

Minimizing capture time with many small traps in heterogeneous media

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We study the problem of optimally placing a large number of small absorbing traps to minimize the mean first-passage time (MFPT) of particles diffusing in a heterogeneous medium with space-dependent diffusivity $D(x)$ and prescribed initial particle distribution $\omega(x)$. In two and three dimensions we identify two distinct regimes, depending on how strongly the trap ensemble depletes the particles. In the weak trapping regime (fewer traps) the optimal trap density ρ is the arithmetic average $\rho = \frac{1}{2}(\mu + \omega)$ of the normalized inverse diffusivity $\mu \propto 1/D$ and the initial particle distribution ω . In the strong trapping regime (more traps), it is proportional to their geometric average, $\rho \propto \sqrt{\mu\omega}$. We revisit the classical Green's function approach and show that it applies to weak trapping only; in 2D this requires the trap size to be exponentially small in the number of traps, so that most applications of interest fall in the strong trapping regime instead. We therefore develop a homogenization approach that captures both regimes. A special choice of initial particle distribution is $\omega \propto 1/D$, which corresponds to the equilibrium particle distribution in the absence of traps according to the Itô interpretation. In this case we show that the optimal trap distribution is the stationary particle distribution itself, regardless of the trapping strength, and this makes the MFPT constant throughout the domain; the same trap distribution also minimizes the worst-case capture time. Finally, in one dimension we find instead $\rho \propto (\mu\omega)^{1/3}$, and a similar analysis covers space-dependent drift and thin domains of variable cross-section. Direct numerical optimization confirms the analytical results.

1. INTRODUCTION

The mean first-passage time (MFPT) of a diffusing particle to a set of small absorbing traps is a classical problem in diffusion theory (also called the narrow escape problem [1]), with applications ranging from cellular signaling and receptor-ligand binding [2–5] to search theory and ecology [6–9]. A recurring question is: given a fixed number N of traps, how should they be arranged in space to minimize the average time it takes a diffusing particle to be captured? For homogeneous media, this question has been studied extensively in various contexts [10–15].

However, most of the natural environments (e.g., the cytoplasm of a living cell) are not homogeneous. Several recent works have looked at the MFPT problem with inhomogeneities [16–30]. Most of these works consider a single or several traps whose locations are fixed. However, the fundamental problem of finding the optimal spatial configuration of traps minimizing the MFPT remains open. When the medium is homogeneous, the optimal configuration of traps is expected to be roughly uniform [12, 31]. In turn, in the presence of heterogeneous diffusion or drift (e.g., advection, external force), the optimal trap location is intuitively expected to have a higher density in areas where particles “linger”, i.e., in areas of lower diffusion or slower advection. The goal of this paper is to develop precise asymptotic descriptions of optimal configurations for several model situations in the limit of many traps.

Consider a bounded domain $\Omega \subset \mathbb{R}^d$ with a smooth boundary $\partial\Omega$. For a smoothly varying space-dependent diffusion coefficient $D(x) > 0$, the Fokker–Planck equation in the Itô interpretation reads

$$p_t = \Delta(D(x)p), \quad (1.1)$$

where Δ is the Laplace operator [32–34]. In turn, the associated MFPT is governed by the adjoint operator (backward form). If the diffusing particle starts from a point $x \in \Omega$, the MFPT $u(x)$ to any of N small non-overlapping spherical traps, all of the same radius ε , located at points $x_j \in \Omega$ ($j = 1 \dots N$), satisfies

$$\begin{cases} \Delta u = -M(x) & x \in \Omega \setminus (\cup_{j=1}^N B_\varepsilon(x_j)), \\ u = 0 & x \in (\cup_{j=1}^N \partial B_\varepsilon(x_j)), \\ \partial_n u = 0, & x \in \partial\Omega, \end{cases} \quad (1.2)$$

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where ∂_n is the normal derivative, $M(x) = 1/D(x)$ (inverse diffusivity or mobility), and $B_\varepsilon(x_j)$ is a ball of radius ε centered at x_j : $B_\varepsilon(x_j) = \{x \in \mathbb{R}^d : |x - x_j| < \varepsilon\}$. We also define

$$|\Omega| = \int_{\Omega} dx, \quad |M| = \int_{\Omega} M(x) dx = \int_{\Omega} \frac{dx}{D(x)}, \quad \mu(x) = \frac{M(x)}{|M|} = \frac{D^{-1}(x)}{|D^{-1}|}. \quad (1.3)$$

Note that $\mu(x)$ is precisely the equilibrium distribution of a particle when there is no trap. Indeed, the probability flux density, $\mathbf{J}_{\text{eq}} = -\nabla(Dp_{\text{eq}})$, is zero at equilibrium, implying $Dp_{\text{eq}} = \text{const}$. Normalizing so that $\int_{\Omega} p_{\text{eq}} = 1$ gives exactly $p_{\text{eq}}(x) = \mu(x)$.

We focus on the average capture time. Let $\omega(x)$ denote a given distribution of the particle's starting location, normalized throughout to be a probability density,

$$\int_{\Omega} \omega(x) dx = 1, \quad \omega \geq 0, \quad (1.4)$$

so that the quantity to be minimized is the ω -averaged MFPT

$$\bar{u}_{\omega} = \int_{\Omega} \omega(x) u(x) dx. \quad (1.5)$$

The uniform choice $\omega = \omega_0 \equiv 1/|\Omega|$ gives the “classical” volume-averaged MFPT $\bar{u} = \int_{\Omega} u dx / |\Omega|$, averaged over all starting locations distributed uniformly. Our main question is the following:

Question: *In the limit of large N and small ε , for a given diffusivity $D(x)$ and a given starting distribution $\omega(x)$, how should the traps be distributed to minimize the ω -averaged MFPT $\bar{u}_{\omega}$?*

We consider this problem in one, two or three dimensions. Let us summarize the results in 2D and 3D first. The answer strongly depends on the relative scaling of N and ε . Define

$$\nu := \begin{cases} 4\pi\varepsilon & \text{in 3D} \\ \frac{2\pi}{\log(1/\varepsilon)} & \text{in 2D} \end{cases}, \quad \kappa := N\nu. \quad (1.6)$$

We refer to $\kappa = N\nu$ as the trapping strength. In particular, we identify two opposite regimes, $\kappa \ll 1$ or $\kappa \gg 1$, which we refer to as weak or strong trapping, respectively.

Our approach starts with a well-known Green's function energy-type formulation for the MFPT in the limit of small traps [11, 35]. Taking a continuum limit as $N \rightarrow \infty$ we then obtain a simple asymptotic description of how the optimal trap density depends on the heterogeneity $\mu(x)$ and on the starting distribution $\omega(x)$ (see § 2):

$$\rho(x) \sim \frac{1}{2} (\mu(x) + \omega(x)), \quad \kappa \ll 1, \quad N \gg 1. \quad (1.7)$$

Here and below, we use $f \sim g$ to mean $f/g \rightarrow 1$ in the indicated limit. For a uniformly distributed starting point, $\omega_0 \equiv 1/|\Omega|$, this is the average of μ and the uniform density. The corresponding optimal $\bar{u}_{\omega}$ is given by (1.9) below.

The optimal density $\rho(x)$ (in distribution sense) is defined as follows. For a fixed N , let $x_1 \dots x_N$ be optimal trap locations that minimize the MFPT for the problem (1.2) in the limit $\varepsilon \rightarrow 0$, and $\rho_N(x) = \frac{1}{N} \sum_{j=1}^N \delta(x - x_j)$. Note $\int_S \rho_N(x) dx$ gives the fraction of N traps inside an arbitrary region $S \subset \Omega$. We then define the limiting trap density as $\rho = \lim_{N \rightarrow \infty} \rho_N$, understood in the weak sense, so that $\int_S \phi(x) \rho_N(x) dx \rightarrow \int_S \phi(x) \rho(x) dx$ as $N \rightarrow \infty$, for any appropriate test function $\phi(x)$ and subset $S \subset \Omega$.

The downside of the Green's function approach is that it is only valid in the weak trapping regime $\kappa \ll 1$. This is particularly restrictive in two dimensions as it requires trap sizes ε to be exponentially small in N , which is unrealistic for a physically or numerically reasonable trap size (e.g. even for $N = 10$, one needs $\varepsilon \ll e^{-2\pi N} \approx 5 \cdot 10^{-28}$). Most realistic 2D situations are therefore in the strong trapping regime $\kappa \gg 1$. In 3D, this restriction is milder, but still relevant under many realistic scenarios (e.g. $\varepsilon = 0.01, N = 100$ gives $\kappa \approx 12.6$).

To overcome this restriction, we make use of a homogenization technique [12, 36–39]. It originates in the study of domains perforated by many small holes, developed by Marchenko and Khruslov [37, 40], by Kac [41] and by Rauch and Taylor [42] for the “crushed ice” problem, by Papanicolaou and Varadhan [43], and by Cioranescu and Murat [36], who coined “strange term” (terme étrange) corresponding to the non-vanishing $O(1)$ effect of the holes in the limit $\kappa = O(1)$. Berezhkovskii, Muratov, Shvartsman and co-workers [38, 39, 44] applied the same idea to surfaces bearing many small traps, and Cheviakov and Zawada [12] to the narrow escape problem. Here the novelty is that

the trap density is neither uniform, nor prescribed, but is the quantity to be optimized. The homogenization limit for this problem, derived in § 3, is

$$\Delta u - \kappa \rho(x) u(x) = -M(x) \text{ in } \Omega, \quad \partial_n u = 0 \text{ on } \partial\Omega. \quad (1.8)$$

In contrast to the Green's function approach, the homogenized formulation is not restricted to $\kappa \ll 1$ and provides an effective description across the weak-, intermediate-, and strong-trapping regimes, subject to the dilute-trap assumptions $\varepsilon^d N \ll 1$, underlying the homogenization limit. It reproduces the Green's function result (1.7) in the weak-trapping case $\kappa \ll 1$, and we further obtain the corresponding ω -averaged MFPT:

$$\bar{u}_\omega = \frac{|M|}{\kappa} - \frac{|M|}{4} \int_{\Omega} |\nabla V_{\omega-\mu}|^2 + O(\kappa), \quad (1.9)$$

where $V_{\omega-\mu}$ is the Poisson potential defined in (2.21).

Moreover, homogenization also gives an explicit answer for $\kappa \gg 1$. In the latter case, we find that the optimal density scales like a *geometric* average of ω and μ :

$$\rho(x) \sim \frac{\sqrt{\omega(x)\mu(x)}}{\int_{\Omega} \sqrt{\omega(x)\mu(x)} dx}, \quad \kappa \gg 1. \quad (1.10)$$

The corresponding optimal $\bar{u}_\omega$ is given by

$$\bar{u}_\omega \sim \frac{|M|}{\kappa} \left(\int_{\Omega} \sqrt{\omega(x)\mu(x)} dx \right)^2, \quad \kappa \gg 1. \quad (1.11)$$

More generally, we derive an optimality system (3.49) valid for any κ . We use this system to validate our results numerically throughout.

A very natural choice is $\omega = \mu$, corresponding to the equilibrium particle distributions in the absence of traps; in this case we simply get $\rho = \mu$, both from (1.7) or (1.10), and $\bar{u}_\mu = \frac{|M|}{\kappa}$ in both regimes. In fact we show that this holds for any κ . This is one of the key findings of the paper which we summarize as follows.

Theorem 1.1. *Consider a Brownian particle diffusing without traps under a heterogeneous diffusivity $D(x)$ in 2D or 3D, whose density is governed by the Fokker–Planck equation (1.1) (in Itô sense). Wait long enough until its distribution equilibrates to $\mu(x)$ given by (1.3). Now turn on the traps. Then the trap density minimizing the mean capture time starting from $\mu(x)$ is precisely $\rho(x) = \mu(x)$: the traps should be distributed exactly like the particle itself. This holds for every $\kappa = \nu N$. At the optimum, the MFPT $u(x)$ is constant, independent of the starting location:*

$$u_{\text{opt}}(x) \equiv \frac{|M|}{\kappa}, \quad (1.12)$$

which is therefore also the mean capture time. Moreover, the optimal density $\rho = \mu$ is the unique global minimum of $\bar{u}_\mu$:

$$\int_{\Omega} \mu u \geq \frac{|M|}{\kappa} \text{ for all densities } \rho \text{ and any } \kappa, \quad (1.13)$$

with equality if and only if $\rho = \mu$.

Instead of minimizing the *average* $\bar{u}_\omega$ for a given ω , one can ask how to minimize the *worst-case capture time* $\max_{x \in \Omega} u(x)$. In fact Theorem 1.1 gives the answer: since $\int \mu u \leq \max u$ (average with respect to any measure is bounded by $\max u$), it then immediately follows from Theorem 1.1 that the choice $\rho = \mu$ solves the mini-max problem to minimize the worst-case (i.e. maximum) MFPT. We state this as a theorem.

