Aktive Brownsche Teilchen: ein physikalisches Multi-Agenten-System zur Modellierung interaktiver Strukturbildung

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Gliederung

Complex Systems

"By complex system, it is meant a system comprised of a (usually large) number of (usually strongly) interacting entities, processes, or agents, the understanding of which requires the development, or the use of, new scientific tools, nonlinear models, out-of equilibrium descriptions and computer simulations."

Journal "Advances in Complex Systems"

"Complex systems are systems with multiple interacting components whose behavior cannot be simply inferred from the behavior of the components.
The study of complex systems spans all scales, from particle fields to the universe. Among the most complex systems with which we are familiar are biological and social systems – including biological macromolecules, biological organisms, ecosystems, and human social and economic structures."

New England Complex Systems Institute

Multi-Agent Systems (MAS)

agent:

- subunit with "intermediate" complexity

⇒ may represent local processes, individuals, species, agglomerates, components, ...

multi-agent system:

- *large number* / *different types* of agents
- interactions between agents:
  – on *different spatial and temporal scales*
  – local / direct interaction
  – global / indirect interactions (coupling via resources)
- "bottom-up approach": no universal equations
  ⇒ self-organization, *emergence* of system properties
- external influences (boundary conditions, in/outflux)

⇒ coevolution, circular causality

minimalistic agent:

- possibly simplest set of rules ⇒ "sufficient" complexity
- no deliberative actions, no specialization, no internal memory
- cooperative interaction instead of autonomous action

Active Brownian Particles

"Active Brownian particles are Brownian particles with internal degrees of freedom. They have the ability to take up energy from the environment, to store it in an internal depot and to convert internal energy to perform different activities, such as metabolism, motion, change of the environment, or signal-response behavior."

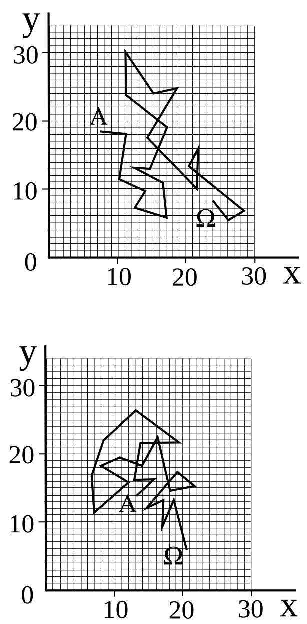
internal degrees of freedom:

1. internal energy depot: $e_i(t)$
   – take-up, storage, conversion of internal energy
   → pumped Brownian particles, Brownian motors
2. discrete internal states: $\theta_i(t)$
   – generation of different components of a self-consistent field
   – sensitivity to different field components
   → *non-linear feedback* ⇒ *interactive structure formation* on the macroscopic level

advantages:

- particle-based approach to structure formation
- complete stochastic dynamics, based on Langevin equations
- consideration of energetic aspects
- interaction between particles via multicomponent field
- external eigendynamics of the field

Observation of Brownian Motion



The position of the Brownian particle (radius 0.4 μm) is documented on a millimeter grid in time intervals $t_0 = 30$ seconds.

Equations for Brownian Particles

- stochastic approach $\Rightarrow$ Langevin equation:

$$\frac{d\boldsymbol{r}_i}{dt} = \boldsymbol{v}_i \quad ; \quad m\frac{d\boldsymbol{v}_i}{dt} = -\gamma_0 \boldsymbol{v}_i + \mathcal{F}^{stoch}$$

γ_0: friction coefficient of motion

$\mathcal{F}^{stoch}$: stochastic force

$$\langle \mathcal{F}^{stoch}(t) \rangle = 0\,; \quad \langle \mathcal{F}^{stoch}(t)\, \mathcal{F}^{stoch}(t') \rangle = 2S\, \delta(t-t')$$

fluctuation-dissipation theorem: $S = k_B T\, \gamma_0$

- overdamped limit: $d\boldsymbol{v}_i/dt = 0$, or $\gamma_0 \to \infty$

$$\frac{d\boldsymbol{r}_i}{dt} = \sqrt{2\, D_n}\, \boldsymbol{\xi}(t) \;\; ; \; D_n = \frac{k_B\, T}{\gamma_0} = \frac{\varepsilon}{\gamma_0}$$

D_n: spatial diffusion coefficient of the particles

$\boldsymbol{\xi}(t)$: white noise, $\left\langle \boldsymbol{\xi}_i(t)\, \boldsymbol{\xi}_j(t') \right\rangle = \delta_{ij}\, \delta(t-t')$.

