## Complex patterns in patricle 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,

$$
\begin{equation*}
\frac{d x_{j}}{d t}=\frac{1}{N} \sum_{\substack{k=1 \ldots N \\ k \neq j}} F\left(\left|x_{j}-x_{k}\right|\right) \frac{x_{j}-x_{k}}{\left|x_{j}-x_{k}\right|}, \quad j=1 \ldots N \tag{1}
\end{equation*}
$$

- Models insect aggregation [Edelstein-Keshet et al, 1998] such as locust swarms [Topaz et al, 2008]; robotic motion [Gazi, Passino, 2004].
- 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 $r$.
- Alternative formulation: (1) is a gradient flow of the minimization problem

$$
\min E\left(x_{1}, \ldots x_{N}\right) \quad \text { where } E=\sum \sum P\left(\left|x_{i}-x_{j}\right|\right) \text { with } F(r)=-P^{\prime}(r)
$$

## Confining vs. spreading

- Consider a Morse interaction force:

$$
\begin{equation*}
F(r)=\exp (-r)-G \exp (-r / L) ; \quad G<1, L>1 \tag{2}
\end{equation*}
$$



- If $G L^{3}>1$, the morse potential is confining (or catastrophic): doubling $N$ doubles the density but cloud volume is unchanged:

$$
G=0.5, \quad L=2
$$



- If $G L^{3}<1$, the system is non-confining (or h -stable): doubling $N$ doubles the cloud volume but density is unchanged:

$$
\begin{aligned}
& r=9.56367 \\
& r=13.3742 \\
& r=19.3298
\end{aligned}
$$

$$
\begin{aligned}
& N=100
\end{aligned}
$$

## Continuum limit

- For confining potentials, we can take the continuum limit as the number of particles $N \rightarrow \infty$.
- We define the density $\rho$ as

$$
\int_{D} \rho(x) d x \approx \frac{\# \text { particles inside domain } D}{N}
$$

- The flow is then characterized by density $\rho$ and velocity field $v$ :

$$
\begin{equation*}
\rho_{t}+\nabla \cdot(\rho v)=0 ; \quad v(x)=\int_{\mathbb{R}^{n}} F(|x-y|) \frac{x-y}{|x-y|} \rho(y) d y \tag{3}
\end{equation*}
$$

- Variational formulation: Let

$$
\begin{equation*}
E[\rho]:=\int_{\mathbb{R}^{n}} \int_{\mathbb{R}^{n}} \rho(x) \rho(y) P(|x-y|) d x d y ; \quad P^{\prime}(r)=-F(r) \tag{4}
\end{equation*}
$$

Then (3) is the gradient flow of $E$; minima of $E$ are stable equilibria of (3).

- Questions

1. Describe the equilibrium cloud shape in the limit $t \rightarrow \infty$
2. What about dynamics?

## Linear force: $F(r)=\min (a r+b, 1-r)$

| $\mathrm{b}=0$ | 0.025 | 0.05 | 0.1 | 0.15 | 0.2 | 0.3 | 0.4 | 0.5 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $a=0$ |  |  |  |  |  |  |  |  |
| 0.2 | 1 | $1$ |  |  |  |  |  |  |
| 0.4 |  |  |  |  |  |  |  |  |
| 0.6 |  |  |  |  |  |  |  |  |
| 0.8 |  |  |  |  |  |  |  |  |
| 1 |  |  | . |  |  |  |  |  |
| 1.4 |  |  | (11) |  |  | 0 |  |  |
| 1.8 |  |  |  |  |  | - |  |  |
| 2.4 |  |  |  |  |  |  |  |  |
| 3 |  |  |  |  |  |  |  |  |

## Ring-type steady states

- Seek steady state of the form $x_{j}=r(\cos (2 \pi j / N), \sin (2 \pi j / N)), j=1 \ldots N$.
- In the limit $N \rightarrow \infty$ the radius of the ring must be the root of

$$
\begin{equation*}
I(r):=\int_{0}^{\frac{\pi}{2}} F(2 r \sin \theta) \sin \theta d \theta=0 \tag{5}
\end{equation*}
$$

- For Morse force $F(r)=\exp (-r)-G \exp (-r / L)$, such root exists whenever $G L^{2}>$ 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 $N \rightarrow \infty$ we obtain

$$
\begin{equation*}
\rho_{t}=\rho \frac{<z_{\alpha}, z_{\alpha t}>}{\left|z_{\alpha}\right|^{2}} ; \quad z_{t}=K * \rho \tag{6}
\end{equation*}
$$

where $z(\alpha ; t)$ is a parametrization of the solution curve; $\rho(\alpha ; t)$ is its density and

$$
\begin{equation*}
K * \rho=\int F\left(\left|z\left(\alpha^{\prime}\right)-z(\alpha)\right|\right) \frac{z\left(\alpha^{\prime}\right)-z(\alpha)}{\left|z\left(\alpha^{\prime}\right)-z(\alpha)\right|} \rho\left(\alpha^{\prime}, t\right) d S\left(\alpha^{\prime}\right) . \tag{7}
\end{equation*}
$$

- 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 (6).
- Agrees with direct simulation of the ODE system (1):



