Asymptotic Methods for PDE Problems in Fluid Mechanics and Related Systems with Strong Localized Perturbations in Two-Dimensional Domains

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CISM Advanced Course; Asymptotic Methods in Fluid Mechanics: Surveys and Recent Advances

Lecture III: Strong Localized Perturbation of Eigenvalue Problems

Outline of Lecture III

Singularly Perturbed Eigenvalue Problems in Domains with Localized Traps

THREE SPECIFIC PROBLEMS CONSIDERED:

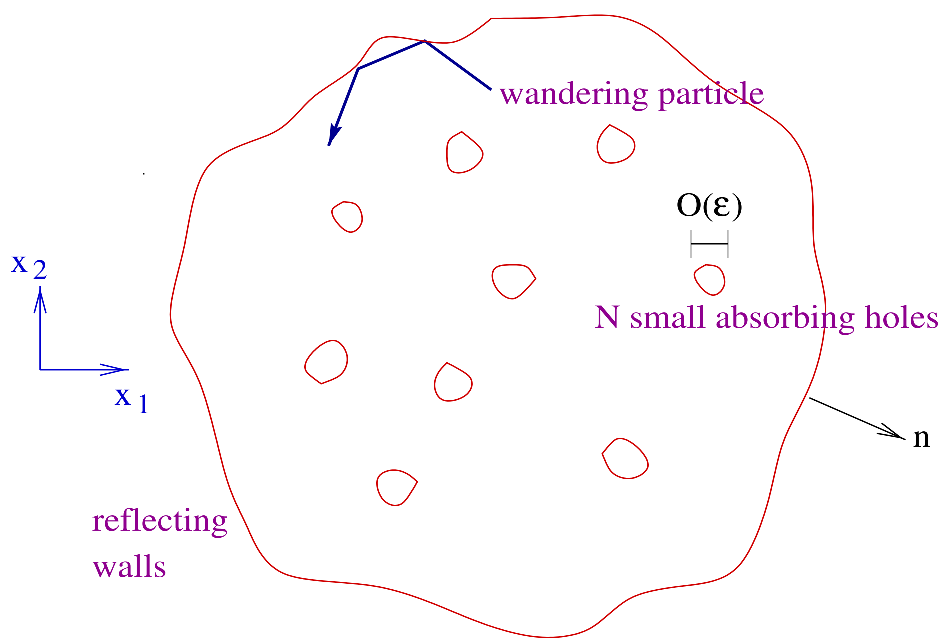
1. Principal Eigenvalue in a Planar Domain
2. Principal Eigenvalue on the Sphere
3. Narrow Escape From Within a Sphere

Eigenvalue Problem with Interior Traps

$$\Delta u + \lambda u = 0\,, \quad \mathbf{x} \in \Omega \backslash \Omega_p\,; \quad \int_{\Omega\backslash\Omega_p} u^2\, d\mathbf{x} = 1\,,$$

$$\partial_n u = 0 \quad \mathbf{x} \in \partial\Omega\,, \quad u = 0\,, \quad \mathbf{x} \in \partial\Omega_p\,.$$

- Here $\Omega_p = \cup_{i=1}^K \Omega_{\varepsilon_i}$ are K interior non-overlapping holes or traps, each of 'radius' $O(\varepsilon) \ll 1$. The holes are assumed to be identical up to a translation and rotation.
- Also $\Omega_{\varepsilon_i} \to \mathbf{x}_i$ as $\varepsilon \to 0$, for $i = 1, \ldots, K$. The centers $\mathbf{x}_i$ are arbitrary.



The Eigenvalue Optimization Problem

Goal: Let $\lambda_0 > 0$ be the fundamental eigenvalue. For $\varepsilon \to 0$ (small hole radius) find the hole locations x_i, for $i = 1, \ldots, K$, that maximize λ_0. In other words, chose the trap locations to minimize the lifetime of a wandering particle in the domain, i.e. where are the best places to fish?

Remarks:

- The average mean first passage time $\bar{v}$ for a Brownian particle with diffusivity D is $\bar{v} \sim 1/(D\lambda_0)$ for $\varepsilon \to 0$.
- For the unit ball $\Omega = |\mathbf{x}| \leq 1$, determine ring-type configurations of holes $\mathbf{x}_1, ..., \mathbf{x}_K$ that maximize λ_0.
- **Ref:** T. Kolokolnikov, M. Titcombe, MJW, Optimizing the Fundamental Neumann Eigenvalue for the Laplacian in a Domain with Small Traps, EJAM Vol. 16, No. 2, (2005), pp. 161-200.

Previous Studies I

For the Neumann problem, with K circular holes each of radius $\varepsilon \ll 1$, Ozawa (Duke J. 1981) proved that

$$\lambda_0 \sim \frac{2\pi K \nu}{|\Omega|} + O(\nu^2), \quad \nu \equiv \frac{-1}{\log \varepsilon} \ll 1 \, .$$

Since this is independent of $\mathbf{x}_i$, $i = 1, \ldots, K$, we need the neglected $O(\nu^2)$ term to optimize λ_0. For the Dirichlet problem, Ozawa (1981) proved

$$\lambda_0 \sim \lambda_{0d} + 2\pi \sum_{i=1}^{K} \left[u_0(\mathbf{x}_i) \right]^2 \nu + O(\nu^2) \, .$$

To optimize λ_0, put the hole at a local maxima of u_0 (Harrell, (SIMA 2001)). For the Dirichlet case, MJW, Henshaw, Keller (SIAP, 1993) showed

$$\lambda_0 \sim \lambda_*(\nu; \mathbf{x}_1, \ldots, \mathbf{x}_K) + O(\varepsilon/\nu) \, ,$$

where λ_* (which "sums" all the log terms) satisfies a PDE that must be solved numerically. Highly accurate results for λ_0, but no analytical insight on how to optimize λ_0 wrt hole locations.

Eigenvalue Asymptotics I

A singular perturbation analysis shows that all of the logarithmic terms are contained in the solution to

$$\Delta u^* + \lambda^* u^* = 0\,, \quad \mathbf{x} \in \Omega \backslash \{\mathbf{x}_1, \ldots, \mathbf{x}_K\}\,,$$
$$\int_\Omega (u^*)^2 d\mathbf{x} = 1\,; \qquad \partial_n u^* = 0\,, \quad x \in \partial\Omega\,,$$
$$u^* \sim A_j\, \nu_j\, \log|\mathbf{x} - \mathbf{x}_j| + A_j\,, \quad \mathbf{x} \to \mathbf{x}_j\,, \;\; j = 1, \ldots, K\,.$$

Here $\nu_j \equiv -1/\log(\varepsilon d_j)$, where d_j is the logarithmic capacitance of the j^{th} hole defined by

$$\Delta_{\mathbf{y}} v = 0\,, \quad \mathbf{y} \notin \Omega_j \equiv \varepsilon^{-1}\Omega_{\varepsilon_j}\,,$$
$$v = 0\,, \quad \mathbf{y} \in \partial\Omega_j\,,$$
$$v \sim \log|\mathbf{y}| - \log d_j + o(1)\,, \quad |\mathbf{y}| \to \infty\,.$$

- Notice that each hole is replaced in the outer region by a singularity structure with pre-specified regular part.
- The highlighted term together with the normalization condition provides $K+1$ constraints for the $K+1$ unknowns λ^* and A_j, for $j = 1, \ldots, K$.

