

*Harmonic measure
and the passivation
of 2D and 3D fractals*

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Outline

- Geometry-adapted fast random walks
- Multifractal properties of the harmonic measure on Von Koch boundaries

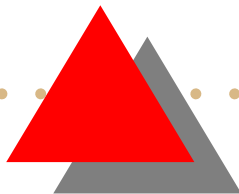
Grebenkov, Lebedev, Filoche, Sapoval, Phys. Rev. E 71, 056121 (2005)

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- Passivation of 2D and 3D fractals

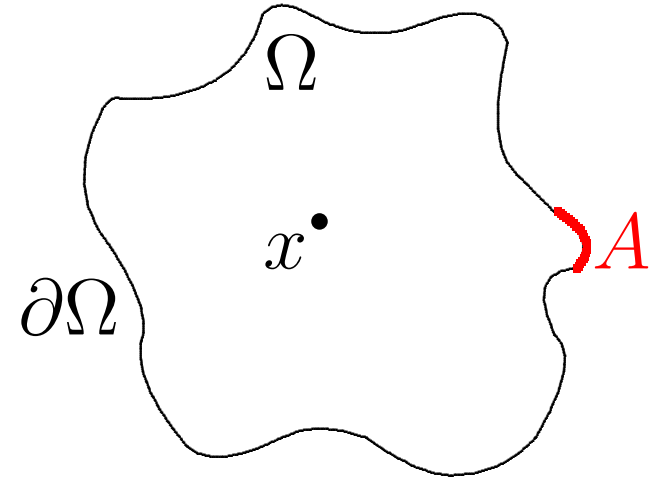
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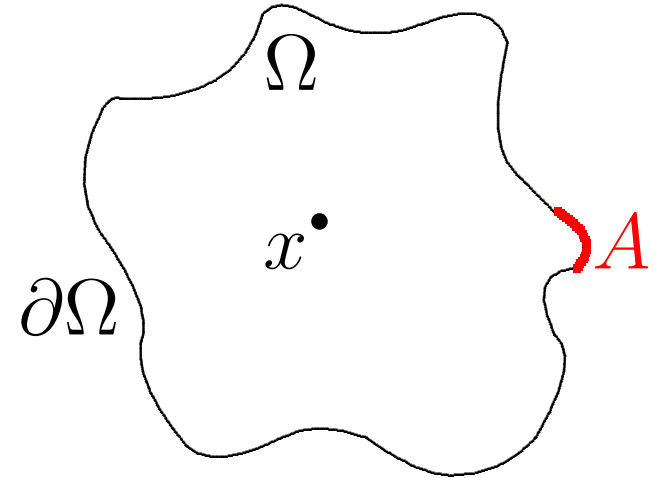
Harmonic measure

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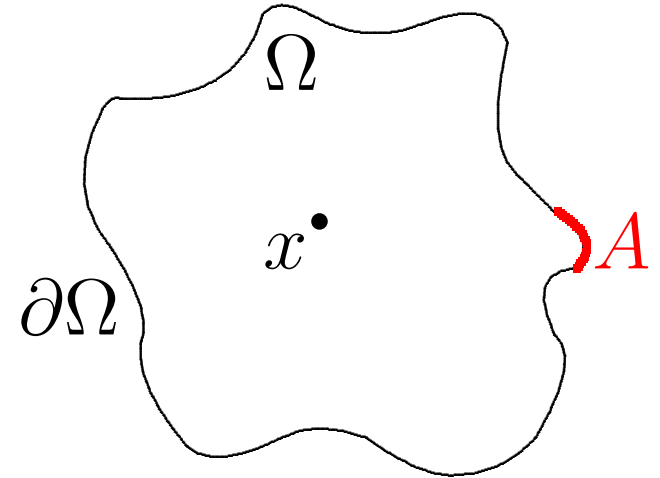
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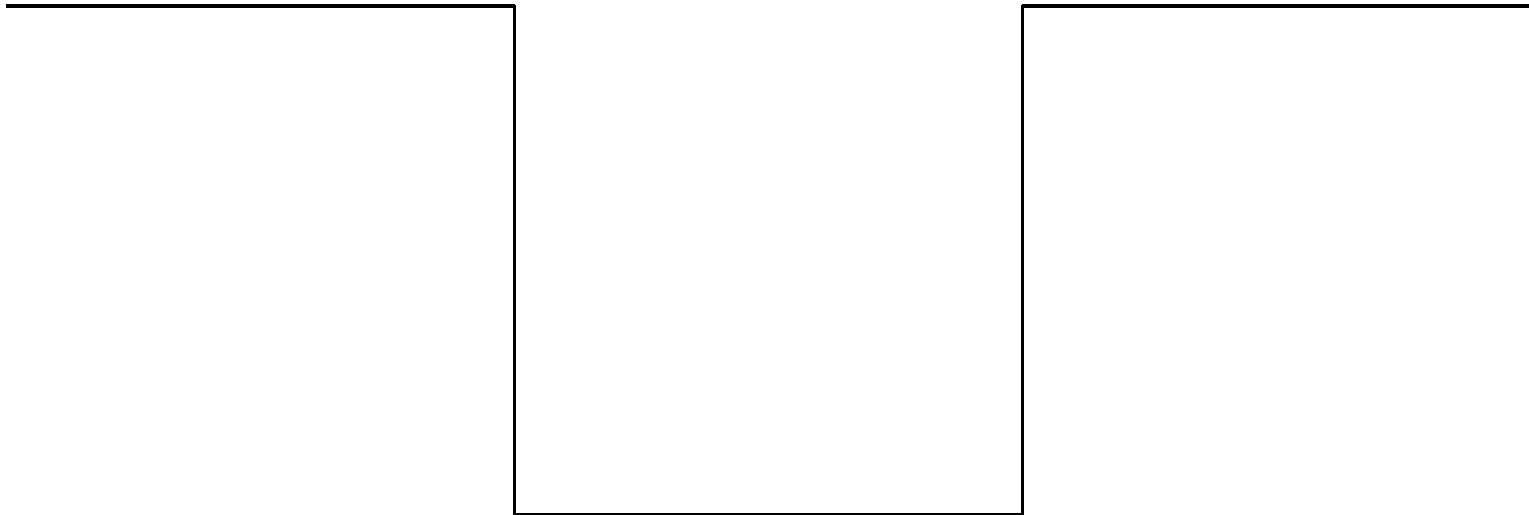
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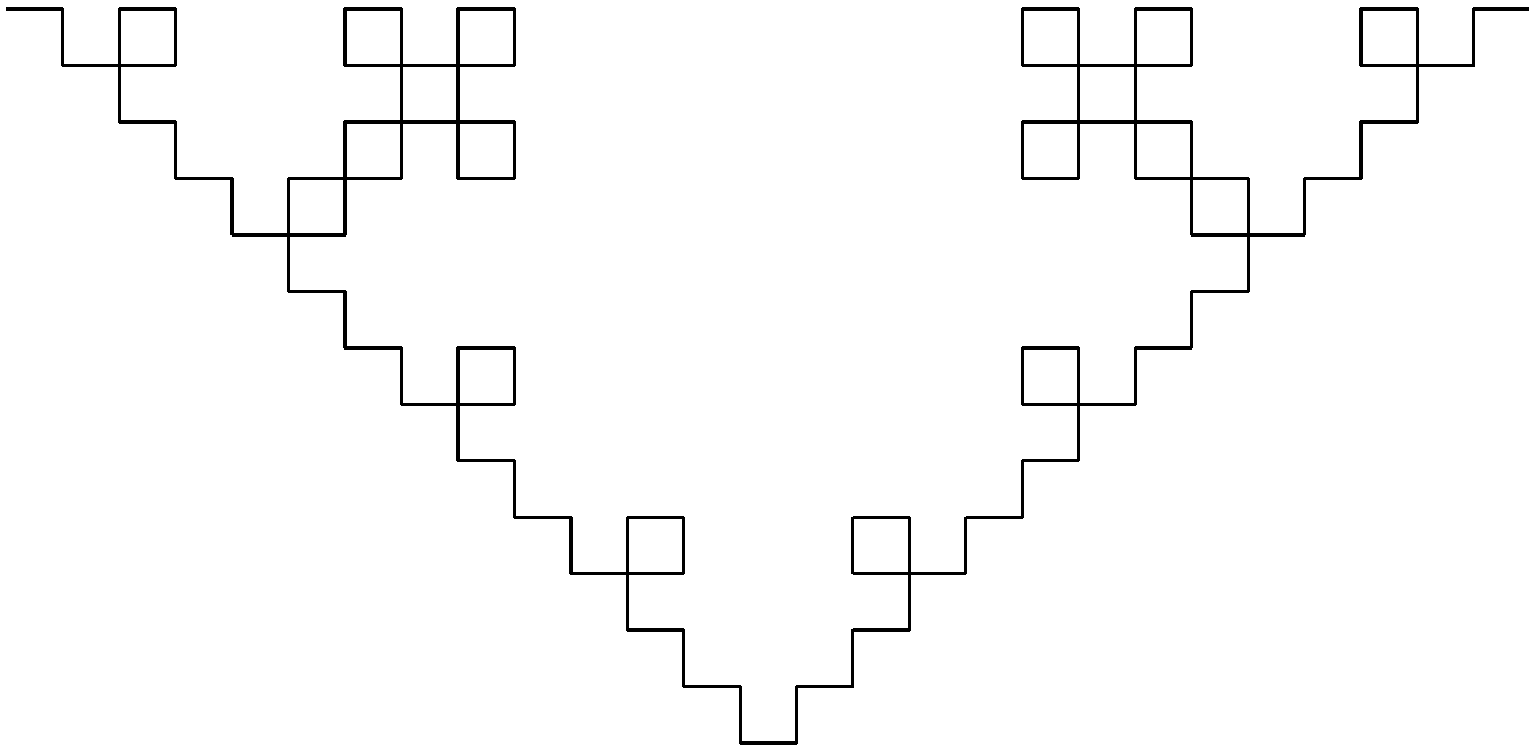
For a smooth surface, there exists a harmonic

measure density $\omega_x(s)$:
$$\omega_x\{A\} = \int_A \omega_x(s) ds$$

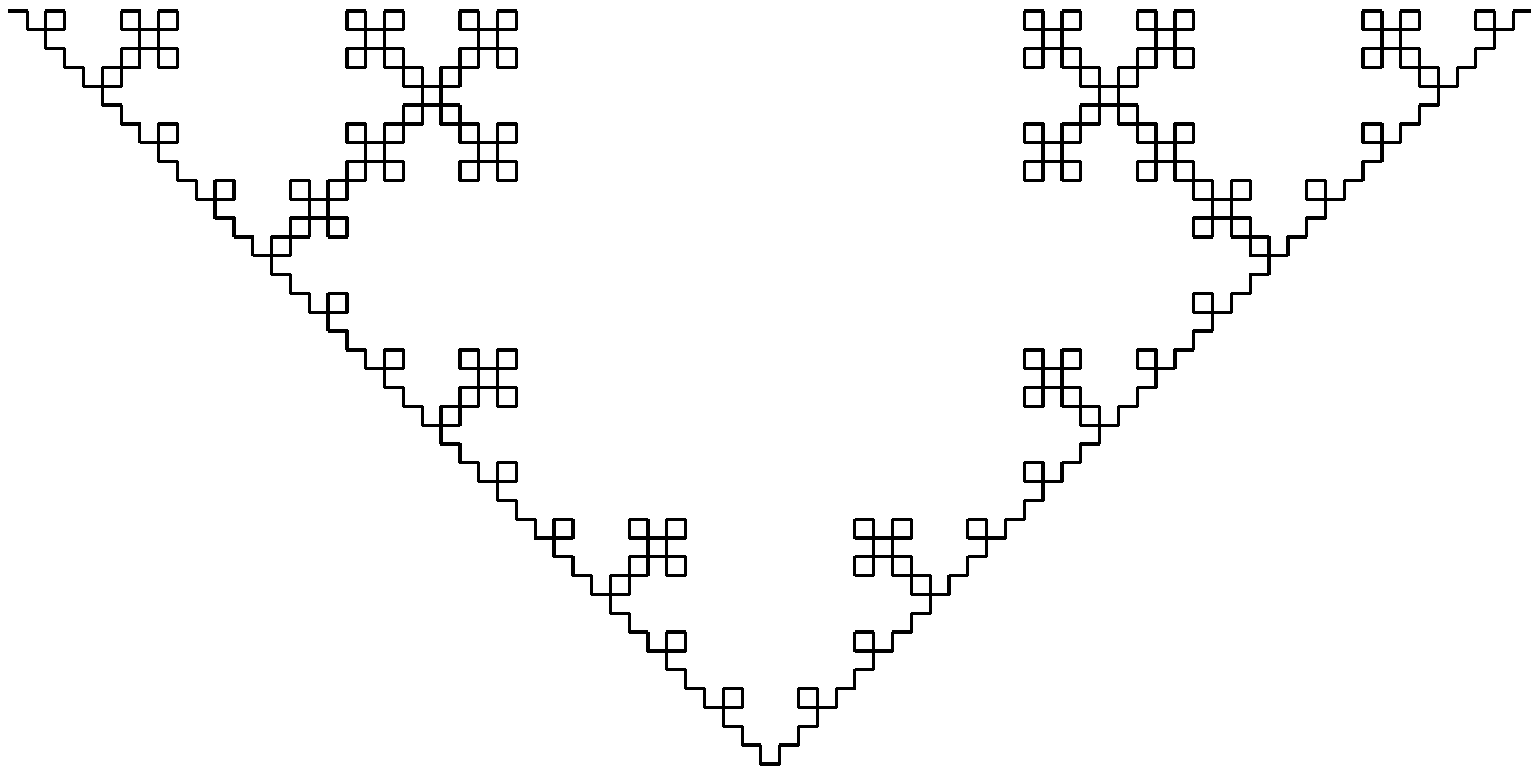
Von Koch boundaries



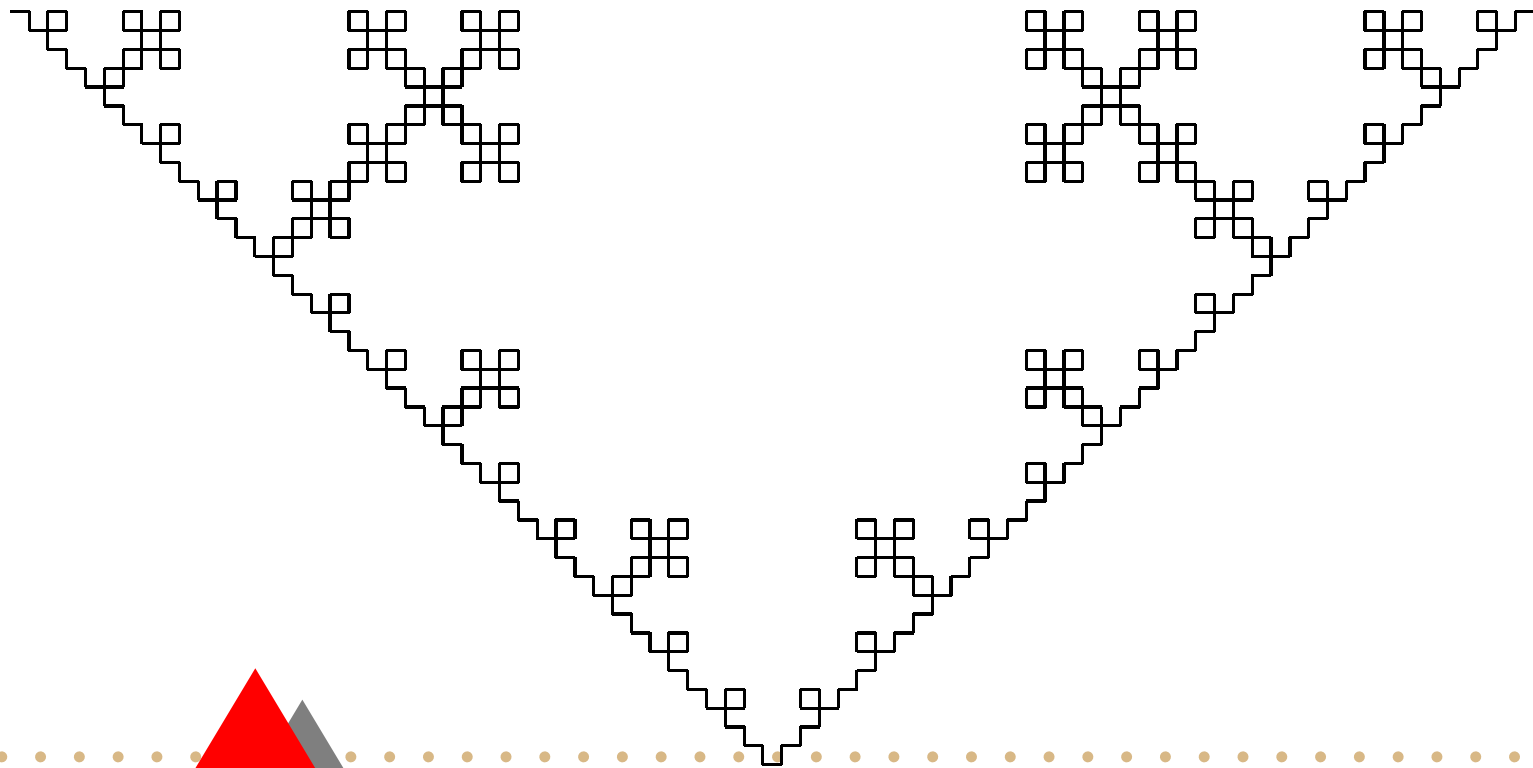
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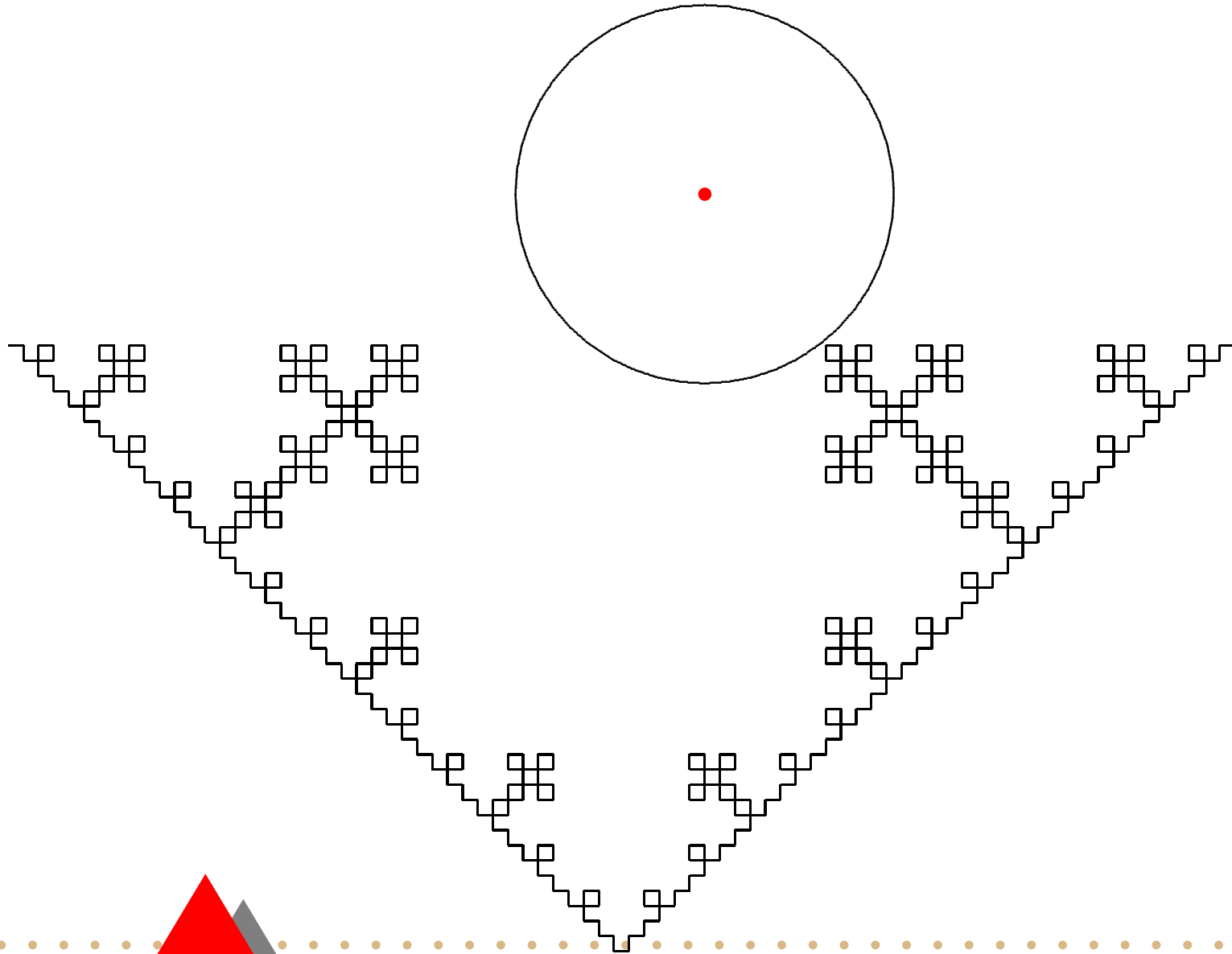


Fast random walks



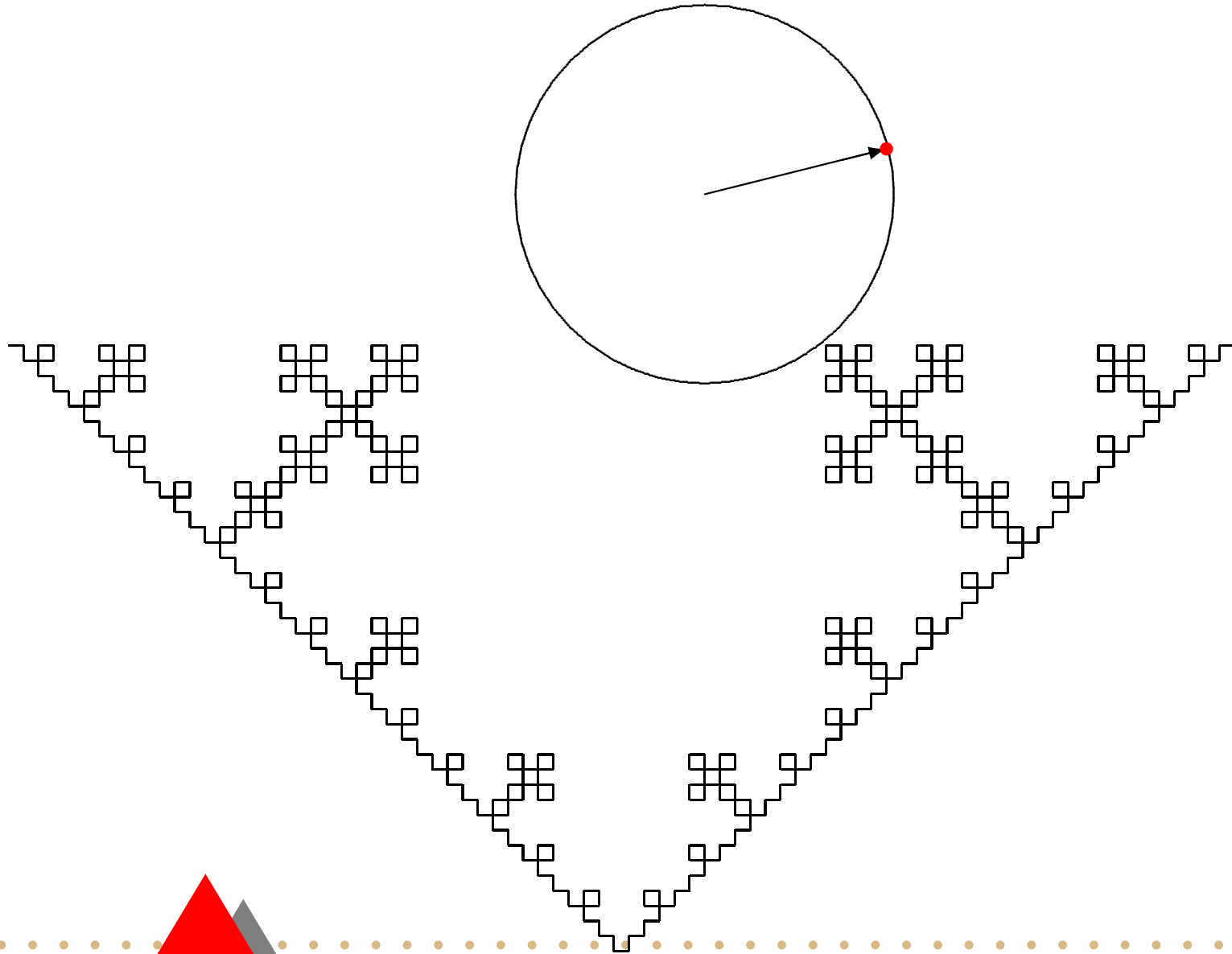
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Fast random walks



