NCN@Purdue-Intel Summer School
Notes on Percolation Theory

Lecture 2
Thresholds, Islands, and Fractals

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Outline of lecture 2

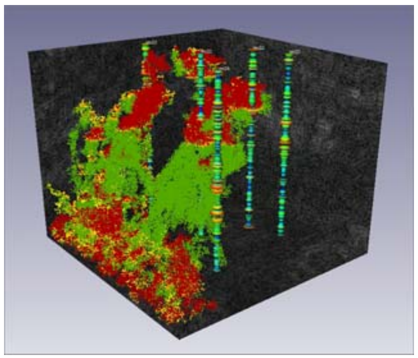
1) **Basic concepts of percolation theory**
2) Percolation threshold and ‘excluded volume’
3) Cluster size distribution, cluster Radius
4) Fractal dimension of a random surface
5) Conclusion

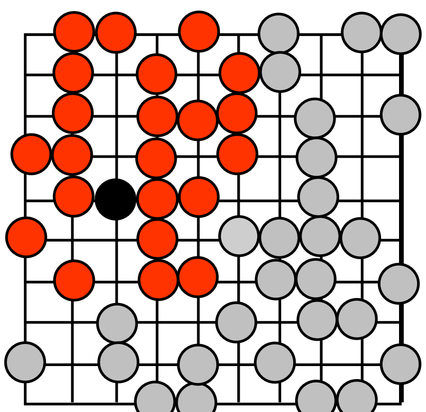
Application Notes: Nanocrystal Flash

Three topics of random systems

Cluster sizes

Oil fields, NC Flash

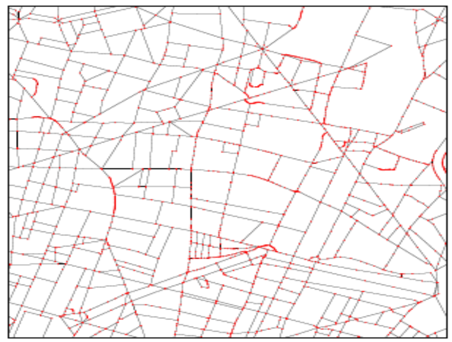


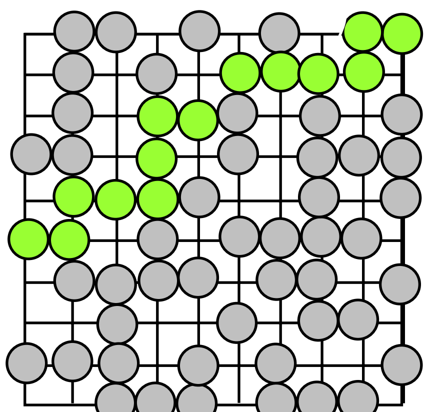


Percolation threshold

epidemics, forest fire, telecom grid, www

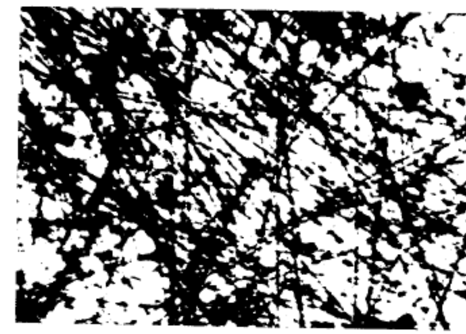
Nanonets, photovoltaics

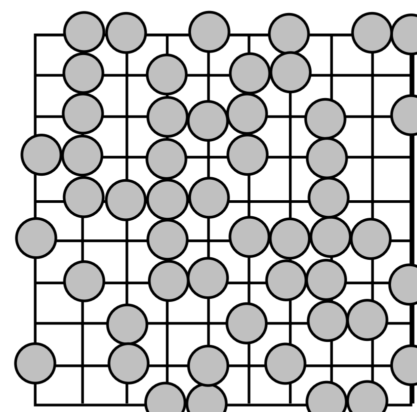




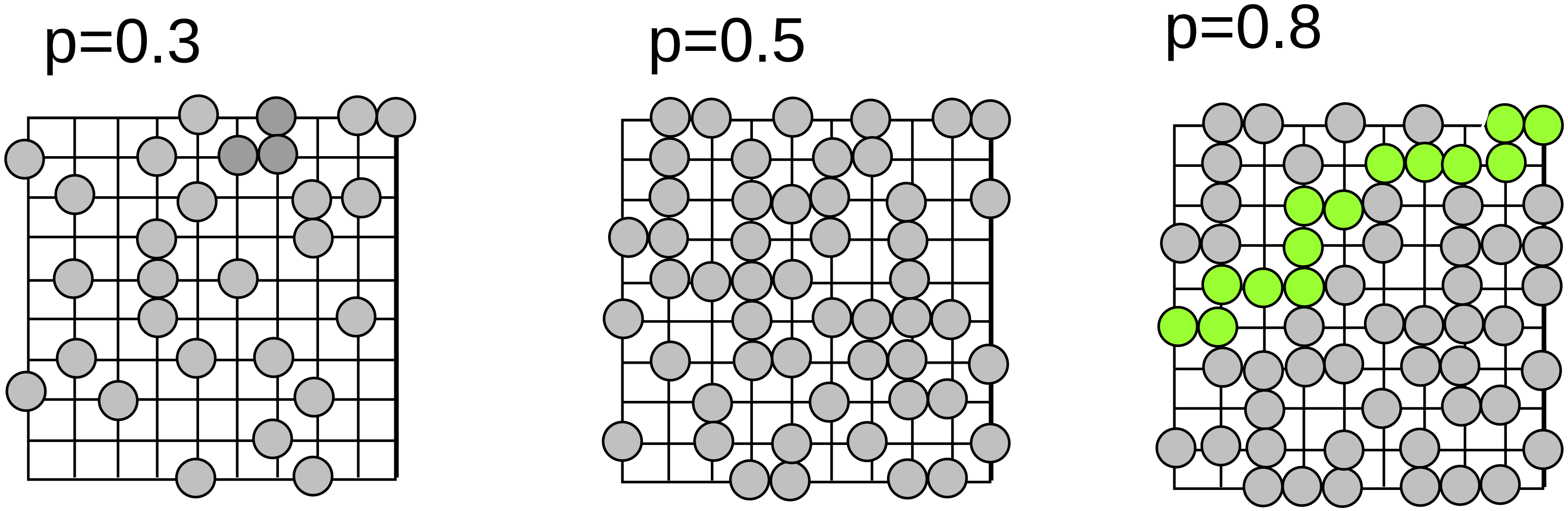
Fractal dimension

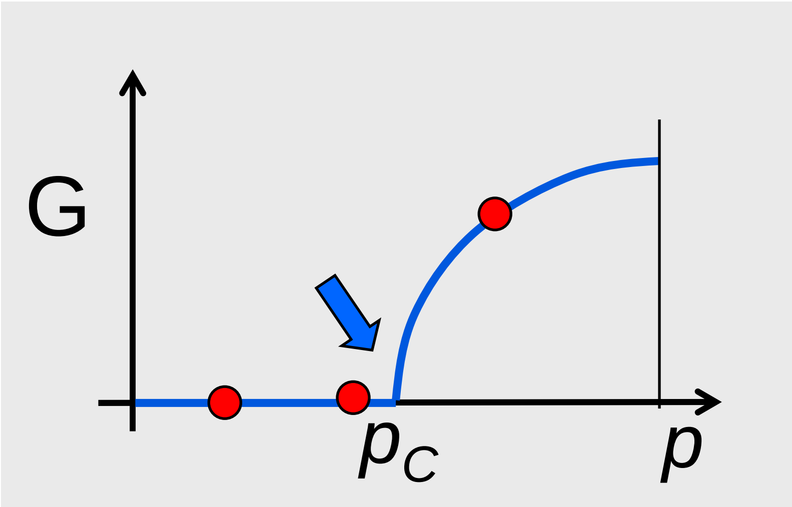
Aerosol, paper, sensors



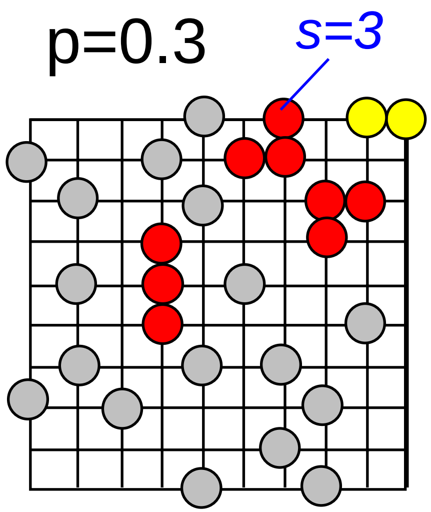


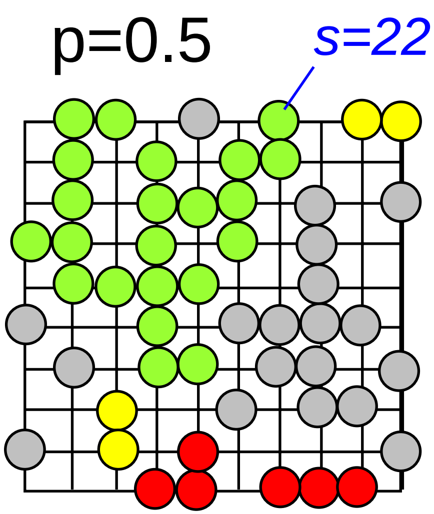
basic concepts: percolation threshold

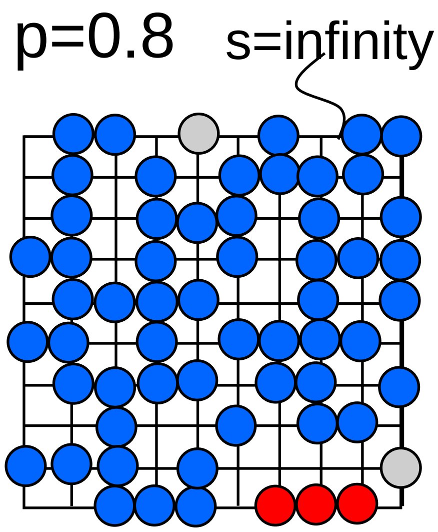


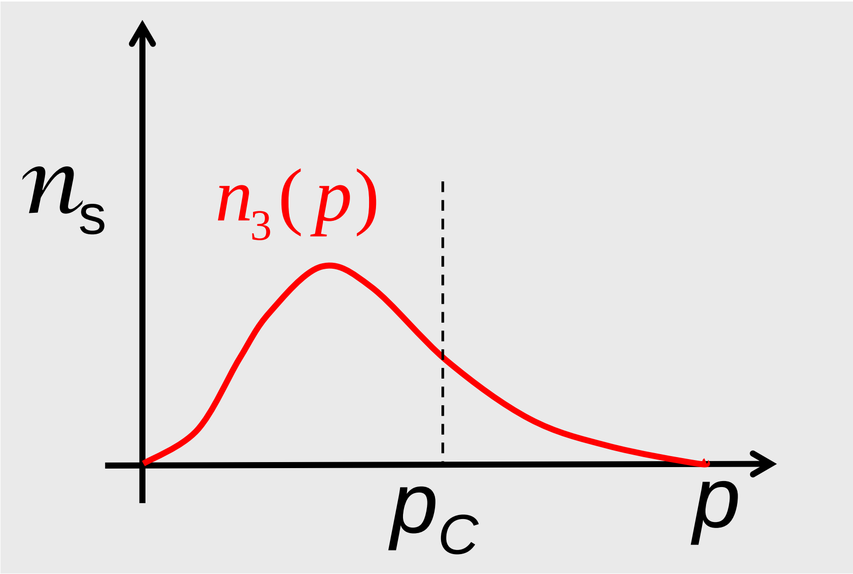