Eigenvalue Asymptotics II

Define the G-function $G_H(\mathbf{x}; \mathbf{x}_0, \lambda^*)$ for the Helmholtz operator as

$$\Delta G_H + \lambda^* G_H = -\delta(\mathbf{x} - \mathbf{x}_0) \,, \quad \mathbf{x} \in \Omega \,; \quad \partial_n G_H = 0 \,, \quad \mathbf{x} \in \partial\Omega \,,$$

$$G_H(\mathbf{x}; \mathbf{x}_0, \lambda^*) = -\frac{1}{2\pi} \log |\mathbf{x} - \mathbf{x}_0| + R_H(\mathbf{x}; \mathbf{x}_0, \lambda^*) \,.$$

Here R_H is its "regular part". Then, $u^* = -2\pi \sum_{i=1}^{K} A_i \nu_i G_H(\mathbf{x}; \mathbf{x}_i, \lambda^*)$.

Satisfying the prescribed regular part condition at each $\mathbf{x}_j$ gives the homogeneous system

$$A_j \left(1 + 2\pi\nu_j R(\mathbf{x}_j; \mathbf{x}_j, \lambda^*)\right) + 2\pi \sum_{\substack{i=1 \\ i \neq j}}^{K} A_i \nu_i G(\mathbf{x}_j; \mathbf{x}_i, \lambda^*) = 0 \,, \quad j = 1, \ldots, K \,.$$

Consider the first eigenvalue for which $\lambda^* \to 0$ as $\varepsilon \to 0$. Set the determinant to zero and then use for $\lambda^* \ll 1$ that

$$G_H(\mathbf{x}; \mathbf{x}_0, \lambda^*) \sim -\frac{1}{|\Omega| \lambda^*} + G(\mathbf{x}; \mathbf{x}_0) \,, \quad R_H(\mathbf{x}; \mathbf{x}_0, \lambda^*) \sim -\frac{1}{|\Omega| \lambda^*} + R(\mathbf{x}; \mathbf{x}_0) \,,$$

where G and R are the Neumann G-function and its regular part.

Eigenvalue Expansion: A Two-Term Result

Principal Result: *For K small circular holes centered at $\mathbf{x}_1, \ldots, \mathbf{x}_K$ with logarithmic capacitances $d_1, \ldots, d_K$, then*

$$\lambda_0(\varepsilon) \sim \lambda^* \,, \quad \lambda^* = \frac{2\pi}{|\Omega|} \sum_{j=1}^{K} \nu_j - \frac{4\pi^2}{|\Omega|} \sum_{j=1}^{K} \sum_{i=1}^{K} \nu_j \nu_i \left(\mathcal{G}\right)_{ji} + O(\nu^3) \,.$$

Here $\nu_j \equiv= -1/\log(\varepsilon d_j)$ and $\left(\mathcal{G}\right)_{jk}$ are the entries of a certain Neumann Green's function matrix $\mathcal{G}$.

Corollary: *For K small circular holes each of radius ε (for which $d_j = 1$), then with $\nu = -1/\log(\varepsilon)$,*

$$\lambda_0(\varepsilon) \sim \lambda^* \,, \quad \lambda^* = \frac{2\pi K \nu}{|\Omega|} - \frac{4\pi^2 \nu^2}{|\Omega|} p(\mathbf{x}_1, \ldots, \mathbf{x}_K) + O(\nu^3) \,,$$

where

$$p(\mathbf{x}_1, \ldots, \mathbf{x}_K) \equiv \sum_{j=1}^{K} \sum_{i=1}^{K} \left(\mathcal{G}\right)_{ji} \,.$$

Remark: For K circular holes and $\nu \ll 1$, λ_0 has a local maximum at a local minimum point of the "Energy-like" function $p(\mathbf{x}_1, \ldots, \mathbf{x}_K)$.

Derivation of the Two-Term Result:

Problem 8: *For the eigenvalue problem (5.1) of the notes, consider the special case of K holes that have a common logarithmic capacitance $d = d_1 = \ldots, d_K$. By introducing two-term expansions directly in equation (5.1) of the notes for the eigenvalue and the outer and inner approximations to the eigenfunction, re-derive the two-term approximation of the Corollary.*

Solution: homework is deferred until...

The Neumann Green's Function

The Neumann Green's function $G(\mathbf{x};\mathbf{x}_0)$, with regular part $R(\mathbf{x};\mathbf{x}_0)$, satisfies:

$$\Delta G = \frac{1}{|\Omega|} - \delta(\mathbf{x}-\mathbf{x}_0)\,, \quad \mathbf{x}\in\Omega\,,$$

$$\partial_n G = 0\,, \quad \mathbf{x}\in\partial\Omega\,; \qquad \int_\Omega G\, d\mathbf{x} = 0\,,$$

$$G(\mathbf{x},\mathbf{x}_0) = -\frac{1}{2\pi}\log|\mathbf{x}-\mathbf{x}_0| + R(\mathbf{x};\mathbf{x}_0)\,;$$

The Green's matrix $\mathcal{G}$ is determined in terms of the hole-interaction term $G(\mathbf{x}_i;\mathbf{x}_j) \equiv G_{ij}$, and the self-interaction $R(\mathbf{x}_i;\mathbf{x}_i) \equiv R_{ii}$ by

$$\mathcal{G} \equiv \begin{pmatrix} R_{11} & G_{12} & \cdots & \cdots & G_{1K} \\ G_{21} & R_{22} & G_{23} & \cdots & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ G_{K1} & \cdots & \cdots & G_{KK-1} & R_{KK} \end{pmatrix}.$$

Multiple Holes in the Unit Disk

Let Ω be the unit circle, so that $|\Omega| = \pi$. Then, G_m and R_m are

$$G_m(\mathbf{x};\boldsymbol{\xi}) = -\frac{1}{2\pi}\log|\mathbf{x}-\boldsymbol{\xi}| + R_m(\mathbf{x};\boldsymbol{\xi})$$

$$R_m(\mathbf{x};\boldsymbol{\xi}) = -\frac{1}{2\pi}\log\left|\mathbf{x}|\boldsymbol{\xi}| - \frac{\boldsymbol{\xi}}{|\boldsymbol{\xi}|}\right| + \frac{(|\mathbf{x}|^2 + |\boldsymbol{\xi}|^2)}{2} - \frac{3}{4}\,.$$

