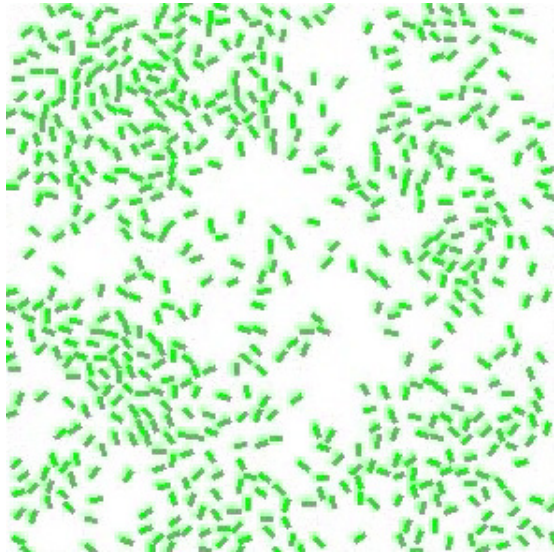
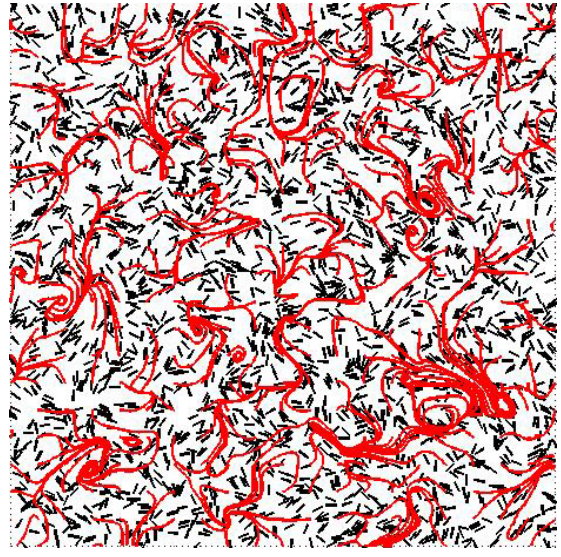
Coherent behaviors in groups of locally interacting particles





Emergent Behaviour in multi-particle systems with non-local interactions
January 22-27, 2012 - Banff International Research Station

Outline

Question: Can collisions, i.e. local interactions at the microscopic scale, lead to collective behaviors at the macroscopic scale?

Outline

Question: Can collisions, i.e. local interactions at the microscopic scale, lead to collective behaviors at the macroscopic scale?

1. **Motivations**
   - Experiments with *Bacillus subtilis*
   - Collisions versus continuous interactions

Outline

Question: Can collisions, i.e. local interactions at the microscopic scale, lead to collective behaviors at the macroscopic scale?

1. **Motivations**
   - Experiments with *Bacillus subtilis*
   - Collisions versus continuous interactions
2. **A collision rule that gives rise to large-scale behaviors**
   - Numerical simulations
   - Quantitative results: emergence of large-scale behaviors

Outline

Question: Can collisions, i.e. local interactions at the microscopic scale, lead to collective behaviors at the macroscopic scale?

1. **Motivations**
   - Experiments with *Bacillus subtilis*
   - Collisions versus continuous interactions
2. **A collision rule that gives rise to large-scale behaviors**
   - Numerical simulations
   - Quantitative results: emergence of large-scale behaviors
3. **Conclusions and perspectives**
   - A new type of complex fluid
   - Lyapunov spectrum and Lyapunov modes

Experiments with *Bacillus subtilis*

- **Dense bacterial colonies on wet agar:** hierarchy of scales and collective behaviors
  - Microscopic level: bacteria (micrometer)
  - Mesoscopic level: whirls and jets (tens of micrometers)
  - Macroscopic level: colony shape (centimeters)

Experiments with *Bacillus subtilis*

- **Dense bacterial colonies on wet agar:** hierarchy of scales and collective behaviors
  - Microscopic level: bacteria (micrometer)
  - Mesoscopic level: whirls and jets (tens of micrometers)
  - Macroscopic level: colony shape (centimeters)

- **Modeling:** different models are appropriate at different scales
  - Reaction-diffusion models: shape of a colony
  - hydrodynamic model [developed with T. Passot]: colony boundary and large-scale structures inside the colony
  - Microscopic level: one needs to model how bacteria interact

Ingredients for a microscopic model

- If the **bacteria do not communicate** through chemical cues or long-range forces, the only way they can interact is through collisions.
- The word collision should be understood in a general sense:
  - Two bacteria come into physical contact.
  - Two bacteria affect one another through mechanical effects.
- In particular, one can model how the fluid displacement created by one swimmer influences the motion of another one.
- The problem is then reduced to the question of the dynamics of a collection of "live" colliding particles.

Systems of colliding particles

Systems of colliding particles are well studied.

- **Molecular gases** consist of particulate systems that undergo elastic collisions. Each collision conserves momentum and kinetic energy. Such systems are typically chaotic.
- **Granular gases** can display incredibly rich and complex behaviors.
- **Self-propelled granular particles** have been shown to organize themselves into vortex structures, and self-propelled needles into jets.
- **Active granular nematics** also display large-scale structures.

Systems of self-propelled particles

There is also an abundant literature on models of **self-propelled interacting particles**.

- Most of these models are in terms of Newton's equations.
- Each group member feels attractive and repulsive forces exerted by other members, often tends to align its direction of motion with the average direction of its neighbors, and may be subject to drag and random forcing.

$$(1)\ m\frac{d\vec{v}_i}{dt} = -\gamma\vec{v}_i + \sum \text{other forces}$$

$$\Longrightarrow \vec{v}_i = \frac{1}{\gamma}\sum \text{other forces.}$$

$$(2)\ m\frac{d\vec{v}_i}{dt} = \text{velocity-dependent friction} + \sum \text{other forces.}$$

- Velocity-dependent friction includes self-propulsion.

Systems of self-propelled particles

- These models assume that each group members continuously feels the presence of its neighbors, through short- and long-range forces.
- Most of these forces are potential, so that one can study equilibrium configurations as the minima of a potential function.
- Such an approach of course only works for agents that can communicate with one another, or sense each other's presence.
- Here, we consider a different situation, where particles only interact through collisions, i.e. such that no long-range forces are present.

Outline

Question: Can collisions, i.e. local interactions at the microscopic scale, lead to collective behaviors at the macroscopic scale?

1. **Motivations**
   - Experiments with *Bacillus subtilis*
   - Collisions versus continuous interactions
2. **A collision rule that gives rise to large-scale behaviors**
   - Numerical simulations
   - Quantitative results: emergence of large-scale behaviors
3. **Conclusions and perspectives**
   - A new type of complex fluid
   - Lyapunov spectrum and Lyapunov modes

Ingredients for a microscopic model

- We are interested in modeling the dynamics of particles of finite size that interact through collisions, and tumble, just like bacteria.
- We first consider hard disks that move on a plane.
- The collision rule however may be more general than for elastic collisions. In particular, it does not have to conserve momentum.
- It should be chosen on the basis of experimental observations or theoretical investigation.
- We consider a collision rule that promotes collinear motion after a collision.

Collision rule

- In mathematical terms, the collision rule is given by $(\vec{v}_1,\, \vec{v}_2) \mapsto (\vec{u}_1,\, \vec{u}_2)$, where

$$\vec{u}_1 = \frac{1}{2}\left(\vec{v}_1 + \vec{v}_2 + \alpha\,\delta\vec{v}\right), \qquad \vec{u}_2 = \frac{1}{2}\left(\vec{v}_1 + \vec{v}_2 - \alpha\,\delta\vec{v}\right),$$
$$\delta\vec{v} = \frac{\vec{v}\cdot\vec{r}}{||\vec{r}||^2}\,\vec{r}, \qquad \vec{r} = \vec{r}_2 - \vec{r}_1, \qquad \vec{v} = \vec{v}_2 - \vec{v}_1, \qquad (1)$$
$$\alpha = \frac{||\vec{v}||}{||\delta\vec{v}||} \text{ if } ||\delta\vec{v}|| \neq 0 \quad \text{and} \quad \alpha = 0 \text{ otherwise.}$$

- For comparison, a binary elastic collision, which conserves momentum and kinetic energy, is given by

$$(\vec{v}_1,\, \vec{v}_2) \mapsto (\vec{u}_1,\, \vec{u}_2), \qquad \vec{u}_1 = \vec{v}_1 + \delta\vec{v}, \qquad \vec{u}_2 = \vec{v}_2 - \delta\vec{v}.$$

Molecular dynamics simulations of live particles

- Initial conditions: N particles of radius $\rho = \sqrt{\frac{L^2\eta}{N\pi}}$ ($L = 1$; η is the packing fraction) are placed on a square lattice. They are assigned random initial velocities (both components of their velocity vector are normally distributed).
- Boundary conditions are periodic.
- Tumbles: particles start tumbling after $t = 0.5$.
  - Tumbling times are uniformly distributed.
  - The velocity of a particle after a tumble has the same Maxwellian distribution as what was used for the initial conditions.
- Techniques used for molecular dynamics simulations can be adapted to simulate such a system. In particular, the codes developed for this work make use of *cell structures* and of *linked lists*, in order to save time and memory space.

Results

- The movies below show the steady state dynamics of the system for different packing fractions, both for the non-elastic collision rule introduced above, and for elastic collisions.

- They confirm that, in contrast with elastic collisions, the proposed collision rule can promote coherent, large-scale motions.

- $\eta = 0.15$: Clusters form and break up.
- $\eta = 0.45$: Clusters are bigger and more coherent.
- $\eta = 0.6$: Coherence is almost system-wide.