## Local stability of a ring

- Linearize: $x_{k}=r_{0} \exp (2 \pi i k / N)\left(1+\exp (t \lambda) \phi_{k}\right)$ where $\phi_{k} \ll 1$.
- Ring is stable of $\operatorname{Re}(\lambda) \leq 0$ 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

$$
\begin{gather*}
M(m):=\left[\begin{array}{cc}
I_{1}(m) & I_{2}(m) \\
I_{2}(m) & I_{1}(-m)
\end{array}\right] ; m=2,3, \ldots  \tag{8}\\
I_{1}(m)=\frac{2}{\pi} \int_{0}^{\frac{\pi}{2}}\left[\frac{F(2 r \sin \theta)}{2 r \sin \theta}+F^{\prime}(2 r \sin \theta)\right] \sin ^{2}((m+1) \theta) d \theta  \tag{9a}\\
I_{2}(m)=\frac{2}{\pi} \int_{0}^{\frac{\pi}{2}}\left[\frac{F(2 r \sin \theta)}{2 r \sin \theta}-F^{\prime}(2 r \sin \theta)\right]\left[\sin ^{2}(m \theta)-\sin ^{2}(\theta)\right] d \theta \tag{9b}
\end{gather*}
$$

- Eigenfunction is a pure fourier mode when projected to the curvilinear coordinates of the circle.


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## Quadratic force $F(r)=r-r^{2}$

- Computing explicitly,

$$
\begin{aligned}
\operatorname{tr} M(m) & =-\frac{\left(4 m^{4}-m^{2}-9\right)}{\left(4 m^{2}-1\right)\left(4 m^{2}-9\right)}<0, \quad m=2,3, \ldots \\
\operatorname{det} M(m) & =\frac{3 m^{2}\left(2 m^{2}+1\right)}{\left(4 m^{2}-9\right)\left(4 m^{2}-1\right)^{2}}>0, \quad m=2,3, \ldots
\end{aligned}
$$

- 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 $\lambda \sim-\frac{3}{8 m^{2}} \rightarrow 0$ as $m \rightarrow \infty$. 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 $p q>1$ 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

$$
\begin{aligned}
0 & =723-594(p+q)-27\left(p^{2}+q^{2}\right)-431 p q+106\left(p q^{2}+p^{2} q\right)+19\left(p^{3} q+p q^{3}\right) \\
& +10\left(p^{3} q^{2}+p^{2} q^{3}\right)+6\left(p^{3}+q^{3}\right)+p^{3} q^{3}
\end{aligned}
$$

- Boundaries for $m=4,5, \ldots$ are similarly expressed in terms of higher order polynomials in $p, q$.



## 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



## Point-concentration (hole) solutions

$$
F(r)=\min \left(a r, r-r^{2}\right)
$$

Solutions consist of $K$ "clusters", where each cluster has $N / K$ points inside. The number $K$ depends on $a$ :


Theorem: $K$ hole solution is guaranteed to be stable if $a \in\left(a_{1}, a_{2}\right)$ whose values are summarized in the following table:

| $K$ | $r$ | $a_{1}$ | $a_{2}$ |
| :---: | :---: | :---: | :---: |
| 3 | $3^{-1 / 2} \approx 0.5773$ | 0 | 0.5 |
| 4 | 0.585786 | 0.171573 | 0.656851 |
| 5 | 0.587785 | 0.309017 | 0.736067 |
| 6 | 0.588457 | 0.411543 | 0.788636 |
| 7 | 0.588735 | 0.489115 | 0.819194 |
| 8 | 0.588867 | 0.549301 | 0.841735 |
| $\gg 1$ | $\frac{3}{16} \pi$ | $1-\frac{3 \pi^{2}}{8 K}$ | $1-\frac{\pi^{2}}{8 K}$ |

## Spots: "degenerate" holes

$$
F(r)=\min (a r+\delta, 1-r) ; \quad \delta \ll 1
$$

- Points degenerate into spots of size $O(\delta)$. eg. $a=0.3, \delta=0.05$ :

- Inside each of the cluster, the reduced problem is:

$$
\phi_{l}^{\prime}=\sum_{j \neq l}^{n} \frac{\phi_{l}-\phi_{j}}{\left|\phi_{l}-\phi_{j}\right|}-n\left[\begin{array}{cc}
\alpha & 0 \\
0 & \beta
\end{array}\right] \phi_{l}
$$

- $\alpha, \beta$ depend only on $F(r)$ not on $N$.


## Reduced problem: stripe or blob??

$$
\phi_{l}^{\prime}=\sum_{j \neq l}^{n} \frac{\phi_{l}-\phi_{j}}{\left|\phi_{l}-\phi_{j}\right|}-n\left[\begin{array}{cc}
\alpha & 0 \\
0 & \beta
\end{array}\right] \phi_{l}
$$

- Admits the steady state consisting of particles located uniformly along a vertical line of length $2 / \beta$, centered at the origin.
- Such "one-dimensional" equilibrium is stable if

$$
\begin{equation*}
1+\frac{1}{2}+\ldots \frac{1}{n-1}<\frac{\alpha}{\beta} \tag{11}
\end{equation*}
$$

unstable otherwise.