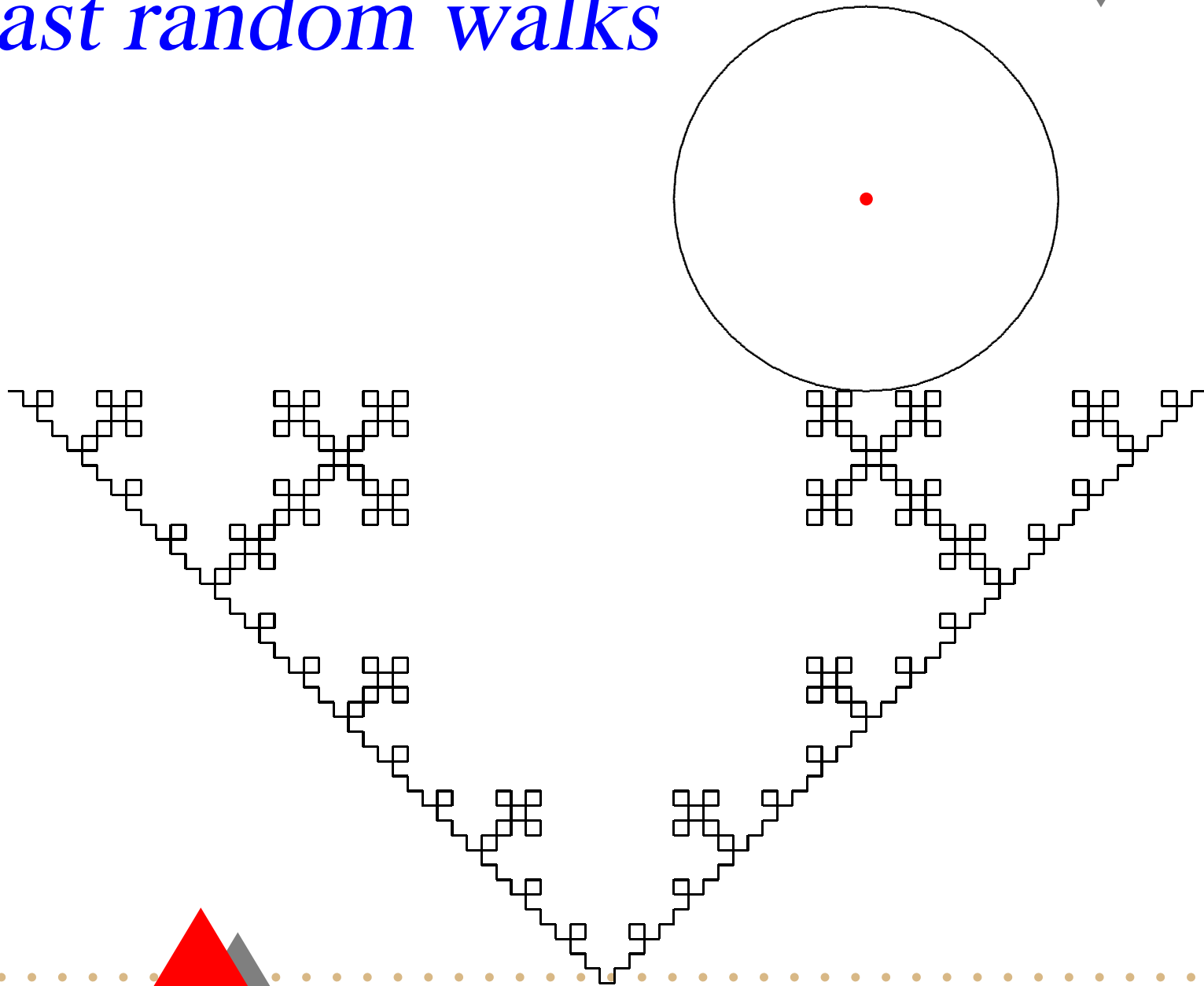
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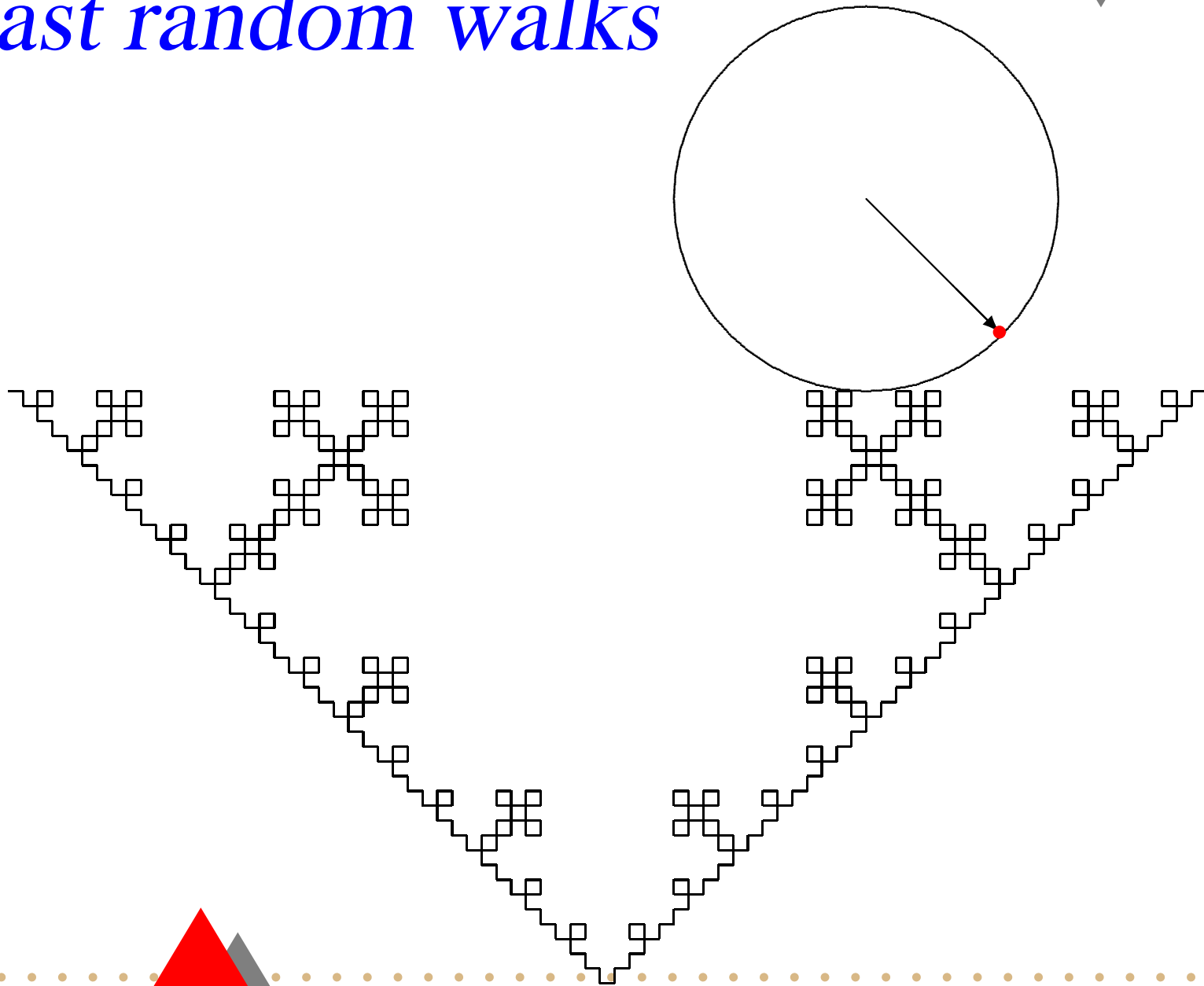
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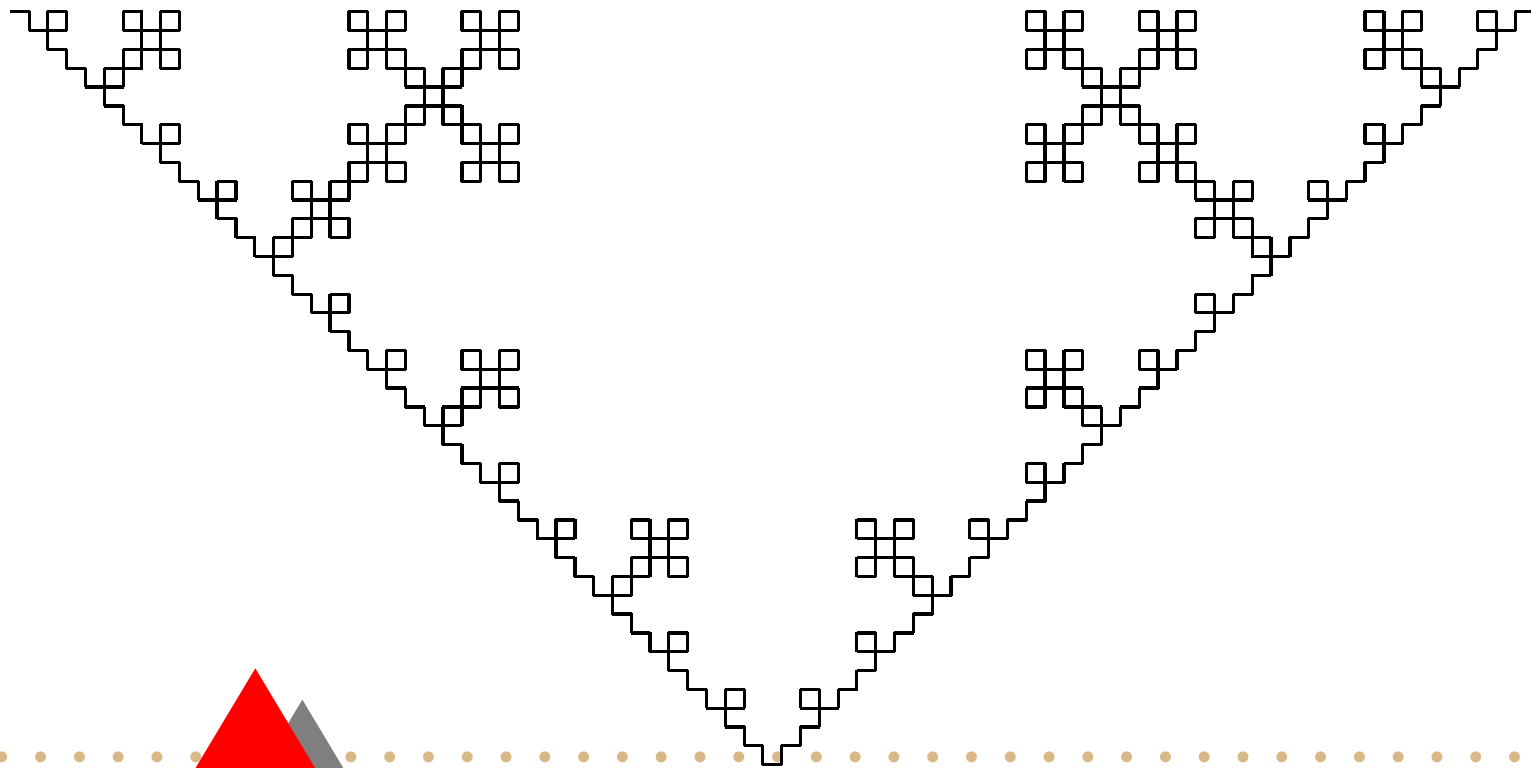
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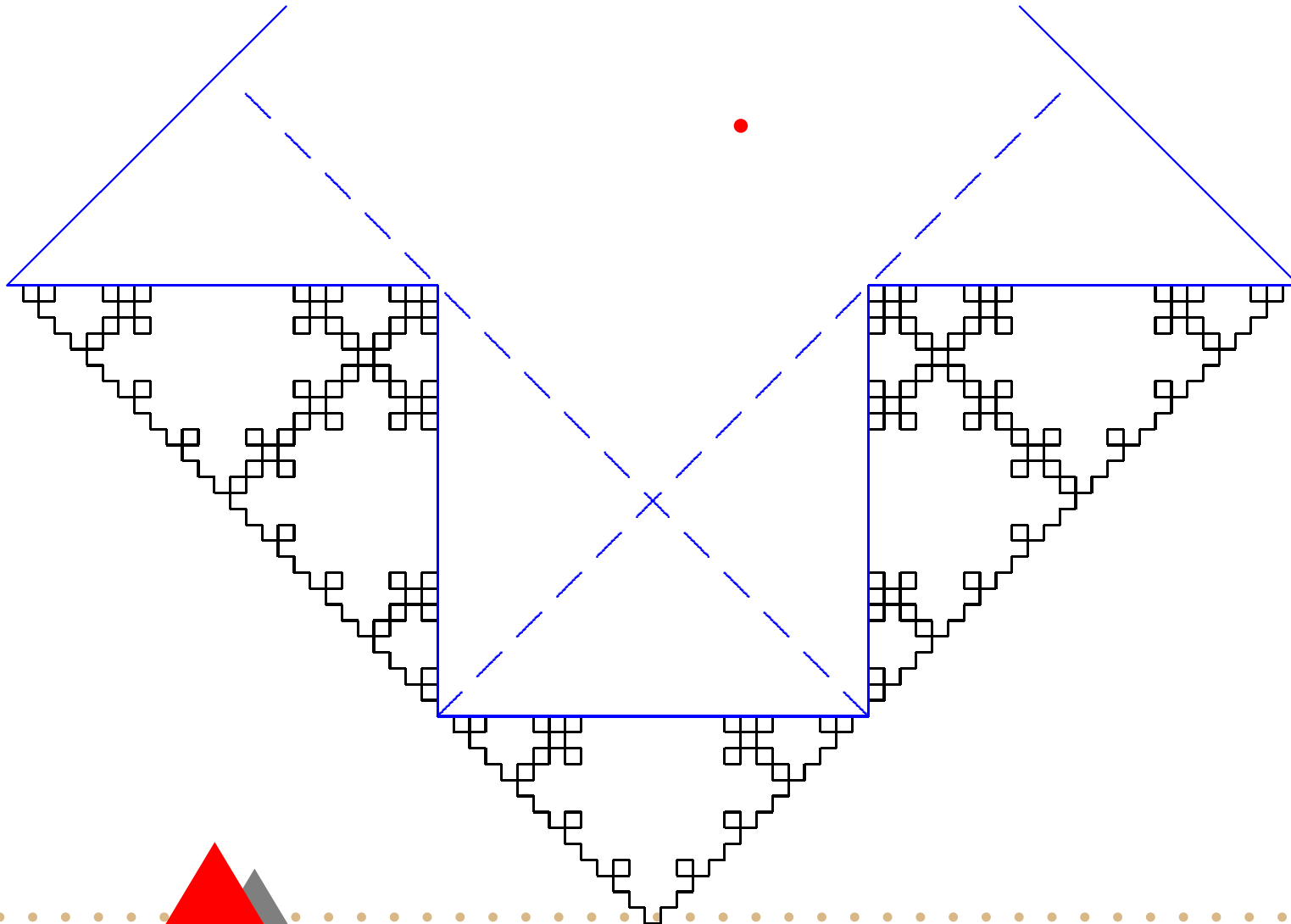
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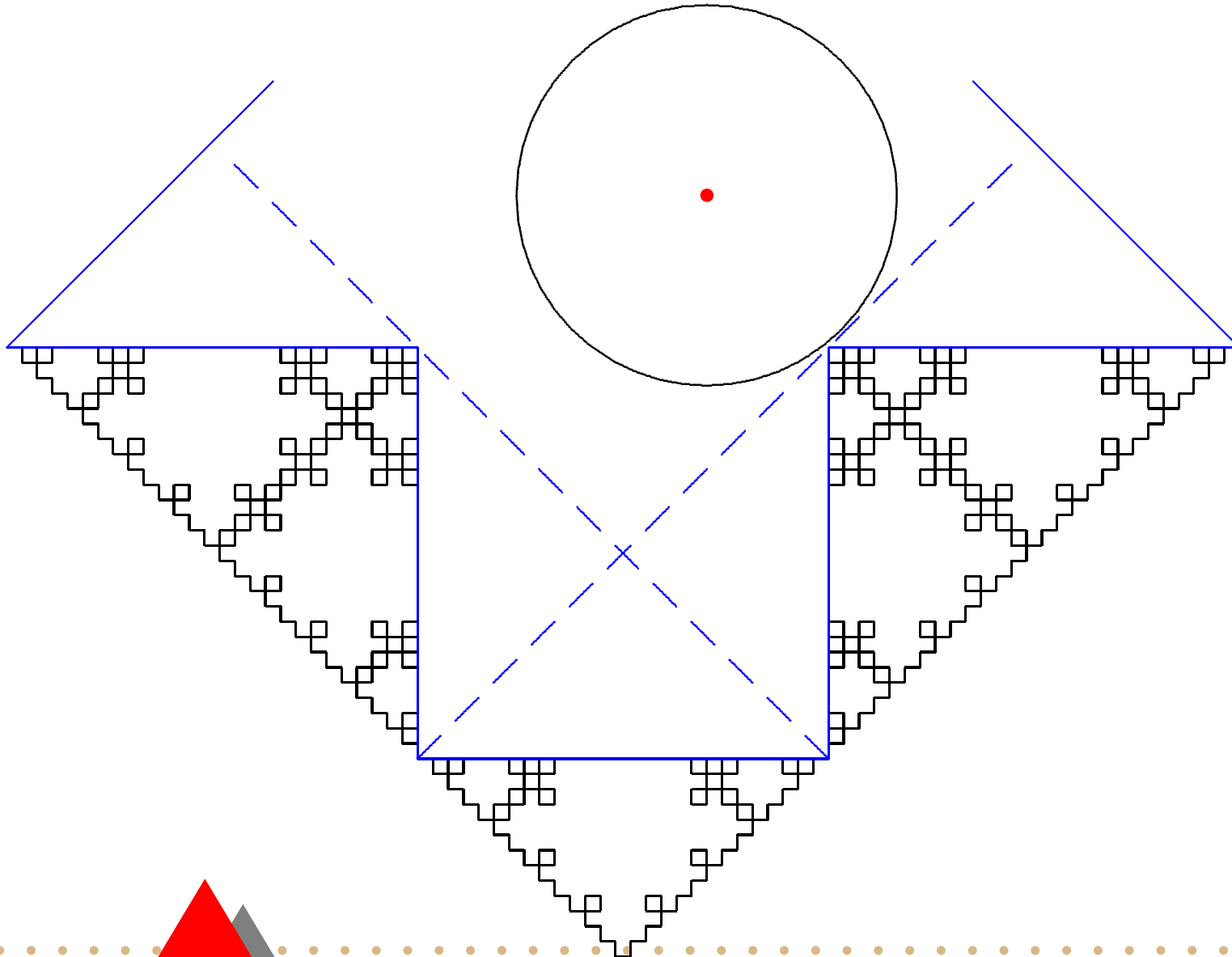
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Calculation of distance



