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Random walks with absorbing boundaries

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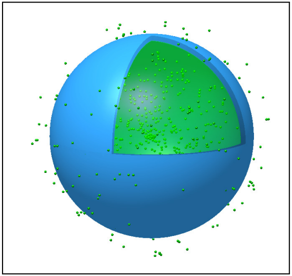
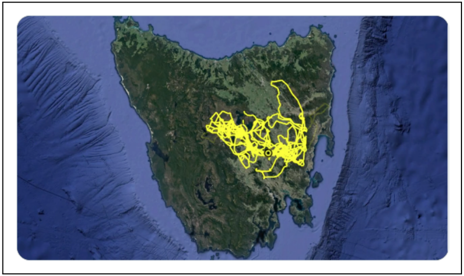


Drug Delivery



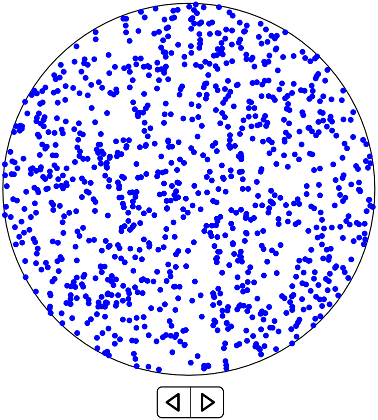
Animal Movement[1]

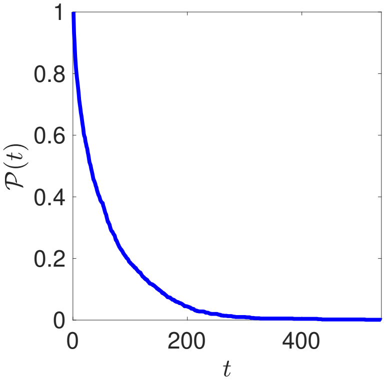
Mathematical questions:

1. What proportion of "particles" remain in the system at a given time?
2. How long does it take for a "particle" to exit given its starting location?

[1] https://twitter.com/JamesMPay/status/1484298706375655426

Proportion of particles remaining
Survival probability





Stochastic Model
Random walk

- Domain: Disc of radius L.
- N_p non-interacting particles
  (initially uniformly-distributed across domain)
- Unbiased random walk:

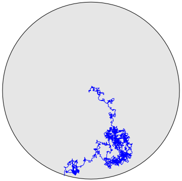
$$\mathbf{x}_j(t+\tau) = \mathbf{x}_j(t) + \delta\,[\cos(\theta_j), \sin(\theta_j)], \quad \theta_j \sim U(0, 2\pi).$$

- Absorbing boundary ($P = 1$) at $r = L$ or
  Semi-absorbing boundary ($0 < P < 1$) at $r = L$.
- Proportion of particles remaining:

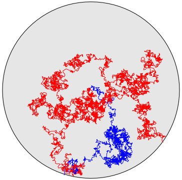
$$\mathcal{P}(t) = \frac{N(t)}{N_p},$$

where $N(t)$ is number of particles remaining at time t.

Absorbing



Semi-absorbing



- Probability a particle is at location (x, y) at time t

$$p(x,y,t) = \int_0^{2\pi} p(x-\delta\cos\theta, y-\delta\sin\theta, t-\tau) f(\theta)\,\mathrm{d}\theta, \qquad f(\theta) = \frac{1}{2\pi}.$$

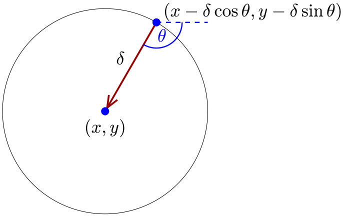
- Expanding in Taylor series

$$p = \int_0^{2\pi} \left[p - \delta\cos\theta \frac{\partial p}{\partial x} - \delta\sin\theta\frac{\partial p}{\partial y} - \tau\frac{\partial p}{\partial t} + \cdots \right] f(\theta)\,\mathrm{d}\theta$$

- Diffusion equation

$$\frac{\partial p}{\partial t} = D\left(\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2}\right) + \text{higher order terms}$$

where $D = \delta^2/(4\tau)$.