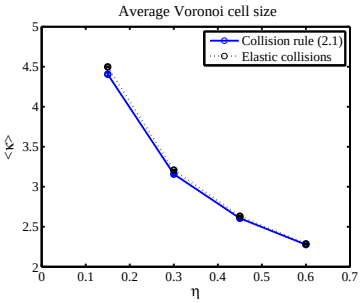
J.L., *Collective Behaviors in Two-Dimensional Systems of Interacting Particles*, SIAM J. Appl. Dyn. Sys. **10**, 1213-1231 (2011)

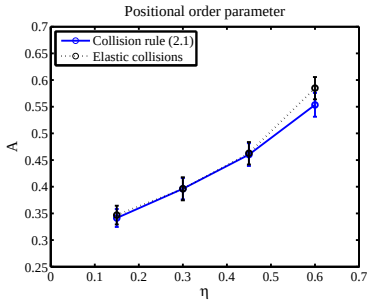
Measuring order and aggregation

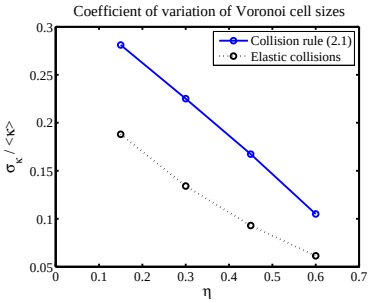
- The **positional order parameter** and the **average Voronoi cell size** measure order but do not differentiate between collision rules.
- The **coefficient of variation** of the distribution of Voronoi cell sizes quantifies the presence of large and small Voronoi cells, corresponding to regions of low and high particle density respectively.
- The **Morisita index** measures the amount of clustering in the system.
- The **total polarization** describes system-wide coherence of the particles.

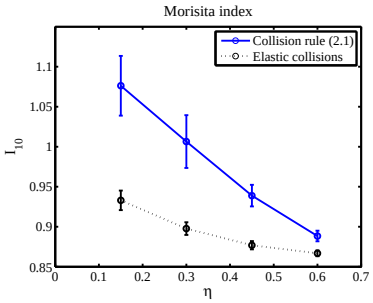
Measuring order and aggregation

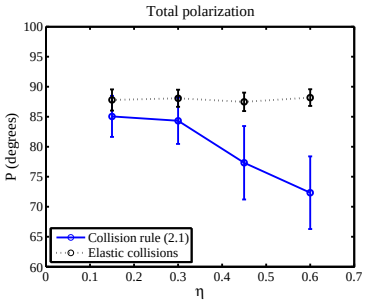
- As the packing fraction η increases,
  - the average Voronoi cell size $< \kappa >$ decreases and the positional order parameter A increases,
  - the coefficient of variation of Voronoi cell sizes $\frac{\sigma_\kappa}{< \kappa >}$ decreases and the Morisita index I_{10} decreases.
- These quantities indicate that the particle positions become more ordered and that clusters disappear as η becomes larger.
- At the same time, the total polarization P decreases, indicating an increase in the system-wide coherence of the direction of motion.











Summary

- Collision rules, defined at the microscopic scale, can affect the dynamics at the macroscopic scale.
- The collision rule introduced here is not elastic and does not conserve momentum.
- It leads to the appearance of large-scale coherent structures that have a characteristic size, but which are short lived.
- To model bacteria, randomness, in the form of tumbling, is also included.
- Only the size of the particles relative to the size of the system (or the packing fraction) is relevant. As a consequence, this approach is not restricted to bacterial systems.

Outline

Question: Can collisions, i.e. local interactions at the microscopic scale, lead to collective behaviors at the macroscopic scale?

1. **Motivations**
   - Experiments with *Bacillus subtilis*
   - Collisions versus continuous interactions
2. **A collision rule that gives rise to large-scale behaviors**
   - Numerical simulations
   - Quantitative results: emergence of large-scale behaviors
3. **Conclusions and perspectives**
   - A new type of complex fluid
   - Lyapunov spectrum and Lyapunov modes

A new type of complex fluid

- The system of particles that we just described can be viewed as a generalization of molecular or granular gases, and is therefore a new type of complex fluid.
- One can thus seek to develop a kinetic theory to describe the dynamics of macroscopic quantities.
- Because it is easier to densely pack rods rather than disks, it might be preferable to follow the same approach with colliding rods.

Lyapunov spectrum and Lyapunov modes

- **The Lyapunov spectrum** of a system of interacting hard disks shows two regions [1]:
  - Small Lyapunov exponents are associated with large-scale modes.
  - Large Lyapunov exponents are associated with modes that are very localized.
- It will be interesting to analyze how changing the collision rule affects the Lyapunov spectrum and modes.
- In particular, can one connect the emergence of collective behaviors with a loss of influence of the strongly localized modes?

[1] J.P. Eckmann, C. Forster, H.A. Posch, & E. Zabey, *Lyapunov modes in hard-disk systems*, J. Stat. Phys. **118**, 813-847 (2005).

Lyapunov spectrum and Lyapunov modes

- **The Lyapunov spectrum** of a system of interacting hard disks shows two regions [1]:
  - Small Lyapunov exponents are associated with large-scale modes.
  - Large Lyapunov exponents are associated with modes that are very localized.
- It will be interesting to analyze how changing the collision rule affects the Lyapunov spectrum and modes.
- In particular, can one connect the emergence of collective behaviors with a loss of influence of the strongly localized modes?

[1] J.P. Eckmann, C. Forster, H.A. Posch, & E. Zabey, *Lyapunov modes in hard-disk systems*, J. Stat. Phys. **118**, 813-847 (2005).

Connection with random matrices

- The flow is the composition of free flight and collision maps.
- Its linearization is the product of matrices comprised of the free flight map and the linearized collision map.
- If we assume the duration of each free flight is random, and the particles that collide are chosen randomly, the result is a random matrix.
- Results on the spectral properties of such random matrices will give information on the Lyapunov spectrum and modes of the dynamics.
- The goal would again be to describe how the collision rule affects the tangent flow.

Granular gases

- Granular gases consist of particles that interact through inelastic collisions.
- Such collisions, which dissipate energy, favor clustering.

Picture from I. Goldhirsch and G. Zanetti, *Clustering instability in dissipative gases*, Phys. Rev. Lett. **70**, 1619-1622 (1993).

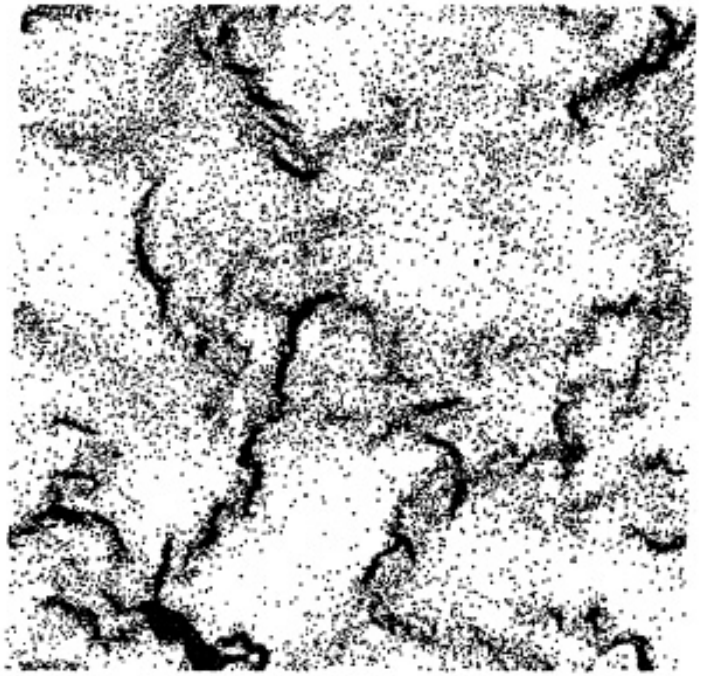
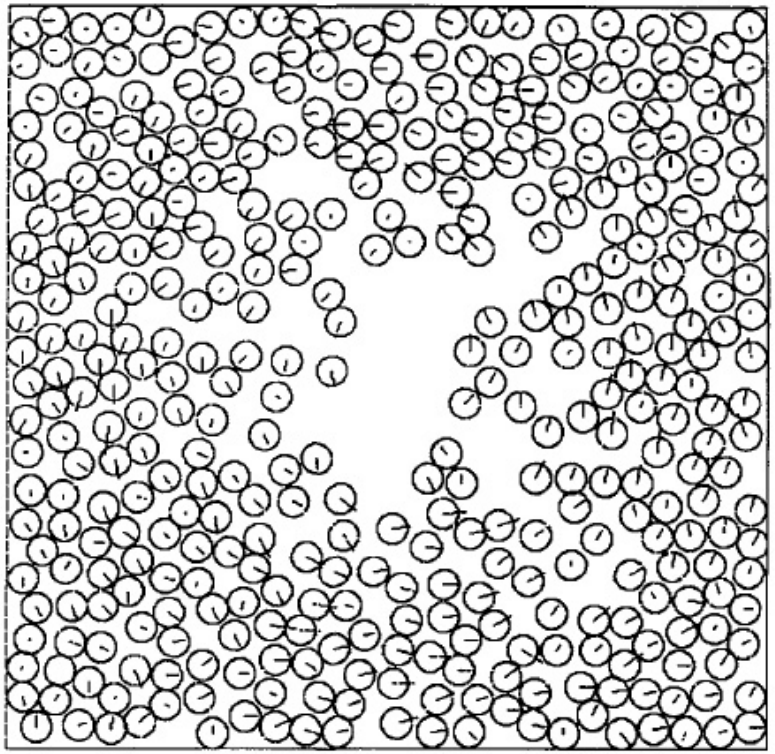


FIG. 3. A typical configuration of particles exhibiting clusters. Here the coefficient of restitution is 0.6, the time corresponds to 500 collisions per particle, and the area fraction is 0.05. The number of particles is 40000.

Back

Self-propelled granular gases

- Vortex structures, of the size of the system, were found in simulations of self-propelled disks that interact through inelastic collisions and are confined to a region of finite extent.

