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PyEscape: A narrow escape problem simulator package for Python

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Summary

In biology, many research questions focus on uncovering the mechanisms that allow particles (molecules, proteins, etc.) to move from one location to another. Often these movements are from one domain to another and these domains are in some way contained. The "narrow escape problem" is a biophysics problem where the solution would provide the average time required for a Brownian particle to escape a bounded domain through a particular opening. Originally proposed by Holcman & Schuss (2004), solutions to this problem have been given and refined over the years (Schuss, Singer, & Holcman, 2007).

Recently, solutions have been given (Kaye & Greengard, 2020) for more complex narrow escape problems, such as arbitrary escape pore patterning and size variation. However, these are provided without easily accessible implementations and confine the problem to a single container shape.

Here, we present a novel Python library that enables stochastic simulations to be run in order to approximate the narrow escape problem for unique scenarios. The mathematical models provided are implementations of random walks in 3 dimensions (Codling, Plank, & Benhamou, 2008). We show that our models are good approximations for analytical solutions (example notebook), and that they can be scaled to many custom problems.

Through this library we provide functionality for both cubical- and spherical-shaped domains. We enable a broad range of simulation variables to control. In the most simple case, a user will select the volume and shape they wish to act as their container, the number and size of escape pores on the container's surface, and the diffusion coefficient of the particle of interest.

Additionally, we give an implementation of Fibonacci spheres that allows for the fast placement of escape pores pseudo-evenly spaced on the surface of a sphere. This is often useful in experiments to test how number of escapes relates to mean escape time.

External libraries used

The models given are implemented through NumPy (van der Walt, Colbert, & Varoquaux, 2011)], results are visualised through Matplotlib (Hunter, 2007)], and documentation has been implemented using Jupyter-notebooks (Kluyver et al., 2016).

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