Heterogeneous Continuous Time Random walks on graphs

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Introduction

Continuous Time Random Walk (CTRW) [1] often has been evoked as a simplified model of transport in porous media [2,3]. The propagator formula $\hat{P}_k(s)$ for CTRW:

$$\hat{P}_k(s)=\frac{1-\tilde{\psi}(s)}{s}\frac{1}{[1-\tilde{\psi}(s)\hat{f}(k)]} \quad (1)$$

Figure 1. Transport in porous media.

$\tilde{\psi}(s)$ is the Laplace transform of PDF of the waiting time between steps, $\hat{f}(k)$ is the characteristic function of the jump distribution in Fourier space.

In practice, pores and channels have a broad distribution of sizes and shapes [4,5,6], hence the heterogeneity of the waiting time distributions is needed.

HCTRW model

Random walker in HCTRW model moves on a graph with the **generalized transition matrix** $Q(t)$:

$Q_{xx'}(t) = Q_{xx'}\,\psi_{xx'}(t)$:

- $Q_{xx'}$ is the **probability of jump** from x to x'
- The **travel time** $\tau_{xx'}$ from one x to x' is random with probability density $\psi_{xx'}(t)$.

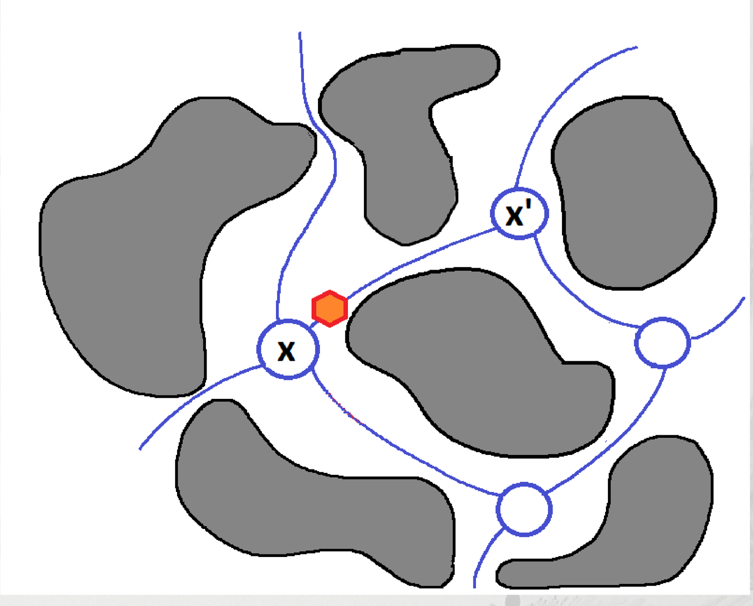

Figure 2. HCTRW model on a porous graph: travel times $\psi_{xx'}(t)$, graph transition Q matrix.

Analytical results

The **propagator of the HCTRW** $P_{x_0x}(t)$ is the probability of reaching x from x_0 in time t. The exact general formula for the propagator $P_{x_0x}(t)$ of the HCTRW in the Laplace domain:

$$\tilde{P}_{x_0x}(s)=\frac{1-\sum_{x'}\tilde{Q}_{xx'}(s)}{s}[I-\tilde{Q}(s)]^{-1}_{x_0x} \quad (2)$$

The spectral representation for (2) is given by

$$\tilde{P}_{x_0x}(s)=\frac{1-\sum_{x'}\tilde{Q}_{xx'}(s)}{s}\sum_{k\geq 0}\frac{u_k(x)v_k(x_0)}{\lambda_k} \quad (3)$$

where λ_k are eigenvalues, dependent on s, u_k, v_k are left-, right- eigenvectors of $H(s)=I-\tilde{Q}(s)$.