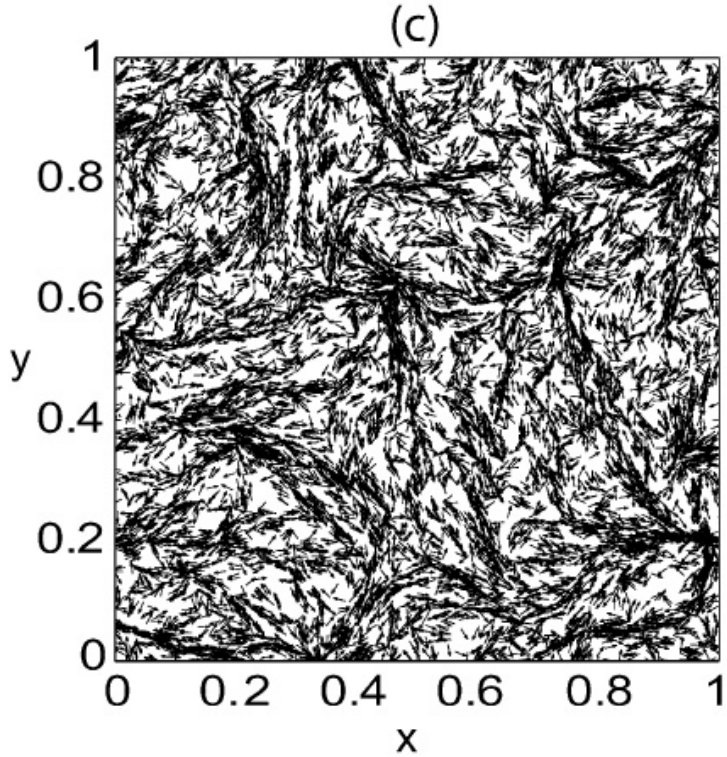


Picture from Y. Limon Duparcmeur, H. Herrmann, and J.P. Troadec, *Spontaneous formation of vortex in a system of self motorised particles*, J. Phys. I France **5**, 1119-1128 (1995).

Back

Self-propelled needles

- Simulations of self-propelled needles that interact through volume exclusion reveal a tendency for the needles to align locally and to create structures in the form of large-scale jets, at size of the system.



Picture from N. Sambelashvili, A.W.C. Lau, D. Cai, *Dynamics of bacterial flow: emergence of spatiotemporal coherent structures*, Phys. Lett. **A 360**, 507-511 (2007).

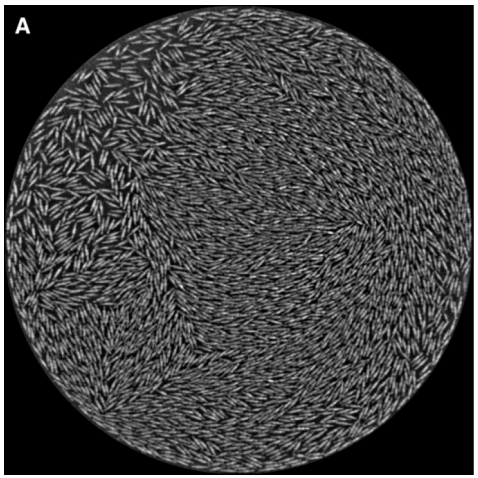
Back

Active granular nematics

- Copper rods etched at both ends, confined to an almost two-dimensional layer, and vibrated vertically, behave as an active granular nematic.

Movie

- The fact that cylindrical (i.e. not tapered at the ends) rods do not form nematic states may be an indication that the collision rule between rods plays an important role in these experiments.



Picture from V. Narayan, S. Ramaswamy, N. Menon, *Long-lived giant number fluctuations in a swarming granular nematic*, Science **317**, 105-108 (2007).

Back

Collective motions in an active granular nematic layer

V. Narayan, S. Ramaswamy, N. Menon, *Long-lived giant number fluctuations in a swarming granular nematic*, Science **317**, 105-108 (2007).

Back

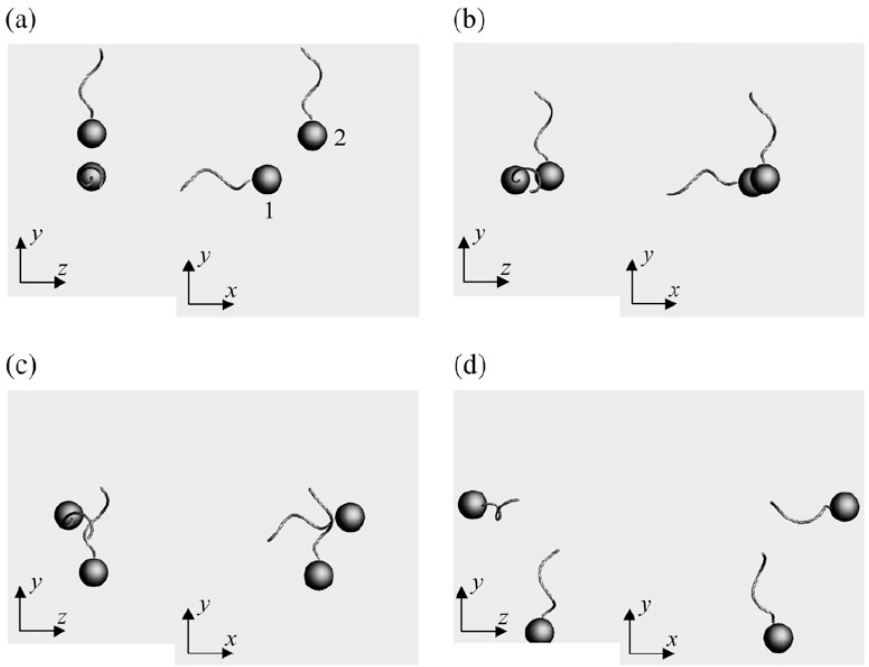
Collision between two bacteria (experiment)

Inelasic collision between two bacteria in a thin fluid film

I.S. Aranson, A. Sokolov, J.O. Kessler, & R.E. Goldstein, *Model for dynamical coherence in thin films of self-propelled microorganisms*, Phys. Rev. **E 75**, 040901 (2007).

Back

Collision between two bacteria (model)



Collision between two bacteria, based on a model taking into account hydrodynamic interactions between swimming cells

T. Ishikawa, G. Sekiya, Y. Imai, & T. Yamaguchi, *Hydrodynamic interactions between two swimming bacteria*, Biophys. J. **93**, 2217-2225 (2007).

▸ Back

Motion of *B. subtilis* on agar

The movie on the right (Cathy Ott, 2001) shows how *Bacillus subtilis* moves on agar.

▸ Larger Movie

▸ E coli movie

- *Bacillus subtilis* is a flagellated rod-like bacterium
  - Length: 2 to 3 μm.
  - Diameter: $\sim$ 0.7 μm.
  - Swimming speed: about 10 times its length per second.
  - It moves by a succession of runs and tumbles.
- In the experiments of Mendelson *et al.*, *B. subtilis*
  - does not form spores;
  - does not secrete a surfactant;
  - does not form a biofilm.

▸ Back

Collective behaviors in colonies of *B. subtilis*

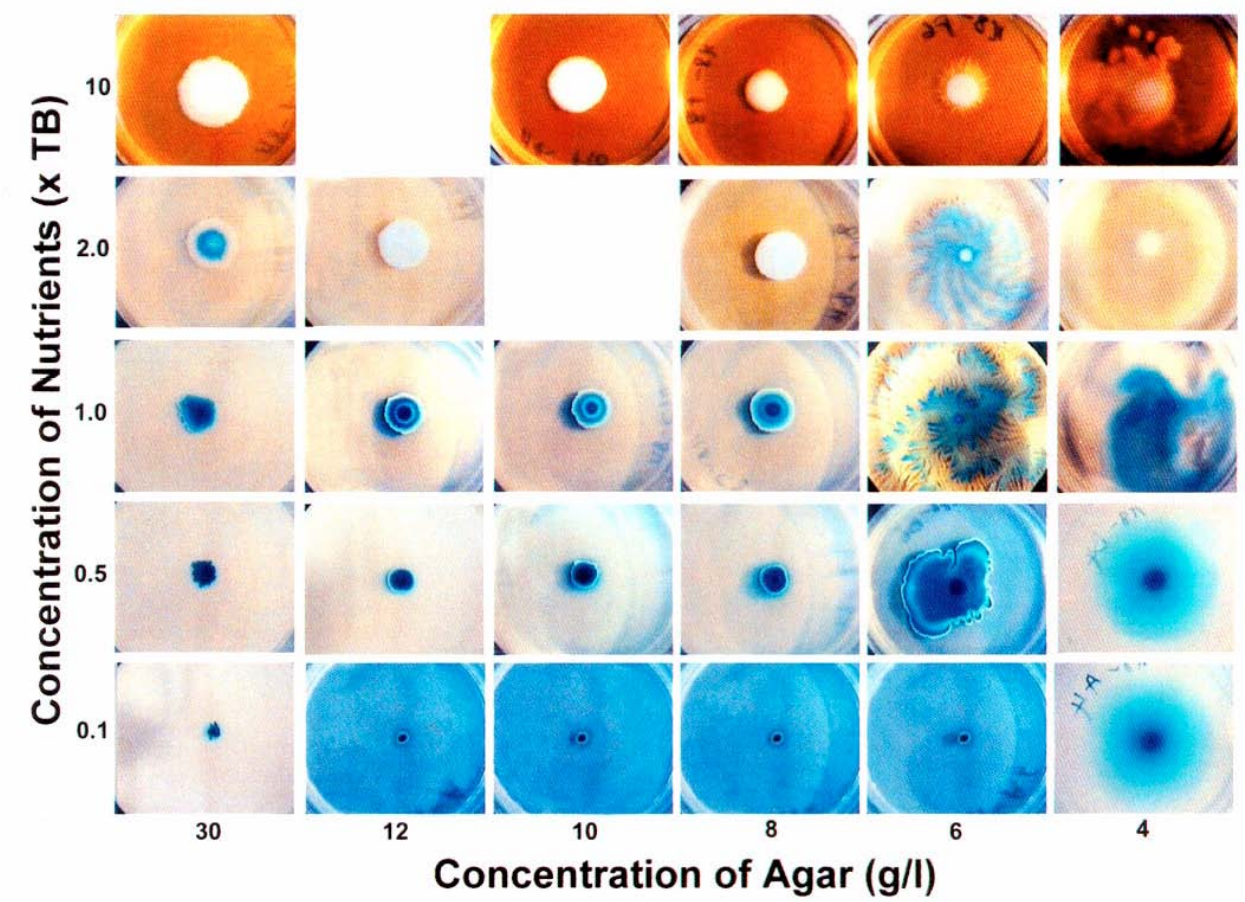
The movie on the right (Cathy Ott, 2001) shows a colony of *Bacillus subtilis* before and after exposure to formaldehyde vapors. ▸ Larger Movie

- Jets and vortices are present inside the colony.
- These motions stop when the bacteria die.
- Bacterial motion in jets is faster than the swimming speed of an isolated bacterium.
- These phenomena involve a broad range of scales.

