Information theory for complex systems

Pattern formation in chemical self-organizing systems

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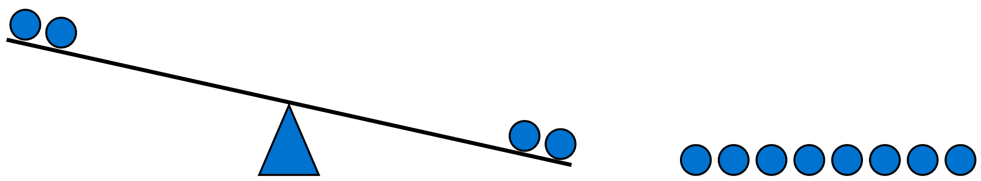
Balance Ball Puzzle

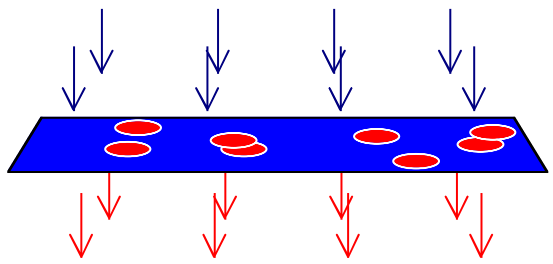
- You have 12 balls, all have the same weight except one that deviates. By using a balance three times you should be able to find the deviating ball, and tell whether it is lighter or heavier. The task is to find such a procedure.



Gray-Scott model (self-replicating spots)

$$U + 2V \rightarrow 3V$$
$$V \rightarrow G$$

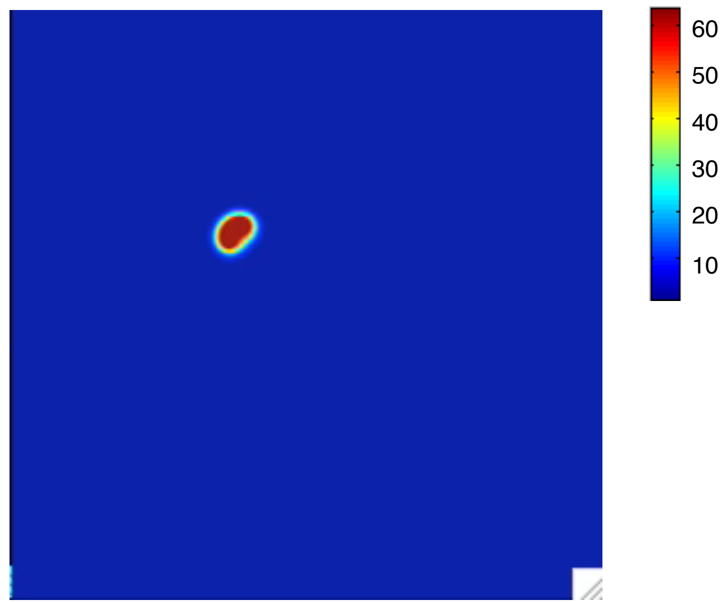
Gray & Scott, *Chem Eng Sci* (1984),
Pearson, *Science* (1993), and Lee et al, (1993).



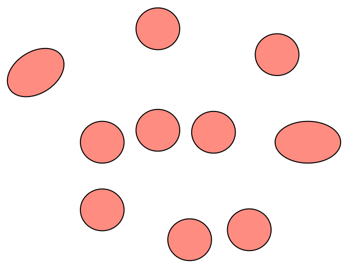
Reaction-diffusion dynamics:

$$\frac{\partial U}{\partial t} = D_u \nabla^2 U - (U - k_{back} V) V^2 + F(1-U)$$

$$\frac{\partial V}{\partial t} = D_v \nabla^2 V + (U - k_{back} V) V^2 - kV - FV$$

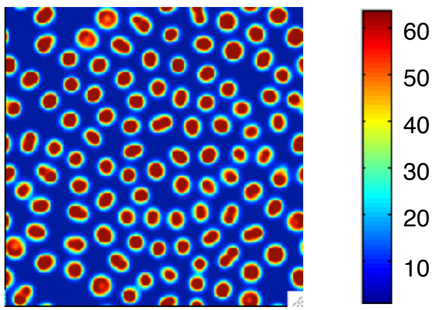


Levels of description



population dynamics of self-replicating spots

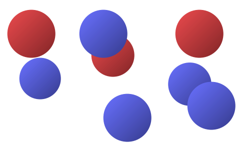
$$\frac{\partial N}{\partial t} = \alpha N(1 - f(N))$$



reaction-diffusion equations

$$\frac{\partial U}{\partial t} = D_u \nabla^2 U - (U - k_{back} V)V^2 + F(1-U)$$

$$\frac{\partial V}{\partial t} = D_v \nabla^2 V + (U - k_{back} V)V^2 - kV - FV$$



mechanistic, single reactions

$$U + 2V \rightarrow 3V$$

Information in pattern formation

Three types of information characteristics

- Information on dynamics (”genetics”), I_{genetics}
- Information from fluctuations or noise (symmetry breaking), I_{noise}
- Information in free energy (driving force), I_{energy}