Theorem 1.2. *The worst-case mean capture time $\max_{x \in \Omega} u(x)$ is minimized by choosing $\rho = \mu$, in which case $u(x)$ is everywhere constant: $u(x) = \frac{|M|}{\kappa}$. In other words, $\rho = \mu$ solves the mini-max problem $\min_{\rho, \text{ density}} \|u\|_\infty$.*

Finally, we have the following generalization of Theorem 1.1 for any starting density ω :

Theorem 1.3. Define $\bar{u}_\omega[\rho] = \int_\Omega \omega(x)u(x)dx$, where u solves (1.8) for a given density ρ . Then

$$\bar{u}_\omega[\rho] \geq \frac{|M|}{\kappa} \left(\int_\Omega \sqrt{\omega\mu} \right)^2 \quad \text{for all densities } \omega, \rho \text{ and any } \kappa. \quad (1.14)$$

Moreover the equality is achieved if and only if $\omega = \rho = \mu$.

Note that the lower bound is the same as in (1.11): it is approached as $\kappa \rightarrow \infty$ but never touched unless $\omega = \rho = \mu$. Indeed, Theorem 1.1 can be viewed as the special case $\omega = \mu$ of Theorem 1.3.

The proofs of Theorems 1.1 and 1.3 are given in § 3.1.

In § 4 we consider the analogous problem in one dimension. Here, the problem simplifies, since one-dimensional traps split the domain into disjoint subintervals. We find that the optimal trap density scales with $\mu^{1/3}$ for the uniform starting distribution. On the other hand if the particle starts from the equilibrium distribution $\omega = \mu$, the optimal distribution becomes proportional to $\mu^{2/3}$. Both are special cases of a single formula: for an arbitrary starting distribution $\omega(x)$, the optimal density in 1D is proportional to $(\mu(x)\omega(x))^{1/3}$, recovering $\mu^{1/3}$ for uniform ω and $\mu^{2/3}$ for $\omega = \mu$. This is in contrast to 2D, where the same choice $\omega = \mu$ makes the optimal density exactly proportional to μ itself, for every value of $\kappa = \nu N$. Finally, we also apply a similar machinery to determine optimal configurations for heterogeneous media with spatially-dependent drift, as well as to “thin” domains.

2. GREEN’S FUNCTION APPROACH

We start by generalizing the classical Green’s function approach to MFPT computations with heterogeneous diffusion and starting positions with the goal of optimizing (1.5) over trap positions in 2D or 3D.

To show our main result (1.7), we first use standard asymptotics to reduce the MFPT to an energy formulation involving Green’s functions [11], which we generalize here to the case of non-constant $M(x)$ and $\omega(x)$. The argument proceeds in two steps: we first derive (following [11]) a discrete pairwise Green’s-function energy $E(x_1, \dots, x_N)$ whose minimizer approximates the optimal trap locations (Lemma 2.1 below), we then pass to the continuum limit $N \rightarrow \infty$ of this energy to obtain the density formula (1.7).

We first introduce some notation. Let $G(x, y)$ denote the Neumann Green’s function on the domain Ω satisfying

$$\begin{cases} \Delta G = \frac{1}{|\Omega|} - \delta(x - y), & x, y \in \Omega \subset \mathbb{R}^d; \\ \partial_n G = 0 & \text{on } \partial\Omega; \quad \int_\Omega G(x, y)dx = 0, \end{cases} \quad (2.15)$$

and let G_μ be the analogous Green’s function with a heterogeneity, defined via

$$\begin{cases} \Delta G_\mu = \mu(x) - \delta(x - y), & x, y \in \Omega \subset \mathbb{R}^d; \\ \partial_n G_\mu = 0 & \text{on } \partial\Omega; \quad \int_\Omega G_\mu(x, y)dx = 0. \end{cases} \quad (2.16)$$

Finally, let R and R_μ be the regular parts of G and G_μ , respectively:

$$R_\mu(x, y) = G_\mu(x, y) - g(x - y), \quad (2.17)$$

$$R(x, y) = G(x, y) - g(x - y), \quad (2.18)$$

where g is the free-space Green’s function in $\mathbb{R}^d$:

$$g(x) = \begin{cases} -\frac{1}{2\pi} \log |x|, & d = 2, \\ \frac{1}{4\pi |x|}, & d = 3. \end{cases} \quad (2.19)$$

It is convenient to introduce, for an arbitrary function ψ on Ω , the potential generated by ψ ,

$$V_\psi(x) := - \int_\Omega \psi(y)G(x, y) dy, \quad (2.20)$$

which, by (2.15), is the unique mean-zero solution of

$$\Delta V_\psi = \psi(x) - \frac{|\psi|}{|\Omega|}, \quad \partial_n V_\psi = 0 \text{ on } \partial\Omega, \quad \int_\Omega V_\psi(x)dx = 0. \quad (2.21)$$

The two densities entering our problem generate the potentials V_μ and V_ω respectively: the first comes from heterogeneity, the second from the starting distribution. Note also that V_ψ is linear in ψ so that e.g. $V_\mu + V_\omega = V_{\mu+\omega}$. For a uniform starting distribution $\omega \equiv 1/|\Omega|$ one has $V_\omega \equiv 0$.

Note that G_μ can be decomposed as follows:

$$G_\mu(x, y) = G(x, y) + V_\mu(x), \quad (2.22)$$

where G satisfies (2.15) and V_μ is given by (2.20) with $\psi = \mu$.

We start with the following asymptotic reduction for $u(x)$. In the outer region, away from the traps x_j , we search for u in the form

$$u(x) \sim T + \sum_{j=1}^N C_j G_\mu(x, x_j), \quad (2.23)$$

where the constants T and C_j are to be found. Note that this estimate is asymptotically valid away from x_j and corresponds to a monopole approximation of the trap; the neglected terms are $O(\varepsilon^2)$ coming from neglecting the dipole terms, and independent of ν to all orders in 2D [45–48].

For $x \notin \{x_1, \dots, x_N\}$, Eqs. (1.2, 2.16) imply $\Delta u = -M(x) = \sum_{j=1}^N C_j \mu(x)$. Integrating over Ω we then obtain

$$\sum_{j=1}^N C_j = -|M|. \quad (2.24)$$

In the inner region near x_k , we change variables $x = x_k + \varepsilon y$, $u(x) = \tilde{u}_k(y)$ to obtain, at leading order, $\Delta_y \tilde{u}_k \sim 0$, which is to be solved outside the unit ball, i.e., $|y| > 1$, with $\tilde{u}_k = 0$ on $|y| = 1$ and $\tilde{u}_k$ growing at most like g at infinity. The admissible solutions are

$$\tilde{u}_k(y) \sim A_k \times \begin{cases} \log |y|, & d = 2, \\ (1 - |y|^{-1}), & d = 3, \end{cases} \quad (2.25)$$

with the factor A_k to be found by matching the inner and outer solution. Writing the outer problem with respect to the inner variables near x_k , we have:

$$\begin{aligned} u(x_k + \varepsilon y) &\sim T + \sum_{j=1}^N C_j G_\mu(x_k + \varepsilon y, x_j) \\ &\sim T + \sum_{j \neq k}^N C_j G_\mu(x_k, x_j) + C_k [g(\varepsilon y) + R_\mu(x_k, x_k)]. \end{aligned} \quad (2.26)$$

Using (2.19) and matching (2.25) and (2.26), one fixes $A_k = -C_k/(2\pi)$ in 2D and $A_k = -C_k/(4\pi\varepsilon)$ in 3D; evaluating at the trap $|y| = 1$ in both cases yields

$$0 = T + \sum_{j \neq k}^N C_j G_\mu(x_k, x_j) + C_k \left[\frac{1}{\nu} + R_\mu(x_k, x_k) \right], \quad k = 1 \dots N, \quad (2.27)$$

with ν defined in (1.6).

There are two ways to proceed. In the first approach, one can consider (2.27) together with (2.24) as a linear system of $N + 1$ equations for the $N + 1$ unknowns T and $C_1, \dots, C_N$, which can be easily solved numerically; this approach is valid for any trapping strength κ . From (2.23) and using $\int_\Omega \omega G_\mu(x, x_j) dx = -V_\omega(x_j) + \int_\Omega \omega V_\mu$ together with (2.24), we then obtain a simplified expression

$$\bar{u}_\omega = T - \sum_{j=1}^N C_j V_\omega(x_j) - |M| \int_\Omega \omega V_\mu. \quad (2.28)$$

This expression is the essence of a *hybrid asymptotic-numerical method* for computing $\bar{u}_\omega$: *numeric* because the coefficients C_j and T must be computed numerically by solving (2.24, 2.27); but *asymptotic* in that the traps in the full problem (1.2) are replaced by sources and the entire solution is approximated by the Neumann Green's functions.

This method has been extensively used by Ward and collaborators [11, 45, 46, 49–51], who coined the term “hybrid”; also referring to it as the “sum-of-logs” when done in 2D. Correspondingly, we shall refer to (2.28), together with (2.27, 2.24), as the **hybrid system**.

The accuracy of approximation (2.28) inherits the accuracy of the approximation (2.23), which is of $O(\varepsilon^2)$, coming from dropping the dipole terms. As a consequence, the error between (2.28) and (1.2) is of $O(\varepsilon^2)$ even in the strong trapping regime $\nu N \gg 1$.

In turn, the second approach corresponds to the asymptotic expansion in $\nu \ll 1$ of the hybrid system (2.28); as we will see it is only valid in the weak trapping regime $\nu N \ll 1$. We now expand in ν ,

$$C_k = C_{k0} + C_{k1}\nu + C_{k2}\nu^2 + \dots, \quad T = \frac{1}{\nu}T_0 + T_1 + \nu T_2 + \dots \quad (2.29)$$

We then obtain from (2.27), at leading order,

$$C_{k0} = -T_0 \quad k = 1, \dots, N.$$

Upon substituting into (2.24) this yields

$$T_0 = \frac{1}{N} |M|, \quad C_{k0} = -\frac{1}{N} |M|, \quad k = 1, \dots, N. \quad (2.30)$$

At the next order in ν , (2.27) yields

$$T_1 + C_{k1} + \sum_{j \neq k}^N C_{j0} G_\mu(x_k, x_j) + C_{k0} R_\mu(x_k, x_k) = 0, \quad k = 1 \dots N, \quad (2.31)$$

and from (2.24) we get

$$\sum_{k=1}^N C_{k1} = 0. \quad (2.32)$$

Summing N equations (2.31) for $k = 1 \dots N$ and using (2.30) and (2.32), we then obtain

$$T_1 = \frac{|M|}{N^2} \sum_{j=1}^N \sum_{k=1}^N G_{\mu kj}, \quad \text{where } G_{\mu kj} = \begin{cases} G_\mu(x_k, x_j), & k \neq j \\ R_\mu(x_k, x_k), & k = j \end{cases}.$$

The decomposition (2.22) also yields

$$T_1 = \frac{|M|}{N^2} \left\{ \sum_{k=1}^N \sum_{j \neq k}^N G(x_k, x_j) + \sum_{k=1}^N R(x_k, x_k) + N \sum_{k=1}^N V_\mu(x_k) \right\}.$$

An analogous expansion shows that

$$T_2 = \frac{|M|}{N^3} \left(\sum_{k=1}^N \sum_{j=1}^N G_{\mu kj} \right)^2 - \frac{|M|}{N^2} \sum_{k=1}^N \sum_{j=1}^N \sum_{l=1}^N G_{\mu jl} G_{\mu kj}, \quad (2.33)$$

so that, generically, $T_2 = O(N)$. It follows that the entire asymptotic procedure is only valid for $\nu N \ll 1$, so as not to contradict the asymptotic orders in (2.29).

It remains to compute $\bar{u}_\omega$. From (2.23), we have

$$\bar{u}_\omega = \int_{\Omega} \omega u = T + \sum_{j=1}^N C_j \int_{\Omega} \omega(x) G_\mu(x, x_j) dx,$$

and by (2.22), (2.20) and the symmetry of G ,

$$\int_{\Omega} \omega(x) G_\mu(x, x_j) dx = -V_\omega(x_j) + \int_{\Omega} \omega V_\mu.$$

Using (2.24) and (2.30), we obtain

$$\bar{u}_\omega \sim T + \frac{|M|}{N} \sum_{k=1}^N V_\omega(x_k) - |M| \int_{\Omega} \omega V_\mu. \quad (2.34)$$

Note that the last two terms in (2.34) are of the same order as the terms in T_1 . Together with $T \sim T_0/\nu + T_1$ this gives the following.