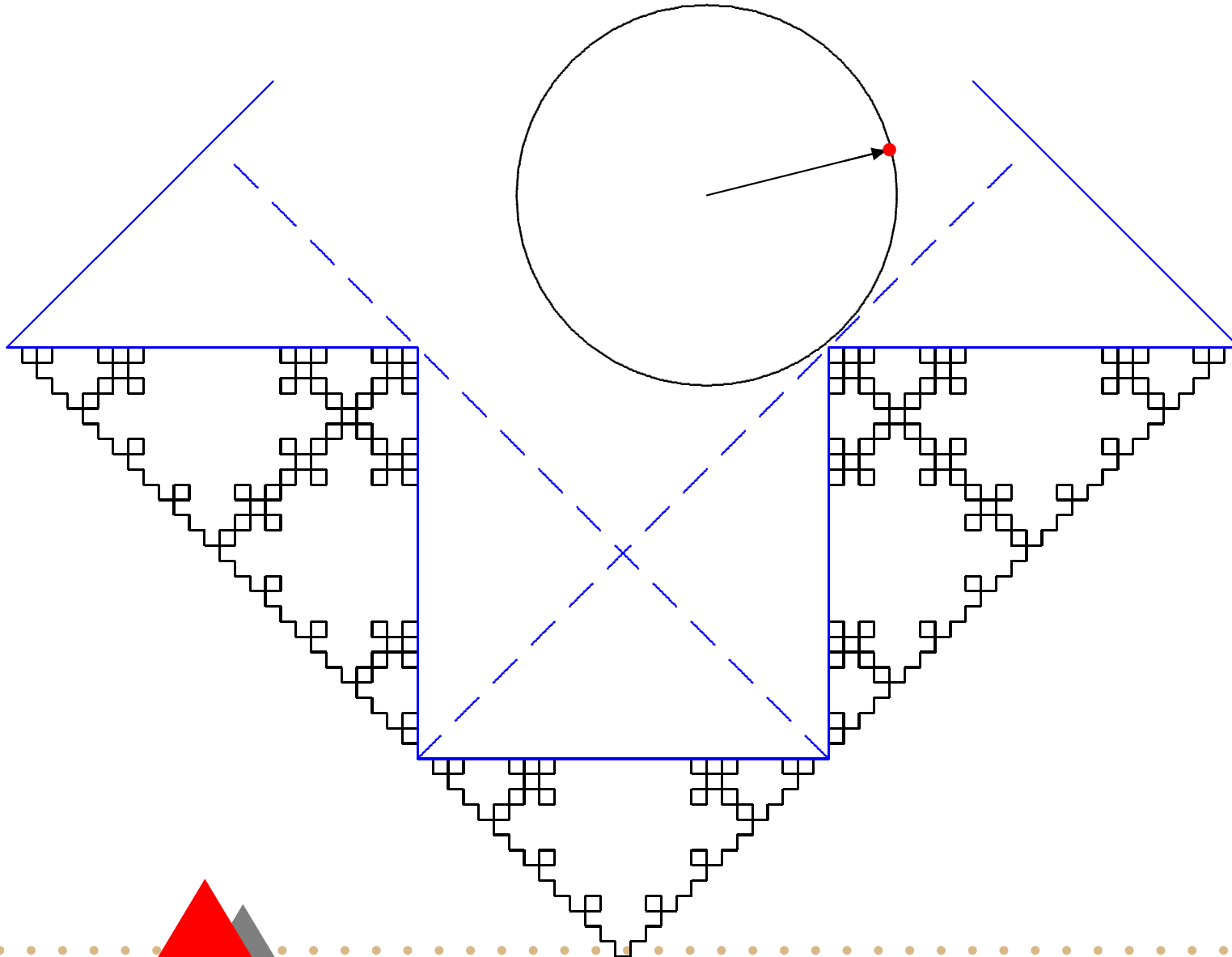
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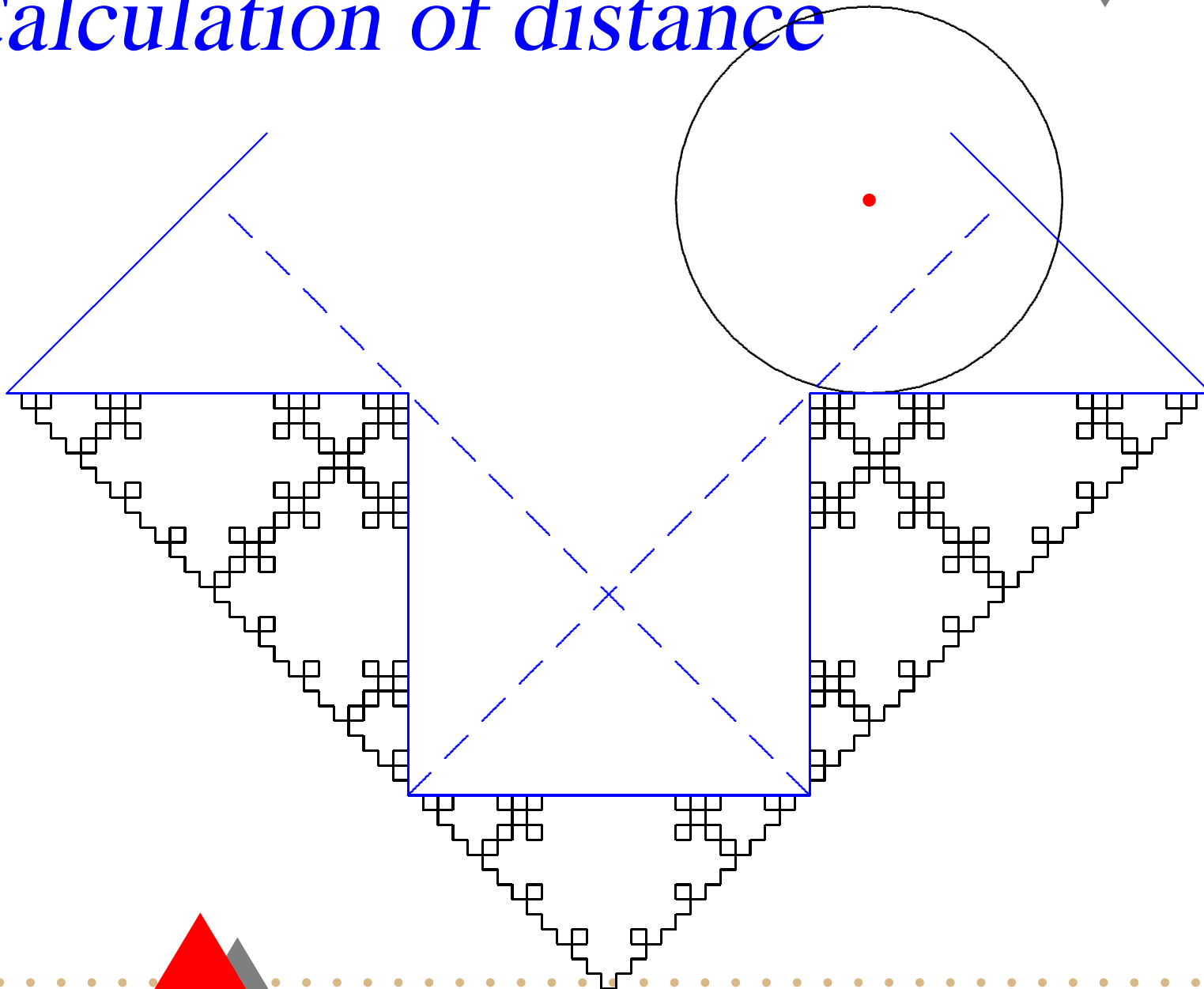
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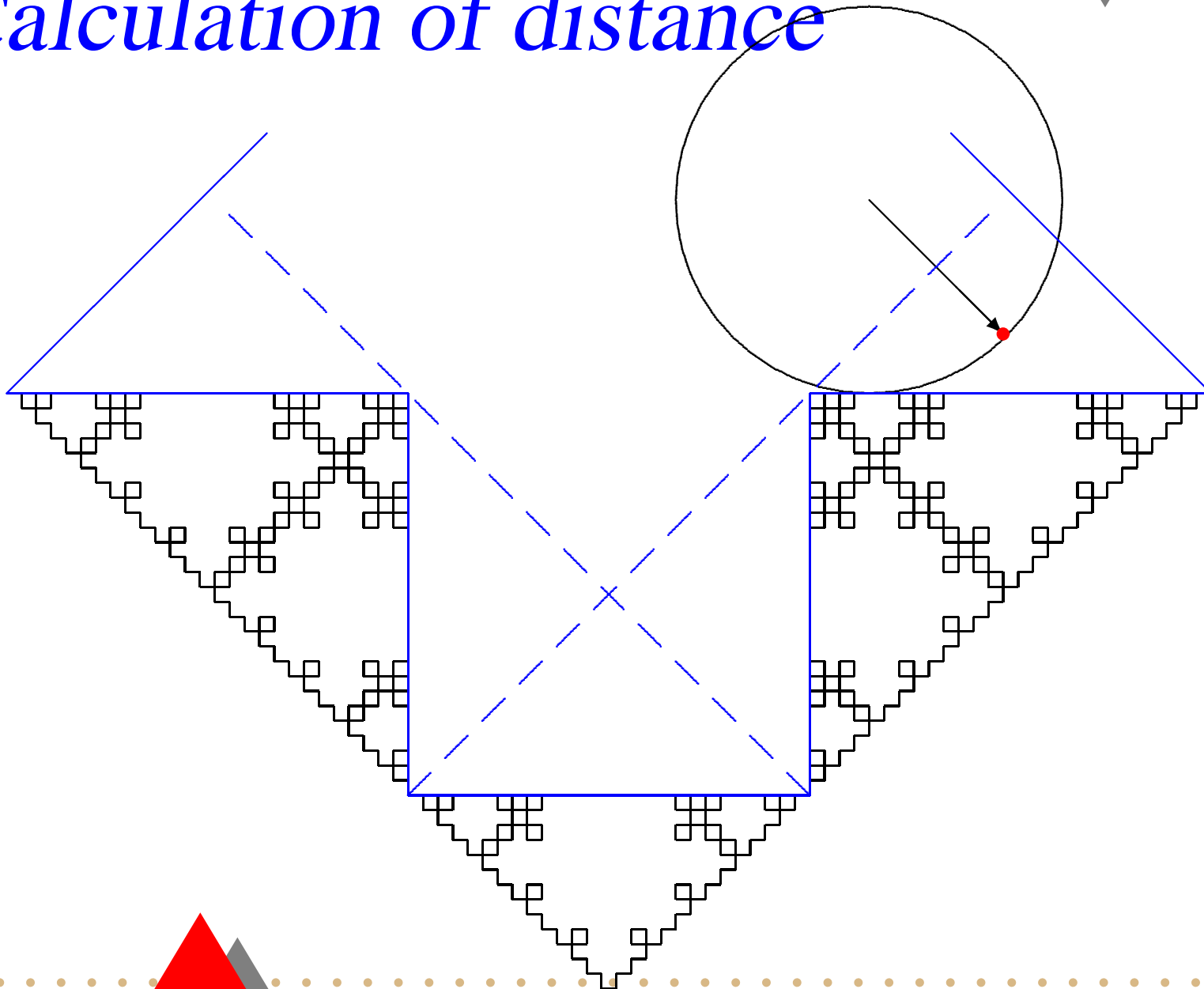
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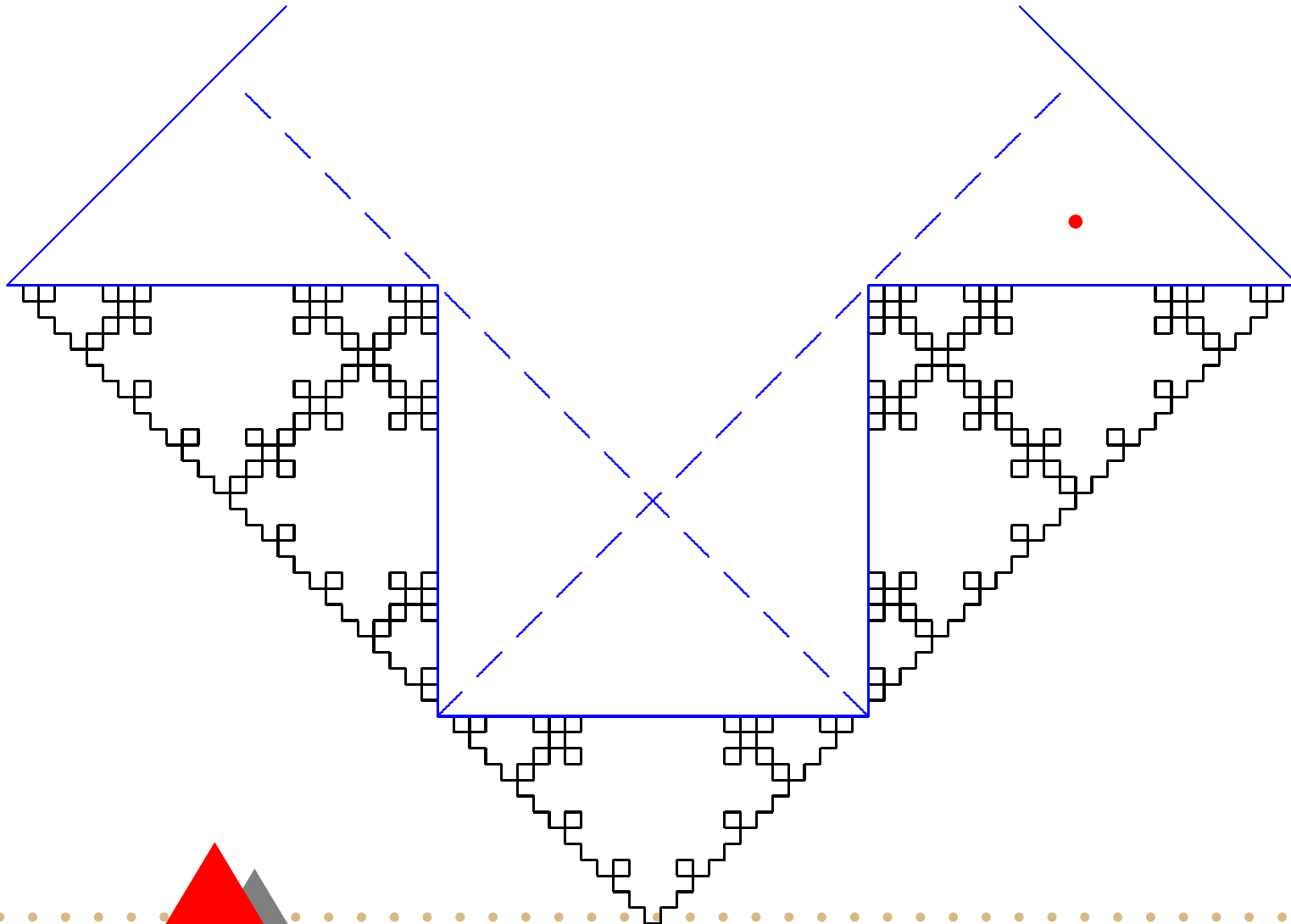
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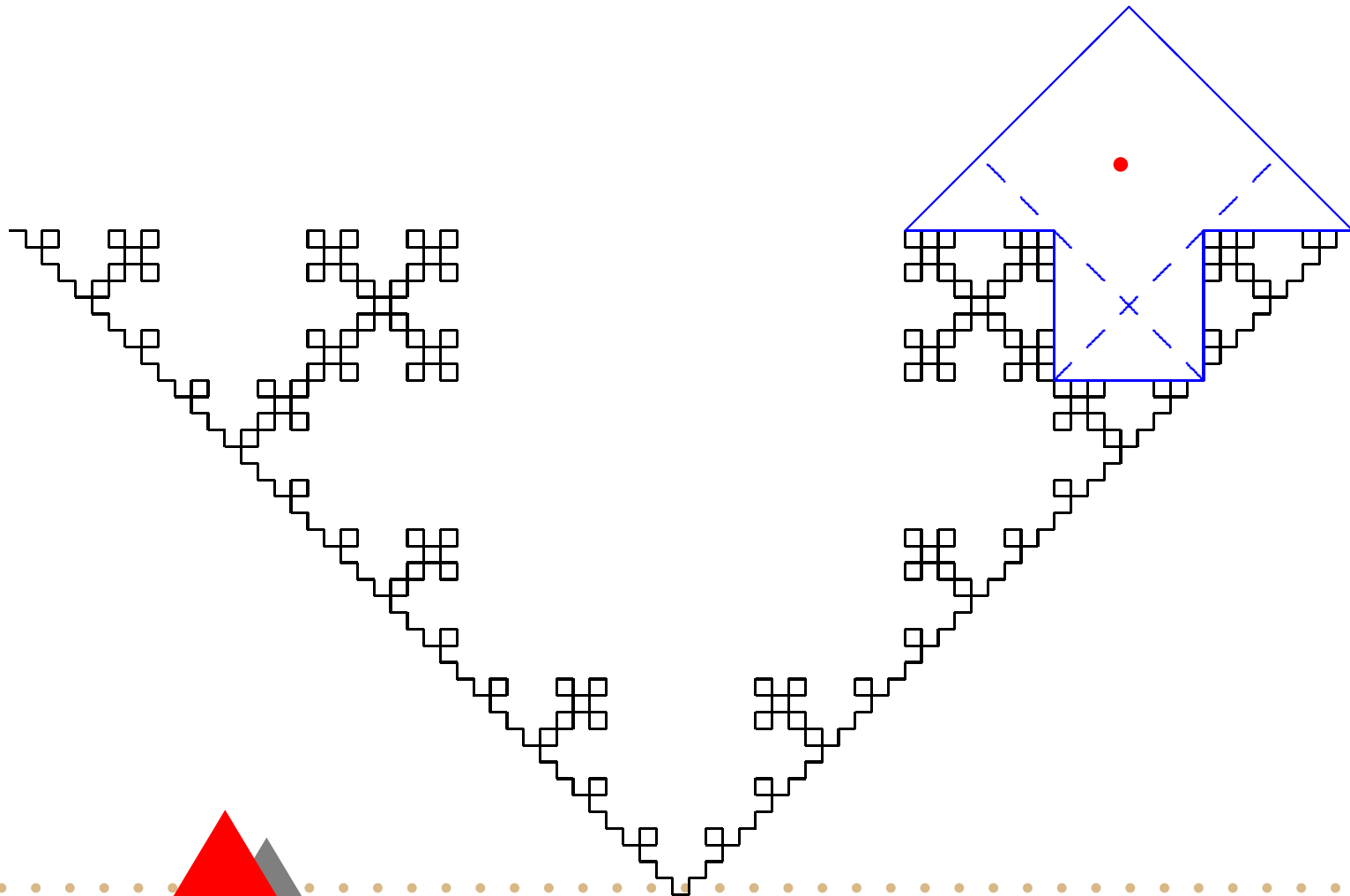
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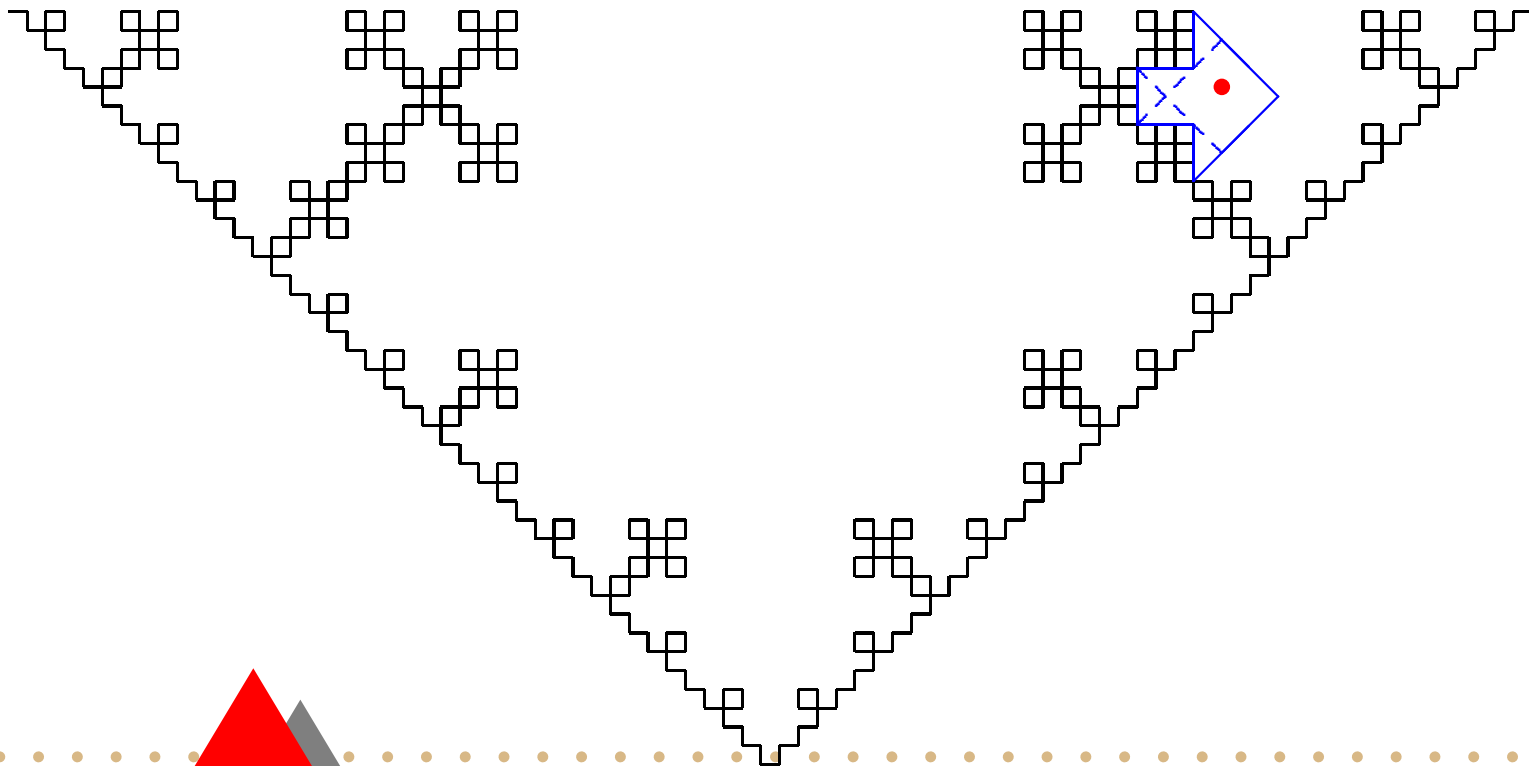
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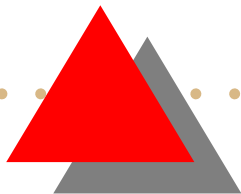
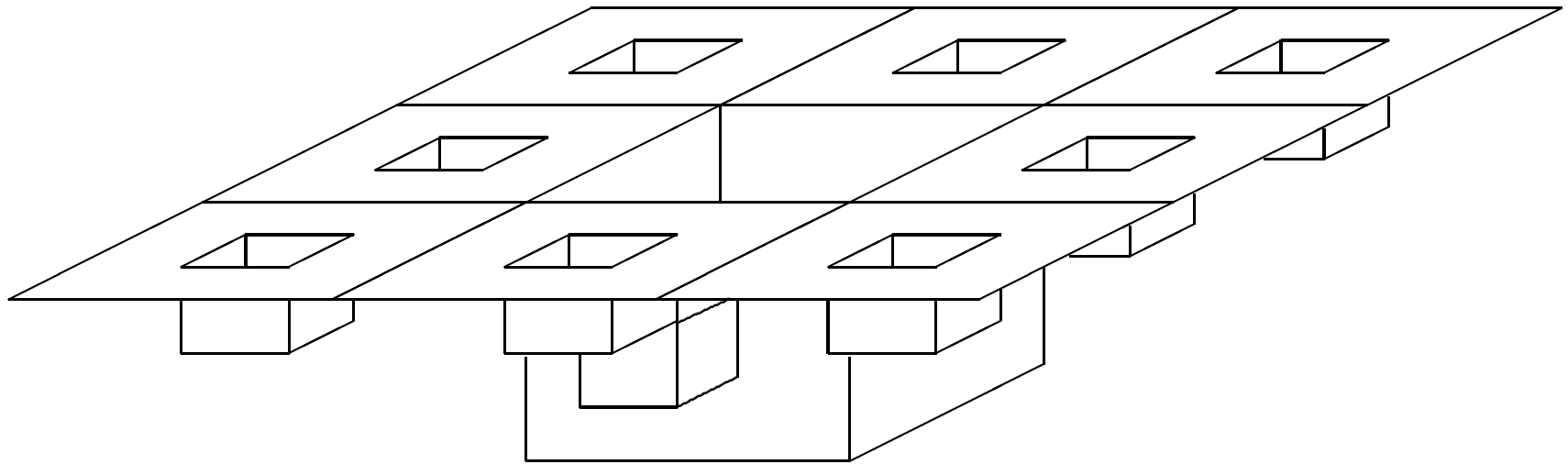
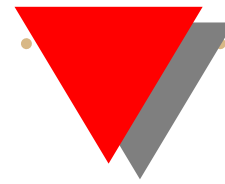
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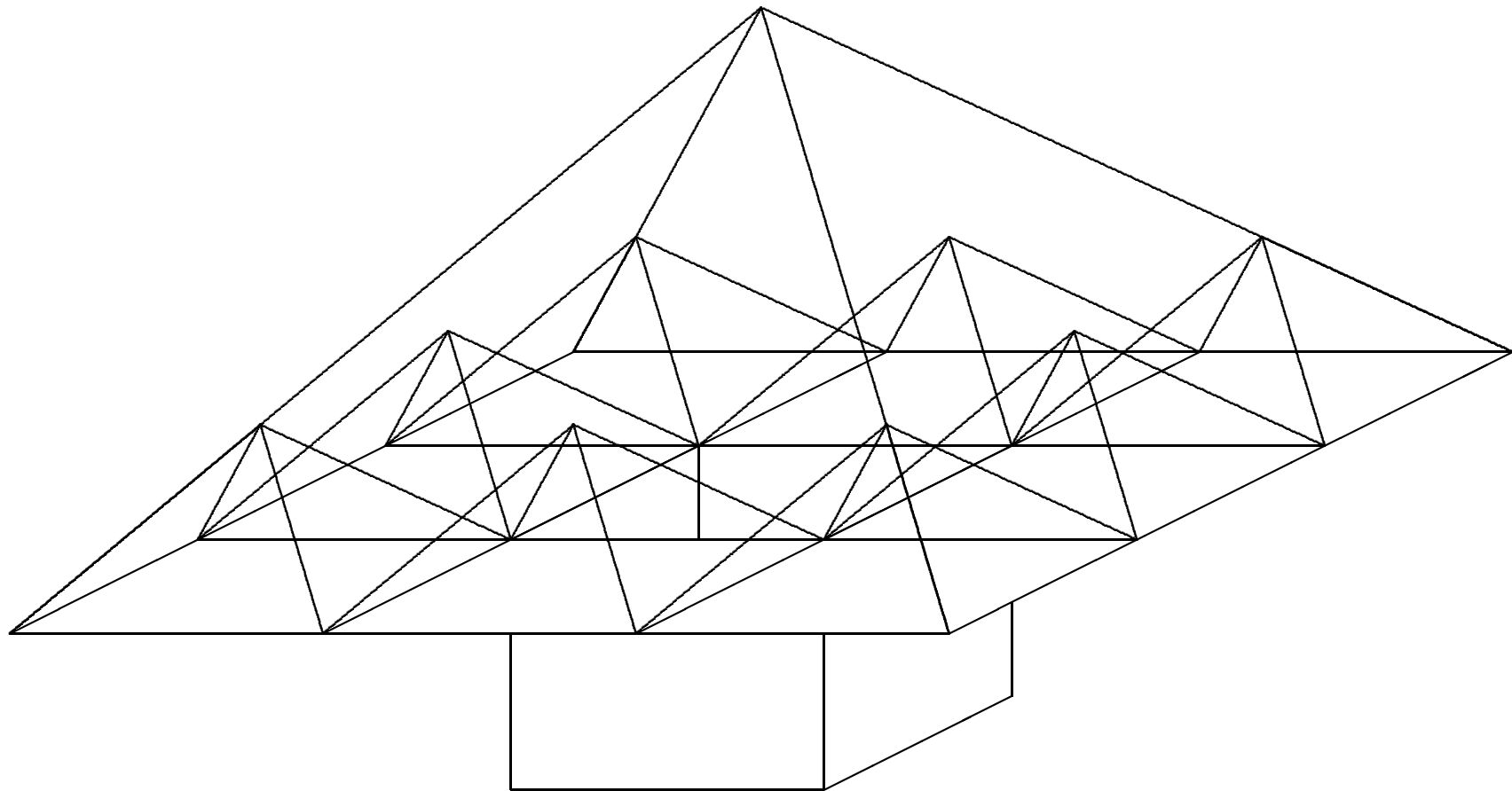


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Realization in 3D



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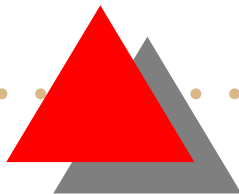
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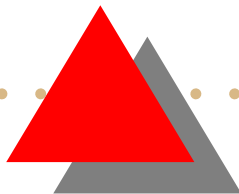
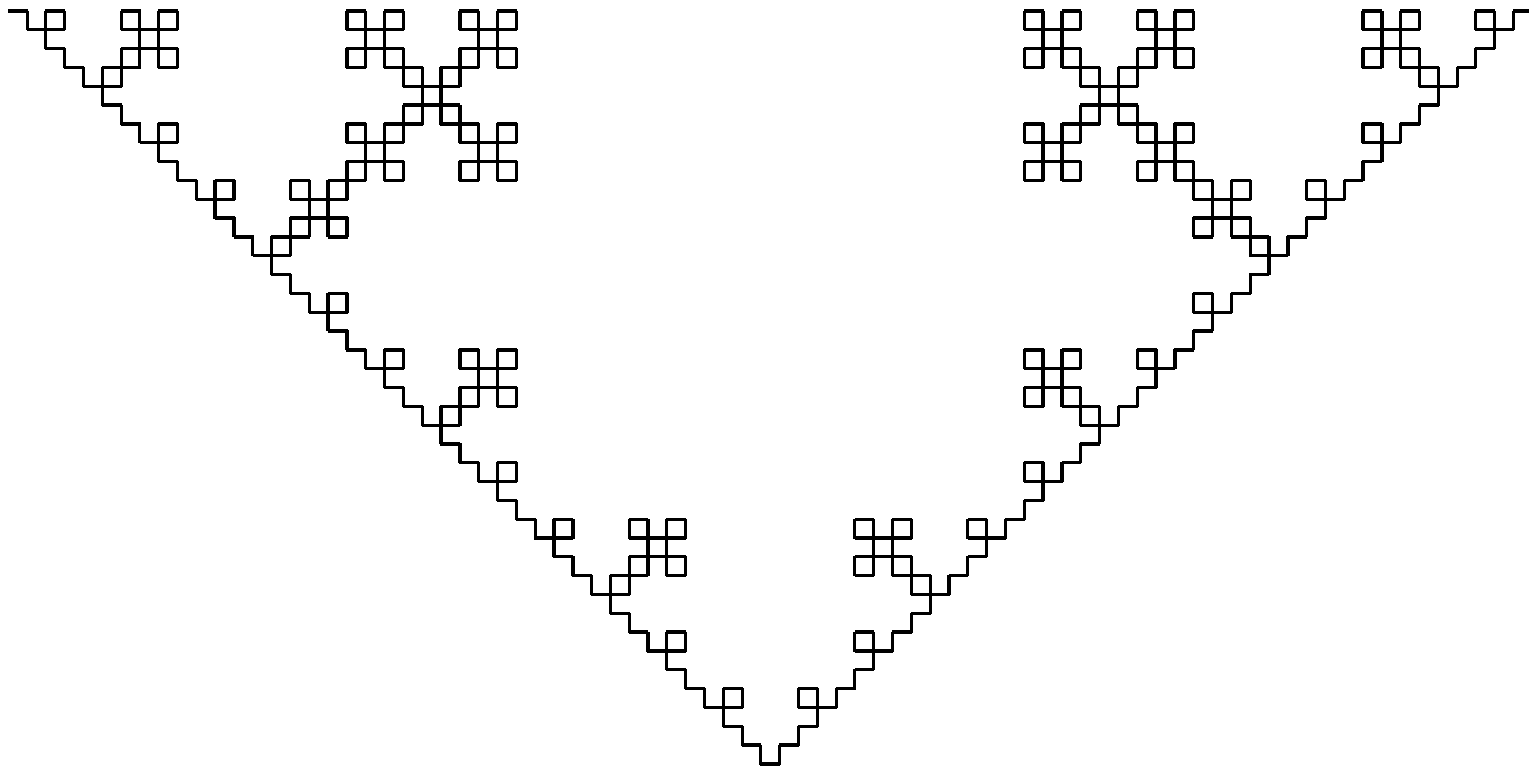
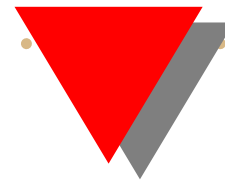
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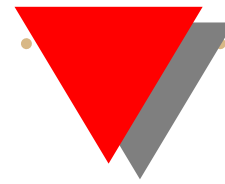
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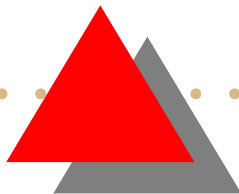
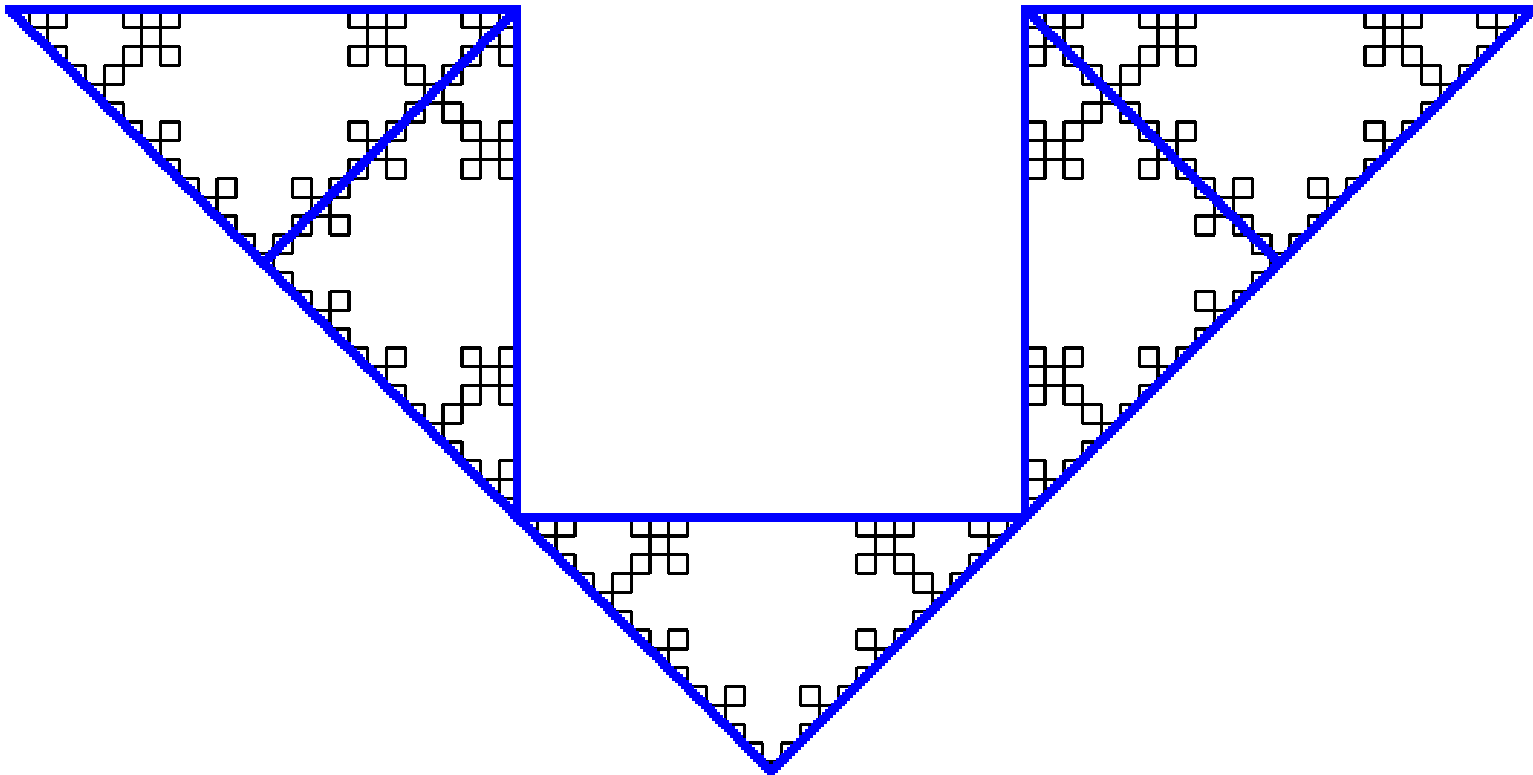
Multifractal analysis: Triangular cover