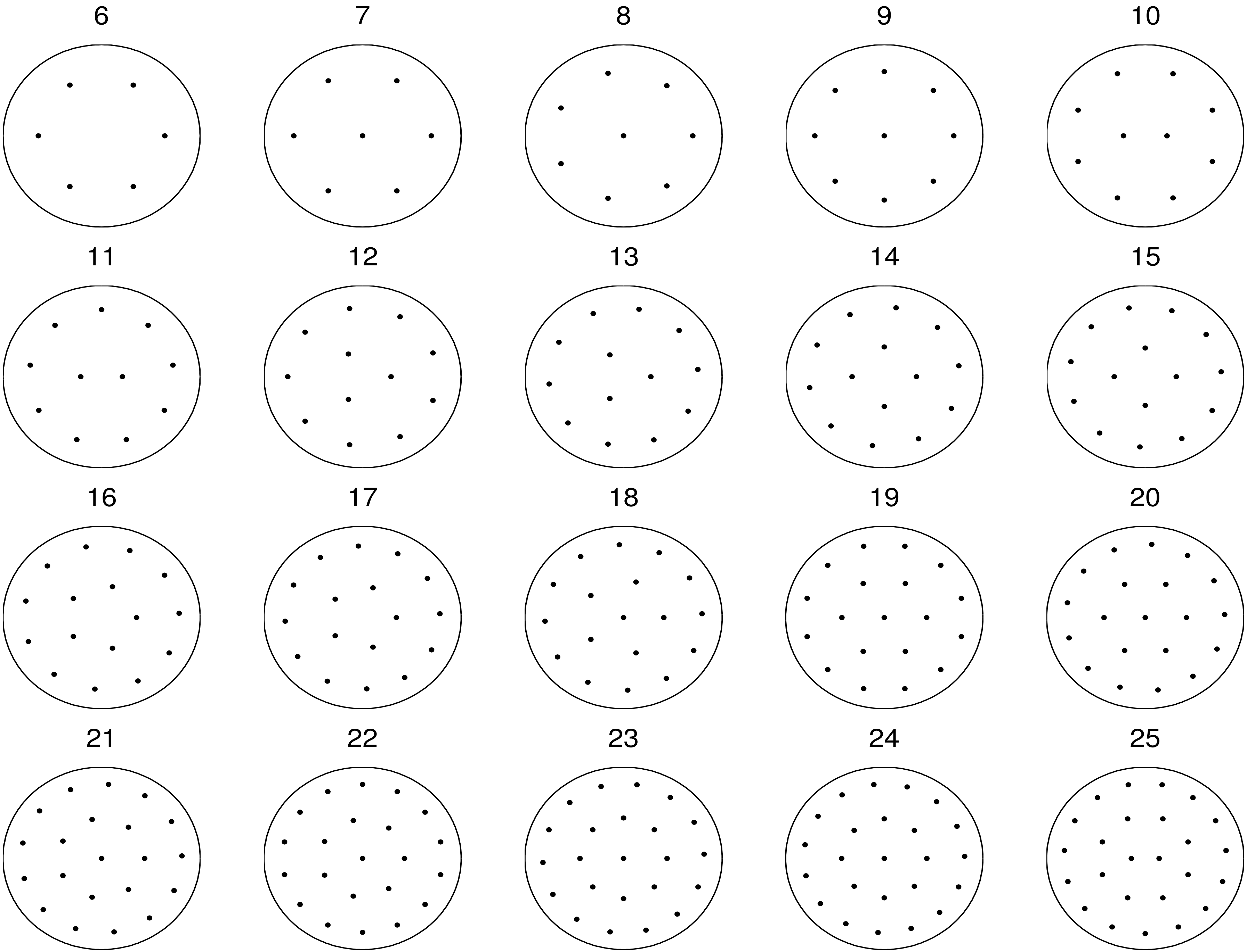
For the unit disk, the problem of minimizing $p(\mathbf{x}_1, \ldots, \mathbf{x}_K)$ is equivalent to the problem of minimizing the function $\mathcal{F}(\mathbf{x}_1, \ldots, \mathbf{x}_K)$ defined by

$$\mathcal{F}(\mathbf{x}_1, \ldots, \mathbf{x}_K) = -\sum_{j=1}^{K}\sum_{\substack{k=1\\k\neq j}}^{K}\log|\mathbf{x}_j - \mathbf{x}_k| - \sum_{j=1}^{K}\sum_{k=1}^{K}\log|1-\mathbf{x}_j\bar{\mathbf{x}}_k| + K\sum_{j=1}^{K}|\mathbf{x}_j|^2\,,$$

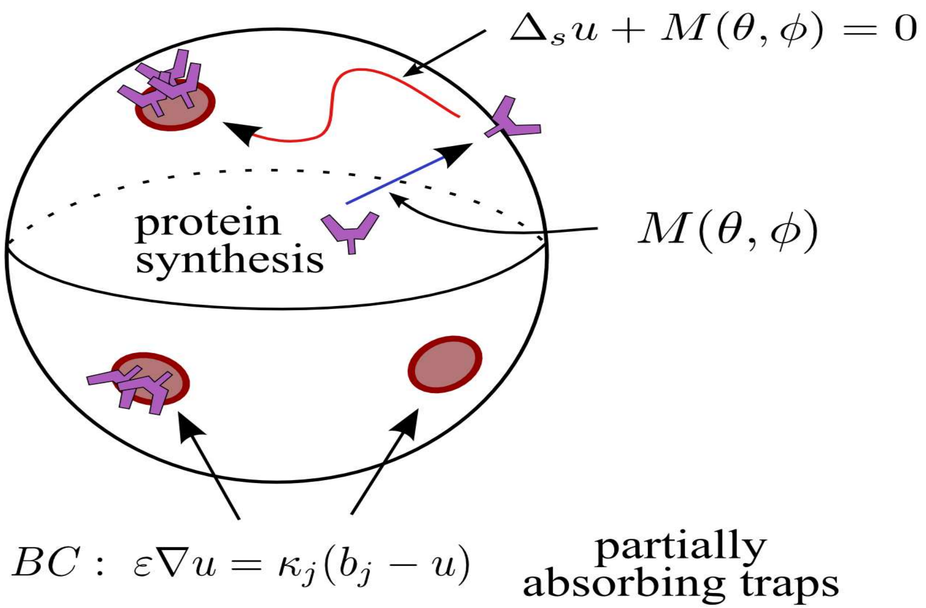
for $|\mathbf{x}_j| < 1$ and $\mathbf{x}_j \neq \mathbf{x}_k$ when $j \neq k$.

Remark 1: Except for the confining potential term this is the same discrete energy as for the equilibrium theory of Ginzburg-Landau vortices.
Remark 2: Compute the optimum configurations for $K = 6$ to $K = 25$ holes. Does the optimal pattern approach a hexagonal lattice structure as $K \to \infty$?

Optimization: Ring Patterns



Diffusion on the Surface of a Sphere: I



Let S be the unit sphere, Ω_{ε_j} be a circular trap of radius $O(\varepsilon)$ on S centered at $\mathbf{x}_j$ with $|\mathbf{x}_j| = 1$. Then, the mean first passage time (MFPT) $v(\mathbf{x})$ satisfies

$$\triangle_s v = -\frac{1}{D}\,, \quad \mathbf{x} \in S_\varepsilon \equiv S \backslash \cup_{j=1}^{N} \Omega_{\varepsilon_j}\,; \quad v = 0\,, \quad \mathbf{x} \in \partial\Omega_{\varepsilon_j}\,.$$

The average MFPT is defined by

$$\bar{v} \equiv \frac{1}{4\pi} \int_S v \, ds\,.$$

Diffusion on the Surface of a Sphere: II

Mean First Passage Time: Consider Brownian motion with diffusivity D on S with a multi-connected absorbing trap-set $\partial\Omega_a$ of measure $O(\varepsilon)$. Let $X(0) = \mathbf{x} \in \Omega$ be the initial point for Brownian motion. Then, the MFPT $v(\mathbf{x}) \equiv E\left[\tau | X(0) = \mathbf{x}\right]$, where τ is the time for capture, satisfies (2.1). The MFPT averaged over a uniform distribution of starting points is $\bar{v} = (4\pi)^{-1} \int_S v\, ds$.

Eigenvalue Problem: The corresponding eigenvalue problem on S is

$$\triangle_s \psi + \sigma \psi = 0 \,, \quad \mathbf{x} \in S_\varepsilon \,; \qquad \psi = 0 \,, \quad \mathbf{x} \in \partial\Omega_{\varepsilon_j} \,.$$

For $\varepsilon \to 0$ then $\bar{v} \sim 1/(D\sigma_1)$.

2-D (Elliptic Fekete Points): minimum point of the logarithmic energy $\mathcal{H}_L$ on the unit sphere

$$\mathcal{H}_L(\mathbf{x}_1, \ldots, \mathbf{x}_N) = -\sum_{j=1}^{N} \sum_{k>j}^{N} \log |\mathbf{x}_j - \mathbf{x}_k| \,, \quad |\mathbf{x}_j| = 1 \,.$$

(References: Smale and Schub, Saff, Sloane, Kuijlaars) Are these points related to minimizing the MFPT for diffusion on the sphere?