- For large $n$, (11) becomes

$$
\begin{equation*}
n<\exp (\alpha / \beta-\gamma) \approx 0.5614 \exp (\alpha / \beta) \tag{12}
\end{equation*}
$$



Take $\alpha=1, \beta=0.25$; then $\mathrm{rhs}(12)=30.6$. Line is stable when $n=30$; unstable for $n=40$.

## Stability of vertical "stripe": key steps

- Perturbations in vertical direction are stable
- In horizontal direction, stability reduces to study of

$$
\begin{equation*}
\lambda \psi_{l}=\sum_{\substack{j=1 \ldots . . n \\ j \neq l}} \frac{\psi_{l}-\psi_{j}}{|l-j|}, \quad l=1 \ldots n \tag{13}
\end{equation*}
$$

- Lemma: The $n$ eigenvalues of (13) are given by $\lambda_{k}=2 \sum_{j=1}^{k} \frac{1}{j}, \quad k=0 \ldots n-1$.
- Proof: Continuum limit yields

$$
\lambda \psi(x)=\int_{0}^{1} \frac{\psi(x)-\psi(y)}{|x-y|} d y
$$

eigenvalues are polynomials of the form $\psi(x)=x^{k}+\ldots ;$ with $\lambda_{k}=2 \sum_{j=1}^{k} \frac{1}{j}, k=$ $0,1,2, \ldots$ The discrete problem is the same except $k=0 \ldots n-1$.

## (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 $[0,2 r]$, then the necessary and sufficient conditions for wellposedness of a ring are:

$$
\begin{align*}
& F(0)=0, \quad F^{\prime \prime}(0)<0 \text { and }  \tag{14}\\
& \int_{0}^{\pi / 2}\left(\frac{F(2 r \sin \theta)}{2 r \sin \theta}-F^{\prime}(2 r \sin \theta)\right) d \theta<0 . \tag{15}
\end{align*}
$$

- Ring solution for the morse force $F(r)=\exp (-r)-G \exp (-r / L)$ is always ill-posed since $F(0)>0$.


## Bifurcation to annulus:

Consider

$$
F(r)=r-r^{2}+\delta, \quad 0 \leq \delta \ll 1
$$

- A ring is stable of radius $R \sim \frac{3 \pi}{16}+\frac{2}{\pi} \delta+O\left(\delta^{2}\right)$ if $\delta=0$ but high modes become unstable for $\delta>0$
- The most unstable mode in the discrete system is $m=N / 2$ and can be stable even if the continuous model is ill-posed!
- Proposition: Let

$$
N_{c} \sim \frac{\pi}{4} e^{4-\gamma} \exp \left(\frac{3 \pi^{2}}{64 \delta}\right) .
$$

The ring is stable if $N<N_{c}$.

- For $N>N_{c}$ but $N \sim N_{c}$, solution consists of two radii $R \pm \varepsilon$ where

$$
R=\frac{3 \pi}{32}\left(1+\sqrt{1+\frac{128}{3 \pi^{2}}} \delta\right) ; \quad \beta \sim 4 R e^{-2} \exp \left(\frac{-4 R^{2}+R \pi / 2}{\delta}\right)
$$

－Example：$\delta=0.35 \Longrightarrow N_{c} \sim 90,2 \beta \sim 0.033$ ．Numerically，we obtain $2 \beta \approx$ 0．036．Good agreement！

| ． | － | $\cdots$ | $\therefore$ | $\because \therefore$ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| － | － | $\therefore$ | $\because$ |  |  |  |  |  |
| － |  | $\because$ |  |  |  |  |  |  |
| － | － | $\cdots$ |  |  |  |  |  |  |
| $\cdot$ |  |  |  |  | ： |  |  |  |
| － | － |  |  |  | ： |  |  |  |
| － | － |  |  |  | ： |  |  |  |
| － |  |  |  |  |  |  | \％ 0 |  |
| － | － |  |  |  | 克 |  | \％ |  |
|  | ．${ }^{\text {－}}$ |  |  | $\therefore \because$ | $\therefore \because \because 0^{\circ}$ |  |  | 为㔚 |
| 80 | 100 | 300 | 400 | 600 | 1200 | 1900 | 2500 | 3000 |

－Increasing $N$ further，more rings appear until we get a thin annulus of width $O(\beta)$ ．


## Annulus: continuum limit $N \gg N_{c}$ :

- $F(r)=r-r^{2}+\delta, \quad 0<\delta \ll 1$
- Main result: In the limit $\delta \rightarrow 0$, the annulus inner and outer radii $R_{1}, R_{2}$ are given by

$$
R \sim \frac{3 \pi}{16}+\frac{2}{\pi} \delta ; \quad R_{1} \sim R-\beta, \quad R_{2} \sim R+\beta
$$

where

$$
\beta \sim 3 \pi e^{-5} \exp \left(-\frac{3 \pi^{2}}{64} \frac{1}{\delta}\right) \ll \delta \ll 1
$$

The radial density profile inside the annulus is

$$
\rho(x) \sim\left\{\begin{array}{c}
\frac{c}{\sqrt{\beta^{2}-(R-|x|)^{2}}}, \quad|R-x|<\beta \ll 1 \\
0, \quad \text { otherwise }
\end{array}\right.
$$

- Annulus is exponentially thin in $\delta \ldots$ note the $1 /$ sqrt singularity near the edges!