Typically:

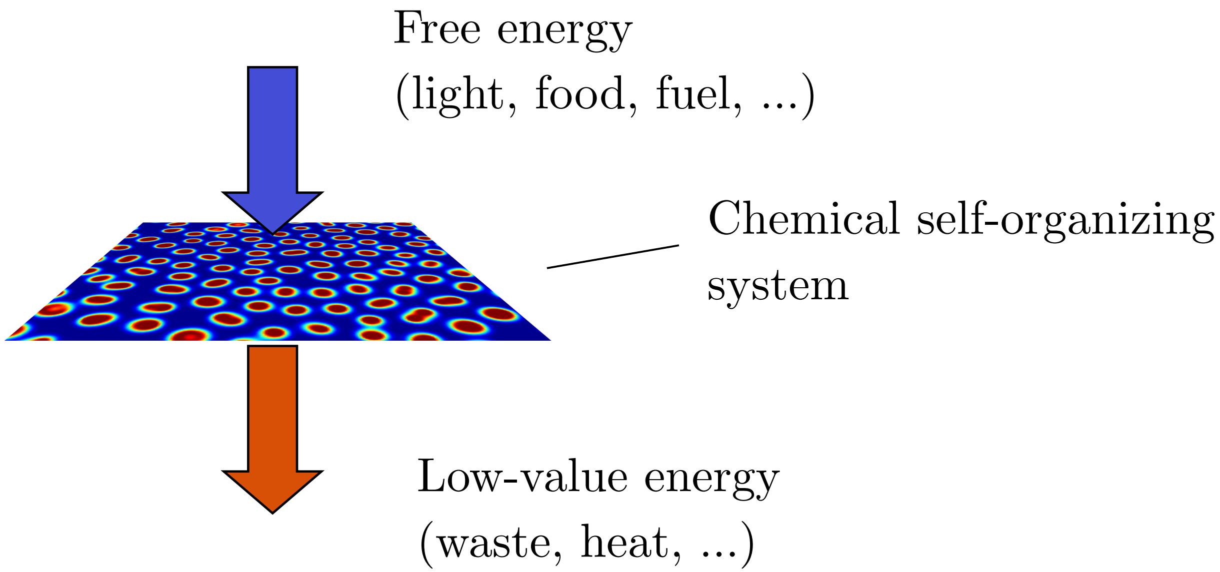
$$I_{\text{genetics}} << I_{\text{noise}} << I_{\text{energy}}$$

Information in a chemical pattern

- The relative information $K[c_0;\, c(x)]$ quantifies the information difference between an a priori description
  - c_{i0} — the equilibrium concentrations c_{i0} of the chemical components i, and
  - $c_i(x)$ — the observed spatially dependent concentrations.
- By integrating over all positions x, we get a total information K in the chemical pattern:

$$K = \int_V dx \sum_{i=1}^{M} c_i(x) \ln \frac{c_i(x)}{c_{i0}}$$

Thermodynamic context



- Second law thermodynamcis: the entropy within the system may decrease, but in total, entropy increases.
- Out-of-equilibrium, low-entropy state maintained by exporting more entropy than what is imported and produced

Free energy and information

The free energy E of a concentration pattern $c_i(x)$ can be related to the information-theoretic relative information K, and under certain conditions this relation can be written:

$$E = k_{\mathrm{B}} T_0 \frac{N}{V} \int_V dx \sum_{i=1}^{M} c_i(x) \ln \frac{c_i(x)}{c_{i0}} = k_{\mathrm{B}} T_0 \frac{N}{V} K$$

where k_{B} is Boltzmann's constant, T_0 the temperature, and N/V the molecular density.

Geometric information theory: Decomposition of information

Goal:

- Decompose the total information (free energy) into contributions from different positions and length scales.