For **HCTRW** with finite first moments of travel times $<\tau_{xx'}>$ we define T: $T_{xx'} = Q_{xx'} <\tau_{xx'}>$. Then for small s the matrix $H(s) \approx I - Q + sT + O(s^2)$, $\lambda_k = \lambda_{0k} + s\lambda_{1k} + o(s)$, $v_k = v_{0k} + s\, v_{1k} + O(s^2)$, $u_k = u_{0k} + s\, u_{1k} + O(s^2)$, where $\lambda_{1k} = (u_{0k}\, T v_{0k}$.) This gives **the long time asymptotic behavior of the HCTRW propagator**:

$$P_{x_0x}(t)=p_x^{st}+t_x\sum_{k>0}\frac{u_{0k}(x)v_{0k}(x_0)}{\lambda_{1k}}e^{-t\lambda_{0k}/\lambda_{1k}} \quad (4)$$

where p_x^{st} is stationary distribution, $t_x=\sum_{x'} T_{xx'}$. The HCTRW propagator with infinite mean of travel time distribution is approximated by:

$$P_{x_0x}(t)=p_x^{st}+t_x\sum_{k>0}\frac{u_{0k}(x)v_{0k}(x_0)}{\lambda_{1k}}E_\alpha(-t^\alpha\lambda_{0k}/\lambda_{1k}) \quad (5)$$

where $E_\alpha(z)$ is the Mittag-Leffler function with parameter α.

Numerical results

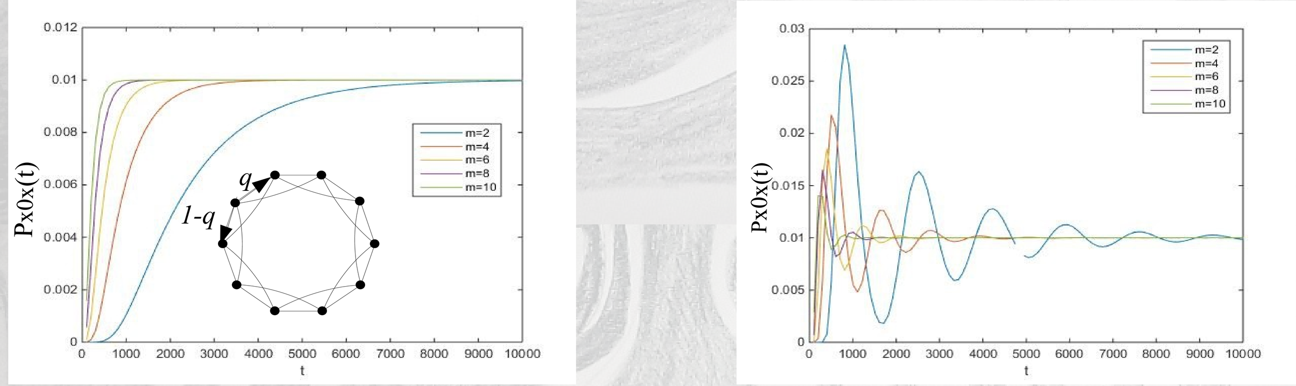

Figure 3. HCTRW propagator $P_{x0x}(t)$ on m-circular graph with $N = 100$ nodes for $m = \{2,4,6,8,10\}$, $\psi_{xx'}(s) = 1/(1+s\tau_{xx'})$, $q = 0.5$ (**left**), $q = 0.6$ (**right**).

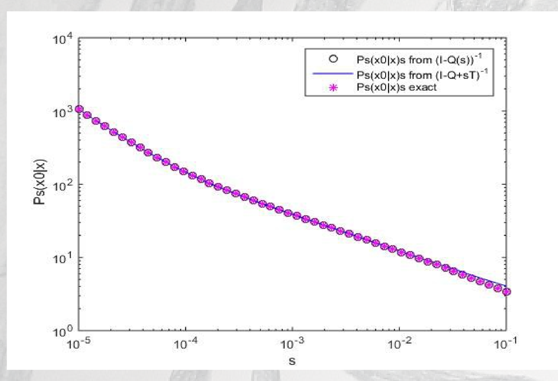

Figure 4. Comparison of HCTRW the analytic Eq. (2), exact solution and approximate solution Eq. (3) of $P_{x0x}(s)$ for a circular graph.