## Key steps for computing annulus <br> profile

- For radially symmetric density, the velocity field reduces to a 1D problem:

$$
\begin{gathered}
v(r)=\int_{0}^{\infty} K(s, r) \rho(s) s d s \\
K(s, r):=\int_{0}^{2 \pi}(r-s \cos \theta) f\left(\sqrt{r^{2}+s^{2}-2 r s \cos \theta}\right) d \theta ; \quad f(r)=1-r+\frac{\delta}{r}
\end{gathered}
$$

- Assume thin annulus; expand all integrals:

$$
r=R+\xi ; \quad s=R+\eta ; \quad \xi, \eta \ll \delta \ll 1
$$

- The singular part " $\delta / r$ " yields a log:

$$
\begin{gathered}
g(t)=2 \int_{0}^{\pi}(t-\cos \theta)\left(1+t^{2}-2 t \cos \theta\right)^{-1 / 2} d \theta \\
g(1+\varepsilon) \sim 4-2 \varepsilon \ln |\varepsilon|+\varepsilon(6 \ln 2-2)+O\left(\varepsilon^{2} \ln |\varepsilon|\right)
\end{gathered}
$$

- It boils down to integral equation

$$
\int_{-\beta}^{\beta} \ln |\eta-\xi| \varrho(\eta) d \eta=1 \text { for all } \xi \in(\alpha, \beta)
$$

- Explicit solution is a special case of Formula 3.4.2 from "Handbook of integral equations" A.Polyanin and A.Manzhirov:

$$
\varrho(\xi)=\frac{C}{\sqrt{\beta^{2}-\xi^{2}}}
$$

- The inverse root law blowup near the boundaries is the same as computed for "radial blobs" by Bernoff et.al. [preprint]


## Annulus for Newtonian repulsion

$$
\begin{gather*}
f(r)=\frac{F(r)}{r}=1-r+\frac{\delta}{r^{2}}, \quad \delta \ll 1  \tag{16}\\
v(r)=\int_{0}^{\infty} K(s, r) \rho(s) s d s \\
K(s, r):=\int_{0}^{2 \pi}(r-s \cos \theta) f\left(\sqrt{r^{2}+s^{2}-2 r s \cos \theta}\right) d \theta
\end{gather*}
$$

Expand

$$
r=R_{0}+\xi ; \quad s=R_{0}+\eta ; \quad \xi, \eta=O(\delta) ; \quad R_{0}=\frac{3}{16} \pi
$$

Annulus inner/outer radii:

$$
R_{1} \sim R_{0}+\alpha ; \quad R_{2} \sim R_{0}+\beta ; \quad \alpha, \beta=O(\delta) \ll 1
$$

then

$$
\begin{gather*}
4 \delta \int_{\alpha}^{\xi} \varrho(\eta) d \eta \sim R_{0} \int_{\alpha}^{\beta}(\xi+3 \eta) \varrho(\eta) d \eta, \quad \xi \in(\alpha, \beta)  \tag{17}\\
4 \delta \varrho(\xi) \sim R_{0} \int_{\alpha}^{\beta} \varrho
\end{gather*}
$$

$$
\begin{aligned}
\rho(x) & \sim \begin{cases}1, & |x| \in\left(R_{0}+\alpha, R_{0}+\beta\right) \\
0, & \text { otherwise }\end{cases} \\
R_{0} & =\frac{3}{16} \pi ; \quad \alpha=-\frac{8}{\pi} \delta ; \quad \beta=\frac{40}{3 \pi} \delta
\end{aligned}
$$



## 3D sphere instabilities

- Radius satisfies: $\int_{0}^{\pi} F\left(2 r_{0} \sin \theta\right) \sin \theta \sin 2 \theta=0$
- Instability can be done using spherical harmonics



## Stability of a spherical shell

Define

$$
g(s):=\frac{F(\sqrt{2 s})}{\sqrt{2 s}}
$$

The spherical shell has a radius given implicitly by

$$
0=\int_{-1}^{1} g\left(R^{2}(1-s)\right)(1-s) \mathrm{d} s
$$

Its stability is given by a sequence of $2 \times 2$ eigenvalue problems

$$
\lambda\binom{c_{1}}{c_{2}}=\left(\begin{array}{cc}
\alpha+\lambda_{l}\left(g_{1}\right) & l(l+1) \lambda_{l}\left(g_{2}\right) \\
\lambda_{l}\left(g_{2}\right) & \frac{l(l+1)}{R^{2}} \lambda_{l}\left(g_{3}\right)
\end{array}\right)\binom{c_{1}}{c_{2}}, \quad l=2,3,4, \ldots
$$

where

$$
\lambda_{l}(f):=2 \pi \int_{-1}^{1} f(s) P_{l}(s) \mathrm{d} s
$$

with $P_{l}(s)$ the Legendre polynomial and

$$
\begin{aligned}
\alpha & :=8 \pi g\left(2 R^{2}\right)+\lambda_{0}\left(g\left(R^{2}\left(1-s^{2}\right)\right)\right. \\
g_{1}(s) & :=R^{2} g^{\prime}\left(R^{2}(1-s)\right)(1-s)^{2}-g\left(R^{2}(1-s)\right) s \\
g_{2}(s) & :=g\left(R^{2}(1-s)\right)(1-s) ; \quad g_{3}(s):=\int_{0}^{R^{2}(1-s)} g(z) d z .
\end{aligned}
$$

