Complex patterns in particle aggregation models of biological formation

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Introduction

- Animals often aggregate in groups
- Biologically, it can provide protection from predators; conserve heat, act without an apparent leader, enable collective behaviour
- Examples include bacteria, ants, fish, birds, bees....
Aggregation model

We consider a simple model of particle interaction,

\[
\frac{dx_j}{dt} = \frac{1}{N} \sum_{k=1, \ldots, N \atop k \neq j} F(|x_j - x_k|) \frac{x_j - x_k}{|x_j - x_k|}, \quad j = 1 \ldots N
\]  

(1)


- Interaction force \( F(r) \) is of attractive-repelling type: the insects repel each other if they are too close, but attract each other at a distance.

- Note that acceleration effects are ignored as a first-order approximation.

- Mathematically \( F(r) \) is positive for small \( r \), but negative for large \( r \).
Commonly, a **Morse interaction force** is used:

\[ F(r) = \exp(-r) - G \exp(-r/L); \quad G < 1, L > 1 \]  

(2)

Under certain conditions on repulsion/attraction, the steady state typically consists of a bounded “particle cloud” whose diameter and is independent of \( N \) in the limit \( N \to \infty \). Then the continuum limit becomes

\[
\rho_t + \nabla \cdot (\rho v) = 0; \quad v(x) = \int_{\mathbb{R}^n} F(|x - y|) \frac{x - y}{|x - y|} \rho(y) dy.
\]

**Questions**

1. Describe the equilibrium cloud shape in the limit \( t \to \infty \)

2. What about dynamics?
Morse force, h-stable vs. catastrophic

- If $GL^{n+1} > 1$, the system is catastrophic: doubling $N$ doubles the density but cloud volume is unchanged:

  $$F(r) = e^{-r} - 0.5e^{-r/2}$$

- If $GL^{n+1} < 1$, the system is h-stable: doubling $N$ doubles the cloud volume: but density is unchanged:

  $$F(r) = e^{-r} - 0.5e^{-r/1.2}$$
Tanh-type force: \( F(r) = \tanh ((1 - r) a) + b \)
Part I: Ring-type steady states

- Seek steady state of the form $x_j = r \left( \cos \left( \frac{2\pi j}{N} \right), \sin \left( \frac{2\pi j}{N} \right) \right), \ j = 1 \ldots N$.

- In the limit $N \to \infty$ the radius of the ring must be the root of

$$I(r) := \int_0^{\frac{\pi}{2}} F(2r \sin \theta) \sin \theta d\theta = 0.$$  \hspace{1cm} (3)

- For Morse force $F(r) = \exp(-r) - G \exp(-r/L)$, such root exists whenever $GL^2 > 1$ [coincides with 1D catastrophic regime]

- For general repulsive-attractive force $F(r)$, a ring steady state exists if $F(r) \leq C < 0$ for all large $r$.

- Even if the ring steady-state exists, the time-dependent problem can be ill-posed!
Continuum limit for curve solutions

- If particles concentrate on a curve, in the limit $N \to \infty$ we obtain
  \[
  \rho_t = \rho \frac{\langle \dot{z}_\alpha, \dot{z}_\alpha t \rangle}{|\dot{z}_\alpha|^2}; \quad z_t = K \ast \rho
  \]  \hspace{1cm} (4)

  where $z(\alpha; t)$ is a parametrization of the solution curve; $\rho(\alpha; t)$ is its density and
  \[
  K \ast \rho = \int F(|z(\alpha') - z(\alpha)|) \frac{z(\alpha') - z(\alpha)}{|z(\alpha') - z(\alpha)|} \rho(\alpha', t) dS(\alpha').
  \]  \hspace{1cm} (5)

- Depending on $F(r)$ and initial conditions, the curve evolution may be **ill-defined!**
  - For example a circle can degenerate into an annulus, gaining a dimension.

- We used a Lagrange particle-based numerical method to resolve (4).
  - Agrees with direct simulation of the ODE system (1):
Local stability of a ring

• Linearize: $x_k = r_0 \exp \left( \frac{2\pi ik}{N} \right) (1 + \exp(t\lambda)\phi_k)$ where $\phi_k \ll 1$.

