Diffusion on disordered fractals

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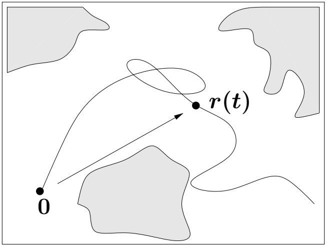
Anomalous Diffusion

Diffusion of particles in disordered materials

- inside a bulk
- on the surface (deposit)



Mean square displacement:

$$\langle r^2(t)\rangle \sim t^{\gamma} \qquad \gamma > 0$$

$\gamma < 1$ subdiffusion
$\gamma = 1$ normal diffusion
$\gamma > 1$ superdiffusion

$r(t)$: Distance a particle has traversed in time t from its origin

Anomalous Diffusion

- Anomalous diffusion of water in biological tissues.
  M. Köpf, et al. *Biophys. J.*, 70(6):2950–2958, 1996.
- Anomalous diffusion of hydrogen in amorphous metals.
  W. Schirmacher, et al.; *Europhys. Lett.*, 13(6):523–529, 1990.
- Submonolayer growth with repulsive impurities.
  S. Liu, et al.; *Phys. Rev. Lett.*, 74(22):4495–4498, 1995.

→ Investigation of diffusion in disordered materials by numerical simulation

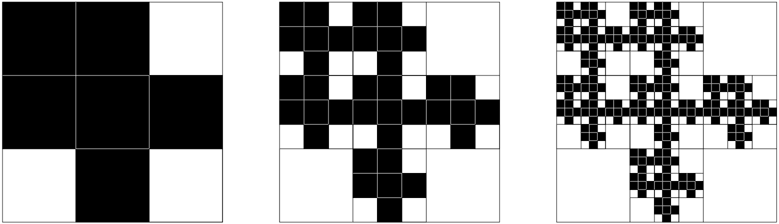
Porous Materials

Properties of porous materials:

- Holes, barriers and connections on all length scales
- Self similar over certain length scales
- At larger length scales $\longrightarrow$ rather homogeneous
- Smallest length scale $\longrightarrow$ at least atom size

$\rightsquigarrow$ Aim: Modelling porous materials by fractals

Regular Sierpinski Carpets



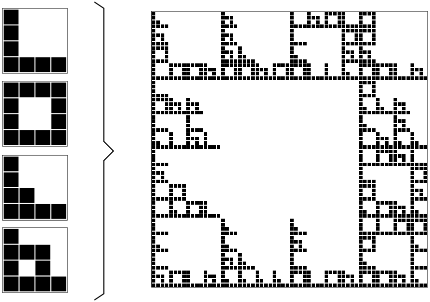
- Iteration repeated ad infinitum → Sierpinski carpet
- k-fold iteration → iterator of depth k

Fractal dimension: $M \sim L^{d_f} \;\rightarrow\; d_f = \frac{\ln M}{\ln L}$

→ Transition from regular to randomized fractals

Randomized Sierpinski Carpets

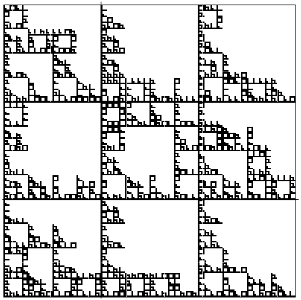
- Random mixing of different generators



- More realistic model

→ But: Real materials are self-similar only at certain length scales

Repeated Randomized Sierpinski Carpets

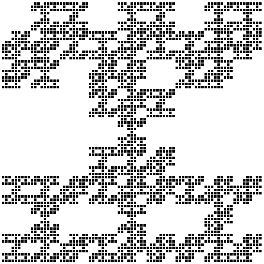


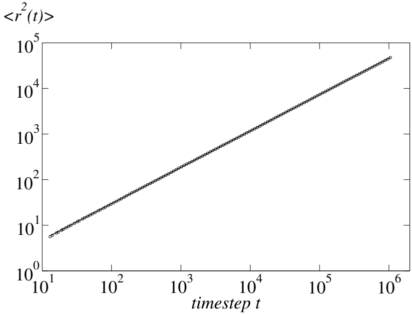
- Combining different iterators to one carpet
- Simulation model exhibit same properties as real materials
  - Smallest length scale
  - Large length scales

→ Discrete space of states for simulation of diffusion by random walk approach

Random Walk Dimension

- Random walk dimension: $d_w = \frac{2}{\gamma}$
  $\rightarrow \langle r^2(t) \rangle \sim t^\gamma \rightarrow t \sim r^{d_w} \rightarrow$ Power law behavior
  $\rightarrow$ also valid for randomized Sierpinski carpets





D. Anh, et al.; *Europhys. Lett.*, 70(1):109-115, 2005

Open Questions

- What happens by mixing different generators with $\langle d_w \rangle$?