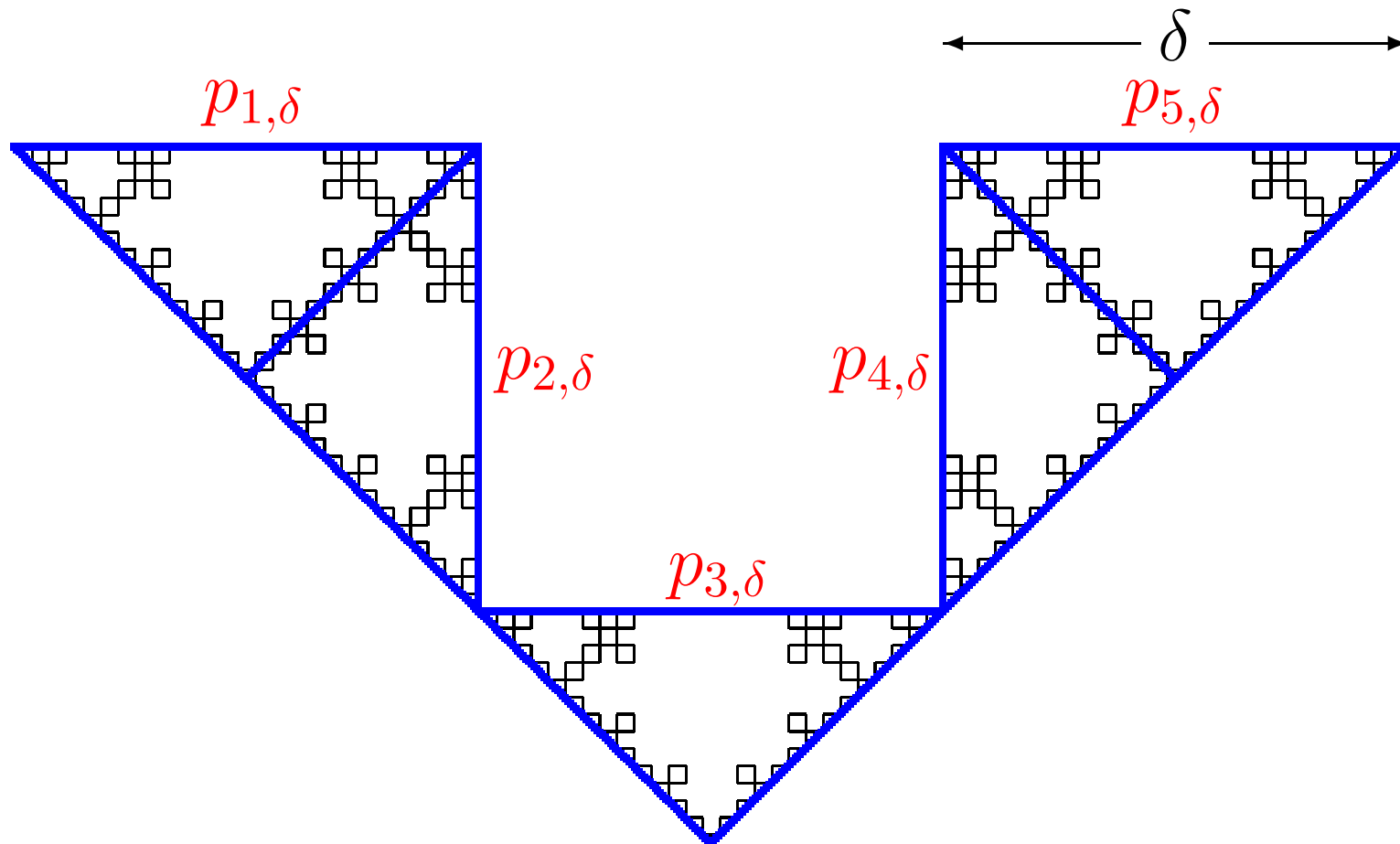
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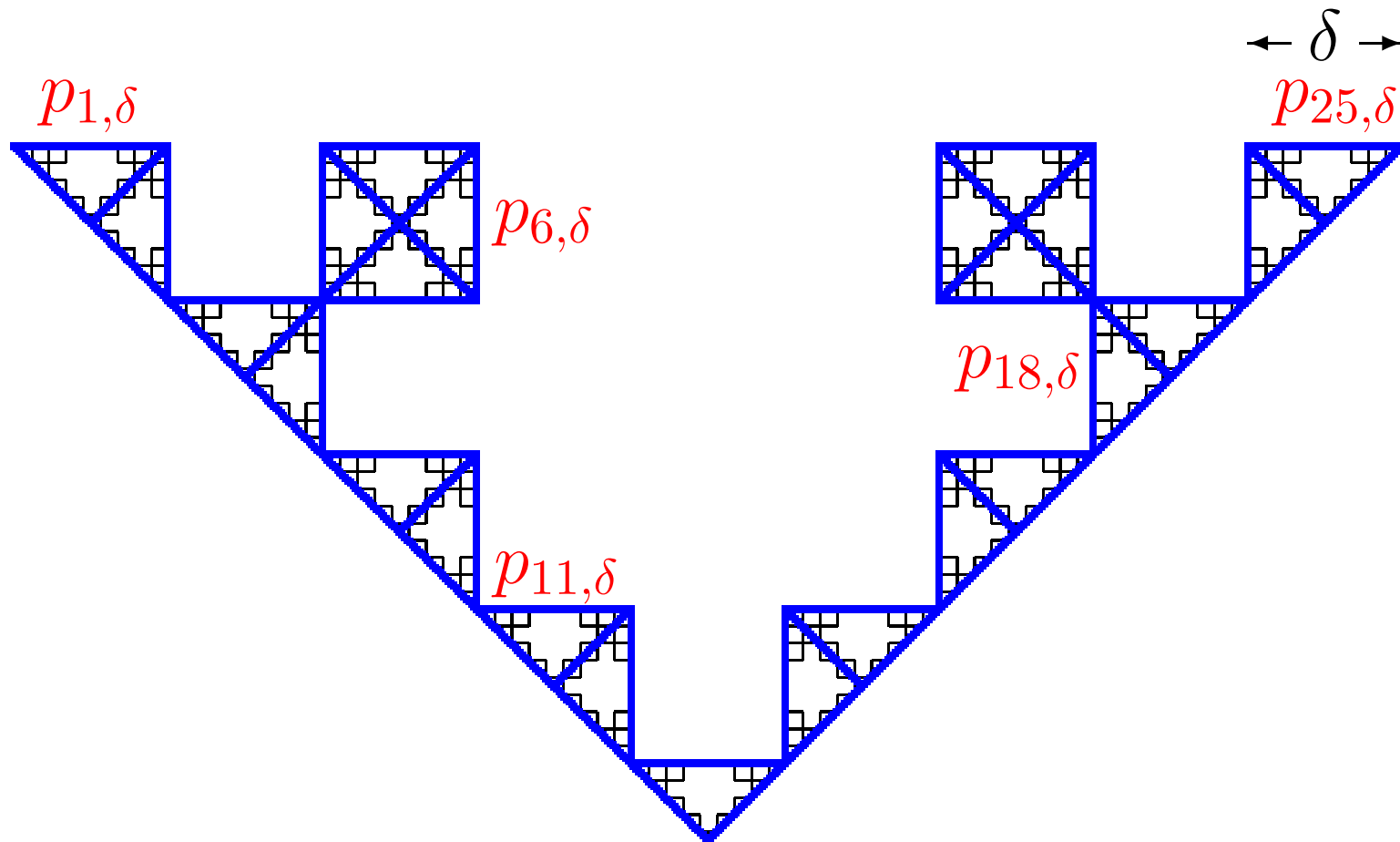
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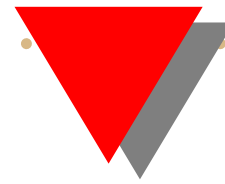
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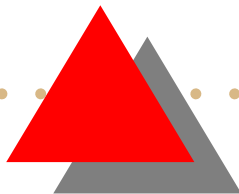
$$D_q = \lim_{\delta \rightarrow 0} D_{q,\delta}$$

Logarithmic development: a smooth boundary

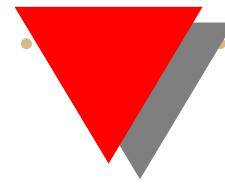


$$p_{k,\delta} \simeq \delta^{d-1} \omega(s_k)$$

$\omega(s)$ is the harmonic
measure density



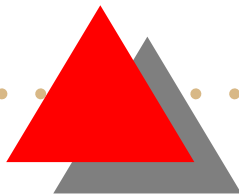
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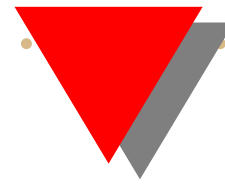
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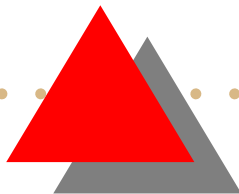
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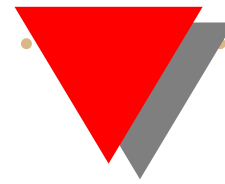
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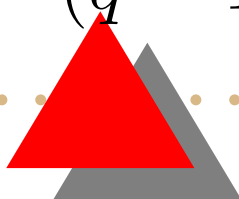


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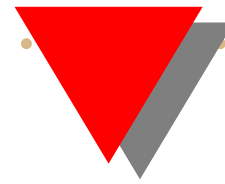
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Grebenkov, Lebedev, Filoche, Sapoval, Phys. Rev. E 71, 056121 (2005)

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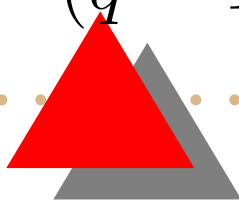


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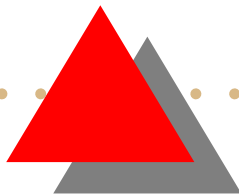


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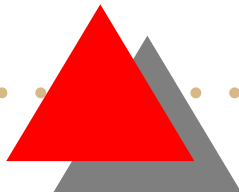


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Logarithmic development: application to fractals

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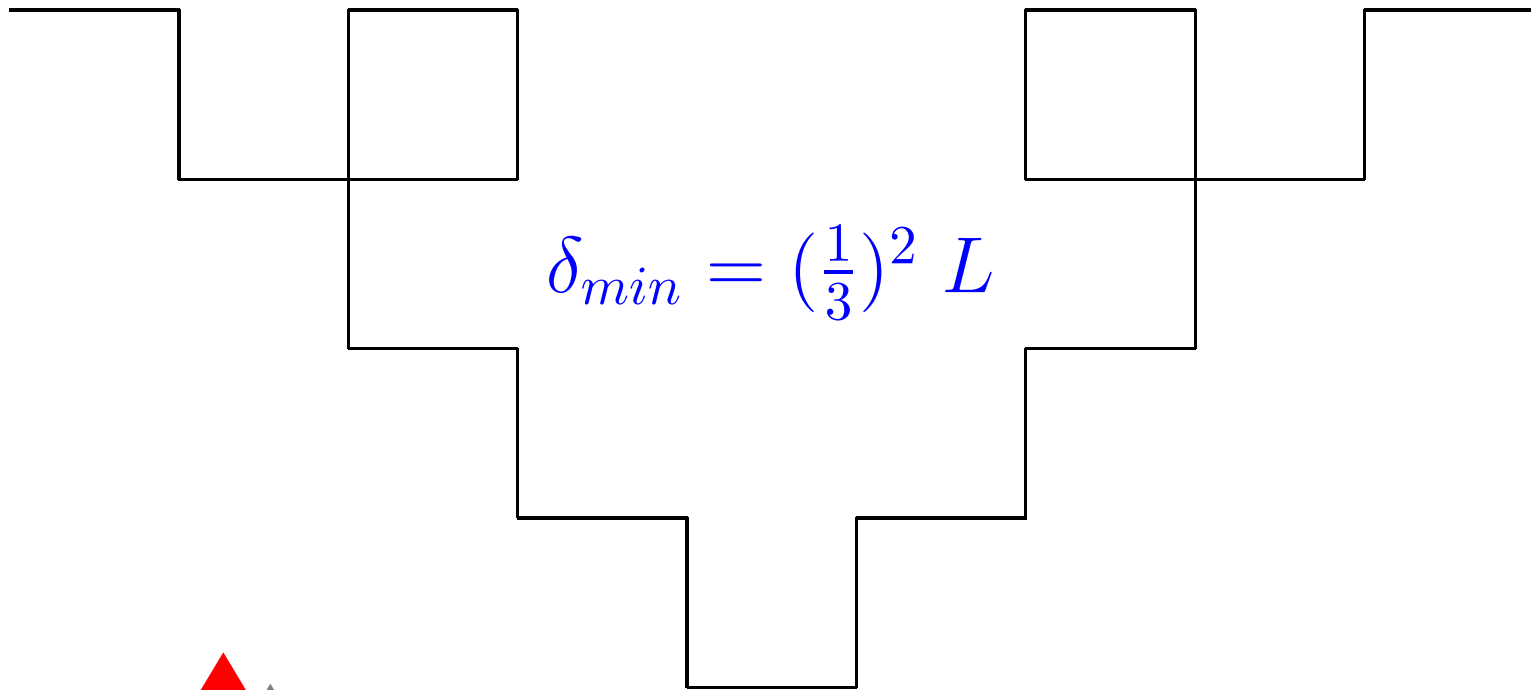
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$$\delta_{min} = \left(\frac{1}{3}\right) L$$

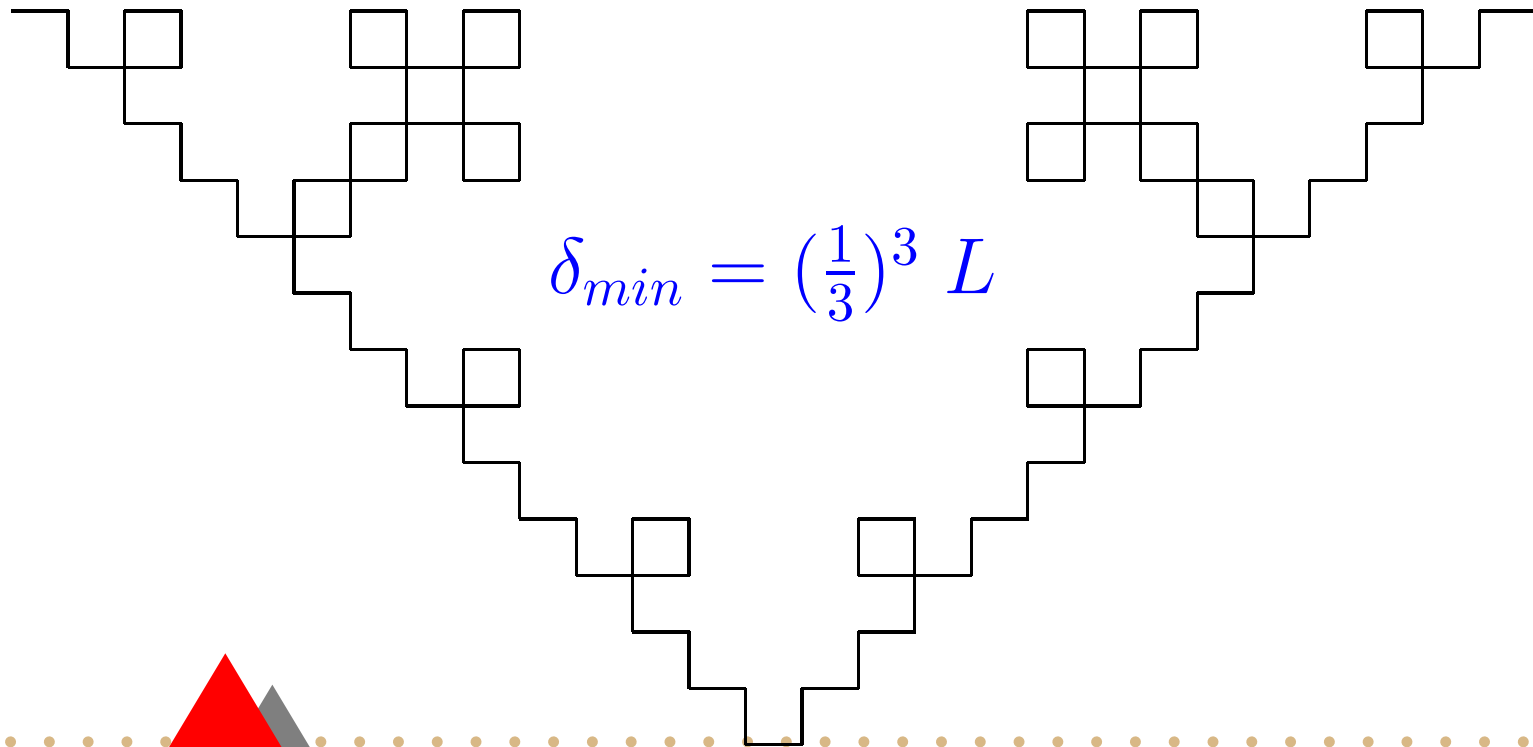
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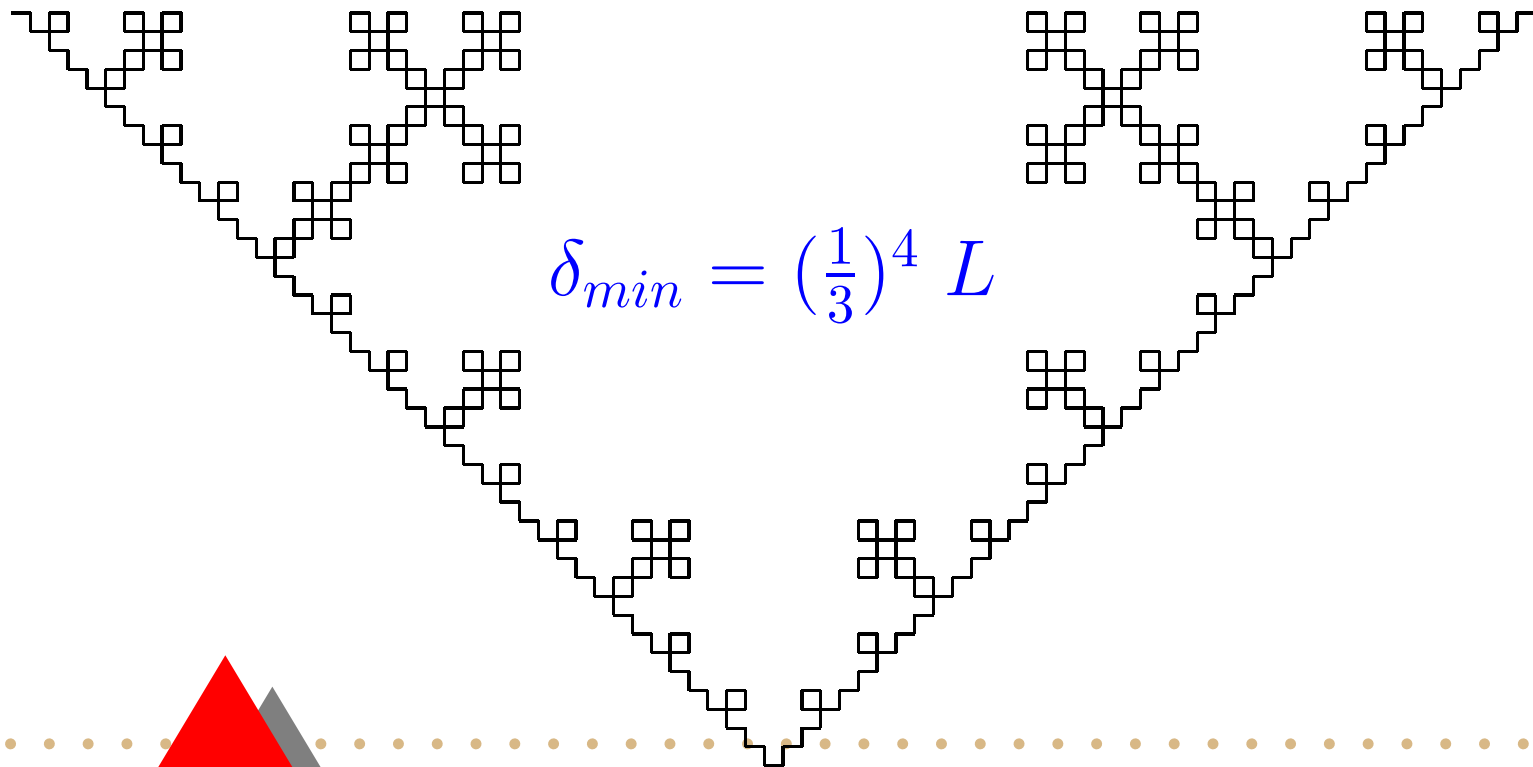
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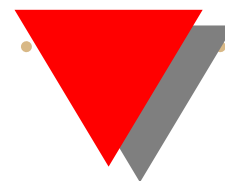
Quadratic Von Koch curve

	$g = 5$
$D_{1,\delta}$	1.0345
$D_{2,\delta}$	0.9263

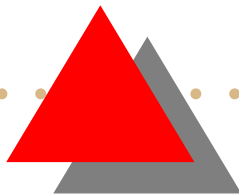
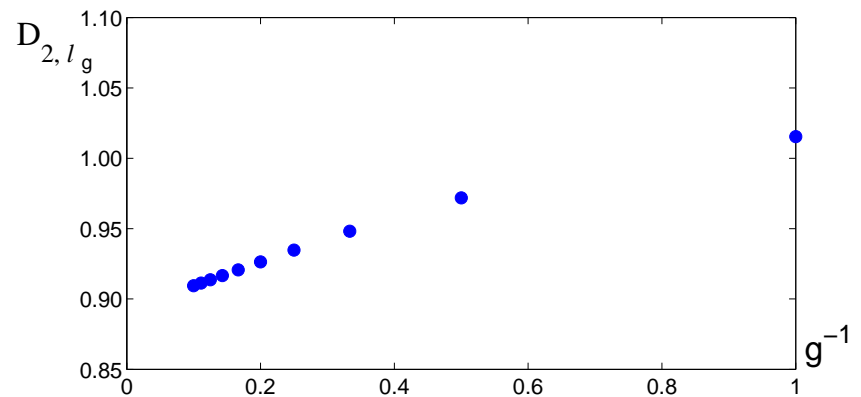
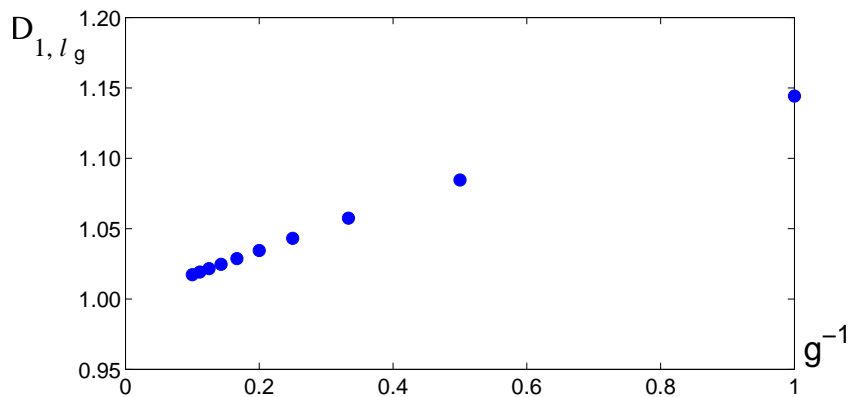
Quadratic Von Koch curve

	$g = 5$	$g = 6$	$g = 7$	$g = 8$	$g = 9$	$g = 10$
$D_{1,\delta}$	1.0345	1.0287	1.0246	1.0215	1.0191	1.0172
$D_{2,\delta}$	0.9263	0.9207	0.9166	0.9136	0.9113	0.9094

