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Interactive Structure Formation in Biological Systems

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Schedule

1. Interactive Structure Formation
2. Model of Active Brownian Particles
3. Swarming
4. Aggregation
5. Coherent Motion on Tracks
6. Conclusions

Biological Patterns

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- found on different levels of biological organization from (intra) cell level to groups of higher organisms

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- example:

  surface patterns:
  insect wings, mammalian coats, sea shells
  $\Rightarrow$ activator-inhibitor systems
  (Murray, Meinhard, Swinney ...)

- **Patterns made by biological creatures**

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- aggregates, clusters (cells, bacteria, insects, human crowds)
- networks (neural networks)
- trail systems (gliding bacteria, ants, hoof animals, pedestrians)
- nest buildings (gregarious insects)
- coherent motion (swarms of bird, schools of fish, herds of hoof animals)

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  emergent properties on the “higher” level:
  new system qualities resulting from the *interaction* of the entities

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- **Answer:**
  universal features in structure formation: *self-organization*
  non-linear interaction between elements
  (provided some suitable boundary conditions)

Interactive Structure Formation

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- biological “creatures” (entities): cells, bacteria, insects, ...
- cause changes in their environment
  generation of chemical fields, consumption of resources, waste ...

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- **Non-linear feedback**
  - environmental changes feed back to their further behavior
  - indirect *communication* process

Model of Active Brownian Particles (ABP)

- moving in an "effective" or *quasi-potential* (environment):

$$U^{\star}(\boldsymbol{r},t) = U(\boldsymbol{r}) - h(\boldsymbol{r},t)$$

$U(\boldsymbol{r})$: external potential
$h(\boldsymbol{r},t)$: adaptive, can be changed by the ABP

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- *internal energy depot* $e(t)$

$$\frac{d}{dt}e(t) = q(\boldsymbol{r}) - c\, e(t) - s - \eta(v^2)\, d_2 v^2\, e(t)$$

- $q(r)$: take-up of energy from the environment
- c: internal dissipation ("metabolism")
- s: environmental changes (generation of $h(\boldsymbol{r},t)$)
- acceleration: conversion rate d_2, efficiency $\eta(v^2)$

Equation of motion:

Langevin-type equation:

$$\dot{\boldsymbol{v}} = -\gamma_0\,\boldsymbol{v} - \frac{1}{m}\boldsymbol{\nabla}[U(\boldsymbol{r}) - h(\boldsymbol{r},t)] + \eta(v^2)\,d_2 e(t)\,\boldsymbol{v} + \sqrt{2\,D}\,\boldsymbol{\xi}(t)$$

considers:

- ➤ stochastic influences (D)
- ➤ spatial differences in $h(\boldsymbol{r},t)$ (“signal-response-behavior”)
- ➤ dissipation / acceleration of motion

Swarming in a Parabolic Potential

- ensemble of N active Brownian particles
- $U(x_1, x_2) = \frac{a}{2}(x_1^2 + x_2^2)$, $\quad q(\boldsymbol{r}) = q_0 = \text{const.}$
- initial conditions: $x_1(0)$, $x_2(0)$, $v_1(0)$ $v_2(0)$, $e(0) = 0$
- parameters: q_0, c, γ_0, d_2, $s = 0$

Film

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Film

result: coherent motion with slow spatial dispersion

- for $q_0 d_2 > \gamma_0 c$: two branches
  (left- and righthand rotation)
- additional coupling (mean velocity, center of mass, ...):
  one branch

Interaction between ABP:

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  example: reaction-diffusion dynamics

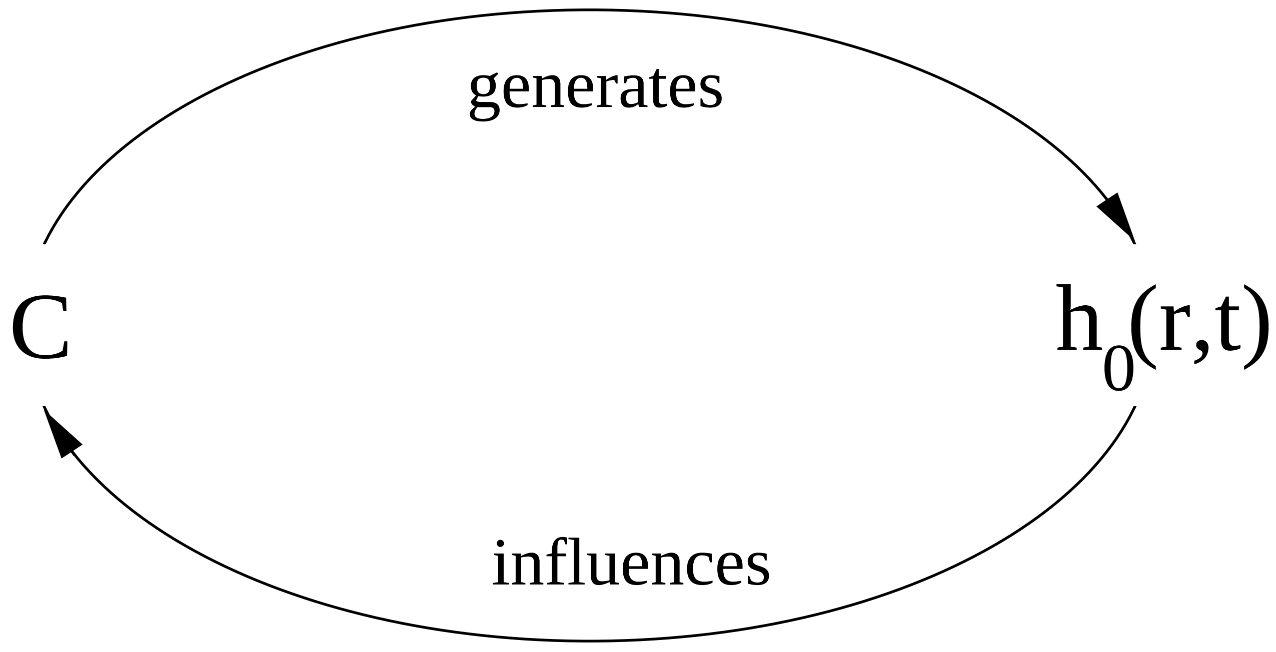
$$\frac{dh_0(\boldsymbol{r},t)}{dt} = s\sum_{i=1}^{N}\delta(\boldsymbol{r}-\boldsymbol{r_i}(t)) \;-k_0\,h_0(\boldsymbol{r},t)\;+\;D_0\,\boldsymbol{\Delta}h_0(\boldsymbol{r},t)$$

- non-linear feedback: Langevin dynamics

$$\frac{d\boldsymbol{v}_i}{dt} = -\gamma_0\boldsymbol{v}_i + \alpha\,\left.\frac{\partial h_0(\boldsymbol{r},t)}{\partial \boldsymbol{r}}\right|_{\boldsymbol{r}_i} + \sqrt{2D}\,\boldsymbol{\xi}_i(t)$$

for $U(\boldsymbol{r}) = \mathrm{const.}$, $d_2 \equiv 0$

Circular Causation:



Application: Biological Aggregation

cells, slime mold amoebae, myxobacteria generate a *chemical field* to communicate

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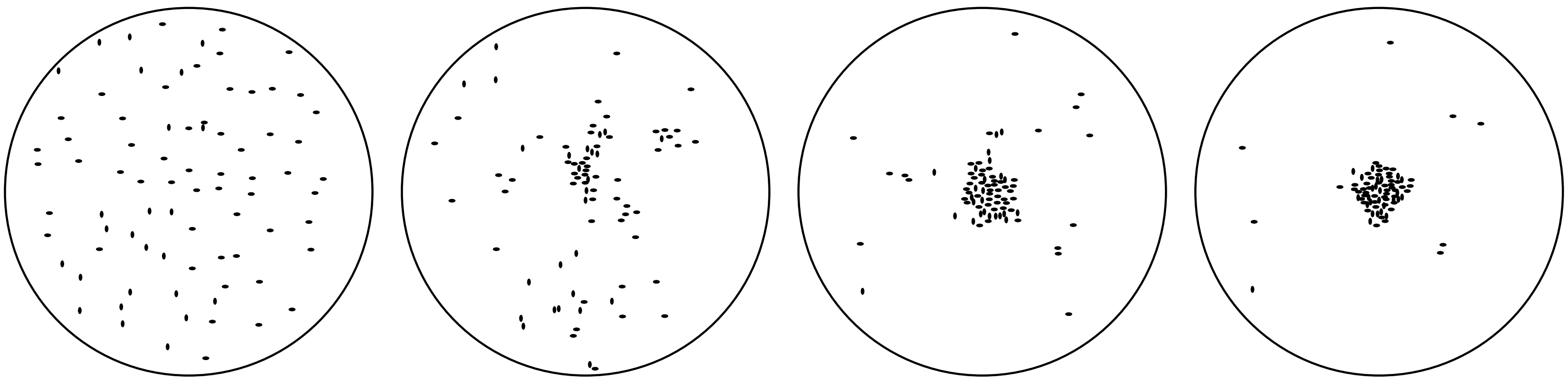
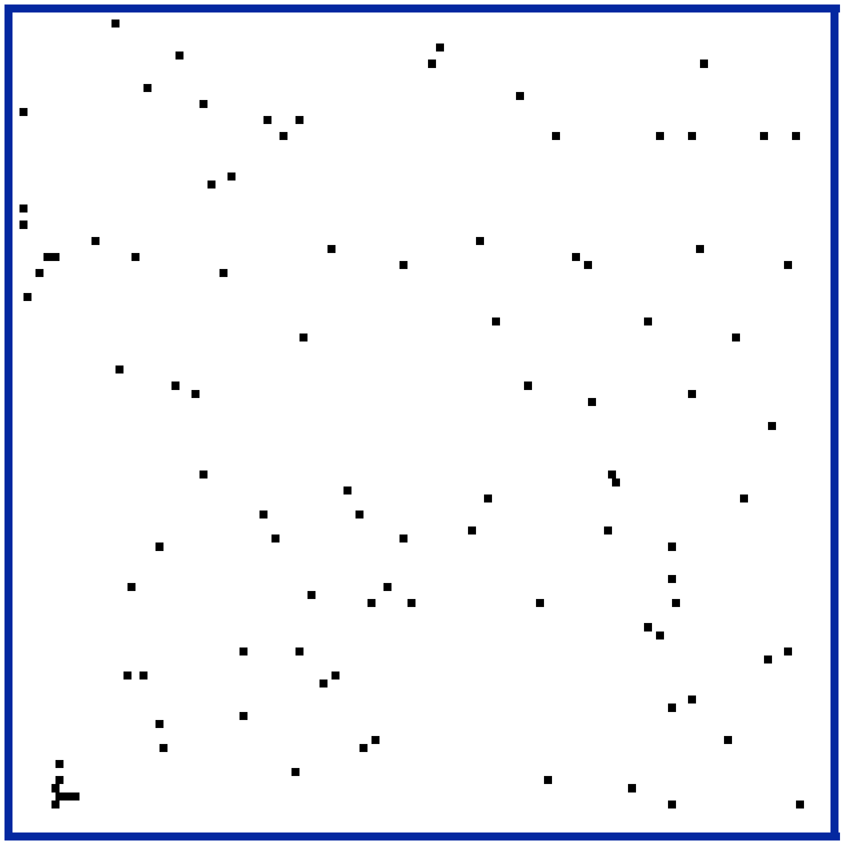


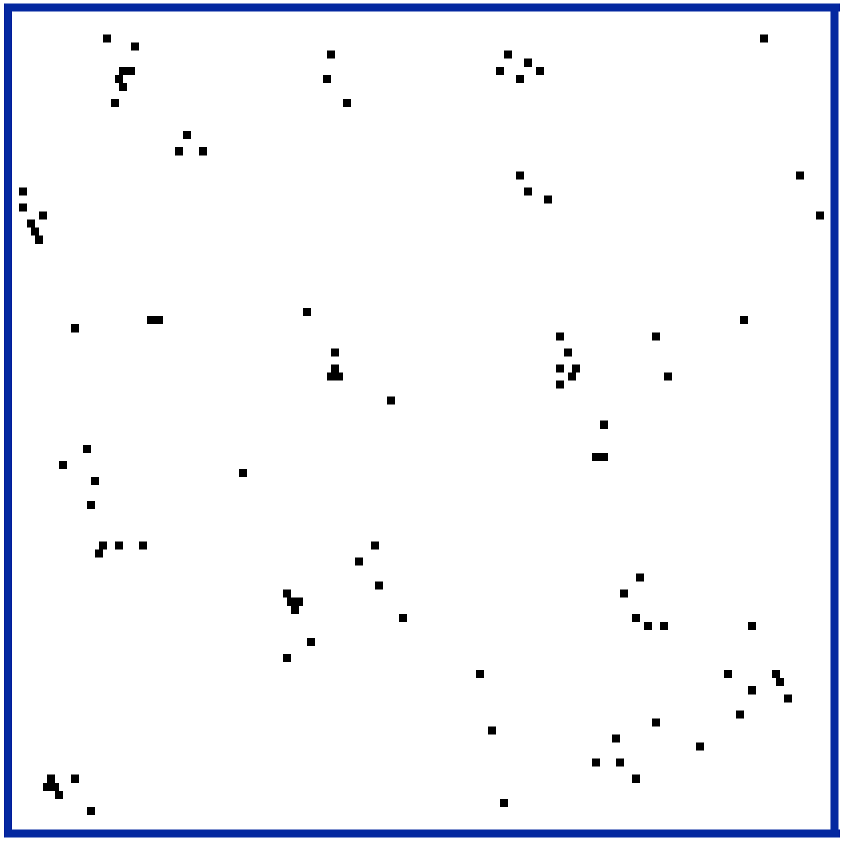
Deneubourg, J. L.; Gregoire, J. C.; Le Fort, E. (1990):