Investigations by Reis with regular random fractals (different from our construction procedure)

F. Reis; *J. Phys.A: Math. Gen.*,29(24):7803-7810, 1996

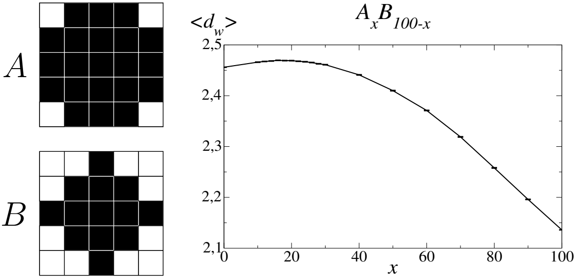
$\longrightarrow$ No significant changes in exponents

$\Rightarrow$ But we obtained quite different results!

Results

D. Anh, et al.; *Europhys. Lett.*, 70(1):109-115, 2005

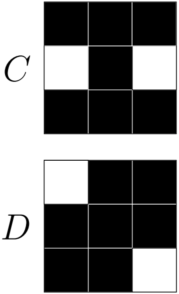
- Mixing pairs of different generators
- Two generators of different d_f and different d_w

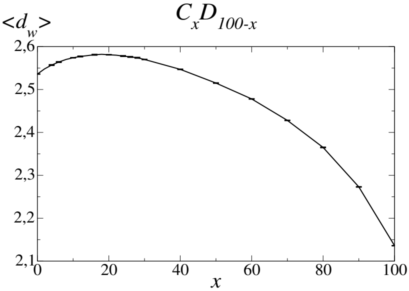


- Maximum of $\langle d_w \rangle$ can be observed

Results

- Two generators with different d_w but same d_f

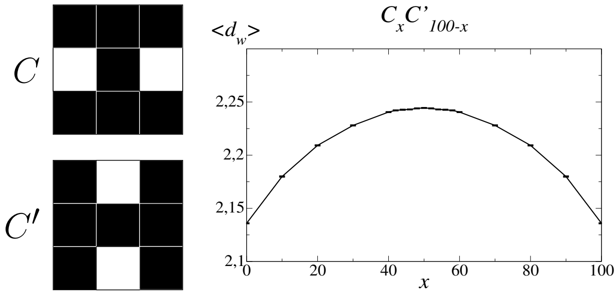




- Maximum of $\langle d_w \rangle$ can be observed

Results

- Two generators with same d_w and same d_f



- Variation even for similar d_w and d_f

Results

- Two generators with same d_w and same d_f

D

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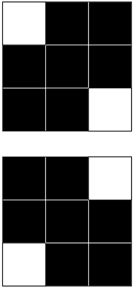
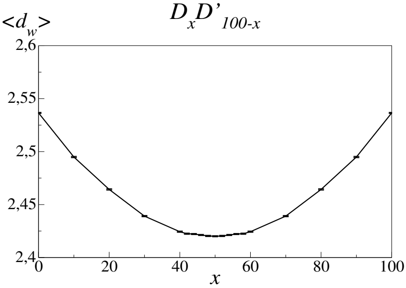




- More disorder can enhance diffusion

Question

Can we predict dynamical properties just by knowing the structure?

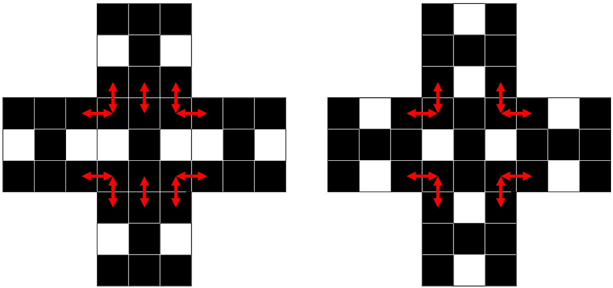
If yes: Analysis porous materials for experiments:

- Mass
- Connectivity
- ...