N.H. Mendelson, A. Bourque, K. Wilkening, K.R. Anderson, and J.C. Watkins, *Organized cell swimming motions in Bacillus subtilis colonies: patterns of short-lived whirls and jets*, J. Bacteriol. **181**, 600-609 (1999).

▸ Back

Colony forms for *B. subtilis*



N.H. Mendelson, and B. Salhi, *Patterns of reporter gene expression in the phase diagram of Bacillus subtilis colony forms*, J. Bacteriol. **178**, 1980-1989 (1996).

(Diameter of petri dishes: 6 cm)

▸ Back

Hydrodynamic model

$$\frac{\partial S}{\partial t} = R_S + D^S \nabla^2 S$$

$$\frac{\partial W}{\partial t} + \nabla \cdot (W \vec{v}) = R_W + \nabla \cdot \left(D^W \nabla W \right) - \nabla \cdot \left(D^N \nabla N \right)$$

$$\frac{\partial N}{\partial t} + \nabla \cdot (N \vec{v}) = R_N + \nabla \cdot \left(D^N \nabla N \right)$$

$$\frac{\partial \vec{v}}{\partial t} = \mathcal{P} \left[- (\vec{v} \cdot \nabla) \vec{v} + \left(\frac{1}{\rho} - \frac{1}{\rho_m} \right) \mathcal{D} \vec{v} - \left(\frac{\eta}{\rho} - \frac{\eta_m}{\rho_m} \right) \vec{v} + \frac{\vec{F}}{\rho} \right]$$
$$- \frac{1}{\rho} \nabla p_c^N + \frac{\mathcal{D} \vec{v}}{\rho_m} - \frac{\eta_m}{\rho_m} \vec{v},$$

where S, W and N are the concentrations of nutrients, water, and bacteria respectively, $\vec{v}$ is the velocity field of the bacteria-water mixture, $\rho = N + W$, $\mathcal{D}\vec{v} = \mu \nabla^2 \vec{v} + \lambda \nabla (\nabla \cdot \vec{v})$, η_m and ρ_m are typical (constant) values of η and ρ in the system, and $\mathcal{P}\vec{v}$ is the projection of $\vec{v}$ on its solenoidal part.

Back

Chemotaxis-like behavior

- Only keep the bacterial pressure term in the equation for $\vec{v}$.
- Neglect diffusion in equation for nutrients and assume $R_S = -k_0 N \varphi$, where φ is an arbitrary function of S.
- Then, the hydrodynamic model may be simplified into

$$\frac{\partial S}{\partial t} = R_S + D^S \nabla^2 S \qquad \vec{v} \simeq \frac{2\gamma}{k_0} \frac{N}{\rho} \frac{\nabla S}{\varphi(S)} = \chi \nabla S$$

$$\frac{\partial W}{\partial t} + \nabla \cdot (W \vec{v}) = R_W + \nabla \cdot \left(D^W \nabla W \right) - \nabla \cdot \left(D^N \nabla N \right)$$

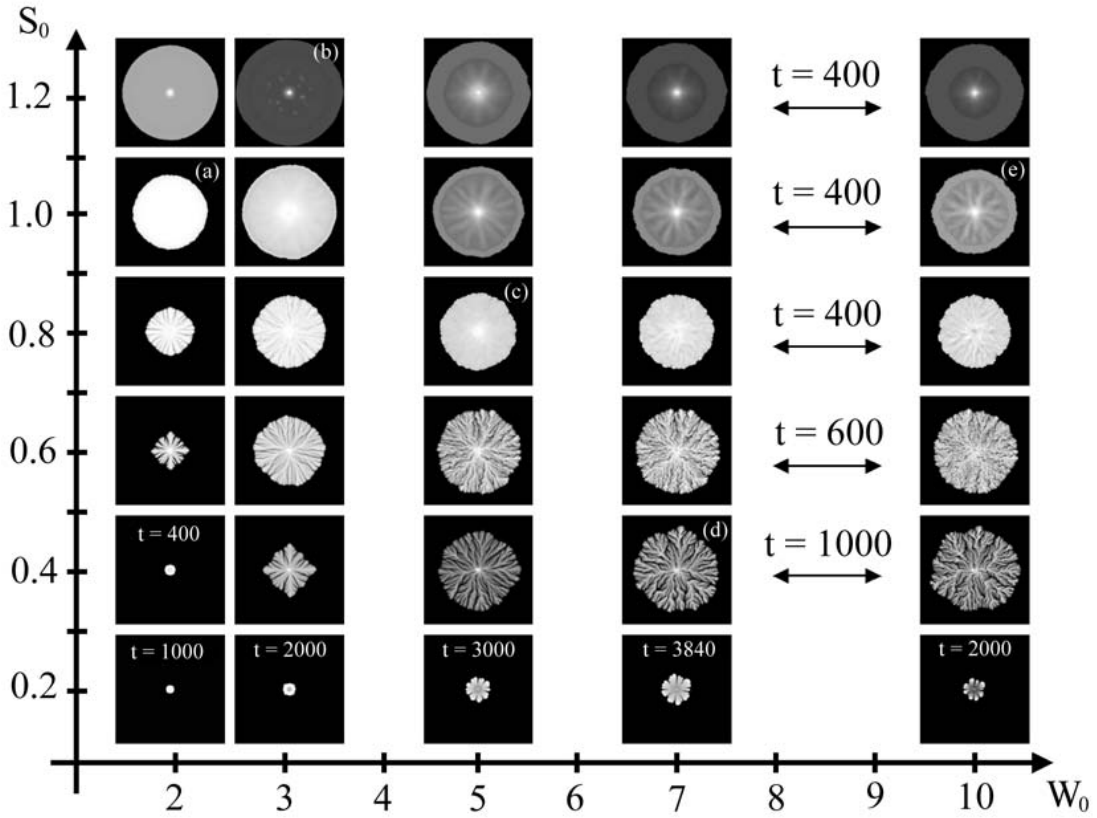
$$\frac{\partial N}{\partial t} + \nabla \cdot (N \vec{v}) = R_N + \nabla \cdot \left(D^N \nabla N \right)$$

The *chemotactic coefficient* $\chi = \dfrac{2\gamma}{k_0} \dfrac{N}{\rho} \dfrac{1}{\varphi(S)}$ matches

- The Keller-Segel model for chemotaxis if $\varphi(S) = S$.
- The "receptor law" for chemotaxis if $\varphi(S) = (1+S)^2$.

Back

Numerical phase diagram



$D^S = 0.002$

$D^W = 0.002$

$D_0 = 0.0004$

$k_0 = 1.0$ $\quad N_0 = 1.0$

$\alpha = 1.0$ $\quad \mu = 0.01$

$f_0 = 0.04$ $\quad \eta = 0.01$

$\gamma_0 = 0.001$ $\quad \lambda_W = 0$

▸ $W_0 = 3$ - $S_0 = 1.2$

▸ $W_0 = 7$ - $S_0 = 0.4$

$$R_S = -k_0 NS|N_0 - N| \quad R_N = \alpha NS(N_0 - N) \quad R_W(N,S,W) = -\lambda_W W$$

$$D^N(N,S,W) = D_0\, f(N,S,W) \qquad F_g(N,S,W) = \rho\, f_0\, f(N,S,W) G$$

$$F_e(N,S,W) = 0 \qquad \gamma(N,S,W) = \gamma_0\, f(N,S,W)$$

$f(N,S,W)$ is small for W_0 or N_0 small, and of order 1 otherwise

▸ Back

Reaction-diffusion models

It is well known that branched colony shapes may be captured by means of reaction-diffusion models

$$\frac{\partial S}{\partial t} = D^S \nabla^2 S - \eta N S$$

S : density of nutrients
N : density of bacteria

- These models often involve nonlinear diffusion

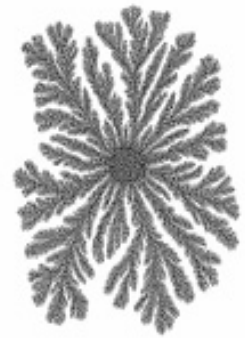
$$\frac{\partial N}{\partial t} = \nabla \left(D^N N^k \nabla N \right) + NS - \mu N$$

S. Kitsunezaki, J. Phys. Soc. Jpn. **66**, 1544-1550 (1997)

- Possibly with a stochastic diffusion coefficient

$$\frac{\partial N}{\partial t} = \nabla \left(D^N (1+\sigma) NS \nabla N \right) + NS$$

K. Kawasaki et al., J. Theor. Biol. **188**, 177-185 (1997)



Images from I. Golding et al., Physica **A 260**, 510-554 (1998).

Back

Collective motions in *B. subtilis* colony

Movie by Cathy Ott

Back

Motion of *B. subtilis* on agar

Movie by Cathy Ott

Back

Swimming of *E. coli* on agar

▸ Back

Turner, L., Ryu, W.S. and Berg, H.C. Real-time imaging of fluorescent flagellar filaments. J. Bacteriol. **182**, 2793-2801 (2000).

Hydrodynamic model, with T. Passot

- Our model is based on a two-phase fluid description of dense colonies growing on agar plates.
- It generalizes classical reaction-diffusion equations with nonlinear diffusion that are used in the literature to model bacterial colonies.
- It describes large-scale collective bacterial behaviors in terms of a hydrodynamic field $\vec{v}$ and reproduces a variety of colony forms observed in experiments.
- Our numerical simulations revealed a non-trivial interaction between hydrodynamic motions within the colony and the dynamics of the colony boundary.

J.L. & T. Passot,
Hydrodynamics of bacterial colonies: a model, Phys. Rev. **E 67**, 031906 (2003);
Hydrodynamics of bacterial colonies: phase diagrams, Chaos **14**, 562-570 (2004);
Hydrodynamics of bacterial colonies, Nonlinearity **20**, C1-C16 (2007).