Lemma 2.1. *Define a pairwise Green's function energy to be*

$$E(x_1, \dots, x_N) = \sum_{k=1}^N \sum_{j \neq k}^N G(x_k, x_j) + \sum_{k=1}^N R(x_k, x_k) + N \sum_{k=1}^N V_{\mu+\omega}(x_k) - N^2 \int_{\Omega} \omega V_\mu, \quad (2.35)$$

where G and R are defined in (2.15, 2.18), $V_{\mu+\omega}$ in (2.20) with $\psi = \mu + \omega$, and ν in (1.6). In the limit $\varepsilon \rightarrow 0$ and for a fixed N , we have

$$\bar{u}_\omega = \int_{\Omega} \omega(x) u(x) dx \sim \frac{|M|}{\nu N} + \frac{|M|}{N^2} E(x_1, \dots, x_N) + \mathcal{O}(\nu N) \quad \text{as } \varepsilon \rightarrow 0. \quad (2.36)$$

The optimal trap locations correspond to the minimum of the pairwise Green's function energy E in (2.35). Note that we must have $\nu N \ll 1$ for the asymptotics to be applicable. This is quite restrictive especially in 2D: ε must be exponentially small in N , see (1.6).

To compute optimal configurations of the energy E , we will study its gradient flow, as was done e.g. in [31, 52–55]. We introduce a time-dependent position $x_k(t)$ (with artificial time t) along with the gradient flow $x'_k(t) = -\partial_{x_k} E(x_1(t), \dots, x_N(t))$. Then $x_k(t) \rightarrow x_k$ as $t \rightarrow \infty$, where x_k is a local minimum of E . We now compute

$$\partial_{x_k} E = 2 \left(\sum_{j \neq k}^N \nabla_x G(x_k, x_j) \right) + 2 \nabla_x R(x_k, x_k) + N \nabla V_{\mu+\omega}(x_k).$$

The associated gradient flow (up to time rescaling by $\frac{1}{2N}$ for convenience) then becomes

$$-x'_k(t) = \frac{1}{N} \left(\sum_{j \neq k} \nabla_x G(x_k, x_j) + \nabla_x R(x_k, x_k) \right) + \frac{1}{2} \nabla V_{\mu+\omega}(x_k). \quad (2.37)$$

The global minimizer of E corresponds to a stable equilibrium of the ODE system (2.37): $x_k = \lim_{t \rightarrow \infty} x_k(t)$. We now look at the continuum density formulation in the limit $N \rightarrow \infty$ of the steady state of (2.37). Following [31, 53], we define a coarse-grained density to be

$$\rho(x, t) = \frac{1}{N} \sum_{j=1}^N \delta(x - x_j(t)).$$

Then (2.37) is equivalent to the continuum density evolution equation $\rho_t + \nabla \cdot (v\rho) = 0$, where v is the associated velocity field:

$$v(x) = \frac{1}{2} \nabla V_{\mu+\omega}(x) + \int_{\Omega} \nabla_x G(x, y) \rho(y) dy. \quad (2.38)$$

At the steady state, we have $v(x) = 0$ so that $\nabla \cdot v = 0$. Applying the divergence to both sides of (2.38) and using (2.21) and (2.15), we obtain

$$0 = \nabla \cdot v = \frac{1}{2} \Delta V_{\mu+\omega}(x) + \int_{\Omega} \Delta G(x, y) \rho(y) dy = \frac{1}{2} (\mu(x) + \omega(x)) - \rho(x).$$

It follows that $\rho(x) = \frac{1}{2} (\mu(x) + \omega(x))$, which is (1.7). ■

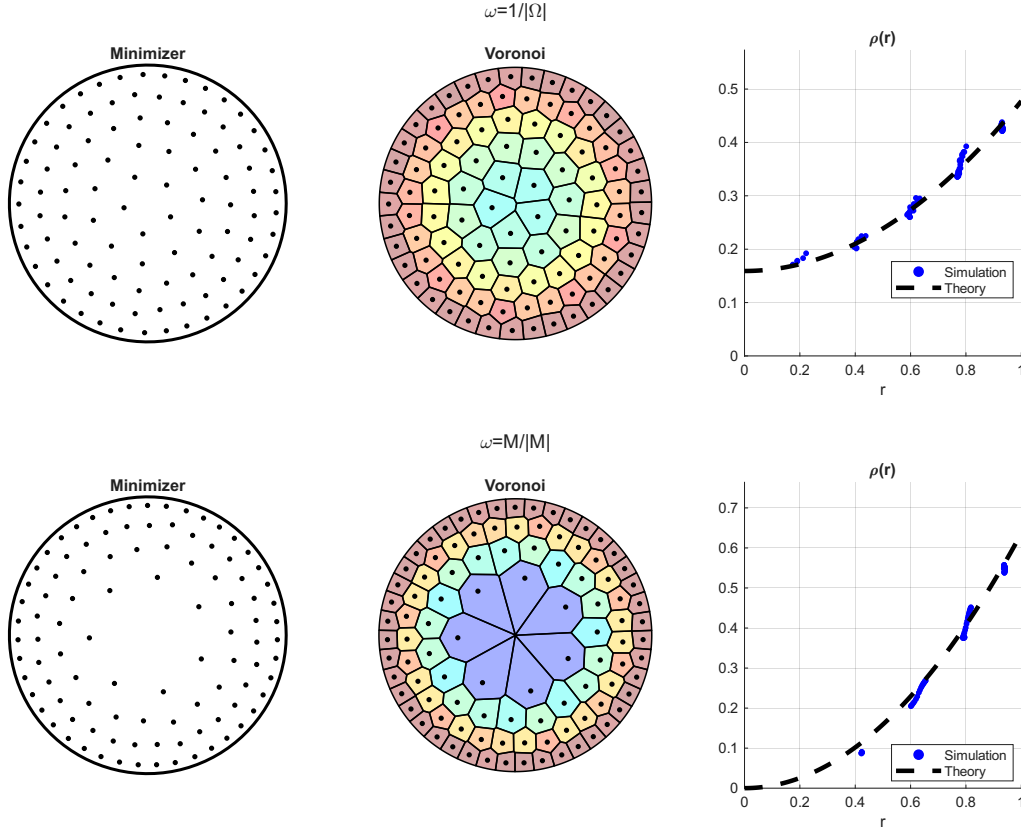


FIG. 1. Optimal trap distribution with $N = 100$ and $M(r) = r^2$ inside a unit disk with (i) $\omega = 1/|\Omega|$ (top) and (ii) $\omega = M/|M|$ (bottom). Left: trap positions that minimize the Green's energy (2.35), computed numerically (see text); Middle: the corresponding Voronoi cells. Right: Comparison of numerical approximation of $\rho(x)$ obtained from the Voronoi diagram (see text) shown as “simulation”, with continuum limit (2.41) shown as “theory”.

2.1. Numerics

We now consider several numerical experiments for a disk and a rectangular domain, for which an efficient computation of the Neumann Green's function G is available.

Disk. When Ω is a unit disk, an explicit expression for the Neumann Green's function is available [56, 57],

$$G(x, y) = -\frac{1}{2\pi} \log(|x - y|) + \frac{1}{4\pi} \left[-\log(|x|^2 |y|^2 + 1 - 2x \cdot y) + |x|^2 + |y|^2 - \frac{3}{2} \right]. \quad (2.39)$$

As an example, we take the radial dependence for both $M(x)$ and $\omega(x)$:

$$M(x) = a|x|^2 + b, \quad \omega(x) = \frac{c|x|^2 + d}{\pi(c/2 + d)}. \quad (2.40)$$

The effective trap density in the large- N limit from (1.7) is then given by

$$\rho(x) = \frac{1}{2\pi} \left[\frac{a|x|^2 + b}{a/2 + b} + \frac{c|x|^2 + d}{c/2 + d} \right]. \quad (2.41)$$

Solving (2.21) using radial coordinates, we find that

$$\begin{aligned} V_{\mu+\omega}(x) &= - \left[\frac{a}{4\pi(a+2b)} + \frac{c}{4\pi(c+2d)} \right] \left(|x|^2 - \frac{|x|^4}{2} - \frac{1}{3} \right), \\ \nabla G(x, y) &= - \frac{1}{2\pi} \frac{x-y}{|x-y|^2} + \frac{1}{2\pi} \left[- \frac{x|y|^2 - y}{|x|^2|y|^2 + 1 - 2x \cdot y} + x \right], \\ \nabla V_{\mu+\omega} &= - \left[\frac{a}{2\pi(a+2b)} + \frac{c}{2\pi(c+2d)} \right] (1 - |x|^2) x, \\ \nabla R(x, y) &= + \frac{1}{2\pi} \left[- \frac{x|y|^2 - y}{|x|^2|y|^2 + 1 - 2x \cdot y} + x \right], \quad \nabla R(x, x) = \frac{1}{2\pi} \left[\frac{|x|^2 - 2}{|x|^2 - 1} \right] x. \end{aligned}$$

With these explicit expressions at hand, it is easy to apply the gradient descent method to ODE (2.37) to compute the optimal trap positions for any given a, b, c, d . We illustrate this for $M(x) = |x|^2$ and for (i) constant $\omega(x) = 1/\pi$ and (ii) $\omega(x) = M/|M| = |x|^2/(\pi/2)$. We used $N = 100$ traps and applied the forward Euler method to compute the steady state of the ODE (2.37). A few minutes on a standard computer is enough to compute the steady state within 10^{-5} , measured as $\max_k |x'_k(t)|$ at the final time. The result is shown in Fig. 1 (left side).

Once the steady state of (2.37) is computed, we construct Voronoi cells (shown in the middle of Fig. 1) to estimate an effective density $\rho(x)$. We use $\rho(x_j) \approx 1/(NS_j)$, where S_j is the area of the Voronoi cell around x_j . This is shown on the scatter plot on the right, where $|x_j|$ is plotted versus the estimated $\rho(x_j)$, $j = 1 \dots N$. For comparison, this scatter plot is superimposed with the explicit formula (2.41) for the effective trap density. Excellent agreement is observed. We emphasize that this is a comparison between the minimization of the Green's energy and our theoretical predictions; both relations are valid only in the limit $\nu \ll 1$. An ultimate validation would require comparison with a numerical solution of the original PDE (1.2). However, as said earlier, the validity condition $\nu \ll 1$ would require dealing with extremely small ε . For this reason, we relegate such a comparison to §3, in which the use of the homogenization technique will relax this condition.

Rectangle. Consider a rectangle $\Omega = (0, L) \times (0, H)$ and take the heterogeneity to be one-dimensional and the weight to be uniform:

$$M(x, y) = f(x), \quad \omega = 1/|\Omega|. \quad (2.42)$$

Then (1.7) yields

$$\rho(x, y) = \frac{1}{2H} \left(\frac{f(x)}{|f|} + \frac{1}{L} \right), \quad |f| := \int_0^L f(x) dx, \quad (2.43)$$

and

$$\nabla V_\mu(x, y) = \left(\frac{1}{H} \left[\frac{F(x)}{|f|} - \frac{x}{L} \right], 0 \right), \quad F(x) := \int_0^x f(s) ds; \quad V_\omega = 0, \quad (2.44)$$

the latter because the starting distribution is uniform, so that $V_{\mu+\omega} = V_\mu$. For $f = ax + b$ this gives

$$\nabla V_\mu(x, y) = \left(\frac{ax^2/2 + bx}{(aL^2/2 + bL)H} - \frac{x}{LH}, 0 \right). \quad (2.45)$$

The Neumann Green's function admits a rapidly convergent Fourier series representation, with a resummation technique used to obtain a rapidly convergent series for its regular part (see [56], Section 4.2 for these explicit formulas that we do not reproduce here). We implemented these formulas in MATLAB and used them for computing the steady state of the energy flow (2.37).