- Derive quantities expressing flows of information that
  – obey a continuity equation for information, and
  – connect with thermodynamic constraints

Resolution – length scale

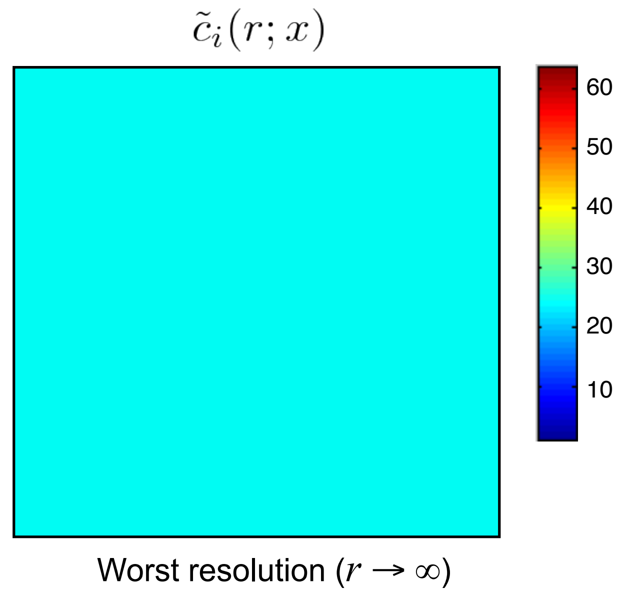
- We define the pattern of a certain component i at resolution r by "kernel smoothing" (convolution) of $c_i(x)$ with a Gaussian of width r

$$\tilde{c}_i(r;x) = \frac{1}{\sqrt{2\pi r}} \int_{-\infty}^{\infty} e^{-w^2/2r^2} c_i(x-w)\, dw$$

- with the properties

$$\tilde{c}_i(0;x) = c_i(x)$$

$$\tilde{c}_i(\infty;x) = \bar{c}_i(x)$$



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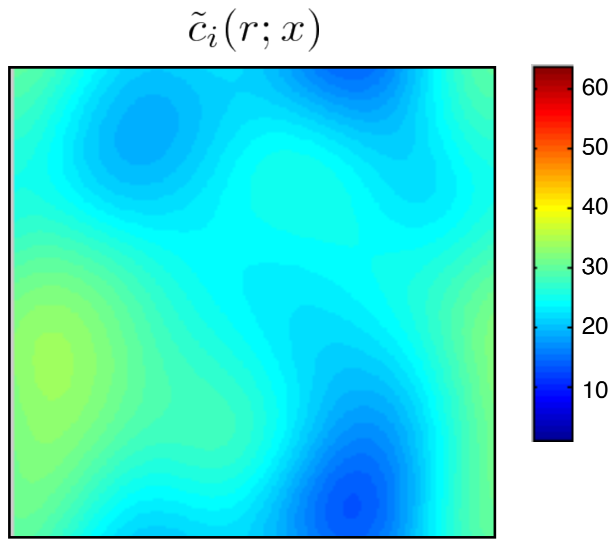

Bad resolution (high r)

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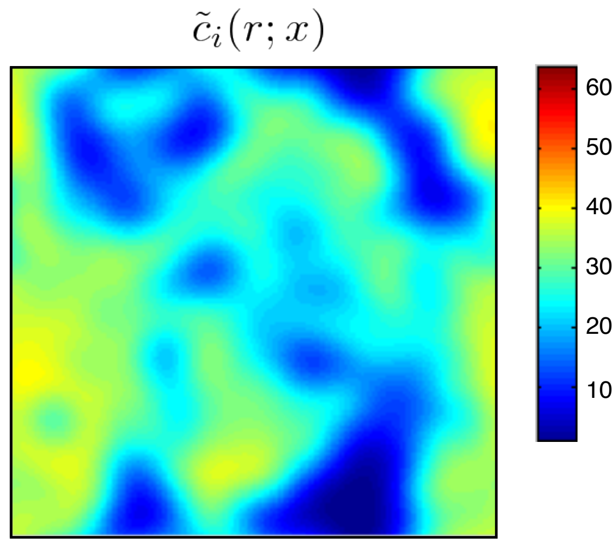

Better resolution (decreasing r)

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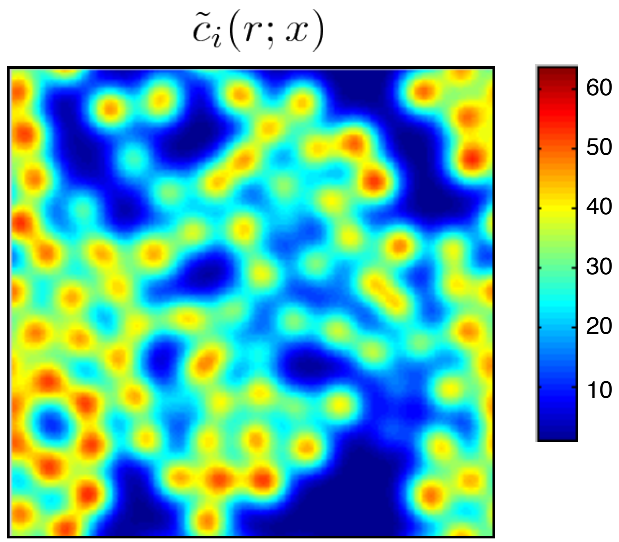

