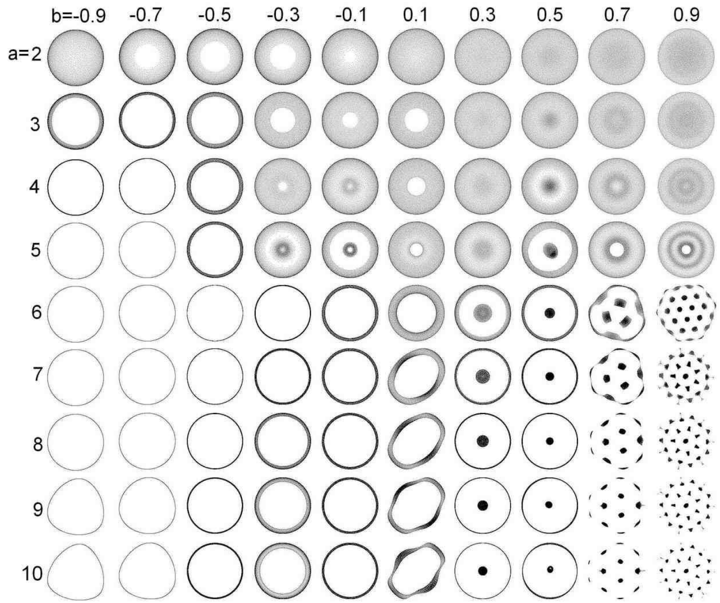
Complex patterns in patricle aggregation models of biological formation



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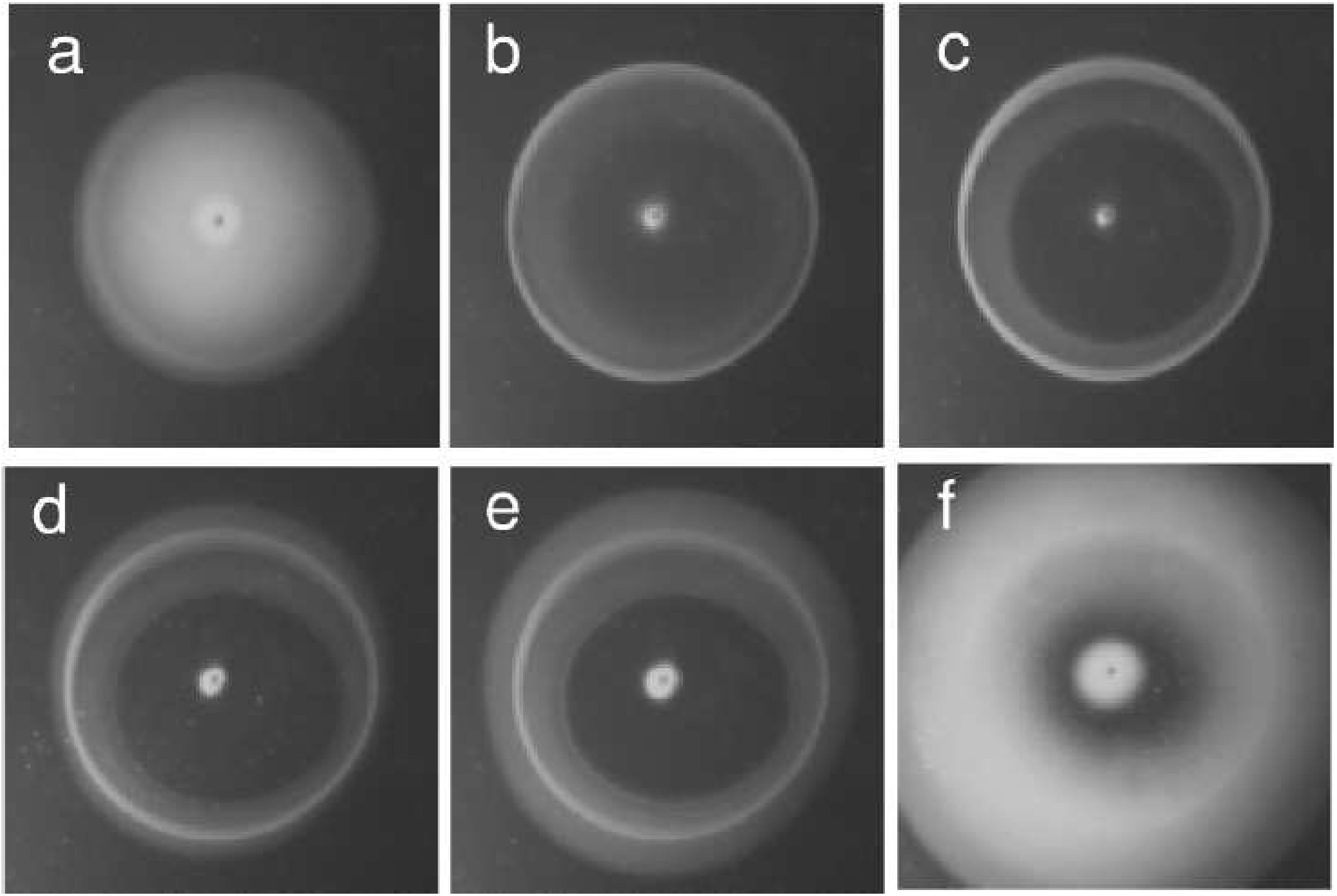
Introduction