• Ring is stable of $\text{Re} (\lambda) \leq 0$ for all pair $(\lambda, \phi)$. There are three zero eigenvalues corresponding to rotation and translation invariance; all other eigenvalues come in pairs due to rotational invariance.

• $\lambda$ is the eigenvalue of

$$M(m) := \begin{bmatrix} I_1(m) & I_2(m) \\ I_2(m) & I_1(-m) \end{bmatrix}; \quad m = 2, 3, \ldots \quad (6)$$

$$I_1(m) = \frac{2}{\pi} \int_0^{\frac{\pi}{2}} \left[ \frac{F(2r \sin \theta)}{2r \sin \theta} + F'(2r \sin \theta) \right] \sin^2 ((m + 1)\theta) \, d\theta; \quad (7a)$$

$$I_2(m) = \frac{2}{\pi} \int_0^{\frac{\pi}{2}} \left[ \frac{F(2r \sin \theta)}{2r \sin \theta} - F'(2r \sin \theta) \right] \left[ \sin^2 (m\theta) - \sin^2 (\theta) \right] \, d\theta. \quad (7b)$$

• Eigenfunction is a pure fourier mode when projected to the curvilinear coordinates of the circle.
Quadratic force \( F(r) = r - r^2 \)

- Computing explicitly,

\[
\text{tr } M(m) = -\frac{(4m^4 - m^2 - 9)}{(4m^2 - 1)(4m^2 - 9)} < 0, \quad m = 2, 3, \ldots
\]

\[
\det M(m) = \frac{3m^2(2m^2 + 1)}{(4m^2 - 9)(4m^2 - 1)^2} > 0, \quad m = 2, 3, \ldots
\]

- Conclusion: **ring pattern corresponding to** \( F(r) = r - r^2 \) **is locally stable**

- For large \( m \), the two eigenvalues are \( \lambda \sim -\frac{1}{4} \) and \( \lambda \sim -\frac{3}{8m^2} \to 0 \) as \( m \to \infty \). The presence of arbitrary small eigenvalues implies the existence of very slow dynamics near the ring equilibrium.
General power force

\[ F(r) = r^p - r^q, \quad 0 < p < q \]

- The mode \( m = \infty \) is stable if and only if \( pq > 1 \) and \( p < 1 \).
- Stability of other modes can be expressed in terms of Gamma functions.
- The dominant unstable mode corresponds to \( m = 3 \); the boundary is given by
  \[ 0 = 723 - 594(p + q) - 27(p^2 + q^2) - 431pq + 106(pq^2 + p^2q) + 19(p^3q + pq^3) \]
  \[ + 10(p^3q^2 + p^2q^3) + 6(p^3 + q^3) + p^3q^3; \]
- Boundaries for \( m = 4, 5, \ldots \) are similarly expressed in terms of higher order polynomials in \( p, q \).
(In)stability of $m \gg 1$ modes

- If $\lambda(m) > 0$ for all sufficiently large $m$, then we call the ring solution **ill-posed**. Otherwise we call it **well-posed**.

- For ill-posed problems, the ring can degenerate into either an annulus (eg. $F(x) = 0.5 + x - x^2$) or discrete set of points (eg $F(x) = x^{1.3} - x^2$)

- , if $F(r)$ is $C^4$ on $[0, 2r]$, then the necessary and sufficient conditions for well-posedness of a ring are:

  \[
  F(0) = 0, \quad F''(0) < 0 \quad \text{and} \quad \int_0^{\pi/2} \left( \frac{F(2r \sin \theta)}{2r \sin \theta} - F'(2r \sin \theta) \right) d\theta < 0.
  \]

- Ring solution for the morse force $F(r) = \exp(-r) - F \exp(-r/L)$ is always ill-posed.
Discrete vs. continuous

• Consider e.g. \( F(r) = \tanh(4(1 - r)) - 0.5 \). The ring for the \textit{continuous model} is ill-posed since \( F(0) > 0 \). But the ring for the \textit{discrete model} is stable with \( N = 120 \) particles!