Kinetics of Larval Gregarious Behavior in the Bark Beetle *J. Insect Behavior* **3/2**, 169-182 (1990)

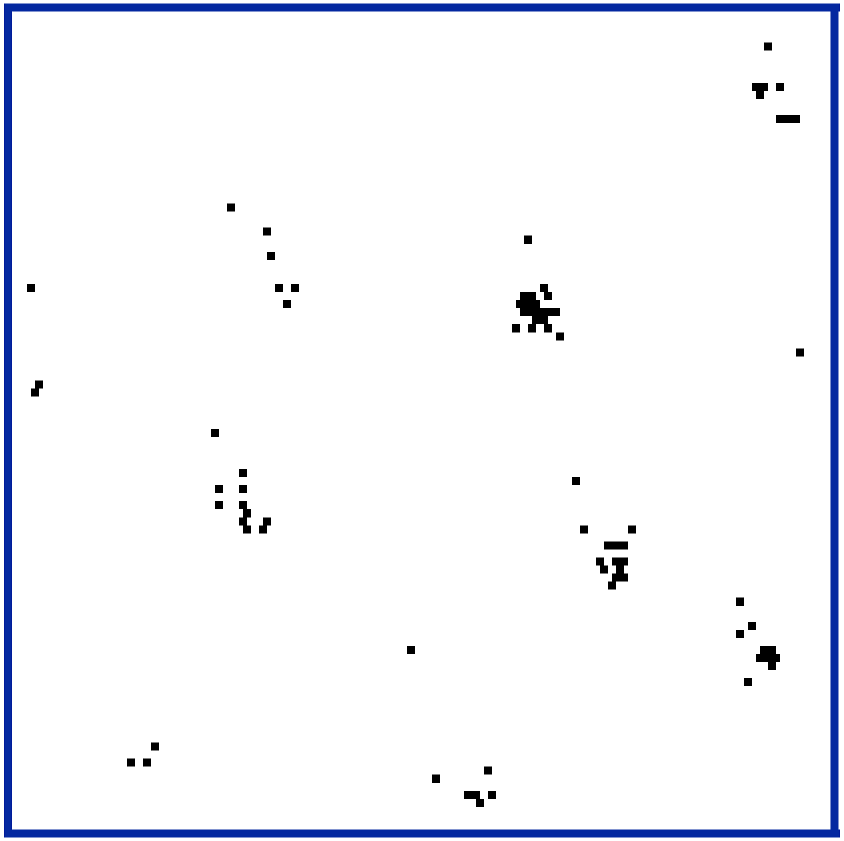
Aggregation of Active Brownian Particles