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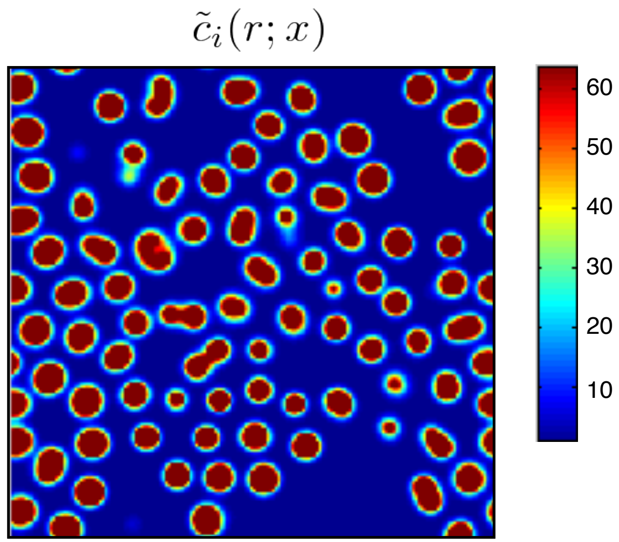
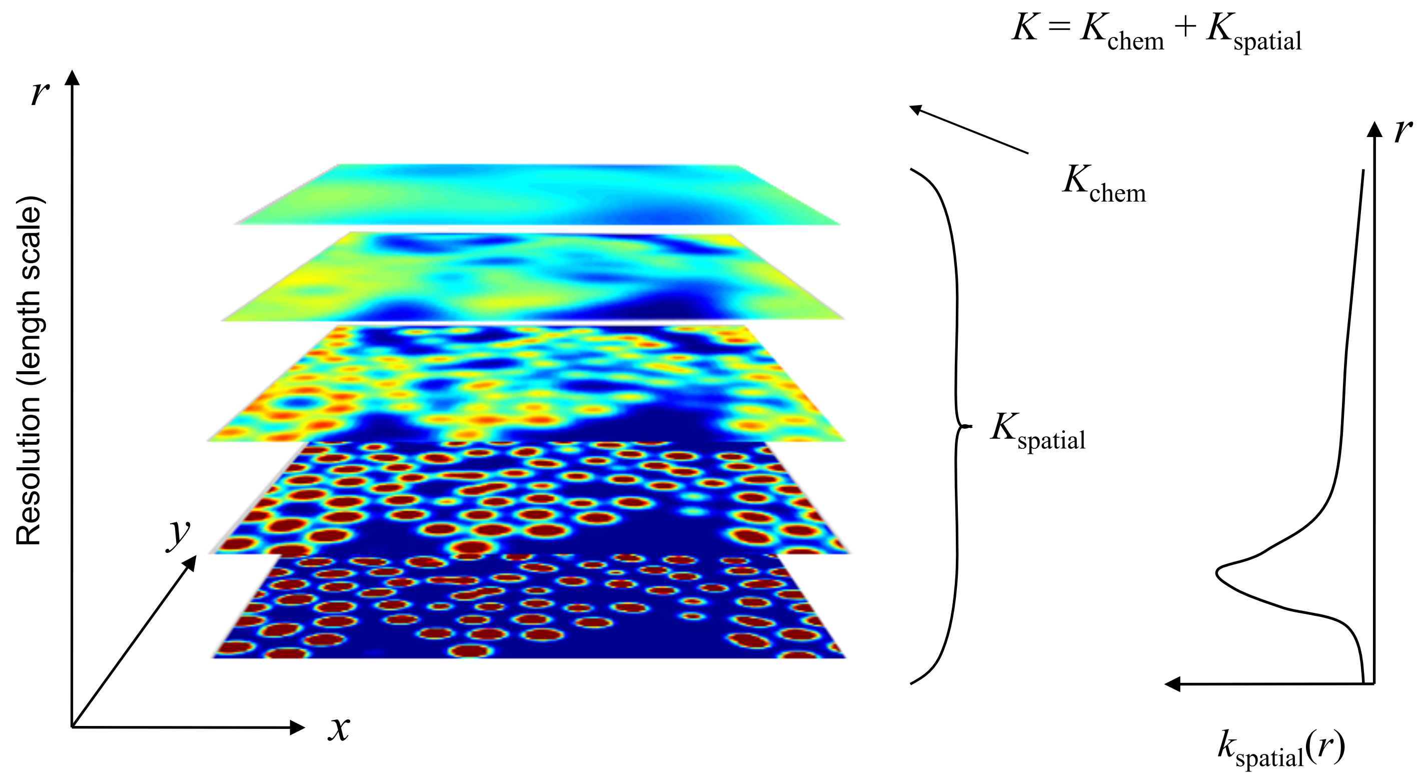