basic concepts: cluster size



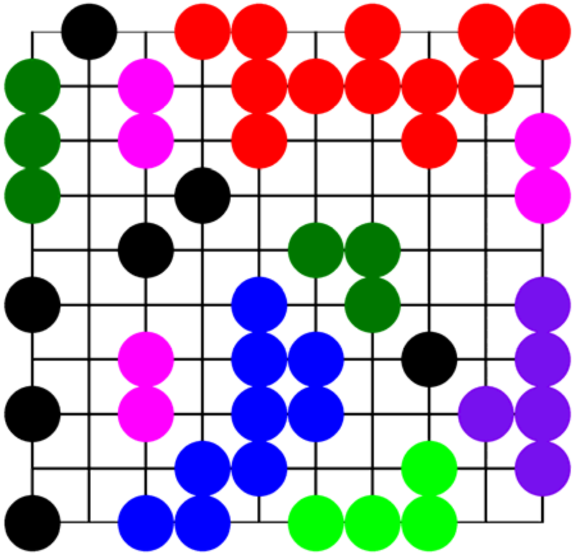






cluster-size distribution and its moments

$n_s(p,L)$ Number of cluster of size s divided by the number of sites

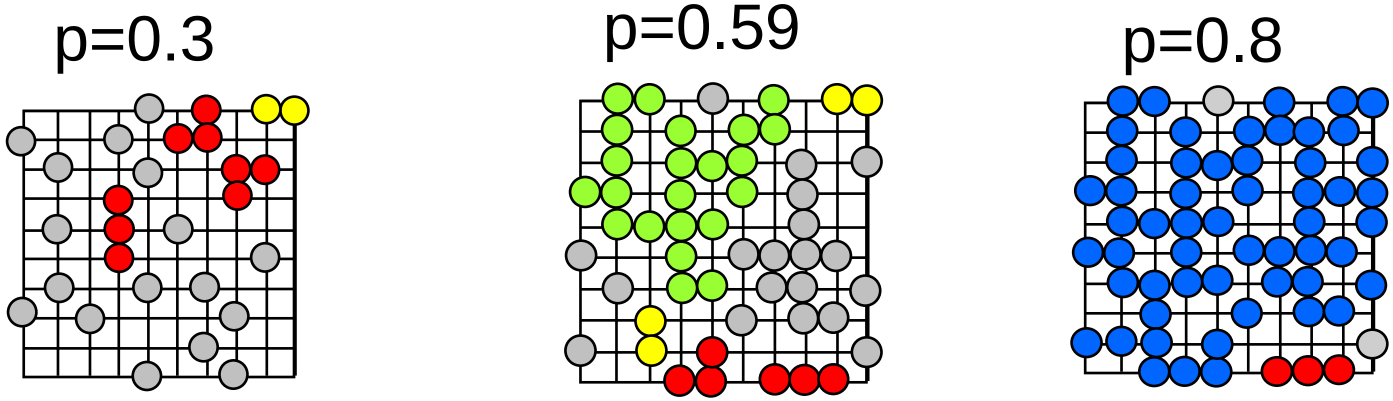


$$p = \sum_{0<s<\infty} s n_s(p)$$

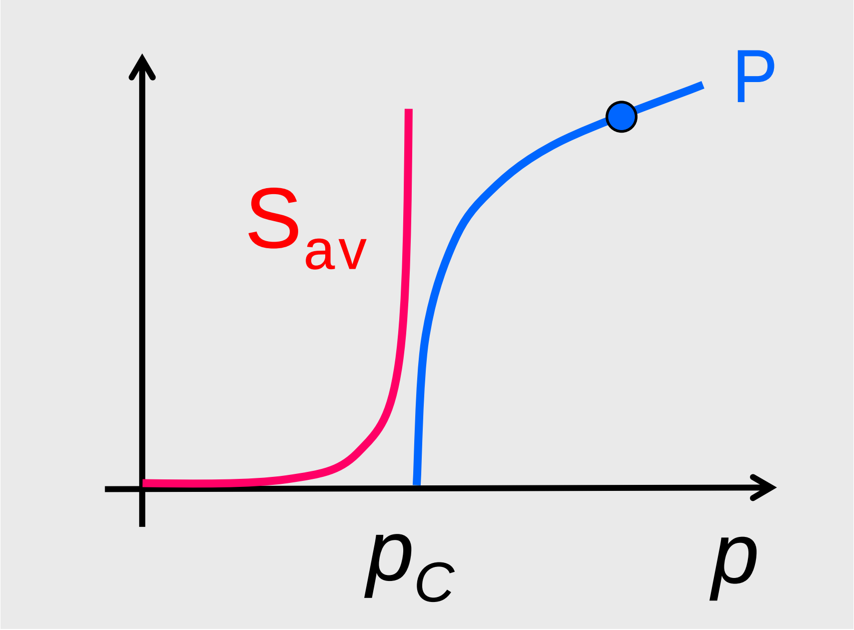
$$s_{avg} = \frac{\sum_{s>0} s^2 n_s(p)}{\sum_{s>0} s n_s(p)}$$

...plays a role similar to Boltzmann distribution f(E)

average cluster vs. infinite cluster



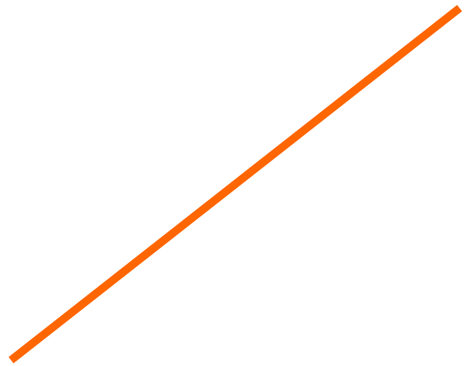
$$s_{avg} = \frac{\sum_{s>0} s^2 n_s(p)}{\sum_{s>0} s n_s(p)}$$



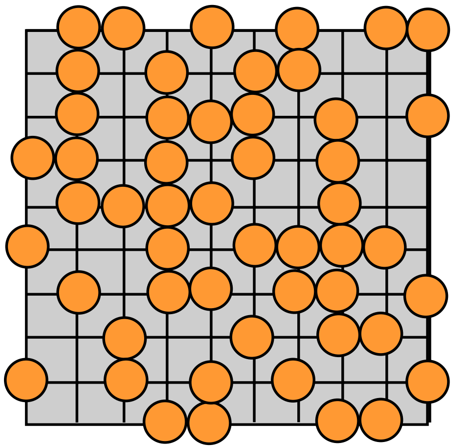
basic concepts: dimension of a surface

D=2

D=1



D=0



D=?

outline

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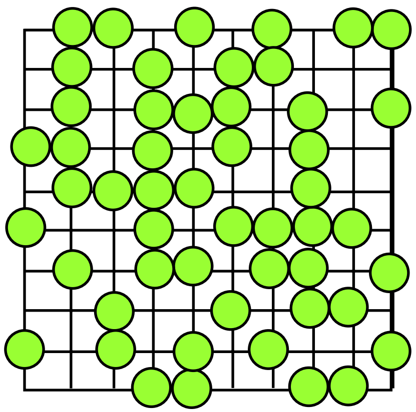
Application Notes: Nanocrystal Flash

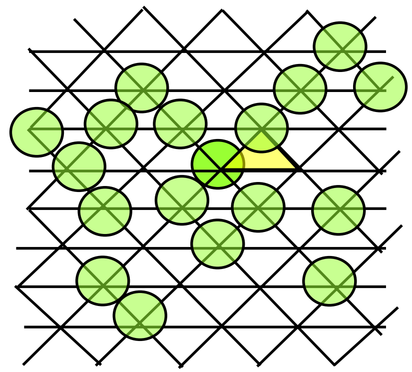
calculation of percolation threshold

Square



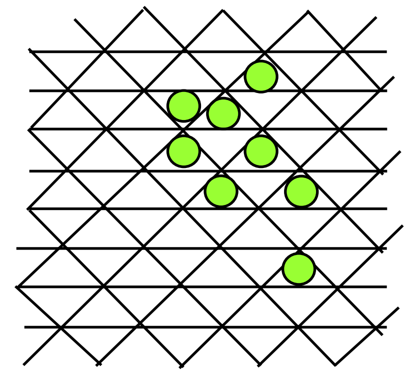
p_c = 0.593

Triangular



p_c = 0.500

Hexagonal

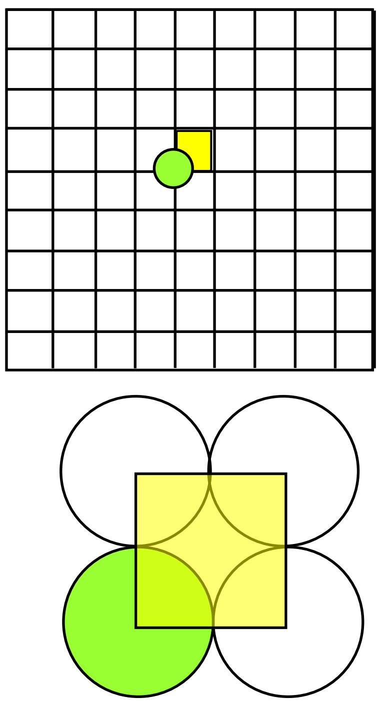


p_c = 0.697

Percolation threshold (p_c=N_c/N_T) depends on lattice, there is something wrong here !