Diffusion on the Surface of a Sphere: III

Principal Result: *Consider N perfectly absorbing circular traps of a common radius $\varepsilon a \ll 1$ centered at $\mathbf{x}_j$, for $j = 1, \ldots, N$ on S. Then, the asymptotics for the MFPT v in the "outer" region $|\mathbf{x} - \mathbf{x}_j| \gg O(\varepsilon)$ for $j = 1, \ldots, N$ is*

$$v(\mathbf{x}) = -2\pi \sum_{j=1}^{N} A_j G(\mathbf{x}; \mathbf{x}_j) + \chi \,, \quad \chi \equiv \frac{1}{4\pi} \int_S v \, ds \,,$$

where A_j for $j = 1, \ldots, N$ with $\mu = -1/\log(\varepsilon a)$ satisfies

$$A_j = \frac{2}{ND} \left[1 + \mu \sum_{\substack{j=1 \\ j \neq i}}^{N} \log |\mathbf{x}_i - \mathbf{x}_j| - \frac{2\mu}{N} p(\mathbf{x}_1, \ldots, \mathbf{x}_N) + O(\mu^2) \right] \,.$$

The average MFPT $\bar{v} = \chi$ and the principal eigenvalue $\sigma(\varepsilon)$ satisfy

$$\bar{v} = \chi = \frac{2}{ND\mu} + \frac{1}{D} \left[(2 \log 2 - 1) + \frac{4}{N^2} p(\mathbf{x}_1, \ldots, \mathbf{x}_N) \right] + O(\mu) \,,$$

$$\sigma(\varepsilon) \sim \frac{\mu N}{2} + \mu^2 \left[-\frac{N^2}{4} (2 \log 2 - 1) - p(\mathbf{x}_1, \ldots, \mathbf{x}_N) \right] + O(\mu^3) \,.$$

Diffusion on the Surface of a Sphere: IV

Here the discrete energy $p(x_1, \ldots, x_N)$ *is the logarithmic energy*

$$p(\mathbf{x}_1, \ldots, \mathbf{x}_N) \equiv -\sum_{i=1}^{N} \sum_{j>i}^{N} \log |\mathbf{x}_i - \mathbf{x}_j| \,.$$

The Green's function $G(\mathbf{x}; \mathbf{x}_0)$ that appears satisfies

$$\triangle_s G = \frac{1}{4\pi} - \delta(\mathbf{x} - \mathbf{x}_0) \,, \quad \mathbf{x} \in S \,; \quad \int_S G \, ds = 0 \,,$$

and is given analytically by

$$G(\mathbf{x}; \mathbf{x}_0) = -\frac{1}{2\pi} \log |\mathbf{x} - \mathbf{x}_0| + R \,, \qquad R \equiv \frac{1}{4\pi} \left[2 \log 2 - 1 \right] \,.$$

- G occurs in study of fluid vortices on a sphere (P. Newton, S. Boatto)
- **Key Point:** $\sigma(\varepsilon)$ is maximized and $\bar{v}$ minimized at the minumum point of p, i.e. at the elliptic Fekete points.
- **Reference:** D. Coombs, R. Straube, MJW, *"Diffusion on a Sphere with Traps..."*, SIAM J. Appl. Math., Vol. 70, No. 1, (2009), pp. 302–332.

Diffusion on the Surface of a Sphere: V

In order to sum the infinite logarithmic series for the principal eigenvalue we must solve

$$\triangle_s \psi + \sigma \psi = 0 \,, \quad \mathbf{x} \in S \backslash \{\mathbf{x}_1, \ldots, \mathbf{x}_K\} \,; \quad \int_S \psi^2 \, ds = 1 \,, \tag{2.1a}$$

$$\psi \sim A_j + \mu_j A_j \log |\mathbf{x} - \mathbf{x}_j| \,, \quad \text{as} \quad \mathbf{x} \to \mathbf{x}_j \,, \quad j = 1, \ldots, K \,. \tag{2.1b}$$

where ψ is singularity-free at the poles $\theta = 0, \pi$ and is 2π periodic in ϕ. Note that the regular part of the singularity structure is prescribed.

To do so we introduce the Helmholtz Green's function $G_H(\mathbf{x}; \mathbf{x}_0, \nu)$ for the Laplace-Beltrami operator, defined as the solution to

$$\triangle_s G_H + \nu(\nu + 1) G_H = -\delta(\mathbf{x} - \mathbf{x}_0) \,, \quad \mathbf{x} \in S \,, \tag{2.2a}$$

$$G_H \quad \text{is } 2\pi \text{ periodic in } \phi \text{ and smooth at } \theta = 0, \pi \,. \tag{2.2b}$$

This Green's function is given explicitly by

$$G_H(\mathbf{x}; \mathbf{x}_0, \nu) = -\frac{1}{4 \sin(\pi \nu)} P_\nu \left(-\mathbf{x} \cdot \mathbf{x}_0 \right) \,, \tag{2.3}$$

where $P_\nu(z)$ is the Legendre function of the first kind of order ν.

Diffusion on the Surface of a Sphere: VI

As $\mathbf{x} \to \mathbf{x}_0$, G_H has the local behavior

$$G_H(\mathbf{x};\mathbf{x}_0,\nu) = -\frac{1}{2\pi}\log|\mathbf{x}-\mathbf{x}_0| + R_h(\nu) + o(1)\,, \quad \text{as } \mathbf{x} \to \mathbf{x}_0\,, \tag{2.4a}$$

$$R_H(\nu) \equiv -\frac{1}{4\pi}\left[-2\log 2 + 2\gamma_e + 2\psi(\nu+1) + \pi\cot(\pi\nu)\right]\,. \tag{2.4b}$$

where $\psi(z)$ is the Digamma function and γ_e is Euler's constant.

The solution to (2.3) is then written as

$$\psi = -2\pi\mu \sum_{i=1}^{K} A_i G_H(\mathbf{x};\mathbf{x}_i,\nu)\,. \tag{2.5}$$

Then, by using (2.6), we can expand ψ as $\mathbf{x} \to \mathbf{x}_j$ for each $j = 1,\ldots,K$ and equate the resulting regular part of this expression with the required regular part in (2.3b).

Diffusion on the Surface of a Sphere: VII

This yields that A_j must satisfy the following homogeneous linear system:

$$A_j + 2\pi\mu A_j R_H + 2\pi\mu \sum_{\substack{i=1 \\ i\neq j}}^{K} A_i G_{Hji} = 0\,, \qquad j = 1, \ldots, K\,. \tag{2.6}$$

We write this problem in matrix form as:

Principal Result: *Consider N perfectly absorbing traps of a common radius εa for $j = 1, \ldots, N$. Let $\nu(\varepsilon)$ be the smallest root of the transcendental equation*

$$\text{Det}\,(I + 2\pi\mu\mathcal{G}_h) = 0\,, \quad \mu = -\frac{1}{\log(\varepsilon a)}\,.$$

Here $\mathcal{G}_h$ is the Helmholtz Green's function matrix with matrix entries

$$\mathcal{G}_{hjj} = R_h(\nu)\,; \qquad \mathcal{G}_{hij} = -\frac{1}{4\sin(\pi\nu)} P_\nu\left(\frac{|x_j - x_i|^2}{2} - 1\right)\,, \quad i \neq j\,.$$

Then, with an error of order $O(\varepsilon)$, we have $\sigma(\varepsilon) \sim \nu(\nu+1)$.