High resolution ($r \approx 0$)

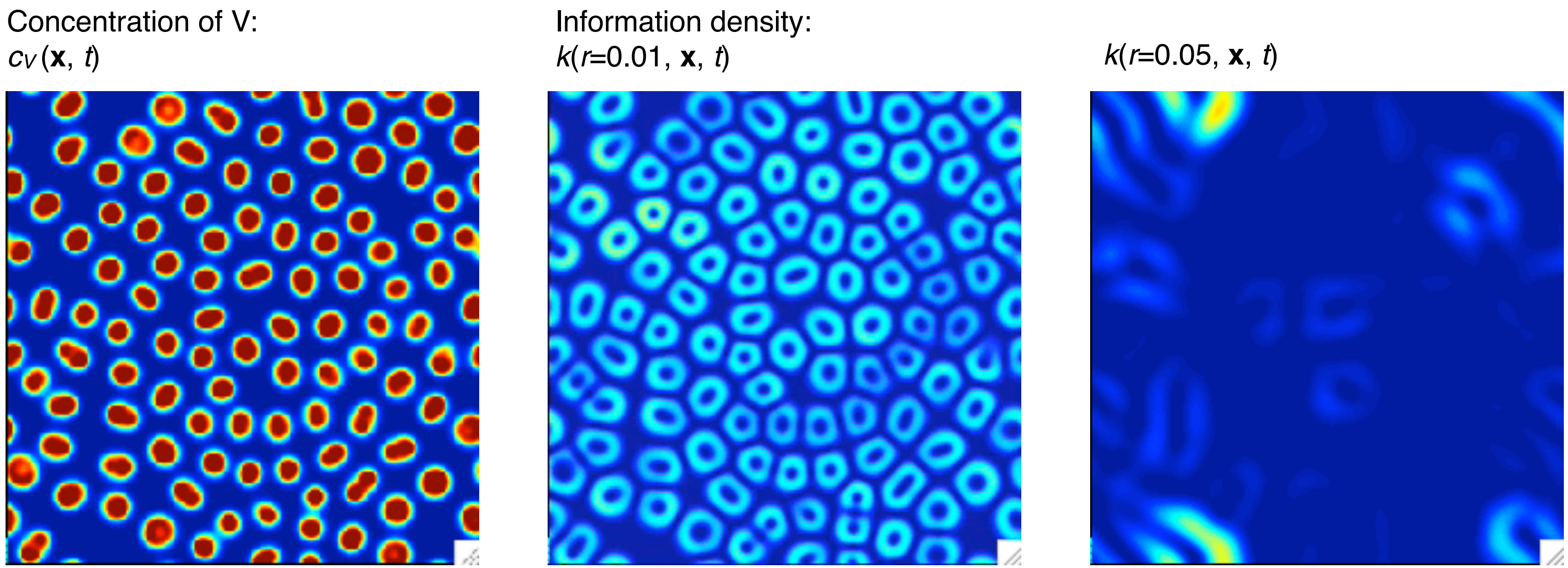
Space spanned by resolution r and position $(x,\ y)$



$$k_{\text{spatial}}(r) = \int dx\ k(r,x) \qquad \text{where} \qquad k(r,x) = \sum_i \tilde{c}_i(r,x)(r\ \nabla \ln \tilde{c}_i(r,x))^2 \geq 0$$