## 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

$$
\text { (i) } \alpha<0 \quad \text { and } \quad \text { (ii) } p_{1} \in(-1,0) \bigcup(1,2) \bigcup(3,4) \ldots
$$

The ring is ill-posed [i.e. $\lambda>0$ for all sufficiently large $l$ ] if either $\alpha>0$ or $p_{1} \notin$ $[-1,0] \bigcup[1,2] \bigcup[3,4] \ldots$

## Key identity to prove well-posedness:

$$
\begin{aligned}
\int_{-1}^{1}(1-s)^{p} P_{l}(s) \mathrm{d} s & =\frac{2^{p+1}}{p+1} \frac{\Gamma(l-p) \Gamma(p+2)}{\Gamma(l+p+2) \Gamma(-p)} \\
& \sim-\frac{1}{\pi} \sin (\pi p) \Gamma^{2}(p+1) 2^{p+1} l^{-2 p-2} \quad \text { as } l \rightarrow \infty
\end{aligned}
$$

Proof:

- Use hypergeometric representation: $P_{l}(s)={ }_{2} F_{1}\left(\begin{array}{c}l+1,-l \\ 1\end{array} ; \frac{1-s}{2}\right)$.
- Use generalized Euler transform:

$$
\begin{aligned}
& A+1 F_{B+1}\left(\begin{array}{c}
a_{1}, \ldots, a_{A}, c \\
b_{1}, \ldots, b_{B}, d
\end{array} ; z\right)=\frac{\Gamma(d)}{\Gamma(c) \Gamma(d-c)} \int_{0}^{1} t^{c-1}(1-t)^{d-c-1}{ }_{A} F_{B}\left(\begin{array}{c}
a_{1}, \ldots, a_{A}, \\
b_{1}, \ldots, b_{B}, a
\end{array}\right. \\
& \text { to get } \int_{-1}^{1}(1-s)^{p} P_{l}(s) \mathrm{d} s=\frac{2 \pi 2^{p+1}}{p+1}{ }_{3} F_{2}\left(\begin{array}{c}
p+1, l+1,-l \\
p+2,1
\end{array} ; 1\right)
\end{aligned}
$$

- Apply the Saalschütz Theorem to simplify

$$
{ }_{3} F_{2}\left(\begin{array}{c}
p+1, l+1,-l \\
p+2,1
\end{array} ; 1\right)=\frac{\Gamma(l-p) \Gamma(p+2)}{\Gamma(l+p+2) \Gamma(-p)} .
$$

## Generalized Lennard-Jones interaction

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

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


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

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

Particle simulation
Linearized solution

## 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?



## Bounded states of constant density

Claim. Suppose that

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

Then the aggregation model

$$
\rho_{t}+\nabla \cdot(\rho v)=0 ; \quad v(x)=\int_{\mathbb{R}^{n}} F(|x-y|) \frac{x-y}{|x-y|} \rho(y) d y .
$$

admits a steady state of the form

$$
\rho(x)=\left\{\begin{array}{ll}
1, & |x|<R \\
0, & |x|>R
\end{array} ; \quad v(x)= \begin{cases}0, & |x|<1 \\
-a x, & |x|>1\end{cases}\right.
$$

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

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

Then we have:

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

so that

$$
v(x)=\int_{\mathbb{R}^{n}} \nabla_{x} G(x-y) \rho(y) d y
$$

Thus we get:

$$
\begin{aligned}
\nabla \cdot v & =\int_{\mathbb{R}^{n}}(2 \pi \delta(x-y)-2) \rho(y) d y \\
& =2 \pi \rho(x)-2 M \\
& =\left\{\begin{array}{cc}
0, & |x|<R \\
-2 M, & |x|>R
\end{array}\right.
\end{aligned}
$$

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 $M=\int_{\mathbb{R}^{n}} \rho(y) d y=M R^{2} \Longrightarrow R=1$.

## Dynamics in 1D with $F(r)=1-r$

Assume WLOG that

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

Then

$$
\begin{aligned}
v(x) & =\int_{-\infty}^{\infty} F(|x-y|) \frac{x-y}{|x-y|} \rho(y) d y \\
& =\int_{-\infty}^{\infty}(1-|x-y|) \operatorname{sign}(x-y) \rho(y) \\
& =2 \int_{-\infty}^{x} \rho(y) d y-M(x+1)
\end{aligned}
$$

and continuity equations become

$$
\begin{aligned}
\rho_{t}+v \rho_{x} & =-v_{x} \rho \\
& =(M-2 \rho) \rho
\end{aligned}
$$

Define the characteristic curves $X\left(t, x_{0}\right)$ by

$$
\frac{d}{d t} X\left(t ; x_{0}\right)=v ; \quad X\left(0, x_{0}\right)=x_{0}
$$

Then along the characteristics, we have $\rho=\rho(X, t)$;

$$
\frac{d}{d t} \rho=\rho(M-2 \rho)
$$

Solving we get:

$$
\rho\left(X\left(t, x_{0}\right), t\right)=\frac{M}{2+e^{-M t}\left(M / \rho_{0}-2\right)} ; \quad \rho\left(X\left(t, x_{0}\right), t\right) \rightarrow M / 2 \text { as } t \rightarrow \infty
$$

