# Alternatives to Monte Carlo Simulations for Fractal Diffusion Models

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# Why Focus on Fractal Diffusion Simulations?

- Fun
- Check validity of analytically derived models
- Obtain simulation-based dimension estimates
- Application in anomalous diffusion research

# Waypoints

- Fractal dynamics introduction
- Graph-based set representation
- Random walk models
- Constraint convolution schema
- Application: oscillation detection

# Diffusion on Fractals

**Mass Scaling**

$$M \sim L^{d_f}$$

**Time Scaling**

$$t \sim L^{d_w}$$

## Observables

- Return probability

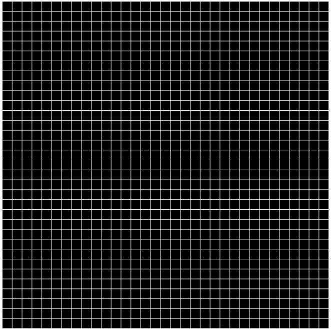
$$\Pr(X_t = \boldsymbol{x}_0) \sim t^{-d_s/2}$$

- Absolute moments

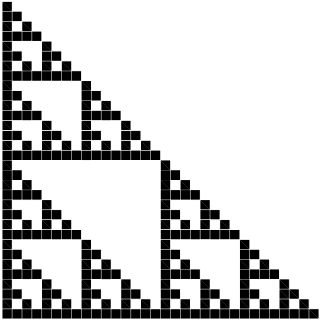
$$\mathrm{E}\,||X_t - \boldsymbol{x}_0||^{\alpha} \sim t^{\alpha/d_w}$$

# Grid Based Models

$d = 2$



$d_f = \log 3 \big/ \log 2$



# Random Walk on Graph

$$\mathcal{G} = (\mathcal{F}, \mathcal{E}), \quad \mathcal{F} \subset \mathbb{Z}^d$$

$$p \in (0,1), \quad c(\boldsymbol{x}) = \operatorname{card} \mathcal{N}(\boldsymbol{x})$$

$$\Pr\left(X_{t+1} = \boldsymbol{y} \mid X_t = \boldsymbol{x}\right) = \begin{cases} p, & \boldsymbol{y} \in \mathcal{N}(\boldsymbol{x}) \\ 1 - c(\boldsymbol{x})\, p, & \boldsymbol{y} = \boldsymbol{x} \\ 0, & \text{otherwise} \end{cases}$$

$$\boldsymbol{x}, \boldsymbol{y} \in \mathcal{F}$$

# Standard Full Space Approach

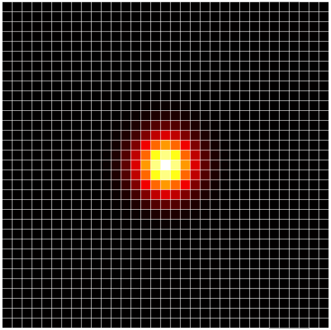
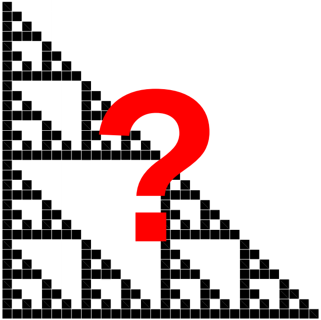
- $\mathsf{P}_t : \mathbb{Z}^d \mapsto [0, 1]$
- $\mathsf{P}_t(\boldsymbol{x}) = \Pr(X_t = \boldsymbol{x} | X_0 = \boldsymbol{x}_0)$
- $\mathsf{P}_0(\boldsymbol{x}) = 1(\boldsymbol{x} = \boldsymbol{x}_0)$

**Full Grid Probability Evolution**

$$\mathsf{P}_{t+1} = \mathsf{N} * \mathsf{P}_t$$

- $\mathsf{N}_{\text{square}} = \begin{pmatrix} 0 & p & 0 \\ p & 1-4p & p \\ 0 & p & 0 \end{pmatrix}$
- $\mathsf{N}_{\text{hexa}} = \begin{pmatrix} p & p & 0 \\ p & 1-6p & p \\ 0 & p & p \end{pmatrix}$

# Random Walk Over Grid Based Models

| $d = 2$ | $d_f = \log 3 / \log 2$ |
|---|---|
|  |  |

# Constrained Convolution Schema

- $\mathrm{P}_t, \mathrm{F}, \mathrm{C} : \mathbb{Z}^d \mapsto \mathbb{R}$
- $\mathrm{P}_t(\boldsymbol{x}) = \Pr(X_t = \boldsymbol{x} | X_0 = \boldsymbol{x}_0)$
- $\mathrm{P}_0(\boldsymbol{x}) = 1(\boldsymbol{x} = \boldsymbol{x}_0)$
- $\mathrm{F}(\boldsymbol{x}) = 1(\boldsymbol{x} \in \mathcal{F})$
- $\mathrm{C} = \mathrm{F}\,(\mathrm{N} * \mathrm{F})$