Quadratic Von Koch curve



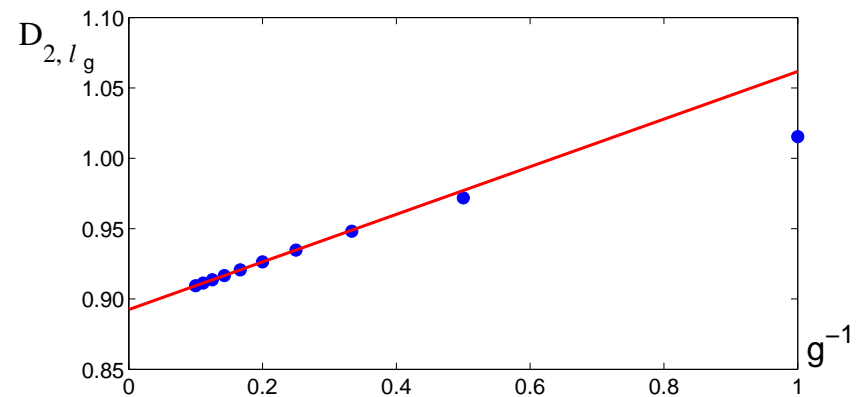
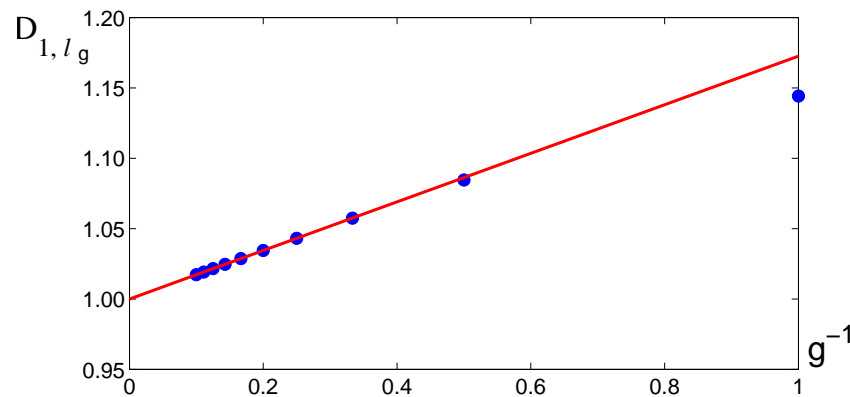
	$g = 5$	$g = 6$	$g = 7$	$g = 8$	$g = 9$	$g = 10$
$D_{1,\delta}$	1.0345	1.0287	1.0246	1.0215	1.0191	1.0172
$D_{2,\delta}$	0.9263	0.9207	0.9166	0.9136	0.9113	0.9094



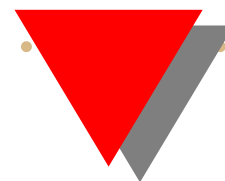
Grebenkov, Lebedev, Filoche, Sapoval, Phys. Rev. E 71, 056121 (2005)

Quadratic Von Koch curve

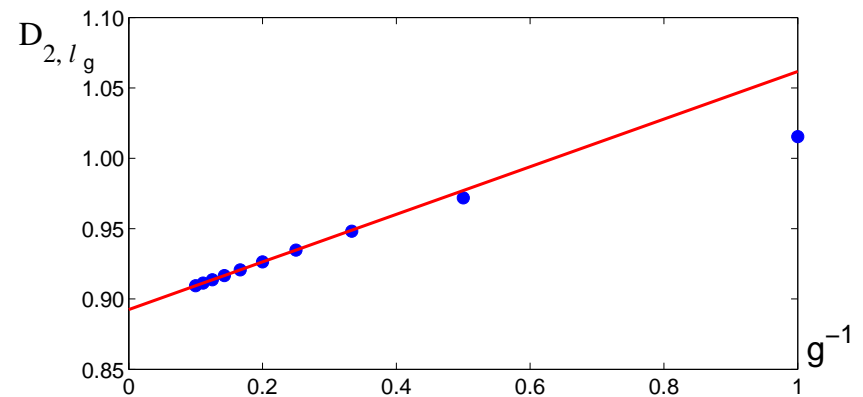
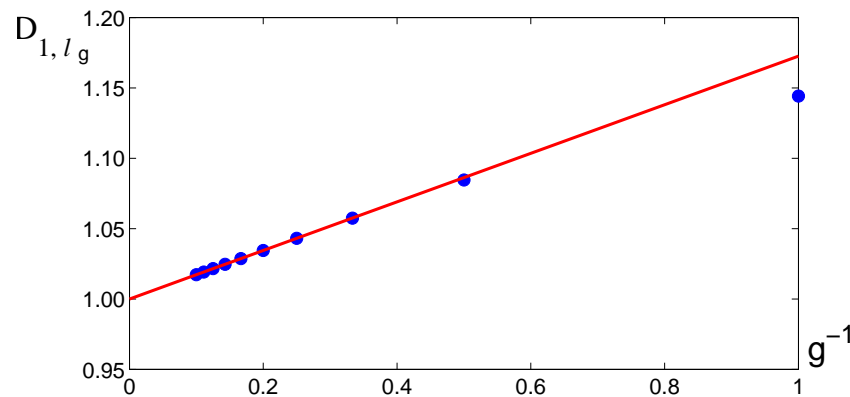
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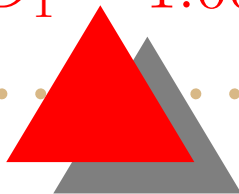


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$$D_1 = 1.0000 \pm 0.0003$$

$$D_2 = 0.8925 \pm 0.0007$$



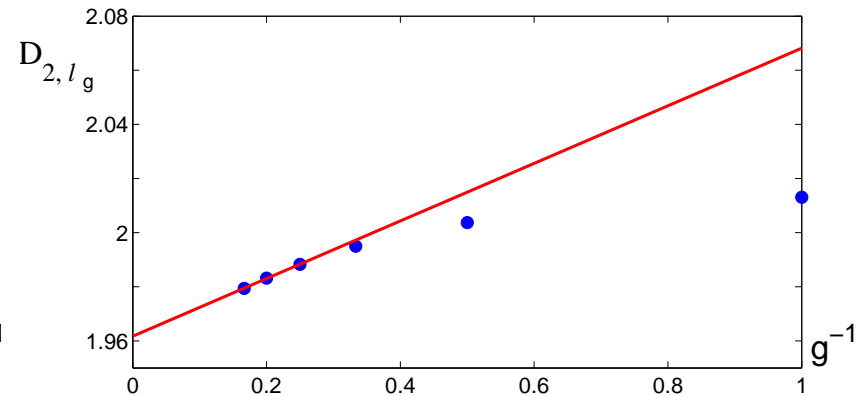
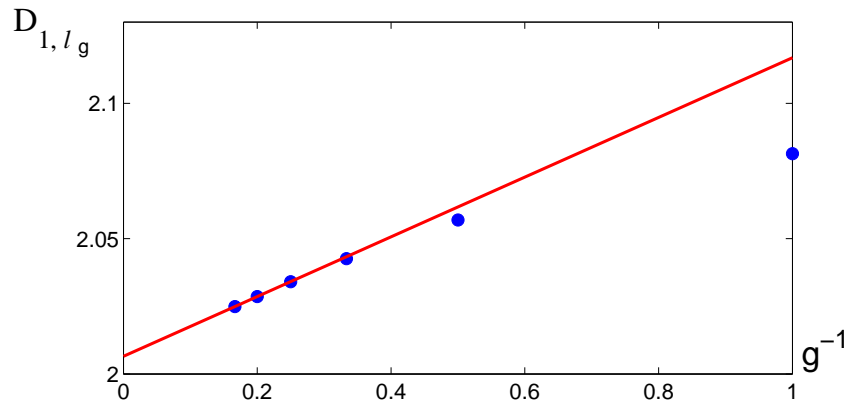
Grebenkov, Lebedev, Filoche, Sapoval, Phys. Rev. E 71, 056121 (2005)

Cubic Von Koch surface

	$g = 1$	$g = 2$	$g = 3$	$g = 4$	$g = 5$	$g = 6$
$D_{1,\delta}$	2.0815	2.0569	2.0426	2.0341	2.0286	2.0249
$D_{2,\delta}$	2.0132	2.0038	1.9951	1.9883	1.9832	1.9794

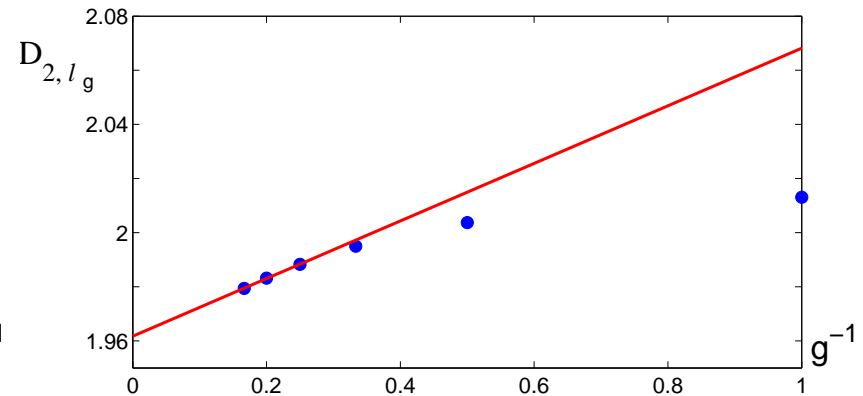
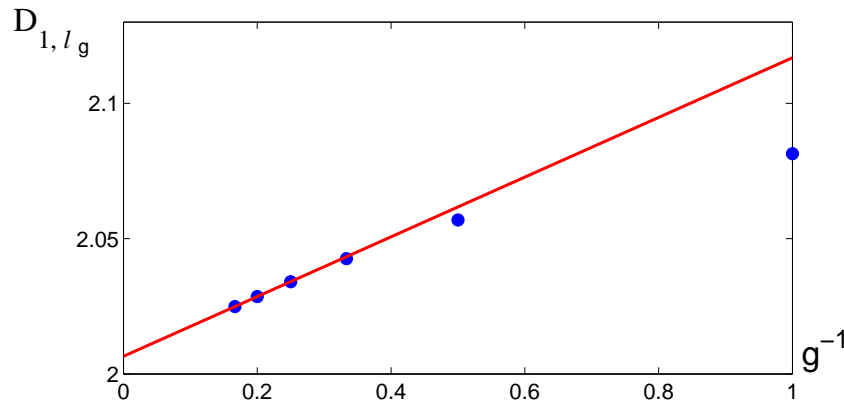
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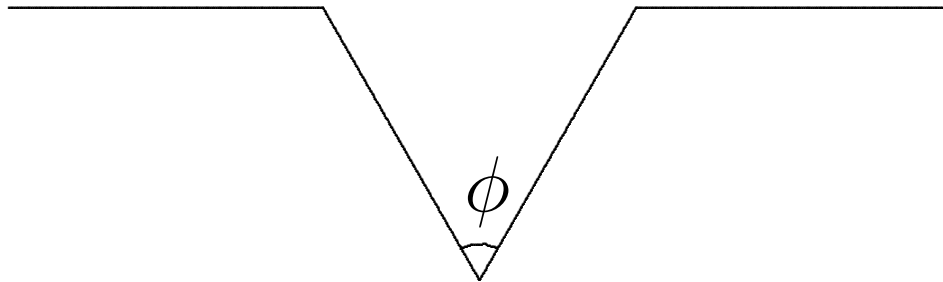


$$D_1 = 2.007 \pm 0.002$$

$$D_2 = 1.963 \pm 0.006$$

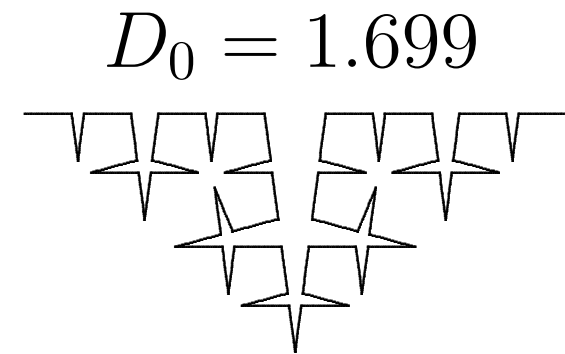
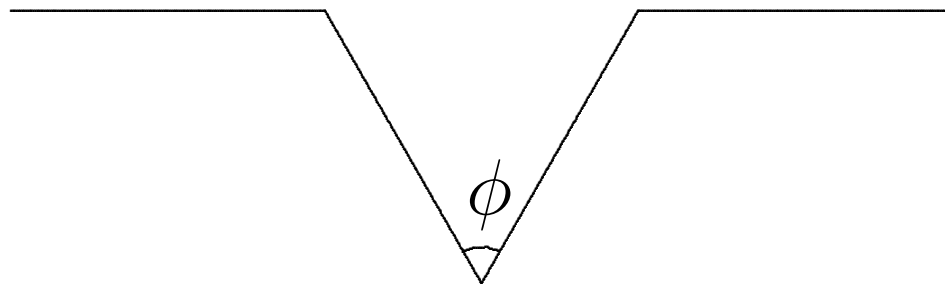
Von Koch curves of variable dimension

$$D_0 = \frac{\ln 4}{\ln 2(1 + \sin \phi/2)}$$

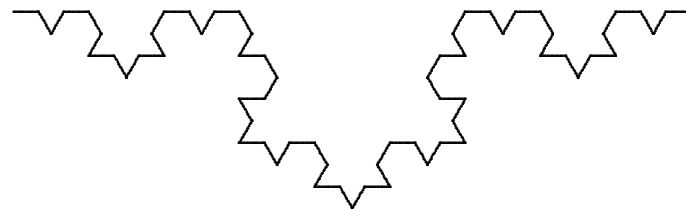


Von Koch curves of variable dimension

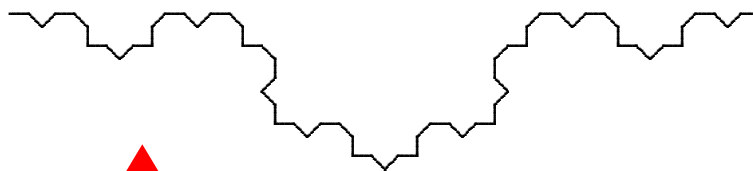
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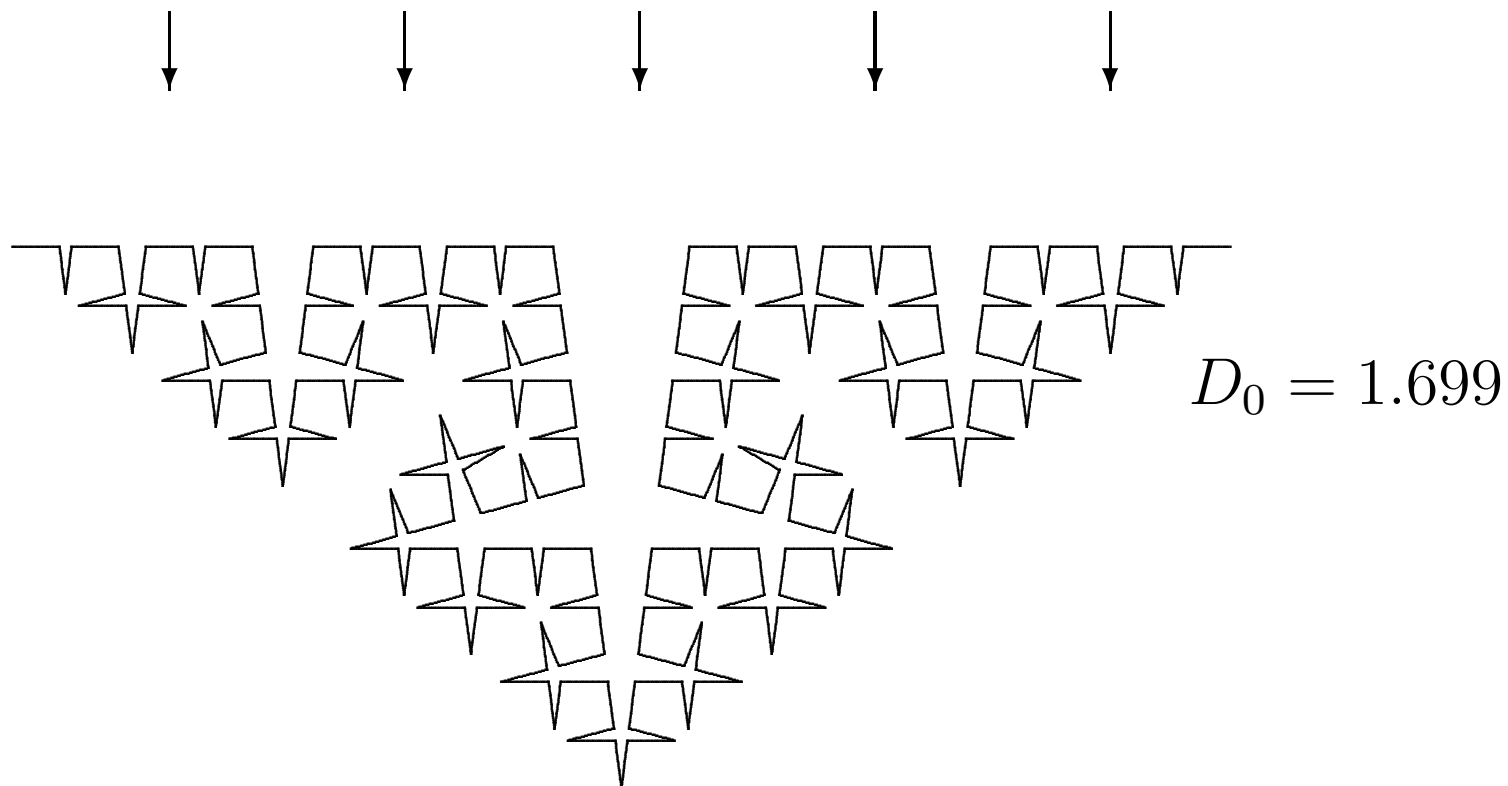
$D_0 = 1.262$