• The most unstable mode in the discrete system is \( m = N/2 \) and can be stable even if the continuous model is ill-posed!

• This can lead to “thin annuli” solutions...
Weakly nonlinear analysis

- Near the instability threshold, higher-order analysis shows a **supercritical pitchfork bifurcation**, whereby a ring solution bifurcates into an $m-$symmetry breaking solution.
- This shows existence of nonlocal solutions.
- Example: $F(r) = r^{1.5} - r^q$; bifurcation $m = 3$ occurs at $q = q_c \approx 4.9696$; nonlinear analysis predicts
  \[
  \max_i |x_i| - \min_i |x_i| = \sqrt{\max 0, \tau(q - q_c)}; \quad \tau \approx 0.109.
  \]
3D sphere instabilities

- Radius satisfies: \[ \int_0^\pi F(2r_0 \sin \theta) \sin \theta \sin 2\theta = 0 \]
- Instability can be done using spherical harmonics
Stability of a spherical shell

Define
\[ g(s) := \frac{F(\sqrt{2s})}{\sqrt{2s}}; \]

The spherical shell has a radius given implicitly by
\[ 0 = \int_{-1}^{1} g(R^2(1 - s))(1 - s)ds. \]

Its stability is given by a sequence of 2x2 eigenvalue problems
\[ \lambda \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} \alpha + \lambda_l(g_1) & l(l + 1)\lambda_l(g_2) \\ \lambda_l(g_2) & \frac{l(l+1)}{R^2}\lambda_l(g_3) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \quad l = 2, 3, 4, \ldots \]

where
\[ \lambda_l(f) := 2\pi \int_{-1}^{1} f(s)P_l(s) \, ds; \]

with \( P_l(s) \) the Legendre polynomial and
\[ \alpha := 8\pi g(2R^2) + \lambda_0(g(R^2(1 - s^2))) \]
\[ g_1(s) := R^2 g'(R^2(1 - s))(1 - s)^2 - g(R^2(1 - s))s \]
\[ g_2(s) := g(R^2(1 - s))(1 - s); \quad g_3(s) := \int_{R^2}^{R^2(1-s)} g(z)\,dz. \]
Well-posedness in 3D

Suppose that \( g(s) \) can be written in terms of the generalized power series as

\[
g(s) = \sum_{i=1}^{\infty} c_i s^{p_i}, \quad p_1 < p_2 < \cdots \quad \text{with} \quad c_1 > 0.
\]

Then the ring is well-posed [i.e. \( \lambda < 0 \) for all sufficiently large \( l \)] if

(i) \( \alpha < 0 \) and (ii) \( p_1 \in (-1, 0) \cup (1, 2) \cup (3, 4) \ldots \)

The ring is ill-posed [i.e. \( \lambda > 0 \) for all sufficiently large \( l \)] if either \( \alpha > 0 \) or \( p_1 \notin [-1, 0] \cup [1, 2] \cup [3, 4] \ldots \)
Key identity to prove well-posedness:

\[
\int_{-1}^{1} (1-s)^p P_l(s) \, ds = \frac{2^{p+1}}{p+1} \frac{\Gamma(l-p)\Gamma(p+2)}{\Gamma(l+p+2)\Gamma(-p)} \Gamma(l-p)\Gamma(p+2) \Gamma(l+p+2) \Gamma(-p) \sim -\frac{1}{\pi} \sin(\pi p) \Gamma^2(p+1)2^{p+1}l^{-2p-2} \quad \text{as } l \to \infty.
\]

Proof:

• Use hypergeometric representation: \( P_l(s) = 2F_1 \left( \begin{array}{c} l+1, -l \\ 1 \end{array} ; \frac{1-s}{2} \right) \).

