Entropic metastability in the narrow escape problem

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PhD under the supervision of Tony Lelièvre, Urbain Vaes & Gabriel Stoltz

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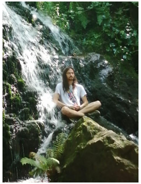
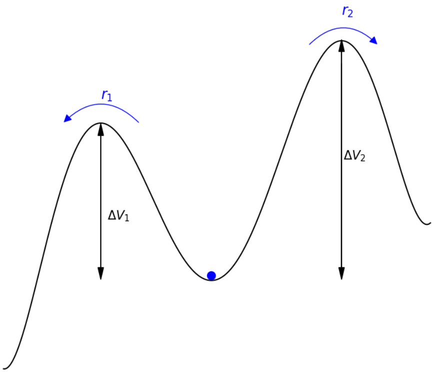


Metastability of **energetic** origin



Thermal particle living in a potential well:

- Slow dynamics between the wells
- Long time to escape. This is a **rare event**

Toy model: Langevin particle in a double-well potential

How much time does it take to **escape** the well?

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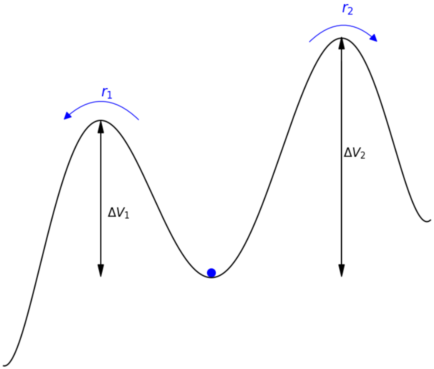

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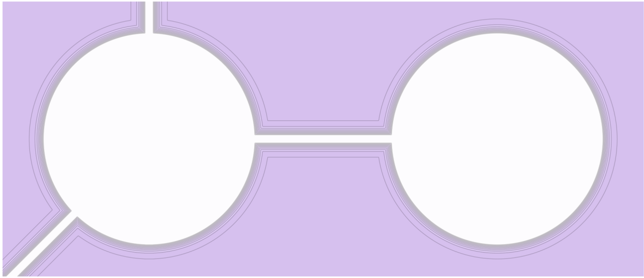
Eyring-Kramers' formula

The escape time is exponentially distributed, with a rate r_i, with $i \in \{1, 2\}$:

$$r_i = C_i \exp\left(-\frac{\Delta V_i}{k_B T}\right)$$

What if energy is not the driving factor?



A potential made of a confining well and a few **narrow canals**:

Still a long time to escape. This is still a **rare event**

Is there an equivalent to the Eyring-Kramers formula in this case?

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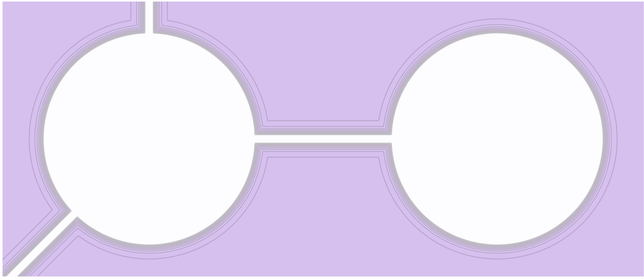

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Applications: Biology (Ion transfer between cells, neurotransmitter), Statistical physics

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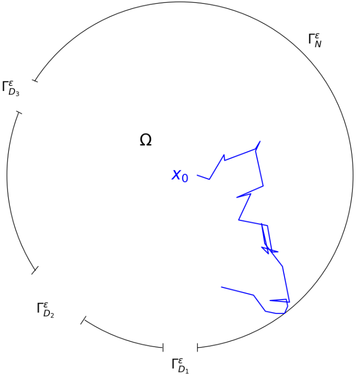
The narrow escape problem

Toy model of the metastability of entropic origin:



Setting:

- Domain Ω with holes Γ^ε_D and reflecting boundary Γ^ε_N
- A Brownian motion starting at x_0 taking a long time to exit $\tau_\varepsilon = \inf\{t \geq 0 \,|\, X_t \notin \overline{\Omega}\}$

$$\mathrm{d}X_t = \sqrt{2}\,\mathrm{d}B_t - \mathbb{1}_{\Gamma^\varepsilon_{\mathrm{D}}}(X_t)n(X_t)\mathrm{d}L_t.$$