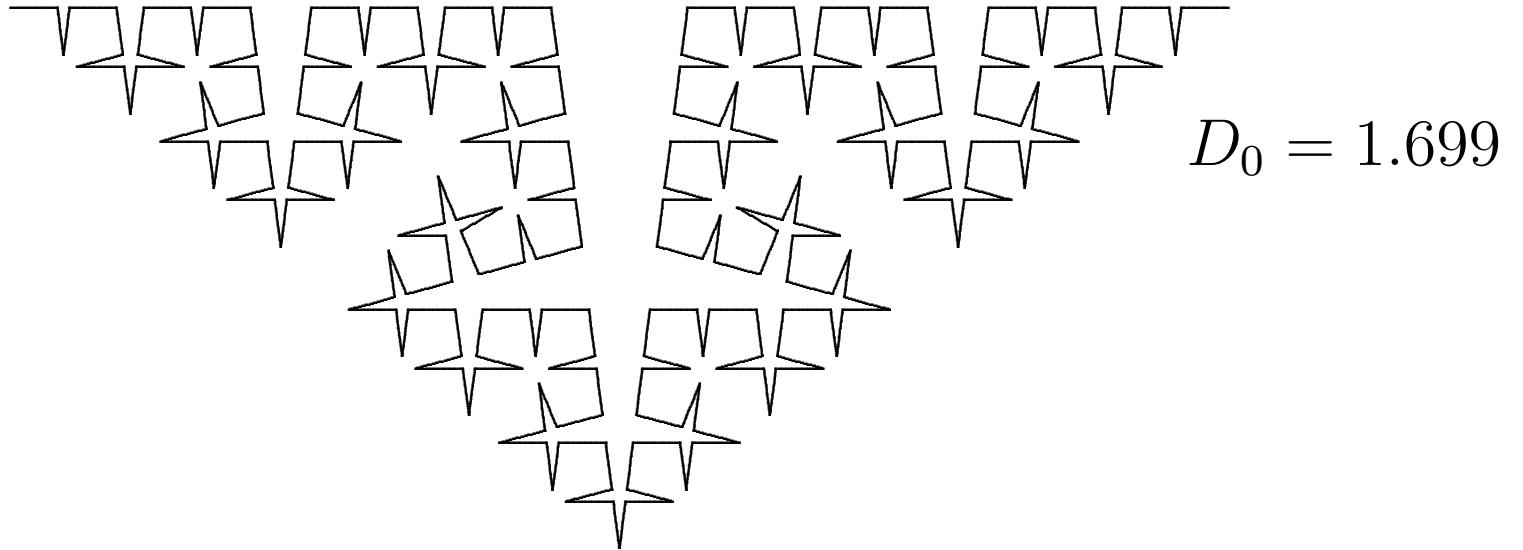
$D_0 = 1.129$



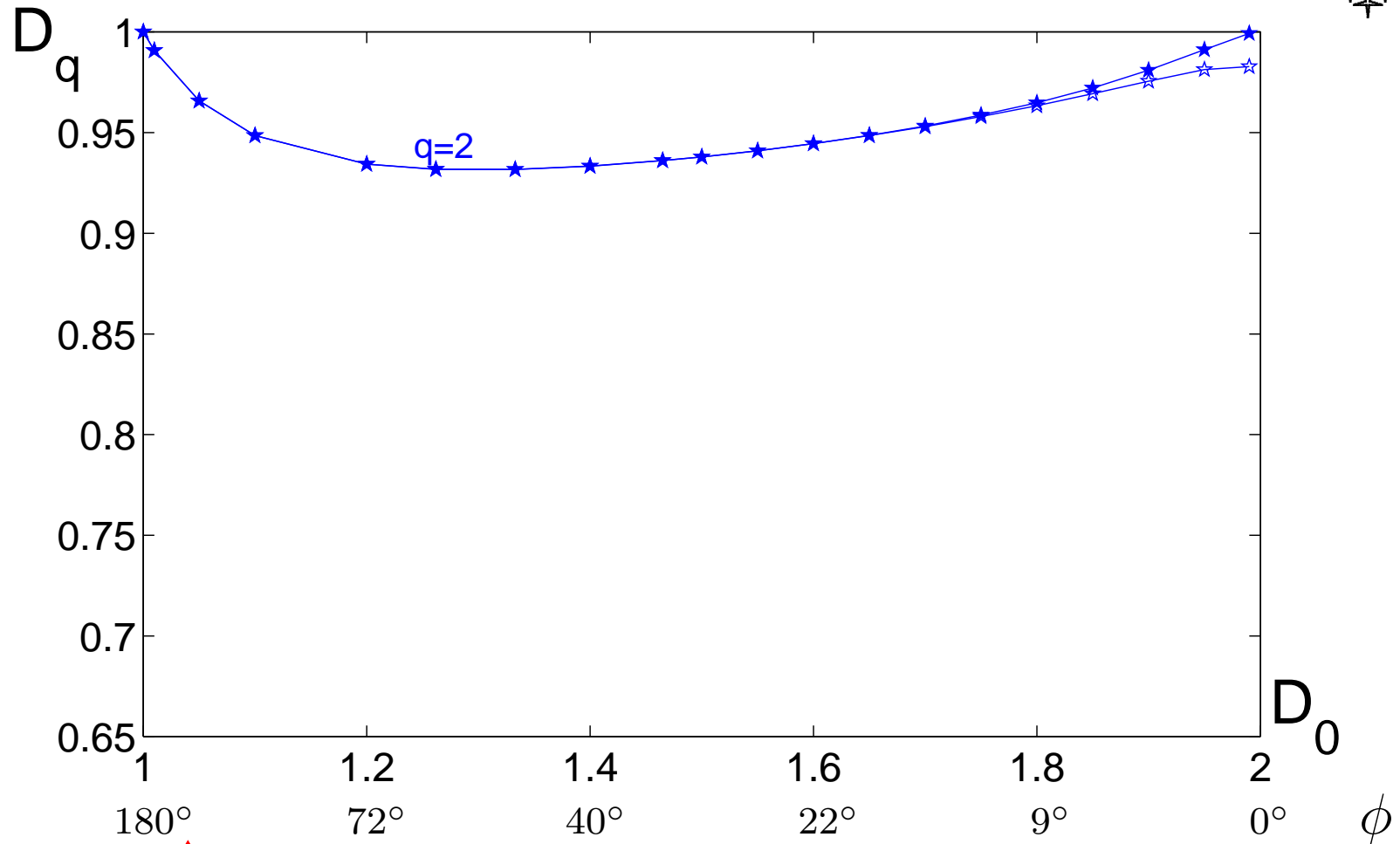
Two families of curves



Two families of curves

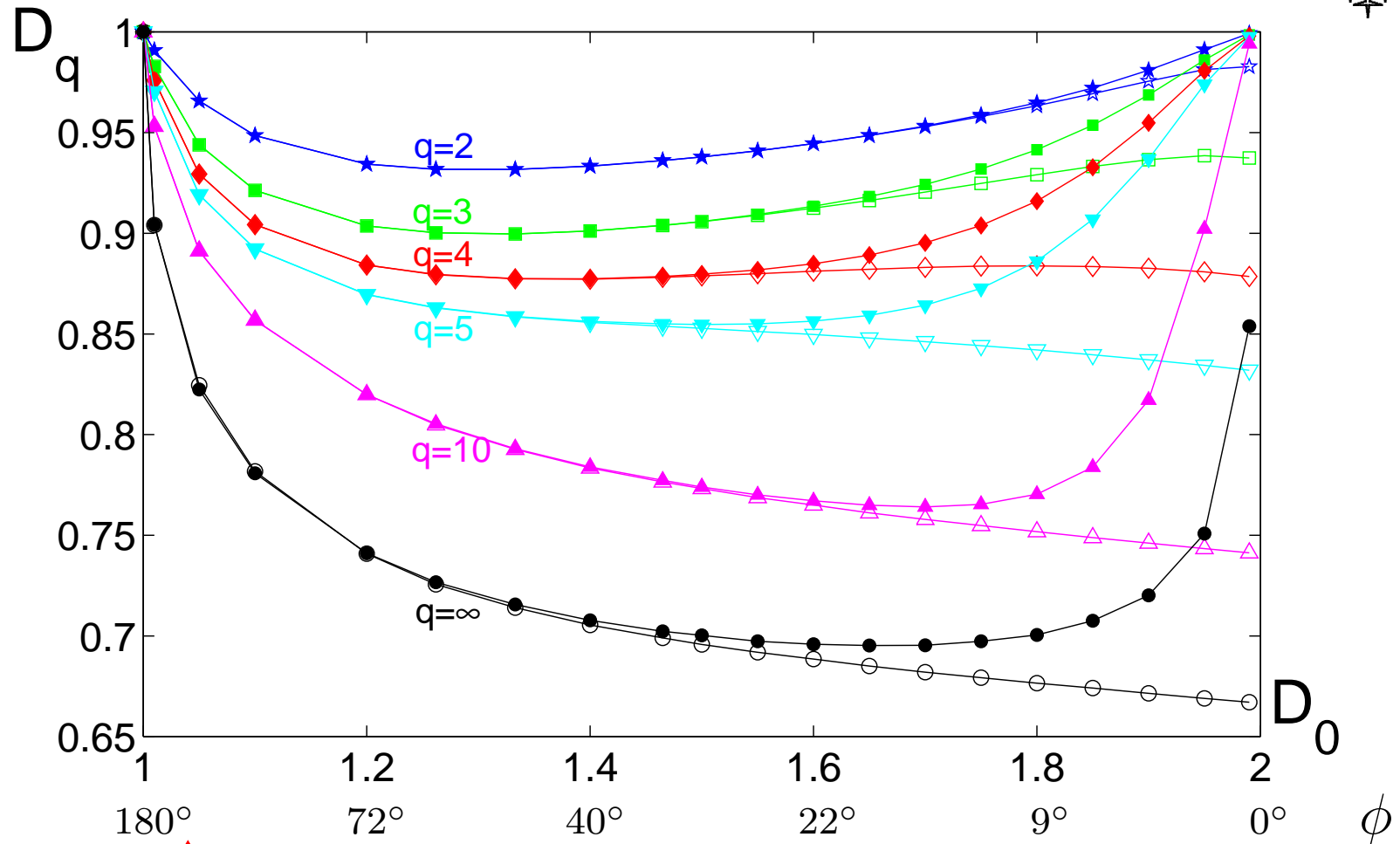


Multifractal dimensions



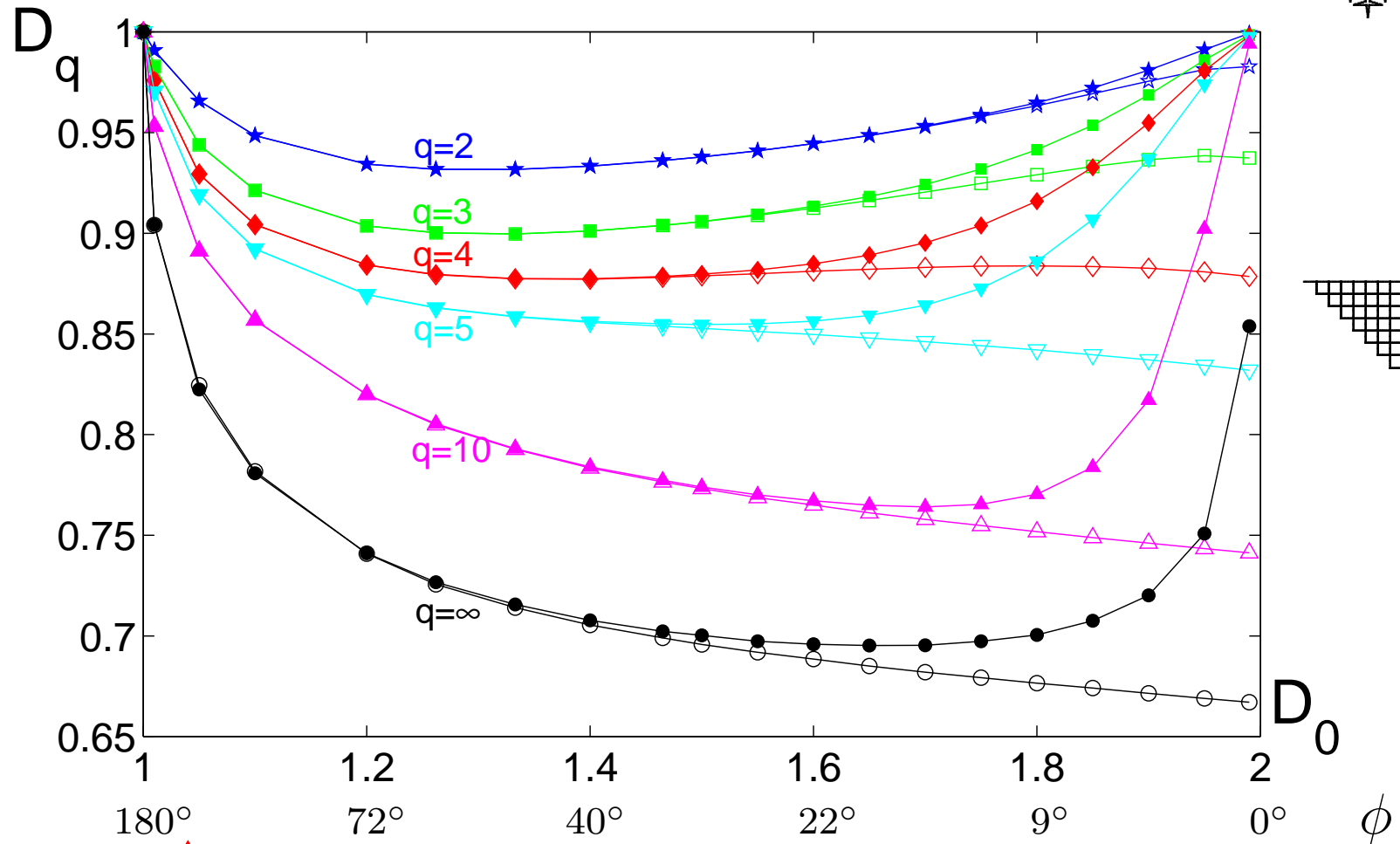
Grebenkov, Phys. Rev. Lett. 95, 200602 (2005)

Multifractal dimensions



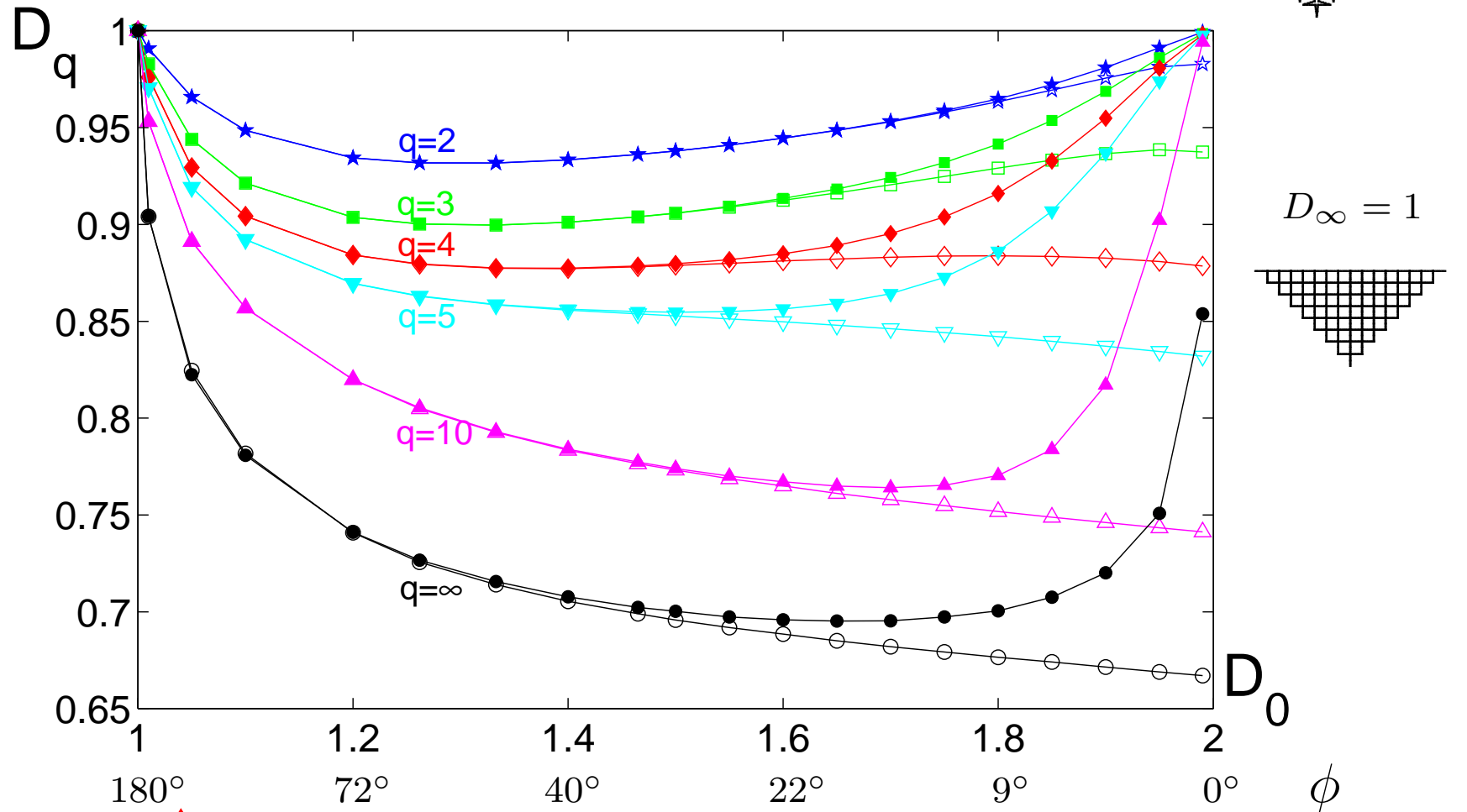
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Multifractal dimensions



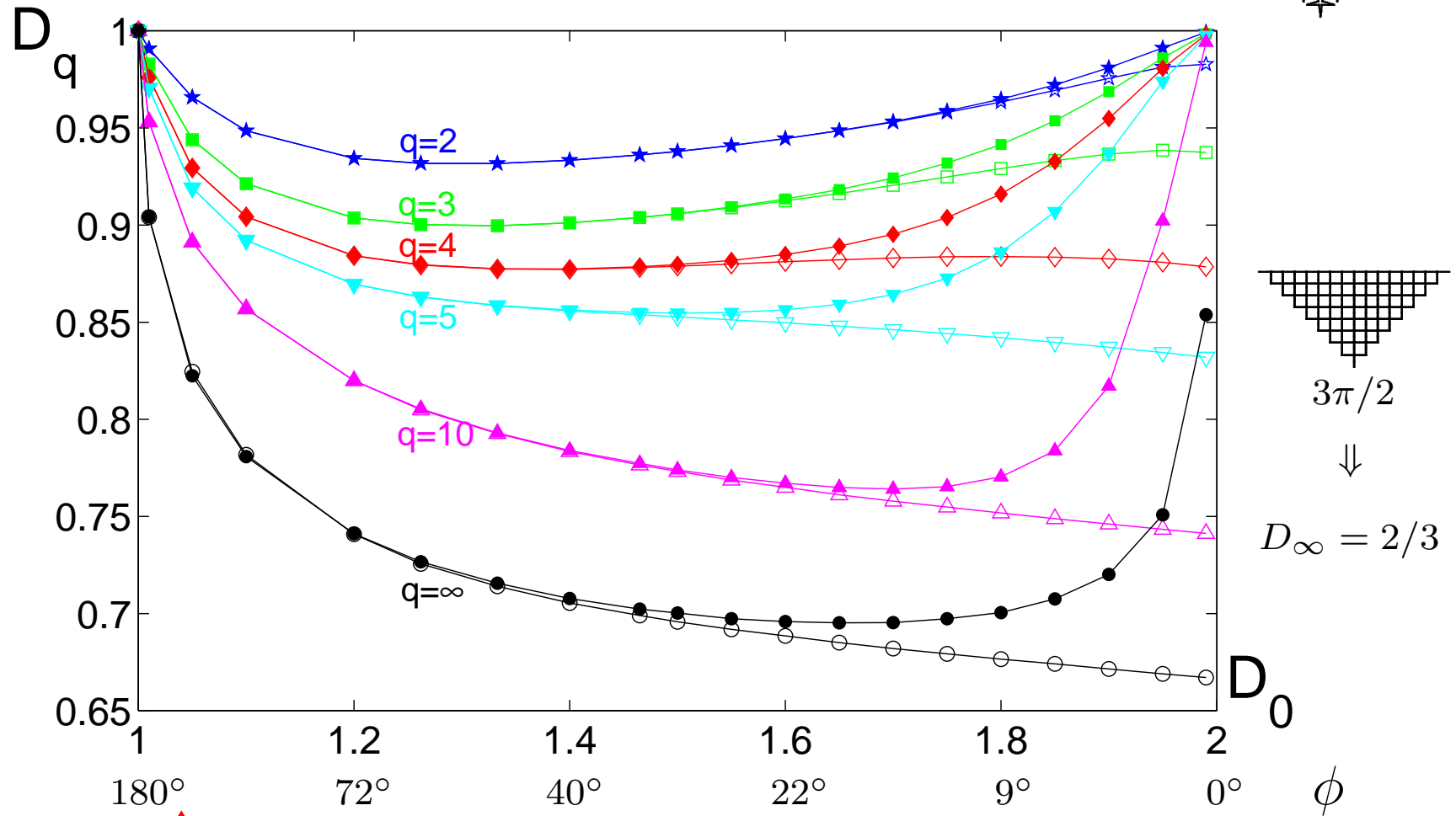
Grebenkov, Phys. Rev. Lett. 95, 200602 (2005)

Multifractal dimensions



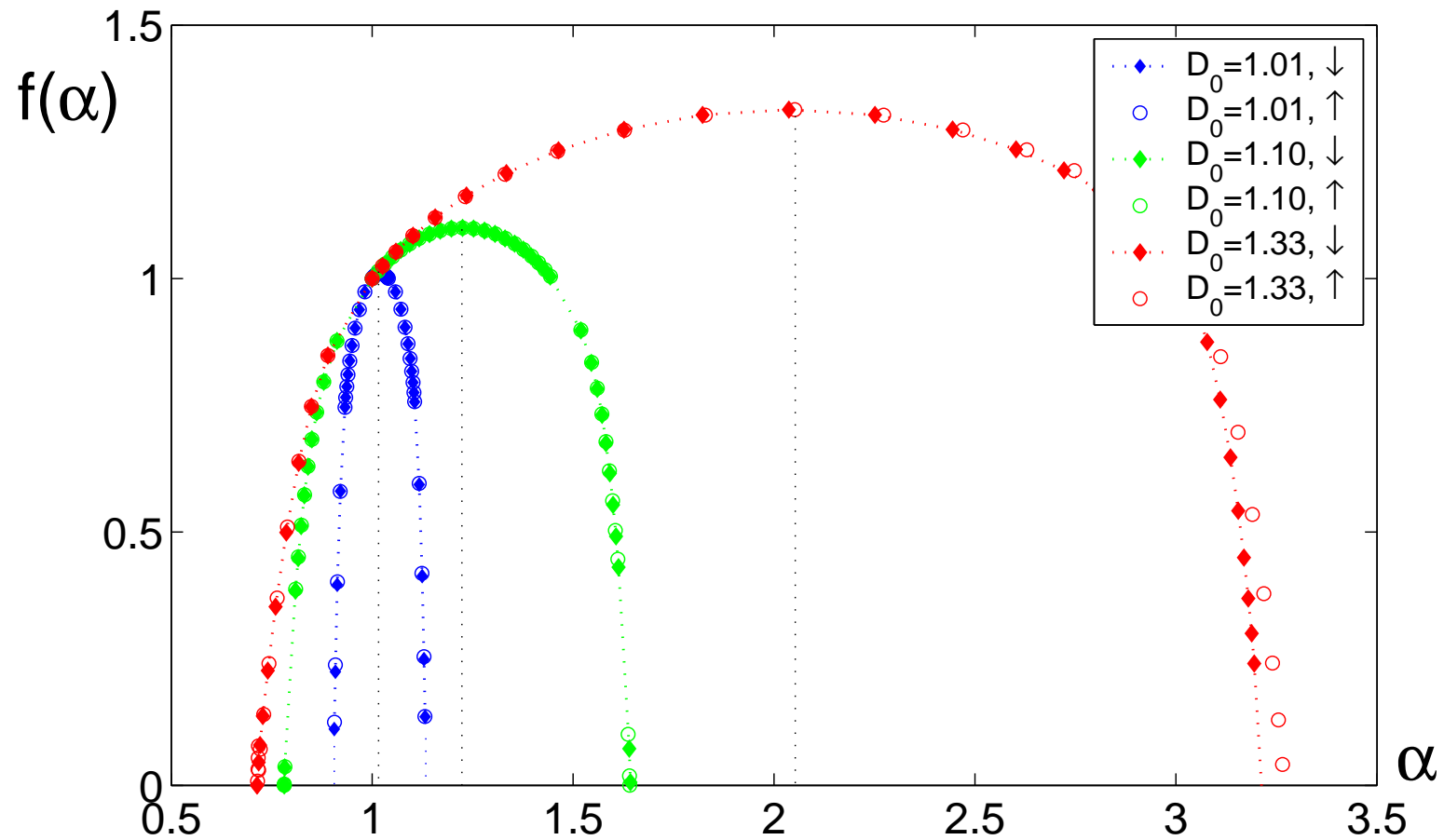
Grebenkov, Phys. Rev. Lett. 95, 200602 (2005)

Multifractal dimensions



Grebenkov, Phys. Rev. Lett. 95, 200602 (2005)

Multifractal spectrum





Outline

- Geometry-adapted fast random walks
- Multifractal properties of the harmonic measure on Von Koch boundaries

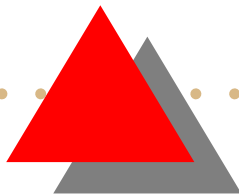
Grebenkov, Lebedev, Filoche, Sapoval, Phys. Rev. E 71, 056121 (2005)

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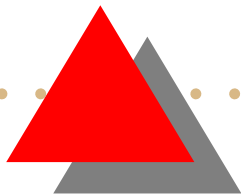
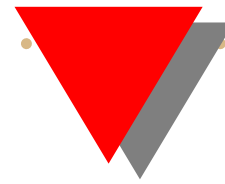
- Passivation of 2D and 3D fractals

Filoche, Grebenkov, Andrade, Sapoval (submitted)

Sapoval, Costa, Andrade, Filoche, Fractals 12, 381 (2004).

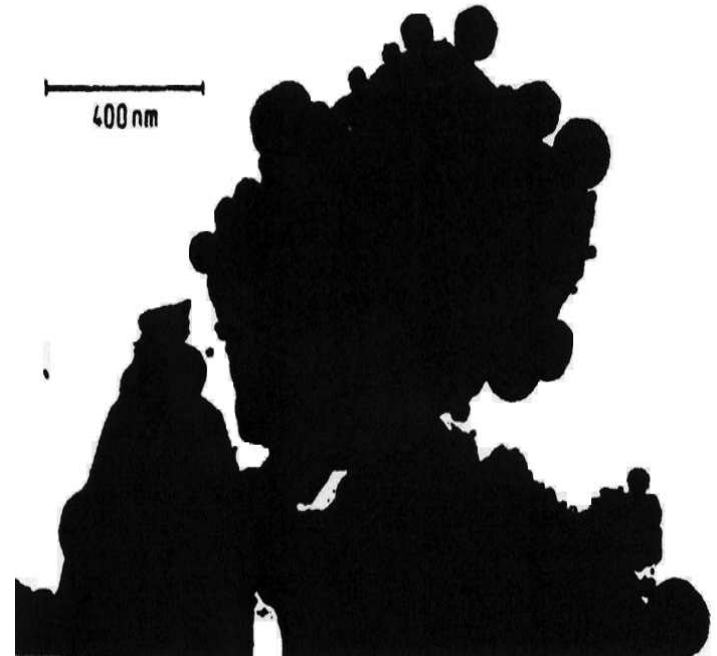
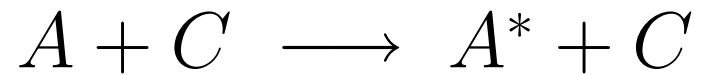


Heterogeneous catalysis



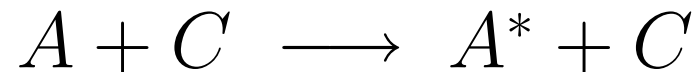
Heterogeneous catalysis

Catalytic reaction
on the boundary



Heterogeneous catalysis

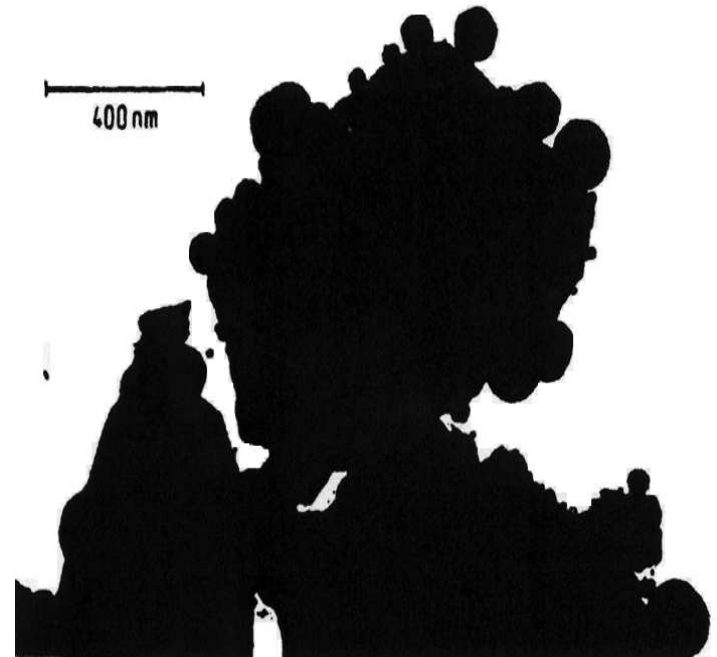
Catalytic reaction
on the boundary



Larger surface

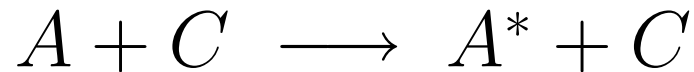


Higher outcome



Heterogeneous catalysis

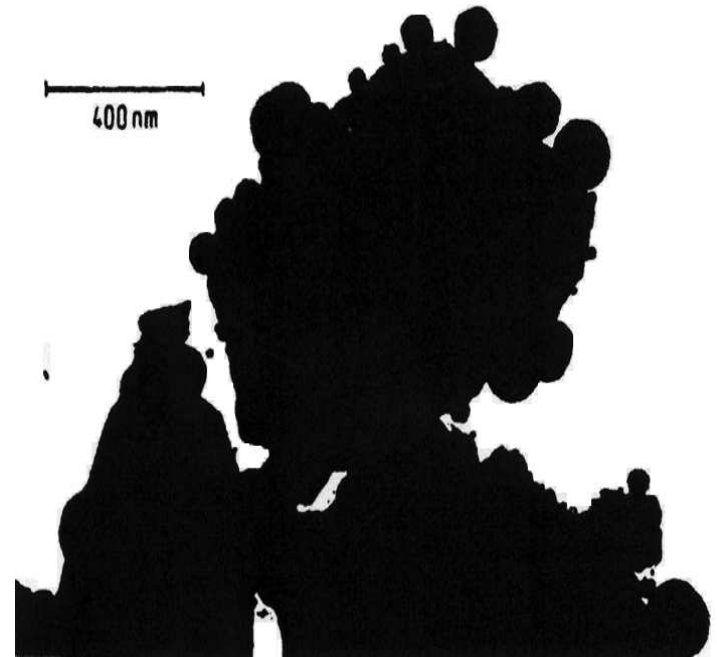
Catalytic reaction
on the boundary



Larger surface



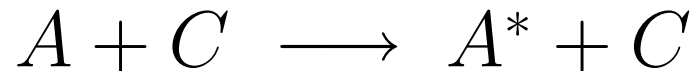
Higher outcome



BUT

Heterogeneous catalysis

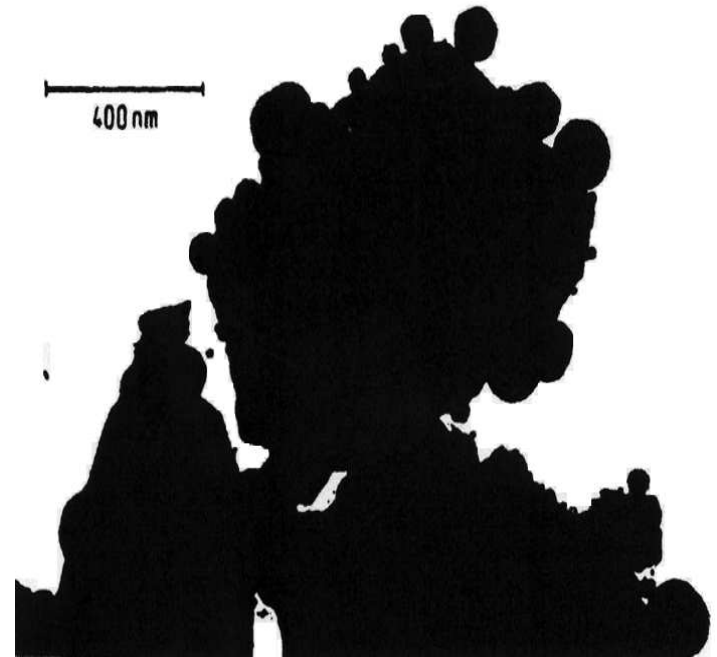
Catalytic reaction
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Larger surface