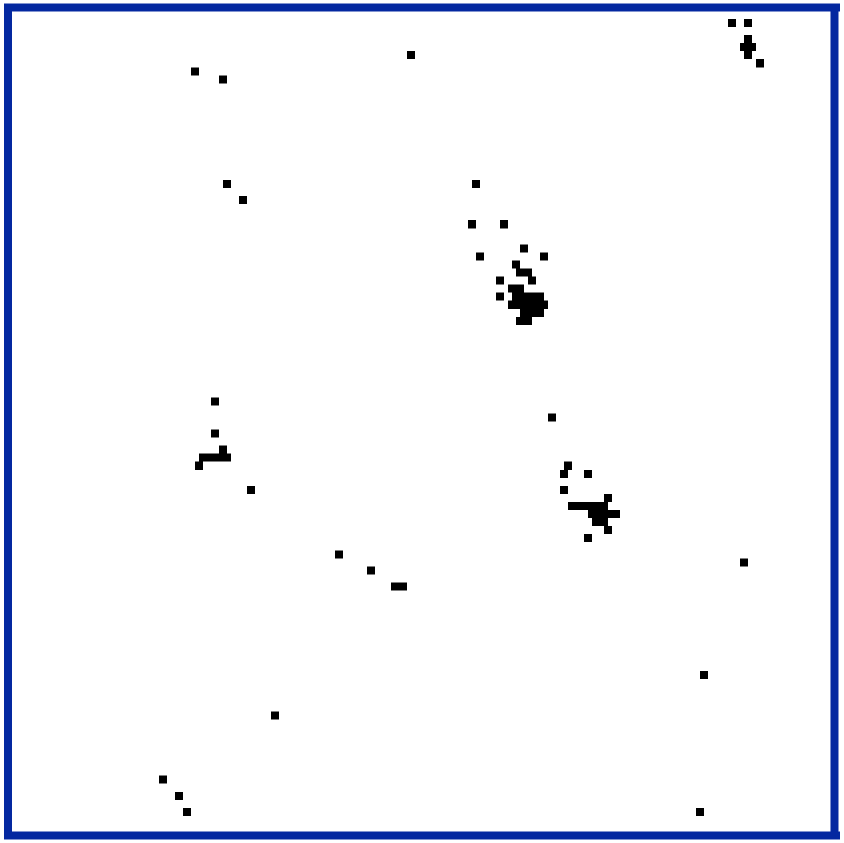
$t = 10^2$



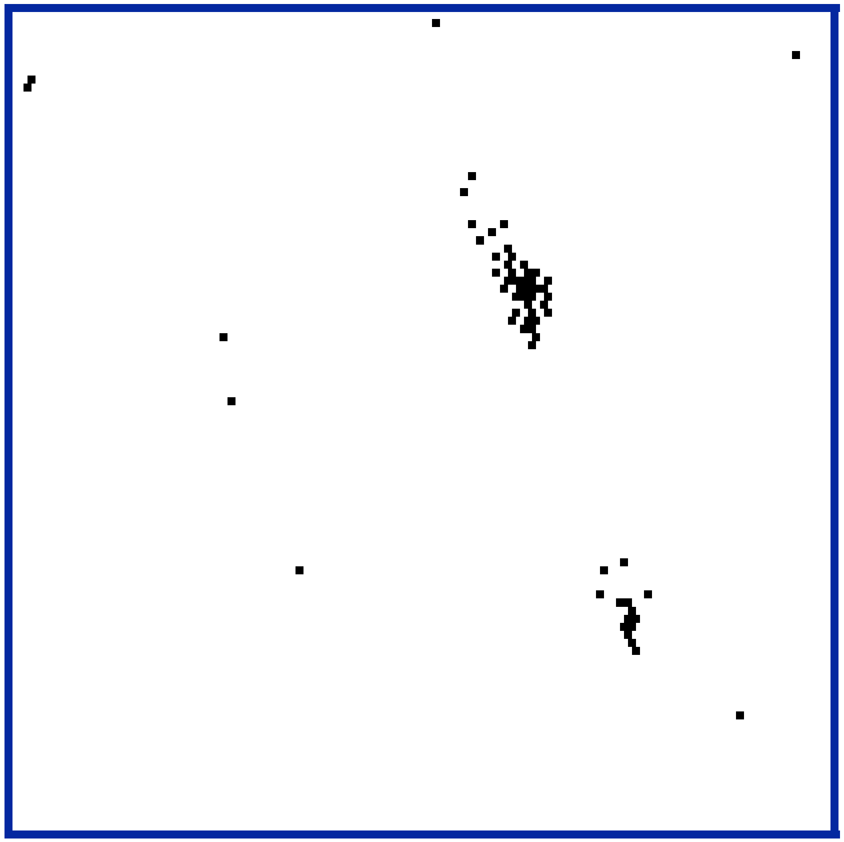
$t = 10^3$



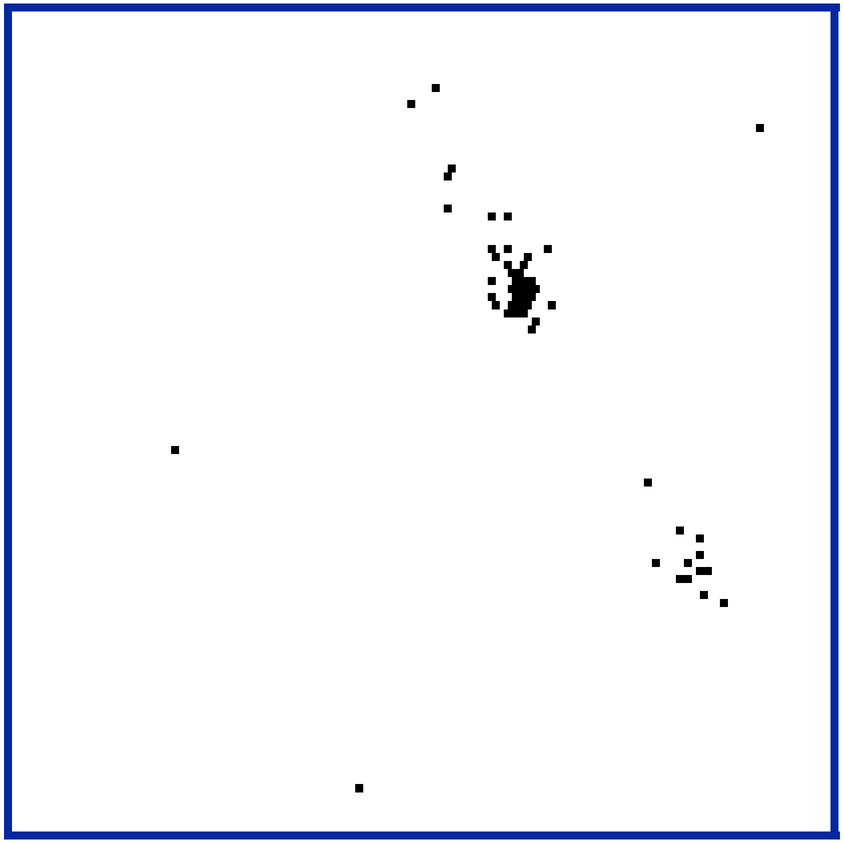
$t = 5 \times 10^3$



$t = 10^4$

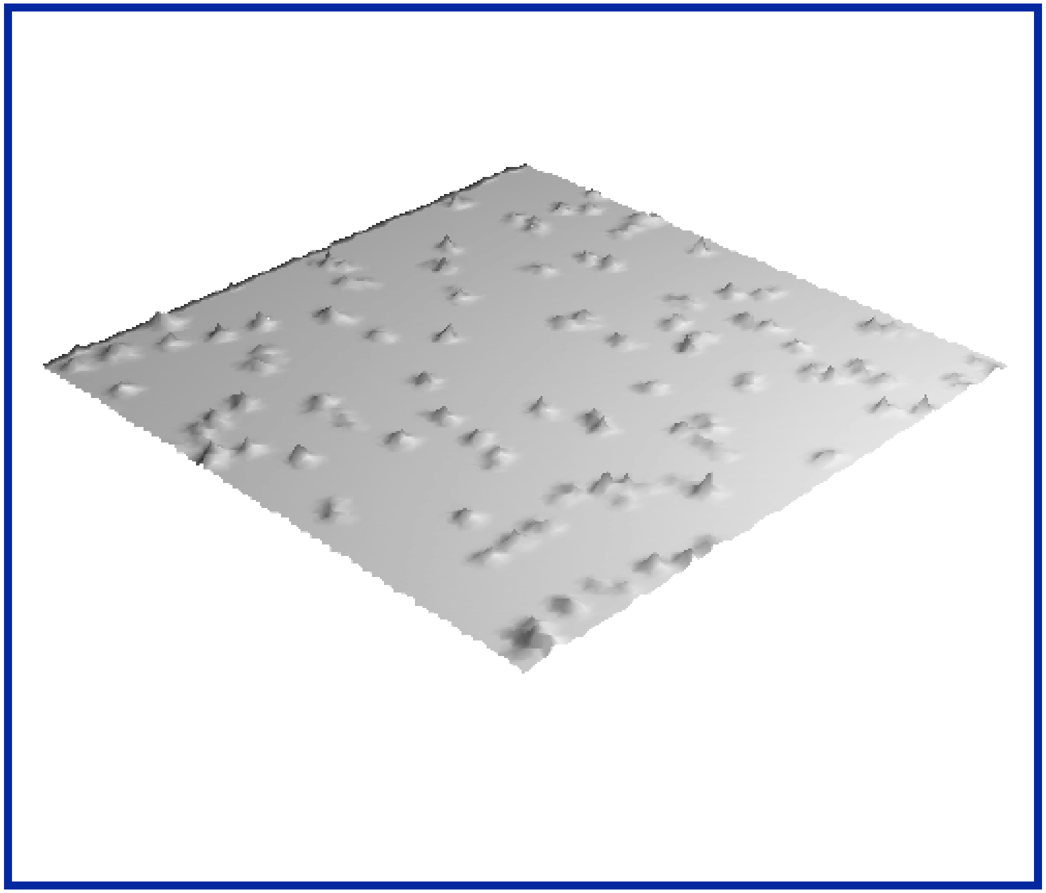


$t = 2.5 \times 10^4$

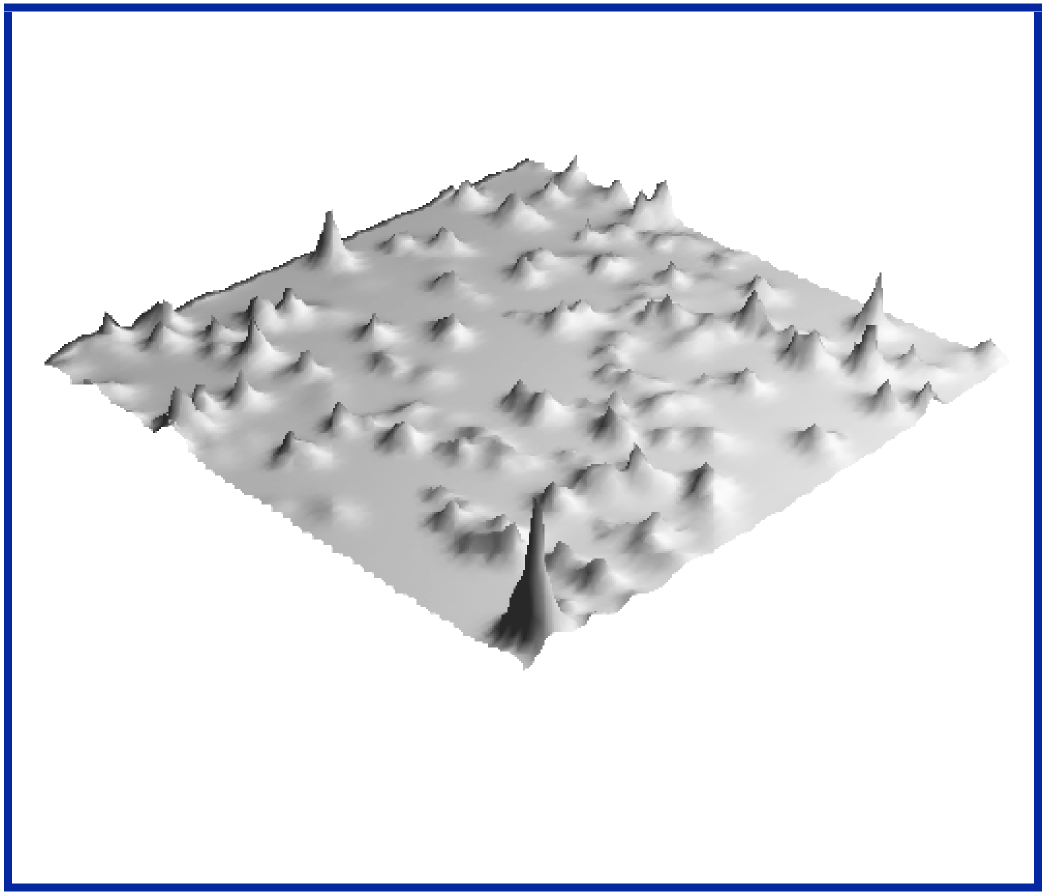