Continuum Model
Initial boundary value problem

- For a disc, dimensionless particle concentration $c(r,t)$ satisfies:

$$\frac{\partial c}{\partial t} = \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right), \quad 0 < r < L,$$

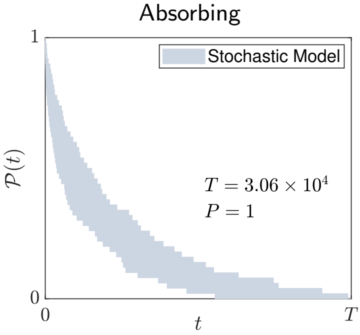
$$c(r,0) = 1,$$

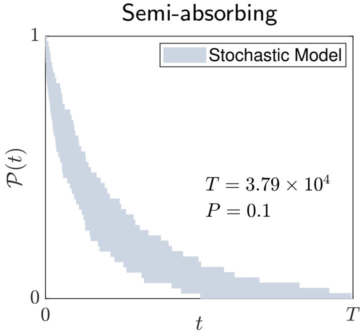
$$\frac{\partial c}{\partial r}(0,t) = 0 \text{ (radial symmetry)}$$

$$c(L,t) = 0 \text{ (absorbing) or } c(L,t) + \frac{\delta}{P}\frac{\partial c}{\partial r}(L,t) = 0 \text{ (semi-absorbing)}$$

- Proportion of particles remaining:

$$\mathcal{P}(t) = \frac{\int_\Omega c(r,t)\,\mathrm{d}A}{\int_\Omega c(r,0)\,\mathrm{d}A} = \frac{2}{L^2}\int_0^L rc(r,t)\,\mathrm{d}r.$$

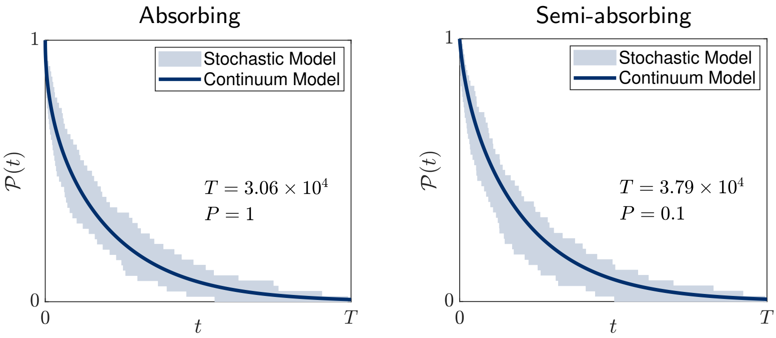




Stochastic: $\mathcal{P}(t) = \dfrac{N(t)}{N_p}$ (100 trials)

Continuum: $\mathcal{P}(t) = \dfrac{2}{L^2} \displaystyle\int_0^L r c(r,t)\,\mathrm{d}r$

Continuum Model
Results



Stochastic: $\mathcal{P}(t) = \dfrac{N(t)}{N_p}$ (100 trials)

Continuum: $\mathcal{P}(t) = \dfrac{2}{L^2}\displaystyle\int_0^L r c(r,t)\,\mathrm{d}r$

$$\mathcal{P}_{\mathrm{c}}(t) = \frac{2}{L^2}\int_0^L rc(r,t)\,\mathrm{d}r$$

Exponential model:

$$\mathcal{P}(t) = e^{-\lambda t}.$$

Choose λ to satisfy:

$$\int_0^\infty \mathcal{P}(t)\,\mathrm{d}t = \int_0^\infty \mathcal{P}_{\mathrm{c}}(t)\,\mathrm{d}t.$$