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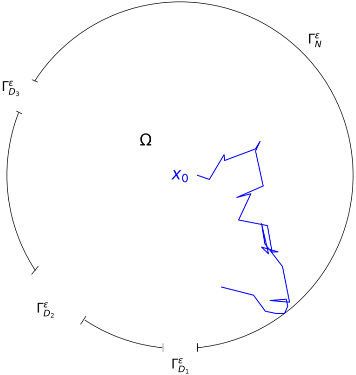

Setting:

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$$\mathrm{d}X_t = \sqrt{2}\,\mathrm{d}B_t - \mathbb{1}_{\Gamma_{\mathrm{D}}^\varepsilon}(X_t)n(X_t)\mathrm{d}L_t.$$

Goal: In the limit of small holes $\varepsilon \to 0$:

- The law of the escape time τ_ε
- The law of exit hole X_{τ_ε}

A spectral approach to solve the narrow escape problem

Let $\rho(x,t)$be the density of probability to be at x at time $t < \tau_\varepsilon$ starting from ρ_0 then it verifies the Fokker-Plank equation:

$$\begin{cases} \partial_t \rho = \Delta \rho & \text{in } \Omega \\ \partial_n \rho = 0 & \text{on } \Gamma_N^\varepsilon \\ \rho = 0 & \text{on } \Gamma_D^\varepsilon \\ \rho(\cdot, 0) = \rho_0 & \text{in } \Omega \end{cases} \tag{1}$$

Idea of the proof: Itô's lemma, the local time is continuous with finite variation

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Idea of the proof: Itô's lemma, the local time is continuous with finite variation

The operator $\mathcal{L}_\varepsilon$ associated to (1) is self-adjoint with compact resolvent

→ there exists an orthonormal basis in $H^1(\Omega)$ of eigenfunctions $(u_\varepsilon^k)_{k\geq 0}$ and eigenvalues $(\lambda_\varepsilon^k)_{k\geq 0}$ ranked in increasing order $\lambda_\varepsilon^0 < \lambda_\varepsilon^1 < \ldots$

$$\rho(x, t) = \sum_{k\geq 0} \langle \rho_0,\, u_\varepsilon^k \rangle \mathrm{e}^{-\lambda_\varepsilon^k t} u_\varepsilon^k(x)$$

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Large time behaviour

If the eigengap $\lambda_\varepsilon^1 - \lambda_\varepsilon^0$ is large, then the large time behaviour of $\rho(x,t)$ is dominated by the first eigenmode

$$\rho(x,t) = \sum_{k\geq 0} \langle \rho_0,\, u_\varepsilon^k \rangle \mathrm{e}^{-\lambda_\varepsilon^k t} u_\varepsilon^k(x) \approx \langle \rho_0,\, u_\varepsilon^0 \rangle \mathrm{e}^{-\lambda_\varepsilon^0 t} u_\varepsilon^0(x)$$

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From the probability, we deduce the behaviour of quantities of interest:

- The exit time distribution is exponentially distributed with parameter λ_ε^0
- The law of the exit hole will be dictated by u_ε^0
- Starting from $\rho_0 \propto u_\varepsilon^0$, these results are exact

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$\Rightarrow$ Rigorous approach: the quasi-stationary distribution [1]

[1] Di Gesù, Lelièvre, Le Peutrec and Nectoux, *Faraday Discussion*, (2016)

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Quasi-stationary distribution (QSD)

Definition

A quasi-stationary distribution ν_ε is a probability measure on $\overline{\Omega}$ such that

$$\text{If } X_0 \sim \nu_\varepsilon, \quad \text{then } \mathrm{Law}(X_t \,|\, t < \tau_\varepsilon) = \nu_\varepsilon$$

Starting from $\rho_0 = u_\varepsilon^0$, for any $x \in \Omega$

$$\rho(x,t) = \mathrm{e}^{-\lambda_\varepsilon^0 t} u_\varepsilon^0(x)$$

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Consequences:

- The quasi-stationary distribution is the first eigenmode up to a renormalisation
- The QSD is the Yaglom limit of the process

$$\text{If } X_0 \in \Omega, \quad \text{then } \lim_{t \to +\infty} \mathrm{Law}(X_t \,|\, t < \tau_\varepsilon) = \nu_\varepsilon$$

First result on the QSD

Theorem [C., Lelièvre, Normand, Stoltz, Vaes]

There exists a unique quasi-stationary distribution ν_ε associated to the process $(X_t)_{t\geq 0}$. It is the L^1-normalised principal eigenfunction of $-\Delta$ with mixed boundary conditions. Furthermore, ν_ε is continuous on $\overline{\Omega}$, and $\partial_n \nu_\varepsilon$ is a measure on $\partial\Omega$.

Corollary

Starting from $X_0 \sim \nu_\varepsilon$, we know

- The exit time $\tau_\varepsilon \sim \mathrm{Exp}(\lambda_\varepsilon^0)$
- The exit place $\mathbb{P}(X_{\tau_\varepsilon} \in \Gamma_k^\varepsilon) = -\frac{1}{\lambda_\varepsilon^0}\partial_n \nu_\varepsilon(\Gamma_k^\varepsilon)$

Furthermore, τ_ε and X_{τ_ε} are independent.

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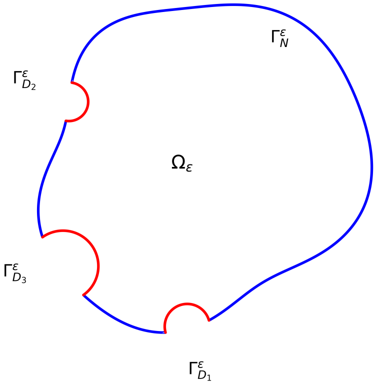
The QSD as an eigenvalue problem



We want to find the QSD ν_ε :

$$\begin{cases} -\Delta \nu_\varepsilon = \lambda_\varepsilon \nu_\varepsilon & \text{in } \Omega_\varepsilon \\ \partial_n \nu_\varepsilon = 0 & \text{on } \Gamma_N^\varepsilon \\ \nu_\varepsilon = 0 & \text{on } \Gamma_D^\varepsilon \end{cases}$$

N holes of radius $r_\varepsilon^{(i)}$ centered at $x^{(i)} \in \partial\Omega$

Already studied in [2] for the disk and the ball

Use of a quasi-mode ansatz to get the asymptotic expansion of ν_ε in the limit $\varepsilon \to 0$

[2] Lelièvre, Rachid and Stoltz, *preprint* (2024)

Results on the exit time

Theorem [Asymptotic of the exit time]

Consider only one hole of radius r_ε. Then there exists a $C_{d,\Omega} > 0$ such that the eigenvalue λ_ε^0 scales as:

$$\lambda_\varepsilon^0 = \Big(\mathbb{E}[\tau_\varepsilon]\Big)^{-1} = \begin{cases} C_{2,\Omega}\left(\log(r_\varepsilon)\right)^{-1} & + \mathrm{O}\left(\left[\log(r_\varepsilon)\right]^{-2}\right) & \text{for } d = 2 \\ C_{3,\Omega}\, r_\varepsilon & + \mathrm{O}({r_\varepsilon}^2 \log(r_\varepsilon)) & \text{for } d = 3 \\ C_{d,\Omega}\, r_\varepsilon^{d-2} & + \mathrm{O}(r_\varepsilon^{d-1}) & \text{for } d > 3 \end{cases}$$

Where does the scaling comes from?

The fundamental solution of the laplacian Λ in dimension d:

$$\lambda_\varepsilon^0 \sim C_{d,\Omega}\Lambda(r_\varepsilon)^{-1} \qquad \text{and} \qquad C_{d,\Omega} = \frac{\max\{d-2,\, 1\}}{2}\,\frac{|\mathscr{C}(0,1)|}{|\Omega|}$$

Results for N exit holes and $d \geq 2$

We define

$$K_\varepsilon^i = -\Lambda(r_i^\varepsilon)^{-1} = \begin{cases} -\dfrac{1}{\log(r_i^\varepsilon)} & \text{if } d = 2 \\ (r_i^\varepsilon)^{d-2} & \text{if } d \geq 3 \end{cases} \qquad \overline{K}_\varepsilon = K_1 + \cdots + K_N$$