Figure 2 shows the results of a numerical experiment on a long rectangle with $L = 10$ and $H = 1$. Here, we fixed $M(x, y) = x$ so that $|f| = 50$ and (2.43) gives $\rho(x, y) = x/100 + 1/20$, and varied N , showing $N = 5, 20$ and 80 . Each row of the figure shows the same N for the two starting distributions: a uniform $\omega = 1/|\Omega|$ on the left, and $\omega = \mu$ on the right, for which (1.7) collapses to $\rho = \mu = x/50$. It is interesting to note that as N is increased, the optimal configuration of traps changes from a single line ($N = 5$) to a mix of one and two rows ($N = 20$), and so on. The optimal configuration is denser on the right (lower diffusivity) and sparser on the left (high diffusivity); note that

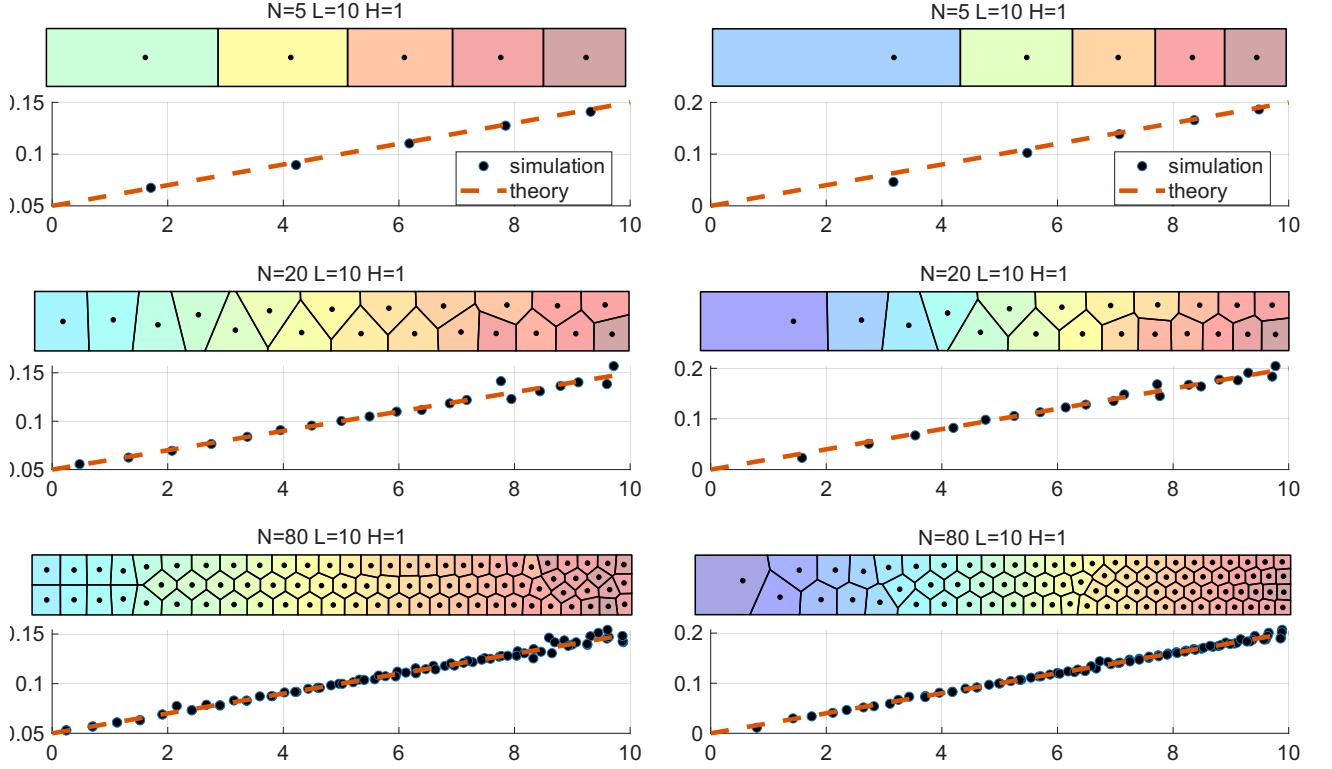


FIG. 2. Optimal trap locations inside an elongated rectangle $(0, 10) \times (0, 1)$ with $M(x, y) = x$, for $N = 5, 20$ and 80 traps, from top to bottom. Left column: uniform starting distribution $\omega \equiv 1/|\Omega|$. Right column: $\omega = \mu = M/|M|$. In each panel the strip shows the optimal trap positions together with their Voronoi cells, and the graph below it compares the effective density obtained from the Voronoi cells (dots) with the asymptotic prediction $\rho(x)$ (dashed) from (1.7): $\rho(x) = x/100 + 1/20$ for the left column and $\rho = \mu = x/50$ for the right. Note that the density is strictly positive everywhere for uniform ω , but vanishes at $x = 0$ for $\omega = \mu$.

(2.43) predicts $\rho \rightarrow 1/(2LH) > 0$ rather than zero density as $x \rightarrow 0$. The variable density results in “coexistence” of multi-row patterns (e.g. from one to four rows when $N = 80$). Regardless of pattern complexity, the overall effective density is in excellent agreement with the theory, even for $N = 5$, where the configuration is essentially one-dimensional.

The two columns differ most near $x = 0$, where diffusion is fastest. For a uniform start the traps do not thin out indefinitely there: (2.43) retains the floor $1/(2LH)$ contributed by ω , and the leftmost trap sits well inside the domain at every N . For $\omega = \mu$ that floor is absent, ρ vanishes linearly as $x \rightarrow 0$, and the left end of the rectangle is left progressively emptier — there is no point placing traps where the particle is unlikely to start. This is the case in which the weak- and strong-trapping predictions agree for every κ , by (1.12), so the agreement seen in the right column does not by itself test the $\kappa \ll 1$ restriction; the left column does.

3. HOMOGENIZATION

As the computation of T_2 in (2.33) shows, the asymptotics we derived in Lemma 2.1 are only valid assuming that $\nu N \ll 1$. This is a particularly severe restriction in 2D (e.g. $\varepsilon = 0.01, N = 10$ yields $\nu N \approx 13.6$). In this section, we develop an alternative approach based on homogenization [12, 36–39, 44]. In the limit of many traps, the problem (1.2) can be homogenized as follows. In 3D, consider the inner region near the trap x_k . As in (2.26), we rescale near x_k : $x = x_k + \varepsilon y$; to leading order we obtain $\Delta_y u \sim 0$, with $u = 0$ at $|y| = 1$. The solution is then given by $u \sim b_k(1 - \frac{1}{|y|}) \sim b_k - \frac{b_k \varepsilon}{|x - x_k|}$, where b_k is to be determined. In the intermediate regime $\varepsilon \ll |x - x_k| \ll 1$ we then obtain $u \rightarrow b_k$.

In the outer region we then replace the trap at x_k by a delta source with strength $4\pi b_k \varepsilon$ in the homogenized

equation:

$$\begin{aligned}\Delta u &= -M(x) + \sum_{j=1}^N 4\pi b_j \varepsilon \delta(x - x_j) \\ &= -M(x) + 4\pi \varepsilon \sum_{j=1}^N u(x_j) \delta(x - x_j).\end{aligned}\tag{3.46}$$

Finally, recall that the density is given by $\rho(x) = \frac{1}{N} \sum_j \delta(x - x_j)$ so we replace $\sum_j u(x_j) \delta(x - x_j) \sim u(x) N \rho(x)$ that leads to the homogenization limit (1.8), with ν given by (1.6). A similar derivation in 2D also yields (3.46) but with $4\pi \varepsilon$ replaced by $\frac{2\pi}{\log(1/\varepsilon)}$.

The minimization problem is to find the optimal $\rho(x)$ subject to $\int_{\Omega} \rho dx = 1$ such that the ω -averaged MFPT $\bar{u}_{\omega} = \int_{\Omega} \omega u$ of (1.5) is minimized. In general, there is no explicit solution, and the optimal density $\rho(x)$ has to be found numerically. However the regimes $\kappa \ll 1$ and $\kappa \gg 1$ can be computed explicitly for an arbitrary ω , as we now show.

Weak trapping limit $\kappa \ll 1$. Note that this corresponds precisely to the validity region $\nu N \ll 1$ of Lemma 2.1; we now rederive this result via homogenization approach.

We expand u in powers of κ as follows

$$u = \frac{1}{\kappa} u_0 + u_1 + \kappa u_2 + \dots$$

so that

$$\Delta u_0 = 0, \quad \Delta u_1 = \rho u_0 - M(x), \quad \Delta u_2 = \rho u_1,$$

subject to the boundary conditions $\partial_n u_i = 0$ on $\partial\Omega$, with $i = 0, 1, 2, \dots$. Then u_0 is constant and integrating the equation for u_1 we obtain $u_0 = |M|$. The Green's second identity yields

$$\begin{aligned}u_1(y) &= -|M| \int_{\Omega} G(x, y) (\rho(x) - \mu(x)) dx + K \\ &= |M| V_{\rho-\mu}(y) + K,\end{aligned}$$

where V_{ψ} is defined in (2.20) and K is a constant that can be determined from the equation for u_2 , yielding $\int_{\Omega} \rho u_1 = 0$, so that

$$u_1(y) = |M| \left(V_{\rho-\mu}(y) - \int_{\Omega} \rho V_{\rho-\mu} \right).$$

We therefore obtain the two-term expansion

$$\bar{u}_{\omega} = \frac{|M|}{\kappa} + |M| \int_{\Omega} (\omega - \rho) V_{\rho-\mu} + O(\kappa).\tag{3.47}$$

The optimal $\rho(x)$ minimizes (3.47) subject to $\int_{\Omega} \rho = 1$. Taking a variational derivative and applying a Lagrange multiplier, the optimal density satisfies

$$V_{\omega} - 2V_{\rho} + V_{\mu} = \lambda.$$

Applying Δ to both sides yields $\omega - 2\rho + \mu = 0$ and recovers (1.7). Finally, substituting $\rho = \frac{1}{2}(\mu + \omega)$ into (3.47), we obtain

$$\bar{u}_{\omega} = \frac{|M|}{\kappa} + \frac{|M|}{4} \int_{\Omega} (\omega - \mu) V_{\omega-\mu} + O(\kappa).$$

The integral can be further simplified using the identity $\int_{\Omega} \psi V_{\psi} = - \int_{\Omega} |\nabla V_{\psi}|^2$, valid for any mean-zero ψ (multiply $\Delta V_{\psi} = \psi$ by V_{ψ} and integrate by parts, the boundary term vanishing by $\partial_n V_{\psi} = 0$), resulting in (1.9). Taking $\omega = \mu$ we get $\rho = \mu$ and $\bar{u}_{\omega} = \frac{|M|}{\kappa}$, recovering (1.12) for the special case of small $\kappa = \nu N$.

Strong trapping limit $\kappa \gg 1$. Here, we expand $u = \frac{1}{\kappa}u_0 + \dots$. At the leading order we then obtain $u_0 = \frac{M}{\rho}$, so that $\bar{u}_\omega \sim \frac{1}{\kappa} \int_\Omega \frac{\omega M}{\rho}$. Minimization under the constraint $\int_\Omega \rho = 1$ using a Lagrange multiplier yields $\frac{\omega M}{\rho^2} = \lambda$, so that

$$\rho = \frac{\sqrt{\omega M}}{\int_\Omega \sqrt{\omega M}}, \quad (3.48)$$

which is identical with (1.10); substituting (3.48) into $\bar{u}_\omega \sim \kappa^{-1} \int_\Omega \omega M / \rho$ yields (1.11). Choosing $\omega = \mu$ again gives $\rho = \mu$, $\bar{u}_\omega \sim \frac{1}{\kappa} |M|$, recovering (1.12) for the special case of large $\kappa = \nu N$.

Arbitrary trapping. For general κ the optimal density has no closed form, but it is characterized by a simple optimality system. We seek to minimize $J[\rho] = \int_\Omega \omega u$. Perturbing $\rho \rightarrow \rho + \delta\rho$ and $u \rightarrow u + \delta u$ yields $\delta J = \int_\Omega \omega \delta u$ which we need to rewrite in terms of $\delta\rho$. We have $\Delta \delta u - \kappa \rho \delta u = \kappa u \delta\rho$. Introduce an adjoint v to satisfy $\Delta v - \kappa \rho v = -\omega$ in Ω , with Neumann boundary condition on $\partial\Omega$. Multiplying this equation by δu and integrating by parts we obtain

$$-\int_\Omega \omega \delta u = \int_\Omega \delta u (\Delta v - \kappa \rho v) = \int_\Omega v (\Delta \delta u - \kappa \rho \delta u) = \int_\Omega v \kappa u \delta\rho.$$

This yields $\delta J / \delta\rho = -\kappa u v$. Finally we introduce a Lagrange multiplier for the constraint $\int_\Omega \rho = 1$ so that stationarity of $\bar{u}_\omega$ requires $\kappa u v = \lambda$. In summary, the optimal density ρ satisfies

$$\begin{cases} \Delta u - \kappa \rho u = -M & \text{in } \Omega, & \partial_n u = 0 \text{ on } \partial\Omega, \\ \Delta v - \kappa \rho v = -\omega & \text{in } \Omega, & \partial_n v = 0 \text{ on } \partial\Omega, \\ u v = \text{const}, & \int_\Omega \rho = 1. \end{cases} \quad (3.49)$$

In particular, if $\omega = \mu$, then $v \propto u$, and the optimality condition reduces to $u = \text{const}$: the optimal density equalizes the MFPT over all starting points, and (1.8) gives $\rho = \mu$ together with $u \equiv |M|/\kappa$, for every κ , which is precisely (1.12). For a homogeneous medium (M constant, ω uniform) this says that the optimal density is uniform, $\rho = 1/|\Omega|$.

3.1. Proofs of Theorems 1.1–1.3

We now give the proofs of Theorems 1.1 and 1.3; Theorem 1.2 follows from Theorem 1.1 as noted in the Introduction.