Explicit formula for λ:

$$\lambda = L^2\left[2\int_0^L rM(r)\,\mathrm{d}r\right]^{-1}$$

$$\text{where } M(r) = \int_0^\infty c(r,t)\,\mathrm{d}t$$

Attraction of this approach is that λ can be calculated explicitly as $M(r)$ satisfies a boundary value problem with a simple closed-form solution...

$$M(r) = \int_0^\infty c(r,t)\,\mathrm{d}t, \quad \frac{\partial c}{\partial t} = \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right)$$

Differential equation:

$$\frac{D}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}M}{\mathrm{d}r}\right) = \int_0^\infty \frac{D}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right)\mathrm{d}t = \int_0^\infty \frac{\partial c}{\partial t}\,\mathrm{d}t = -1.$$

Boundary conditions:

$$\frac{\mathrm{d}M}{\mathrm{d}r}(0) = 0 \text{ (radial symmetry)}$$

$$M(L) = 0 \text{ (absorbing) or } M(L) + \frac{\delta}{P}\frac{\mathrm{d}M}{\mathrm{d}r}(L) = 0 \text{ (semi-absorbing)}$$

Solution:

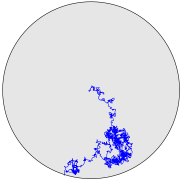
$$M(r) = \frac{L^2 - r^2}{4D} \text{ (absorbing)}$$

$$M(r) = \frac{L^2 - r^2}{4D} + \frac{L\delta}{2DP} \text{ (semi-absorbing)}$$

Absorbing boundary

$$\mathcal{P}(t) = \exp\left(\frac{-8Dt}{L^2}\right), \quad D = \frac{\delta^2}{4\tau}$$

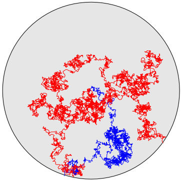
Absorbing



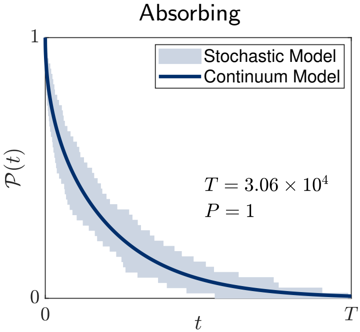
Semi-absorbing boundary

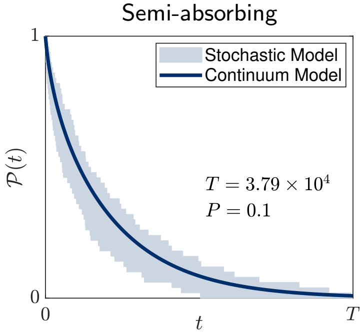
$$\mathcal{P}(t) = \exp\left(\frac{-8Dt}{L^2 + 4\delta L/P}\right)$$

Semi-absorbing



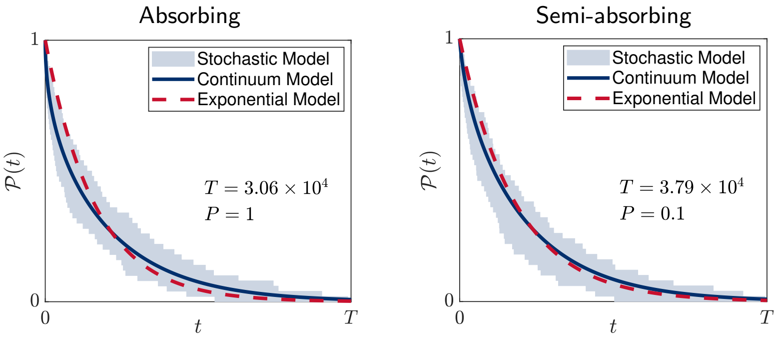
Exponential Model
Results





Stochastic: $\mathcal{P}(t) = \dfrac{N(t)}{N_p}$ (100 trials)