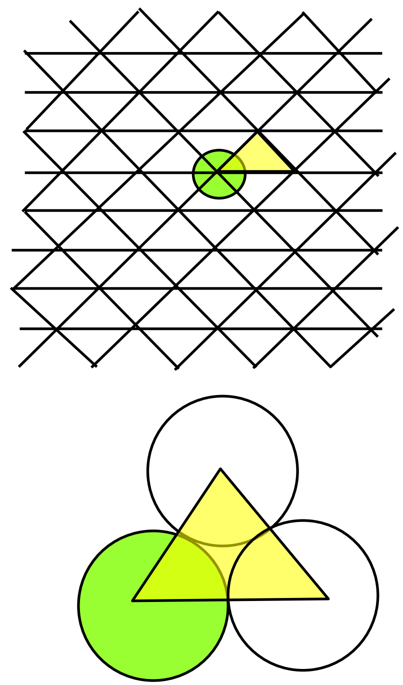
area fraction fill-factor $F \equiv A_{element} / A_{cell}$

Square



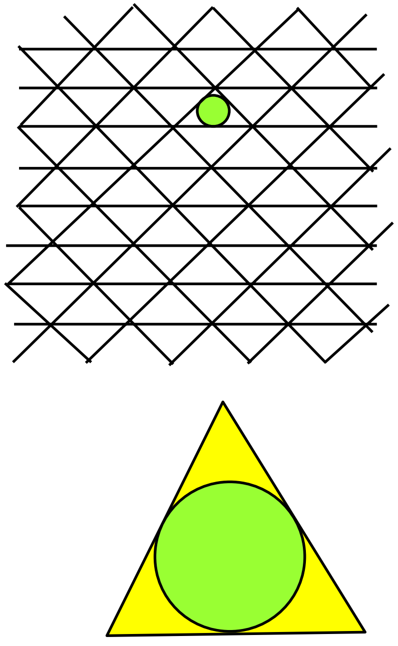
$$F = \frac{\pi}{4}$$

Triangular



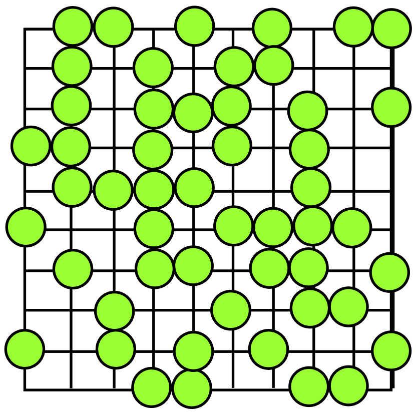
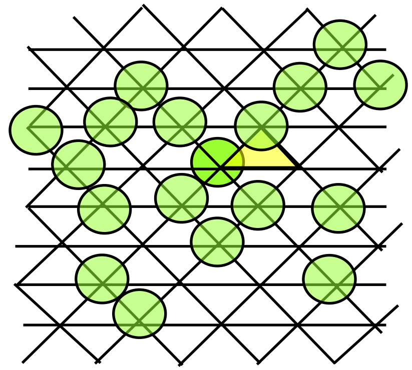
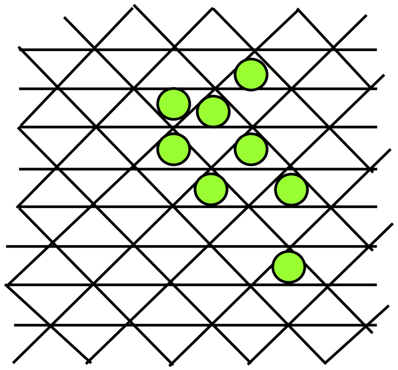
$$F = \frac{\pi}{2\sqrt{3}}$$

Hexagonal



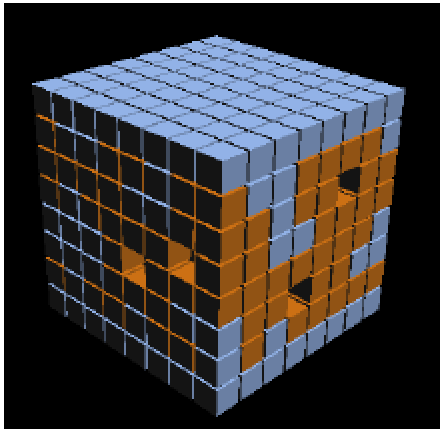
$$F = \frac{\pi}{3\sqrt{3}}$$

(F x p_c) is universal ….

Square	Triangular	Hexagonal
		
p_c = 0.593	p_c = 0.500	p_c = 0.697
$F = \frac{\pi}{4}$	$F = \frac{\pi}{2\sqrt{3}}$	$F = \frac{\pi}{3\sqrt{3}}$
Fp_c ~ 0.45	Fp_c ~ 0.45	Fp_c ~ 0.42

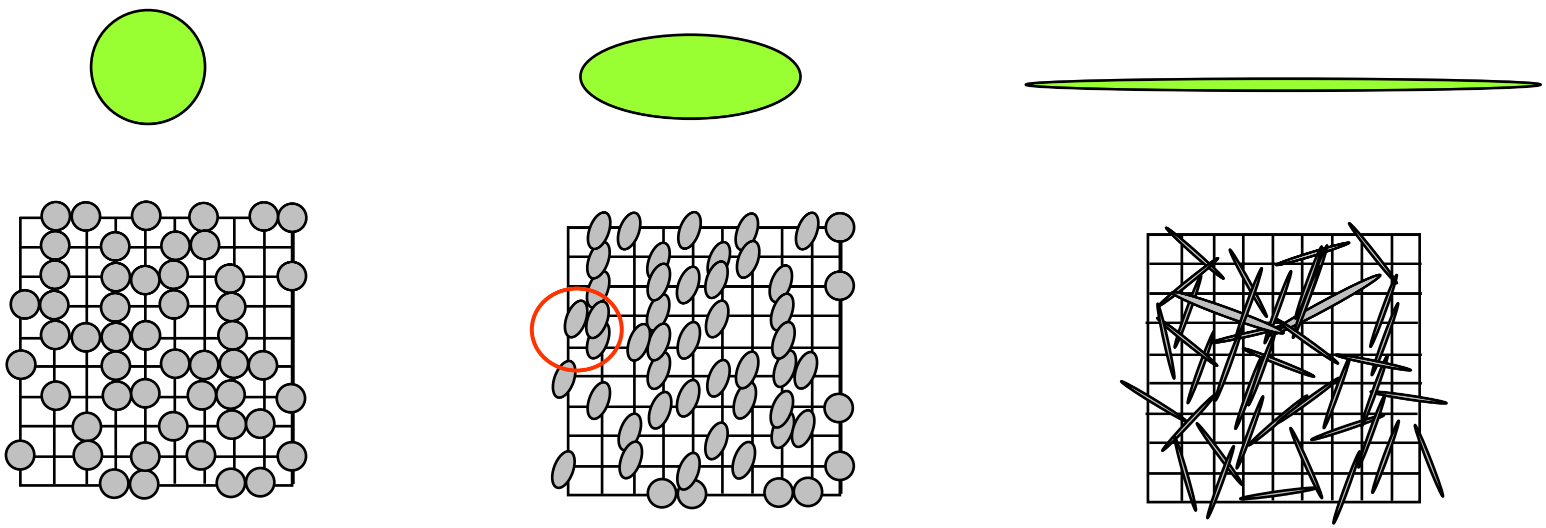
HW: Percolation in 3D lattices

For simple cubic lattice site percolation, $Fp_c \sim 0.16$ and $p_c \sim 0.311$. Here F is the volume fill fraction, not area fill fraction.



Use the universality of Fp_c to show that the percolation threshold for FCC lattice must be approximately 0.1

percolation involving other shapes

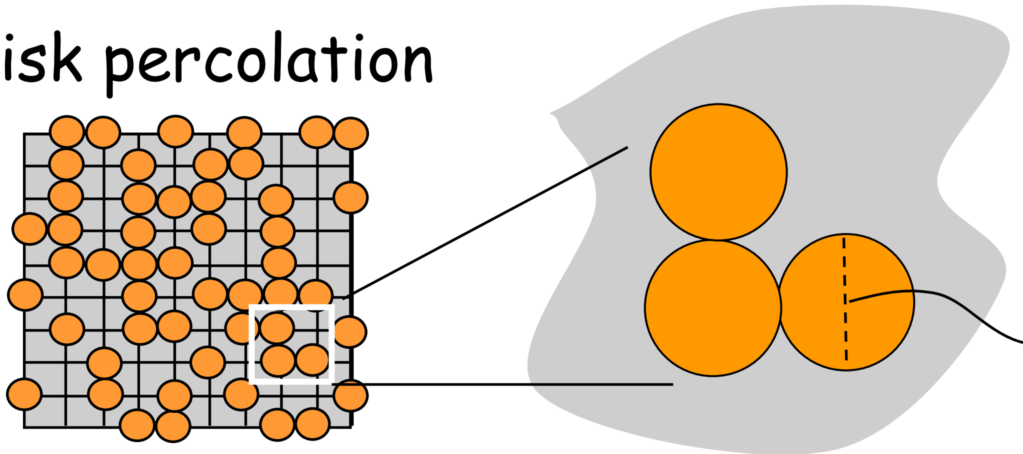


How do I determine the percolation threshold?

$Fxp_c \sim 0.45$ will not work, unfortunately !

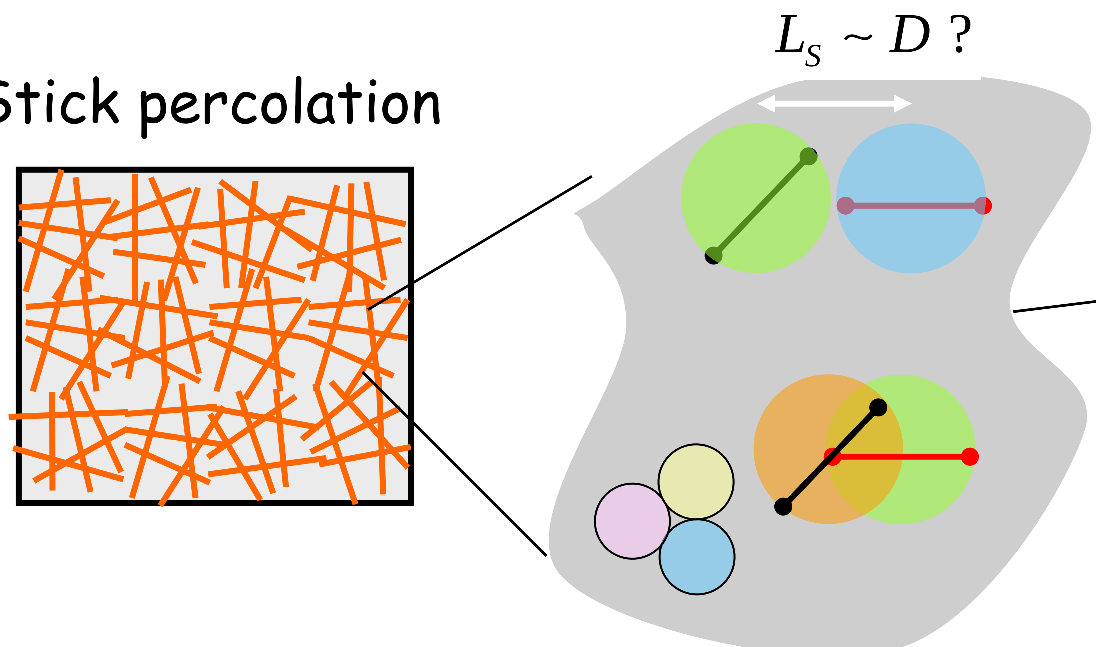
excluded area … first an intuitive result

Disk percolation



$$N_C \approx \frac{1}{\frac{\pi D^2}{4}} = \frac{4}{\pi D^2}$$

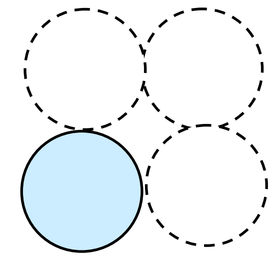
Stick percolation



$$N_C \approx \frac{1}{\frac{\pi\left(L_S/2\right)^2}{4}} = \frac{4^2}{\pi L_S^2}$$

$$N_{C,exact} = \frac{4.26^2}{\pi L_S^2}$$

the concept of excluded area .....