- 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....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Aggregation model

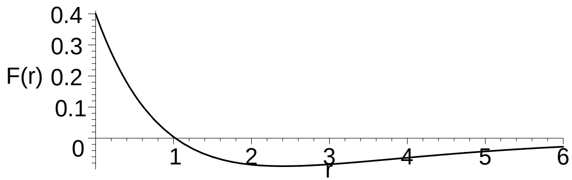
We consider a simple model of particle interaction,

$$\frac{dx_j}{dt} = \frac{1}{N} \sum_{\substack{k=1...N \\ k \neq j}} F\left(|x_j - x_k|\right) \frac{x_j - x_k}{|x_j - x_k|}, \quad j = 1 \dots N \tag{1}$$

- 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.

- Commonly, a ***Morse interaction force*** is used:

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



- 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

$$\rho_t + \nabla \cdot (\rho v) = 0; \qquad v(x) = \int_{\mathbb{R}^n} F\left(|x-y|\right) \frac{x-y}{|x-y|} \rho(y) dy.$$

- Questions

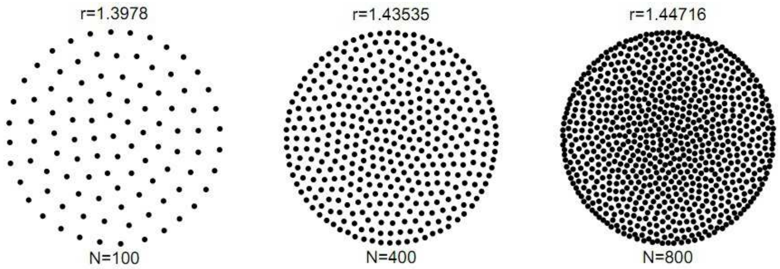
  1. Describe the equilibrium cloud shape in the limit $t \to \infty$

  2. What about dynamics?

Morse force, h-stable vs. catastrophic

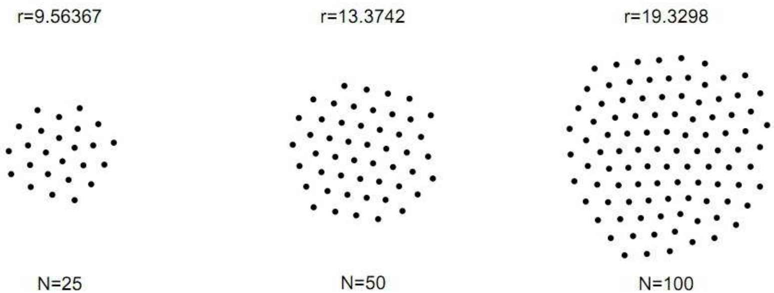
- If $GL^{n+1} > 1$, the system is ***catastrophic:*** doubling N doubles the density but cloud volume is unchanged:

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

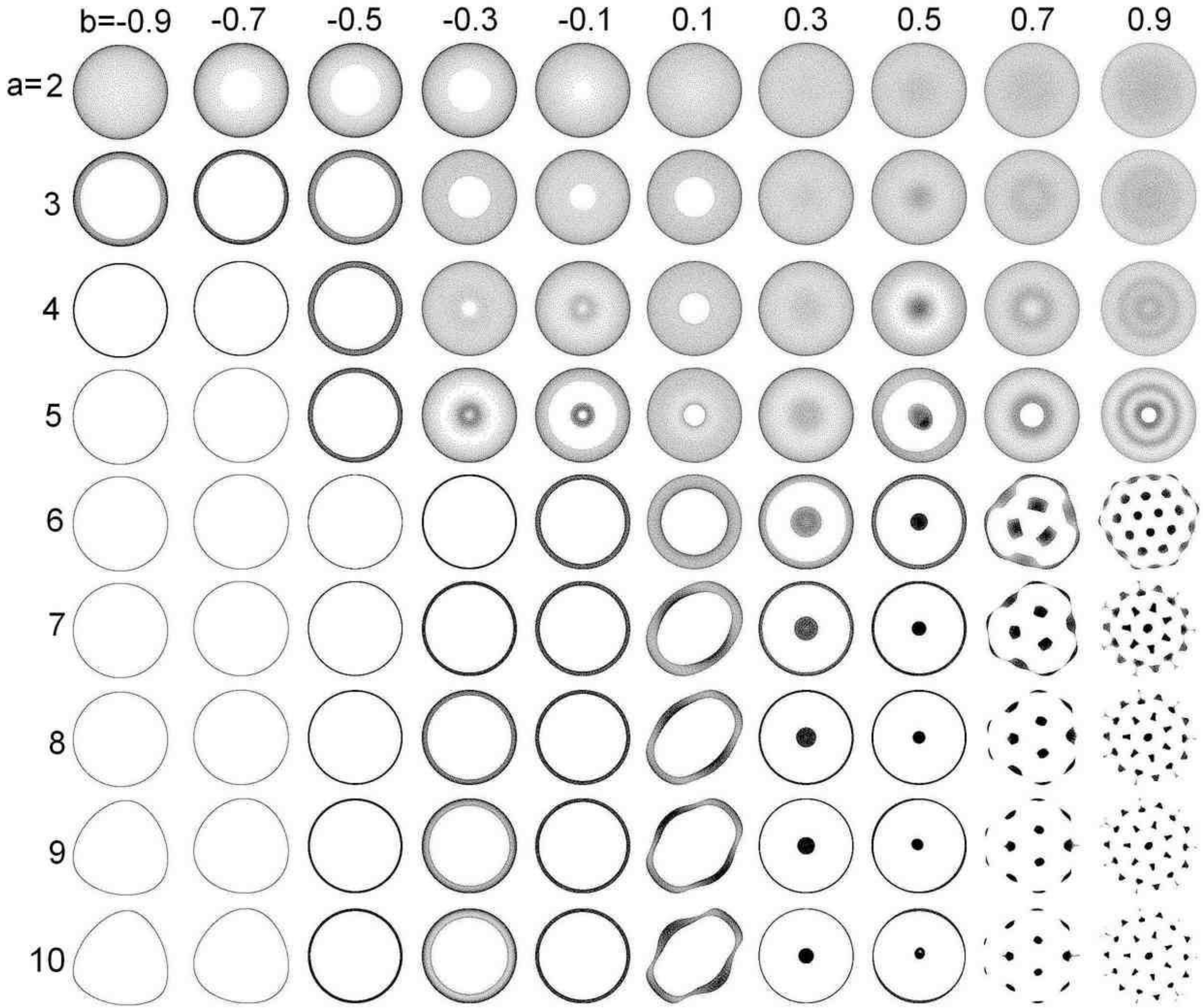


- If $GL^{n+1} < 1$, the system is ***h-stable:*** doubling N doubles the cloud volume: but density is unchanged:

$$F(r) = e^{-r} - 0.5e^{-r/1.2}$$



Tanh-type force: $F(r) = \tanh\left((1-r)\,a\right) + b$



Part I: Ring-type steady states

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

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

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

- 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

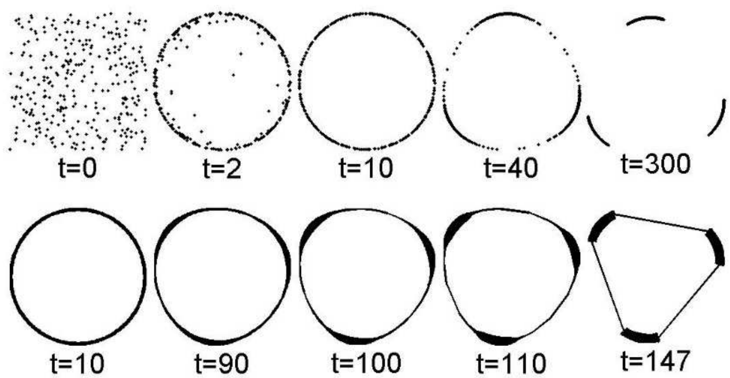
- If particles concentrate on a curve, in the limit $N \to \infty$ we obtain

$$\rho_t = \rho \frac{< z_\alpha, z_{\alpha t} >}{|z_\alpha|^2}; \quad z_t = K * \rho \tag{4}$$