Proof of Theorem 1.1. Multiply (1.8) by u and integrate to obtain

$$\begin{aligned} |M| \int_\Omega \mu u &= \kappa \int_\Omega \rho u^2 - \int_\Omega u \Delta u \\ &= \kappa \int_\Omega \rho u^2 + \int_\Omega |\nabla u|^2 \\ &\geq \kappa \int_\Omega \rho u^2. \end{aligned}$$

By Cauchy–Schwarz, $\int_\Omega \rho u^2 \geq (\int_\Omega \rho u)^2$ (recall that $\rho \geq 0$ and $\int_\Omega \rho = 1$), and integrating (1.8) we obtain $\int_\Omega \rho u = |M|/\kappa$. Putting these together yields

$$\int_\Omega \mu u \geq \frac{|M|}{\kappa}.$$

Equality requires both $\int_\Omega |\nabla u|^2 = 0$ and $\int_\Omega \rho u^2 = (\int_\Omega \rho u)^2$. The former implies that u is constant, which in turn implies the latter. Substituting a constant u into (1.8) gives $\rho \propto \mu$, hence $\rho = \mu$ by normalization, and then $u = |M|/\kappa$. Conversely, for $\rho = \mu$ the constant $u \equiv |M|/\kappa$ solves (1.8), so equality holds. ■

Proof of Theorem 1.3. Since $M > 0$ and $\rho \geq 0$, the maximum principle gives $u > 0$ in Ω . Dividing (1.8) by u and integrating by parts, using $\int_\Omega \rho = 1$, we obtain

$$\int_\Omega \frac{M}{u} = \kappa - \int_\Omega \frac{\Delta u}{u} = \kappa - \int_\Omega \left| \frac{\nabla u}{u} \right|^2 \leq \kappa. \quad (3.50)$$

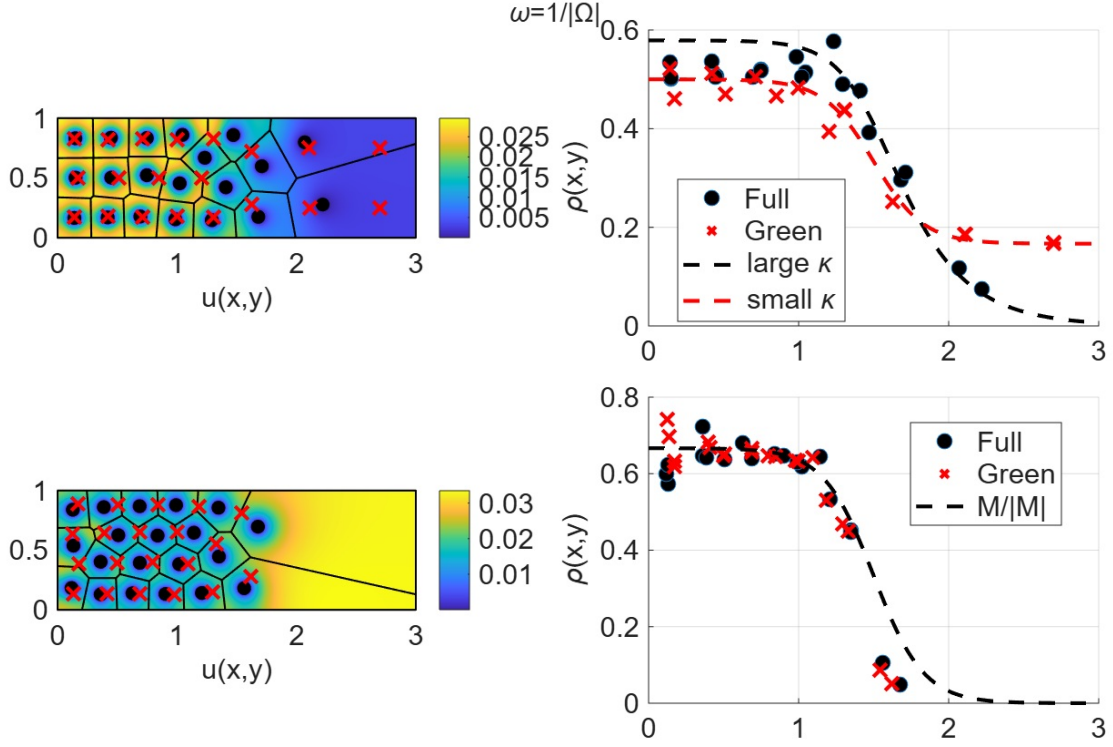


FIG. 3. Top: Optimal trap locations inside a rectangle $(0, 3) \times (0, 1)$, with $M(x, y) = \tanh(3(1.5 - x)) + 1$ (slow on the left, fast on the right), $\omega = 1/|\Omega|$, and with $N = 20, \varepsilon = 0.05$ (so that $\kappa = \nu N \approx 42$). Black dots ('full') correspond to minimizing the full problem (1.2) numerically. Red crosses ('Green') correspond to the minimization of the Green's energy (2.35). Top left: color plot shows the corresponding solution $u(x, y)$ of the full problem (1.2) with optimal trap locations, and the corresponding Voronoi cells. Optimal trap locations computed via Green's energy minimization are also shown. Top right: effective trap density obtained from the two computed configurations, compared with the small- κ prediction (1.7) and the large- κ prediction (3.48). Since $\kappa \approx 42$ here, the large- κ formula is the relevant one, and it is the one the full numerics follows. Bottom: same parameters as top, except $\omega = M/|M|$. Both full and Green's function optimizations approximate the continuum density $\rho = M/|M|$.

Next, use the Cauchy–Schwarz inequality in the form $\int a^2 \geq (\int ab)^2 / \int b^2$. Choosing $a = \sqrt{\omega u}$ and $b = \sqrt{M/u}$ yields

$$\int_{\Omega} \omega u \geq \frac{\left(\int_{\Omega} \sqrt{\omega M} \right)^2}{\int_{\Omega} M/u}. \quad (3.51)$$

From (3.50) the right-hand side is at least $\left(\int_{\Omega} \sqrt{\omega M} \right)^2 / \kappa = \frac{|M|}{\kappa} \left(\int_{\Omega} \sqrt{\omega \mu} \right)^2$, which yields the inequality (1.14). This inequality becomes an equality when we take $\omega = \rho = \mu$ (since in this case the solution is $u = |M|/\kappa$). Conversely, suppose that $\int_{\Omega} \omega u = \frac{|M|}{\kappa} \left(\int_{\Omega} \sqrt{\omega \mu} \right)^2$. This is only possible if the inequalities (3.50) and (3.51) both become equalities. The former implies $\nabla u = 0$, so that u is constant; the latter is the Cauchy–Schwarz inequality, which becomes an equality only if $\sqrt{\omega u} = C \sqrt{|M| \mu/u}$ for some constant $C > 0$. With u constant this forces $\omega = C_2 \mu$ for some constant C_2 ; since μ and ω are both densities, this implies $\omega = \mu$; and then, exactly as in the proof of Theorem 1.1, a constant u in (1.8) forces $\rho = \mu$. ■

3.2. Numerics

Rectangle in 2D. To test the homogenization theory against the original problem (1.2), we used Claude AI to implement a 2D numerical solver as well as a trap location optimizer based on the original full problem (1.2). Details of the implementation are given in Appendix A.

$$M(r) = \tanh(10(0.4 - r)) + 1.1, \quad \kappa = 20$$

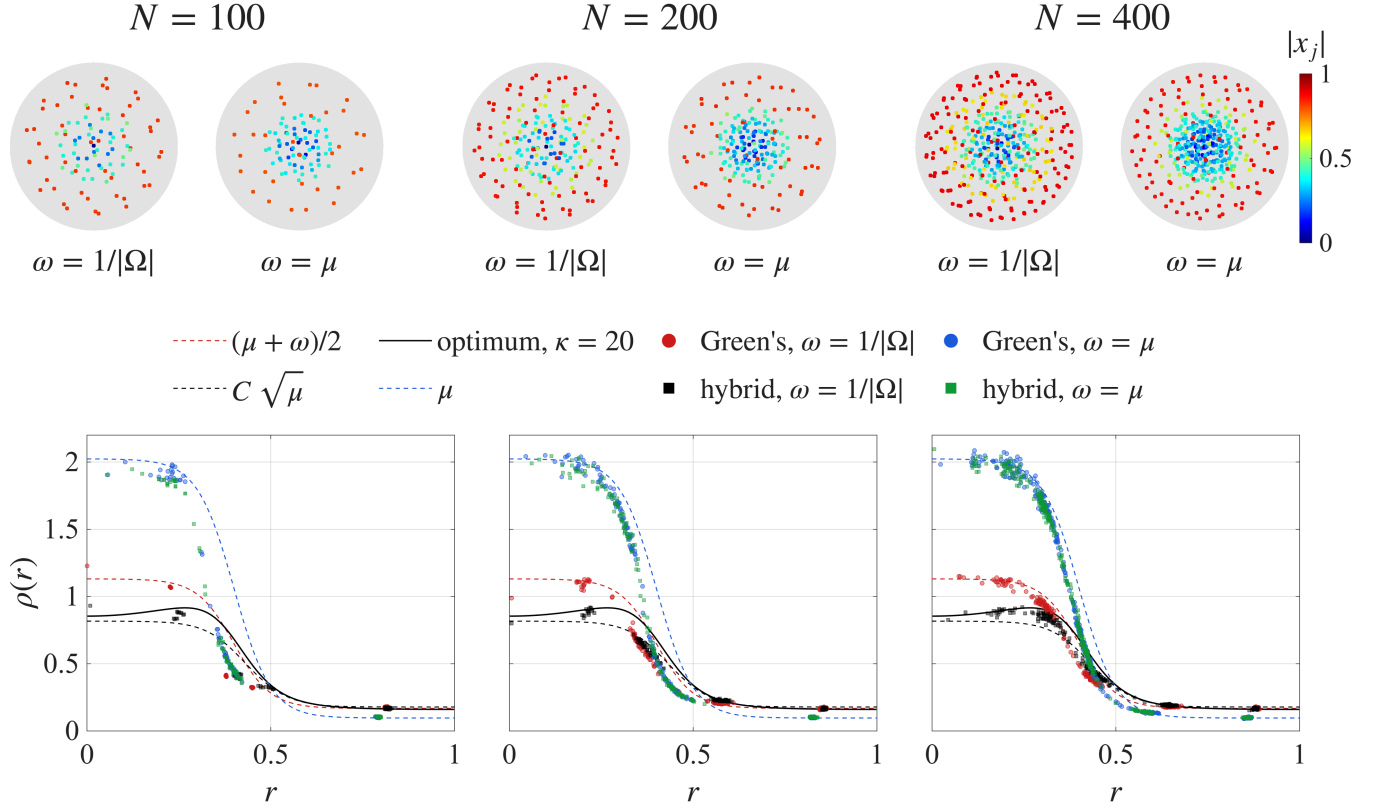


FIG. 4. Optimal trap configurations in the unit ball for $M(r) = \tanh(10(0.4 - r)) + 1.1$ (a slow core inside a fast shell, with an interface of width ~ 0.1 at $r = 0.4$), with $N = 100, 200$ and 400 traps (left to right), all at $\kappa = \nu N = 20$, i.e., the strong-trapping regime. Top: the minimizers of the hybrid objective (2.28) for the uniform starting distribution $\omega \equiv 1/|\Omega|$ and for $\omega = \mu$, colored according to $|x_j|$. Bottom: the effective densities $\rho(x_j) \approx 1/(N|\mathcal{V}_j|)$ from the Voronoi cells, plotted against $|x_j|$, for the minimizers of the Green's energy (2.35) (circles) and of the hybrid objective (2.28) (squares), for $\omega \equiv 1/|\Omega|$ (red and black) and for $\omega = \mu$ (blue and green). For $\omega \equiv 1/|\Omega|$ the curves are: the small- κ prediction (1.7), $(\mu + \omega)/2$ (red dashed); the large- κ prediction (3.48), here $\propto \sqrt{\mu}$ (black dashed); and the optimum of the optimality system (3.49) at $\kappa = 20$ (black solid); for $\omega = \mu$ all predictions coincide at $\rho = \mu$ (blue dashed), by (1.12). The Green's-energy minimizer follows the small- κ curve even though $\kappa = 20$, while the hybrid solution follows the finite- κ optimum, which at this κ is already close to the large- κ limit; for $\omega = \mu$ the two objectives give indistinguishable configurations and densities. The interface at $r = 0.4$ is thinner than the trap spacing at $N = 100$, which is why the measured densities lag the predictions there; the lag disappears as N grows and the core is resolved by several shells of traps.

Figure 3(top) illustrates the two regimes for $\Omega = (0, 3) \times (0, 1)$ with $M(x, y) = \tanh(3(1.5 - x)) + 1$, $N = 20$ and $\varepsilon = 0.05$, with $\omega \equiv 1/|\Omega|$, a uniform starting distribution. Then $\kappa = \nu N \approx 42$, corresponding to the strong-trapping regime. As expected, the full numerics follow the strong-trapping limit (3.48) rather than the weak-trapping limit (1.7), which corresponds to the Green's energy. This clearly illustrates that homogenization theory is usually a superior choice to the Green's function energy (Lemma 2.1) for most parameter values in 2D.