For disks on arbitrary grid ...

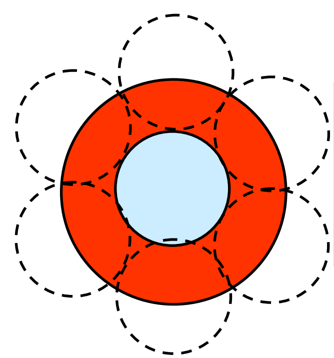
$$F \times p_c = \frac{A_{element}}{A_{cell}} \bullet \frac{N_C}{N_T} \approx 0.45$$

$$A_{element} = \frac{\pi}{4}(D)^2$$

X 4

For arbitrary shape on arbitrary grid ...

$$\frac{A_{ex}}{A_{cell}} \bullet \frac{N_C}{N_T} \approx$$

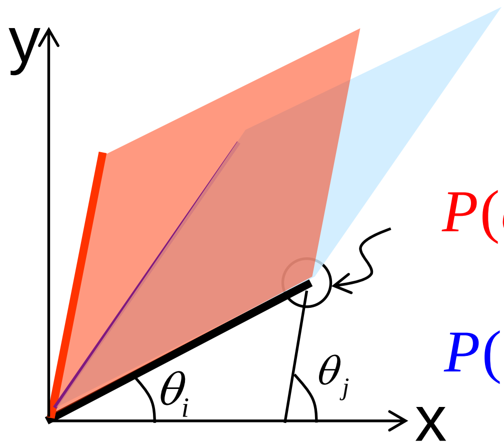


$$A_{ex} = \frac{\pi}{4}(2 \bullet D)^2$$

Percolation begins when excluded volume is routinely breached

excluded volume for a stick ....

$$A_{\theta_i,\theta_j} = L_S \; L_S \; \sin(\theta_i - \theta_j)$$



$$P(\theta_i) = \frac{1}{\pi}$$

$$P(\theta_j) = \frac{1}{\pi}$$

$$A_{ex} = \int_{-\pi/2}^{\pi/2} d\theta_i P(\theta_i) \int_{-\pi/2}^{\pi/2} d\theta_j P(\theta_j) \times A_{\theta_i,\theta_j}$$

$$= \frac{2}{\pi} L_S^2$$

excluded volume for a stick ....

$$\frac{A_{ex}}{A_{cell}} \bullet \frac{N_C}{N_T} \approx 1.8$$

$$A_{ex} N_C = 1.8$$

$$\frac{2L_S^2}{\pi} \frac{N_C}{A_{cell} N_T} \approx 1.8$$

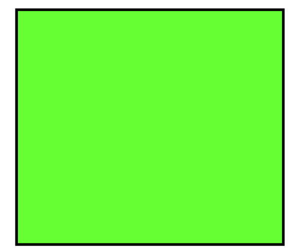
$$N_C \approx \frac{0.9\pi}{L_S^2} \text{ area}^{-1}$$

percolation threshold correct within a factor of 2 !

HW: excluded volume for other shapes ..

curved stick ...

square ...



Ans. $$A_{ex} = \frac{2}{\pi} L_{chord}^2$$

$$(\text{if } L_{chord} < \frac{R}{2})$$

$$A_{ex} = 2L^2 \left(1 + 2/\pi + 4/\pi^2\right)$$

Hint. Compare with circle

Hint.
Use the stick algorithm

For general shape, use the Monte Carlo code posted

outline

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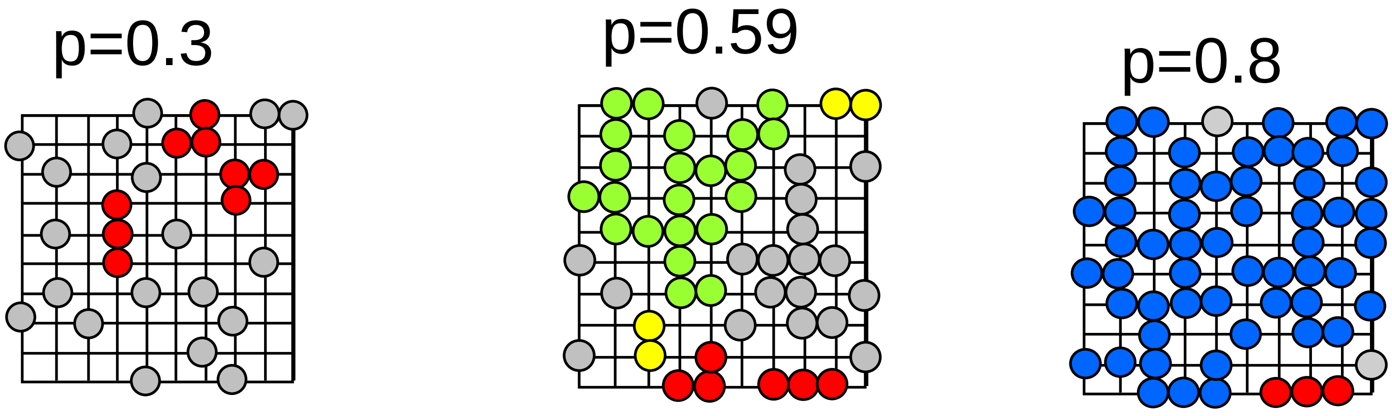
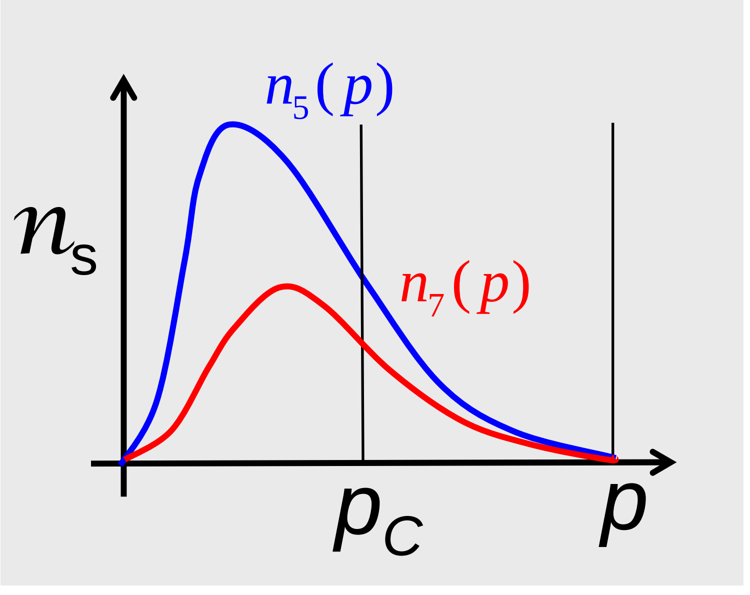
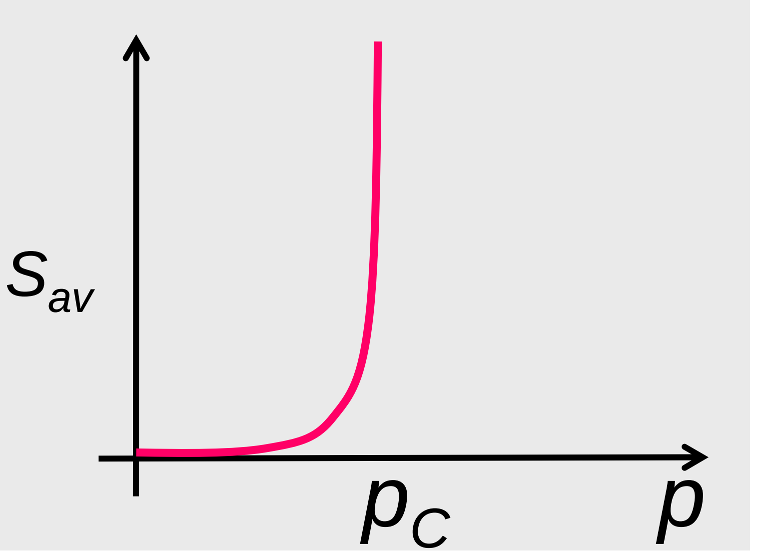
Application Notes: Nanocrystal Flash