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

$$K * \rho = \int F(|z(\alpha') - z(\alpha)|) \frac{z(\alpha') - z(\alpha)}{|z(\alpha') - z(\alpha)|} \rho(\alpha', t) dS(\alpha'). \tag{5}$$

- 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

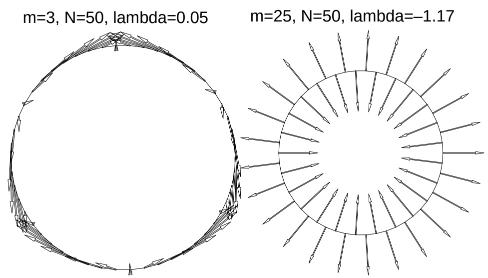
- Linearize: $x_k = r_0 \exp\left(2\pi i k/N\right)\left(1+\exp(t\lambda)\phi_k\right)$ where $\phi_k \ll 1$.
- Ring is stable of $\mathrm{Re}\left(\lambda\right) \leq 0$ for all pair (λ, ϕ). There are three zero eigenvalues corresponding to rotation and translation invariance; all other eigenvalues come in pairs due to rotational invariance.
- λ is the eigenvalue of

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

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

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

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



Quadratic force $F(r) = r - r^2$

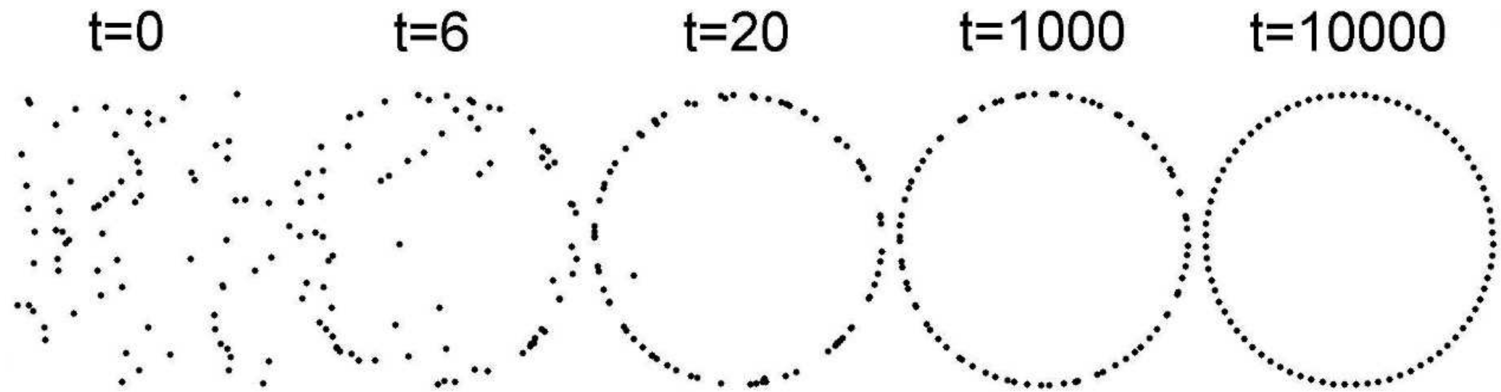
- Computing explicitly,

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

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

- 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.