Higher outcome

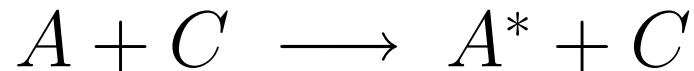


BUT

- Laplacian screening
- Passivation of the catalyst

Heterogeneous catalysis

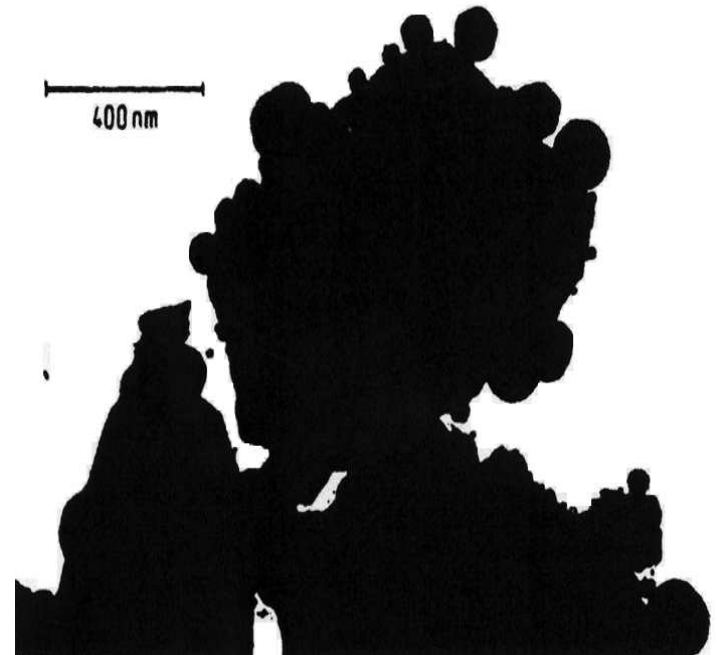
Catalytic reaction
on the boundary



Larger surface



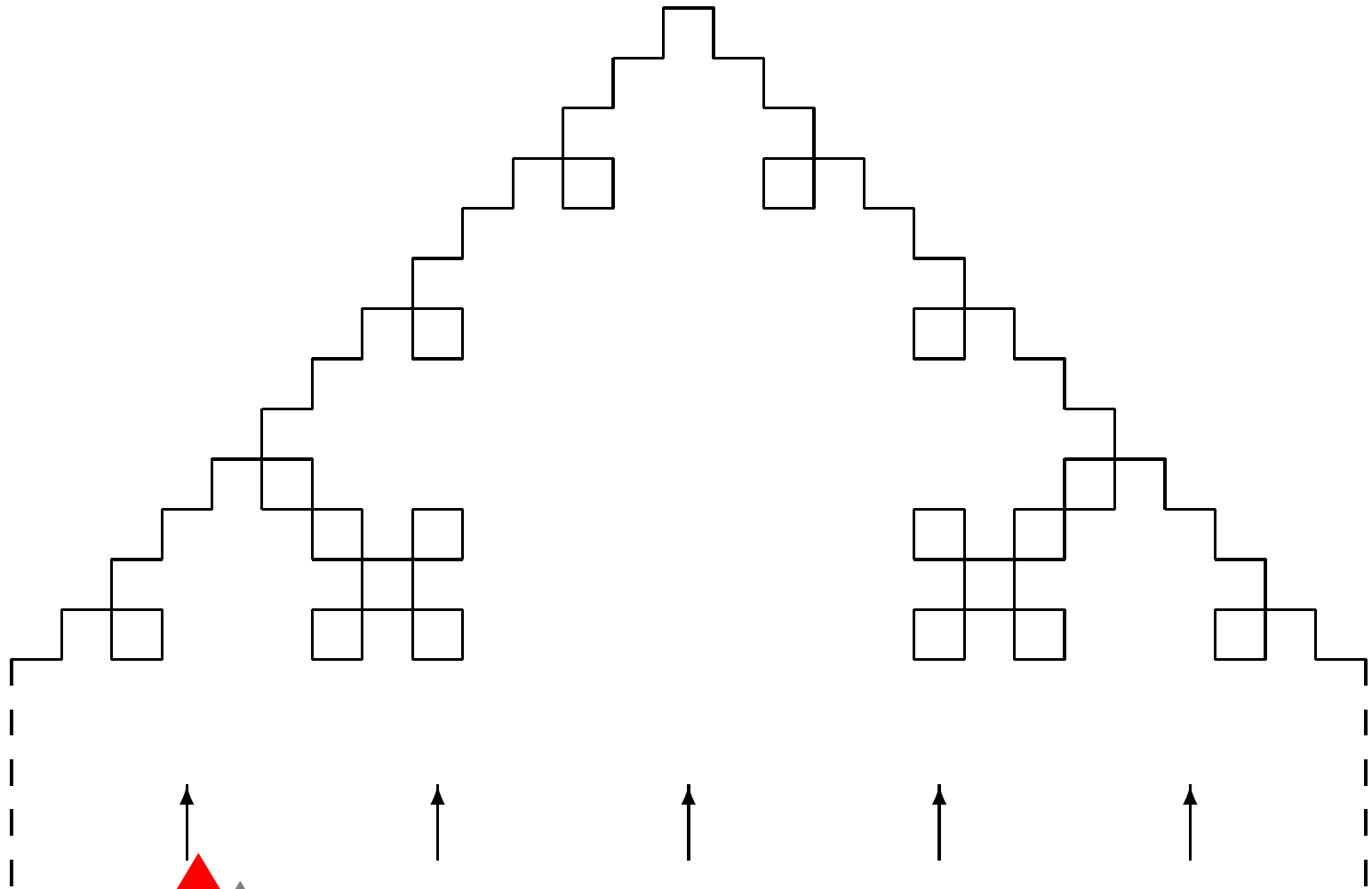
Higher outcome



BUT

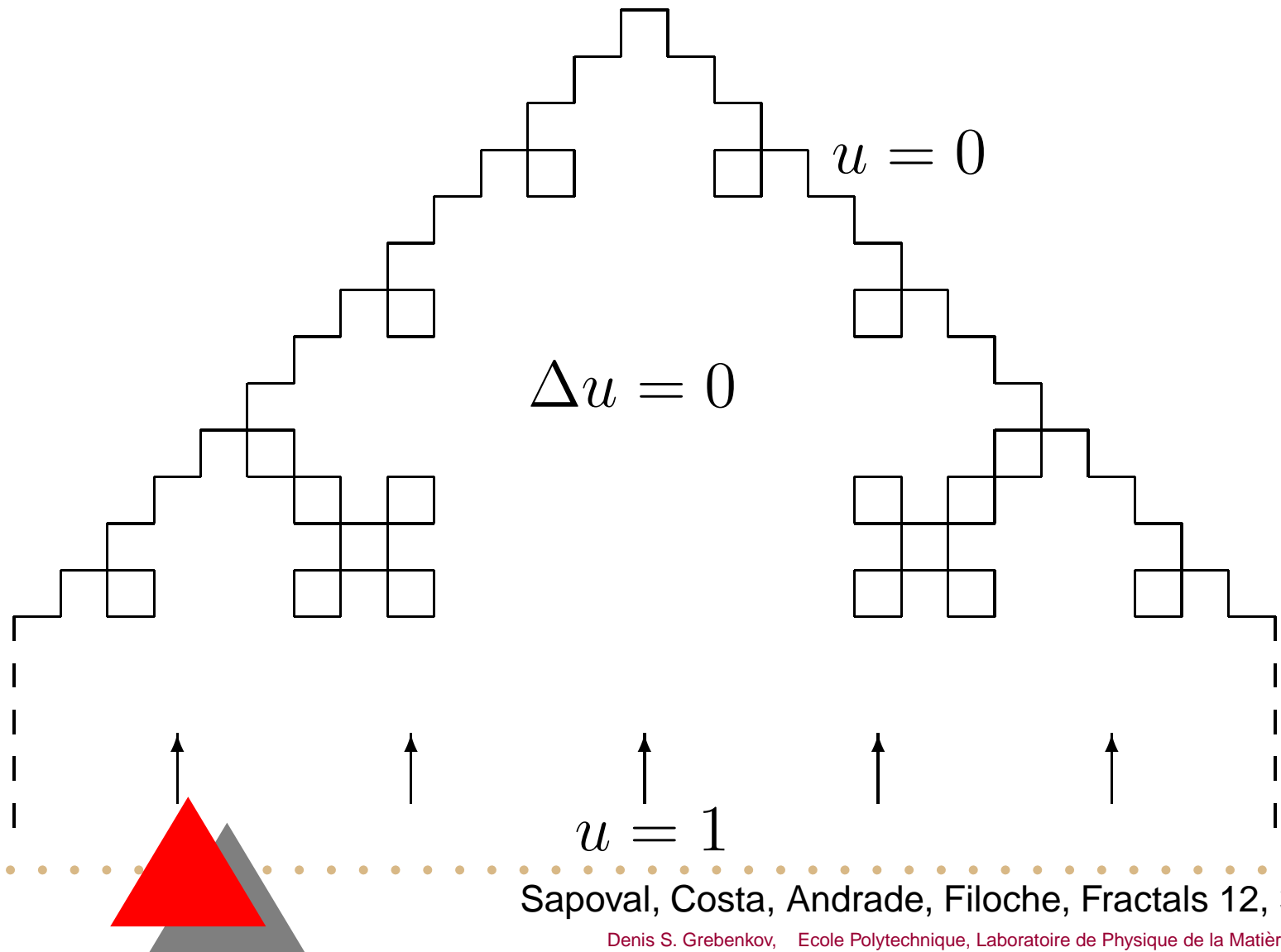
- Laplacian screening
- Passivation of the catalyst

Passivation process



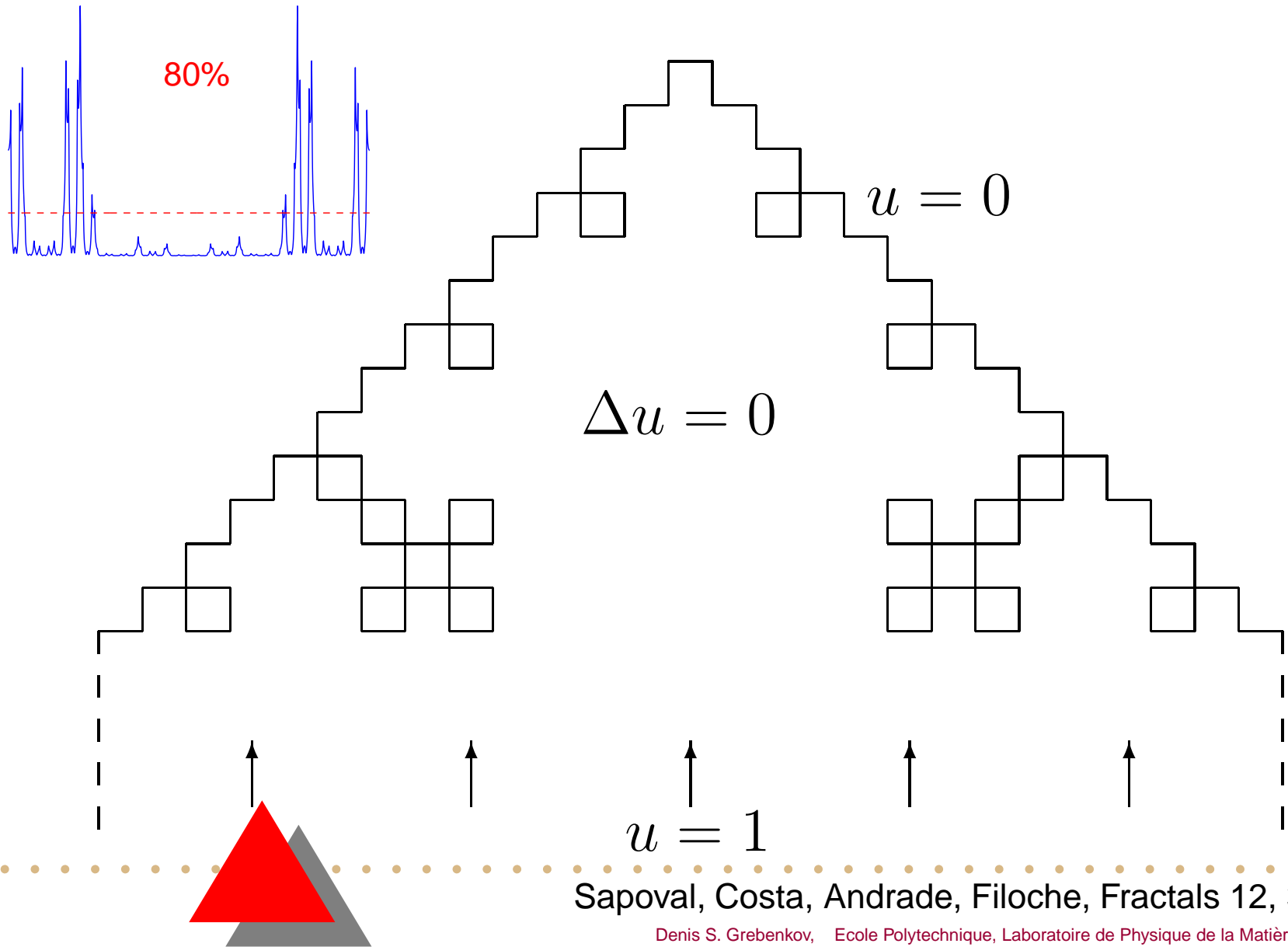
Sapoval, Costa, Andrade, Filoche, *Fractals* 12, 381 (2004).

Passivation process



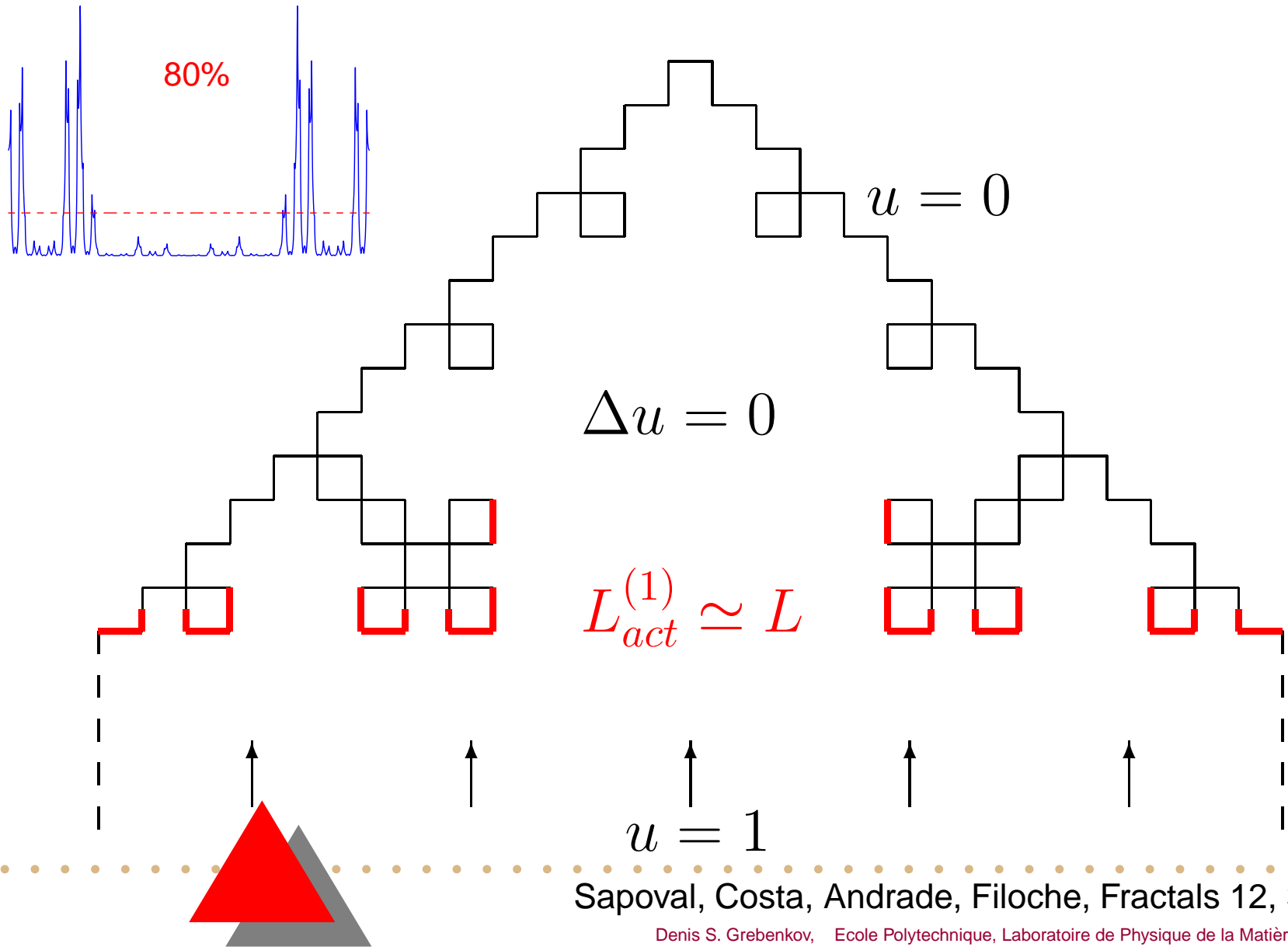
Sapoval, Costa, Andrade, Filoche, *Fractals* 12, 381 (2004).

Passivation process



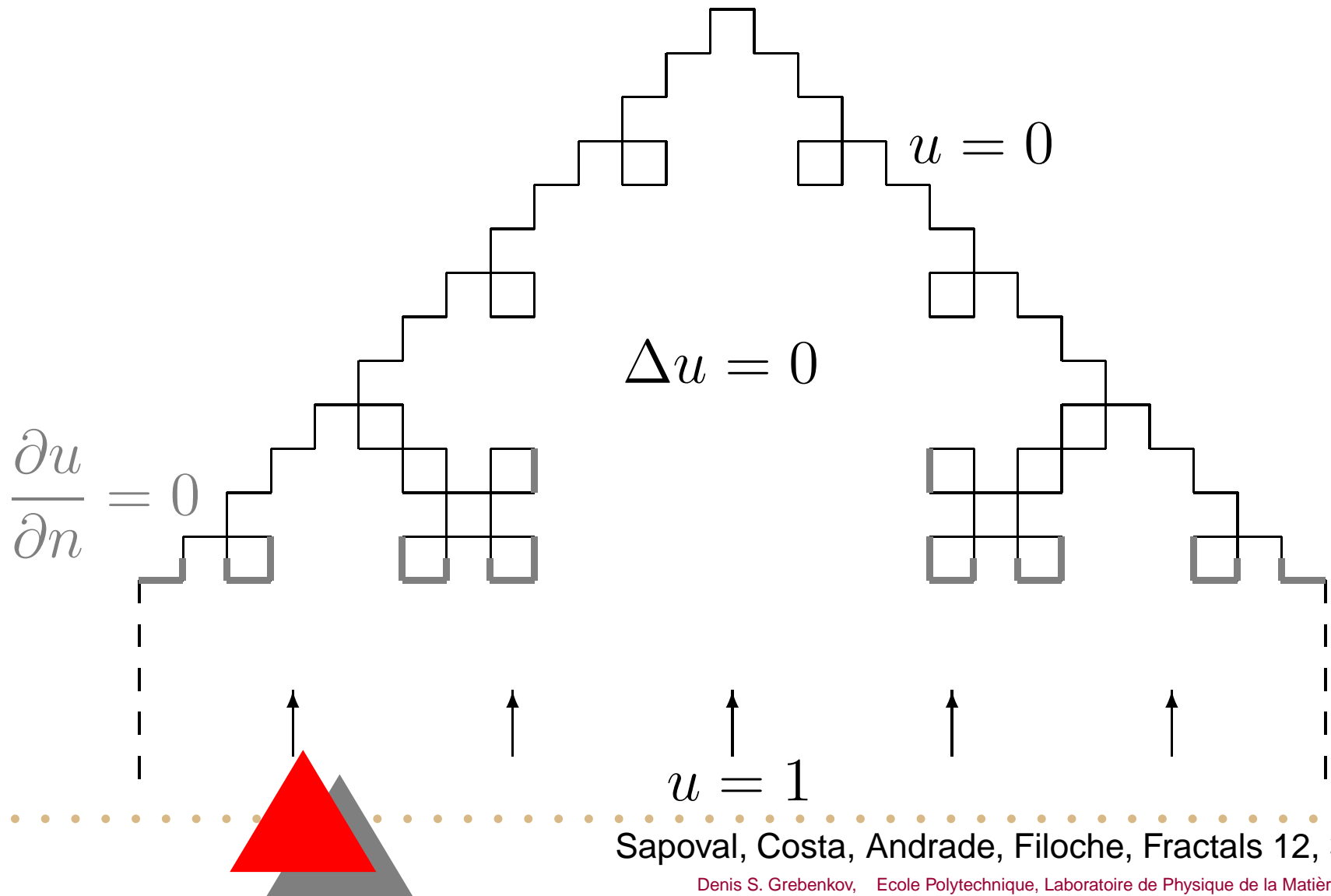
Sapoval, Costa, Andrade, Filoche, *Fractals* 12, 381 (2004).

Passivation process



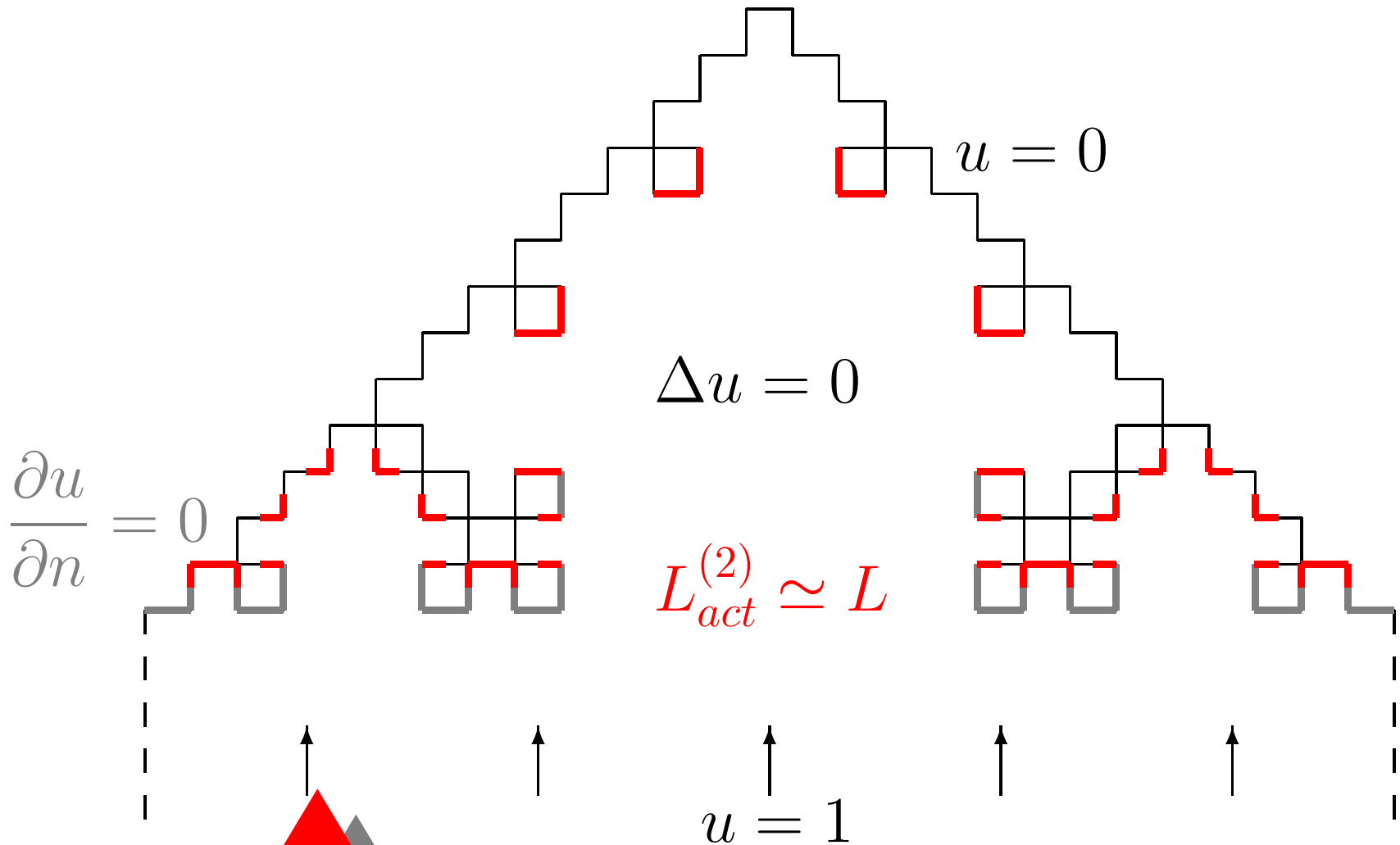
Sapoval, Costa, Andrade, Filoche, *Fractals* 12, 381 (2004).

Passivation process



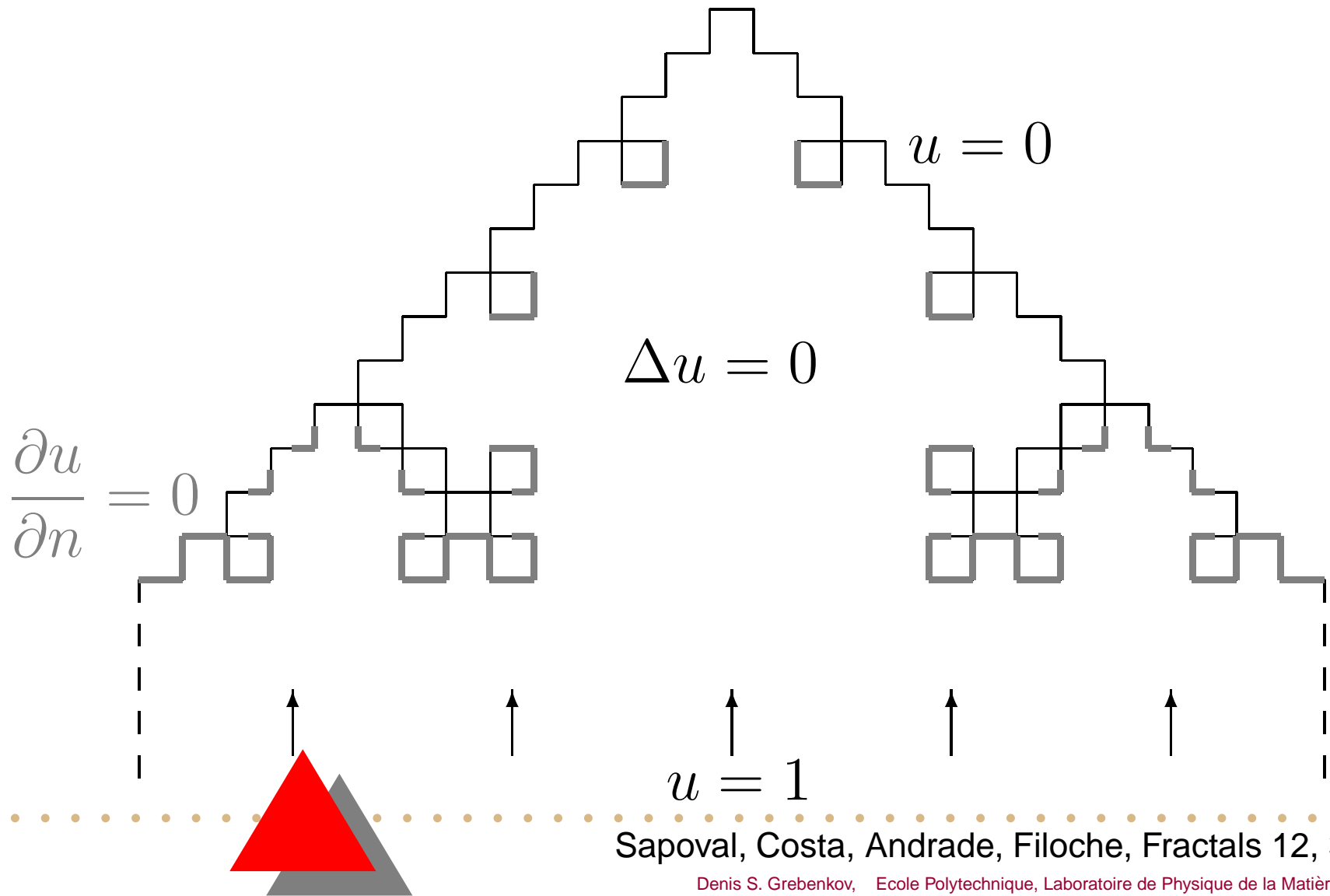
Sapoval, Costa, Andrade, Filoche, *Fractals* 12, 381 (2004).