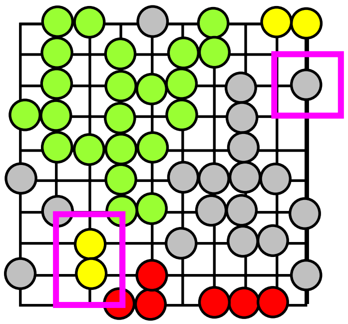
cluster-size distribution

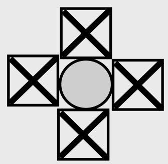




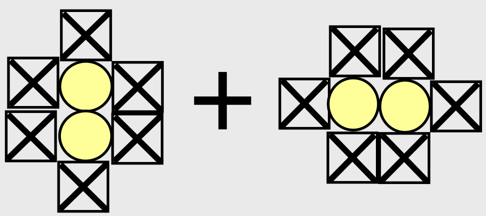


small-cluster size distribution

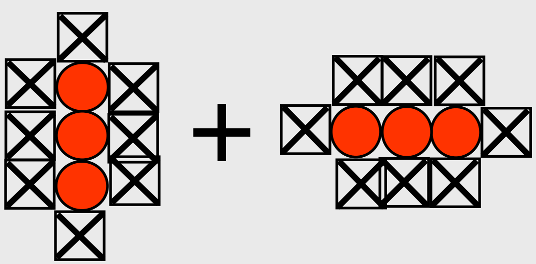




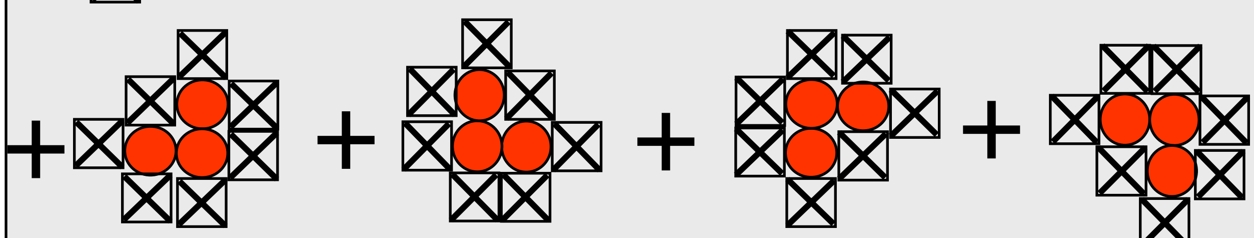
$$n_1(p) = 1 \times p \times (1-p)^4$$



$$n_2(p) = 2 \times p^2 \times (1-p)^6$$



$$n_3(p) = 2 \times p^3 \times (1-p)^8$$



$$+\, 4 \times p^3 \times (1-p)^7$$

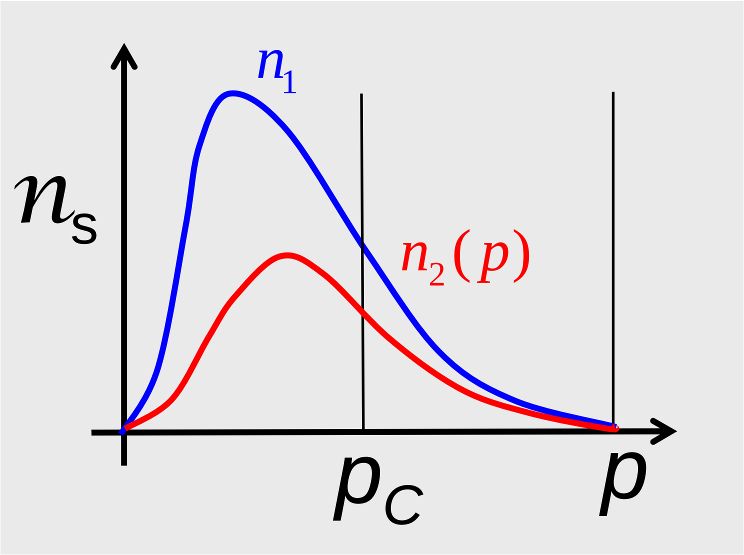
features of cluster-size distribution

$$n_1 = 1 \times p \times (1-p)^4$$

$$n_2 = 2 \times p^2 \times (1-p)^6$$

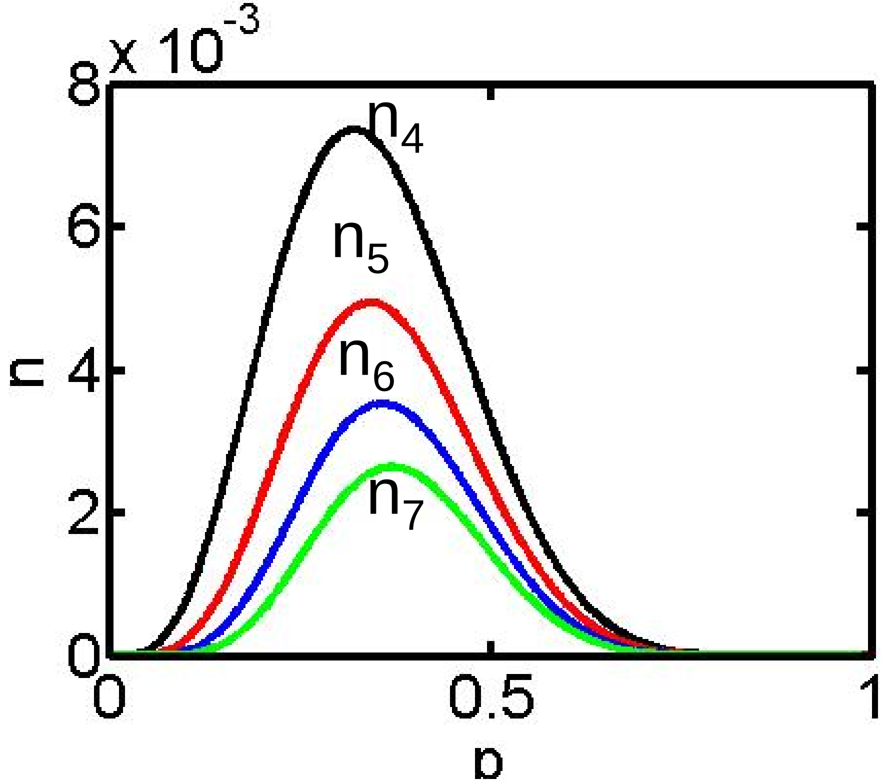
$$n_3 = 2 \times p^3 \times (1-p)^8$$
$$+4 \times p^3 \times (1-p)^7$$

- 'Zeros' at p=0,1 with single peak
- Peak shifts towards p_c with s (e.g. s=1 is 0.2, s=2 is 0.25; s=3 is 0.29)
- General form: $n_s(p) = \sum_t g_{st} \times p^s \times (1-p)^t$
  : g_{st} increases exponentially.

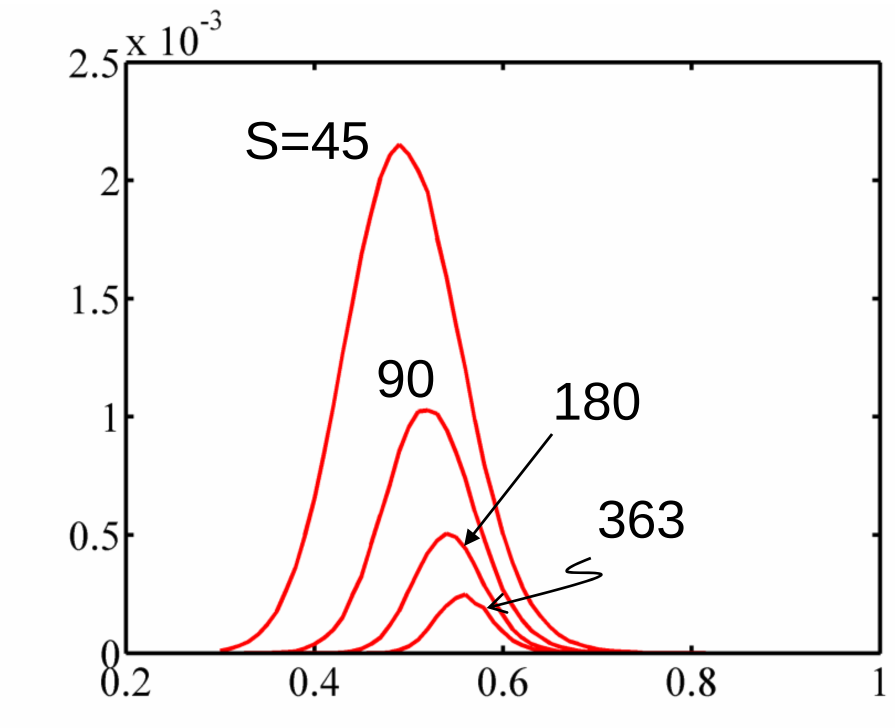


numerical plots for cluster-size distribution

Analytically ...

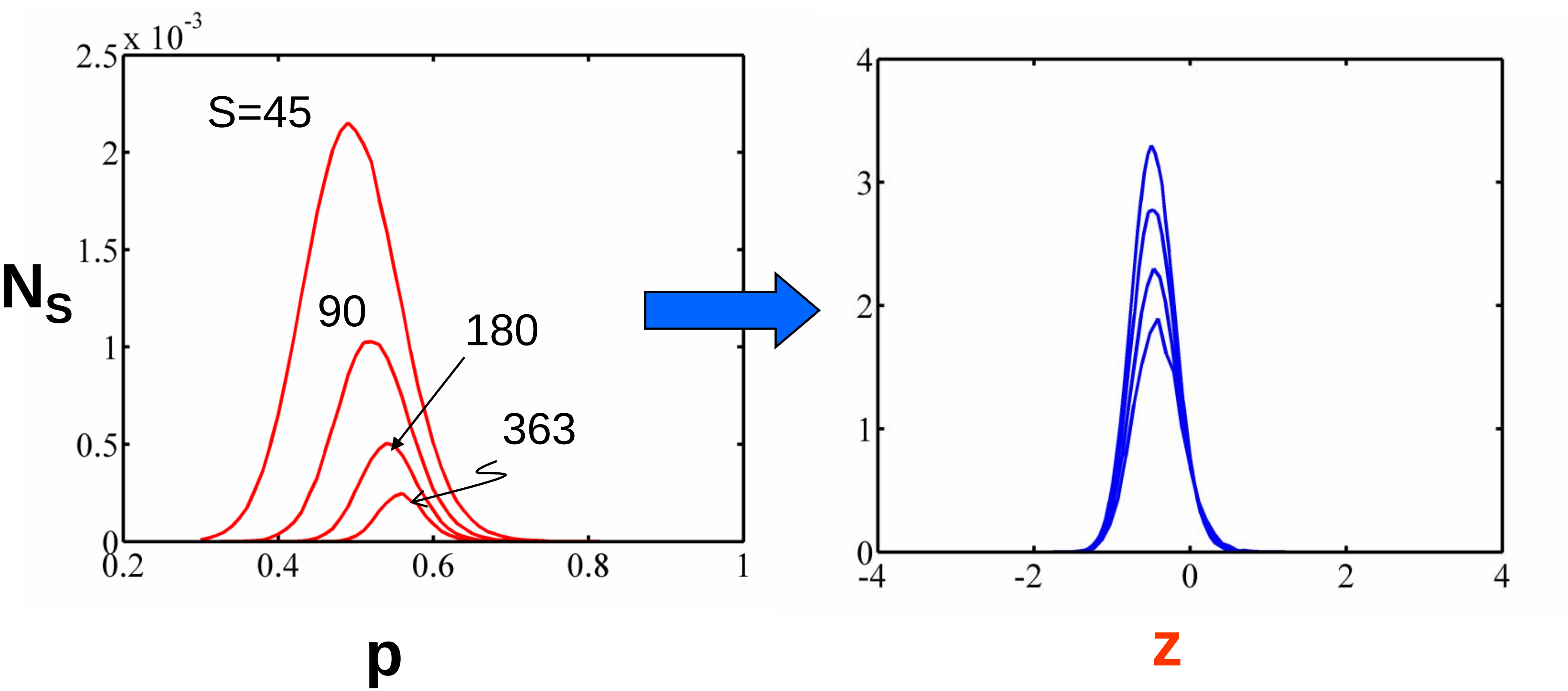


by computer ...