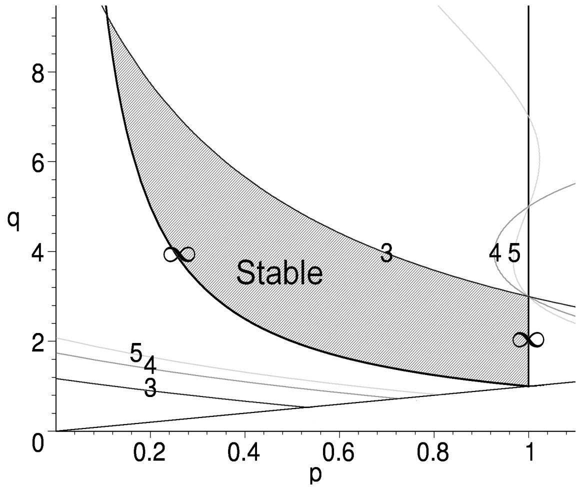
General power force

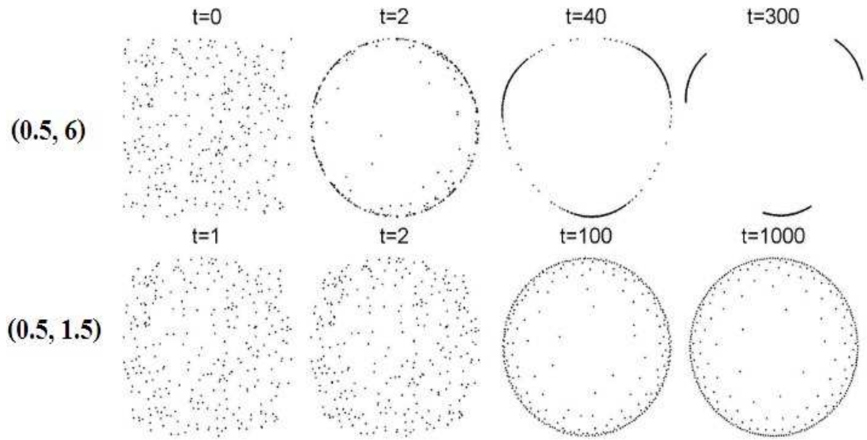
$$F(r) = r^p - r^q, \;\; 0 < p < q$$

- 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

$$0 = 723 - 594(p+q) - 27(p^2+q^2) - 431pq + 106\left(pq^2+p^2q\right) + 19\left(p^3q+pq^3\right)$$
$$+\,10\left(p^3q^2+p^2q^3\right) + 6\left(p^3+q^3\right) + p^3q^3;$$

- 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:**

$$F(0) = 0, \quad F''(0) < 0 \text{ and} \tag{8}$$

$$\int_0^{\pi/2} \left(\frac{F(2r\sin\theta)}{2r\sin\theta} - F'(2r\sin\theta) \right) d\theta < 0. \tag{9}$$

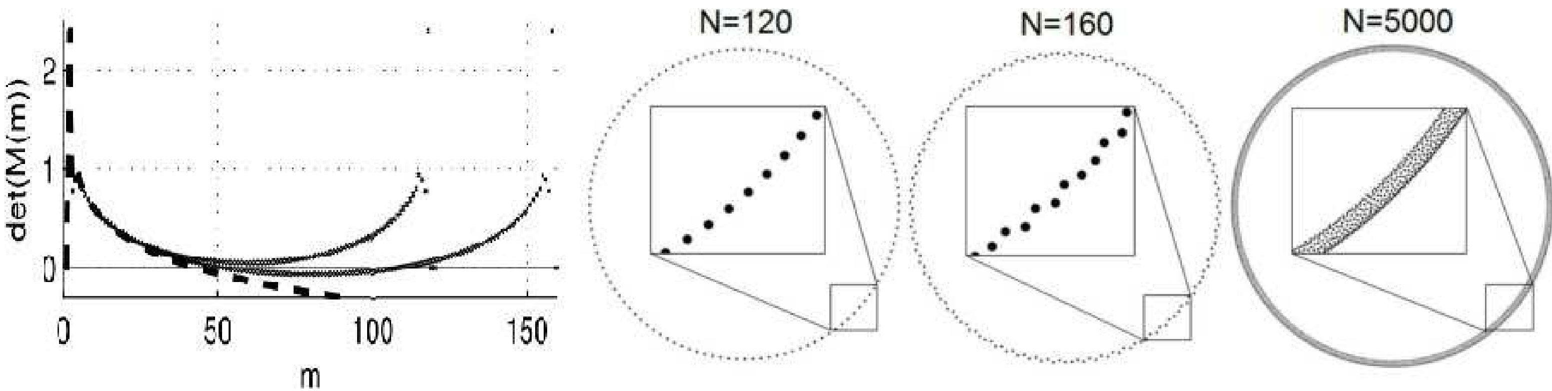
- Ring solution for the morse force $F(r) = \exp(-r) - F\exp(-r/L)$ is always ill-posed.

Discrete vs. continuous

- Consider e.g. $F(r) = \tanh(4(1-r)) - 0.5$. The ring for the ***continuous model*** is ill-posed since $F(0) > 0$. But the ring for the ***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!

