Complex systems: Self-organization vs chaos assumption

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numerical simulations by R. Chatelin
Summary

1. Examples
2. Chaos property in particle systems
3. Binary particle dynamics on $S^1$: the CLD & BDG dynamics
4. Chaos property for CLD & BDG
5. Conclusion
1. Examples
Complex system

- System with locally interacting agents
  - emergence of spatio-temporal coordination
  - patterns, structures, correlations, synchronization
  - No leader / only local interactions
Time-discrete model:

\[ t^n = n \Delta t \]

\[-\] k-th individual

\[-\] \( X^n_k \): position at \( t^n \)

\[-\] \( \omega^n_k \): velocity with \( |\omega^n_k| = 1 \)

\[ X^{n+1}_k = X^n_k + \omega^n_k \Delta t \]

\[ \omega^{n+1}_k = \bar{\omega}^n_k + \text{noise (uniform in small angle interval)} \]

\[ \bar{\omega}^n_k = \frac{J^n_k}{|J^n_k|}, \quad J^n_k = \sum_{j, |X^n_j - X^n_k| \leq R} \omega^n_j \]

Alignment to neighbours’ mean velocity plus noise
Phase transition [Vicsek et al, PRL 95]

- Phase transition to disorder

- Order parameter
  \[ \alpha = \left| N^{-1} \sum_j \omega_j \right|^2 \]
  \[ N = \text{particle number} \]
  \[ 0 \leq \alpha \leq 1 \]

- Measures alignment

\[ \alpha \sim 1: \omega \text{ aligned} \]
\[ \alpha \ll 1: \omega \text{ random} \]
Phase transition to aligned state

As noise decreases
[Vicsek et al, PRL 95]

As density increases
[Vicsek et al, PRL 95]

Band formation [Chaté et al]

Particle positions

\( \rho \) (black) and \( \alpha \) (red) (cross section)
Vicsek dynamics exhibits
- self-organization & emergence of coherent structures
- supposes the build-up of correlations between particles

Kinetic and Hydrodynamic models rely on the chaos assumption
- When $N$ is large, particles are statistically independent

Question: are kinetic and hydrodynamic models relevant for Complex Systems?
- Goal: provide illustrative examples
2. Chaos property in particle systems
Construct the Master equation

- Tells us the passage $F_N(t^n) \rightarrow F_N(t^{n+1})$
- where $F_N(v_1, \ldots, v_N) = \text{N-particle probability distribution}$
- Note: $F_N$ invariant under permutations of $\{v_1, \ldots, v_N\}$

Compute the marginals

$$F_N^{(j)}(v_1, \ldots, v_j) = \int F_N \, dv_{j+1} \ldots dv_N$$

- Master eq. $\Rightarrow$ eq. for the marginals
- Eqs. for the marginals not closed (BBGKY hierarchy)
- Marginals: fixed number of variables when $N \rightarrow \infty$
Binary interactions

- Hierarchy:

\[ F_N^{(j)}(t^{n+1}) = \mathcal{J}^{(j)}(F_N^{(j+1)}(t^n)) \]

- Taking the limit \( N \to \infty \) ‘simplifies’ the problem
  - If \( N \) large, system is not influenced by the state of one given particle

- Particles become independent

\[ F^{(j)}(v_1, \ldots, v_j) = \prod_{k=1}^{j} F^{(1)}(v_k) \]

Chaos assumption
Binary interactions (cont)

- Suppose at $t = 0$: particles are independent

$$F^{(j)}(v_1, \ldots, v_j)|_{t=0} = \prod F^{(1)}(v_k)|_{t=0}$$

- If $N$ finite: Dynamics builds up correlations instantaneously

- If $N \to \infty$, correlations tend to 0
  - for Hard-Sphere Dynamics [Lanford], $\exists T$ s.t. $\forall t \in [0, T]$

$$F^{(j)}(v_1, \ldots, v_j)|_t \to \prod F^{(1)}(v_k)|_t \quad \text{as} \quad N \to \infty$$

- BBGKY hierarchy 'converges' to the Boltzmann eq.
As $N \to \infty$:
- Dynamics becomes irreversible
- $\exists$ entropy functional $H$ which $\searrow$ in time
- Dissipation
- Equilibria $=$ states of maximal disorder

For classical systems (e.g. rarefied gases)
- strong relation between these concepts

Is this still true for self-organization processes?
- will some of these concepts survive while others won’t?
3. Binary particle dynamics on $S^1$: the CLD & BDG dynamics
Setting

- \( N \) particles with velocities \( v_k \in \mathbb{S}^1 \)
- i.e. \( v_k \in \mathbb{R}^2 \) with \( |v_k| = 1 \)
- Space homogeneous problem \( \Rightarrow \) kein \( x \) !!!
- All particles can interact