In Figure 3(bottom), we use the same parameters except that we start with the equilibrium distribution $\omega = \mu$. In this case, both strong- and weak-trapping limits coincide; both yield $\rho = \mu$. Correspondingly, both the full solver (black dots) and the Green's energy optimizer (red crosses) converge to the $\rho = \mu$ curve as expected. Note that the shown solution $u(x, y)$ for $N = 20$ is not yet constant over the domain, as it should be in the limit $N \rightarrow \infty$.

Unit sphere in 3D. For a 3D unit ball, an explicit formula for the Neumann Green's function is available [58]:

$$G(x, y) = \frac{1}{4\pi} \left[\frac{1}{|x - y|} + \frac{1}{\sqrt{1 - 2x \cdot y + |x|^2 |y|^2}} + \log \frac{2}{1 - x \cdot y + \sqrt{1 - 2x \cdot y + |x|^2 |y|^2}} + \frac{|x|^2 + |y|^2}{2} - \frac{14}{5} \right]. \quad (3.52)$$

The regular part (2.18) is

$$R(x, x) = \frac{1}{4\pi} \left[\frac{1}{1 - |x|^2} - \log(1 - |x|^2) + |x|^2 - \frac{14}{5} \right]. \quad (3.53)$$

This makes it easy to optimize the Green's energy formulation. However, solving the full optimization problem with relatively large N (say, few hundred) is still a difficult task. For this reason, we use the hybrid formulation (2.27), rather than its two-term series expansion as given by Lemma 2.1. In other words, we solve a linear system of $N + 1$ equations to get the unknowns T and $C_1, \dots, C_N$ that determine $\bar{u}_\omega$ via (2.28). We then minimize (2.28) over the trap positions using gradient descent with Barzilai–Borwein step lengths and an analytic gradient obtained from the adjoint, as described in Appendix A. The Green's-energy configurations shown for comparison are produced by the same minimization applied to E of (2.35), and the effective densities are estimated from Voronoi cell volumes as in 2D, $\rho(x_j) \approx 1/(N |\mathcal{V}_j|)$ with $|\mathcal{V}_j|$ being the volume of the Voronoi cell of x_j clipped to the unit ball.

Figure 4 illustrates the results for $M(r) = \tanh(10(0.4 - r)) + 1.1$, which models a slow core surrounded by a fast shell, with a sharp interface of width about 0.1 at $r = 0.4$. The three columns correspond to $N = 100, 200$ and 400 traps, all at the same trapping strength $\kappa = 20$ (so that ε is halved from one column to the next). For a uniform starting distribution the two objectives give visibly different configurations: the Green's-energy minimizer (valid only when $\nu N \ll 1$) follows the small- κ prediction (1.7), whereas the minimizer of the hybrid system (2.28) follows the finite- κ optimum of (3.49), which at $\kappa = 20$ already lies close to the large- κ limit (3.48). For $\omega = \mu$ the two objectives produce the same configuration, with density $\rho = \mu$, as (1.12) predicts for every κ .

The agreement between the discrete configurations and the continuum densities is spatially non-uniform, and depends on how the interface width compares with the distance between neighbouring traps. At $N = 100$ the interface is under-resolved, resulting in a significant leftward shift of the trap density near the interface. The agreement is visibly improved as N grows. Similar improvement can be observed by making the interface less sharp (not shown). We invite the reader to experiment with this effect in 2D using the web app [59].

4. ONE-DIMENSIONAL SETTING

We now consider several MFPT problems in one dimension, including inhomogeneous diffusion, advection, and a one-dimensional approximation of a thin-domain problem. Unlike the two-dimensional case, a one-dimensional trap splits the interval into two subintervals that can be solved independently, and then combined to compute the overall MFPT. This gives a significant simplification for the analysis. In fact, all of the problems we consider will reduce to minimizing the “energy” of the general form

$$E(x_1, x_2, \dots, x_N) = \sum_{k=0}^N f(l_k, x_k), \quad l_k = x_{k+1} - x_k, \quad (4.54)$$

inside an interval $[0, L]$ with $0 = x_0 < x_1 < \dots < x_N < x_{N+1} = L$ (for simplicity, we assumed here that the boundaries $x_0 = 0$ and $x_{N+1} = L$ are also trapping). Here, $f(l, x)$ is some function that depends on the specific problem and approximates the contribution of an interval of length l located near x to the objective (here, the MFPT), weighted by the starting distribution when the latter is non-uniform. We are interested in computing the minimizer $x_1, \dots, x_N$ in the limit $N \rightarrow \infty$. In this limit, define a continuous function $\ell(x)$ such that $l_k \rightarrow \ell(x_k)$ as $N \rightarrow \infty$.

Proposition 4.1. *Let $(x_1, x_2, \dots, x_N)$ be the minimizer of (4.54), i.e.,*

$$(x_1, x_2, \dots, x_N) = \arg \min_{0 < x'_1 < \dots < x'_N < L} \{E(x'_1, x'_2, \dots, x'_N)\}. \quad (4.55)$$

Let $\ell(x)$ solve

$$f(\ell, x) - \ell f_\ell(\ell, x) = \lambda, \quad (4.56)$$

where the constant λ (a Lagrange multiplier) is determined by the integral condition

$$N = \int_0^L \frac{1}{\ell(x)} dx. \quad (4.57)$$

Here and below, subscripts on f denote partial derivatives with respect to its first argument ℓ and its second argument x ; l_k continues to denote the discrete gaps and $\ell(x)$ their continuum limit. Then $x_{j+1} - x_j \sim \ell(x_j)$ for $N \gg 1$.

Proof. We pass to the continuum directly. Since $dx/\ell(x_k) \sim dk$, the sum (4.54) becomes

$$E = \sum_{k=0}^N f(l_k, x_k) \sim \int_0^N f(\ell(x_k), x_k) dk \sim \int_0^L f(\ell(x), x) \frac{dx}{\ell(x)},$$

while the number of traps is $\int_0^L dk = \int_0^L \frac{dx}{\ell(x)} = N$. The large- N limit of (4.54) is therefore the constrained variational problem

$$\min_{\ell(x)} \int_0^L f(\ell(x), x) \frac{dx}{\ell(x)} \quad \text{subject to} \quad \int_0^L \frac{dx}{\ell(x)} = N, \quad \ell(x) > 0. \quad (4.58)$$

Introducing a Lagrange multiplier λ for the constraint, this is equivalent to

$$\min_{\ell(x), \lambda} \int_0^L \frac{f(\ell(x), x) - \lambda}{\ell(x)} dx.$$

The integrand depends on ℓ pointwise and not on its derivatives, so the variational derivative is an ordinary derivative,

$$\frac{\partial}{\partial \ell} \left(\frac{f(\ell, x) - \lambda}{\ell} \right) = 0 \iff \ell f_\ell - (f - \lambda) = 0,$$

which is (4.56); the constraint in (4.58) is (4.57). ■

We now investigate several problems by using this framework.

4.1. Heterogeneous diffusion

Consider a Brownian particle governed by a stochastic ODE $dx_t = \sqrt{2D(x_t)} dW_t$, where $D(x) > 0$ is a position-dependent diffusivity. The corresponding Fokker–Planck equation is

$$p_t = (D^\theta (D^{1-\theta} p)_x)_x, \quad (4.59)$$

where the parameter $0 \leq \theta \leq 1$ depends on the stochastic interpretation, see [29, 30, 60, 61] for details. In particular, the Itô interpretation corresponds to $\theta = 0$, whereas the Stratonovich interpretation corresponds to $\theta = 1/2$.

Assuming $0 = x_0 < x_1 < \dots < x_{N+1} = L$, the MFPT problem with N traps reads

$$D^{1-\theta} (D^\theta u_x)_x = -1 \quad \text{on } (x_j, x_{j+1}), \quad u(x_j) = 0 \quad (j = 0, \dots, N), \quad (4.60)$$

and, as in 2D and 3D, we are interested in minimizing the ω -averaged MFPT

$$\bar{u}_\omega = \int_0^L \omega(x) u(x) dx, \quad \int_0^L \omega = 1, \quad \omega \geq 0, \quad (4.61)$$

as a function of trap locations x_j ; the uniform choice $\omega \equiv 1/L$ recovers the global MFPT $T = \int_0^L u(x) dx/L$. Our goal is to find the optimal density distribution of the trap locations as a function of $D(x)$ and $\omega(x)$, in the limit of large N .

The ODE (4.60) for each interval (x_j, x_{j+1}) can be easily solved in terms of quadratures:

$$u(x) = C_j \int_{x_j}^x D^{-\theta}(y) dy - \int_{x_j}^x dy_1 D^{-\theta}(y_1) \int_{x_j}^{y_1} dy_2 D^{\theta-1}(y_2) \quad x \in (x_j, x_{j+1}), \quad (4.62)$$

where the constant

$$C_j = \left(\int_{x_j}^{x_{j+1}} D^{-\theta}(y) dy \right)^{-1} \int_{x_j}^{x_{j+1}} dy_1 D^{-\theta}(y_1) \int_{x_j}^{y_1} dy_2 D^{\theta-1}(y_2) \quad (4.63)$$

ensures the boundary condition $u(x_{j+1}) = 0$. In the following, we deduce more explicit asymptotic results, assuming that $l_k = x_{k+1} - x_k$ is small.

Let $x = x_k + l_k y$ and $u(x) = l_k^2 U(y)$. Then at leading order we obtain

$$D_0 U_{0,yy} = -1 \quad \text{on } (0, 1), \quad U_0(0) = U_0(1) = 0,$$

with $D_0 = D(x_k)$. This yields

$$U_0(y) = \frac{1}{2D_0}(y - y^2).$$

Since ω varies on the $O(1)$ scale while $l_k = O(1/N)$, it is constant across an interval at leading order, so that in original variables the contribution of $[x_k, x_k + l_k]$ to $\bar{u}_\omega$ in (4.61) is

$$\int_{x_k}^{x_k+l_k} \omega u dx \sim \omega(x_k) l_k^3 \int_0^1 U_0(y) dy = \frac{\omega(x_k) l_k^3}{12D(x_k)}.$$

It follows that optimal trap locations correspond to the minimum of the energy

$$E = \sum_{k=0}^N \omega(x_k) \frac{l_k^3}{D(x_k)}, \quad l_k = x_{k+1} - x_k. \quad (4.64)$$

From Proposition 4.1 with $f(\ell, x) = \omega \ell^3 / D$ we obtain $\frac{\omega \ell^3}{D} - \frac{3\omega \ell^3}{D} = -\frac{2\omega \ell^3}{D} = \lambda$, so that

$$\ell(x) = C \left(\frac{D(x)}{\omega(x)} \right)^{1/3}, \quad \text{with } C = \frac{1}{N} \int_0^L \left(\frac{\omega(x)}{D(x)} \right)^{1/3} dx \quad (4.65)$$

being determined via (4.57). The effective trap density is given by $\rho(x) \sim 1/\ell(x)$, so that

$$\rho(x) \propto (\omega(x) M(x))^{1/3} = \left(\frac{\omega(x)}{D(x)} \right)^{1/3}. \quad (4.66)$$

In particular, a uniform starting distribution $\omega \equiv 1/L$ gives $\rho \propto M^{1/3} = D^{-1/3}$, while the stationary choice $\omega = M/|M|$ gives $\rho \propto M^{2/3}$ – in contrast to 2D and 3D, where that same choice yielded $\rho \propto M$ for every νN .

We remark that this result is independent of the choice of θ (Itô vs. Stratonovich).

Example. Suppose that

$$D(x) = \exp(-ax), \quad (4.67)$$

and take the starting distribution to be uniform, $\omega \equiv 1/L$. Then

$$\ell(x) = \frac{3}{Na} (\exp(La/3) - 1) \exp(-ax/3). \quad (4.68)$$

Figure 5 shows a comparison between a full numerical optimization of the problem (4.64) with $a = 1$ and $L = 4$, versus a full optimization of (4.60), and the asymptotic result (4.68). Note that the distribution of the traps is denser on the right, where the diffusion coefficient $D(x)$ is smaller. Good agreement is observed, which improves for larger N .