Theorem [Asymptotic of the exit time]

The mean exit time when $X_0 \sim \nu_\varepsilon$ is given by $\mathbb{E}_{\nu_\varepsilon}[\tau] = \frac{1}{\lambda_\varepsilon}$, where

$$\lambda_\varepsilon = C_{d,\Omega}\overline{K}_\varepsilon + \begin{cases} \mathrm{O}\left(\overline{K}_\varepsilon^2\right) & \text{for } d = 2 \\ \mathrm{O}\left(\overline{K}_\varepsilon^2 \log\left(\overline{K}_\varepsilon\right)\right) & \text{for } d = 3 \\ \mathrm{O}\left(\overline{K}_\varepsilon^{\frac{d-1}{d-2}}\right) & \text{for } d \geq 4 \end{cases}$$

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Exit time for N exit holes and $d \geq 2$

Theorem [Exit hole distribution]

The probability to exit through hole $i \in \{1, \dots, N\}$is given by:

$$\mathbb{P}_\varepsilon(X_\tau \in \Gamma^\varepsilon_{D_i}) = \frac{K^i_\varepsilon}{\overline{K_\varepsilon}} + \begin{cases} \mathrm{O}(\overline{K_\varepsilon}), & \text{for } d = 2 \\ \mathrm{O}(\overline{K_\varepsilon} \log(\overline{K_\varepsilon})), & \text{for } d = 3 \\ \mathrm{O}(\overline{K_\varepsilon}^{\frac{1}{d-2}}) & \text{for } d \geq 4 \end{cases}$$

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Exit point for 2 exit holes and $d \geq 2$

Theorem [Exit hole distribution]

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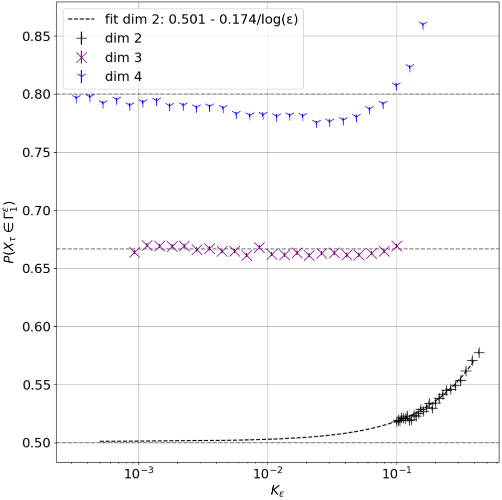
Example: with $N = 2$, scaling as $r^{(1)}_\varepsilon = \varepsilon$ and $r^{(2)}_\varepsilon = 2\varepsilon$

- in dimension 2, $\mathbb{P}_{\nu_\varepsilon}(X_\tau \in \Gamma^\varepsilon_{D_1}) \approx \frac{1}{2}$ equal to $\mathbb{P}_{\nu_\varepsilon}(X_\tau \in \Gamma^\varepsilon_{D_2})$
- in dimension 3, $\mathbb{P}_{\nu_\varepsilon}(X_\tau \in \Gamma^\varepsilon_{D_1}) \approx \frac{1}{3}$ twice smaller than $\mathbb{P}_{\nu_\varepsilon}(X_\tau \in \Gamma^\varepsilon_{D_2})$
- in dimension 4, $\mathbb{P}_{\nu_\varepsilon}(X_\tau \in \Gamma^\varepsilon_{D_1}) \approx \frac{1}{5}$ four times smaller than $\mathbb{P}_{\nu_\varepsilon}(X_\tau \in \Gamma^\varepsilon_{D_2})$

Numerics for the exit point



- Monte Carlo simulation of the exit hole for a unit ball in dimension $\{2, 3, 4\}$
- Two holes, one twice bigger than the other
- Averaged over 64000 realisations
- The asymptotic regime is hard to reach in dimension 2 and 4

Monte Carlo simulation of the narrow escape problem

Given $X_0^1, \dots, X_0^M$, repeat the following steps:

1. Propose move by Euler–Maruyama discretization:

$$\widehat{X}_{n+1} = X_n + \sqrt{2\Delta t}\,\xi_n, \qquad \xi_n \sim \mathcal{N}(0, \mathrm{I}_d)$$

2. If $\widehat{X}_{n+1} \in B(x_i, r_i^\varepsilon)$, register exit event for door $i \in \{1, \dots, N\}$. **Done**
3. Else if $\widehat{X}_{n+1} \notin \Omega$, reject move (*reflecting boundary*)
4. Else, set $X_{n+1} = \widehat{X}_{n+1}$

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This approach is computationally expensive

- Time step should be small compared to $(r_i^\varepsilon)^2$ for $i \in \{1, \dots, N\}$
- Mean exit time increases as $\varepsilon \to 0$

Example: in dimension 3 with $r_i^\varepsilon \propto \varepsilon$, the mean exit time scales as $\frac{1}{\varepsilon}$
$\rightsquigarrow$ Simulation cost of M exit events scales as $M\varepsilon^{-3}$

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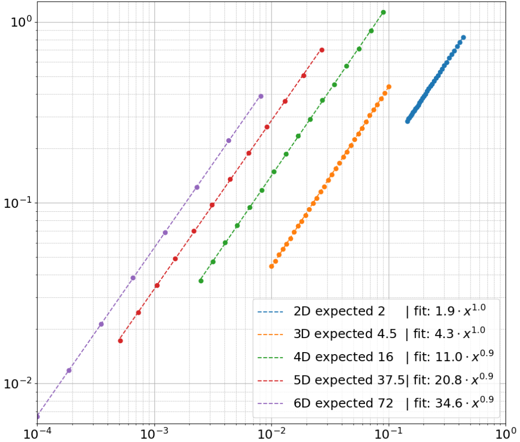
Measure of the exit time in high dimension



- Monte Carlo simulation of the exit time τ_ε for a unit ball in dimension $\{2, 3, 4, 5\}$
- Correct scaling in K_ε, but:

Dimension	C_d^{ball}	C_d^{ball} (simu)
2	2	1.9
3	4.5	4.3
4	16	11
5	32.5	20.8
6	72	34.6

Computation time:

1 week on the Cermics cluster

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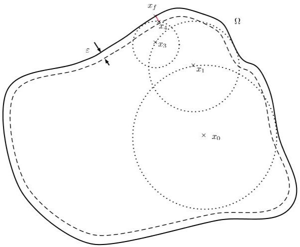
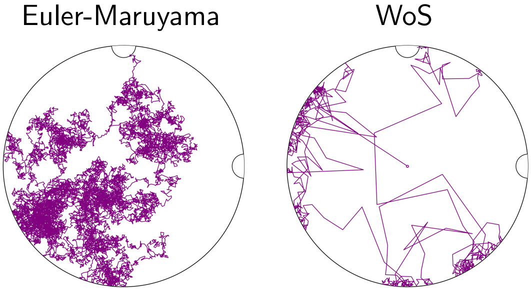
A more efficient simulation method: walk-on-spheres

When far from the boundary, instead of Euler–Maruyama we use *walk-on-spheres*

- Compute radius $r_n = \mathrm{dist}(X_n, \partial\Omega_\varepsilon)$.
- Sample the exit point X_{n+1} from $B(X_n, r_n)$, uniformly on $\partial B(X_n, r_n)$
- Sample exit time $\Delta t_n \sim \mathcal{T}_{r_n}$, with $\mathcal{T}_{r_n}$ the law of first exit time from the ball
- Update time: $t_{n+1} = t_n + \Delta t_n$





Walk on star algorithm

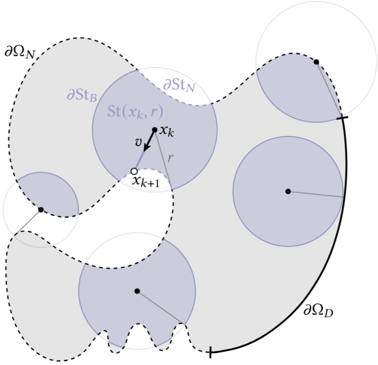


Figure from the original article *Walk on Stars: A Grid-Free Monte Carlo Method for PDEs with Neumann Boundary Conditions* by Sawhney and al. (2023)