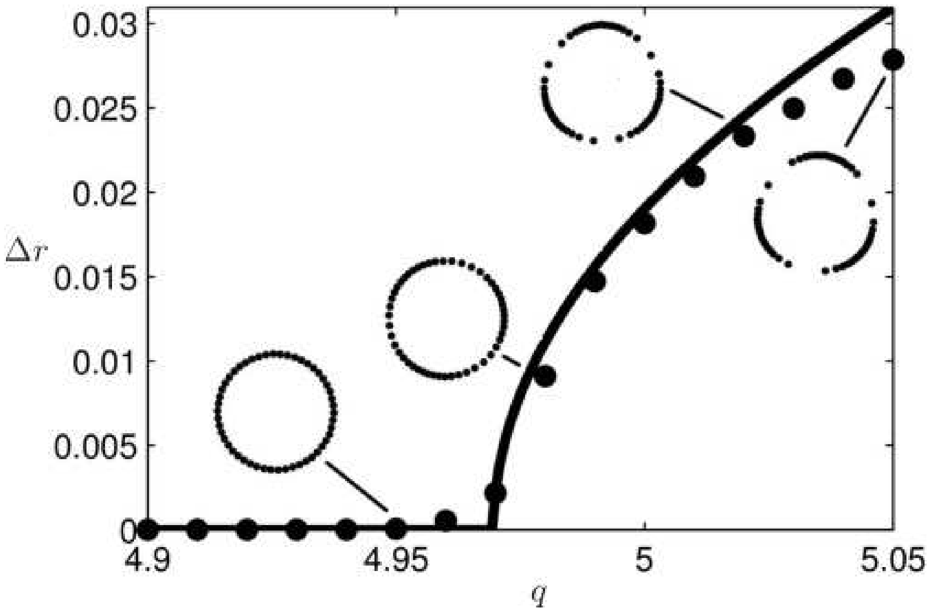
- This can lead to "thin annuli" solutions...



Weakly nonlinear analysis

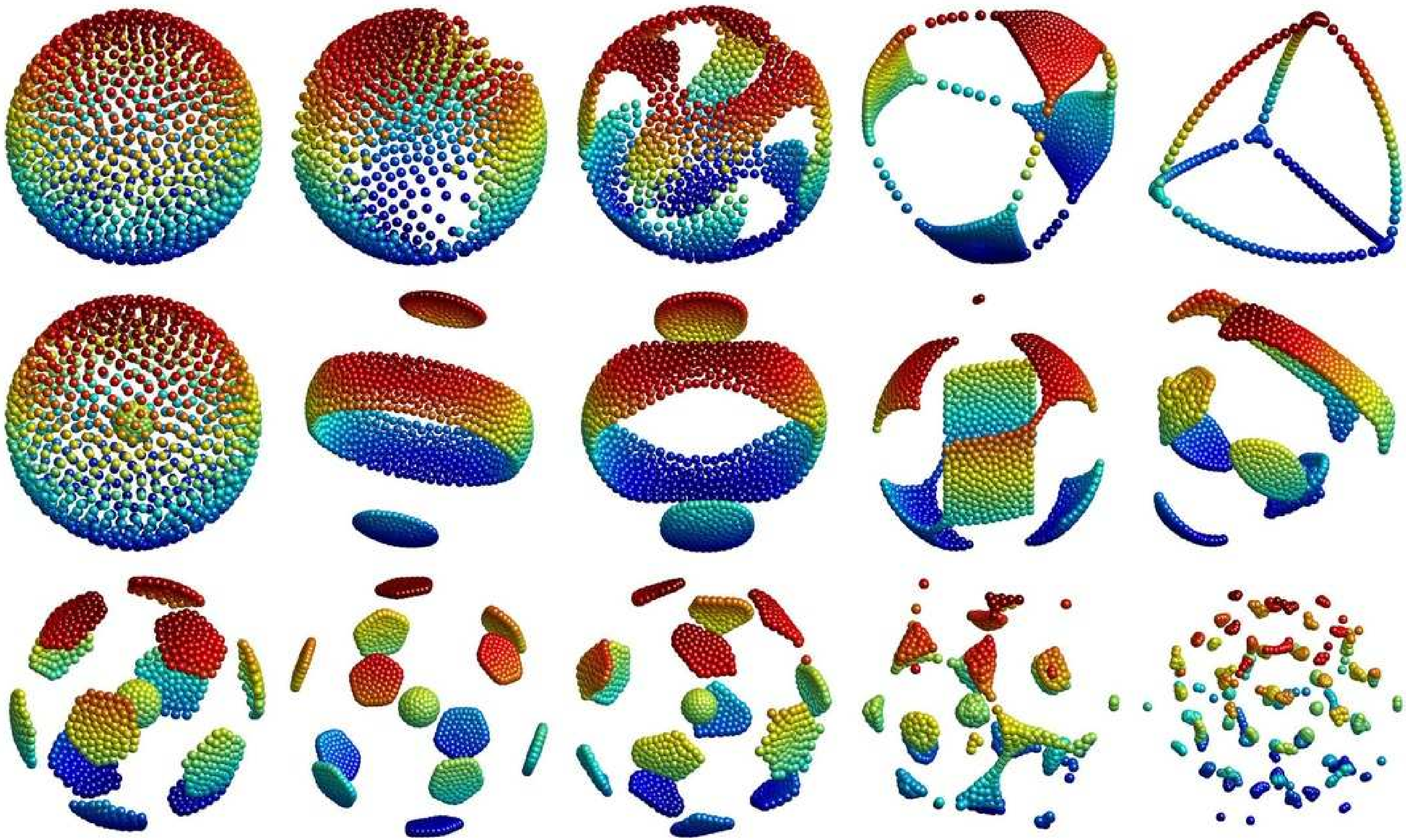
- Near the instability threshold, higher-order analysis shows a **supercritical pitchfork bifurcation,** whereby a ring solution bifurcates into an $m-$symmetry breaking solution
- This shows existence of nonlocal solutions.
- Example: $F(r) = r^{1.5} - r^q$; bifurcation $m = 3$ occurs at $q = q_c \approx 4.9696$; nonlinear analysis predicts

