEM solution in the center of each square;
3. Velocity field for the SDE piece-wise constant;

At each step only a matrix evaluation
$\rightarrow$ huge gain in computational cost

Darcy's problem with stochastic particles

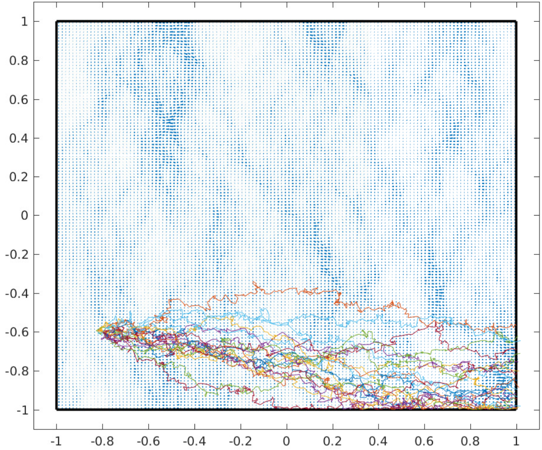


Figure : Velocity field and transported particles. Reflections on the lower boundary and absorbtion on the right boundary are clear.

Estimation of the mean exit time

Estimate the mean exit time $\rightarrow$ nested Montecarlo simulation
M_d realizations of Darcy's problem, M_t trajectories.

Algorithm 1 Estimation of the mean exit time $\bar{\tau}$

for $i = 1$ to M_d **do**
  Generate A;
  Solve the Darcy's problem;
  Interpolate velocity field u on a grid of size Δ_u;
  for $j = 1$ to M_t **do**
    Estimate $(\tau_h)_{i,j}$ using DEM or CEM with step size $h \sim \Delta_u$;
  end for
end for
return $\bar{\tau} = \frac{1}{M_d M_t} \sum_{j=1}^{M_d} \sum_{j=1}^{M_t} (\tau_h)_{i,j}$

This algorithm gives consistent result with satisfying performances.

Conclusion

- We verified the properties of three numerical methods for estimating the mean exit time and the exit probability.
- The Continuous Euler-Maruyama offers the best performances and accuracy among the studied methods.
- We studied the effect of a perturbation term in the analytic and numerical solution of an SDE.
- If an interpolation step is performed, the step size for time integration must be balanced with the interpolation grid size.
- We applied the studied techniques to the Darcy's problem, leading to a stable and efficient nested Montecarlo simulation.
- Future developments could regard integrating MLMC techniques in outer or inner Montecarlo estimation, as well as integrating the modeling of extraction wells.