Brownian Particle with Internal Energy Depot

Depot $e(t) \Rightarrow$ internal storage of energy

$$\frac{d}{dt}e(t) = q(\boldsymbol{r}) - c\,e(t) - d(\boldsymbol{v})\,e(t)$$

$q(\boldsymbol{r})$: *gain* $\Rightarrow$ space-dependent take-up of energy

c: *loss* $\Rightarrow$ internal dissipation

$d(\boldsymbol{v})$: *conversion* of internal into kinetic energy
simple ansatz: $d(\boldsymbol{v}) = d_2 v^2;\ d_2 > 0$

Stochastic equation for Brownian particles with energy depot

$$m\dot{\boldsymbol{v}} + \gamma_0 \boldsymbol{v} + \nabla U(\boldsymbol{r}) = d_2 e(t)\boldsymbol{v} + \mathcal{F}(t)$$

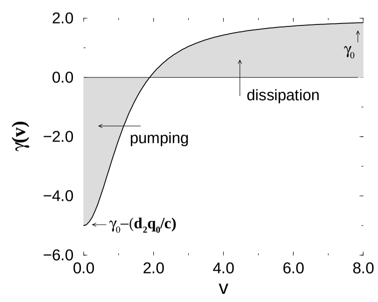
Non-linear Friction Function

equations of motion:

$$\dot{\boldsymbol{v}} + \gamma_0 \boldsymbol{v} + \nabla U(\boldsymbol{r}) = d_2 e(t)\boldsymbol{v} + \mathcal{F}(t)$$
$$\frac{d}{dt}e(t) = q(\boldsymbol{r}) - c\,e(t) - d(\boldsymbol{v})\,e(t)$$
$$\Rightarrow \quad \gamma(\boldsymbol{v}) = \gamma_0 - d_2\,e(t)$$

assumptions: $q(\boldsymbol{r}) \equiv q_0$; $\quad d(\boldsymbol{v}) = d_2 v^2$; $\quad \dot{e}(t) = 0$

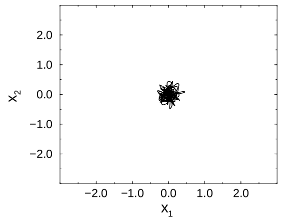
$$e_0 = \frac{q_0}{c + d_2 v^2}$$
$$\Rightarrow \quad \gamma(\boldsymbol{v}) = \gamma_0 - \frac{q_0\,d_2}{c + d_2 v^2} \qquad \text{zero: } v_0^2 = \frac{q_0}{\gamma_0} - \frac{c}{d_2}$$

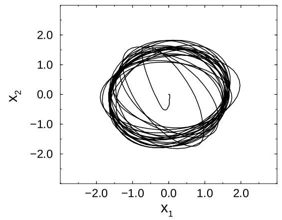


Critical Supply of Energy

assumption: motion in two dimensions

$$q(x_1, x_2) = q_0 \qquad U(x_1, x_2) = \frac{a}{2}(x_1^2 + x_2^2)$$





$q_0 = 0.0$: simple Brownian motion;
$q_0 = 1.0$: motion on a stochastic limit cycle

Brownian particle as micro–motor:

- efficiency ratio:

$$\sigma = \frac{dE_{out}/dt}{dE_{in}/dt} = \frac{d_2\, e\, v^2}{q_0}$$

- energy depot in quasi-stationary equilibrium: $e = \dfrac{q_0}{c + d_2 v^2}$
- $\boldsymbol{v}$ approximated by the stationary velocity:

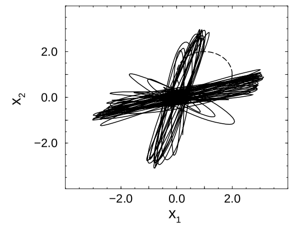
$$v_0^2 = \left(v_1^2 + v_2^2\right) = \frac{q_0}{\gamma_0} - \frac{c}{d_2}$$

$\Rightarrow$ $\boxed{\sigma = 1 - \dfrac{c\,\gamma_0}{d_2\, q_0}}$ $\quad \sigma > 0$ only if: $q_0 > q_0^{crit} = \dfrac{\gamma_0 c}{d_2}$

Localized Energy Sources

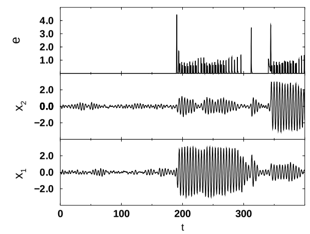
- parabolic potential: $U(x_1, x_2) = \frac{a}{2}(x_1^2 + x_2^2)$
- take-up of energy in a restricted area:

$$q(x_1, x_2) = \begin{cases} q_0 & \text{if } [(x_1 - b_1)^2 + (x_2 - b_2)^2] \le R^2 \\ 0 & \text{else} \end{cases}$$



- motion into the energy area becomes accelerated

$\Rightarrow$ oscillatory movement with fixed direction



- intermittent type of motion
- new cycles start with a burst of energy
- increase in d_2 abridges the cycle $\Rightarrow$ directed motion more susceptible to become Brownian motion

Active Brownian Particles Responding to a Field

active particles:

- characterized by an internal degree of freedom: $\theta_i(t)$, which can be changed: $w(\theta_i'|\theta_i)$
- Langevin equation:

$$\frac{d\boldsymbol{r}_i}{dt} = \boldsymbol{v}_i \, ; \; \frac{d\boldsymbol{v}_i}{dt} = -\gamma \boldsymbol{v}_i + \alpha_i \left. \frac{\partial h^e(\boldsymbol{r},t)}{\partial \boldsymbol{r}} \right|_{\boldsymbol{r}_i} + \sqrt{2\,\varepsilon_i\,\gamma}\,\boldsymbol{\xi}_i(t)$$

overdamped limit:

$$\frac{d\boldsymbol{r}_i}{dt} = \frac{\alpha_i}{\gamma} \left. \frac{\partial h^e(\boldsymbol{r},t)}{\partial \boldsymbol{r}} \right|_{\boldsymbol{r}_i} + \sqrt{\frac{2\varepsilon_i}{\gamma}}\,\boldsymbol{\xi}_i(t)$$

$h^e(\boldsymbol{r},t)$: effective field

- "individual" parameters (may depend on θ_i) :

α_i: individual response to the field
– attraction: $\alpha_i > 0$, or repulsion: $\alpha_i < 0$
– threshold h_0: $\alpha_i = \Theta[h^e(\boldsymbol{r},t) - h_0]$, $\Theta[y] = 1$, if $y > 0$
– internal value θ: $\alpha_i = \delta(\theta_i - \theta)$

ε_i: individual intensity of noise
– measure of the *sensitivity* s_i of the particle: $s_i \propto 1/\varepsilon_i$.

Effective Field

- Langevin eq.: particles respond to the gradient of $h^e(\boldsymbol{r},t)$
- effective field: a specific function of the different field components $h_\theta(\boldsymbol{r},t)$:

$$\boldsymbol{\nabla} h^e(\boldsymbol{r},t) = \boldsymbol{\nabla} h^e(\ldots, h_\theta(\boldsymbol{r},t), h_{\theta'}(\boldsymbol{r},t), \ldots)$$

- particles with internal parameter θ generate a field $h_\theta(\boldsymbol{r},t)$ which obeys a reaction-diffusion equation:

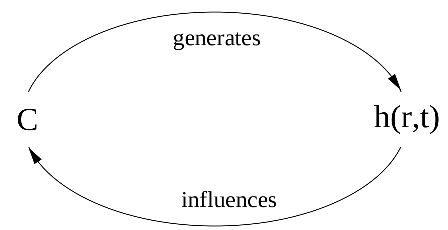
$$\frac{dh_\theta(\boldsymbol{r},t)}{dt} = -k_\theta\, h_\theta(\boldsymbol{r},t) + D_\theta\, \boldsymbol{\Delta} h_\theta(\boldsymbol{r},t) + \sum_{i=1}^{N} q_i(\theta_i,t)\,\delta(\theta-\theta_i(t))\,\delta(\boldsymbol{r}-\boldsymbol{r}_i(t))$$

spatio-temporal evolution of the field, $h_\theta(\boldsymbol{r},t)$:
(i) decay with rate k_θ
(ii) diffusion (coefficient D_θ)
(iii) production with individual rate $q_i(\theta_i,t)$

Complete Dynamics for N Active Particles

- N active Brownian particles:
  internal parameters $\theta_1, ..., \theta_N$; positions $\boldsymbol{r}_1, ..., \boldsymbol{r}_N$
  canonical N-particle distribution function:
  $$P(\underline{r}, \underline{\theta}, t) = P(\boldsymbol{r}_1, \theta_1, \ldots, \boldsymbol{r}_N, \theta_N, t)$$
- changes:
  (i) movement: $r_i \to r_i'$
  (ii) transition: $\theta_i \to \theta_i'$ with probability $w(\theta_i'|\theta_i)$
- multivariate master equation:
  limit of strong damping: $\gamma_0 \to \infty$, and $\alpha_i = \alpha$, $\varepsilon_i = \varepsilon$:
  $$\begin{aligned} \frac{\partial}{\partial t} P(\underline{r}, \underline{\theta}, t) \;=\; & -\sum_{i=1}^{N} \{ \boldsymbol{\nabla}_i \left((\alpha/\gamma_0)\, \boldsymbol{\nabla}_i h^e(\boldsymbol{r}, t)\, P(\underline{\theta}, \underline{r}, t) \right) \\ & - D_n\, \boldsymbol{\Delta}_i P(\underline{r}, \underline{\theta}, t) \} \\ & + \sum_{i=1}^{N} \sum_{\theta_i' \neq \theta_i} \{ w(\theta_i|\theta_i') P(\theta_i', \underline{\theta}^\star, \underline{r}, t) \\ & - w(\theta_i'|\theta_i) P(\theta_i, \underline{\theta}^\star, \underline{r}, t) \} \end{aligned}$$
- dynamics of the effective field $h^e(\boldsymbol{r}, t)$

Examples of Circular Causation

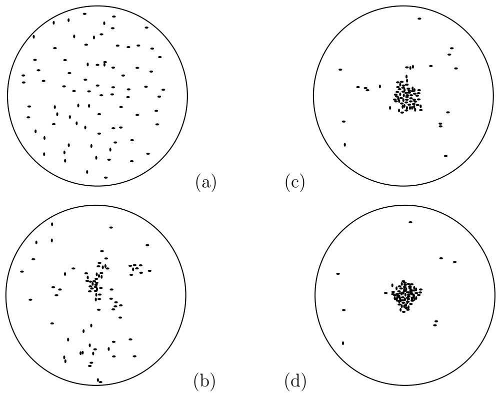


- active particles are identical $\Rightarrow$ no transitions
  $\alpha_i = \alpha > 0$, $\varepsilon_i = \varepsilon$, $\theta_i = 0$, $q_i(\theta_i, t) = q_0 = \text{const.}$
- one-component field:
  $$\begin{aligned} \boldsymbol{\nabla}_i h^e(\boldsymbol{r}, t) &= \boldsymbol{\nabla}_i h(\boldsymbol{r}, t) \\ \frac{dh(\boldsymbol{r}, t)}{dt} &= -k_0\, h(\boldsymbol{r}, t) + D_0\, \boldsymbol{\Delta} h_\theta(\boldsymbol{r}, t) + q_0 \sum_{i=1}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_i(t)) \end{aligned}$$

applications:

- biological aggregation:
  cells, slime mold amoebae, myxobacteria generate a *chemical field* to communicate
- track formation:
  bacteria, pedestrians mark their track, which can be reinforced by other individuals (ususally $D_0 = 0$)

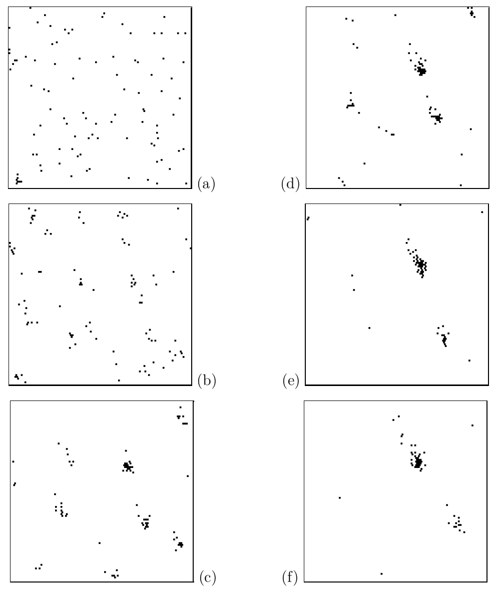
Aggregation of Larvae



Aggregation of larvae of the bark beetle *Dendroctonus micans*.
Total population 80 larvae, density 0.166 larvae/cm^2.
Time in minutes: (a) $t = 0$, (b) $t = 5$, (c) $t = 10$, (d) $t = 20$.

Deneubourg, J. L.; Gregoire, J. C.; Le Fort, E.: Kinetics of Larval Gregarious Behavior in the Bark Beetle *Dendroctonus micans* (Coleoptera: Scolytidae), *J. Insect Behavior* **3/2**, 169-182 (1990)

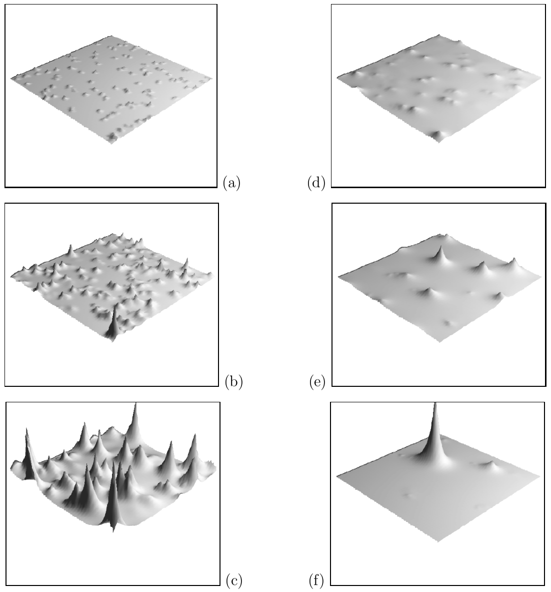
Aggregation of Active Brownian Particles



Position of 100 active Brownian particles moving on a triangular lattice (size: $A = 100 \times 100$).
Time in simulation steps: (a) $t = 100$, (b) $t = 1.000$, (c) $t = 5.000$, (d) $t = 10.000$, (e) $t = 25.000$, (f) $t = 50.000$.

Schweitzer, F.; Schimansky-Geier, L.: Clustering of Active Walkers in a Two-Component System, *Physica A* **206**, (1994) 359-379

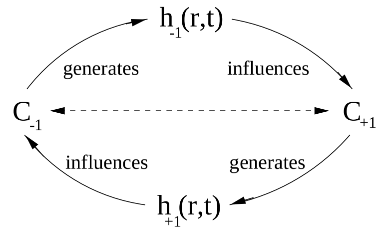
Evolution of the Self-Consistent Field



Time in simulation steps. (left side) Growth regime: (a) $t = 10$, (b) $t = 100$, (c) $t = 1.000$, (right side) Competition regime: (d) $t = 1.000$, (e) $t = 5.000$, (f) $t = 50.000$. The scale of the right side is 10 times the scale of the left side. Hence, Fig. (d) is the same as Fig. (c).