Diffusion on the Surface of a Sphere: VIII

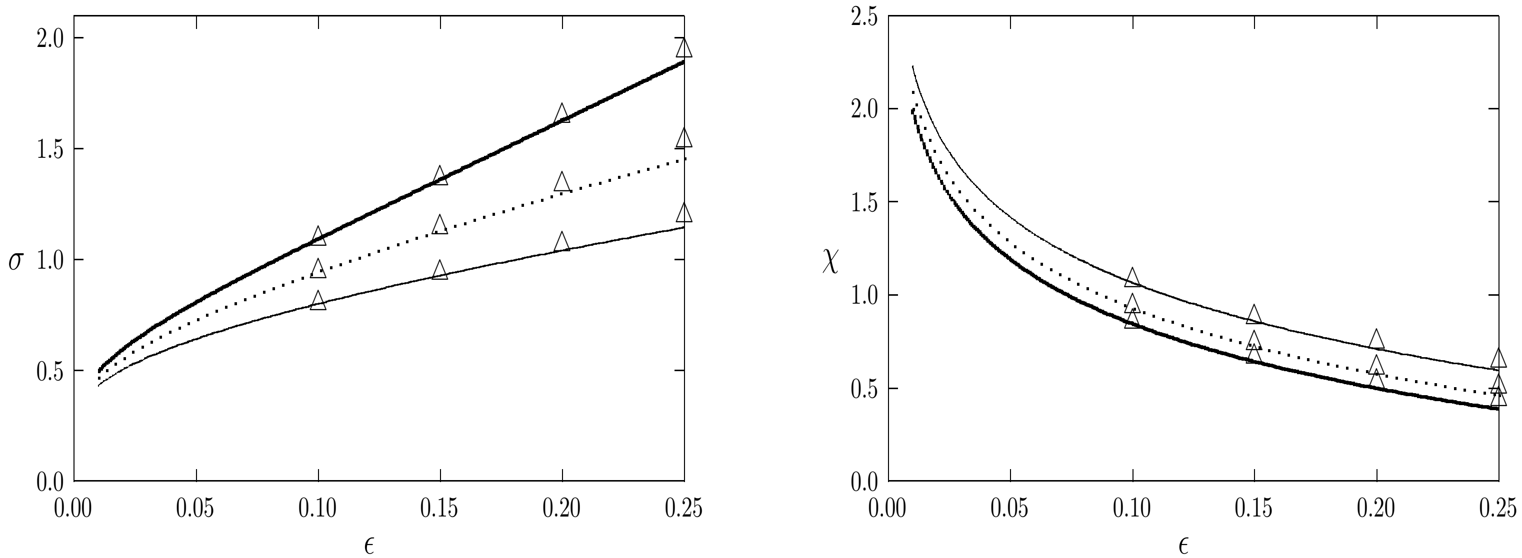
Table 1: Smallest eigenvalue $\sigma(\varepsilon)$ for the 2- and 5-trap configurations. For the 2-trap case the traps are at $(\theta_1, \phi_1) = (\pi/4, 0)$ and $(\theta_2, \phi_2) = (3\pi/4, 0)$. Here, σ is the numerical solution found by COMSOL; σ^* corresponds to summing the log expansion; σ_2 is calculated from the two-term expansion.

	5 traps			2 traps		
ε	σ	σ^*	σ_2	σ	σ^*	σ_2
0.02	0.7918	0.7894	0.7701	0.2458	0.2451	0.2530
0.05	1.1003	1.0991	1.0581	0.3124	0.3121	0.3294
0.1	1.5501	1.5452	1.4641	0.3913	0.3903	0.4268
0.2	2.5380	2.4779	2.3278	0.5177	0.5110	0.6060

Note: For $\varepsilon = 0.2$ and $N = 5$, we get 5% trap area fraction. The agreement is still very good: 2.4% error (summing logs) and 8.3% error (2-term).

Diffusion on the Surface of a Sphere: IX

EFFECT OF SPATIAL ARRANGEMENT OF $N = 4$ IDENTICAL TRAPS:



Note: $\varepsilon = 0.1$ corresponds to 1% trap surface area fraction.

Plots: Results for $\sigma(\varepsilon)$ (left) and $\chi(\varepsilon)$ (right) for three different 4-trap patterns with perfectly absorbing traps and a common radius ε. **Heavy solid:** $(\theta_1, \phi_1) = (0, 0)$, $(\theta_2, \phi_2) = (\pi, 0)$, $(\theta_3, \phi_3) = (\pi/2, 0)$, $(\theta_4, \phi_4) = (\pi/2, \pi)$; **Solid:** $(\theta_1, \phi_1) = (0, 0)$, $(\theta_2, \phi_2) = (\pi/3, 0)$, $(\theta_3, \phi_3) = (2\pi/3, 0)$, $(\theta_4, \phi_4) = (\pi, 0)$; **Dotted:** $(\theta_1, \phi_1) = (0, 0)$, $(\theta_2, \phi_2) = (2\pi/3, 0)$, $(\theta_3, \phi_3) = (\pi/2, \pi)$, $(\theta_4, \phi_4) = (\pi/3, \pi/2)$. The marked points are computed from finite element package COMSOL.

Diffusion on the Surface of a Sphere: X

For $N \to \infty$, the optimal energy for elliptic Fekete points gives

$$\max\left[-p(x_1,\ldots,x_N)\right] \sim \frac{1}{4}\log\left(\frac{4}{e}\right)N^2 + \frac{1}{4}N\log N + l_1 N + l_2\,, \quad N \to \infty\,,$$

with $l_1 = 0.02642$ and $l_2 = 0.1382$.

Reference: E. A. Rakhmanov, E. B. Saff, Y. M. Zhou, (1994); B. Bergersen, D. Boal, P. Palffy-Muhoray, J. Phys. A: Math Gen., **27**, No. 7, (1994).

This yields a key scaling law for the minimum of the averaged MFPT as

Principal Result: *For $N \gg 1$, and N circular disks of common radius εa, and with small trap area fraction $N\varepsilon^2 a^2 \ll 1$ with $|S| = 4\pi$, then*

$$\min \bar{v} \sim \frac{1}{ND}\left[-\log\left(\frac{\sum_{j=1}^{N}|\Omega_{\varepsilon_j}|}{|S|}\right) - 4l_1 - \log 4 + O(N^{-1})\right].$$

Diffusion on the Surface of a Sphere: XI

Application: Estimate the averaged MFPT T for a surface-bound molecule to reach a molecular cluster on a spherical cell.

Physical Parameters: The diffusion coefficient of a typical surface molecule (e.g. LAT) is $D \approx 0.25\mu$m^2/s. Take $N = 100$ (traps) of common radius 10nm on a cell of radius 5μm. This gives a 1% trap area fraction:

$$\varepsilon = 0.002 \,, \qquad N\pi\varepsilon^2/(4\pi) = 0.01 \,.$$

Scaling Law: The scaling law gives an asymptotic lower bound on the averaged MFPT. For $N = 100$ traps, the bound is 7.7s, achieved at the elliptic Fekete points.