▸ Back

Techniques of molecular dynamics simulations

- In a system of hard disks, one needs to estimate collision times between particles. This is typically resource consuming, especially when the number of particles N is large.
- The problem is similar for soft potentials, since one would have to calculate the contribution of each particle to the potential experienced by any other particle.
- The above process is greatly simplified by dividing the computational box into cells, so that collisions take place between particles that are either in the same or in neighboring cells.
- The price to pay is that one then has to correctly describe what happens when a particle leaves a cell and keep track of which cell each particle occupies (in particular when collisions occur on the boundary between two cells).

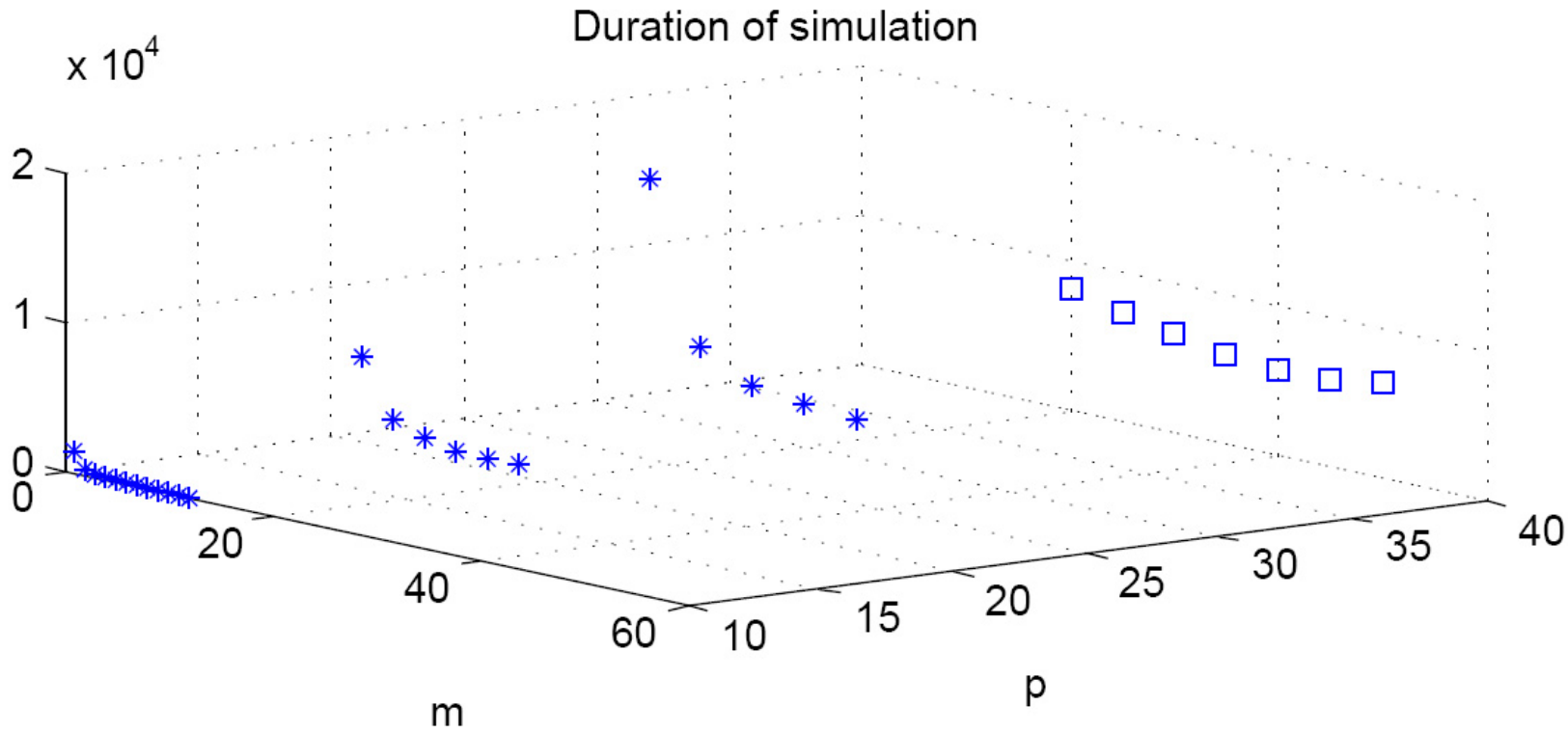
Techniques of molecular dynamics simulations

This can be accomplished as follows.

- Define a `head` matrix, of size equal to the number of cells, such that the j^{th} entry of `head` is the index of a particle in cell j. If that cell is empty, then $\texttt{head}(j) = 0$.
- Define a linked list that keeps track of particles in a same cell, such that
  1. $\texttt{list}(j) = i$ means that particle i is in the same cell as particle j.
  2. $\texttt{list}(j) = 0$ means that there are no other particles in that cell.
- It is then easy to
  1. Find all of the particles in a given cell;
  2. Update the `head` and `list` matrices when a particle moves from one cell to another.

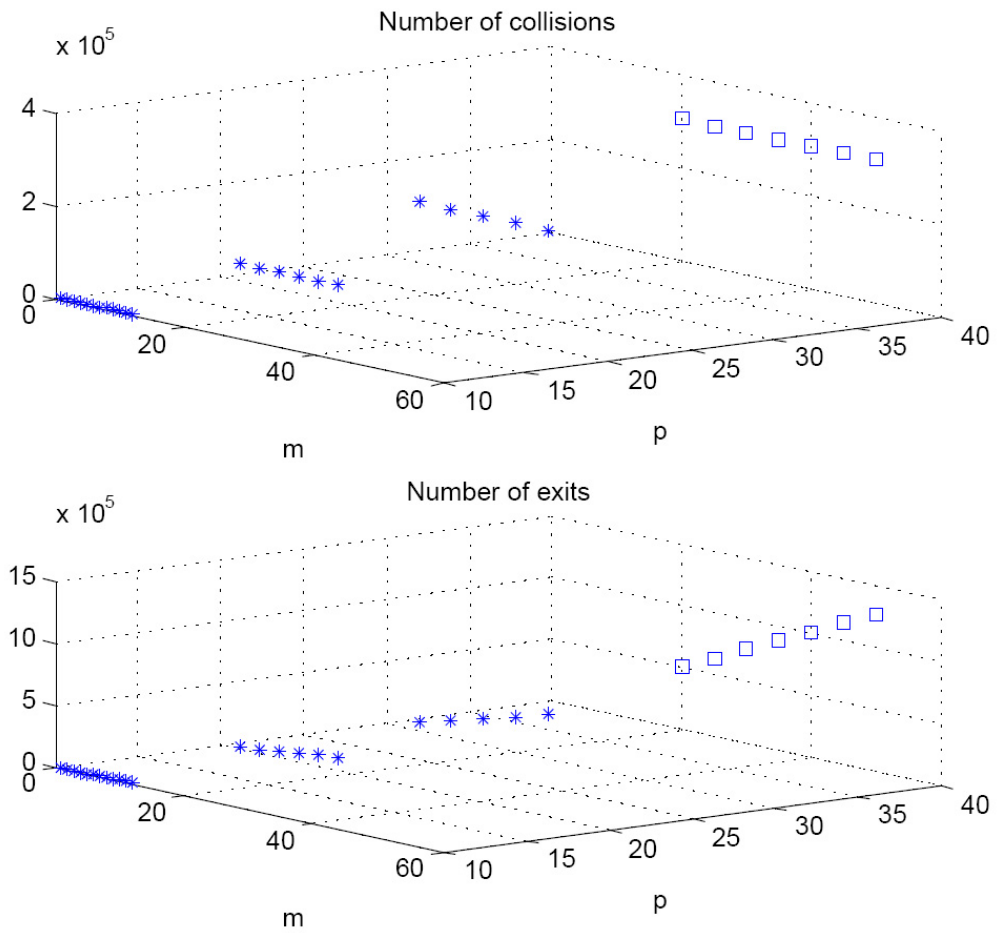
Techniques of molecular dynamics simulations

The simulation time decays faster than exponentially as the number of cells increases.



Simulation time as a function of the number of particles p and the number of cells m.

Techniques of molecular dynamics simulations



Number of collisions (top) and number of exits (bottom) as functions of the number of particles p and the number of cells m.

Back

Numerical simulation - $\eta = 0.15$

Left: non-elastic collisions. Right: elastic collisions

Back

Numerical simulation - $\eta = 0.6$

Left: non-elastic collisions. Right: elastic collisions

Back

Numerical simulation - $\eta = 0.45$

Left: non-elastic collisions. Right: elastic collisions

Back

Numerical simulation - $W_0 = 3$ - $S_0 = 1.2$

Movie from $t = 340$ to $t = 400$, with a frame shown every unit of time

Back

Numerical simulation - $W_0 = 7$ - $S_0 = 0.4$

Movie from $t = 0$ to $t = 1000$, with a frame shown every 20 units of time

Back

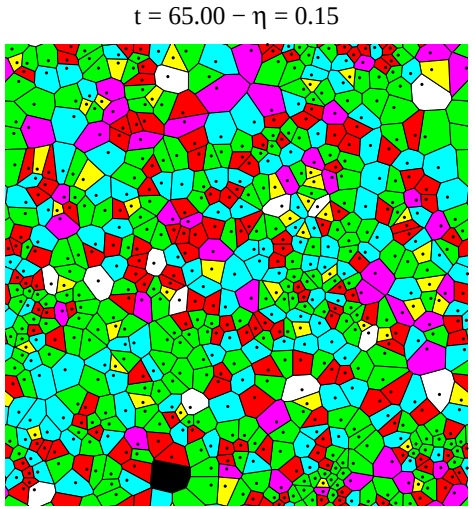
Numerical simulation - $W_0 = 5$ - $S_0 = 0.8$ - $\gamma_0 = 10^{-10}$