Schweitzer, F.; Schimansky-Geier, L.: Clustering of Active Walkers in a Two-Component System, *Physica A* **206**, (1994) 359-379

Examples of Circular Causation



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

$$q_i(\theta_i,t) = \frac{\theta_i}{2}[(1+\theta_i)\, q_i(+1,t) \;-\; (1-\theta_i)\, q_i(-1,t)-1]$$

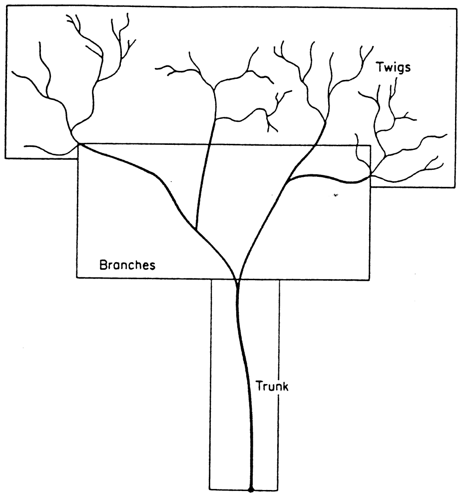
- two-component field

$$\begin{aligned} \boldsymbol{\nabla}_{\boldsymbol{i}} h^e(\boldsymbol{r},t) &= \frac{\theta_i}{2}\left[(1+\theta_i)\, \boldsymbol{\nabla}_{\boldsymbol{i}} h_{-1}(\boldsymbol{r},t) \;-\; (1-\theta_i)\, \boldsymbol{\nabla}_{\boldsymbol{i}} h_{+1}(\boldsymbol{r},t)\right] \\ \frac{dh_\theta(\boldsymbol{r},t)}{dt} &= -k_\theta\, h_\theta(\boldsymbol{r},t) + \sum_{i=1}^{N} q_i(\theta_i,t)\, \delta(\theta-\theta_i(t))\, \delta(\boldsymbol{r}-\boldsymbol{r_i}(t)) \end{aligned}$$

applications:

- exploitation of food sources:
  ants mark trails from food sources to the nest with additional chemicals to guide nestmates to resources
- self-assembling of networks:
  particles responding to two different fields, link nodes with opposite potential

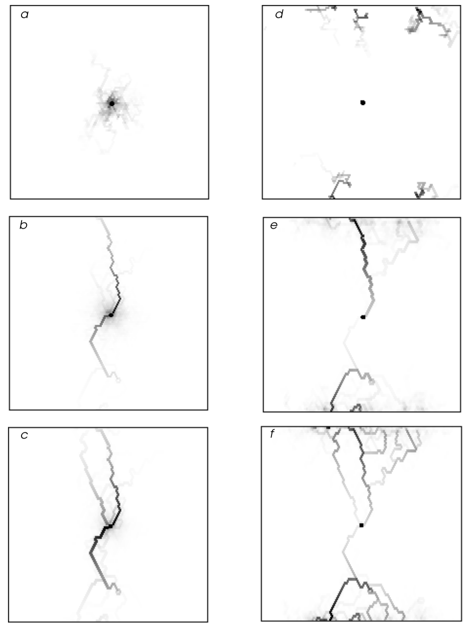
Foraging Route of Ants (*Pheidole milicida*)



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

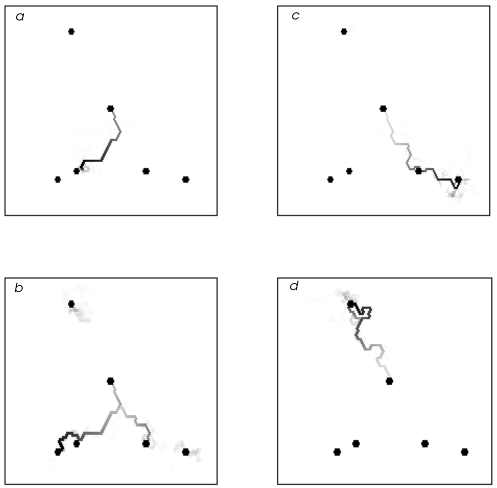
Trunk Trail Formation to Extended Forage Areas



Formation of trails from a nest (middle) to a line of food at the top and the bottom of a lattice. (a-c) show the distribution of chemical component (+1), and (d-f) show the distribution of chemical component (−1). Time in simulation steps: (a), (d) $t = 1.000$, (b), (e) $t = 5.000$, (c), (f) $t = 10.000$.