Continuum: $\mathcal{P}(t) = \dfrac{2}{L^2}\displaystyle\int_0^L rc(r,t)\,\mathrm{d}r$



Stochastic: $\mathcal{P}(t) = \dfrac{N(t)}{N_p}$ (100 trials)

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Exponential: $\mathcal{P}(t) = e^{-\lambda t}$

$$\mathcal{P}_\mathrm{c}(t) = \frac{2}{L^2}\int_0^L r c(r,t)\,\mathrm{d}r$$

Weibull model:

$$\mathcal{P}(t) = e^{-(\lambda t)^\alpha}.$$

Match the zeroth and first moments of $\mathcal{P}(t)$ and $\mathcal{P}_\mathrm{c}(t)$:

$$\int_0^\infty t^k \mathcal{P}(t)\,\mathrm{d}t = \int_0^\infty t^k \mathcal{P}_\mathrm{c}(t)\,\mathrm{d}t, \quad \text{for } k = 0, 1.$$

Two coupled nonlinear equations for λ and α:

$$\frac{\Gamma(\frac{k+1}{\alpha})}{\alpha\lambda^{k+1}} = \frac{2}{L^2}\int_0^L r M_k(r)\,\mathrm{d}r, \quad k = 0, 1,$$

where $M_k(r) = \int_0^\infty t^k c(r,t)\,\mathrm{d}t$.

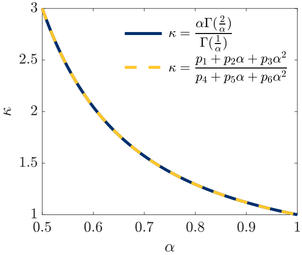
As for the exponential model, $M_k(r)$ satisfies a boundary value problem with simple closed-form polynomial solutions.

Combine two nonlinear equations

$$\frac{\alpha\Gamma(\frac{2}{\alpha})}{\Gamma(\frac{1}{\alpha})^2} = \kappa.$$

Padé approximation

$$\frac{p_1 + p_2\alpha + p_3\alpha^2}{p_4 + p_5\alpha + p_6\alpha^2} = \kappa.$$



Approximate explicit formulas for α and λ

$$\alpha = \frac{p_5\kappa - p_2 - \sqrt{(p_5\kappa - p_2)^2 - 4(p_3 - p_6\kappa)(p_1 - p_4\kappa)}}{2(p_3 - p_6\kappa)}$$

$$\lambda = L^2\left[\frac{2\alpha}{\Gamma(\frac{1}{\alpha})}\int_0^L r M_0(r)\,\mathrm{d}r\right]^{-1}$$

$$\mathcal{P}(t) = e^{-(Dt/\lambda)^{\alpha}}$$

Absorbing boundary

$$\kappa = 4/3$$
$$\alpha = 0.78258$$
$$\lambda = 0.10856L^2$$

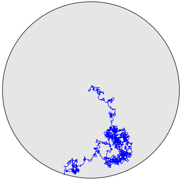
Semi-absorbing boundary

$$\kappa = \frac{4[L^2 + 6\delta(L + 2\delta/P)/P]}{3(L + 4\delta/P)^2}$$

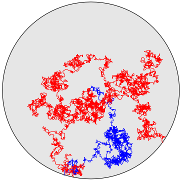
$$\alpha = \frac{p_5\kappa - p_2 - \sqrt{(p_5\kappa - p_2)^2 - 4(p_3 - p_6\kappa)(p_1 - p_4\kappa)}}{2(p_3 - p_6\kappa)}$$