$\Rightarrow$ Explanation of dynamics due to structural properties

Connection Points

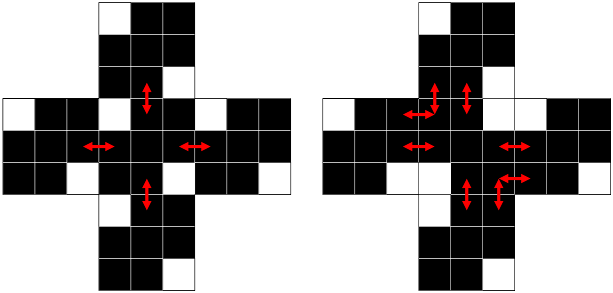
Structural property: Connection points between generators



→ Slowing down of diffusion

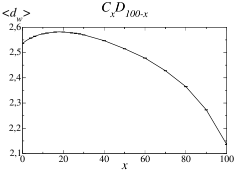
Connection Points

Structural property: Connection points between generators



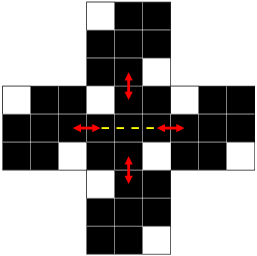
→ Enhancement of diffusion

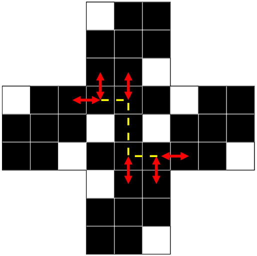
Shortest Path

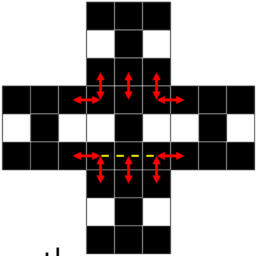


Structural property:

Shortest path through generators





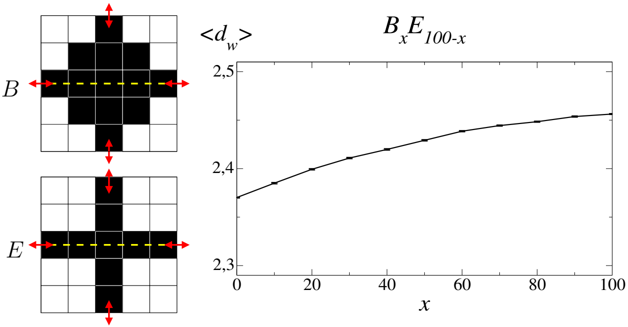


More connection points but longer shortest path

$\longrightarrow$ Slowing down of diffusion

Results

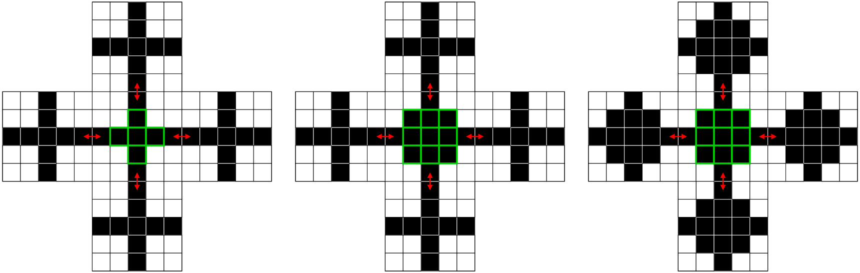
But how can we explain this behaviour?



- Equal number of connection points and path length
- But changing of $\langle d_{\mathrm{w}} \rangle$

Active Sites

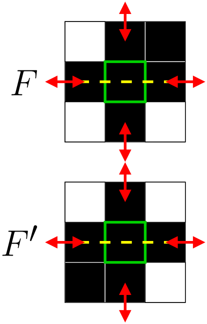
Different number of actives sites inside the generators

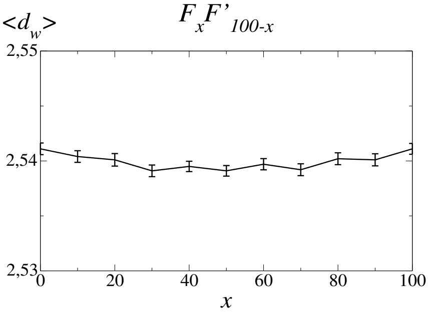


→ More active sites slows diffusive process down

Results

Test: Same number of connection points, shortest path length and number of active sites





→ Nearly no change for $\langle d_w \rangle$

Summary

From structure to dynamics:

- Increasing number of connection points $\longrightarrow$ enhancement of diffusion
- For longer shortest paths $\longrightarrow$ diffusion slows down
- More active sites inside a generator $\longrightarrow$ diffusion slows down

$\leadsto$ Number of connection point, shortest path length and number of active sites are important for $\langle d_w \rangle$

Acknowledgement

Thank you for your attention!