State of the system at the \( n \)-th iterate

- \( Z_N(t^n) = (v_1, \ldots, v_N)(t^n) \in (\mathbb{S}^1)^N \)
- \( t^n = n\Delta t \)
- Discrete stochastic dynamics \( Z_N(t^n) \longrightarrow Z_N(t^{n+1}) \)
Ex. 1: Space-homogeneous Vicsek dynamics

- Compute average direction
  \[ \bar{v} = \frac{\sum_k v_k}{|\sum_k v_k|} \]

- Add independent noise
  \[ v'_k = \bar{v} w_k \]
  - \( g(z) \) proba on \( S^1 \), symmetric \( g(z) = g(z^*) \)
  - \( w_k: N \) independent random var. drawn according to \( g \)

- Note:
  - Multiplicative group structure of \( S^1 \)
  - Also use phases \( \theta \) s.t. \( v = e^{i\theta} \)
  - All particles interact \( \Rightarrow \) no reduction using marginals
After [Bertin, Droz, Gregoire]

Pick a pair \{i, j\} at random

- probability \( P_{ij} = \frac{2}{N(N - 1)} \)
- average direction: \( v_{ij} = \frac{(v_i + v_j)}{|v_i + v_j|} \)

Add independent noise drawn according to \( g \):

- \( v_i' = v_{ij}w_i \quad v_j' = v_{ij}w_j \)
- All particles but \{i, j\} unchanged

Variant (acceptor-rejection)

- Collision performed with probability \( h(v_iv_j^*) \) s.t. \( 0 \leq h \leq 1 \)
Ex 3. 'Choose the Leader' (CLD)

- Pick an ordered pair \((i, j)\) at random
  - Probability \(P_{ij} = \frac{1}{N(N - 1)}\)

- Then, \(i\) joins \(j\) plus noise \(w\) drawn according to \(g\)
  \[ v'_i = v_j w \]

- All particles but \(i\) unchanged
4. Chaos property in BDG and CLD dynamics
Noise scaling

Outline

- Compute the masters eq. and the marginals
- Let $N \to \infty$ while scaling noise variance appropriately

Assumptions on noise distribution as $N \to \infty$:

$$g_N \to \delta(v)$$

$$\text{Var}(g_N) = \frac{\sigma^2}{N} \quad \text{i.e.} \quad \text{MSD}(g_N) = O\left(\frac{1}{\sqrt{N}}\right)$$

Goal: find eqs. for the marginals as $N \to \infty$ and $\Delta t = O\left(\frac{1}{N^2}\right)$ (continuous time limit)
Master eq: methodology

⇒ Take any observable \( \phi(v_1, \ldots, v_N) \)

⇒ Denote \( Z_N(t^n) = (v_1, \ldots, v_N)(t^n) \) the state of the system at time \( t^n \)

⇒ Markov transition operator

\[
Q^* \phi(v_1, \ldots, v_N) = \mathbb{E}\{\phi(Z_N(t^{n+1})) \mid Z_N(t^n) = (v_1, \ldots, v_N)\}
\]

⇒ Denote \( F_N(v_1, \ldots, v_N) = \) N-particle proba:

\[
\mathbb{E}\{\phi(Z_N(t^{n+1}))\} = \int \phi \ F_N(t^{n+1}) \ dZ = \int (Q^* \phi) \ F_N(t^n) \ dZ
\]

⇒ \( F_N(t^{n+1}) = QF_N(t^n) \) where \( Q = \) adjoint of \( Q^* \)
Example: CLD

\[ Q^* \phi(v_1, \ldots, v_N) = \]
\[ \frac{1}{N(N-1)} \sum_{i \neq j} \int_{S^1} \phi(v_1, \ldots, wv_j, \ldots, v_j, \ldots, v_N) g(w) \, dw \]

\[ QF_N(v_1, \ldots, v_N) = \]
\[ \frac{1}{N(N-1)} \sum_{i \neq j} g(v_j v_i^*) \int_{S^1} F_N(v_1, \ldots, w_i, \ldots, v_N) \, dw_i \]
Example: BDG

\[ Q^* \phi(v_1, \ldots, v_N) = \frac{2}{N(N-1)} \sum_{i<j} \left\{ \int_{S^1} h(\sqrt{v_i v_j^*}) \times \right. \\
\left. \times \phi(v_1, \ldots, v'_i, \ldots, v'_j, \ldots, v_N) g(v_{ij}^*v'_i)g(v_{ij}^*v'_j) \, dv'_i \, dv'_j \\
+ (1 - h(\sqrt{v_i v_j^*})) \phi(v_1, \ldots, v_N) \right\} \\
\]

with mid-direction \( v_{ij} \) defined by

\[ v_{ij} = (v_i + v_j) / |v_i + v_j| \]
\[ N \to \infty \text{ in CLD} \]

- **Small noise limit**
  \[ g_N \to \delta \quad \text{Var}(g_N) = \frac{\sigma^2}{N} \quad \Delta t = O(1/N^2) \]