## Solving for characteristic curves

Let

$$
w:=\int_{-\infty}^{x} \rho(y) d y
$$

then

$$
v=2 w-M(x+1) ; \quad v_{x}=2 \rho-M
$$

and integrating $\rho_{t}+(\rho v)_{x}=0$ we get:

$$
w_{t}+v w_{x}=0
$$

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

$$
\frac{d}{d t} X=2 w_{0}-M(X+1) ; \quad X\left(0 ; x_{0}\right)=x_{0}
$$

## Summary for $F(r)=1-r$ in 1D:

$$
\begin{aligned}
X & =\frac{2 w_{0}\left(x_{0}\right)}{M}-1+e^{-M t}\left(x_{0}+1-\frac{2 w_{0}\left(x_{0}\right)}{M}\right) \\
w_{0}\left(x_{0}\right) & =\int_{-\infty}^{x_{0}} \rho_{0}(z) d z ; \quad M=\int_{-\infty}^{\infty} \rho_{0}(z) d z \\
\rho(X, t) & =\frac{M}{2+e^{-t M}\left(M / \rho_{0}\left(x_{0}\right)-2\right)}
\end{aligned}
$$

Example: $\rho_{0}(x)=\exp \left(-x^{2}\right) / \sqrt{\pi} ; \quad M=1$ :



## Global stability

In limit $t \rightarrow \infty$ we get:

$$
X=\frac{2 w_{0}}{M}-1 ; \quad w_{0}=0 \ldots M ; \quad \rho(X, \infty)=\frac{M}{2}
$$

We have shown that as $t \rightarrow \infty$, the steady state is

$$
\rho(x, \infty)=\left\{\begin{array}{c}
M / 2,|x|<1  \tag{18}\\
0,|x|>1
\end{array}\right.
$$

- This proves the global stability of (18)!
- 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,

$$
\begin{aligned}
\nabla \cdot v & =2 \pi \rho(x)-4 \pi M ; \\
\rho_{t}+v \cdot \nabla \rho & =-\rho \nabla \cdot v \\
& =-\rho(\rho-2 M) 2 \pi
\end{aligned}
$$

- Along the characterisitics:

$$
\frac{d}{d t} X\left(t ; x_{0}\right)=v ; \quad X\left(0, x_{0}\right)=x_{0}
$$

we still get

$$
\begin{gather*}
\frac{d}{d t} \rho=2 \pi \rho(2 M-\rho) \\
\rho\left(X\left(t ; x_{0}\right), t\right)=\frac{2 M}{1+\left(\frac{2 M}{\rho\left(x_{0}\right)}-1\right) \exp (-4 \pi M t)} \tag{19}
\end{gather*}
$$

- Continuity equations yield:

$$
\rho\left(X\left(t ; x_{0}\right), t\right) \operatorname{det} \nabla_{x_{0}} X\left(t ; x_{0}\right)=\rho_{0}\left(x_{0}\right)
$$

- Using (19) we get

$$
\operatorname{det} \nabla_{x_{0}} X\left(t ; x_{0}\right)=\frac{\rho_{0}\left(x_{0}\right)}{2 M}+\left(1-\frac{\rho_{0}\left(x_{0}\right)}{2 M}\right) \exp (-4 \pi M t)
$$

- If $\rho$ is radially symmetric, characteristics are also radially symmetric, i.e.

$$
X\left(t ; x_{0}\right)=\lambda\left(\left|x_{0}\right|, t\right) x_{0}
$$

then

$$
\operatorname{det} \nabla_{x_{0}} X\left(t ; x_{0}\right)=\lambda(t ; r)\left(\lambda(t ; r)+\lambda_{r}(t ; r) r\right), \quad r=\left|x_{0}\right|
$$

so that

$$
\begin{gathered}
\lambda^{2}+\lambda_{r} \lambda r=\frac{\rho_{0}\left(x_{0}\right)}{2 M}+\left(1-\frac{\rho_{0}\left(x_{0}\right)}{2 M}\right) \exp (-4 \pi M t) \\
\lambda^{2} r^{2}=\frac{1}{M} \int_{0}^{r} s \rho_{0}(s) d s+2 \exp (-4 \pi M t) \int_{0}^{r} s\left(1-\frac{\rho(s)}{2 M}\right) d s
\end{gathered}
$$

So characteristics are fully solvable!!

- This proves global stability in the space of radial initial conditions $\rho_{0}(x)=$ $\rho_{0}(|x|)$.
- More general global stability is still open.