$$\left[p_{\max}(s) - p_c \right] s^{0.395} \approx 0.45 \qquad p_c \sim 0.6$$

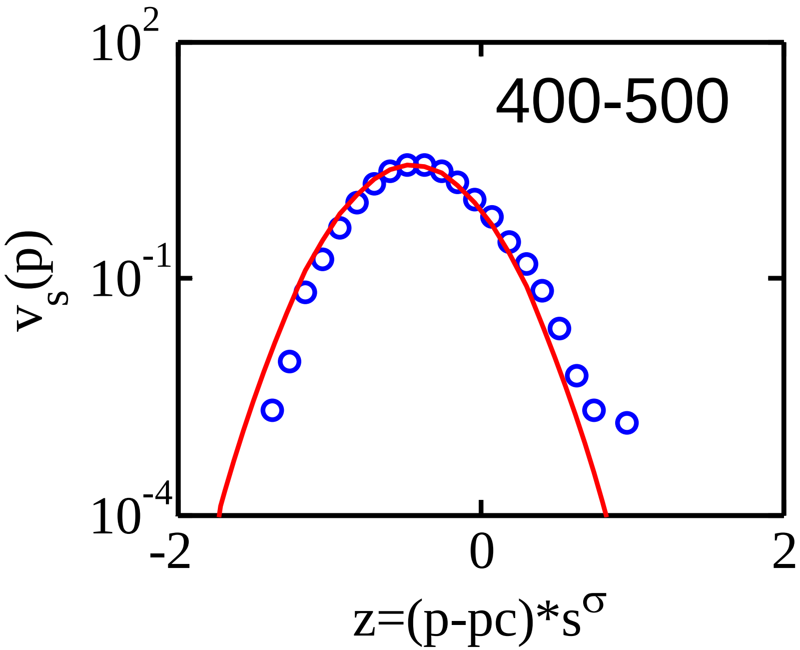
scaling of cluster sizes

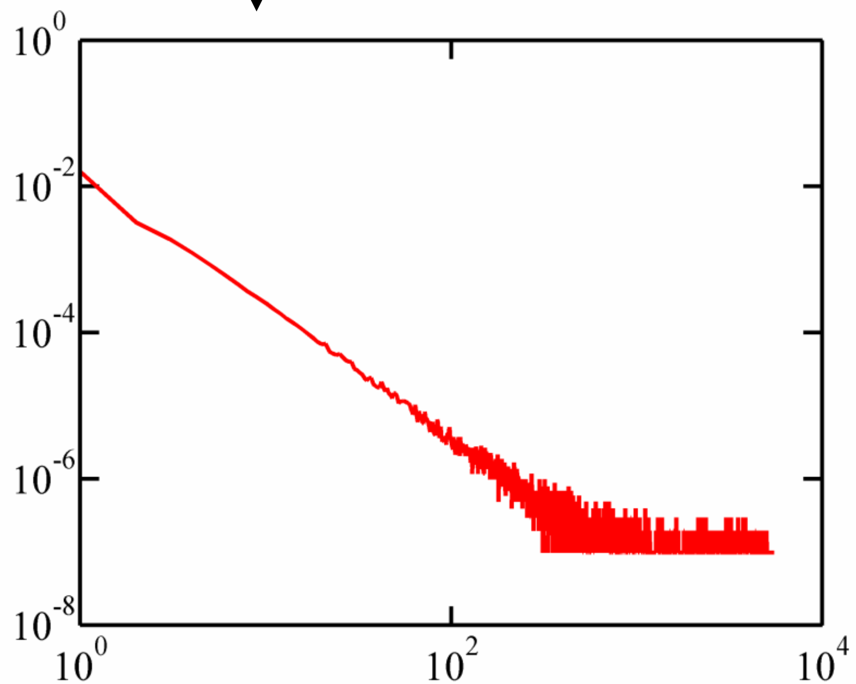


$$z \equiv \left[p(s) - p_c \right] s^{0.395}$$

for reasonably large cluster-sizes (s>20)

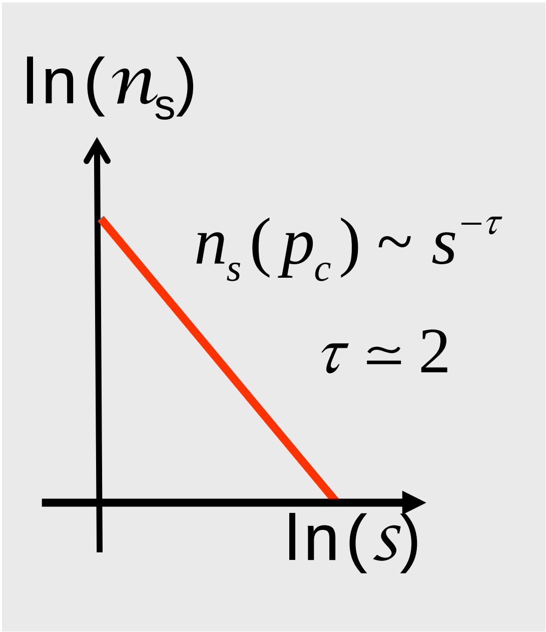
$$n_s(p) \approx e^{-c\left[(p-p_c)s^{\sigma}+0.45\right]^{\alpha}} \; n_s(p_c)$$



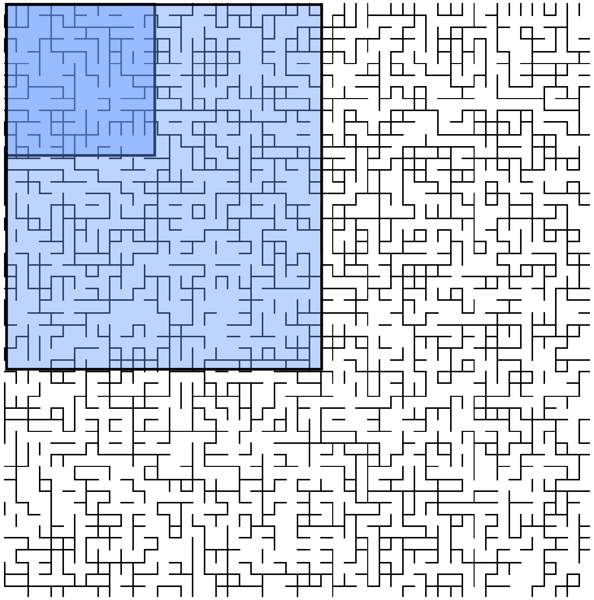


self-similarity and scale-invariance

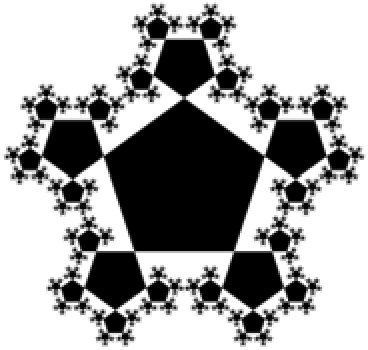
self-similarity

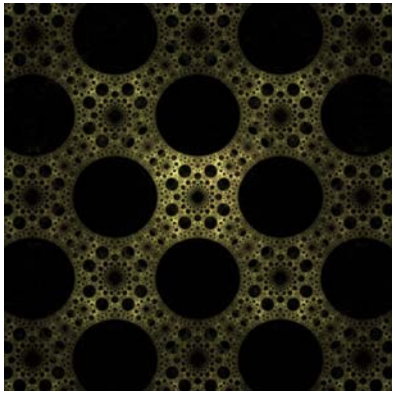


irregular self-similarity



regular self-similarity





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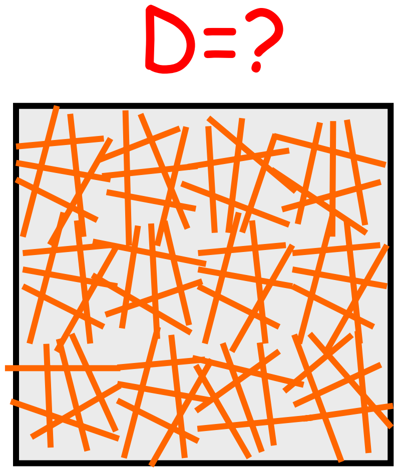
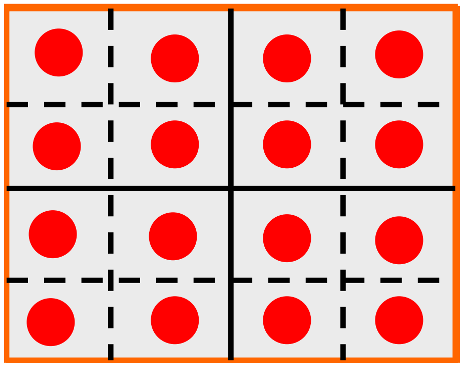
Application Notes: Nanocrystal Flash

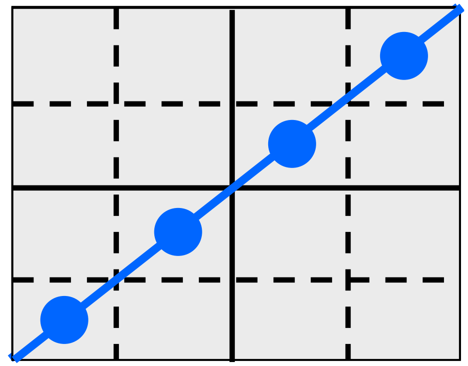


classification of surfaces…

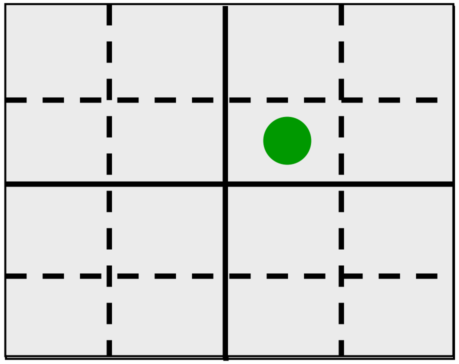
Fractal Dimension (D_F)- Box counting technique