$t = 5 \times 10^4$

Evolution of the Self-Consistent Field



$t = 10^1$



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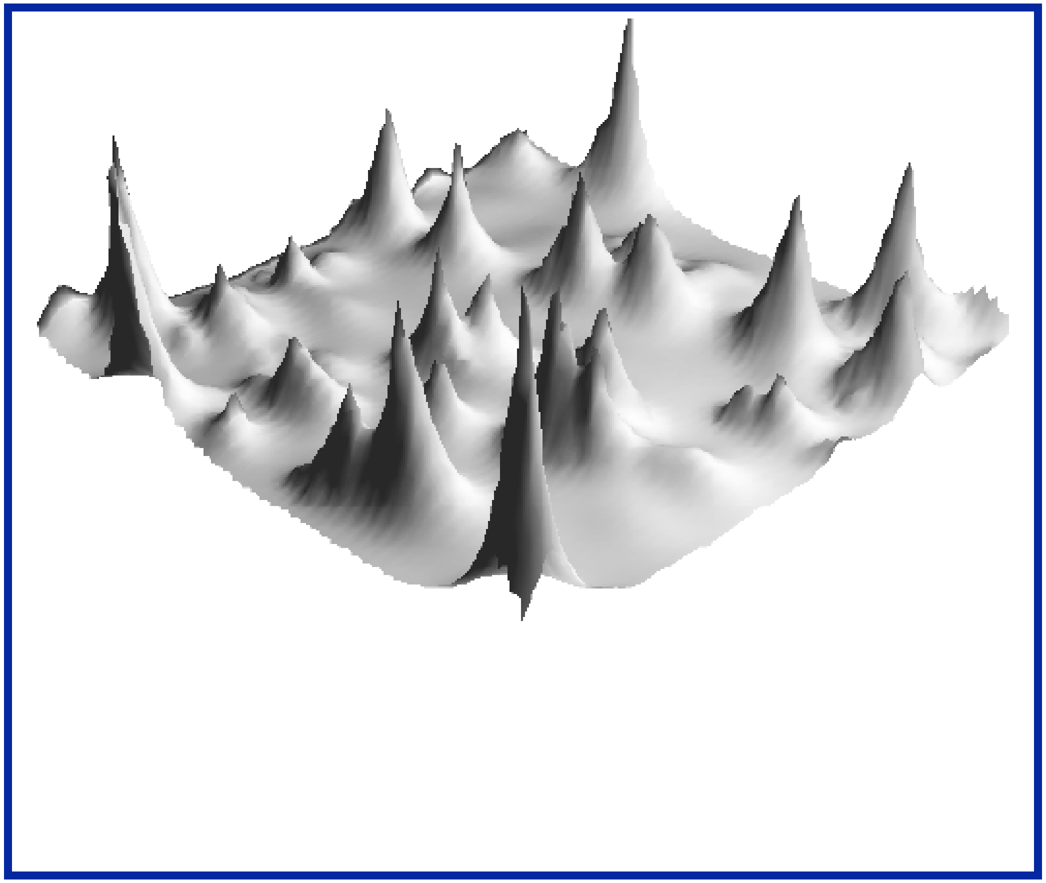

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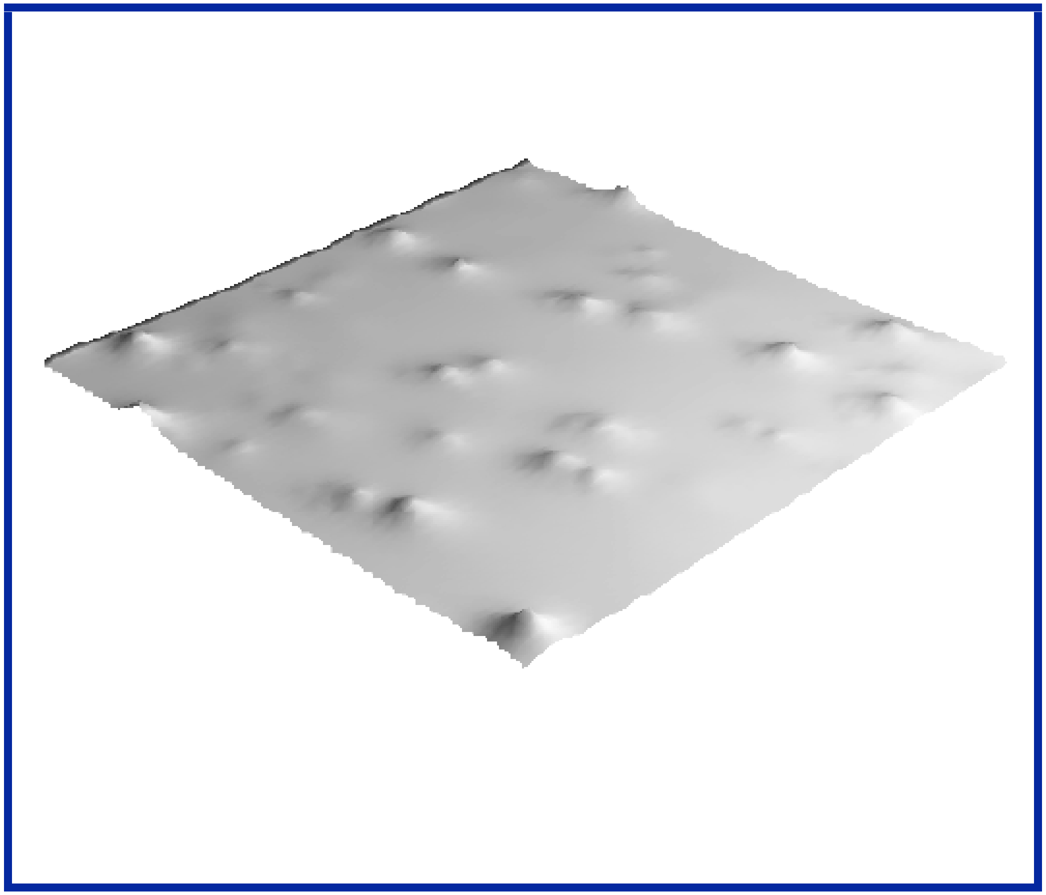

