The Mathematical Model for the Narrow Escape Problem

The Narrow Escape Problem concerns the calculation of the mean first passage time (MFPT) required for a Brownian particle confined in a bounded domain $\Omega \subset \mathbb{R}^d$ (two or three dimensional spaces) to escape through one of finitely many small boundary windows, or traps. The domain boundary $\partial \Omega = \partial \Omega_1 \cup \partial \Omega_2$, is almost entirely reflecting ($\partial \Omega_1$), except for traps ($\partial \Omega_2$).

The MFPT $v(x)$ satisfies the mixed Dirichlet-Neumann problem

$$\Delta v = \frac{1}{\sigma} \varepsilon, \quad x \in \Omega; \quad v = 0, \quad x \in \partial \Omega_2; \quad \frac{\partial v}{\partial \nu} = 0, \quad x \in \partial \Omega_1,$$

where $D$ is constant diffusivity. An important integral characteristic of escape times from a domain with a prescribed trap arrangement is the Average MFPT:

$$\bar{v}(x) = \frac{1}{|\Omega|} \int_{\Omega} v(x, dx),$$

where $|\Omega|$ is the measure of the domain.

**Approximate asymptotic solutions** of (1) have been obtained for various 3D domains WLOG, the physical problem (1) can be re-scaled:

- $d \bar{a}m \Omega = 1$,
- $D = 1$.

The MFPT $v(x)$ for the unit sphere with $N$ non-equal traps was obtained in Ref. [1] using the method of matched asymptotic expansions, and is given by

$$v(x) = \bar{v} - \frac{2D}{\sigma} \sum_{j=1}^{N} a_j G_j(x; x_j) + O(\log \varepsilon).$$

Correspondingly, the average MFPT $\bar{v}$ is given by

$$\bar{v} = \frac{1}{2D\sigma} \sum_{j=1}^{N} a_j \log \left( \frac{1}{\bar{a}m \Omega} \frac{1 + \varepsilon \log \varepsilon}{2N} \sum_{j=1}^{N} a_j \right) \varepsilon^2 \sum_{j=1}^{N} a_j \gamma_j + O(\varepsilon^2 \log \varepsilon).$$

Here $p_l(x_1, \ldots, x_N)$ is a *repulsive potential* depending on the specific trap arrangement [1].

MATLAB Code for Brownian Simulations

- A MATLAB code was developed that can be to trace the trajectories of Brownian particles starting from a given point up to their escape through a trap.
- Code takes into account boundary reflections.
- Parameters were chosen to match asymptotic MFPT results.

**Parameters used in the code**

- $\sigma = 6 \times 10^{-4}$
- $D = 1$
- $\varepsilon = 10^{-2}$

**Specification of the machine used to run the simulations**

- OS: Red Hat Linux 7.6
- Memory: 128 GB
- Processor: Intel Xeon(R) E5-2687W (3.100GHz) × 16

**Comparison Between Asymptotic and Numerical Simulation Results**

- Brownian numerically simulated MFPT is computed by averaging escape times of $N$ Brownian particles launched from the same starting point:

$$\bar{v}_N(x) = \frac{1}{N} \sum_{i=1}^{N} v_i(x),$$

where $v_i(x)$ is the $i$th MFPT.

- Number of Brownian particle runs from each starting location: $N = 20000$

**Averaged Escape Time vs Asymptotic Results for Trajectories of 4000 Brownian Particles Launched from Various Points $(x, r), 0 \leq r \leq 1$ with Each Tuple Specifying a Point of Launch**

**Averaged Brownian Escape Times: the Effect of Number of Launches**

- $N$ Brownian particles are launched from the sphere center, $v_N(0)$ is computed, and compared with the asymptotic value of $v(0)$:

$$\delta v(0) = \left| \frac{v(0) - v_N(0)}{v(0)} \right| \times 100\%.$$

<table>
<thead>
<tr>
<th>Number of Launches</th>
<th>Percentage Difference</th>
</tr>
</thead>
<tbody>
<tr>
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</tr>
<tr>
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<tr>
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<tr>
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</tr>
</tbody>
</table>

**Discussion**

- Efficient and flexible, fully parallelized Matlab code was developed and tested; can be applied to study diffusion processes/average values as well as multiple other statistical characteristics for Brownian motion-based diffusion processes.
- A comprehensive study of results obtained from the simulations showed that averages of $\sim 10^3$ single-particle simulations are sufficient to closely match the asymptotic MFPT values for the unit sphere.
- Time spent by Brownian particles near the boundary was studied; it was shown that irrespective of initial conditions and relative trap location, time near the domain boundary remains about 4.5% of the particle’s lifetime.

**What Next**

1. The developed code can be used to study the dynamics of Brownian particles in any 3D domains, for instance:
   - nanoparticle diffusion within *inverse opals* [2] and related man-made materials with cavities;
   - *domains with long necks* [3].

2. The code may be further optimized, and possibly improved by taking into account particle velocity-based simulated Brownian motion.

**References**