• Use generalized Euler transform:

\[
\begin{align*}
A_{+1}F_{B+1} \left( \begin{array}{c} a_1, \ldots, a_A, c \\ b_1, \ldots, b_B, d \end{array} ; z \right) &= \frac{\Gamma(d)}{\Gamma(c)\Gamma(d-c)} \int_0^1 t^{c-1}(1-t)^{d-c-1} A_{B+1}F_{A+1} \left( \begin{array}{c} a_1, \ldots, a_A, c \\ b_1, \ldots, b_B, d \end{array} ; z \right) dt,
\end{align*}
\]

to get \( \int_{-1}^{1} (1-s)^p P_l(s) \, ds = \frac{2\pi 2^{p+1}}{p+1} 3F_2 \left( \begin{array}{c} p+1, l+1, -l \\ p+2, 1 \end{array} ; 1 \right) \).

• Apply the Saalschütz Theorem to simplify

\[
3F_2 \left( \begin{array}{c} p+1, l+1, -l \\ p+2, 1 \end{array} ; 1 \right) = \frac{\Gamma(l-p)\Gamma(p+2)}{\Gamma(l+p+2)\Gamma(-p)}.
\]
Generalized Lennard-Jones interaction

\[ g(s) = s^{-p} - s^{-q}; \quad 0 < p, q < 1; \quad p > q \]

- Well posed if \( q < \frac{2p-1}{2p-2} \); ill-posed if \( q > \frac{2p-1}{2p-2} \).

Example: steady state with \( N = 1000 \) particles. (a) \((p, q) = (1/3, 1/6)\). Particles concentrate uniformly on a surface of the sphere, with no particles in the interior. (b) \((p, q) = (1/2, 1/4)\). Particles fill the interior of a ball. The particles are color-coded according to their distance from the center of mass.
Custom-designed kernels

- In 3D, we can design force $F(r)$ which is stable for all modes except specified mode.

- EXAMPLE: Suppose we want only mode $m = 5$ to be unstable. Using our algorithm, we get

$$F(r) = \left\{ 3 \left( 1 - \frac{r^2}{2} \right)^2 + 4 \left( 1 - \frac{r^2}{2} \right)^3 - \left( 1 - \frac{r^2}{2} \right)^4 \right\} r + \varepsilon; \quad \varepsilon = 0.1.$$
Part II: Constant-density swarms

- Biological swarms have sharp boundaries, relatively **constant internal population**.

- Question: *What interaction force leads to such swarms?*

- More generally, can we deduce an interaction force from the swarm density?
Claim. Suppose that

\[ F(r) = \frac{1}{r^{n-1}} - r, \quad \text{where } n \equiv \text{dimension} \]

Then the aggregation model

\[ \rho_t + \nabla \cdot (\rho v) = 0; \quad v(x) = \int_{\mathbb{R}^n} F(|x-y|) \frac{x-y}{|x-y|} \rho(y) dy. \]

admits a steady state of the form

\[ \rho(x) = \begin{cases} 1, & |x| < R \\ 0, & |x| > R \end{cases}; \quad v(x) = \begin{cases} 0, & |x| < 1 \\ -ax, & |x| > 1 \end{cases}. \]

where \( R = 1 \) for \( n = 1, 2 \) and \( a = 2 \) in one dimension and \( a = 2\pi \) in two dimensions.
Proof for two dimensions

Define

\[ G(x) := \ln |x| - \frac{|x|^2}{2}; \quad M = \int_{\mathbb{R}^n} \rho(y) dy \]

Then we have:

\[ \nabla G = F(|x|) \frac{x}{|x|} \quad \text{and} \quad \Delta G(x) = 2\pi \delta(x) - 2. \]

so that

\[ v(x) = \int_{\mathbb{R}^n} \nabla_x G(x - y) \rho(y) dy. \]

Thus we get:

\[ \nabla \cdot v = \int_{\mathbb{R}^n} (2\pi \delta(x - y) - 2) \rho(y) dy \]

\[ = 2\pi \rho(x) - 2M \]

\[ = \begin{cases} 
0, & |x| < R \\
-2M, & |x| > R 
\end{cases} \]

The steady state satisfies \( \nabla \cdot v = 0 \) inside some ball of radius \( R \) with \( \rho = 0 \) outside such a ball but then \( \rho = M/\pi \) inside this ball and \( M = \int_{\mathbb{R}^n} \rho(y) dy = MR^2 \implies R = 1. \)
Dynamics in 1D with $F(r) = 1 - r$

