Optimal Arrangements and Homogenization Limit for Traps on the Sphere

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The Narrow Escape Problem

Consider a particle that undergoes Brownian motion while confined to the interior of a domain Ω. The boundary of this domain is made up of almost entirely a reflecting portion, $\partial\Omega_r$ and a relatively small absorbing portion, $\partial\Omega_a$. Define $v(\mathbf{x}), \mathbf{x}\in\Omega$ as the expectation time a particle will stay in the domain starting at point $\mathbf{x}$.

Dirichlet-Neumann Boundary Problem

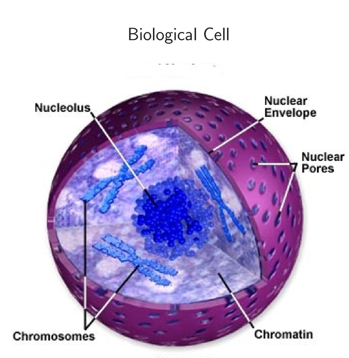
$$\Delta v = -\frac{1}{D}, \mathbf{x}\in\Omega \quad v=0, \mathbf{x}\in\partial\Omega_a \quad \partial_r v = 0, \mathbf{x}\in\partial\Omega_r, \tag{1}$$

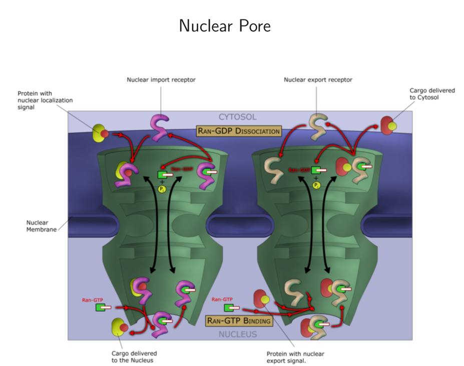
where D is the diffusion constant for the system.

Mean First Passage Time (MFPT):

$$\bar{v} = \int v(\mathbf{x})d\mathbf{x} \tag{2}$$

Applications





- Nuclear export of messenger RNA through nuclear pores
- Reciprical of MFPT acts as a first order rate constant

The Asymptotic Solution For the Unit Sphere

An asymptotic solution was derived for the unit sphere with traps located at $\mathbf{x}_i$ using the method of matched asymptotic expansions.

Assumptions:

- Small trap sizes, $\epsilon \ll 1$
- Well separated traps, $|\mathbf{x}_i - \mathbf{x}_j| \ll \epsilon$

$$\bar{v} = \frac{|\Omega|}{4\epsilon DN}\left[1+\frac{\epsilon}{\pi}\log\left(\frac{2}{\epsilon}\right)+\frac{\epsilon}{\pi}\left(-\frac{9N}{5}+2(N-2)\log 2+\frac{3}{2}+\frac{4}{N}\mathcal{H}(x_1,\dots,x_N)\right)\right] \tag{3}$$

$\mathcal{H}(x_1,\dots,x_N)$ is the interaction energy defined by

$$\mathcal{H}(x_1,\dots,x_N) = \sum_{i=1}^{N}\sum_{j=i+1}^{N}\left(\frac{1}{|x_i-x_j|}-\frac{1}{2}\log|x_i-x_j|-\frac{1}{2}\log(2+|x_i-x_j|)\right) \tag{4}$$

More generally, for unequal trap lengths the MFPT was found to be

$$\bar{v} = \frac{|\Omega|}{2\pi\epsilon DN\bar{c}}\left[1+\epsilon\log\left(\frac{2}{\epsilon}\right)\frac{\sum_{j=1}^{N}c_j^2}{2N\bar{c}}+\frac{2\pi\epsilon}{N\bar{c}}\mathcal{C}^T\mathcal{G}\mathcal{C}-\frac{\epsilon}{N\bar{c}}\sum_{j=1}^{N}c_j\kappa_j\right], \tag{5}$$

where c_j are the elements of the capacitance vector $\mathcal{C}$, given by $c_j = 2a_j/\pi$ where $a_j\epsilon$ is the radius of the trap corresponding to index j. $\bar{c}$ is the mean of the capacitance vector, and $\mathcal{G}$ is the surface Green's function matrix given by

$$\mathcal{G}_{ij} = G_s(x_i;x_j) = \frac{1}{2\pi|x_i-x_j|}+\frac{1}{4\pi}\log\left(\frac{2}{1-\cos\gamma+|x_i-x_j|}\right)-\frac{9}{20\pi}, \; i\neq j, \qquad \mathcal{G}_{ii} = \frac{-9}{20\pi}, \tag{6}$$

where γ is the angle between traps $\mathbf{x}_i$ and $\mathbf{x}_j$.