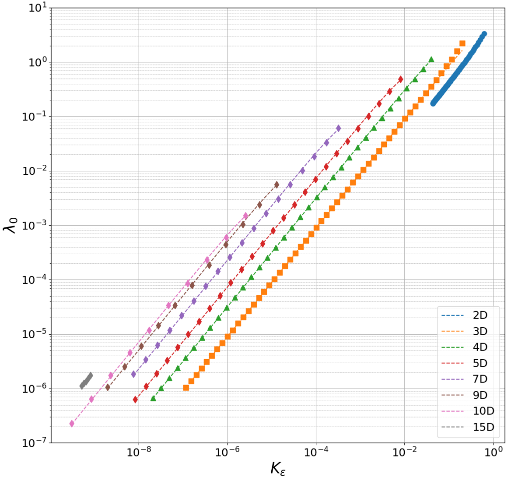
Key idea: Walk on sphere on star-shaped domains

Algorithm: WalkOnStars$(x, \eta, r_{\min})$

Initialise $\tau = 0$

- Compute distance $d_D = \mathrm{dist}(x, \Gamma^{\varepsilon}_{\mathrm{D}})$
- If $d_D < \eta$: **return** $(\tau,\ k)$ such that $x \in \Gamma^{\varepsilon}_{D_k}$
- Set radius $r \leftarrow \max(r_{\min},\ d_D)$
- Sample direction v uniformly on $\mathbb{S}^{d-1}$
- Set next point $p \leftarrow x + rv$
- Sample source point y on $[x, p]$ with density $G_{B(x,r)}(x, \cdot\,)\mathbb{1}_{\Omega}$
- Compute the contribution$\tau \leftarrow \tau + |G_{B(x,y)}|$

Walk of stars results: escape time



Dimension	C_d^{ball}	C_d^{ball} (simu)
2	4	3.95
3	9	8.95
4	32	31.7
5	75	73.4
7	245	229.2
9	567	509
10	800	717
15	2925	2255

Computation time:

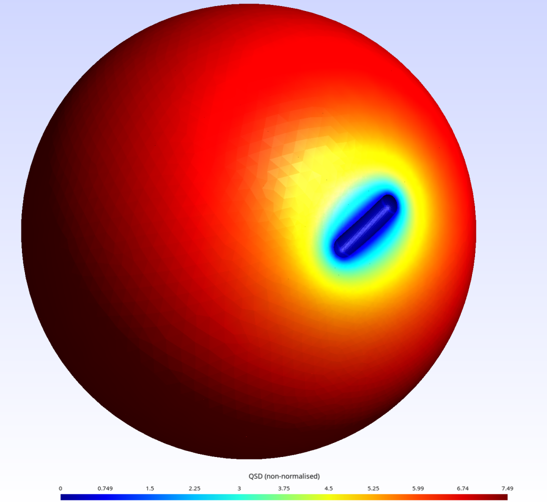
1 night on the Cermics cluster

Conclusion

- The narrow escape is a toy model of metastability of entropic origin
- With our approach we can solve it for any (locally) smooth domain in any dimension
- We get the scaling of the escape time and the law of exit hole

Future work:

- Study the influence of the hole geometry on the escape event → the slit



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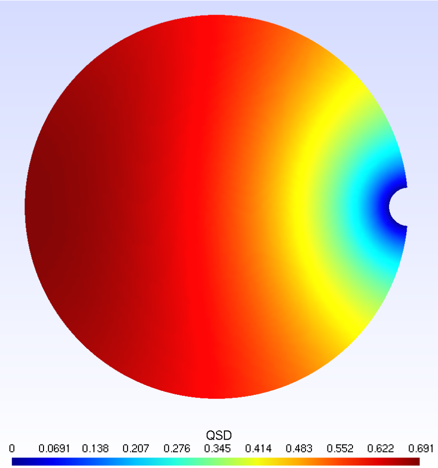
How to build the quasimode (1 hole)?