Assume WLOG that

$$\int_{-\infty}^{\infty} x \rho(x) = 0; \quad M := \int_{-\infty}^{\infty} \rho(x) \, dx$$

Then

$$v(x) = \int_{-\infty}^{\infty} F(|x - y|) \frac{x - y}{|x - y|} \rho(y) \, dy$$

$$= \int_{-\infty}^{\infty} (1 - |x - y|) \text{sign}(x - y) \rho(y)$$

$$= 2 \int_{-\infty}^{x} \rho(y) \, dy - M(x + 1).$$

and continuity equations become

$$\rho_t + v \rho_x = -v_x \rho$$

$$= (M - 2\rho) \rho$$

Define the characteristic curves $X(t, x_0)$ by

$$\frac{d}{dt} X(t; x_0) = v; \quad X(0, x_0) = x_0$$
Then along the characteristics, we have \( \rho = \rho(X, t); \)

\[
\frac{d}{dt} \rho = \rho(M - 2\rho)
\]

Solving we get:

\[
\rho(X(t, x_0), t) = \frac{M}{2 + e^{-Mt}(M/\rho_0 - 2)}; \quad \rho(X(t, x_0), t) \to M/2 \text{ as } t \to \infty
\]
Let

\[ w := \int_{-\infty}^{x} \rho(y) dy \]

then

\[ v = 2w - M(x + 1); \quad v_x = 2\rho - M \]

and integrating \( \rho_t + (\rho v)_x = 0 \) we get:

\[ w_t + vw_x = 0 \]

Thus \( w \) is constant along the characteristics \( X \) of \( \rho \), so that characteristics \( \frac{d}{dt}X = v \) become

\[ \frac{d}{dt}X = 2w_0 - M(X + 1); \quad X(0; x_0) = x_0 \]
Summary for $F(r) = 1 - r$ in 1D:

$$X = \frac{2w_0(x_0)}{M} - 1 + e^{-Mt} \left( x_0 + 1 - \frac{2w_0(x_0)}{M} \right)$$

$$w_0(x_0) = \int_{-\infty}^{x_0} \rho_0(z)dz; \quad M = \int_{-\infty}^{\infty} \rho_0(z)dz$$

$$\rho(X, t) = \frac{M}{2 + e^{-tM}(M/\rho_0(x_0) - 2)}$$

Example: $\rho_0(x) = \exp \left( -x^2 \right) / \sqrt{\pi}$; $M = 1$:

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**Diagram:**
- X vs. t
- Density vs. x for different time steps.

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Global stability

In limit \( t \to \infty \) we get:

\[
X = \frac{2w_0}{M} - 1; \quad w_0 = 0 \ldots M; \quad \rho(X, \infty) = \frac{M}{2}
\]

We have shown that as \( t \to \infty \), the steady state is

\[
\rho(x, \infty) = \begin{cases} 
    M/2, & |x| < 1 \\
    0, & |x| > 1
\end{cases}
\]  \hspace{1cm} (10)

- This **proves the global stability** of (10)!

- Characteristics intersect at \( t = \infty \); solution forms a shock at \( x = \pm 1 \) at \( t = \infty \).
Dynamics in 2D, \( F(r) = \frac{1}{r} - r \)

- Similar to 1D,

\[
\nabla \cdot v = 2\pi \rho(x) - 4\pi M; \\
\rho_t + v \cdot \nabla \rho = -\rho \nabla \cdot v = -\rho (\rho - 2M) 2\pi
\]

- Along the characteristics:

\[
\frac{d}{dt}X(t; x_0) = v; \quad X(0, x_0) = x_0
\]

we still get

\[
\frac{d}{dt} \rho = 2\pi \rho (2M - \rho); \\
\rho(X(t; x_0), t) = \frac{2M}{1 + \left(\frac{2M}{\rho(x_0)} - 1\right) \exp(-4\pi M t)} \quad (11)
\]