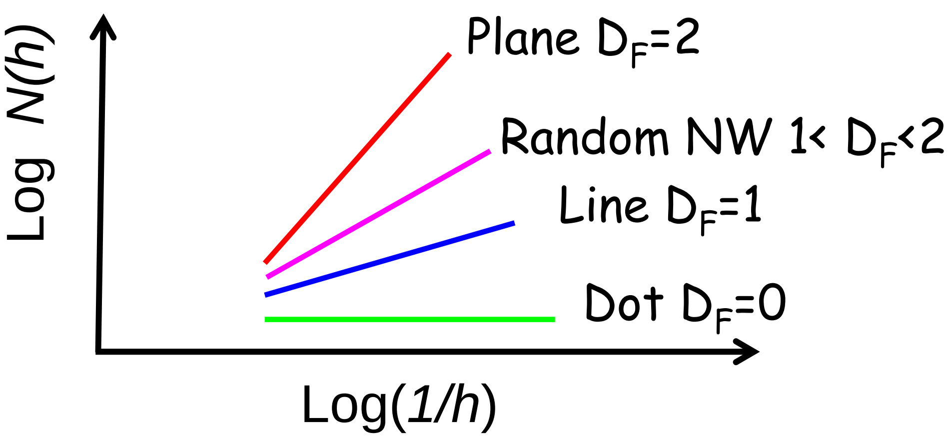
$N(h) \sim h^2$



$N(h) \sim h^1$



$N(h) \sim h^0$



dimension of Cantor dust

h	1/3
N	2

h	1/9
N	4

h	1/27
N	8

h	$1/3^n$
N	2^n

$$D_{F,1} = \frac{\log(N)}{\log(1/h)} = \frac{\log(2^n)}{\log(3^n)} = 0.63$$

Bigger than point,
but smaller than line

$$\text{In general, } D_{F,1} = \frac{\log(m)}{\log(n)}$$

.... keep m piece

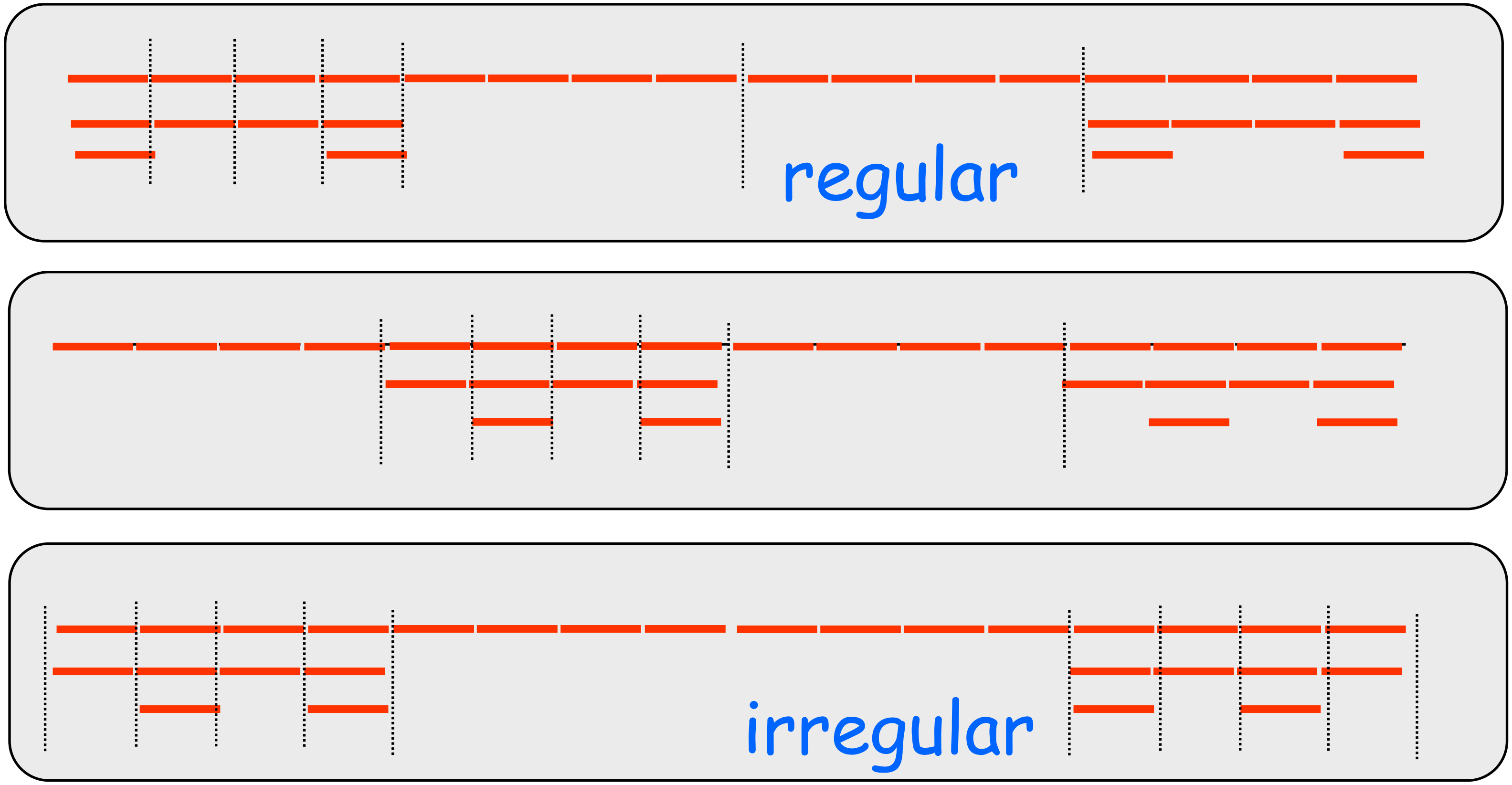
of n pieces

regular and irregular fractals

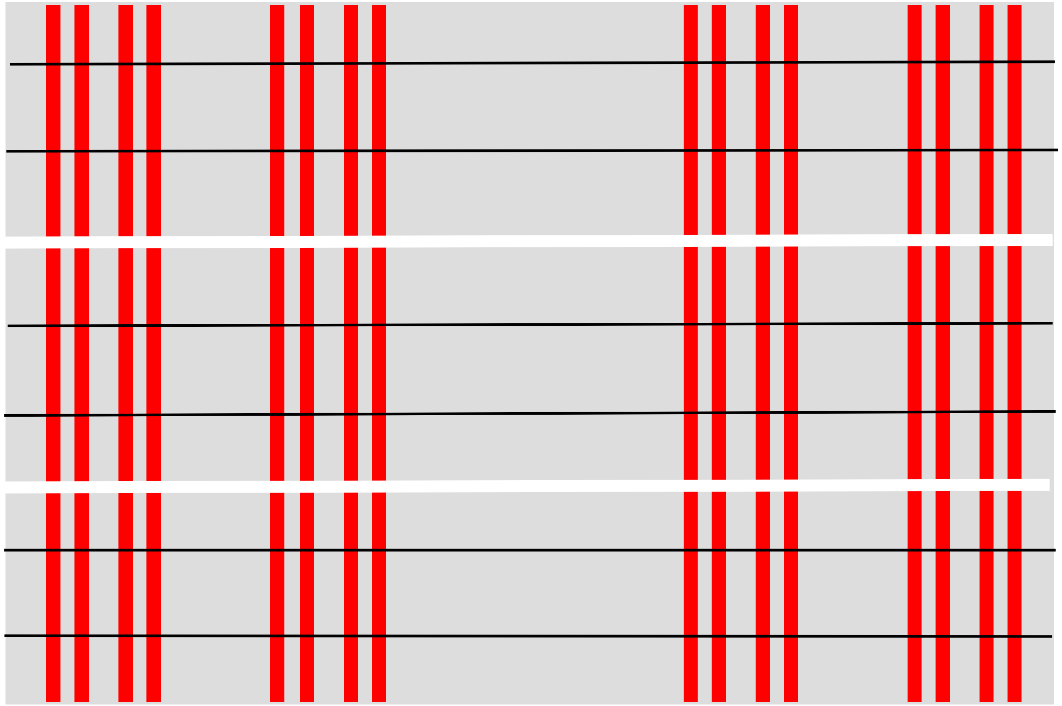
$$D_{F,1} = \frac{\log(m)}{\log(n)}$$

.... keep m piece

of n pieces



dimension of quasi-2D cantor stripes



h	1/3
N	6

h	1/9
N	36

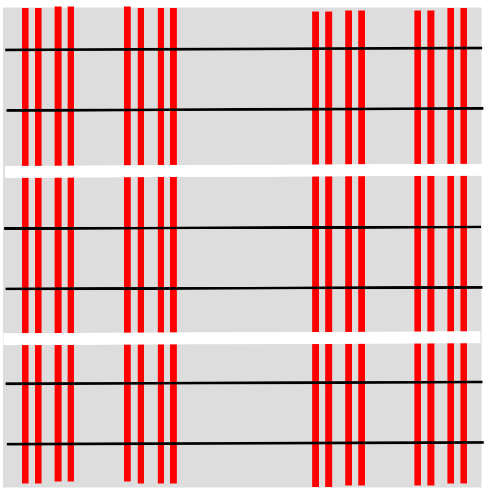
h	1/27
N	216

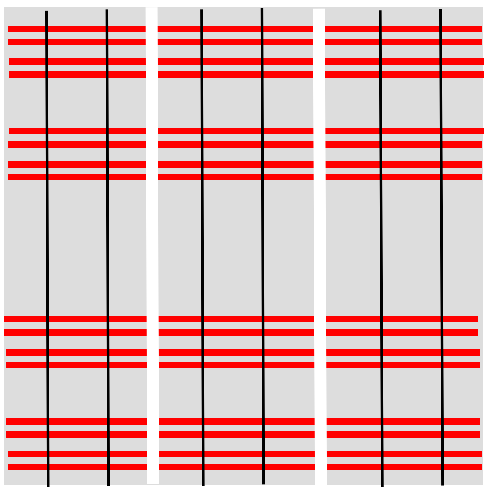
h	$1/3^n$
N	$3^n 2^n$

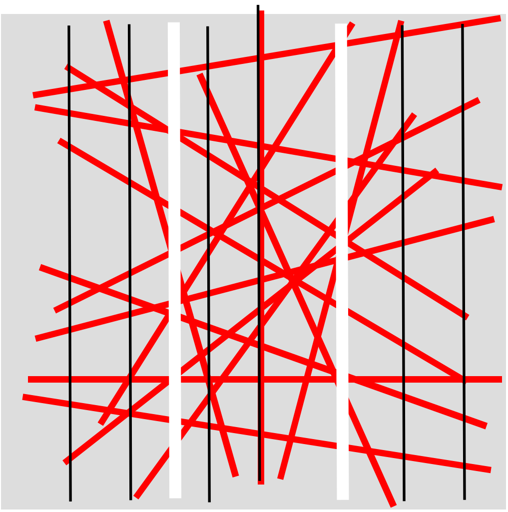
$$D_{F,2} = \frac{\log(N)}{\log(1/h)} = \frac{\log(3^n) + \log(2^n)}{\log(3^n)} = 1 + \frac{\log(2^n)}{\log(3^n)} = 1 + DF_x$$