Information density in the Gray-Scott model

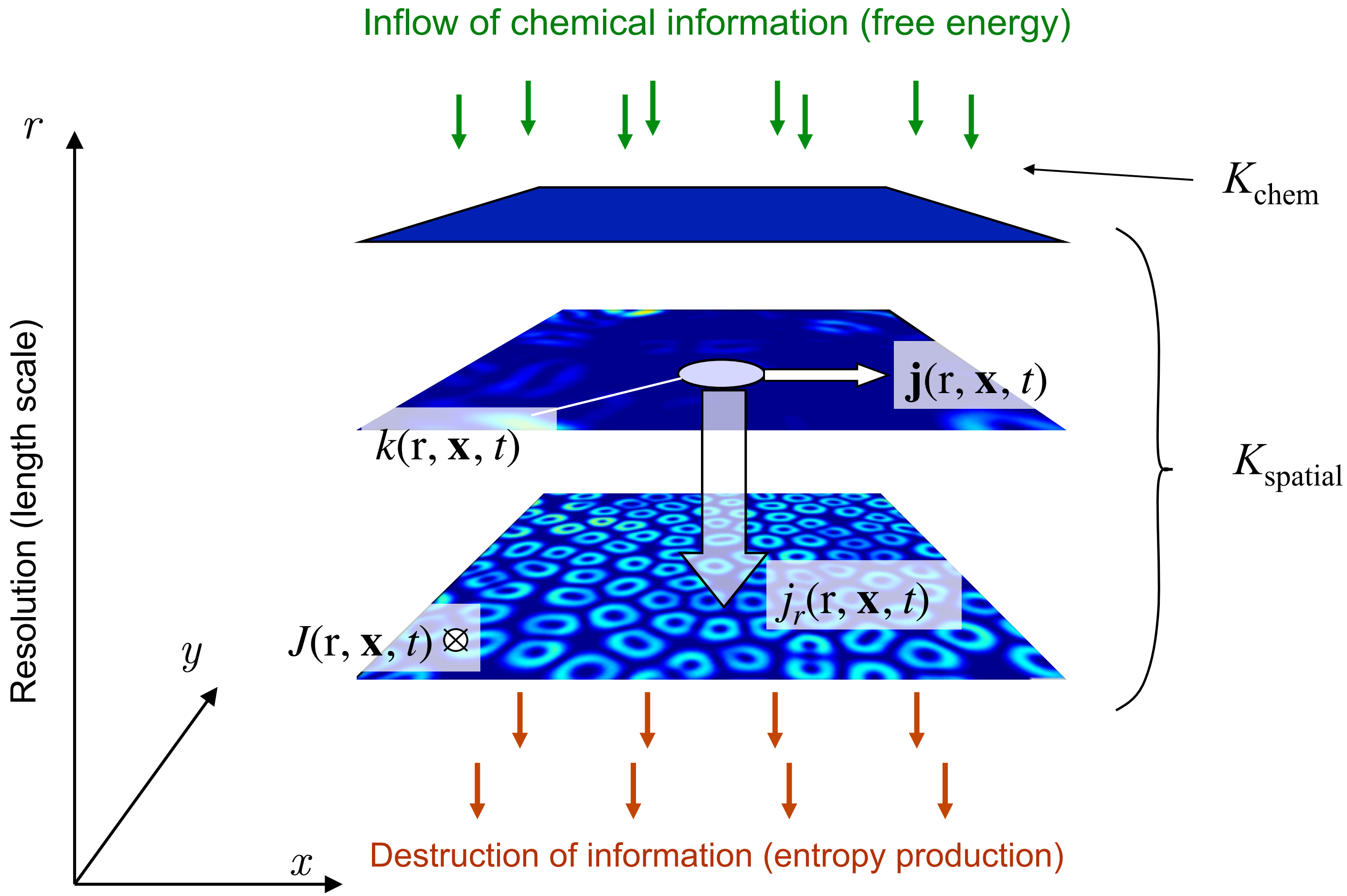
- The information density for two resolution levels r illustrates the presence of spatial structure at different length scales.



Good resolution

Worse resolution

Continuity equation for information



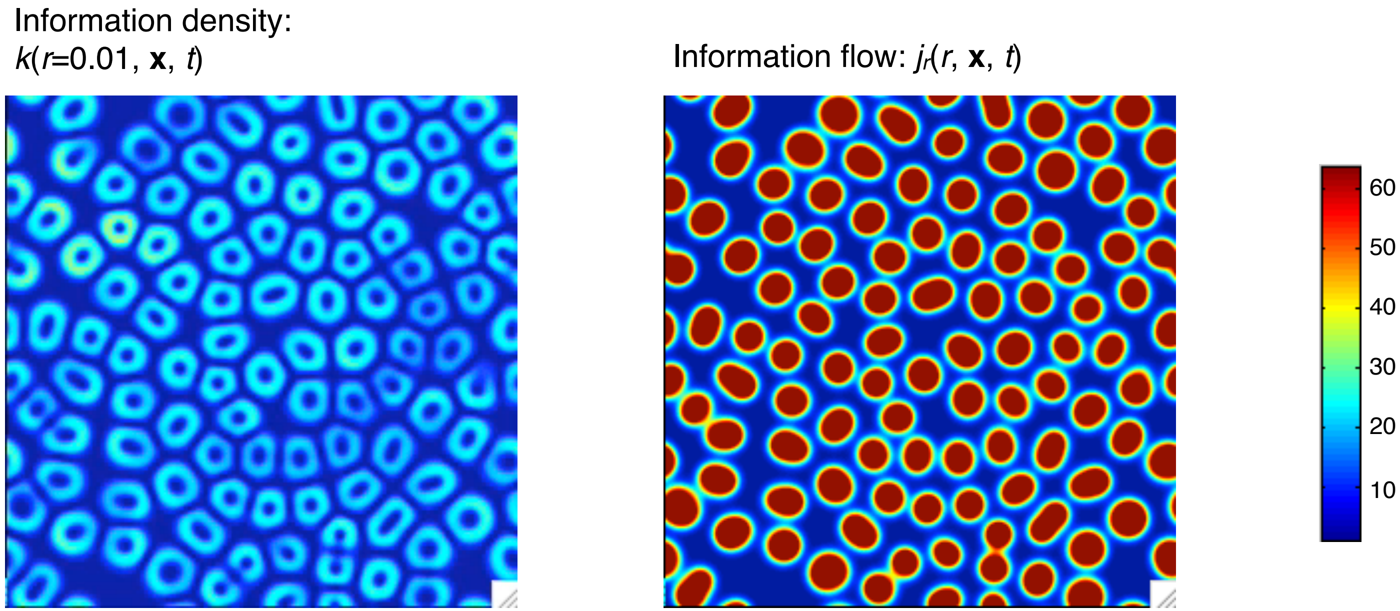
Flow in scale — Sinks (open system)