Passivation process



Sapoval, Costa, Andrade, Filoche, *Fractals* 12, 381 (2004).

Passivation process

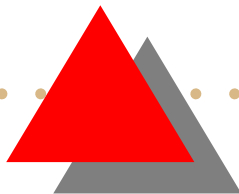


Sapoval, Costa, Andrade, Filoche, *Fractals* 12, 381 (2004).



Numerical scheme and hints

- *Calculate the arrival probabilities on totally active boundary using GAFRW algorithm*



Numerical scheme and hints

- Calculate the arrival probabilities on totally active boundary using GAFRW algorithm
- Determine the most accessible regions (supporting 80% of the total flux) and passivate them $\rightarrow L_{act}^{(1)}$



Numerical scheme and hints

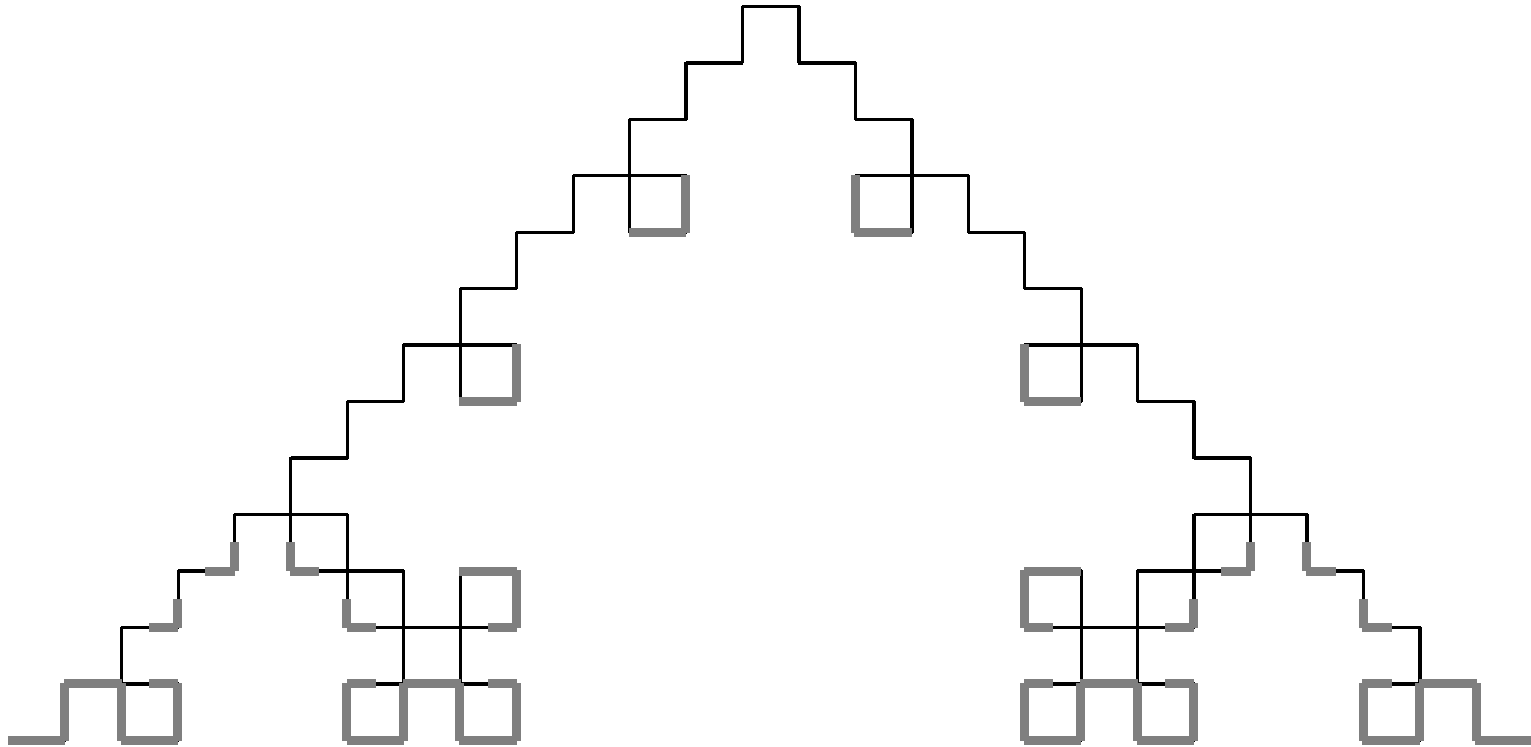
- Calculate the arrival probabilities on totally active boundary using GAFRW algorithm
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- Calculate the arrival probabilities on partially passivated boundary using GAFRW algorithm



Numerical scheme and hints

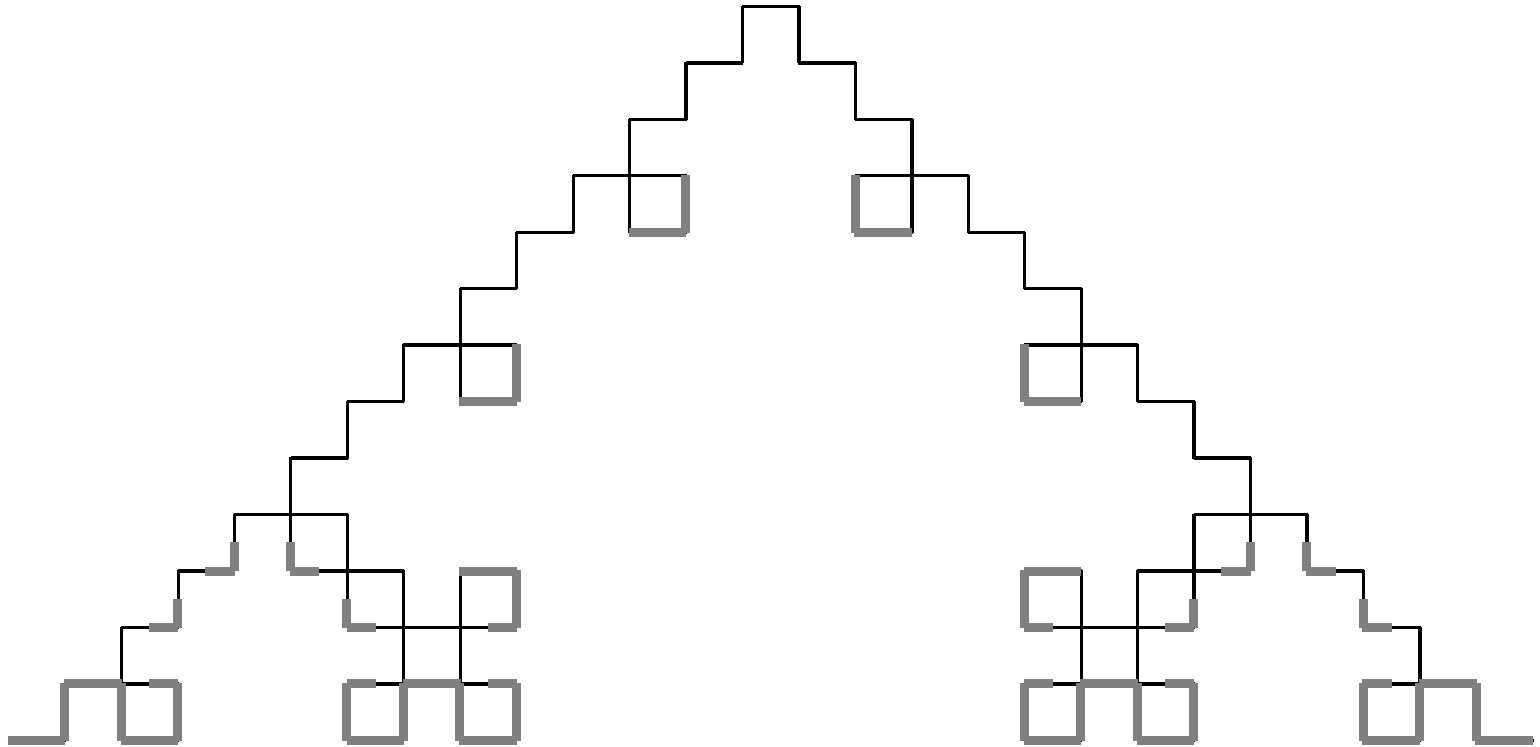
- Calculate the arrival probabilities on totally active boundary using GAFRW algorithm
- Determine the most accessible regions (supporting 80% of the total flux) and passivate them $\rightarrow L_{act}^{(1)}$
- Calculate the arrival probabilities on partially passivated boundary using GAFRW algorithm
- Determine the most accessible regions (supporting 80% of the total flux) and passivate them $\rightarrow L_{act}^{(2)}$
- etc.

Numerical scheme and hints



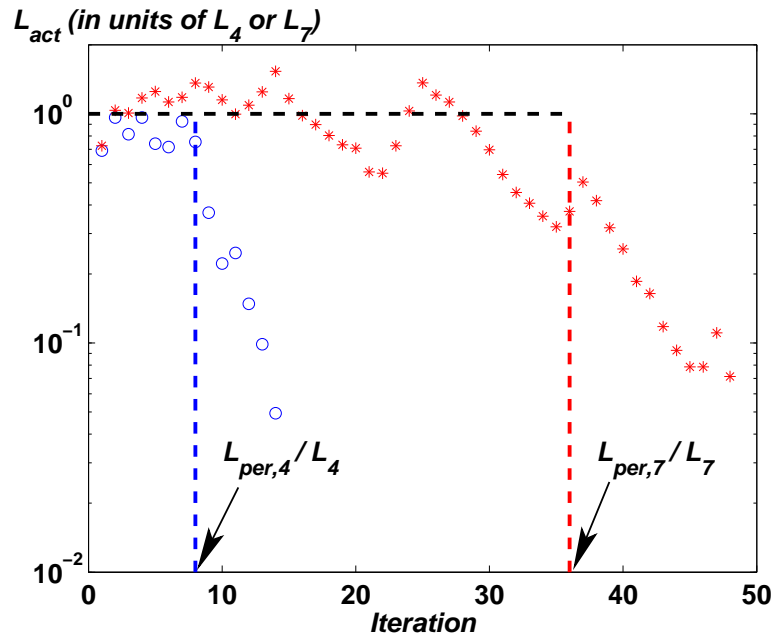
*The most accessible regions are passivated,
the other regions are harder and harder to access*

Numerical scheme and hints

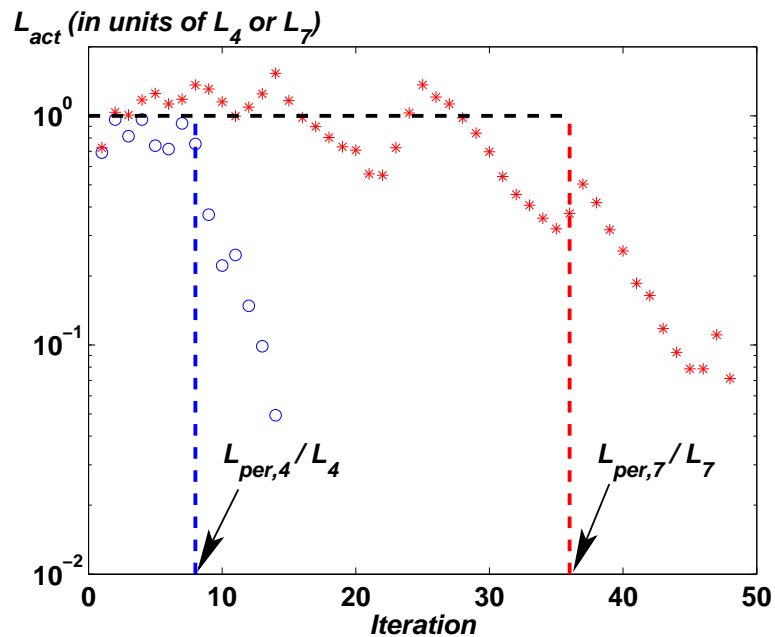


*Use the arrival probability distribution at stage $n - 1$
as an effective source of particles for the stage n*

Passivation in 2D/3D



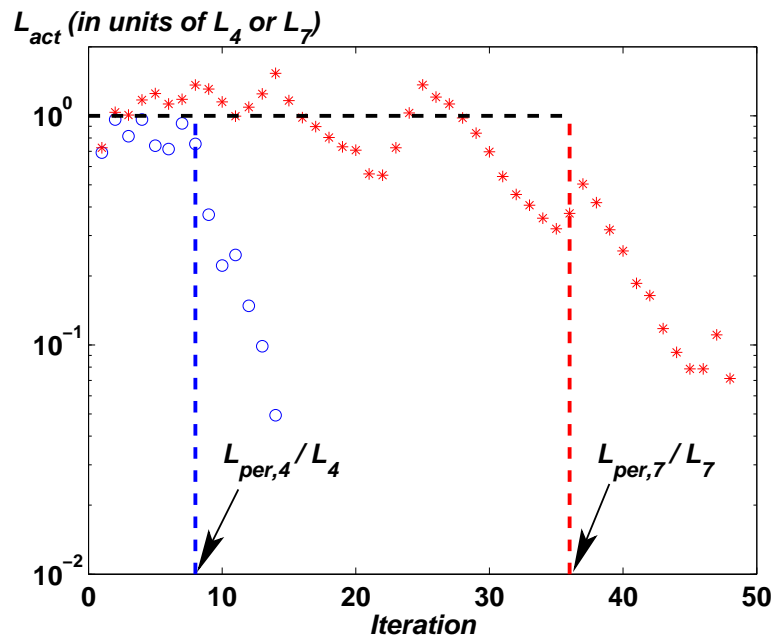
Passivation in 2D/3D



$$L_{act}^{(k)} \simeq L$$

$$n \simeq L_{tot}/L = (5/3)^g$$

Passivation in 2D/3D



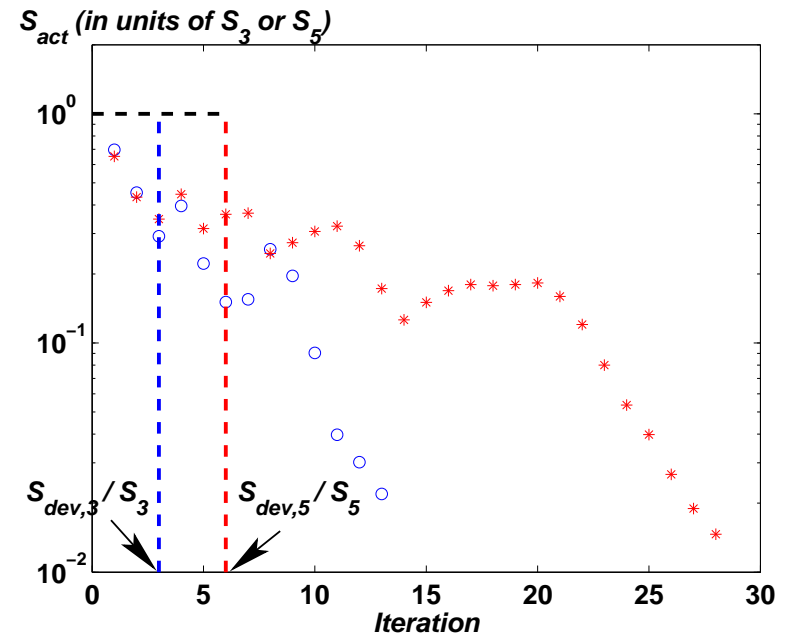
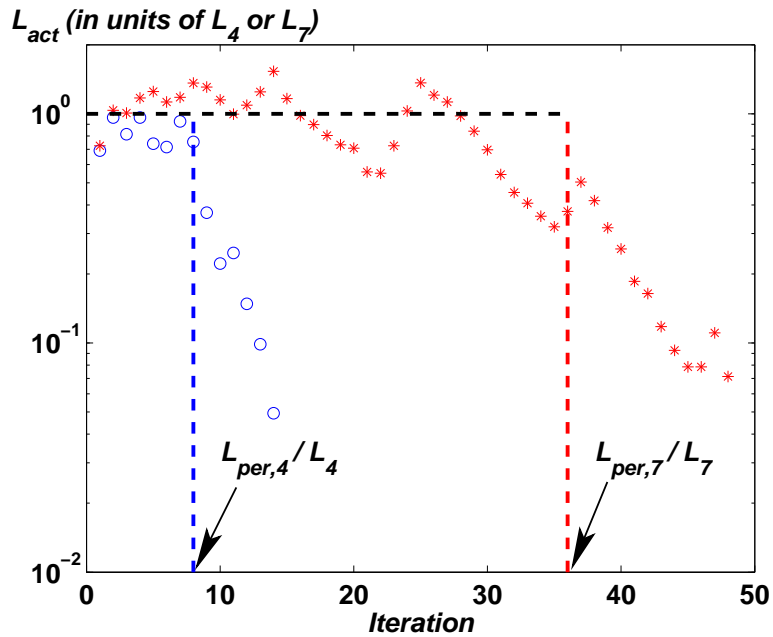
$$L_{act}^{(k)} \simeq L$$

$$n \simeq L_{tot}/L = (5/3)^g$$

$$S_{act}^{(k)} \simeq S$$

$$n \simeq S_{tot}/S = (13/3)^g$$

Passivation in 2D/3D



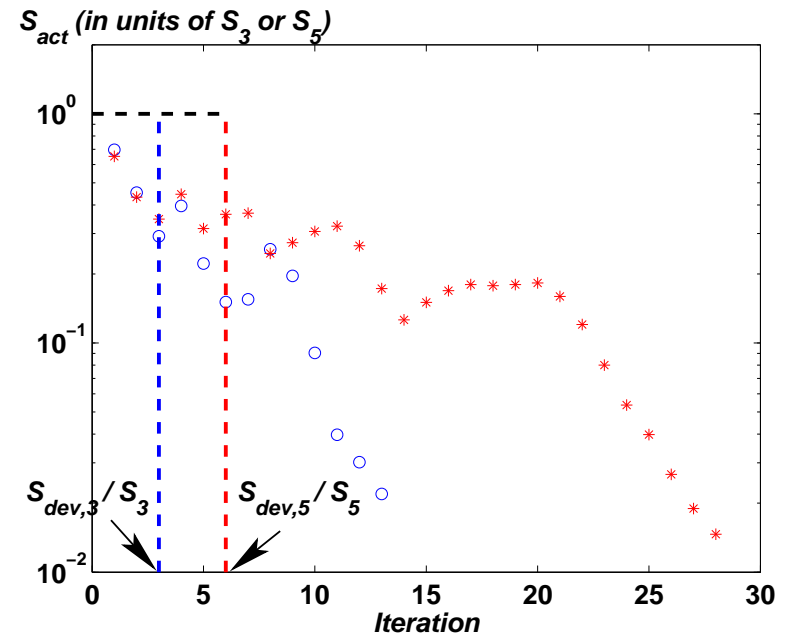
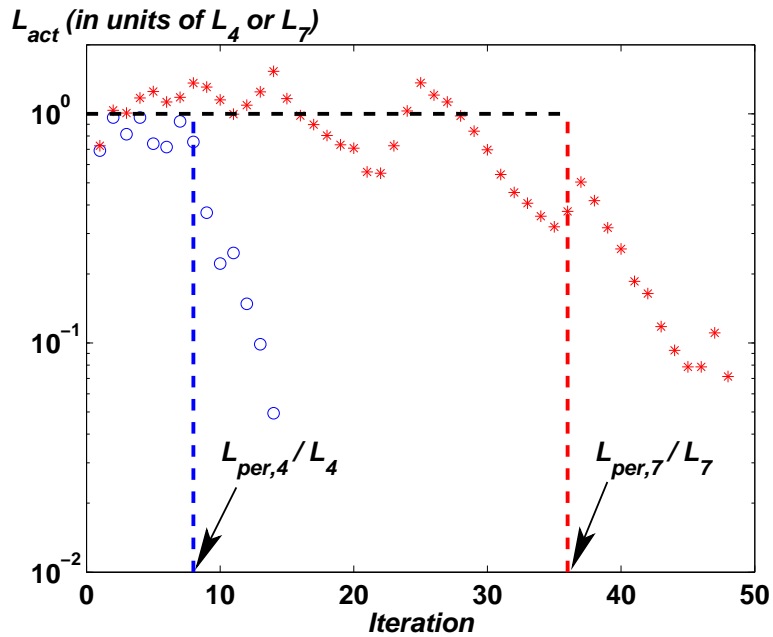
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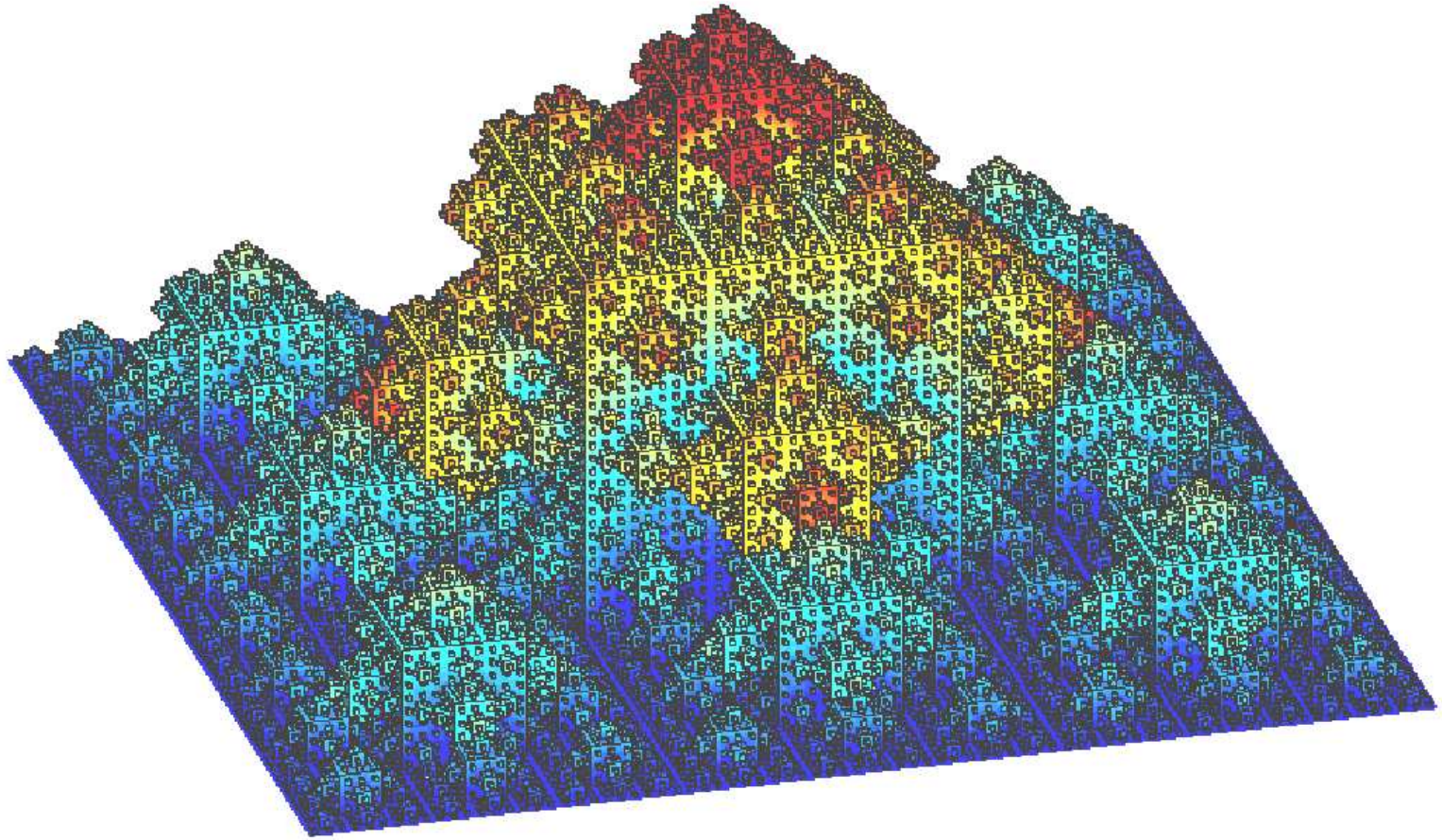
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$$n \simeq L_{tot}/L = (5/3)^g$$

~~$$S_{act}^{(k)} \simeq S$$~~

~~$$n \simeq S_{tot}/S = (13/3)^g$$~~

Passivation in 3D



Passivation in 3D

In sharp contrast with 2D:

- active zones progressively decrease
- passivation is much longer
- catalyst may still contain worth matter and behave as exhausted

Summary

- *Geometry-adapted fast random walk algorithm*

Summary

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- *Accurate computation of the multifractal dimensions of the harmonic measure on Von Koch boundaries*

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Summary

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Summary

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- *Accurate computation of the multifractal dimensions of the harmonic measure on Von Koch boundaries*
 - *In 2D, the scaling properties of the harmonic measure are very close for two families of triangular Von Koch curves, although their geometries are apparently different*
 - *In 3D, the information dimension is slightly larger than 2*
- *Passivation is very different in 2D and 3D*



END