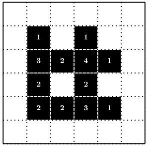
**Sparse Grid Probability Evolution**

$$\mathrm{P}_{t+1} = \mathrm{P}_t\,(1 - p\,\mathrm{C}) + p\,\mathrm{F}\,(\mathrm{N} * \mathrm{P}_t)$$

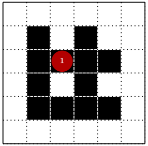
Proof is soon to be published

- $\mathrm{N}_{\text{square}} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$
- $\mathrm{N}_{\text{hexa}} = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$

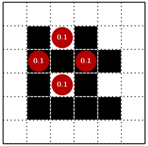
# Square Topology



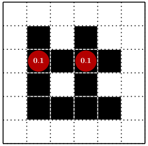

F, C



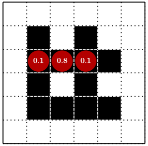

$P_0$



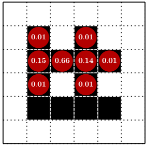

$p\left(P_0 * N\right)$




$p\,F\left(P_0 * N\right)$



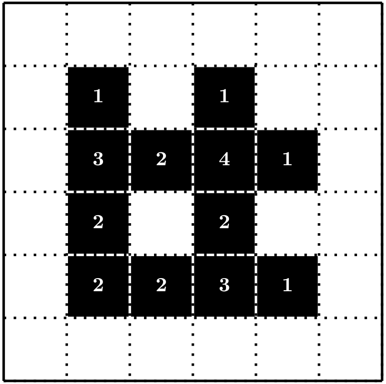

$P_1$




$P_2$

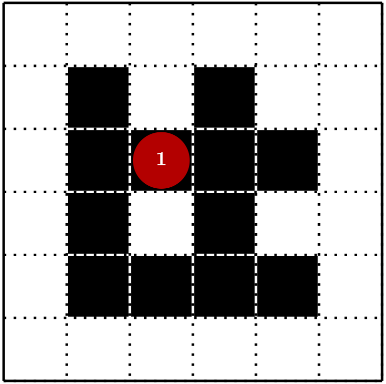
# Square Topology

- Set F with number of neighbours C



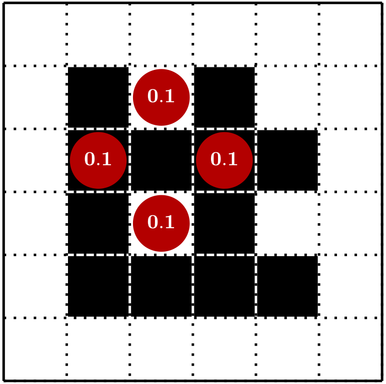
# Square Topology

- Initial distribution: $P_0$



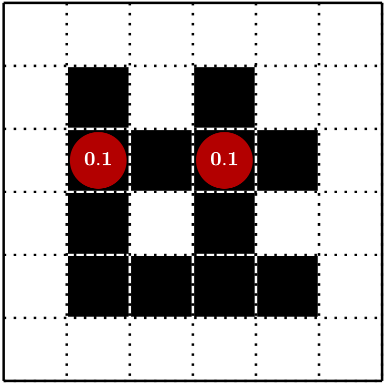
# Square Topology

- Intermediate step: $p\left(\mathrm{P}_0 * \mathrm{N}\right), p = 0.1$



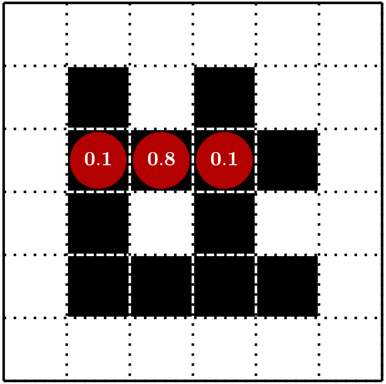
# Square Topology

- Intermediate step: $p\,\mathsf{F}\left(\mathsf{P}_0 * \mathsf{N}\right)$



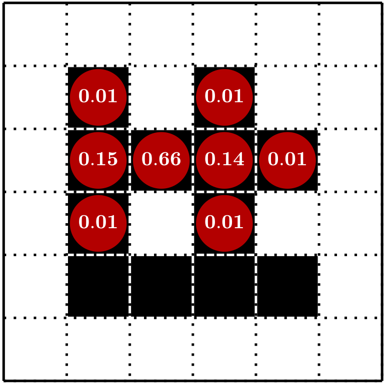