$$\frac{d}{dt}k(r,\mathbf{x},t) = r\frac{\partial}{\partial r}j_r(r,\mathbf{x},t) - \nabla\cdot\mathbf{j}(r,\mathbf{x},t) + J(r,\mathbf{x},t)$$

Information density — Flow in space

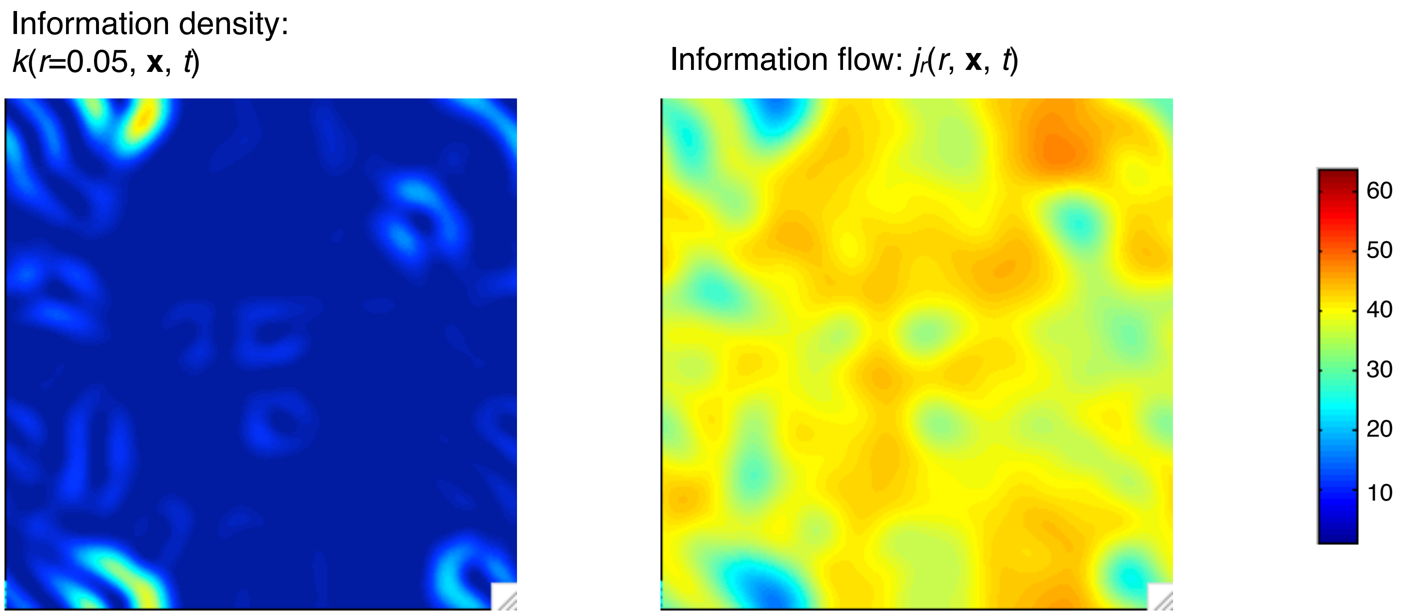
Information density k and information flow j_r