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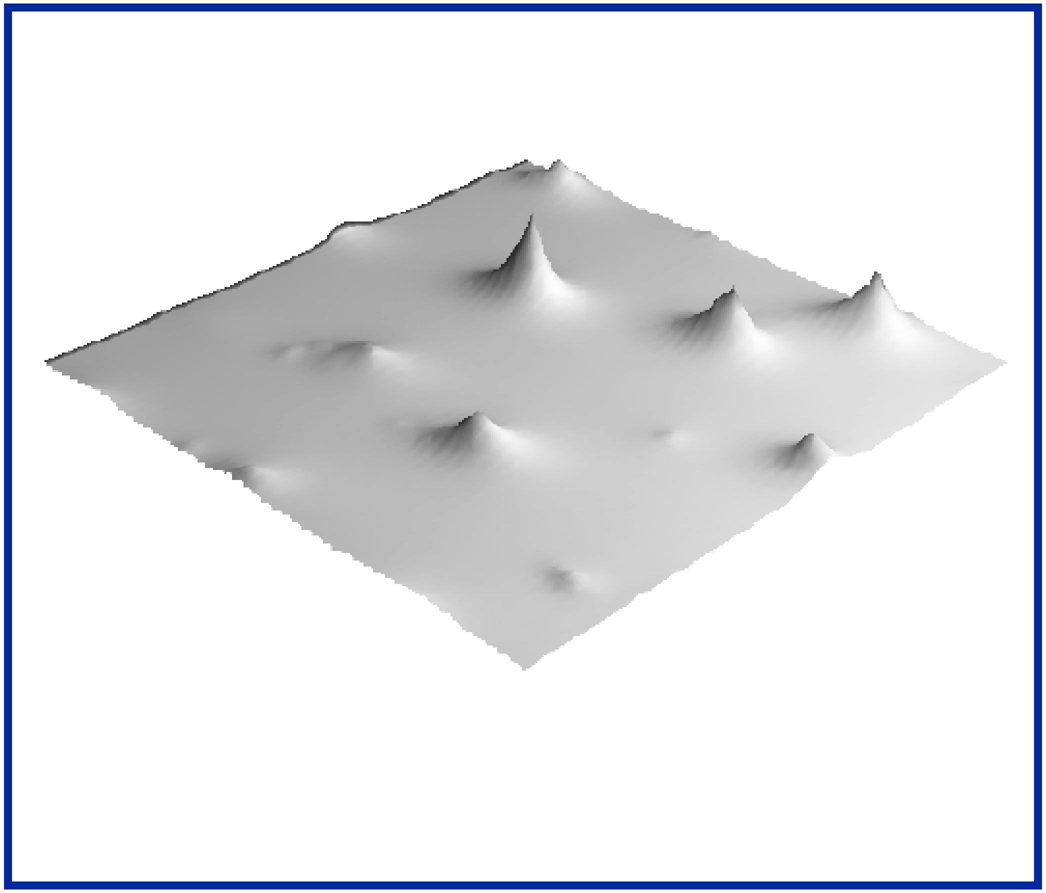

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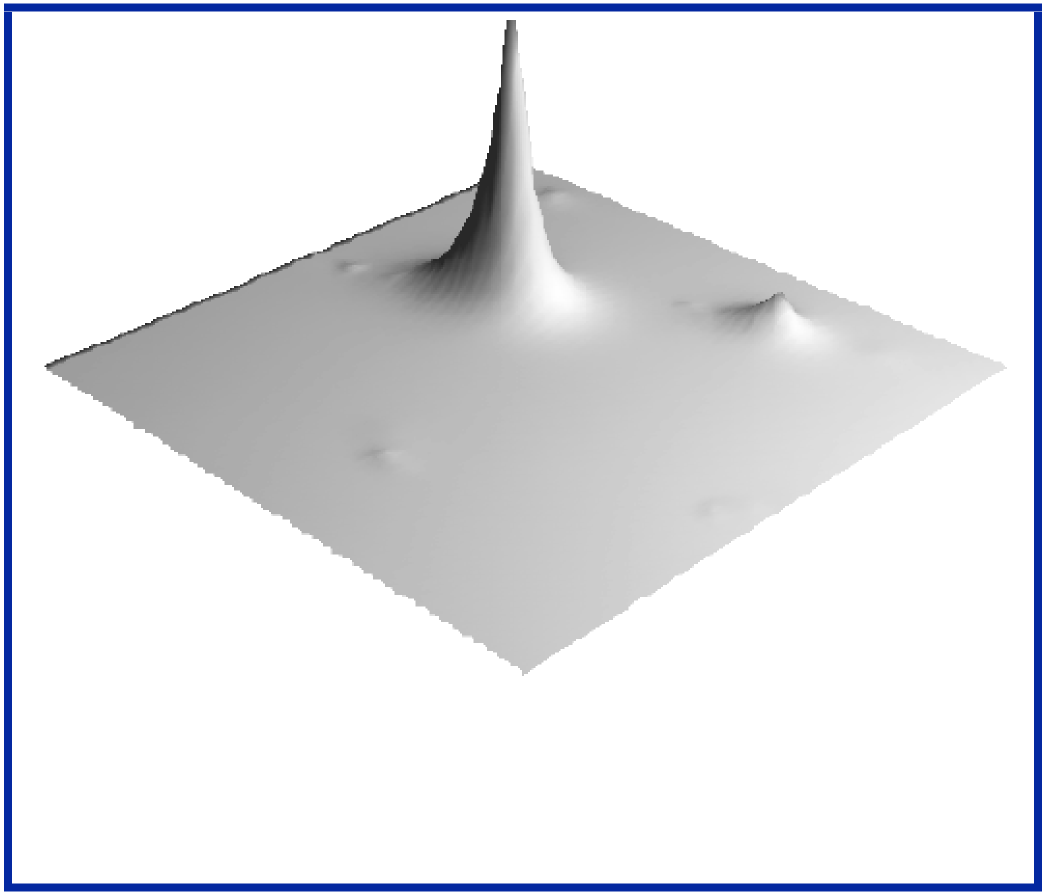