- Continuity equations yield:

\[
\rho(X(t; x_0), t) \det \nabla_{x_0}X(t; x_0) = \rho_0(x_0)
\]
Using (11) we get
\[
\det \nabla_{x_0} X(t; x_0) = \frac{\rho_0(x_0)}{2M} + \left(1 - \frac{\rho_0(x_0)}{2M}\right) \exp(-4\pi Mt).
\]

- If \(\rho\) is \textbf{radially symmetric}, characteristics are also radially symmetric, i.e.
\[
X(t; x_0) = \lambda(|x_0|, t) x_0
\]
then
\[
\det \nabla_{x_0} X(t; x_0) = \lambda(t; r) (\lambda(t; r) + \lambda_r(t; r)r), \quad r = |x_0|
\]
so that
\[
\lambda^2 + \lambda_r \lambda r = \frac{\rho_0(x_0)}{2M} + \left(1 - \frac{\rho_0(x_0)}{2M}\right) \exp(-4\pi Mt)
\]
\[
\lambda^2 r^2 = \frac{1}{M} \int_0^r s \rho_0(s) ds + 2 \exp(-4\pi Mt) \int_0^r s \left(1 - \frac{\rho(s)}{2M}\right) ds
\]
So \textbf{characteristics are fully solvable}!!

- This proves \textbf{global stability in the space of radial initial conditions} \(\rho_0(x) = \rho_0(|x|)\).

- More general global stability is still open.
The force $F(r) = \frac{1}{r} - rq^{-1}$ in 2D

- If $q = 2$, we have explicit ode and solution for characteristics.

- For other $q$, no explicit solution is available but we have **differential inequalities**:

  Define
  \[
  \rho_{\text{max}} := \sup_x \rho(x, t); \quad R(t) := \text{radius of support of } \rho(x, t)
  \]

  Then
  \[
  \frac{d\rho_{\text{max}}}{dt} \leq (aR^{q-2} - b\rho_{\text{max}})\rho_{\text{max}}
  \]
  \[
  \frac{dR}{dt} \leq c\sqrt{\rho_{\text{max}}} - dR^{q-1},
  \]

  where $a, b, c, d$ are some [known] positive constants.

- It follows that if $R(0)$ is sufficiently big, then $R(t), \rho_{\text{max}}(t)$ remain bounded for all $t$. [using bounding box argument]

- **Theorem**: For $q \geq 2$, there exists a bounded steady state [uniqueness??]
Inverse problem: Custom-designer kernels: 1D

**Theorem.** In one dimension, consider a radially symmetric density of the form

\[
\rho(x) = \begin{cases} 
    b_0 + b_2x^2 + b_4x^4 + \ldots + b_{2n}x^{2n}, & |x| < R \\
    0, & |x| \geq R 
\end{cases}
\]  

(12)

Define the following quantities,

\[
m_{2q} := \int_0^R \rho(r)r^{2q}dr. 
\]

(13)

Then \(\rho(r)\) is the steady state corresponding to the kernel

\[
F(r) = 1 - a_0r - \frac{a_2}{3}r^3 - \frac{a_4}{5}r^5 - \ldots - \frac{a_{2n}}{2n+1}r^{2n+1}
\]

(14)

where the constants \(a_0, a_2, \ldots, a_{2n}\), are computed from the constants \(b_0, b_2, \ldots, b_{2n}\) by solving the following linear problem:

\[
b_{2k} = \sum_{j=k}^{n} a_{2j} \binom{2j}{2k} m_{2(j-k)}, \quad k = 0 \ldots n.
\]

(15)
Example: custom kernels 1D

Example 1: $\rho = 1 - x^2$, $R = 1$, then $F(r) = 1 - \frac{9}{5}r + \frac{1}{2}r^3$.

Example 2: $\rho = x^2$, $R = 1$, then $F(r) = 1 + \frac{9}{5}r - r^3$.