Good resolution: $r = 0.01$

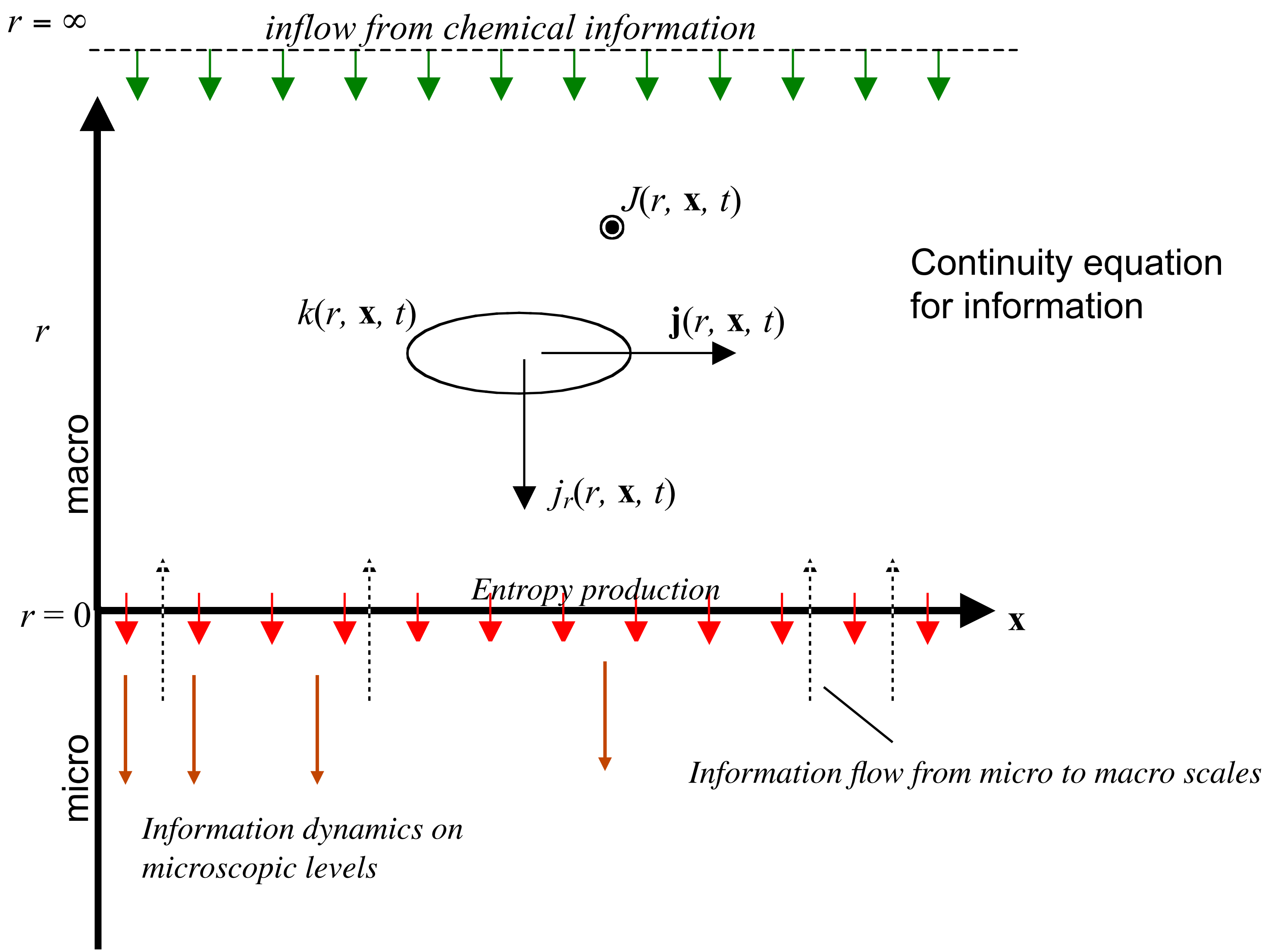


Information density k and information flow j_r

Worse resolution: $r = 0.05$



Summary



r = ∞
inflow from chemical information
J(r, x, t)
Continuity equation
for information
k(r, x, t)
j(r, x, t)
r
macro
j_r(r, x, t)
Entropy production
r = 0
x
micro
Information flow from micro to macro scales
Information dynamics on
microscopic levels

Spots Puzzle

In a far away land, there is an unusual tribe of 300 perfectly logical and perfectly intelligent people. Each member has a visible spot on the back of his or her head, some are red and some are black. Nobody knows the color of their own spot, but they do know the color of everyone else's.

If a person in the tribe ever realizes the color of his or her own spot it is strict custom for that person to publicly commit suicide at noon the following day, so that everybody else notice this. Thus, they never mention spot colors, and there are no mirrors.

But then one day a tourist visits this land and learns about all this. On his day of departure, since he has seen several with red spots and several with black spots, he is sure that it is safe to say to the entire tribe: "I can see that at least one of you has a red spot." The tourist leaves and returns a year later. What has happened?

More information...

- Lecture notes (draft) available on course web site:

  http://studycas.com/node/114

  (Several papers can be provided on request.)