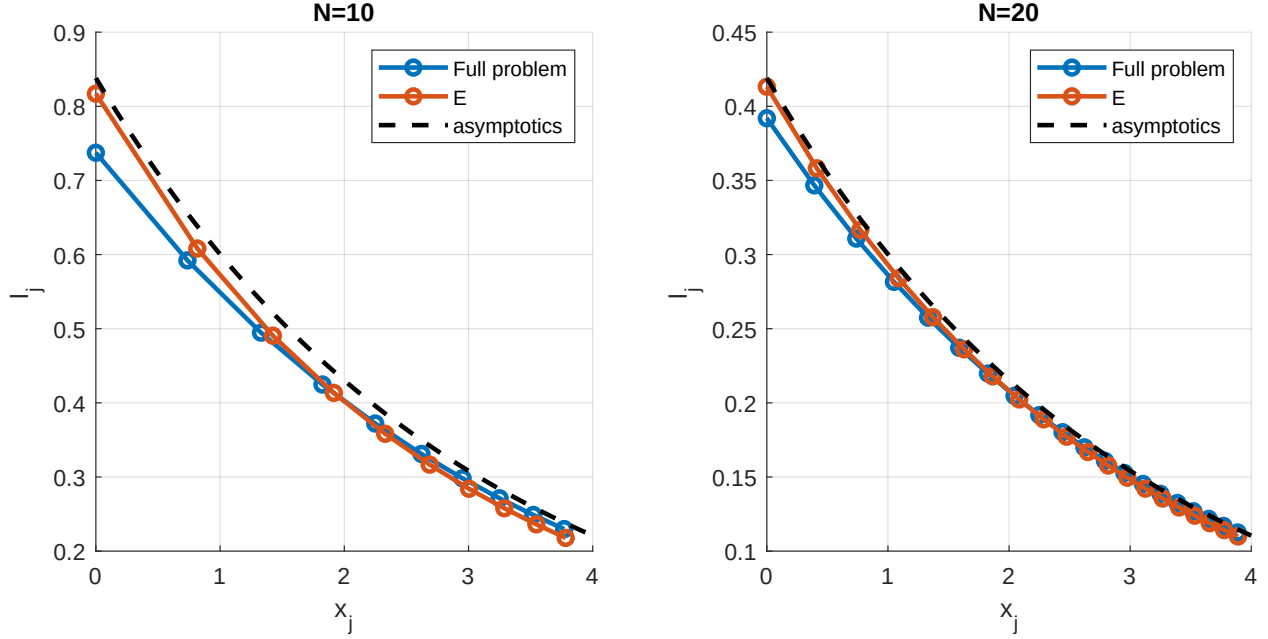


FIG. 5. Optimal trap distribution which minimizes the global MFPT (uniform ω) for the problem (4.60) with $D(x) = \exp(-x)$, $\theta = 0$, $L = 4$, and with $N = 10$ traps (left) and $N = 20$ traps (right). The graphs show a comparison between the numerical minimization of the original problem (4.60) (labeled “full problem”), numerical minimization of the simplified energy E given by (4.64) (labeled “E”), and the asymptotic formula (4.68) (labeled “asymptotics”).

4.2. Heterogeneous drift or thin domain

Consider a particle undergoing a Brownian motion in a one-dimensional medium with space-dependent velocity $v(x)$. The associated Fokker-Planck equation reads

$$p_t + (vp)_x = D_0 p_{xx}. \quad (4.69)$$

Our goal is to distribute N traps at locations x_j within a domain $[0, L]$ to minimize the mean capture time. Rescaling $D_0 = 1$, the associated MFPT problem becomes

$$u_{xx} + v(x)u_x = -1 \quad \text{on } (x_j, x_{j+1}), \quad u(x_j) = 0, \quad j = 0 \dots N. \quad (4.70)$$

Note that the same problem appears in the context of thin domains of variable thickness, with traps that transversally span the domain. A standard approximation via the integral over the transversal direction leads to the problem (4.70) with $v(x) = \frac{\sigma'(x)}{\sigma(x)}$, where $\sigma(x)$ is the cross-sectional area along the transversal direction (see [62, 63] and references therein).

As in § 4.1, here we are interested in finding optimal trap locations minimizing the ω -averaged MFPT $\bar{u}_\omega$ from (4.61). We consider two regimes: $v(x) = O(1)$ and $v(x) = O(N)$.

Case A: $v(x) = O(1)$. We proceed as in § 4.1. Expand along an interval $[x_k, x_k + l_k]$, with $l_k \ll 1$. Rescaling $u(x) = l_k^2 U(y)$, $x = x_k + yl_k$, we obtain, at leading order, that $U_{yy} \sim -1$. As such, the minimization problem is the same as (4.64) with $D(x) = 1$, so that (4.66) gives the leading-order density

$$\rho(x) \propto \omega^{1/3}(x), \quad \ell(x) \propto \omega^{-1/3}(x). \quad (4.71)$$

The drift therefore has no effect at the leading order. Note that this is typically the case for a thin domain, where the geometry is independent of N .

Case B: $v(x) = O(N)$. Assume as before that $x_{k+1} - x_k = O(1/N)$. Let $x_{k+1} = x_k + l_k$, where $l_k = O(1/N)$. Along an interval $[x_k, x_k + l_k]$, with $l_k \ll 1$, we rescale $u(x) = l_k^2 U(y)$, $x = x_k + yl_k$ to obtain the problem

$$U_{yy} + v_0 U_y \sim -1 \quad \text{on } (0, 1), \quad U(0) = 0 = U(1), \quad (4.72)$$

where $v_0 = l_k v(x_k) = O(1)$. After some algebra we then obtain

$$F(v_0) := \int_0^1 U(y) dy = -\frac{1}{v_0^2} + \frac{1}{2v_0} \coth(v_0/2).$$

Consequently, weighting each interval by $\omega(x_k)$ as in (4.64), we seek to minimize the energy

$$E = \sum_{k=0}^N \omega(x_k) l_k^3 F(v(x_k) l_k). \quad (4.73)$$

Equation (4.56) of Proposition 4.1 is equivalent to

$$\omega \frac{z^3}{v^3} (2F(z) + zF'(z)) = \lambda, \quad z = \ell v.$$

After some algebra we find

$$2F(z) + zF'(z) = \frac{1}{2z} \frac{\sinh z - z}{\cosh z - 1},$$

so that

$$\frac{\sinh z - z}{\cosh z - 1} z^2 = C \frac{v^3}{\omega}, \quad z = v\ell.$$

This yields a parametric solution

$$\ell = C \left(\frac{z}{\omega} \frac{\cosh z - 1}{\sinh z - z} \right)^{1/3}, \quad v = z/\ell, \quad (4.74)$$

where the constant C is chosen according to (4.57). As a check, $\frac{\cosh z - 1}{\sinh z - z} \sim 3/z$ as $z \rightarrow 0$, so that $\ell \rightarrow C(3/\omega)^{1/3}$, recovering the $\rho \propto \omega^{1/3}$ of (4.71).

For example, take $\omega \equiv 1/L$ and set $z = x$, $L = 6$; the constant ω is absorbed into C , leaving

$$\ell = \frac{C_0}{N} x^{1/3} \left(\frac{\cosh x - 1}{\sinh x - x} \right)^{1/3}, \quad v = \frac{N}{C_0} \left(\frac{\sinh x - x}{\cosh x - 1} x^2 \right)^{1/3}, \quad (4.75)$$

where

$$C_0 = \int_0^6 x^{-1/3} \left(\frac{\cosh x - 1}{\sinh x - x} \right)^{-1/3} dx \approx 3.7883. \quad (4.76)$$

Figure 6 shows excellent agreement between the formula (4.75) and full numerics, as N is increased.

5. DISCUSSION

In this paper we have obtained the asymptotics of the optimal trap density that minimizes the MFPT $\bar{u}_\omega$ for a generic heterogeneous diffusivity $D(x)$ and starting distribution ω of Brownian particles.

The key quantity is the trapping strength $\kappa = N\nu$ defined in (1.6); the optimal density is the arithmetic average $\rho = \frac{1}{2}(\mu + \omega)$ for weak trapping $\kappa \ll 1$ and is the geometric average $\rho \propto \sqrt{\mu\omega}$ for strong trapping $\kappa \gg 1$. When $\omega = \mu$ (corresponding to the equilibrium particle distribution in the absence of traps), we obtain $\rho = \mu$ for *any* κ , with $u(x)$ being constant in this case. In 2D, the “classical” approach using Green’s functions works only in a very restricted regime where $1 \ll N \ll \log \varepsilon^{-1}$; the restriction is milder in 3D but still significant ($N \ll \varepsilon^{-1}$). For a more realistic regime $N \gtrsim \log \varepsilon^{-1}$, we use a homogenization technique and derive the optimality system (3.49) that determines the optimal density; the geometric average occurs precisely in the asymptotic limit $N \gg \log \varepsilon^{-1}$. Numerical simulations of the full problem (1.2) are shown to agree with the homogenization theory.

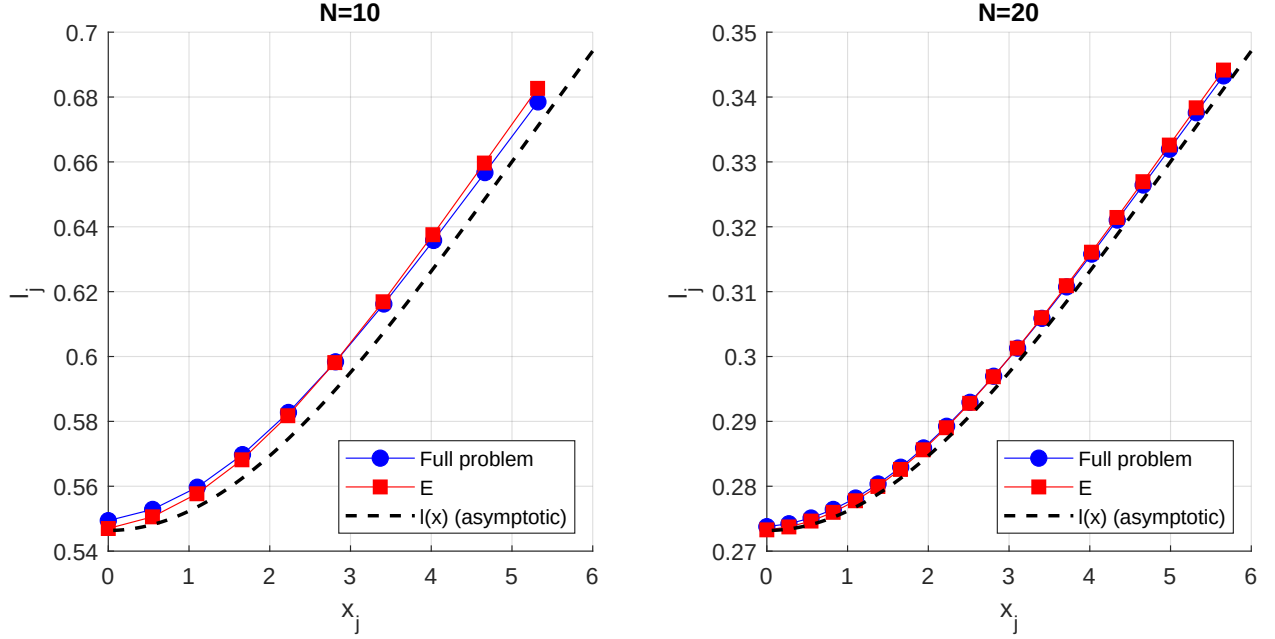


FIG. 6. Optimal trap distribution which minimizes $\int_0^L u(x)dx$ (uniform ω) for the problem (4.70) with $v(x)$ as given in (4.75), $L = 6$, and with $N = 10$ traps (left) and $N = 20$ traps (right). The graphs show a comparison between the numerical minimization of the original problem (4.70) (labeled “full problem”), numerical minimization of the simplified energy E given by (4.73) (labeled “E”), and the asymptotic formula (4.75) (labeled “asymptotics”).

κ	0.1	0.5	1	5	10	50	100	500	1000	5000	∞
gain for $\omega = \mu$, rectangle of Fig. 3	1.022	1.098	1.172	1.449	1.563	1.715	1.743	1.770	1.774	1.777	1.778
gain for $\omega = \mu$, ball of Fig. 4	1.003	1.013	1.026	1.127	1.241	1.870	2.301	3.224	3.468	3.731	3.814
gain for $\Omega = (0, 1)$, $\mu = 1$, $\omega = 2 \cdot \mathbf{1}_{x < 1/2}$	1.002	1.010	1.020	1.082	1.139	1.344	1.449	1.677	1.755	1.879	2

TABLE I. Gain of optimal trap configuration vs. uniform, for different settings.

The results also apply to homogeneous diffusion, but with a non-homogeneous initial distribution. For example, suppose that the particles start uniformly in the left half of the domain, and diffusion is homogeneous. In the weak-trapping limit $\kappa \ll 1$, the optimal trap distribution from (1.7) corresponds to placing 75% of the traps on the left, and 25% on the right, both uniformly. The strong-trapping limit $\kappa \gg 1$ (1.10), by contrast, calls for placing all of the traps on the left side of the domain and none on the right. Figure 3 (top) is an illustration of that, but with the roles of ω and μ reversed (note that all the density formulas are symmetric with respect to swapping $\mu \leftrightarrow \omega$). Interestingly, these results do not “feel” the shape of the domain at leading order, at least in the strong- or weak-trapping limits.