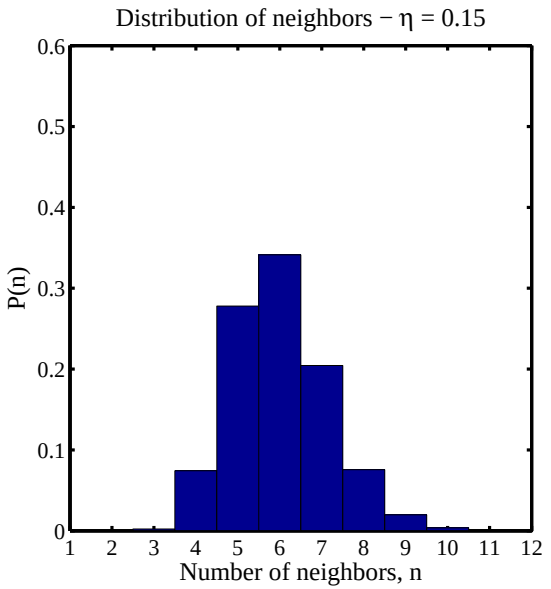
Movie from $t = 400$ to $t = 410$, with a frame shown every 0.1 unit of time

Back

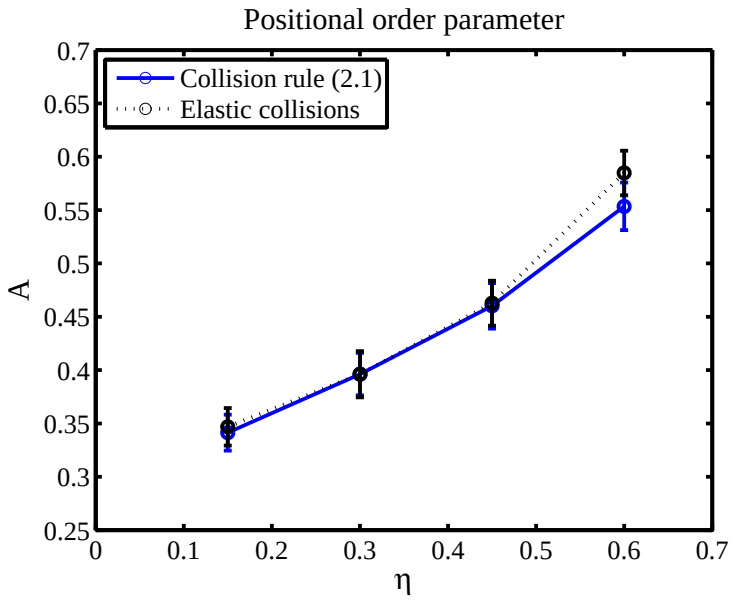
Positional order parameter and average Voronoi cell size

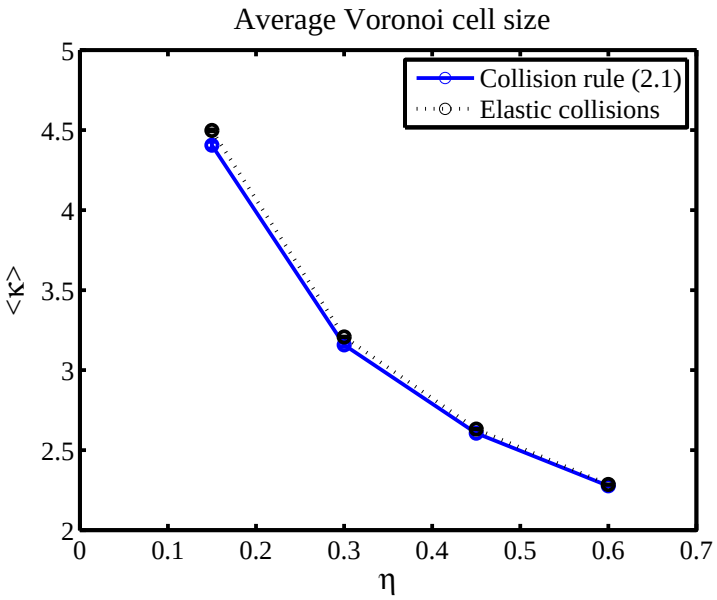
- A measure of order is given by how close the system is to a hexagonal lattice.
- Voronoi tessellations are used to count the number of neighbors of each particle. We define the positional order parameter as the probability for a particle to have 6 neighbors.
- Clusters of particles correspond to small Voronoi cells, while regions of low particle density are associated with larger Voronoi cells.





Positional order parameter and average Voronoi cell size

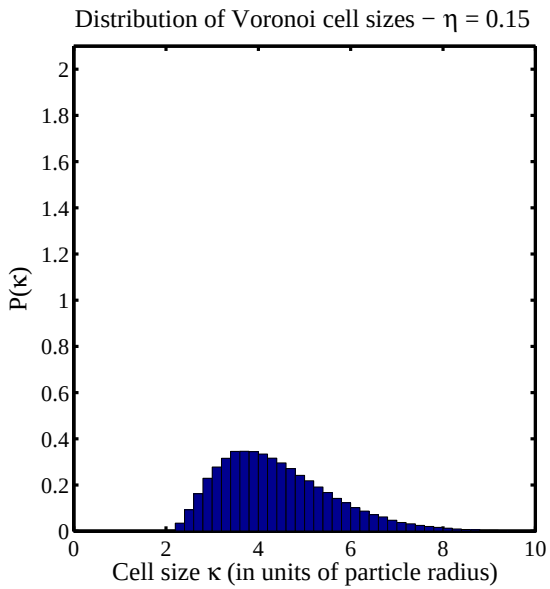


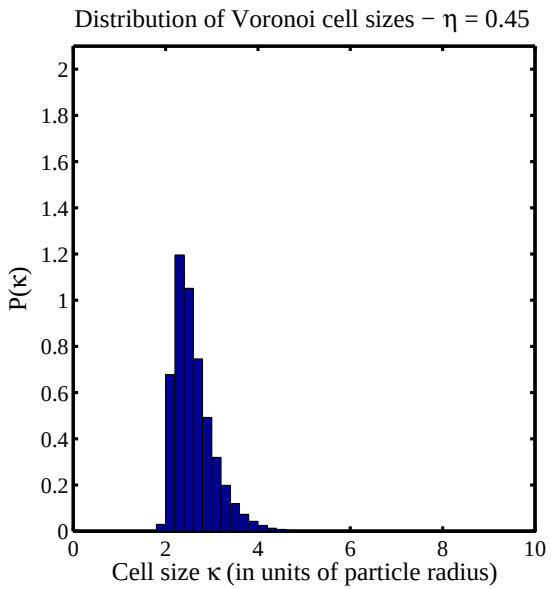


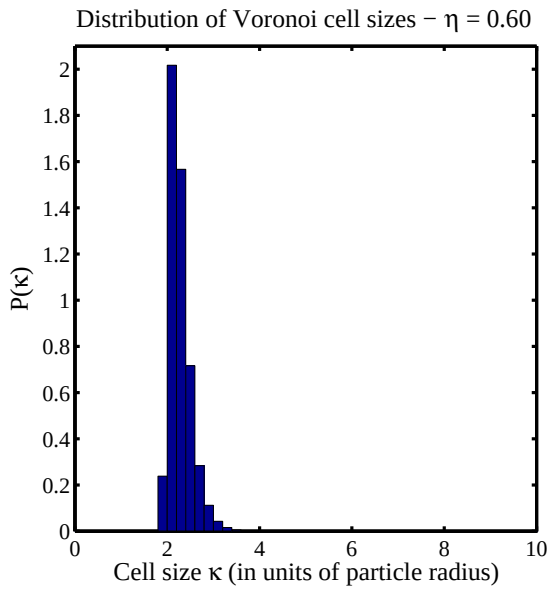
Positional order parameter (left) and average Voronoi cell size (right) as functions of the packing fraction η, for both types of collision rules. Error bars correspond to one standard deviation above and below the mean.

Back

Distribution of Voronoi cell sizes

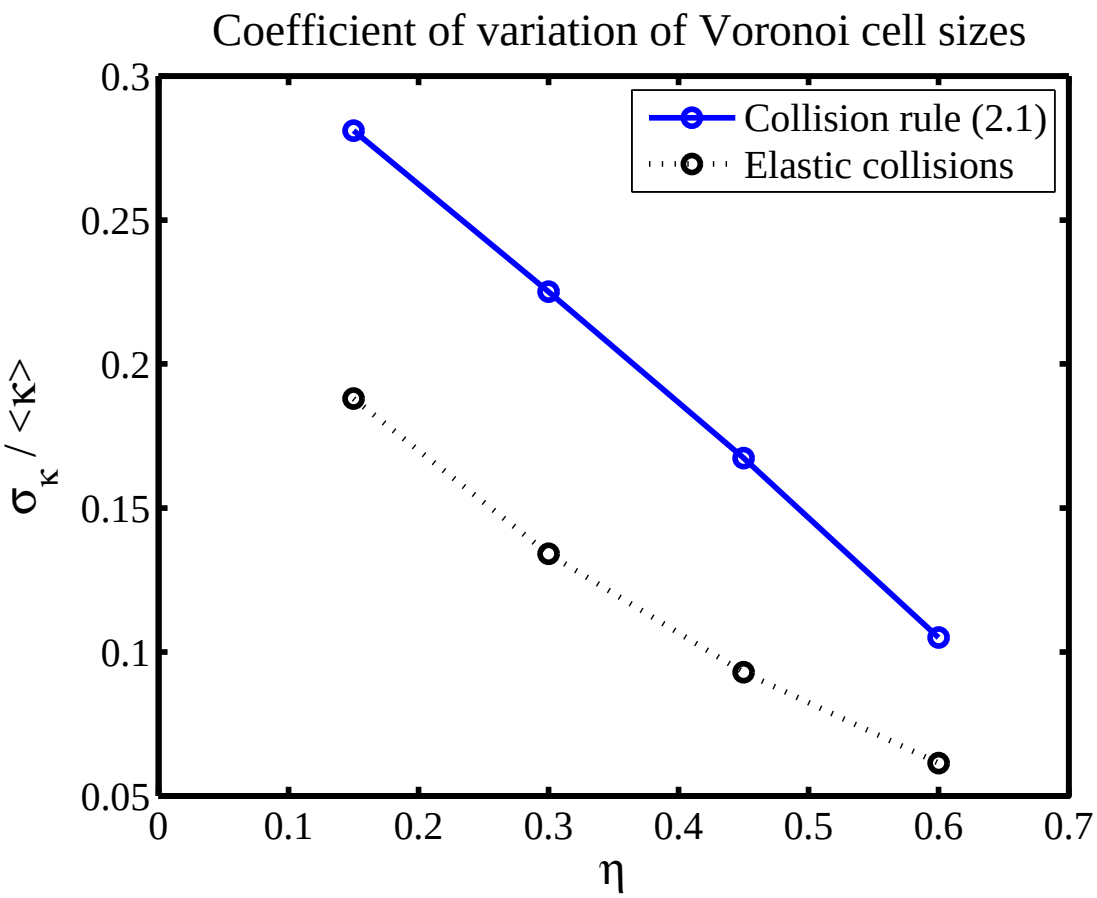






Probability distribution functions for Voronoi cell sizes at given values of the packing fraction η.