Schweitzer, F.; Lao, K.; Family, F.: Active Random Walkers Simulate Trunk Trail Formation by Ants, *BioSystems* **41** (1997) 153-166

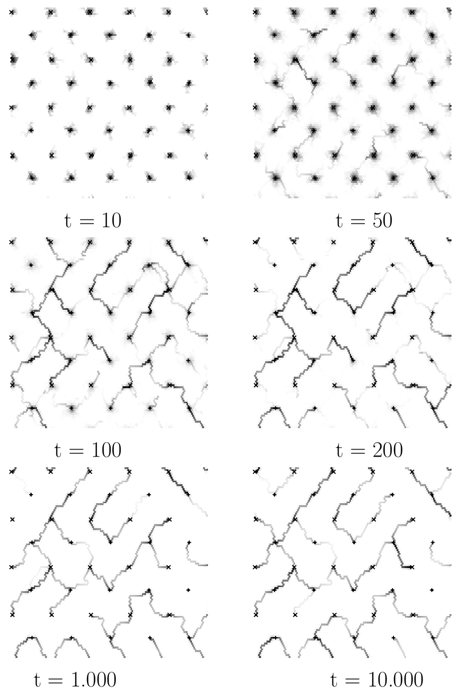
Trunk Trail Formation to Separate Food Items



Formation of trails from a nest (middle) to five randomly placed food clusters. The distribution of chemical component (-1) is shown after (a) 2000, (b) 4000, (c) 8500, and (d) 15000 simulation time steps, respectively.

Schweitzer, F.; Lao, K.; Family, F.: Active Random Walkers Simulate Trunk Trail Formation by Ants, *BioSystems* **41** (1997) 153-166

Formation of Networks



Time series of the evolution of a network (time in simulation steps). Lattice size 100×100, 5.000 particles, 40 nodes, $z_+ = 20$, $z_- = 20$. Parameters: $q_0 = 10.000$, $k_h = 0.03$, $\beta = 0.2$.

Conclusions

1. Model of Active Brownian Particles:

- particle-based model for interactive structure formation
- relation to biology:

(a) energy consumption for metabolism and motion

(b) interaction with the environment due to a self-consistent multicomponent field ⇒ non-linear feedback

2. Conversion of Brownian Motion into Directed Motion:

(a) quasiperiodic movement of the particles between energy sources and "home"

(b) directed movement in a asymetric periodic potential
⇒ direction depends on conversion parameter d_2 and noise D

(c) chemotactic response to a self-consistent chemical field two-component field ⇒ directed forward / backward motion

3. Advantage of the Active Brownian Particles Model:

- stochastic approach to directed movement and structure formation
- efficient and stable simulation algorithm: instead of integrating PDE ⇒ simulation of the Langevin equation
- applicable to systems where only small particle numbers govern the system dynamics

Self-Organization

Self-organization is the process by which individual subunits achieve, through their cooperative interactions, states characterized by new, emergent properties transcending the properties of their constitutive parts.

Biebricher, C. K.; Nicolis, G.; Schuster, P.: Self-Organization in the Physico-Chemical and Life Sciences, EU Report 16546 (1995)

Self-organization is defined as spontaneous formation, evolution and differentiation of complex order structures forming in non-linear dynamic systems by way of feedback mechanisms involving the elements of the systems, when these systems have passed a critical distance from the statical equilibrium as a result of the influx of unspecific energy, matter or information.

SFB 230 "Natural Constructions", Stuttgart, 1984 - 1995