The Homogenization Problem

The homegenization problem deals with the limit of many equally spaced traps that cover a fixed percentage, σ, of the boundary. In this limit, it is possible to replace the Dirchlet-Neumann boundary conditions with an equivalent

Robin Boundary Condition Problem:

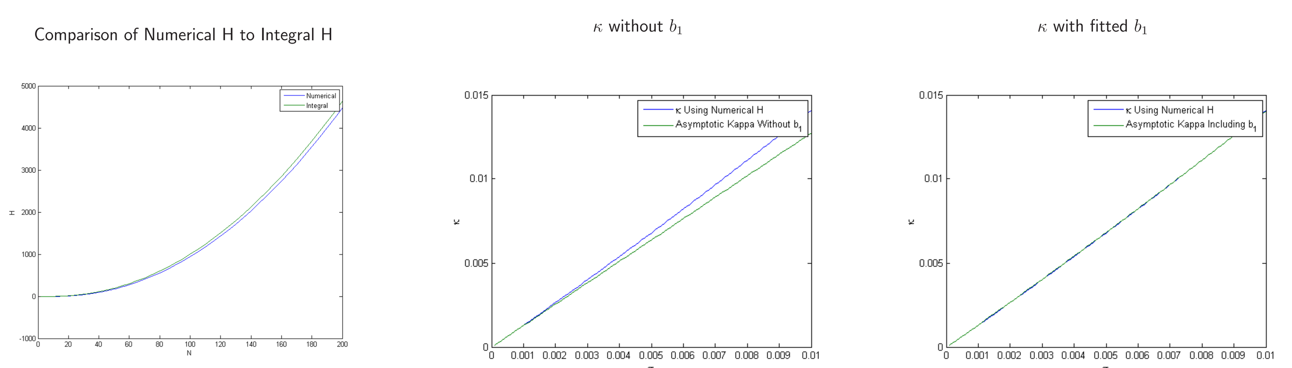
$$\Delta v_H = -\frac{1}{D}, \quad v_H\in\Omega; \quad \epsilon\partial_r v_H + \kappa v_H = 0, \quad v\in\partial\Omega, \tag{7}$$

where κ is a factor that depends on the geometry of the domain. This equation can be solved immediately for the sphere; from (2), one gets

$$\bar{v}_H = \frac{1}{15D}+\frac{1}{3D}\frac{\epsilon}{\kappa}. \tag{8}$$

- $\mathcal{H}$ can be estimated by replacing the sum with an integral over the sphere. One gets

$$\bar{v} \approx \frac{|\Omega|}{4\epsilon DN}\left[1-\frac{\epsilon}{\pi}\log\epsilon+\frac{\epsilon N}{\pi}\left(\frac{1}{5}+\frac{4b_1}{\sqrt{N}}\right)\right]. \tag{9}$$



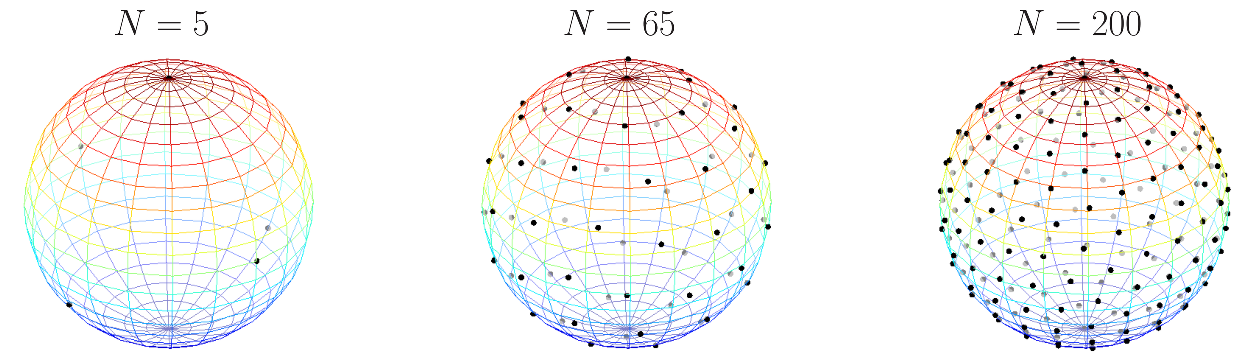
- Expect leading order term is correct.
- Consider leading order terms $\mathcal{H}\approx N^2\frac{1}{2}(1-\log 2)+b_1N^{3/2}$ where b_1 is a constant.
- Equate $\bar{v}$ and $\bar{v}_H$ in the limit $N\to\infty$ to estimate κ:

$$\kappa = \frac{4\sigma}{\pi+8b_1\sqrt{\sigma}}. \tag{10}$$

Fitting κ to the full numerical results for $\mathcal{H}$ gives us $b_1 = -0.3672$, because of the reasonable agreement shown above (3) provides a quick way to estimated $\bar{v}$ in the high N, low σ limit.

Optimal Trap Locations on the Unit Sphere

The optimal trap configuration corresponds to the minimized MFPT, or maximized diffusion rate. Examples of optimal configurations:



Using global optimization software (GANSO, LGO), results were computed up to $N=200$. The computations take a long time since this is minimizing a function in $(2N-3)$-dimensional space.

The Topological Derivative

In [3], the notion of a topological derivative is developed. Consider a functional $\mathcal{J}:\Omega\mapsto\mathbb{R}$; define the topological derivative as

$$\mathfrak{T}(\mathbf{x}) = \lim_{\rho\to0}\frac{\mathcal{J}(\Omega\setminus\overline{B_\rho(\mathbf{x})})-\mathcal{J}(\Omega)}{|B_\rho(\mathbf{x})|}, \tag{11}$$

where $B_\rho(\mathbf{x})$ is a ball of radius ρ located at point $\mathbf{x}\in\Omega$.

- Example:

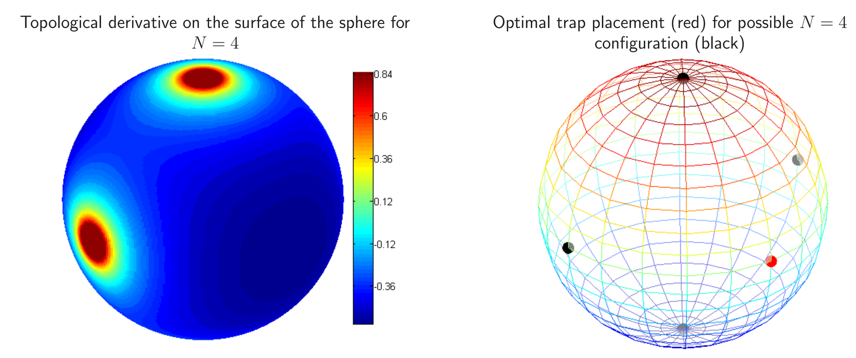
Topological Derivative for Narrow Escape on Unit Sphere

In our case the shape functional $\mathcal{J}$ is $\bar{v}$, the MFPT and $B_\rho(\mathbf{x})$ is a trap of radius ρ centered at point $\mathbf{x}$ on the sphere.

- Topological derivative calculated using (5)

$$\mathfrak{T}(\mathbf{x}) = \frac{|\Omega|}{2\pi\epsilon DN\bar{c}}\left[-\log\left(\frac{2}{\epsilon}\right)\left(\frac{1}{\pi N^2}\right)+\frac{3-4\log 2}{2\pi N^2}+\frac{8N\sum_{j=1}^{N}\mathcal{G}_{j(N+1)}-4\sum_{i,j}^{N}\mathcal{G}_{ij}}{N^2}\right] \tag{12}$$

- Optimal trap location is when $\mathfrak{T}(\mathbf{x})$ is minimized
- Topological derivative is minimized when $\sum_{j=1}^{N}\mathcal{G}_{j(N+1)}$ is minimized



We iterate this process to obtain a rough estimate for the minimum energy.