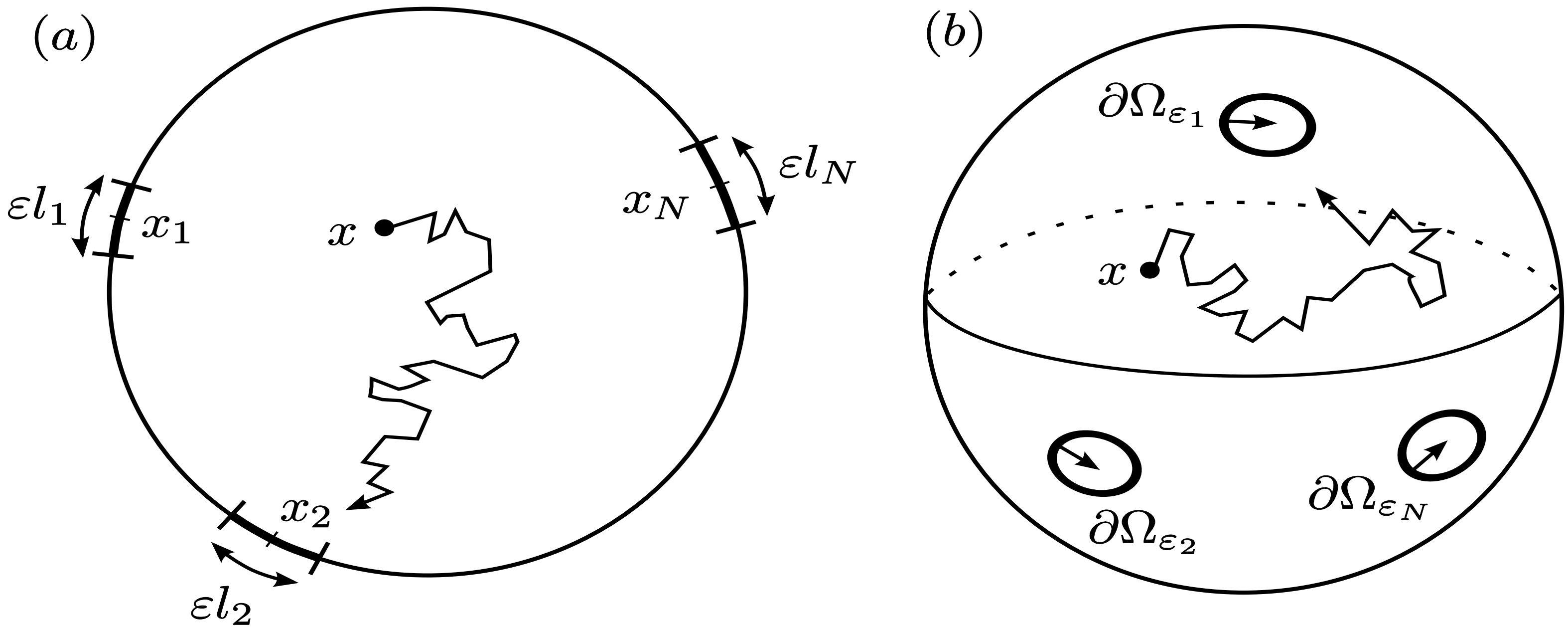
One Big Trap: As a comparison, for one big trap of the same area the averaged MFPT is 360s, which is very different.

Bounds: Therefore, for any other arrangement, 7.7s $< T < 360$s.

Conclusion: Both the Spatial Distribution and Fragmentation Effect of Localized Traps are Rather Significant even at Small Trap Area Fraction

Narrow Escape Problem I

Narrow Escape: Brownian motion with diffusivity D in Ω with $\partial\Omega$ insulated except for an (multi-connected) absorbing patch $\partial\Omega_a$ of measure $O(\varepsilon)$. Let $\partial\Omega_a \to x_j$ as $\varepsilon \to 0$ and $X(0) = x \in \Omega$ be initial point for Brownian motion.



The MFPT $v(x) = E\left[\tau | X(0) = x\right]$ satisfies (Z. Schuss (1980))

$$\Delta v = -\frac{1}{D}, \quad x \in \Omega,$$

$$\partial_n v = 0 \quad x \in \partial\Omega_r; \quad v = 0, \quad x \in \partial\Omega_a = \cup_{j=1}^{N} \partial\Omega_{\varepsilon_j}.$$

Narrow Escape Problem II

KEY GENERAL REFERENCES:

- Z. Schuss, A. Singer, D. Holcman, *The Narrow Escape Problem for Diffusion in Cellular Microdomains*, PNAS, **104**, No. 41, (2007), pp. 16098-16103.
- O. Bénichou, R. Voituriez, *Narrow Escape Time Problem: Time Needed for a Particle to Exit a Confining Domain Through a Small Window*, Phys. Rev. Lett, **100**, (2008), 168105.
- S. Condamin, et al., Nature, **450**, 77, (2007)
- S. Condamin, O. Bénichou, M. Moreau, Phys. Rev. E., **75**, (2007).

RELEVANCE OF NARROW ESCAPE TIME PROBLEM IN BIOLOGY:

- time needed for a reactive particle released from a specific site to activate a given protein on the cell membrane
- biochemical reactions in cellular microdomains (dendritic spines, synapses, microvesicles), consisting of a small number of particles that must exit the domain to initiate a biological function.
- determines reaction rate in Markov model of chemical reactions

Some Recent Results

RECENT 3-D RESULTS:

- For one circular trap of radius ε on the unit sphere Ω with $|\Omega| = 4\pi/3$,

$$\bar{v} \sim \frac{|\Omega|}{4\varepsilon D}\left[1 - \frac{\varepsilon}{\pi}\log\varepsilon + O\left(\varepsilon\right)\right] \,,$$

  Ref: A. Singer et al. J. Stat. Phys., **122**, No. 3, (2006).

- For arbitrary Ω with smooth $\partial\Omega$ and one circular trap at $x_0 \in \partial\Omega$

$$\bar{v} \sim \frac{|\Omega|}{4\varepsilon D}\left[1 - \frac{\varepsilon}{\pi} H \log\varepsilon + O\left(\varepsilon\right)\right] \,.$$

  Here H is the mean curvature of $\partial\Omega$ at $x_0 \in \partial\Omega$. **Ref:** A. Singer, Z. Schuss, D. Holcman, Phys. Rev. E., **78**, No. 5, 051111, (2009).

Main Goal: Calculate a higher-order expansion for $v(x)$ and $\bar{v}$ as $\varepsilon \to 0$ in 3-D to determine the significant effect on $\bar{v}$ of the spatial configuration $\{x_1, \cdots, x_N\}$ of multiple absorbing boundary traps for a fixed area fraction of traps. Minimize $\bar{v}$ with respect to $\{x_1, \cdots, x_N\}$.

Electrons on a Sphere: Fekete Points

3-D (Fekete Points): Let Ω be the unit sphere with N-circular absorbing patches on $\partial\Omega$ of a common radius. Is minimizing $\bar{v}$ equivalent to minimizing the Coulomb energy $\mathcal{H}_C(x_1, \ldots, x_N)$ defined by

$$\mathcal{H}_C(x_1, \ldots, x_N) = \sum_{j=1}^{N} \sum_{k>j}^{N} \frac{1}{|x_j - x_k|}, \quad |x_j| = 1 .$$

Such points are **Fekete points.** They correspond to finding the minimal energy configuration of “electrons” on a sphere boundary. (References: J.J. Thomson, E. Saff, N. Sloane, A. Kuijlaars etc..)

Narrow Escape From a Sphere: I

The surface Neumann G-function, G_s, is central:

$$\triangle G_s = \frac{1}{|\Omega|}\,, \quad x \in \Omega\,; \qquad \partial_r G_s = \delta(\cos\theta - \cos\theta_j)\delta(\phi - \phi_j)\,, \quad x \in \partial\Omega\,,$$

Lemma: *Let* $\cos\gamma = x \cdot x_j$ *and* $\int_\Omega G_s\, dx = 0$. *Then* $G_s = G_s(x; x_j)$ *is*

$$G_s = \frac{1}{2\pi|x - x_j|} + \frac{1}{8\pi}(|x|^2 + 1) + \frac{1}{4\pi}\log\left[\frac{2}{1 - |x|\cos\gamma + |x - x_j|}\right] - \frac{7}{10\pi}\,.$$

Define the matrix $\mathcal{G}_s$ using $R = -\frac{9}{20\pi}$ and $G_{sij} \equiv G_s(x_i; x_j)$ as

$$\mathcal{G}_s \equiv \begin{pmatrix} R & G_{s12} & \cdots & G_{s1N} \\ G_{s21} & R & \cdots & G_{s2N} \\ \vdots & \vdots & \ddots & \vdots \\ G_{sN1} & \cdots & G_{sN,N-1} & R \end{pmatrix},$$