Example 3: $\rho = \frac{1}{2} + x^2 - x^4$, $R = 1$; then $F(r) = 1 + \frac{209425}{336091}r - \frac{4150}{2527}r^3 + \frac{6}{19}r^5$. 
**Inverse problem: Custom-designer kernels: 2D**

**Theorem.** In two dimensions, consider a radially symmetric density \( \rho(x) = \rho(|x|) \) of the form

\[
\rho(r) = \begin{cases} 
  b_0 + b_2r^2 + b_4r^4 + \ldots + b_{2n}r^{2n}, & r < R \\
  0, & r \geq R 
\end{cases}
\]  
(16)

Define the following quantities,

\[
m_{2q} := \int_0^R \rho(r)r^{2q}dr.
\]  
(17)

Then \( \rho(r) \) is the steady state corresponding to the kernel

\[
F(r) = \frac{1}{r} - \frac{a_0}{2}r - \frac{a_2}{4}r^3 - \ldots - \frac{a_{2n}}{2n + 2}r^{2n+1}
\]  
(18)

where the constants \( a_0, a_2, \ldots, a_{2n} \) are computed from the constants \( b_0, b_2, \ldots, b_{2n} \) by solving the following linear problem:

\[
b_{2k} = \sum_{j=k}^{n} a_{2j} \binom{j}{k}^2 m_{2(j-k)+1}; \quad k = 0 \ldots n.
\]  
(19)

This system always has a unique solution for provided that \( m_0 \neq 0 \).
Numerical simulations, 1D

- First, use standard ODE solver to integrate the corresponding discrete particle model,
  \[
  \frac{dx_j}{dt} = \frac{1}{N} \sum_{k=1 \ldots N, k \neq j} F(|x_j - x_k|) \frac{x_j - x_k}{|x_j - x_k|}, \quad j = 1 \ldots N.
  \]

- How to compute \( \rho(x) \) from \( x_i \)? [Topaz-Bernoff, 2010]
  - Use \( x_i \) to approximate the cumulative distribution, \( w(x) = \int_{-\infty}^{x} \rho(z) dz \).
  - Next take derivative to get \( \rho(x) = w'(x) \)

[Figure taken from Topaz+Bernoff, 2010 preprint]
Numerical simulations, 2D

• Solve for $x_i$ using ODE particle model as before [$2N$ variables]

• Use $x_i$ to compute Voronoi diagram;

• Estimate $\rho(x_j) = 1/a_j$ where $a_j$ is the area of the voronoi cell around $x_j$.

• Use Delanay triangulation to generate smooth mesh.

• Example: Take

$$\rho(r) = \begin{cases} 
1 + r^2, & r < 1 \\
0, & r > 0 
\end{cases}$$

Then by Custom-designed kernel in 2D is:

$$F(r) = \frac{1}{r} - \frac{8}{27}r - \frac{r^3}{3}.$$

Running the particle method yeids...
Numerical solutions for radial steady states for \( F(r) = \frac{1}{r} - r^{q-1} \)

- Radial steady states of radius \( R \) satisfy
  \[
  \rho(r) = 2q \int_0^R (r' \rho(r')) I(r, r') dr'
  \]
  where \( c(q) \) is some constant and
  \[
  I(r, r') = \int_0^\pi (r^2 + r'^2 - 2rr' \sin \theta) q/2^{-1} d\theta.
  \]

- To find \( \rho \) and \( R \), we adjust \( R \) until the operator \( \rho \rightarrow c(q) \int_0^R (r' \rho(r')) K(r, r') dr' \) has eigenvalue 1; then \( \rho \) is the corresponding eigenfunction.
Discussions/open problems

- **Constant density states with** $F(r) = r^{1-n} - r$. What is the biological mechanism to minimizes overcrowding?

- Open question: **global stability** for $F(r) = r^{1-n} - r$? [can show for $n = 1$ or for radial initial conditions if $n \geq 2$.]

- Connection to Thompson problem and ball-packing problems:
  - Equilibrium is a hexagonal lattice with “defects”. Can we study these??

- Most of the results generalize to $n$ dimensions.

- This talk and related papers are downloadable from my website
  [http://www.mathstat.dal.ca/~tkolokol/papers](http://www.mathstat.dal.ca/~tkolokol/papers)

Thank you!