# Square Topology

- Distribution $P_1 = P_0 \left(1 - p\,C\right) + p\,F\left(P_0 * N\right)$

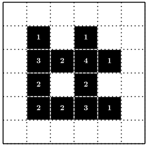


# Square Topology

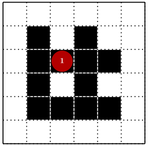
- Distribution $P_2$



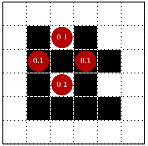
# Square Topology



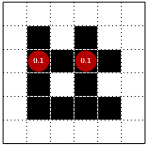

$F, C$



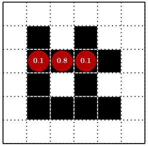

$P_0$



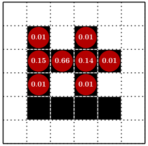

$p\left(P_0 * N\right)$




$p\,F\left(P_0 * N\right)$

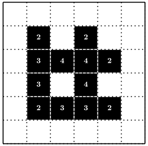



$P_1$

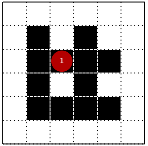



$P_2$

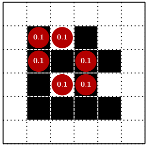
# Hexagonal Topology



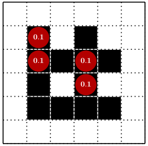

$F, C$



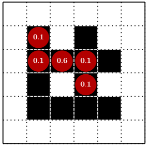

$P_0$



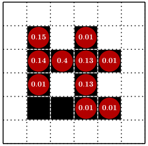

$p\left(P_0 * N\right)$




$p\,F\left(P_0 * N\right)$

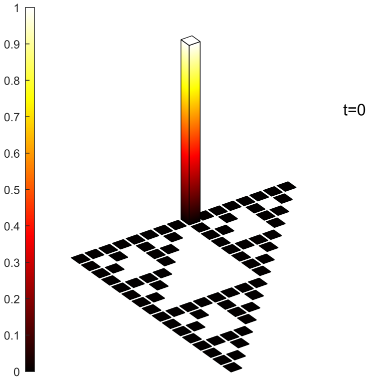



$P_1$

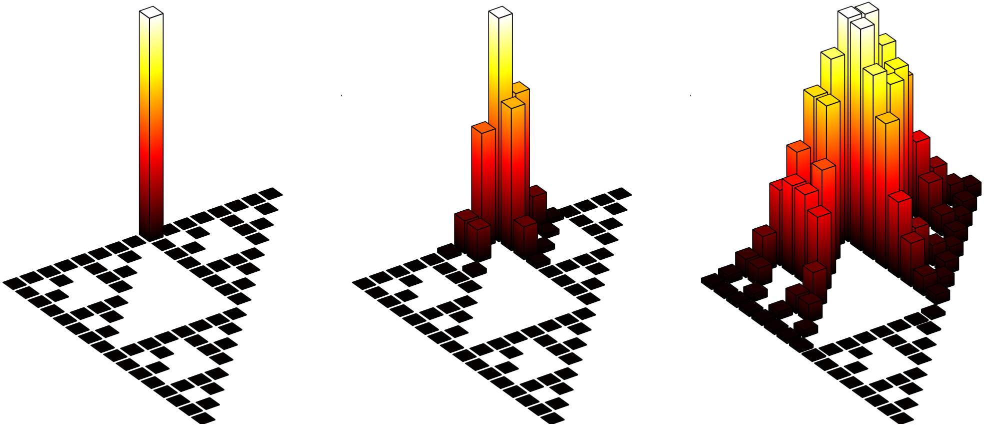



$P_2$

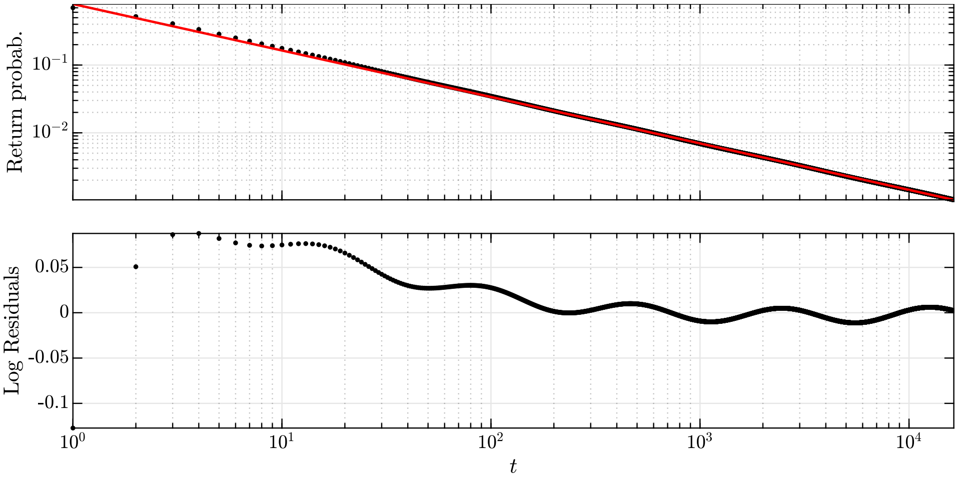
# Probability on Sierpinski Gasket



# Probability on Sierpinski Gasket



# Return Probability



- Random walk "simulation" without noise
- Calculation of full distribution $\mathrm{P}_t$
- Computationaly friendly form
- Random walk analysis tool

# Thank you for your attention!