Coefficient of variation of Voronoi cell sizes



Coefficient of variation of the distribution of Voronoi cell sizes, for both types of collisions.

Back

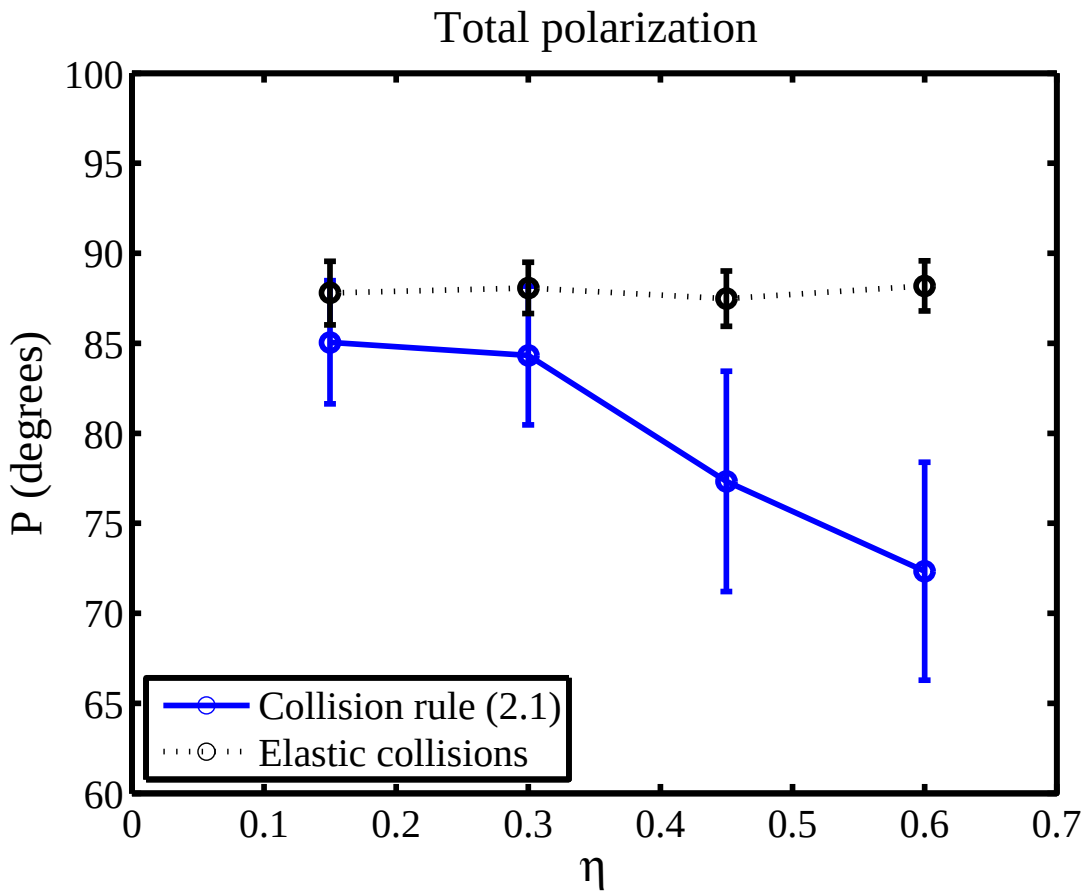
Polarization

- The polarization of a group of agents (e.g. fish in a school) is defined as "the average of the angle deviation of each fish to the mean swimming direction of the school. For $p = 0^{\circ}$ the school is optimally parallel, for $p = 90^{\circ}$ the school is maximally confused."
- Here, we define the polarization P as the average of the absolute value of the angle ($\in [-\pi,\ \pi]$) between the direction of motion of each particle and the average direction of motion of the group

$$P = \left\langle \sum_{i=1}^{N_g} |\theta_i(t) - \theta(t)| \right\rangle_t .$$

A. Huth, C. Wissel, *The simulation of fish schools in comparison with experimental data*, Ecological Modelling **75**, 135-145 (1994).

Polarization



Polarization as a function of the packing fraction η, for both types of collision rules. Error bars represent one standard deviation below and above the mean.

Back

The Morisita index

- The Morisita index I_δ of a population of N individuals divided into δ units is defined as

$$I_\delta = \delta \frac{\sum_{i=1}^{\delta} x_i(x_i - 1)}{N(N-1)},$$

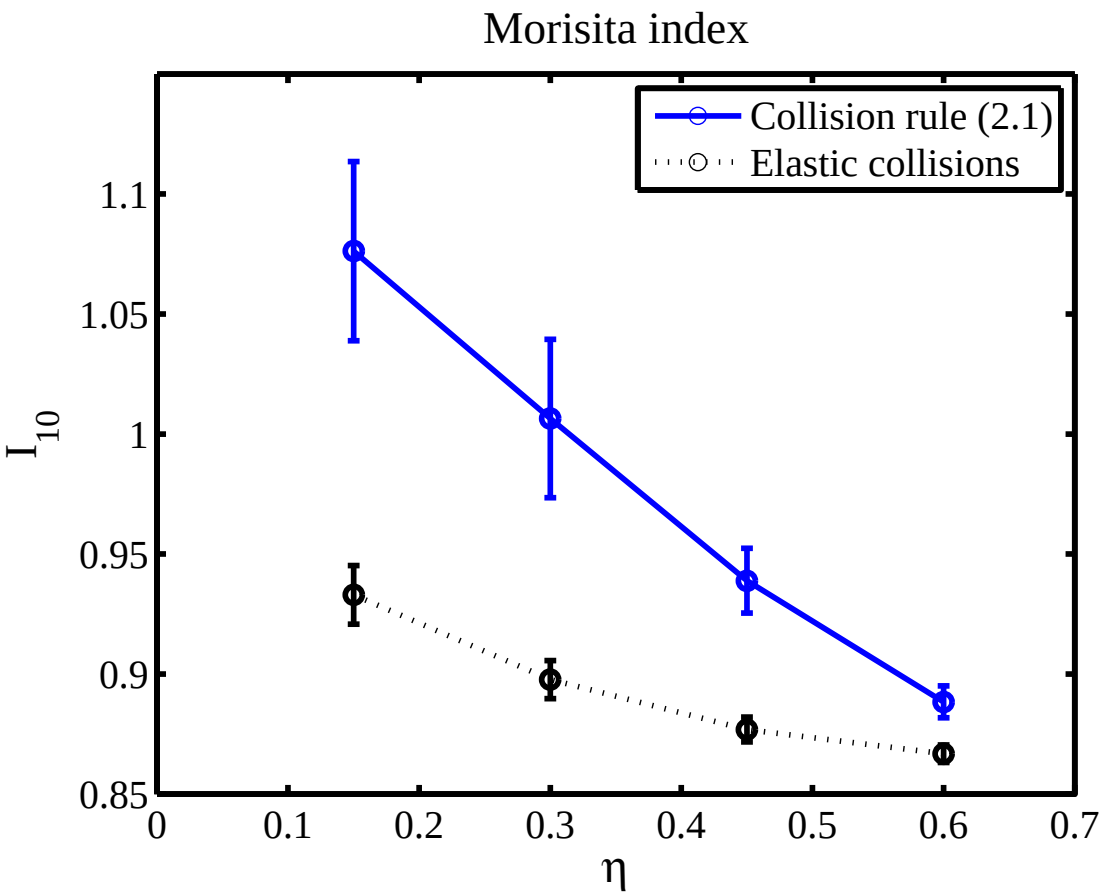
  where x_i is the number of individuals in unit i.

- I_δ measures the probability of having two individuals together in any one of the δ units, divided by that same probability if the individuals were grouped randomly.

- If the units are the cells in a square lattice covering the region where the population is distributed, then I_δ measures clustering.

M. Morisita, *Application of I_δ-index to sampling techniques*, Res. Popul. Ecol. **VI**, 43-53 (1964).

The Morisita index

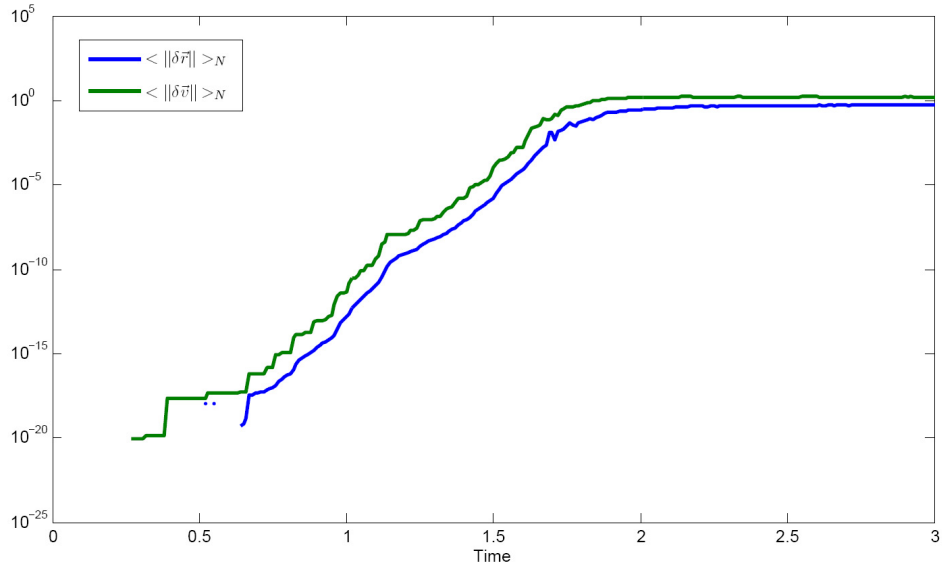


Morisita index I_{10} as a function of the packing fraction η, for both types of collision rules. Error bars represent one standard deviation below and above the mean.