$$\lambda = \frac{8D\Gamma(1/\alpha)}{\alpha(L^2 + 4\delta L/P)}$$

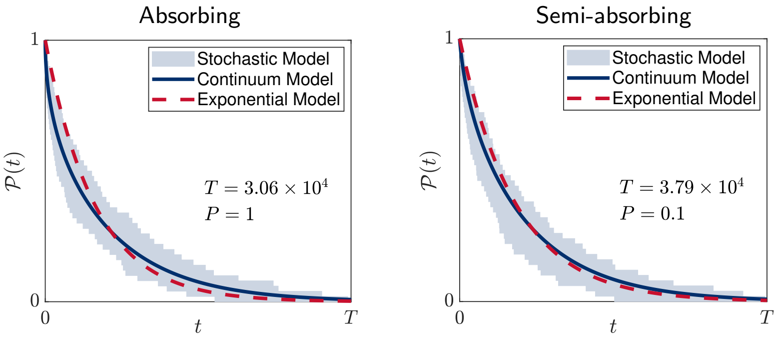
Absorbing



Semi-absorbing



Weibull Model
Results



Stochastic: $\mathcal{P}(t) = \dfrac{N(t)}{N_p}$ (100 trials)

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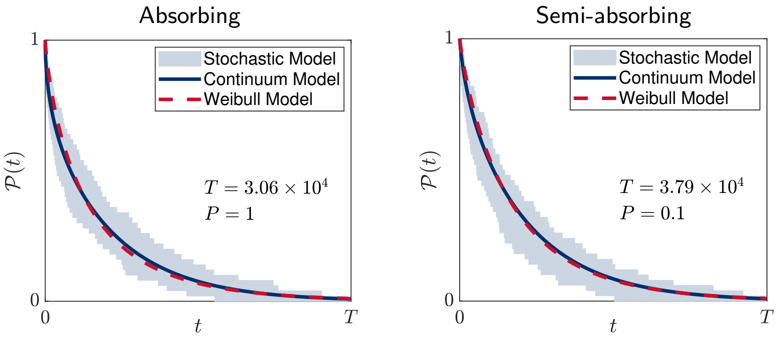

Stochastic: $\mathcal{P}(t) = \dfrac{N(t)}{N_p}$ (100 trials)

Weibull: $\mathcal{P}(t) = e^{-(\lambda t)^{\alpha}}$

Continuum: $\mathcal{P}(t) = \dfrac{2}{L^2}\displaystyle\int_0^L rc(r,t)\,\mathrm{d}r$

Publication, preprint and code
Carr (2022)

Physica A 605 (2022) 127985

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journal homepage: www.elsevier.com/locate/physa

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Exponential and Weibull models for spherical and spherical-shell diffusion-controlled release systems with semi-absorbing boundaries

Elliot J. Carr

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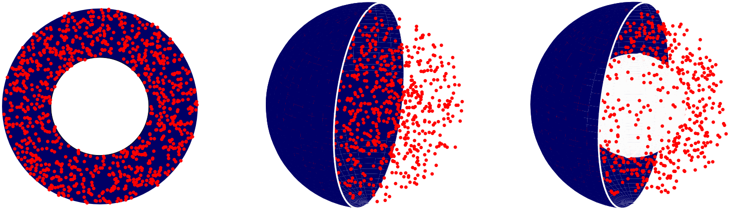
Article: Physica A: Statistical Mechanics and its Applications.
Preprint: arxiv.org/abs/2107.04759.
MATLAB Code: github.com/elliotcarr/Carr2022b.

- Simple one-term models on a disc.
- Models are valid in the continuum limit (small values of δ and τ).
- Exponential model: very simple but moderate accuracy.
- Weibull model: less simple but higher accuracy.
- Models have also been developed for other related problems.