From the simulations, u_ε^0 is almost constant far from the hole:



We can approximate the solution u_ε^0 by a quasimode (semi-classical technique):

$$u_0^\varepsilon \simeq \varphi_\varepsilon = 1 + K_\varepsilon f$$

with K_ε the approximation of the eigenvalue and f the solution when the hole is a point:

$$\begin{cases} -\Delta f = 1 & \text{in } \Omega \\ \partial_n f = 0 & \text{on } \partial\Omega \backslash \{x^{(h)}\} \end{cases}$$

with $x^{(h)}$ the center of the hole.

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Construction of the quasimode

By the compatibility equation

$$|\Omega| = \int_{\Omega} \Delta f = \int_{\partial\Omega} \partial_n f$$

But $\partial_n f = 0$ on $\partial\Omega \backslash \{x^{(h)}\}$, so $\partial_n f$ is not a function but a distribution. A part of my PhD is to have approximation of the singularity of the solution of in the weak $W^{1,p}(\Omega)$ sense:

$$\begin{cases} -\Delta f = 1 & \text{in } \Omega \\ \partial_n f = -|\Omega| \delta_{x^{(h)}} & \text{on } \partial\Omega \end{cases}$$

with $f \in \left\{ u \in W^{1,p}(\Omega),\ \Delta u = 1 \in L^p(\Omega), \partial_n u = -|\Omega|\delta_{x^{(h)}} \in W^{-\frac{1}{p},p}(\Omega) \right\}$

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Construction of the quasimode

Explicit expressions for simple geometries [1], ex: the unit sphere with one hole on $x^{(h)}$

$$\varphi_\varepsilon(x) = 1 + \frac{1}{\sqrt{3\pi}} K_\varepsilon^{(h)} \left[\frac{1}{|x - x^{(h)}|} - \frac{1}{2} \log\left(1 - x \cdot x^{(h)} + \left|x - x^{(h)}\right|\right) + \frac{|x|^2}{4} \right]$$

But in the general case, we have been able to do expansions around the singularity only in the following settings:

- **dimension** 2, any smooth domain for flat holes
- **dimension** 2 **and above**, any C^2 domain, locally smooth, with circular holes
- **dimension** 3, any smooth domain for slit-like holes

I will focus in the dimension 3 setting with N circular holes

Properties of the quasimode

Theorem [Quasimode properties]

One can construct a quasimode $\varphi_\varepsilon \in H^1(\Omega_\varepsilon)$ that satisfies:

- An approximate eigenvalue equation: with $C_{3,\Omega} \in \mathbb{R}^+$

$$\left\| -\Delta \varphi_\varepsilon - C_{3,\Omega} \overline{r_\varepsilon} \varphi_\varepsilon \right\|_{L^2(\widetilde{\Omega}_\varepsilon)} = \mathrm{O}\left((\overline{r_\varepsilon})^2 \right)$$

- The Neumann condition:

$$\partial_n \varphi_\varepsilon = 0 \quad \text{on } \Gamma_N^\varepsilon$$

- An approximate Dirichlet condition:

$$\left\| \varphi_\varepsilon \right\|_{L^\infty(\widetilde{\Gamma}_D^\varepsilon)} = \mathrm{O}\left(\overline{r_\varepsilon} \log\left(\overline{r_\varepsilon} \right) \right)$$

where $\overline{r_\varepsilon} = r_\varepsilon^{(1)} + \cdots + r_\varepsilon^{(N)}$

From the quasimode to the eigenvalue

With Green identity

$$\begin{aligned}\lambda_\varepsilon^0 = \frac{\langle \varphi_\varepsilon,\, -\Delta u_0^\varepsilon \rangle_{\widetilde{\Omega}_\varepsilon}}{\langle \varphi_\varepsilon,\, u_0^\varepsilon \rangle_{\widetilde{\Omega}_\varepsilon}} &= \frac{\langle -\Delta \varphi_\varepsilon,\, u_0^\varepsilon \rangle_{\widetilde{\Omega}_\varepsilon} + \langle \partial_n \varphi_\varepsilon,\, u_0^\varepsilon \rangle_{\partial\widetilde{\Omega}_\varepsilon} - \langle \varphi_\varepsilon,\, \partial_n u_0^\varepsilon \rangle_{\partial\widetilde{\Omega}_\varepsilon}}{\langle \varphi_\varepsilon,\, u_0^\varepsilon \rangle_{\widetilde{\Omega}_\varepsilon}} \\ &= C_{3,\Omega}\overline{r_\varepsilon} + \mathrm{O}\left((\overline{r_\varepsilon})^2 \right) - \frac{\langle \varphi_\varepsilon,\, \partial_n u_0^\varepsilon \rangle_{\widetilde{\Gamma}_D^\varepsilon}}{\langle \varphi_\varepsilon,\, u_0^\varepsilon \rangle_{\widetilde{\Omega}_\varepsilon}}\end{aligned}$$