## The force $F(r)=\frac{1}{r}-r^{q-1}$ 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

$$
\rho_{\max }:=\sup _{x} \rho(x, t) ; \quad R(t):=\text { radius of support of } \rho(x, t)
$$

Then

$$
\begin{aligned}
\frac{d \rho_{\max }}{d t} & \leq\left(a R^{q-2}-b \rho_{\max }\right) \rho_{\max } \\
\frac{d R}{d t} & \leq c \sqrt{\rho_{\max }}-d R^{q-1}
\end{aligned}
$$

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

- It follows that if $R(0)$ is sufficiently big, then $R(t), \rho_{\max }(t)$ 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, conisder a radially symmetric density of the form

$$
\rho(x)=\left\{\begin{array}{c}
b_{0}+b_{2} x^{2}+b_{4} x^{4}+\ldots+b_{2 n} x^{2 n}, \quad|x|<R  \tag{20}\\
0, \quad|x| \geq R
\end{array}\right.
$$

Define the following quantities,

$$
\begin{equation*}
m_{2 q}:=\int_{0}^{R} \rho(r) r^{2 q} d r \tag{21}
\end{equation*}
$$

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

$$
\begin{equation*}
F(r)=1-a_{0} r-\frac{a_{2}}{3} r^{3}-\frac{a_{4}}{5} r^{5}-\ldots-\frac{a_{2 n}}{2 n+1} r^{2 n+1} \tag{22}
\end{equation*}
$$

where the constants $a_{0}, a_{2}, \ldots, a_{2 n}$, are computed from the constants $b_{0}, b_{2}, \ldots, b_{2 n}$ by solving the following linear problem:

$$
\begin{equation*}
b_{2 k}=\sum_{j=k}^{n} a_{2 j}\binom{2 j}{2 k} m_{2(j-k)}, \quad k=0 \ldots n \tag{23}
\end{equation*}
$$

## Example: custom kernels 1D

Example 1: $\rho=1-x^{2}, \quad R=1$, then $F(r)=1-9 / 5 r+1 / 2 r^{3}$.
Example 2: $\rho=x^{2}, \quad R=1$, then $F(r)=1+9 / 5 r-r^{3}$.
Example 3: $\rho=1 / 2+x^{2}-x^{4}, \quad R=1$; 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, conisder a radially symmetric density $\rho(x)=\rho(|x|)$ of the form

$$
\rho(r)=\left\{\begin{array}{c}
b_{0}+b_{2} r^{2}+b_{4} r^{4}+\ldots+b_{2 n} r^{2 n}, \quad r<R  \tag{24}\\
0, \quad r \geq R
\end{array}\right.
$$

Define the following quantities,

$$
\begin{equation*}
m_{2 q}:=\int_{0}^{R} \rho(r) r^{2 q} d r \tag{25}
\end{equation*}
$$

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

$$
\begin{equation*}
F(r)=\frac{1}{r}-\frac{a_{0}}{2} r-\frac{a_{2}}{4} r^{3}-\ldots-\frac{a_{2 n}}{2 n+2} r^{2 n+1} \tag{26}
\end{equation*}
$$

where the constants $a_{0}, a_{2}, \ldots, a_{2 n}$, are computed from the constants $b_{0}, b_{2}, \ldots, b_{2 n}$ by solving the following linear problem:

$$
\begin{equation*}
b_{2 k}=\sum_{j=k}^{n} a_{2 j}\binom{j}{k}^{2} m_{2(j-k)+1} ; \quad k=0 \ldots n \tag{27}
\end{equation*}
$$

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,

$$
\frac{d x_{j}}{d t}=\frac{1}{N} \sum_{\substack{k=1 \ldots N \\ k \neq j}} F\left(\left|x_{j}-x_{k}\right|\right) \frac{x_{j}-x_{k}}{\left|x_{j}-x_{k}\right|}, \quad j=1 \ldots N
$$

- How to compute $\rho(x)$ from $x_{i}$ ? [Topaz-Bernoff, 2010]
- Use $x_{i}$ to approximate the cumulitive distribution, $w(x)=\int_{-\infty}^{x} \rho(z) d z$.
- Next take derivative to get $\rho(x)=w^{\prime}(x)$

[Figure taken from Topaz+Bernoff, 2010 preprint]


## Numerical simulations, 2D

- Solve for $x_{i}$ using ODE particle model as before [ $2 N$ variables]
- Use $x_{i}$ to compute Voronoi diagram;
- Estimate $\rho\left(x_{j}\right)=1 / a_{j}$ where $a_{j}$ is the area of the voronoi cell around $x_{j}$.
- Use Delanay triangulation to generate smooth mesh.
- Example: Take

$$
\rho(r)=\left\{\begin{array}{c}
1+r^{2}, r<1 \\
0, r>0
\end{array}\right.
$$

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 $\rho(r)=2 q \int_{0}^{R}\left(r^{\prime} \rho\left(r^{\prime}\right) I\left(r, r^{\prime}\right) d r^{\prime}\right.$ where $c(q)$ is some constant and $I\left(r, r^{\prime}\right)=\int_{0}^{\pi}\left(r^{2}+r^{\prime 2}-2 r r^{\prime} \sin \theta\right)^{q / 2-1} d \theta$.
- To find $\rho$ and $R$, we adjust $R$ until the operator $\rho \rightarrow c(q) \int_{0}^{R}\left(r^{\prime} \rho\left(r^{\prime}\right) K\left(r, r^{\prime}\right) d r^{\prime}\right.$ has eigenvalue 1 ; then $\rho$ is the corresponding eigenfunction.