Carr (2022), Physica A: Statistical Mechanics and its Applications

Summary

Part 1: Proportion of particles remaining

- Simple one-term models on a disc.
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- Exponential model: very sim racy.
- Weibull model: less simple b
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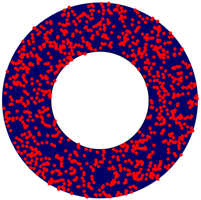

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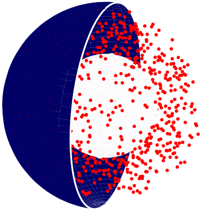

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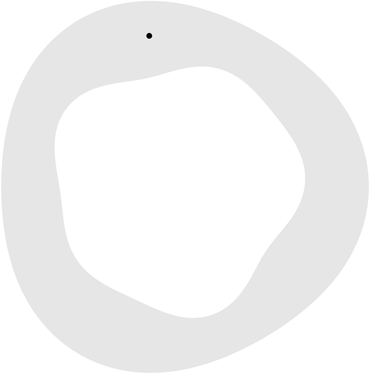
Mean Exit Time

Expected time for a particle to exit the system



Stochastic Model
Random walk

- Irregular annulus domain.
- At least one absorbing boundary.
- Unbiased random walk:

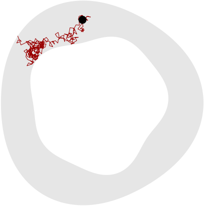
$$\mathbf{x}(t+\tau) = \mathbf{x}(t) + \delta\,[\cos(\theta), \sin(\theta)], \quad \theta \sim U(0, 2\pi).$$

- N repeated trials for each starting position (x, y).
- Mean exit time:

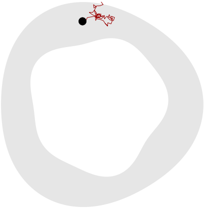
$$T(x, y) = \frac{1}{N}\sum_{i=1}^{N} t_i(x, y),$$

where $t_i(x, y)$ is time taken to exit for ith trial.

Trial 1



Trial 2



- Mean exit time:

$$T(x,y) = \sum_{k=0}^{\infty} t_k p(x,y,t_k), \qquad t_k = k\tau.$$

- Probability a particle starting at location (x, y) exits after k time steps:

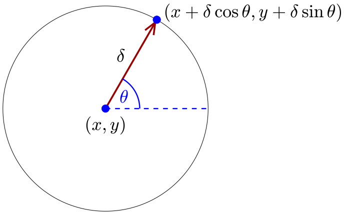
$$p(x,y,t_k) = \int_0^{2\pi} p(x+\delta\cos\theta, y+\delta\sin\theta, t_{k-1}) f(\theta)\,\mathrm{d}\theta, \qquad f(\theta) = \frac{1}{2\pi}.$$

- Combining and expanding in Taylor series:

$$-1 = D\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + \text{higher order terms}$$

- Diffusivity:

$$D = \frac{\delta^2}{4\tau}$$



Continuum Model
Boundary value problem

- Poisson equation for the mean exit time $T(r,\theta)$:

$$D\nabla^2 T = -1$$

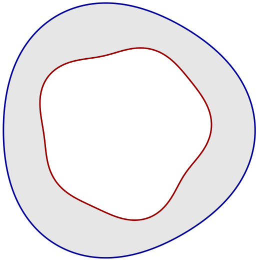
- Reflecting inner boundary:

$$\nabla T(r,\theta)\cdot \mathbf{n}(\theta) = 0 \qquad \text{on } r = \mathcal{R}_1(\theta)$$

- Absorbing outer boundary:

$$T(r,\theta) = 0 \qquad \text{on } r = \mathcal{R}_2(\theta)$$

$$\mathcal{R}_1(\theta) < r < \mathcal{R}_2(\theta)$$



Exact solution for an annulus ($\mathcal{R}_1(\theta) = R_1$, $\mathcal{R}_2(\theta) = R_2$) is trivial. Can we develop an (approximate) analytical solution for the case where the irregular domain is given by a small perturbation of an annulus?