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Since $\varphi_\varepsilon = 1 + \mathrm{O}_{L^2(\widetilde{\Omega}_\varepsilon)}(\overline{r_\varepsilon})$ and $\varphi_\varepsilon = \mathrm{O}_{L^\infty(\widetilde{\Gamma}_{\mathrm{D}}^\varepsilon)}(\overline{r_\varepsilon}\log(\overline{r_\varepsilon}))$

$$\frac{\langle \varphi_\varepsilon,\, \partial_n u_0^\varepsilon \rangle_{\widetilde{\Gamma}_D^\varepsilon}}{\langle \varphi_\varepsilon,\, u_0^\varepsilon \rangle_{\widetilde{\Omega}_\varepsilon}} = \frac{\langle 1,\, \partial_n u_0^\varepsilon \rangle_{\widetilde{\Gamma}_D^\varepsilon}}{\int_{\widetilde{\Omega}_\varepsilon} u_0^\varepsilon}\, \mathrm{O}(\overline{r_\varepsilon}\log(\overline{r_\varepsilon})) = \lambda_0^\varepsilon\, \mathrm{O}(\overline{r_\varepsilon}\log(\overline{r_\varepsilon}))$$

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Then

$$\lambda_0^\varepsilon = C_{3,\Omega}\overline{r_\varepsilon} + \mathrm{O}\left((\overline{r_\varepsilon})^2\log(\overline{r_\varepsilon})\right)$$

Proof of the result on the exit hole distribution (back in dimension 3)

Consider the quasimode $\varphi_\varepsilon^{(-j)}$ without the hole j, it verifies on $\Gamma_{\mathrm{D}}^{\varepsilon}$

$$\varphi_\varepsilon^{(-j)} = \mathbb{1}_{\Gamma_{\mathrm{D}_j}^{\varepsilon}} + \mathrm{O}_{L^\infty}(\overline{K_\varepsilon}\log(\overline{K_\varepsilon}))$$

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Then the probability can be writen as

$$\mathbb{P}_{\nu_\varepsilon}(X_\tau \in \Gamma_{D_j}^\varepsilon) = -\frac{\langle \partial_n u_0^\varepsilon, \mathbb{1}_{\Gamma_{\mathrm{D}_i}^\varepsilon} \rangle_{\Gamma_D^\varepsilon}}{\langle \partial_n u_0^\varepsilon, 1 \rangle_{\Gamma_D^\varepsilon}} = -\frac{\langle \partial_n u_0^\varepsilon, \varphi_\varepsilon^{(-j)} \rangle_{\Gamma_D^\varepsilon}}{\langle \partial_n u_0^\varepsilon, 1 \rangle_{\Gamma_D^\varepsilon}} + \mathrm{O}(\overline{K_\varepsilon} \log(\overline{K_\varepsilon}))$$

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Using the Green identity,

$$\begin{aligned}\mathbb{P}_{\nu_\varepsilon}(X_\tau \in \Gamma_{D_j}^\varepsilon) &= -\frac{\langle \Delta u_0^\varepsilon, \varphi_\varepsilon^{(-j)} \rangle_\Omega - \langle u_0^\varepsilon, \Delta \varphi_\varepsilon^{(-j)} \rangle_\Omega}{\langle \partial_n u_0^\varepsilon, 1 \rangle_{\Gamma_D^\varepsilon}} + \mathrm{O}(\overline{K_\varepsilon} \log(\overline{K_\varepsilon})) \\ &= \frac{C_{3,\Omega}}{\lambda_0^\varepsilon} K_\varepsilon^j + \mathrm{O}(\overline{K_\varepsilon} \log(\overline{K_\varepsilon}))\end{aligned}$$