## Swarming on random networks

- Particles are nodes in a graph; two nodes communicate iff they are connected by an edge:

$$
\begin{aligned}
& \frac{d x_{i}}{d t}=\sum_{k} c_{i, j} F\left(\left|x_{i}-x_{i}\right|\right) \frac{x_{i}-x_{j}}{\left|x_{k}-x_{j}\right|}, j=1 \ldots N ; \\
& c_{i, j}= \begin{cases}1, & \text { if vertices } i, j \text { are connected by an edge } \\
0, & \text { otherwise }\end{cases}
\end{aligned}
$$

- Consider the case of Erdős-Rényi random graph:

$$
c_{i, j}=\left\{\begin{array}{l}
1, \text { with probability } p \\
0, \text { with probability } 1-p
\end{array}\right.
$$

- Question: How does the connectivity affect the cohesion of the swarm??
- Erdős-Rényi ( $\sim 1960$ ): a p-random graph is connected with high probability if $p>\frac{\ln n}{n}+o(1)$; disconnected if $p<\frac{\ln n}{n}-\frac{c}{n}$.
- The swarm will lose cohesion if $p<\frac{\ln n}{n}-\frac{c}{n}$.
- This bound is too lax for most swarms!
- Simplest (non-trivial) case: a 1D swarm consisting of two equal clusters:

$$
\begin{aligned}
F(r) & =\min (a r, 1-r), \quad a>0 \\
x_{1} \ldots x_{n / 2} & =0 ; \quad x_{n / 2+1} \ldots x_{n}=1
\end{aligned}
$$

- Linearized problem: $n=N / 2$;

$$
\left\{\begin{array}{c}
\lambda \phi_{i}=\sum_{j=1}^{n} a c_{i j}\left(\phi_{j}-\phi_{i}\right)+\sum_{j=1}^{n} c_{i, j+n}\left(\psi_{j}-\phi_{i}\right)  \tag{28}\\
\lambda \psi_{i}=\sum_{j=1}^{n} a c_{i+n, j+n}\left(\psi_{j}-\psi_{i}\right)+\sum_{j=1}^{n} c_{i+n, j}\left(\phi_{j}-\psi_{i}\right)
\end{array}\right.
$$

- If $p=1$ (full connectivity), then $\lambda=0,-n(1-a)$ [multiplicity $2 n-2$ ] and $-2 n$, eigenvalues of

$$
L_{\text {full }}=\left[\begin{array}{cccccc}
2 a-3 & -a & -a & 1 & 1 & 1 \\
-a & 2 a-3 & -a & 1 & 1 & 1 \\
-a & -a & 2 a-3 & 1 & 1 & 1 \\
1 & 1 & 1 & 2 a-3 & -a & -a \\
1 & 1 & 1 & -a & 2 a-3 & -a \\
1 & 1 & 1 & -a & -a & 2 a-3
\end{array}\right], \quad N=6
$$

$\Longrightarrow$ two clusters are stable if $0<a<1$ when $p=1$.

- Main result: Consider the two-cluster solution for $F(r)=\min (a r, 1-r), 0<a<$ 1. Let $S(p)$ be the probability that such solution is stable. Suppose that

$$
p=p_{0} \frac{\ln N}{N}
$$

and define

$$
p_{0 c}:=4 \frac{a^{2}+1}{(1-a)^{2}}
$$

Then

Corrollary: The transition of a two-cluster swarm from instability to stability occurs when

$$
p=p_{c}=4 \frac{a^{2}+1}{(1-a)^{2}} \frac{\ln N}{N} .
$$

It is unstable (resp. stable) if $p<p_{c}$ (resp. $p>p_{c}$ ) with very high probability.

$$
a=0.5
$$



- Ingredients in proof:
- Estimate Bernoulli by Normal distribution (C.L.T.): $c_{i, j} \sim p+\sqrt{p(1-p)} \mathcal{N}$;
- Decompose linear problem as $L=L_{\text {full }}+\sqrt{p(1-p) N} A+\sqrt{p(1-p) N} D$ where $L_{\text {full }}$ is a deterministic matrix corresponding to $p=1$; $A$ is full random matrix; $D$ is a diagonal random matrix
- Use elementary probability to bound spectrum of $D$
- Use random matrix theory (Wigner's circle law) to bound spectrum of $A$. It turns out the $A$ term can be thrown out!
- Consensus model on graph is a well-studied model in IEEE literature; corresponds to $F(r)=r$ :

$$
\lambda \phi_{i}=\sum_{j=1}^{n} c_{i j}\left(\phi_{j}-\phi_{i}\right)
$$

- Aggregation is the nonlinear generalization of consensus model; multiple consensus possible!


## Discussions/open problems

- Spots+annuli form basic building blocks from which it is possible to construct more complex solutions...
- Stability?? Multiple rings???
- Conjecture:
- Swarms on networks: more complex swarms; small-world networks?
- Connection to Thompson problem and ball-packing problems:
- Equilibrium is a hexagonal lattice with "defects". Can we study these??
- Constant density states with $F(r)=r^{1-n}-r$. What is the biological mechanism to minimizes overcrowding?
- Forces with sharp transition can produce exotic patterns for example:
- Flower: $F(x)=\max \left(\min \left(1.6,(1-x)^{*} 4\right),-0.1\right)$
- Exotic fish: $F(x)=\max \left(\min \left(1.6,(1-x)^{*} 6\right),-0.3\right)$
- Fuzzball: $F(x)=\max \left(\min \left(1.6,(1-x)^{*} 10\right),-0.05\right)$
- This talk and related papers are downloadable from my website http://www.mathstat.dal.ca/~tkolokol/papers

Thank you!