Remark: As $x \to x_j$, G_s has a subdominant logarithmic singularity:

$$G_s(x; x_j) \sim \frac{1}{2\pi|x - x_j|} - \frac{1}{4\pi}\log|x - x_j| + O(1)\,.$$

Narrow Escape From a Sphere: II

Principal Result: *For $\varepsilon \to 0$, and for N circular traps of radii εa_j centered at x_j, for $j = 1, \ldots, N$, the averaged MFPT $\bar{v}$ satisfies*

$$\bar{v} = \frac{|\Omega|}{2\pi\varepsilon D N\bar{c}} \left[1 + \varepsilon \log\left(\frac{2}{\varepsilon}\right) \frac{\sum_{j=1}^{N} c_j^2}{2N\bar{c}} + \frac{2\pi\varepsilon}{N\bar{c}} p_c(x_1, \ldots, x_N) - \frac{\varepsilon}{N\bar{c}} \sum_{j=1}^{N} c_j \kappa_j + O(\varepsilon^2 \log \varepsilon) \right] .$$

Here $c_j = 2a_j/\pi$ is the capacitance of the j^{th} circular absorbing window of radius εa_j, $\bar{c} \equiv N^{-1}(c_1 + \ldots + c_N)$, $|\Omega| = 4\pi/3$, and κ_j is defined by

$$\kappa_j = \frac{c_j}{2} \left[2 \log 2 - \frac{3}{2} + \log a_j \right] .$$

Moreover, $p_c(x_1, \ldots, x_N)$ is a quadratic form in terms $\mathcal{C}^t = (c_1, \ldots, c_N)$

$$p_c(x_1, \ldots, x_N) \equiv \mathcal{C}^t \mathcal{G}_s \mathcal{C} .$$

Remarks: 1) A similar result holds for non-circular traps. 2) The logarithmic term in ε arises from the subdominant singularity in G_s.

Narrow Escape From a Sphere: III

- **One Trap:** Let $N = 1$, $c_1 = 2/\pi$, $a_1 = 1$, (compare with Holcman et al)

$$\bar{v} = \frac{|\Omega|}{4\varepsilon D}\left[1 + \frac{\varepsilon}{\pi}\log\left(\frac{2}{\varepsilon}\right) + \frac{\varepsilon}{\pi}\left(-\frac{9}{5} - 2\log 2 + \frac{3}{2}\right) + \mathcal{O}(\varepsilon^2\log\varepsilon)\right].$$

- **N Identical Circular Traps:** of common radius ε:

$$\bar{v} = \frac{|\Omega|}{4\varepsilon D N}\left[1 + \frac{\varepsilon}{\pi}\log\left(\frac{2}{\varepsilon}\right) + \frac{\varepsilon}{\pi}\left(-\frac{9N}{5} + 2(N-2)\log 2 + \frac{3}{2} + \frac{4}{N}\mathcal{H}(x_1,\ldots,x_N)\right) + \mathcal{O}(\varepsilon^2\log\varepsilon)\right],$$

with discrete energy $\mathcal{H}(x_1,\ldots,x_N)$ given by

$$\mathcal{H}(x_1,\ldots,x_N) = \sum_{i=1}^{N}\sum_{k>i}^{N}\left(\frac{1}{|x_i - x_k|} - \frac{1}{2}\log|x_i - x_k| - \frac{1}{2}\log\left(2 + |x_i - x_k|\right)\right).$$

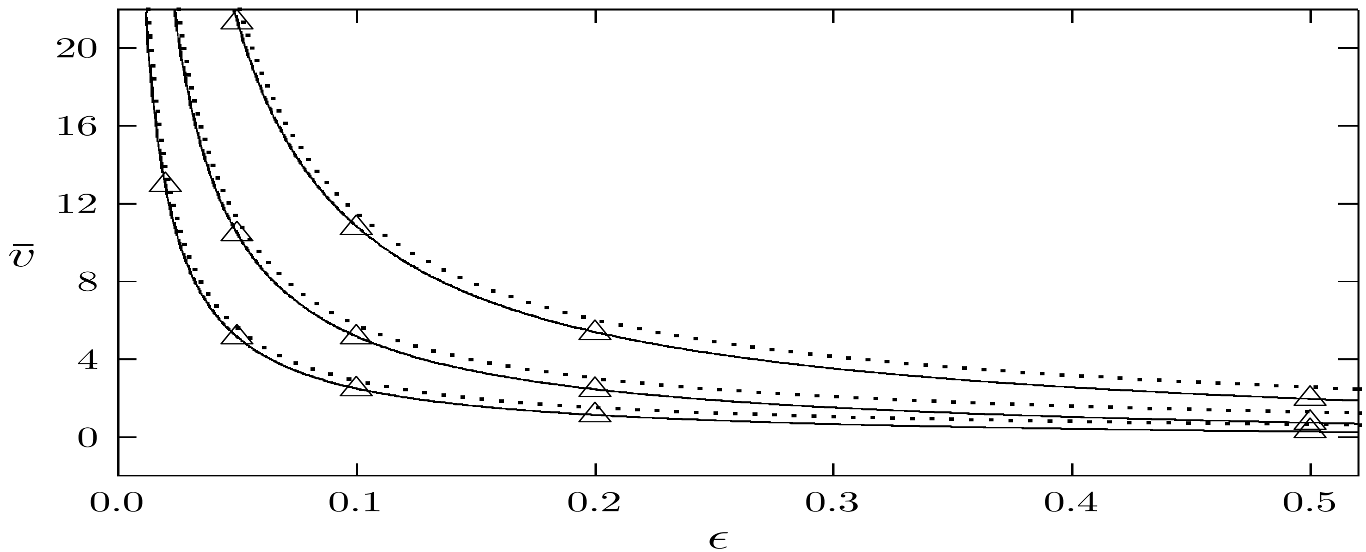
- **Key point:** Minimizing $\bar{v}$ corresponds to minimizing $\mathcal{H}$. This discrete energy is a generalization of the purely Coulombic or logarithmic energies associated with Fekete points.

Narrow Escape From a Sphere: IV

KEY STEPS IN DERIVATION OF MAIN RESULT

- The Neumann G-function has a subdominant logarithmic singularity on the boundary (related to surface diffusion)
- Tangential-normal coordinate system used near each trap.
- Asymptotic expansion of global (outer) solution and local (inner solutions near each trap.
- Leading-order local solution is electrified disk problem in a half-space, with capacitance c_j.
- Logarithmic switchback terms in ε needed in global solution (ubiquitous in Low Reynolds number flow problems in 3-D situations)
- Need corrections to the tangent plane approximation in the inner region, i.e. near the trap. This determines κ_j.
- Asymptotic matching and solvability conditions (Divergence theorem) determine v and $\bar{v}$