$t = 5 \times 10^4$

Theoretical Investigations

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active Brownian particles: density $n(\boldsymbol{r},t)$

$$\frac{\partial}{\partial t}\,n(\boldsymbol{r},t) = \frac{\partial}{\partial \boldsymbol{r}}\left\{-\frac{\alpha}{\gamma_0}\frac{\partial h_0(\boldsymbol{r},t)}{\partial \boldsymbol{r}}n(\boldsymbol{r},t)\;+\;D\frac{\partial n(\boldsymbol{r},t)}{\partial \boldsymbol{r}}\right\}$$

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self-consistent field $h_0(\boldsymbol{r}, t)$:

$$\frac{\partial}{\partial t}\, h_0(\boldsymbol{r}, t) = s_0\, n(\boldsymbol{r}, t) - k_0\, h_0(\boldsymbol{r}, t) + D_0\, \frac{\partial^2 h_0(\boldsymbol{r}, t)}{\partial r^2}$$

Derivation of Selection Equation:

$$\frac{\partial h_0(\boldsymbol{r},t)}{\partial t} = \frac{k_0\,\bar{h}_0}{\langle \exp\{(\alpha/k_BT)\,h_0(\boldsymbol{r},t)\}\rangle_A}\,h_0(\boldsymbol{r},t) \times \left[\frac{\exp\{(\alpha/k_BT)\,h_0(\boldsymbol{r},t)\}}{h_0(\boldsymbol{r},t)} - \frac{\langle \exp\{(\alpha/k_BT)\,h_0(\boldsymbol{r},t)\}\rangle_A}{\bar{h}_0}\right] + D_0\,\Delta h_0(\boldsymbol{r},t)$$

compare to Fisher-Eigen equation:

$$\frac{dx_i}{dt} = x_i\left[E_i - \langle E_i\rangle\right] \;;\quad \langle E_i\rangle = \frac{\sum_i E_i\,x_i}{\sum_i x_i}$$

Derivation of Effective Diffusion Equation:

$$\frac{\partial n(\boldsymbol{r},t)}{\partial t} = \frac{\partial}{\partial \boldsymbol{r}} \left\{ D_{\text{eff}} \frac{\partial n(\boldsymbol{r},t)}{\partial \boldsymbol{r}} \right\}; \quad D_{\text{eff}} = \frac{1}{\gamma_0} [k_B T - \alpha \, h_0(\boldsymbol{r},t)]$$

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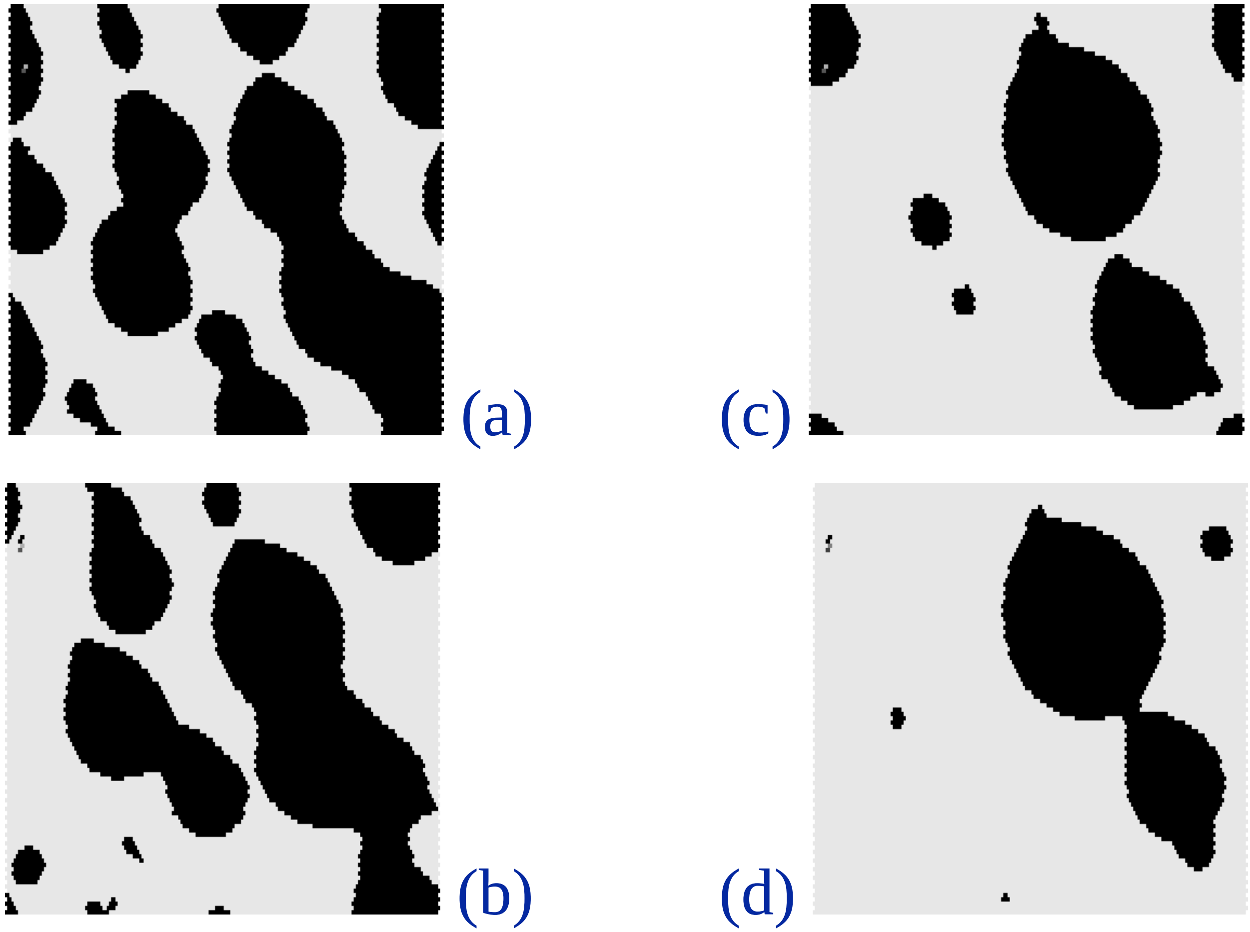
define local supersaturation: $h_0(\boldsymbol{r},t)/h_0^{\text{eq}}(T)$

$$\sigma(\boldsymbol{r},t,\eta) = 1 - \frac{h_0(\boldsymbol{r},t)}{\eta} \frac{k_0}{s_0\,\bar{n}}; \qquad \eta = \frac{T}{T_c}; \qquad T_c = \frac{\alpha}{k_B} \frac{s_0}{k_0} \frac{N}{A}$$



Effective duffusion coefficient $\sigma(\boldsymbol{r}, t, \eta)$

Time in simulation steps: (a) $t = 5.000$, (b) $t = 10.000$, (c) $t = 25.000$, (d) $t = 50.000$

Coherent Motion via Chemical Communication

- active particles with two different states $\theta \in \{-1, +1\}$, transitions possible