- Poisson equation for mean exit time:

$$D\nabla^2 T = -1$$

- Assume perturbation solution:

$$T(r,\theta) = \sum_{k=0}^{\infty} \varepsilon^k T_k(r,\theta)$$

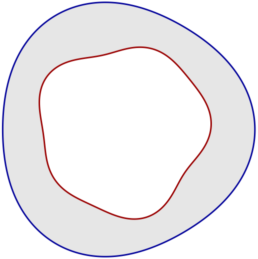
- Substitute and match powers of ε.
- Leading order term ($k = 0$):

$$D\nabla^2 T_0 = -1$$

- Higher order terms ($k = 1, 2, \ldots, N$):

$$\nabla^2 T_k = 0$$

$\mathcal{R}_1(\theta) = R_1(1 + \varepsilon g_1(\theta))$
$\mathcal{R}_2(\theta) = R_2(1 + \varepsilon g_2(\theta))$



Perturbation Solution
Absorbing outer boundary

- Absorbing outer boundary:

$$T(r,\theta) = 0 \qquad \text{on} \quad r = \mathcal{R}_2(\theta).$$

- Expand in Taylor series:

$$\sum_{i=0}^{\infty} \frac{(\varepsilon R_2 g_2(\theta))^i}{i!} \frac{\partial^i T}{\partial r^i}(R_2,\theta) = 0$$

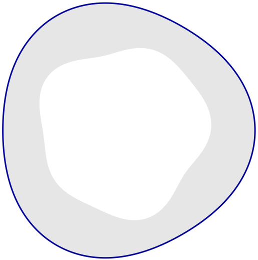
- Introduce perturbation expansion:

$$\sum_{i=0}^{\infty}\sum_{k=1}^{\infty} \frac{\varepsilon^{i+k}(R_2 g_2(\theta))^i}{i!} \frac{\partial^i T_k}{\partial r^i}(R_2,\theta) = 0$$

- Match powers of ε:

$$T_k(R_2,\theta) = b_k(\theta)$$

where $b_k(\theta)$ depends on partial derivatives of $T_0,\ldots,T_{k-1}$ with respect to r.



- Reflecting inner boundary:

$$\nabla T(r,\theta)\cdot \mathbf{n}(\theta) = 0 \qquad \text{on} \quad r = \mathcal{R}_1(\theta).$$

- Normal vector:

$$\mathbf{n}(\theta) = -\mathcal{R}_1(\theta)\mathbf{e}_r + \mathcal{R}_1'(\theta)\mathbf{e}_\theta$$

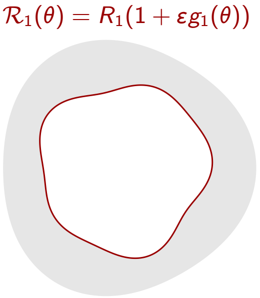
- Reflecting inner boundary:

$$-[\mathcal{R}_1(\theta)]^2\frac{\partial T}{\partial r}(r,\theta) + \mathcal{R}_1'(\theta)\frac{\partial T}{\partial \theta}(r,\theta) = 0.$$

- Expand in Taylor series, introduce expansion and match powers of ε

$$\frac{\partial T_k}{\partial r}(R_1,\theta) = a_k(\theta)$$

where $a_k(\theta)$ depends on partial and mixed derivatives of $T_0,\ldots,T_{k-1}$ with respect to r and θ.

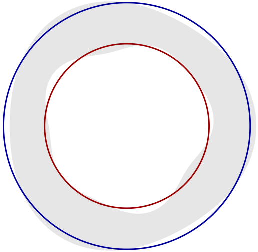


- Leading order term ($k = 0$):

$$\frac{D}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}T_0}{\mathrm{d}r}\right) = -1, \quad R_1 < r < R_2,$$
$$\frac{\mathrm{d}T_0}{\mathrm{d}r}(R_1) = 0, \quad T_0(R_2) = 0.$$

$$\boxed{T_0(r) = \frac{R_2^2 - r^2}{4D} + \frac{R_1^2}{2D}\log(r/R_2)}$$

Unperturbed domain
($R_1 < r < R_2$)