Back

Molecular gases are chaotic

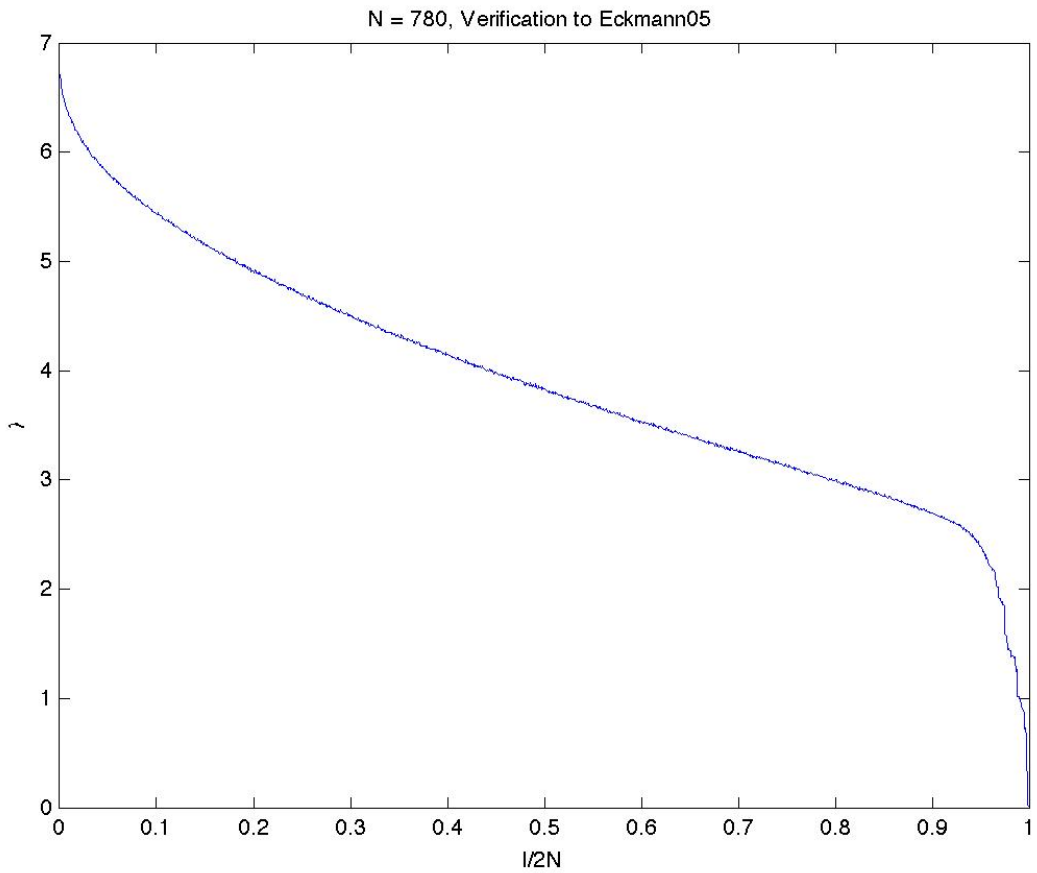
Systems of interacting hard disks are typically chaotic. This is well known for the case of standard molecular dynamics simulations, with collision rules that conserve momentum and energy.



Simulations with 100 particles. Random components of size 10^{-18} are added to each velocity vector after each collision. (Left) The circles show the particles in the absence of noise, and the stars in the presence of noise. (Right) The distance between the two sets of particles first increases exponentially with time, and then saturates.

▸ Back

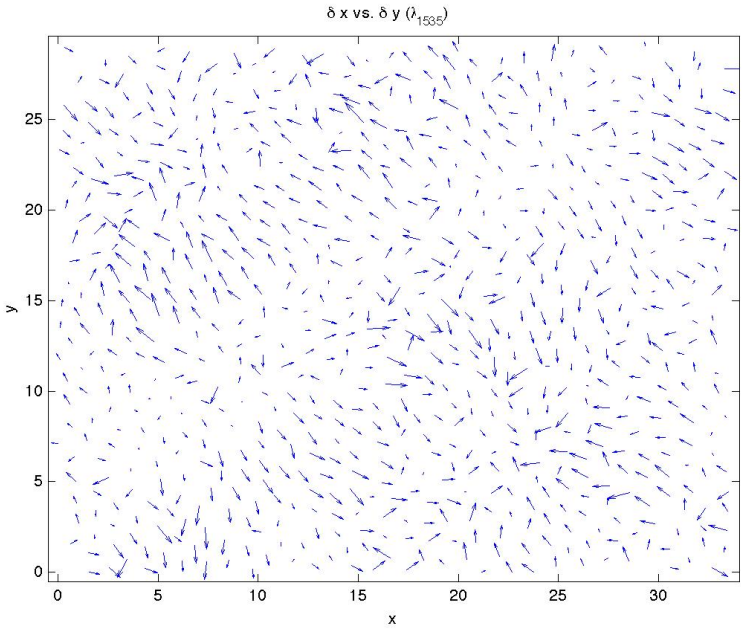
Lyapunov Spectrum

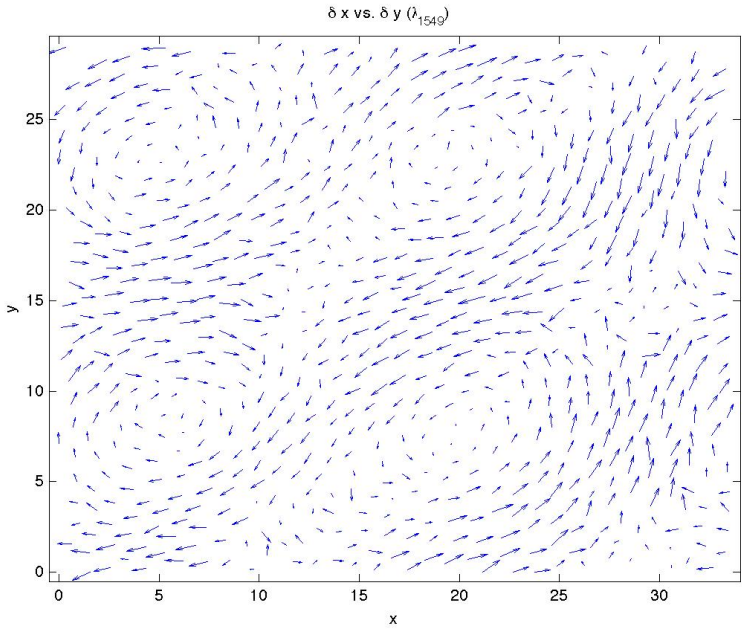


Lyapunov spectrum for a system of 780 hard disks, as in the work of Eckmann et al. (2005). Simulations by Joe Dinius.

▸ Back

Lyapunov Modes

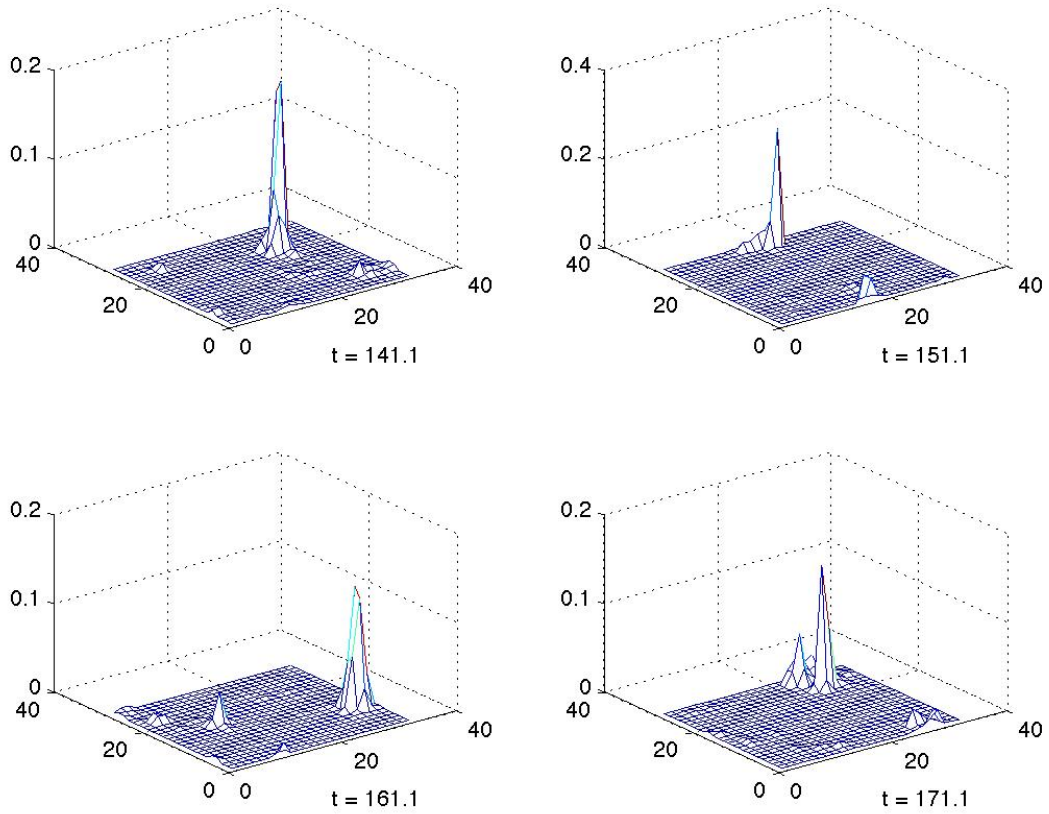




Large-scale Lyapunov modes for a system of 780 hard disks, as in the work of Eckmann et al. (2005). Simulations by Joe Dinius.

▸ Back

Lyapunov Modes



Mode associated with the largest Lyapunov exponent, for a system of 780 hard disks, as in the work of Eckmann et al. (2005). Simulations by Joe Dinius.

▸ Back