In general, $D_{F,3} = DF_x + DF_y + DF_z$

same DF, but different geometry



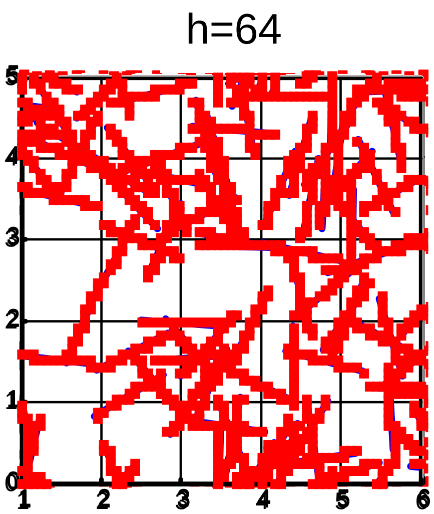


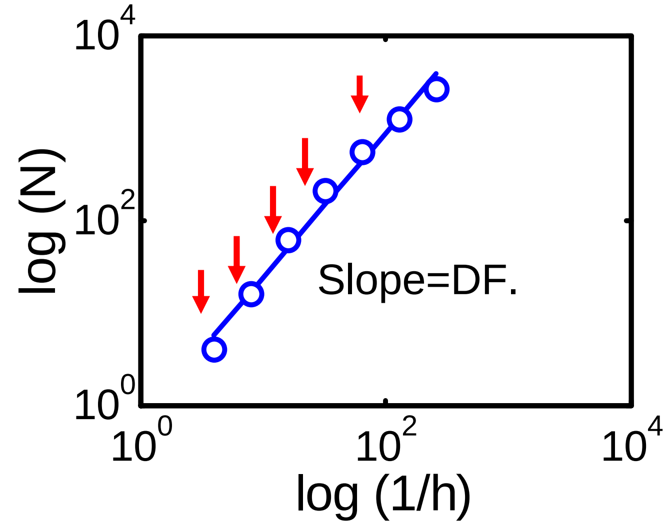


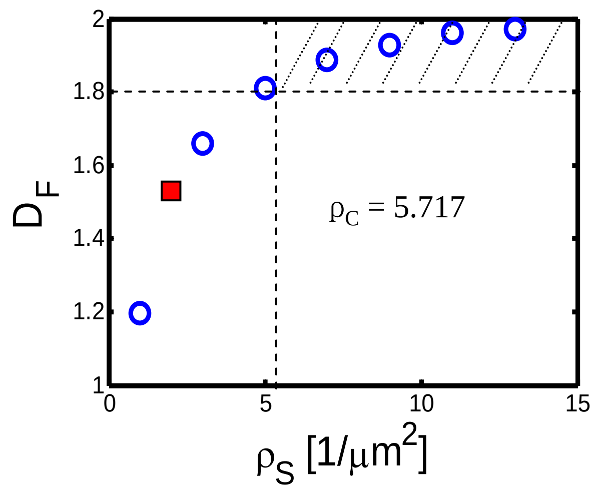
same dimension,
because DF=log(m)/log(n)

What about this
irregular fractal?

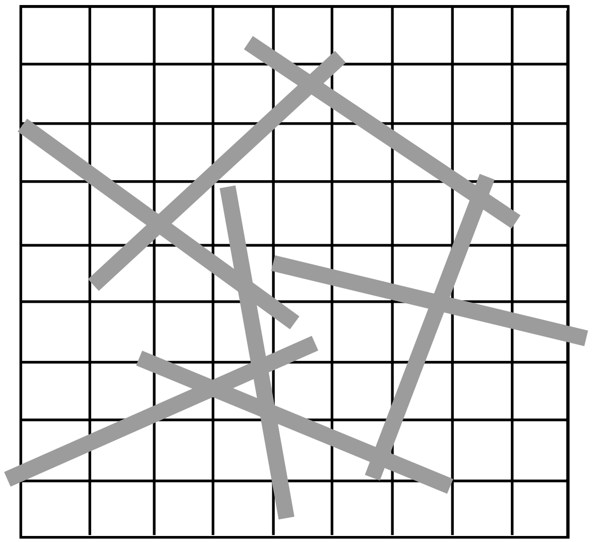
dimension of a irregular fractal

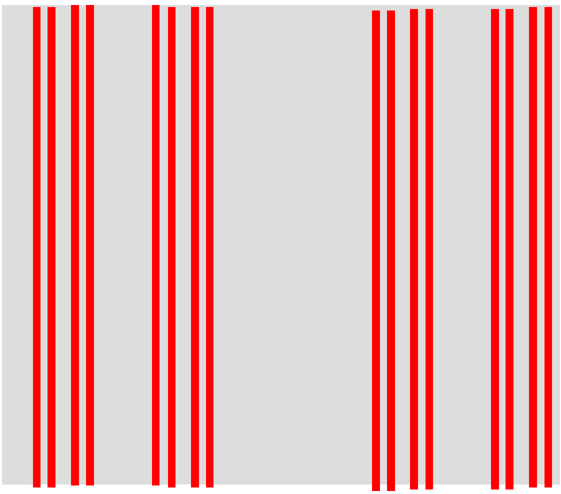






cantor transform

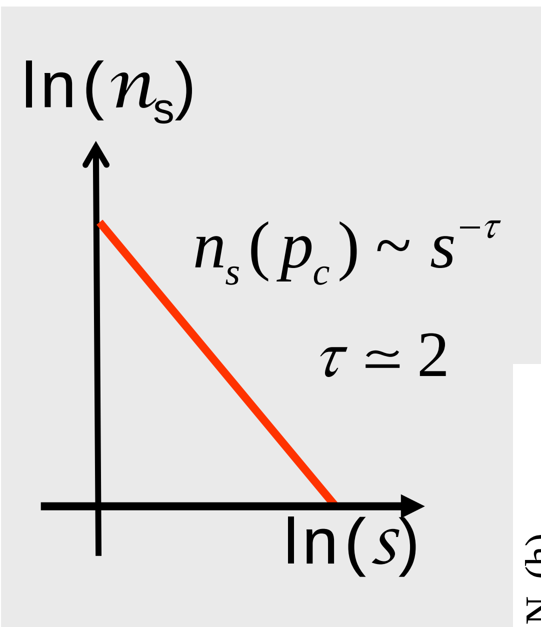


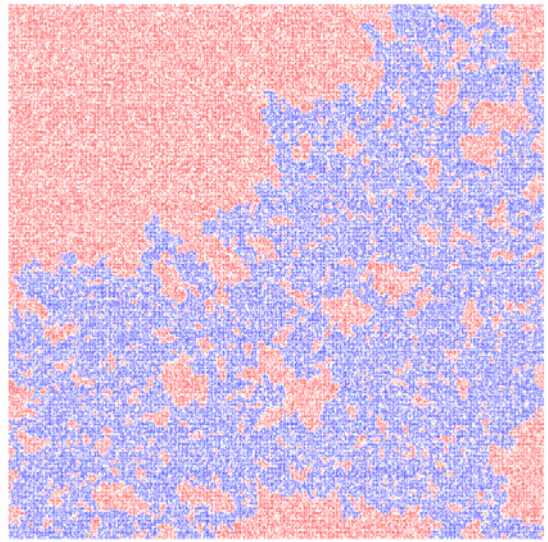


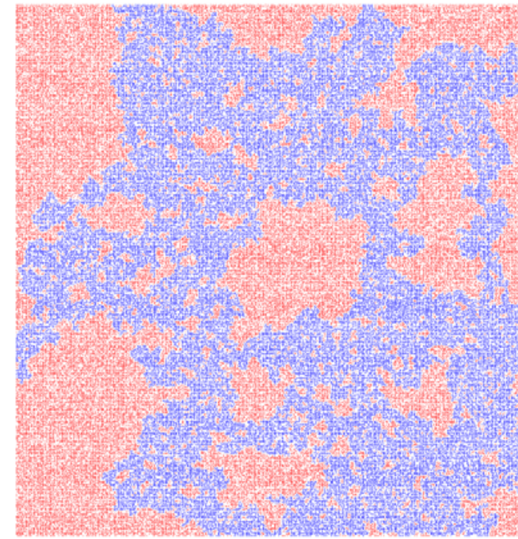
Preserve D_F during transformation

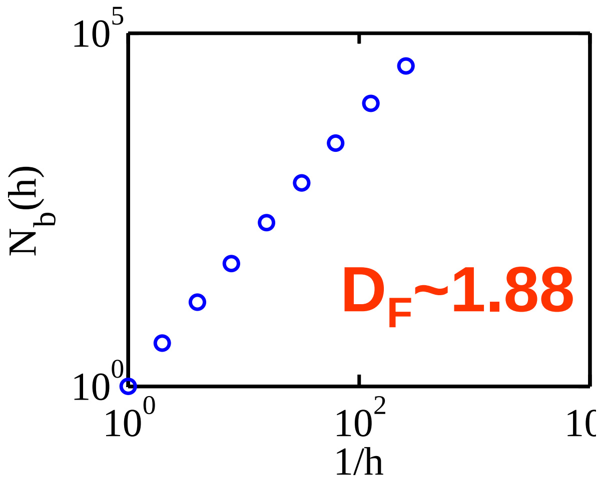
fractal dimension at percolation

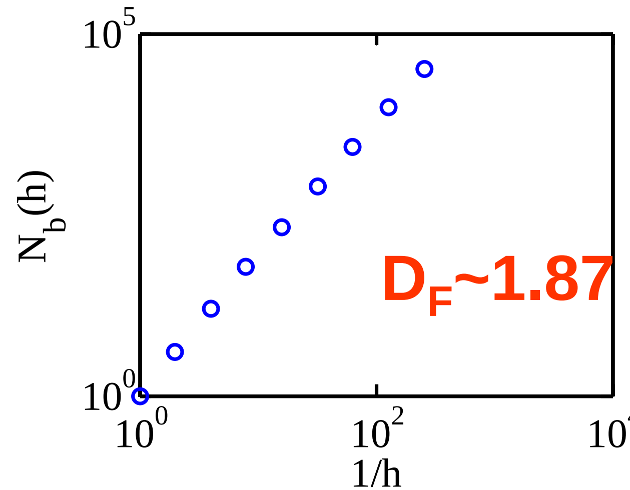
self-similarity











Summary

- Discussed three key concepts of percolative transport: percolation threshold, island size distribution, and fractal dimension

- The concept of excluded volume provides a (nearly) geometry independent way for calculating the percolation threshold for arbitrarily shaped objects on arbitrary grid.

- Distribution of island sizes is also described by simple formula with universal constants. At percolation threshold, the island sizes are self-similar and scale invariant.

- Fractal dimension provides a generalized technique to describe the dimension of any surfaces, even those defined by randomly oriented sticks.