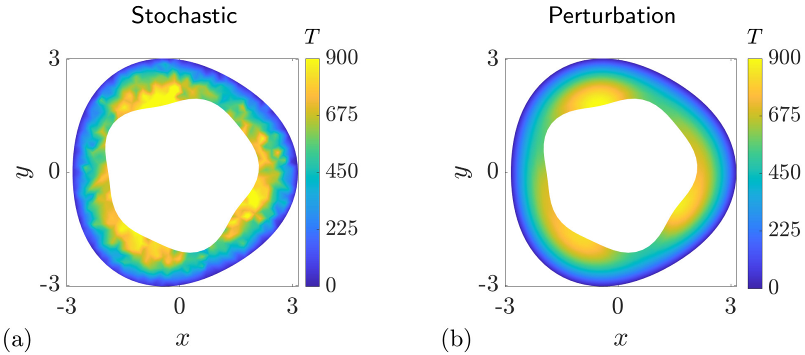


- Higher order terms ($k = 1, 2, \ldots$):

$$\nabla^2 T_k = 0, \quad R_1 < r < R_2,$$
$$\frac{\partial T_k}{\partial r}(R_1, \theta) = a_k(\theta), \quad T_k(R_2, \theta) = b_k(\theta).$$

$T_k(r, \theta)$ can be found using separation of variables.

Reflecting inner boundary and absorbing outer boundary

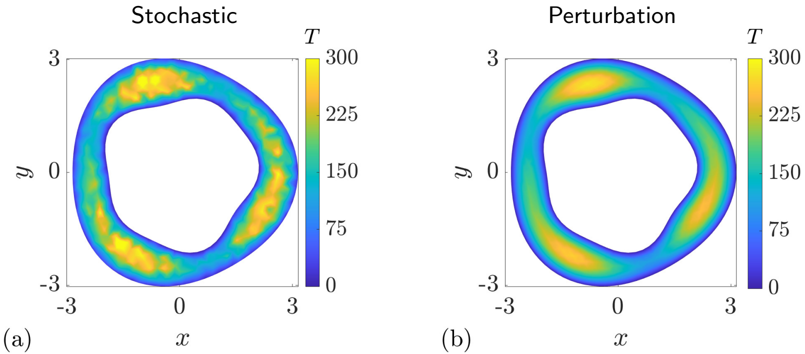


Stochastic: $T(r,\theta) = \frac{1}{N}\sum_{i=1}^{N} t_i(r,\theta)$ $(N = 50)$

Perturbation: $T(r,\theta) = T_0(r) + \varepsilon T_1(r,\theta) + \varepsilon^2 T_2(r,\theta)$

$g_1(\theta) = \sin(3\theta) + \cos(5\theta)$

$g_2(\theta) = \cos(3\theta), \quad \varepsilon = 0.05$



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Publication, preprint and code
Carr et al (2022)

IOP Publishing — Journal of Physics A: Mathematical and Theoretical
J. Phys. A: Math. Theor. **55** (2022) 105002 (21pp) https://doi.org/10.1088/1751-8121/ac4a1d

Mean exit time in irregularly-shaped annular and composite disc domains

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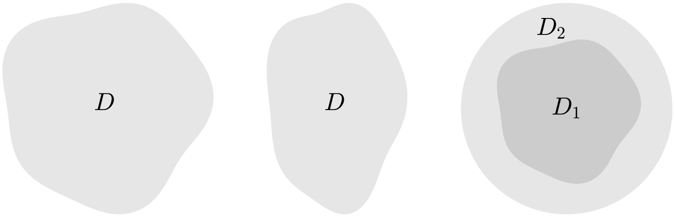
Article: Journal of Physics A: Mathematical and Theoretical.
Preprint: arxiv.org/abs/2108.03816.
MATLAB Code: github.com/ProfMJSimpson/Exit_time.

Summary

- Approximate analytical solutions for the mean exit time on an irregular annulus.
- Solutions are valid in the continuum limit (small values of δ and τ).
- Solutions are valid for domains given by a small perturbation of a perfect annulus.
- Perturbation solutions have also been developed for other related problems.



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