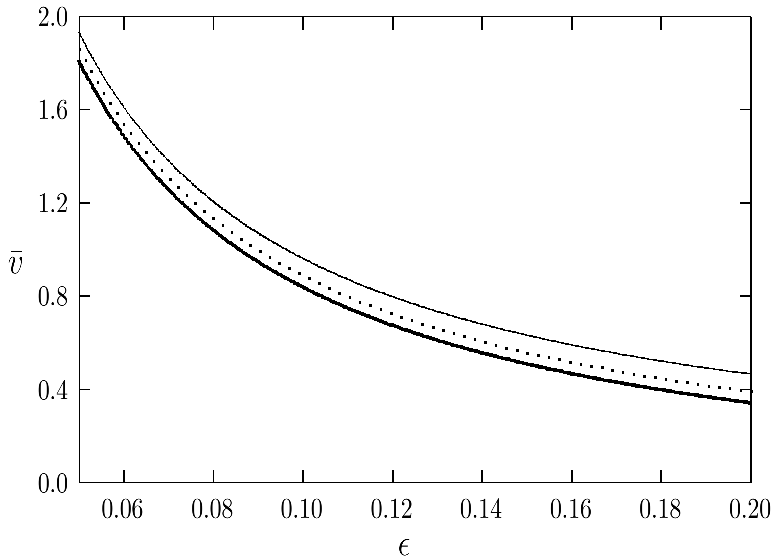
Narrow Escape From a Sphere: V

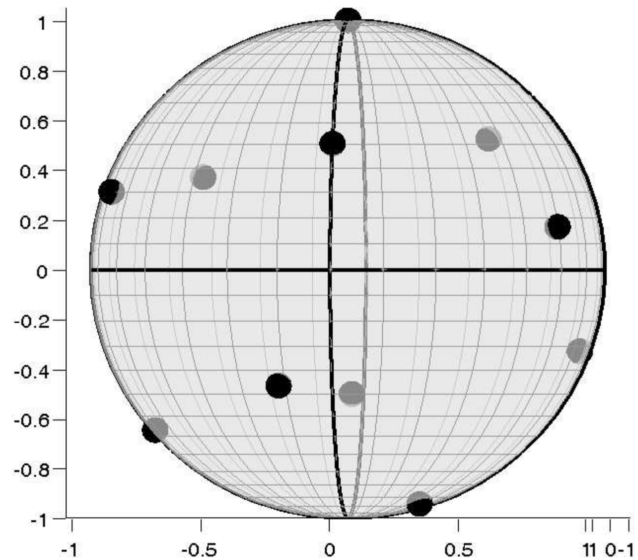


Plot: $\bar{v}$ vs. ε with $D = 1$ and either $N = 1, 2, 4$ equidistantly spaced circular windows of radius ε. **Solid:** 3-term expansion. **Dotted:** 2-term expansion. **Discrete:** COMSOL. **Top:** $N = 1$. **Middle:** $N = 2$. **Bottom:** $N = 4$.

	$N=1$			$N=2$			$N=4$		
ε	$\bar{v}_2$	$\bar{v}_3$	$\bar{v}_n$	$\bar{v}_2$	$\bar{v}_3$	$\bar{v}_n$	$\bar{v}_2$	$\bar{v}_3$	$\bar{v}_n$
0.02	53.89	53.33	52.81	26.95	26.42	26.12	13.47	13.11	12.99
0.05	22.17	21.61	21.35	11.09	10.56	10.43	5.54	5.18	5.12
0.10	11.47	10.91	10.78	5.74	5.21	5.14	2.87	2.51	2.47
0.20	6.00	5.44	5.36	3.00	2.47	2.44	1.50	1.14	1.13
0.50	2.56	1.99	1.96	1.28	0.75	0.70	0.64	0.28	0.30

Narrow Escape From a Sphere: VI

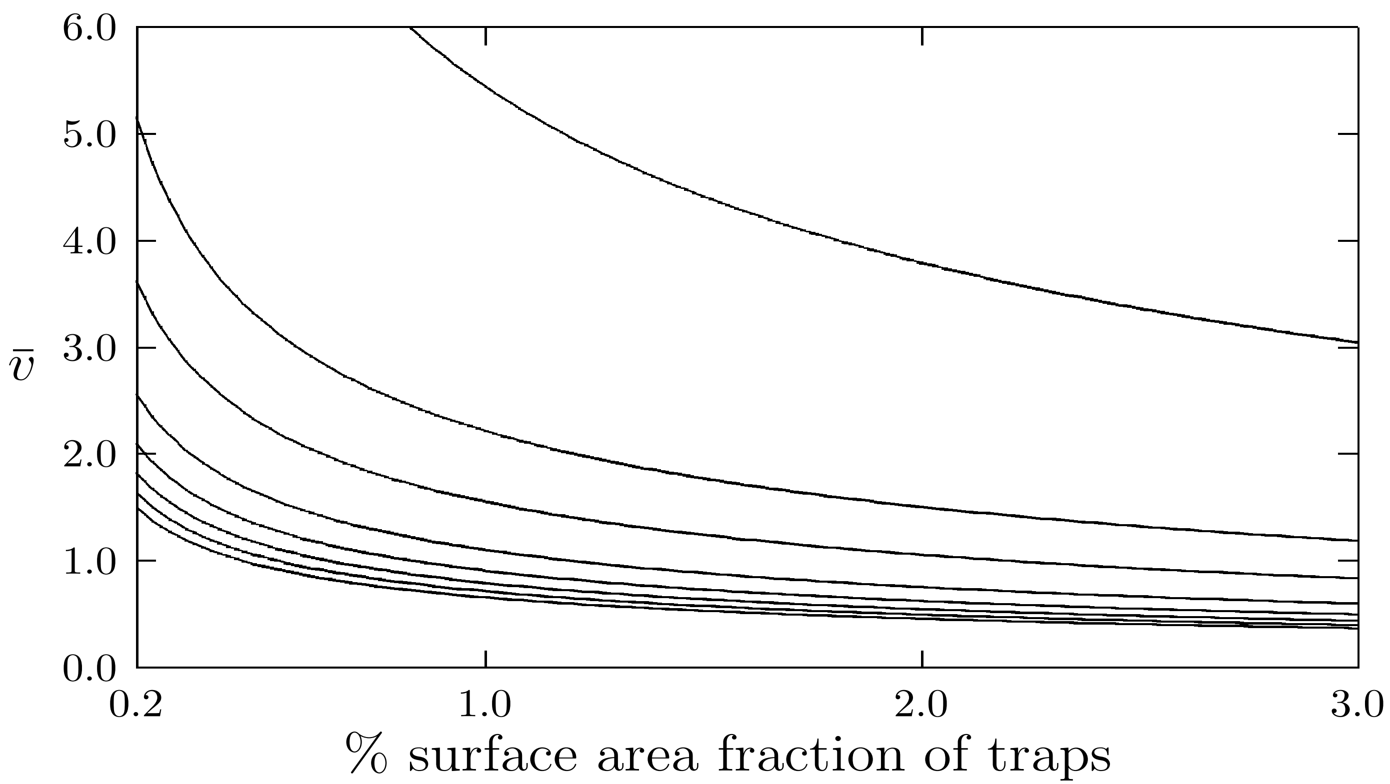




Plot: $\bar{v}(\varepsilon)$ for $D = 1$, $N = 11$, and three trap configurations. **Heavy:** global minimum of $\mathcal{H}$ (right figure). **Solid:** equidistant points on equator. **Dotted:** random.

- Table: $\bar{v}$ agrees well with COMSOL even at $\varepsilon = 0.5$. For $\varepsilon = 0.5$ and $N = 4$, absorbing windows occupy $\approx 20\%$ of the surface. Still, the 3-term asymptotics for $\bar{v}$ differs from COMSOL by only $\approx 7.5\%$.
- For $\varepsilon = 0.1907$, $N = 11$ traps occupy $\approx 10\%$ of surface area; optimal arrangement gives $\bar{v} \approx 0.368$. For a single large trap with a 10% surface area, $\bar{v} \approx 1.48$; a result 3 times larger.

Narrow Escape From a Sphere: VII



Plot: averaged MFPT $\bar{v}$ versus % trap area fraction for $N = 1, 5, 10, 20, 30, 40, 50, 60$ (top to bottom) at optimal trap locations.

- **fragmentation** effect of traps on the sphere is a significant factor.
- **only marginal benefit** by increasing N when N is already large.

References

My Papers Available at: http://www.math.ubc.ca/ ward/prepr.html

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