- **First marginal:**
  \[ \partial_t f^{(1)} - \left( \frac{\sigma^2}{2} \right) \partial_{\theta_1}^2 f^{(1)} = 0 \]

- **Second marginal:**
  \[ \partial_t f^{(2)} - \left( \frac{\sigma^2}{2} \right) \Delta_{\theta_1,\theta_2} f^{(2)} + 2 f^{(2)} = (f^{(1)}(\theta_1) + f^{(1)}(\theta_2)) \delta(\theta_2 - \theta_1) \]
Stationary states as $t \to \infty$

- $f^{(1)} \to f_{\text{eq}}^{(1)} = 1$: uniform distribution on $S^1$

- $f^{(2)} \to f_{\text{eq}}^{(2)}$ the unique solution of

  \[-(\sigma^2/2)\Delta_{\theta_1,\theta_2}f + 2f = 2\delta(\theta_2 - \theta_1)\]

- $f_{\text{eq}}^{(2)}(\theta_1, \theta_2) \neq f_{\text{eq}}^{(1)}(\theta_1) f_{\text{eq}}^{(1)}(\theta_2)$
  \quad $\Rightarrow$ Chaos assumption violated

- $f_{\text{eq}}^{(2)}$ peaked at $\theta_1 = \theta_2$
  \quad $\Rightarrow$ coherent motion
  \quad $\Rightarrow$ but no preferred mean direction

\[\begin{array}{c}
\text{x} \times 10^{-3} \\
\hline
\text{2pi} & \text{3pi/2} \\
\text{0} & \text{pi/2} & \text{pi} & \text{3pi/2} \\
\end{array}\]
Numerical simulations

Experimental protocol

- simulations with $N = 10^2, 10^3, 10^4 \& 10^5$ particles
- wait until 'stationary state'
- Pick one $i$ and a pair $(i, j)$ at random
- Redo the simulation $M$ times to avoid correlations
- Plot histograms of $\theta_1$ and $(\theta_1, \theta_2)$ of these $M$ samples
- Compare with theoretical $f_{eq}^{(1)}$ and $f_{eq}^{(2)}$
$f_{eq}^{(1)} \text{ and } f_{eq}^{(2)}$: experiments $N = 10^3$

$\sigma = \pi$

$\sigma = \pi/10$

$\sigma = \pi/100$
$f_{\text{eq}}^{(2)}$ : experiments vs theory

$N = 10^3$

$\sigma = \pi$

$\sigma = \pi/10$

$\sigma = \pi/100$
$N \to \infty$ in BDG

- **Small noise limit and continuous time limit**
  - $g_N \to \delta \quad \text{Var}(g_N) = \sigma^2/N \quad \Delta t = O(1/N^2)$

- **Strong bias (‘grazing collisions’)**
  - $h_N/\int h_N \to \delta \quad \text{Var}(h_N/\int h_N) = \tau^2/N$

- **Goal: in the limit $N \to \infty$:**
  - Compare the relative influence of the noise $\sigma$ and the grazing bias $\tau$
Explicit hierarchy

\[ \partial_t f^{(1)} = (\sigma^2 - \tau^2) \partial^2_{\theta} f^{(2)}(\theta, \theta)|_{\theta=\theta_1} \]

\[ \partial_t f^{(2)} = (\sigma^2 - \tau^2)(\partial^2_{\theta} f^{(3)}(\theta, \theta_2, \theta)|_{\theta=\theta_1} + \partial^2_{\theta} f^{(3)}(\theta_1, \theta, \theta)|_{\theta=\theta_2}) \]

\[ \vdots \]

\[ \partial_t f^{(j)} = (\sigma^2 - \tau^2) \sum_{k=1}^{j} \partial^2_{\theta} f^{(j+1)}(\theta_1, \ldots, \theta_{k-1}, \theta, \theta_{k+1}, \ldots, \theta_j, \theta)|_{\theta=\theta_k} \]
If chaos assumption holds, $f^{(1)}(\theta)$ satisfies

$$\partial_t f = (\sigma^2 - \tau^2) (f^2)'' = 2(\sigma^2 - \tau^2) (f f')'$$

- nonlinear heat equation
- $\sigma > \tau$: well-posed; noise added wider than initial spread
- $\sigma < \tau$: ill-posed; noise added narrower: concentration?

**BUT:** Chaos assumption does not hold

Existence for hierarchy?
- infinitely many stationary states
5. Conclusion
Observations & Future work

- 'Simple’ dynamics of aggregation do not satisfy chaos assumption
  - How can kinetic theory survive this situation?
  - Requires rethinking of classical concepts (entropy, dissipation, irreversibility, equilibria, …)

- Spatialization
  - Kinetic & fluid models
  - Application to practical systems (swarming, trail formation, construction, …)