Application of Topological Derivative to Computation of Optimal Arrangements

For two particles, the interaction energy is a strictly decreasing function in terms of the separation distance $|\mathbf{x}_i-\mathbf{x}_j|$. We introduce the pseudo-force vector

$$\vec{F}_{ij} = \left(\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|}-\log(|\mathbf{x}_i-\mathbf{x}_j|)-\log(2+|\mathbf{x}_i-\mathbf{x}_j|)\right)\mathbf{e}_{ij} \tag{13}$$

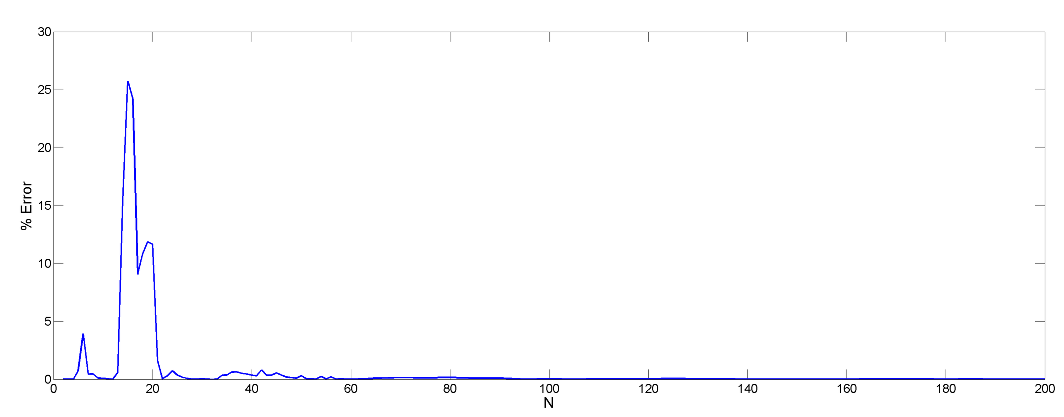
And the total force on a trap $\mathbf{x}_i$ is thus

$$\vec{\mathcal{F}}_i = \sum_{j=1, j\neq i}^{N}\vec{F}_{ij} \tag{14}$$

We start by introducing a new particle in the point of the minimal topological derivative. Then we move each particle a distance proportional to $\vec{\mathcal{F}}_i$. Each particle is subsequently pushed back to the sphere in the normal direction. This process is iterated until a local energy minimum is achieved, which may or may not be the global energy minimum.

Testing the Simulation against Known Results

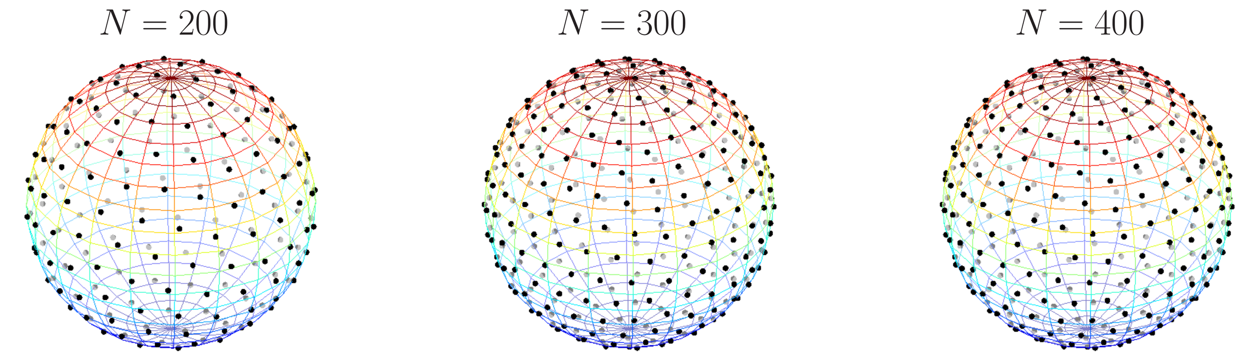
Results for the values of $\mathcal{H}$ from the above simulation were compared against the numerical global optimization results:



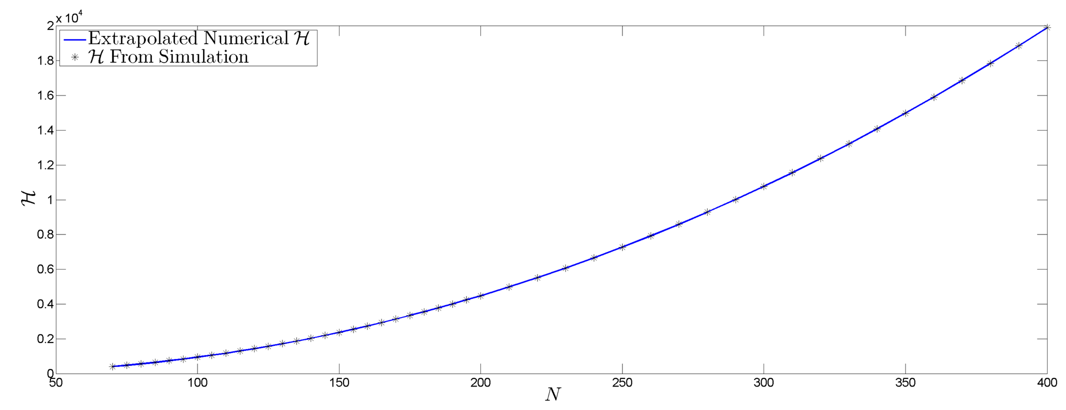
The topological derivative-based simulation showed to be accurate within 0.01% for $N\geq100$. The simulation is naturally much faster compared to full global optimization.

Simulation Results

Optimal trap locations were computed up to $N=400$ in steps of 10.



The interaction energies from the simulation results were compared against a polynomial extrapolation of the $N=2..200$ numerical results up to N=400:



Simulation $\mathcal{H}$ matches extrapolated numerical $\mathcal{H}$ within 0.005%.

N^2 Conjecture

Asymptotic Motivation:

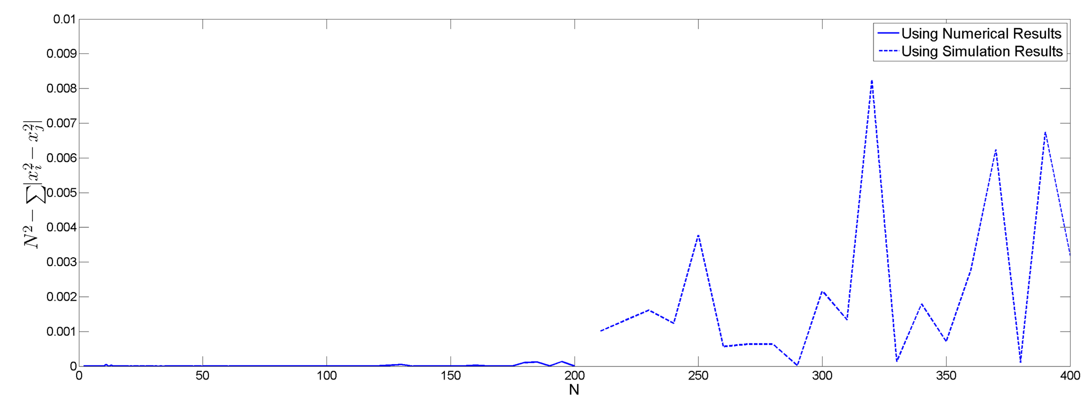
- In the limit of many traps we can approximate the sum of the trap square distances as an integral

$$\sum|\mathbf{x}_i-\mathbf{x}_j|^2 \approx \frac{N^2}{8\pi}\int_0^{\pi}\int_0^{2\pi}(2-2\cos\theta)\cdot\sin\theta\, d\phi\, d\theta = N^2. \tag{15}$$

We conjecture that for an arrangement of traps in the minimal energy configuration,

$$N^2 = \sum|x_i-x_j|^2 \tag{16}$$

The difference between N^2 and numerical/simulation $\mathcal{H}$ was plotted up to $N=400$:



Since the absolute differences were less than 0.01 for all computed N, we conclude that the conjecture holds at least for $N\leq400$.

Conclusions

- An estimate of κ was obtained for the unit sphere.
- Simulation results shown to match previous results within 0.01% for the $N\geq100$ region.
- Topological derivative-based Simulation provides a faster method of computing the optimal trap arrangement on the sphere.
- $N^2-\sum|\mathbf{x}_i-\mathbf{x}_j|^2 < 0.01$ for all computed N.

Further Research Directions / Open Problems

- Rigorous derivation of κ for the homogenization limit.
- Simulation could be programmed with higher precision.
- Computing the topological derivative without the use of the asymptotic formula for $\mathcal{H}$.
- Rigorous justification for N^2 conjecture.
- Asymptotic solution of the narrow escape problem for on an arbitrary domain $\Omega\in\mathbb{R}^3$.

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