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- active particles with two different states $\theta \in \{-1, +1\}$, transitions possible
- state dependent production rate

$$s_i(\theta_i, t) = \frac{\theta_i}{2} \Big[\; (1 + \theta_i)\, s^0_{+1} \; \exp\{-\beta_{+1}\,(t - t^i_{n+})\} - \; (1 - \theta_i)\, s^0_{-1} \; \exp\{-\beta_{-1}\,(t - t^i_{n-})\} \Big]$$

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- two-component field

$$\frac{dh_\theta(\boldsymbol{r}, t)}{dt} = -k_\theta\, h_\theta(\boldsymbol{r}, t) + \sum_{i=1}^{N} s_i(\theta_i, t)\, \delta(\theta - \theta_i(t))\, \delta(\boldsymbol{r} - \boldsymbol{r_i}(t))$$

➤ *overdamped Langevin equation:*

$$\frac{d\boldsymbol{r}_i}{dt} = \alpha \left.\frac{\partial h^e(\boldsymbol{r},t)}{\partial \boldsymbol{r}}\right|_{r_i,\theta_i} + \sqrt{\frac{2k_B T}{\gamma_0}}\boldsymbol{\xi}_i(t)$$

$$\boldsymbol{\nabla}_{\boldsymbol{i}} h^e(\boldsymbol{r},t) = \frac{\theta_i}{2}\left[(1+\theta_i)\,\boldsymbol{\nabla}_{\boldsymbol{i}} h_{-1}(\boldsymbol{r},t) - (1-\theta_i)\,\boldsymbol{\nabla}_{\boldsymbol{i}} h_{+1}(\boldsymbol{r},t)\right]$$

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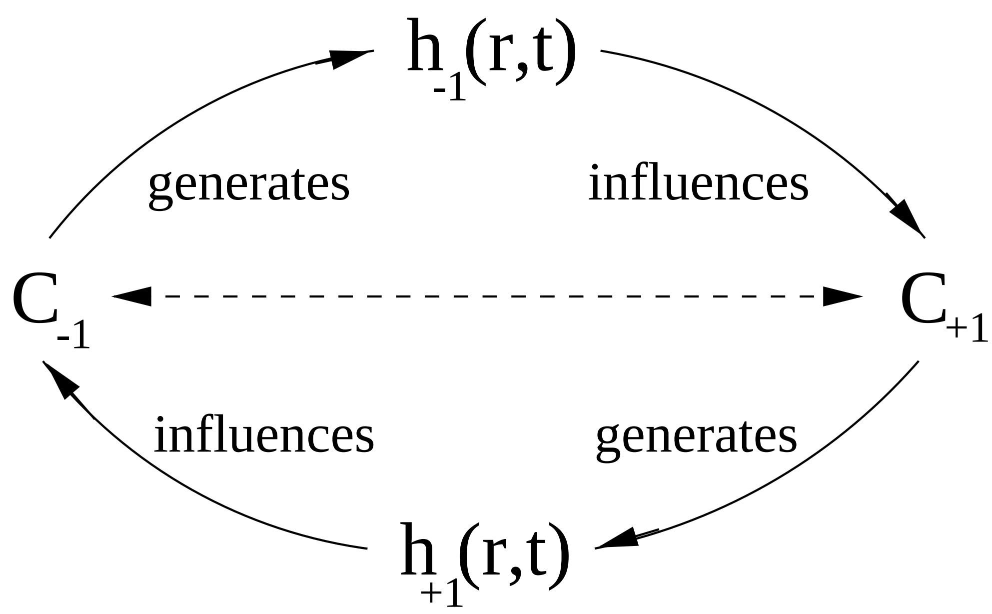

applications:

- exploitation of food sources:
  ants mark trails from food sources to the nest with additional chemicals to guide nestmates to resources

Film

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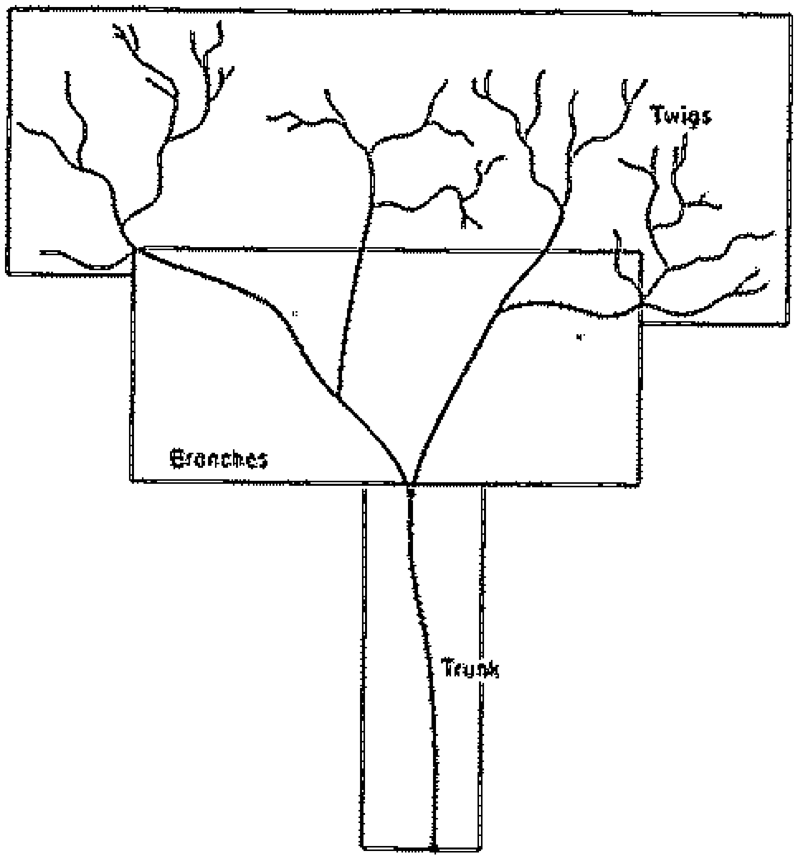
- self-wiring of networks:
  particles link nodes by creating their own “navigation” field

  Film

Foraging Route of Ants (*Pheidole milicida*)



Schematic representation of the complete foraging route of *Pheidole milicida*, a harvesting ant of the southwestern U.S. deserts. Each day tens of thousands of workers move out to the dendritic trail system, disperse singly, and forage for food.

Hölldobler, B. and Möglich, M.: The foraging system of *Pheidole militicida (Hymenoptera: Formicidae), Insectes Sociaux* **27/3** (1980) 237-264

Conclusions

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  indirect communication, exchange of information
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Examples:

- coherent motion (“swarming”)
- aggregation
- directed motion (“foraging behavior”)

Model of Active Brownian Particles:

➤

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- particle-based stochastic approach to complex motion and interactive structure formation
-

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-

Model of Active Brownian Particles:

- particle-based stochastic approach to complex motion and interactive structure formation
- gradual transition from "physical" to "biological" phenomena
- can be extended towards biological Multi-Agent Systems: *example:* information exchange in biological "many-particle" systems