Let us contrast the optimal trap density with the uniform density. Define the gain $= \bar{u}_\omega[\rho_{\text{uni}}]/\bar{u}_\omega[\rho_{\text{opt}}]$, by which an optimal trap arrangement is better than the uniform one; here we use ρ_{opt} to denote the optimal density ρ as found by solving the optimality system (3.49). Table I gives gain as a function of κ for three examples: the equilibrium start $\omega = \mu$ with the space-dependent diffusivity of Figures 3 and 4, and a homogeneous medium on $\Omega = (0, 1)$ with the particles released uniformly in the left half.

When starting from the equilibrium particle density, $\omega = \mu$, we have $\bar{u}_\omega[\kappa; \rho_{\text{opt}}] = \frac{|M|}{\kappa}$ by (1.12), whereas $\bar{u}_\omega[\kappa; \rho_{\text{uni}}]$ is obtained by solving (1.8) with $\rho \equiv 1/|\Omega|$ and evaluating $\int_\Omega \mu u$. Moreover gain $\rightarrow 1$ as $\kappa \rightarrow 0$, since then $u \sim |M|/\kappa$ irrespective of ρ ; in turn, as $\kappa \rightarrow \infty$, we have $u \sim M/(\kappa\rho)$ and thus

$$\text{gain}(\infty) = \frac{|\Omega| \int_\Omega M^2}{\left(\int_\Omega M\right)^2} \geq 1. \quad (5.77)$$

By Cauchy–Schwarz, the equality can only hold for constant M and the gain is highest for highly concentrated M . For the examples of Figures 3 and 4, we find that the optimal placement is 71% better than a uniform arrangement of the same traps for the rectangle ($\kappa = 42$, gain = 1.71) and 44% better for the ball ($\kappa = 20$, gain = 1.44). The

gain increases faster with κ for the rectangle at first but ultimately is more pronounced for the ball example for even larger κ .

The third row is the homogeneous example discussed above, with the particles released in the left half only. Here ρ_{uni} gives $u \equiv 1/\kappa$ exactly, and ρ_{opt} is computed by direct minimization of $\bar{u}_\omega$ over ρ , see Appendix A. The last entry is the strong-trapping limit (1.10), which puts every trap in the left half and gives $\text{gain}(\infty) = 1/(\int \sqrt{\omega\mu})^2 = 2$. This limit is approached very slowly, likely due to the discontinuity of ω at $x = 1/2$. Numerics for high κ indicate a “rampart” of high density near the interface $x = 1/2$, suggesting an optimal placement of traps akin to “border guards” on the boundary of the area where the particles start. We leave further investigations into this phenomenon as an open problem.

An interesting question is how a transition from the 1D scaling ($\rho \propto (\omega\mu)^{1/3}$) to a 2D scaling ($\rho \propto (\omega\mu)^{1/2}$ or $\rho \propto \omega + \mu$) occurs. Consider a thin strip of width $O(h)$, with $h \ll 1$. If we take traps that span the entire transversal direction, then their distribution satisfies a 1D scaling $\rho \propto (\omega\mu)^{1/3}$. On the other hand, if we take traps that are disks whose radius $\varepsilon \ll h$, we obtain a 2D scaling, as shown for example in Figure 2 (top row, $N = 5$). What if we take disks of radius commensurate with the channel width, $\varepsilon = O(h)$? One can expect a transition between different scaling regimes as the disk radius is increased. This is an interesting avenue for future exploration.

We showed that the 1D scaling $\rho \propto (\omega\mu)^{1/3}$ is independent (to leading order) of the choice of the stochastic interpretation (Itô vs. Stratonovich), i.e., of the parameter θ in (4.59). At the same time, our 2D analysis explicitly requires $\theta = 0$. An interesting open problem is to derive the 2D scaling laws when $\theta > 0$. In this case, the equilibrium particle distribution without traps is $p_{\text{eq}} \propto [D(x)]^{\theta-1} \propto \mu^{1-\theta}$, which is different from μ for $\theta > 0$. In particular, the initial particle distribution $\omega = \mu$ does not necessarily lead to the optimal trap density. Finally, it would be interesting to extend the 1D results for particles with drift to a two-dimensional setting.

In conclusion, heterogeneity does not simply attract traps toward regions of low diffusivity. The optimal distribution reflects a competition between where particles accumulate and where they are initially supplied. This competition leads to arithmetic averaging in the weak-trapping regime and geometric averaging in the strong-trapping regime. The equilibrium preparation $\omega = \mu$ is exceptional: these two principles coincide, yielding an optimal trap distribution identical to the particle distribution and a spatially uniform MFPT for arbitrary trapping strength.

Acknowledgements

We are grateful to Sean Lawley for interesting discussions and for suggesting to look at a non-uniform ω . Claude AI (Opus version 5) significantly assisted the elaboration of homogenization technique in §3, the optimality system for general κ (3.49), as well as Theorems 1.2–1.3. It was also used for developing numerics for the full problem (1.2) in 2D to validate the “hybrid” system and density optimization (Fig. 3), as well as for creating a web application showcasing 2D results visually [59]. The algorithms and the reported numerical results for the full problem in 2D have been independently verified by the authors. Appendix A was written by AI and edited by authors, whereas the remaining text was written by authors. The authors assume full responsibility for all content.

Appendix A: Details of the numerical implementation

The full problem in 2D. Equation (1.2) is discretized by finite differences on a cell-centred Cartesian grid. The reflecting condition on $\partial\Omega$ is imposed through the mirror ghost value $u_{\text{ghost}} = u_P$, which on a cell-centred grid is exactly no-flux and second-order accurate. The trap boundaries are resolved by the Shortley–Weller construction [64]: on a grid line cut by $\partial B_\varepsilon(x_j)$ the regular spacing h is replaced by the true distance to the interface and the Dirichlet value moved to the right-hand side, which avoids staircasing the traps; cut fractions are clamped from below to keep the matrix well conditioned. The resulting non-symmetric sparse matrix is factorized directly. The integral $\int_\Omega \omega u$ was computed by using the midpoint rule weighted by the fraction of each cell’s area that lies outside the traps; without this weighting the quadrature loses an order of accuracy along every trap boundary.

Optimization over trap locations in 2D. The objective $J(x_1, \dots, x_N) = \int_\Omega \omega u$ is minimized by gradient descent, each trial step being followed by a projection of the centers back to at least 1.2ε from every wall and 2.6ε from one another, center to center. The gradient is obtained from the adjoint. Introduce v , the solution of the same boundary value problem as u but with the source density ω in place of M :

$$\Delta v = -\omega \quad \text{in } \Omega \setminus (\cup_j B_\varepsilon(x_j)), \quad v = 0 \quad \text{on } \cup_j \partial B_\varepsilon(x_j), \quad \partial_n v = 0 \quad \text{on } \partial\Omega. \quad (\text{A.1})$$

This is the discrete counterpart of the adjoint v of the optimality system (3.49): there v carries the sensitivity of $\bar{u}_\omega$ to the homogenized density ρ , here to the position of an individual trap. Moving $\partial B_\varepsilon(x_k)$ with normal velocity V_n

changes J by the Hadamard shape derivative for a Dirichlet boundary [65],

$$\delta J = - \int_{\partial B_\varepsilon(x_k)} \partial_n u \partial_n v V_n ds, \quad (\text{A.2})$$

where n is the outward normal of the domain, i.e. pointing into the trap. Translating the trap rigidly by a unit vector e means $V_n = e \cdot n$, and on the circle $ds = \varepsilon d\vartheta$, so that taking e along each coordinate direction in turn gives the two components of

$$\frac{\partial J}{\partial x_k} = -\varepsilon \int_0^{2\pi} \partial_r u \partial_r v (\cos \vartheta, \sin \vartheta) d\vartheta, \quad (\text{A.3})$$

the integral being over $\partial B_\varepsilon(x_k)$. Equation (A.3) is the exact, finite- ε counterpart of the gradient of the Green's energy (2.35): expanding it as $\varepsilon \rightarrow 0$ reproduces $\partial E / \partial x_k$, and hence the velocity field of the flow (2.37).

The step length is chosen by the two-point rule of Barzilai and Borwein [66]. Writing $s^{(i)} = x^{(i)} - x^{(i-1)}$ and $y^{(i)} = g^{(i)} - g^{(i-1)}$ for the changes in the configuration and in its gradient between successive iterates,

$$t^{(i)} = \frac{s^{(i)} \cdot s^{(i)}}{s^{(i)} \cdot y^{(i)}}, \quad x^{(i+1)} = x^{(i)} - t^{(i)} g^{(i)}, \quad (\text{A.4})$$

whenever $s^{(i)} \cdot y^{(i)} > 0$, and $t^{(i)} = 2t^{(i-1)}$ otherwise; the first step is scaled so that the largest trap moves a prescribed small distance. The quotient in (A.4) is a Rayleigh quotient of the Hessian along the last step, so it carries curvature information without any second derivative ever being formed. The raw Barzilai-Borwein iteration is not monotone, so each step is accepted only if it satisfies an Armijo condition [67], $J(x - tg) \leq J(x) - c_1 t \|g\|^2$ with $c_1 = 10^{-4}$, and the step is halved until it does; this costs one extra objective evaluation per backtrack, and makes the objective history decrease monotonically. A nonmonotone acceptance window was tried and was slower on these problems.

The ball. All three-dimensional results are computed from the hybrid system (2.27): for a given configuration, T and $C_1, \dots, C_N$ follow from a single $(N+1) \times (N+1)$ solve, which delivers $\bar{u}_\omega$ through (2.28). The trap centers are then optimized by the same Barzilai-Borwein descent (A.4) with Armijo backtracking, the gradient being computed analytically from the adjoint of that linear system. No constraint keeping the traps apart or inside the ball is needed here: the objective is its own barrier, since $R(x, x)$ diverges at the boundary and $G(x_j, x_k)$ as two traps merge. We minimize the Green's energy (2.35) first, from random initial conditions, and use its minimizer as the starting point for the hybrid objective; the descent is stopped when $\max_k |\partial \bar{u}_\omega / \partial x_k|$ falls below 10^{-8} . Effective densities are estimated from Voronoi cell volumes clipped to the unit ball. As an independent check, (1.2) was also solved directly in the ball by a cell-centred finite-volume scheme on a uniform Cartesian grid; resolving the traps needs $n = 8/\varepsilon$ cells per side, so this is affordable only at the largest radii and smallest N , and where both are available the two agree to within 1% for $\varepsilon \leq 0.05$.

The optimal density at finite κ . The solid curves of Figure 4 and the third row of Table I are minimizers of $\bar{u}_\omega = \int_\Omega \omega u$ over densities $\rho \geq 0$ with $\int_\Omega \rho = 1$, where u solves the homogenized problem (1.8). In all considered cases, $\bar{M}$ and ω depend on one coordinate only, so (1.8) is a two-point boundary value problem, either in the radial coordinate r for the ball, or in x for the rectangle; we discretize it by cell-centred finite volumes ($n = 400$ cells, zero flux at both ends), so that one evaluation of $\bar{u}_\omega$ is one tridiagonal solve.

The gradient is available from the adjoint: with v solving (1.8) with ω in place of M , a variation $\delta \rho$ changes the objective by $\delta \bar{u}_\omega = -\kappa \int_\Omega uv \delta \rho$, so the descent direction is κuv , at the cost of a second tridiagonal solve. This is the same quantity that appears in the optimality system (3.49), whose condition $uv = \text{const}$ on the support of ρ is exactly stationarity of $\bar{u}_\omega$ under the mass constraint. Positivity and normalization are built in by optimizing over $\theta(x)$ with $\rho(x) = e^{\theta(x)} / \int_\Omega e^\theta$, which turns the constrained problem into an unconstrained one; the chain rule gives $\partial \bar{u}_\omega / \partial \theta_i = \rho_i (G_i - \sum_j w_j \rho_j G_j)$ with $G_i = -\kappa w_i u_i v_i$ and w_i the cell volumes, i.e. the gradient with its ρ -weighted mean removed.

The descent itself is the Barzilai-Borwein iteration described above, (A.4) with Armijo backtracking, applied to θ : no Hessian is formed, and the two-point step carries the curvature information that a plain gradient method would lack. We continue in κ , starting from the closed-form small- κ optimum (1.7) and using the minimizer at each κ as the starting point for the next; the iteration is stopped when the gradient norm falls below 10^{-6} relative to the objective, which takes between a few and two hundred steps per κ , and an entire κ column of Table I takes well under a minute. For $\omega = \mu$ the method returns $\rho = \mu$ and $\bar{u}_\omega = |M|/\kappa$ to the tolerance used, as (1.12) requires, and doubling n

changes the reported values of the gain in the fourth digit at most.

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