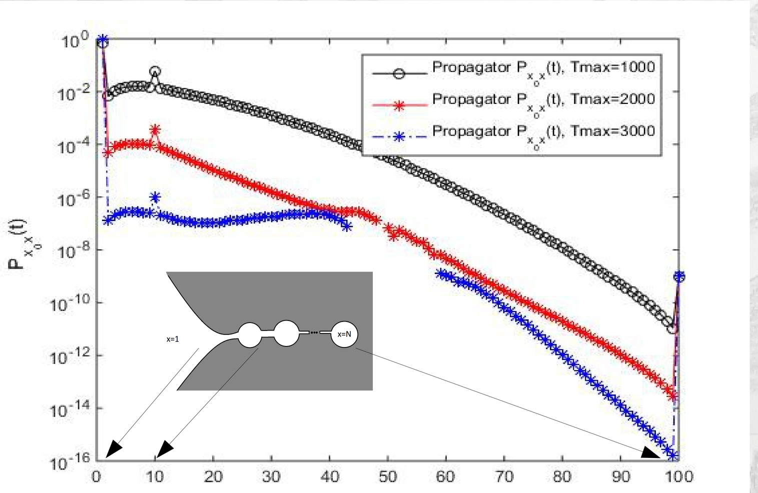

Figure 5. Propagators for HCTRW on the interval with absorbing, reflecting nodes. For all nodes $\tilde{\psi}_{xx'}(s) = 1/(1+s\tau_{xx'})$ with $\tau_{xx'} = 5,1$, except in heterogeneous node $x_h = 10$: $\tau_{xx'} = 20,10$. $q = 0.6$ is the parameter of transition matrix Q .

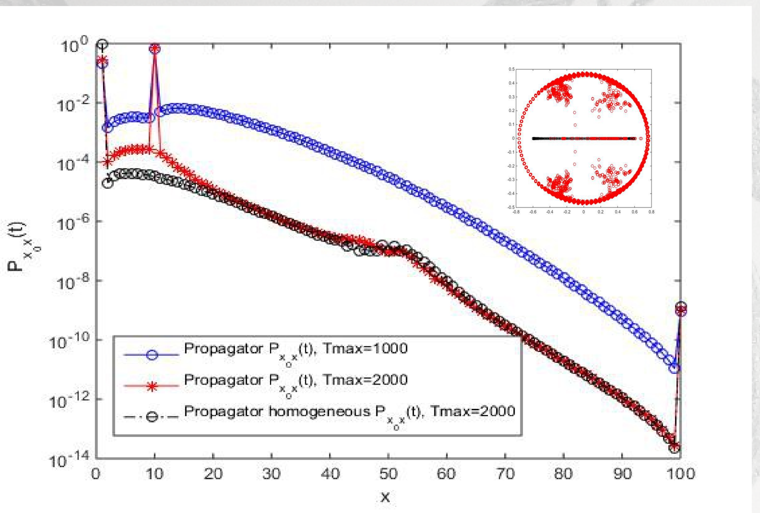

Figure 6. Propagators for HCTRW on the interval with the absorbing, reflecting, heterogeneous node with $\tilde{\psi}_{x_hx'}(s) = 1/(1+s^\alpha\tau^\alpha)$, $\alpha=0.1$, other travel times are $\tilde{\psi}_{xx'}(s) = 1/(1+s\tau_{xx'})$.

Conclusions

Analytic formula for HCTRW on a graph is derived with its spectral representation and asymptotic limit.

Analytic framework for HCTRW links **structural** properties of underlying graph, **spectral** properties of the generalized transition matrix and **dynamical** properties of HCTRW.

HCTRW with finite and infinite mean of travel times applies to graph with absorbing nodes (traps x^*): propagator $P_{x0x^*}(t)$ is interpreted as the cumulative probability distribution of the first passage time (FPT) to the sink site (or to the absorbing boundary).

Open questions:

What are limits of HCTRW on large graphs and macroscopic analogue? How to "encode" the microstructure of a porous medium through $Q(t)$? [4,5,6] ?

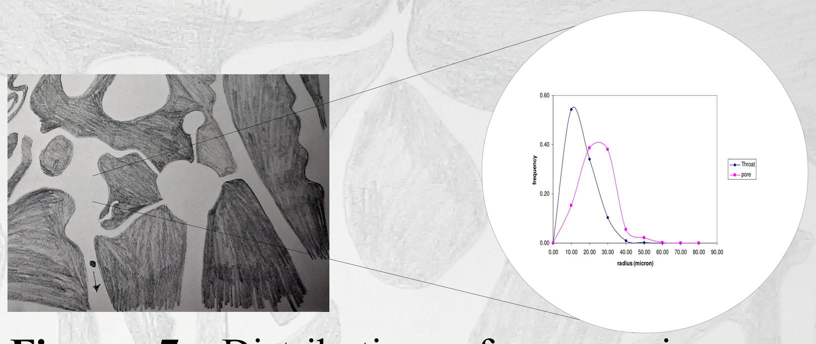

Figure 7. Distribution of pores sizes distributions and their frequency in Berea model of the porous media.

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