$$\max_i |x_i| - \min_i |x_i| = \sqrt{\max\left(0, \tau(q - q_c)\right)}; \quad \tau \approx 0.109.$$



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

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

Its stability is given by a sequence of 2x2 eigenvalue problems

$$\lambda \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} \alpha + \lambda_l(g_1) & l(l+1)\lambda_l(g_2) \\ \lambda_l(g_2) & \frac{l(l+1)}{R^2}\lambda_l(g_3) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}, \qquad l = 2, 3, 4, \ldots$$

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

$$\alpha := 8\pi g(2R^2) + \lambda_0(g(R^2(1-s^2)))$$

$$g_1(s) := R^2 g'(R^2(1-s))(1-s)^2 - g(R^2(1-s))s$$

$$g_2(s) := g(R^2(1-s))(1-s); \qquad g_3(s) := \int_0^{R^2(1-s)} g(z)dz.$$

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

$$\text{(i)} \;\; \alpha < 0 \quad \text{and} \quad \text{(ii)} \;\; p_1 \in (-1,0)\bigcup(1,2)\bigcup(3,4)\ldots$$

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:

$$\int_{-1}^{1}(1-s)^p P_l(s)\,\mathrm{d}s = \frac{2^{p+1}}{p+1}\frac{\Gamma(l-p)\Gamma(p+2)}{\Gamma(l+p+2)\Gamma(-p)}$$

$$\sim -\frac{1}{\pi}\sin(\pi p)\,\Gamma^2(p+1)2^{p+1}l^{-2p-2} \quad \text{as } l \to \infty.$$

Proof:

- Use hypergeometric representation: $P_l(s) = {}_2F_1\left(\begin{matrix} l+1, -l \\ 1 \end{matrix}; \frac{1-s}{2}\right).$
- Use **generalized Euler transform**:

$$ {}_{A+1}F_{B+1}\left(\begin{matrix} a_1,\ldots,a_A, c \\ b_1,\ldots,b_B, d \end{matrix}; z\right) = \frac{\Gamma(d)}{\Gamma(c)\Gamma(d-c)}\int_0^1 t^{c-1}(1-t)^{d-c-1}\,{}_AF_B\left(\begin{matrix} a_1,\ldots,a_A, c \\ b_1,\ldots,b_B, \end{matrix}\right.$$

to get $\int_{-1}^{1}(1-s)^p P_l(s)\,\mathrm{d}s = \frac{2\pi 2^{p+1}}{p+1}{}_3F_2\left(\begin{matrix} p+1, l+1, -l \\ p+2, 1 \end{matrix}; 1\right).$

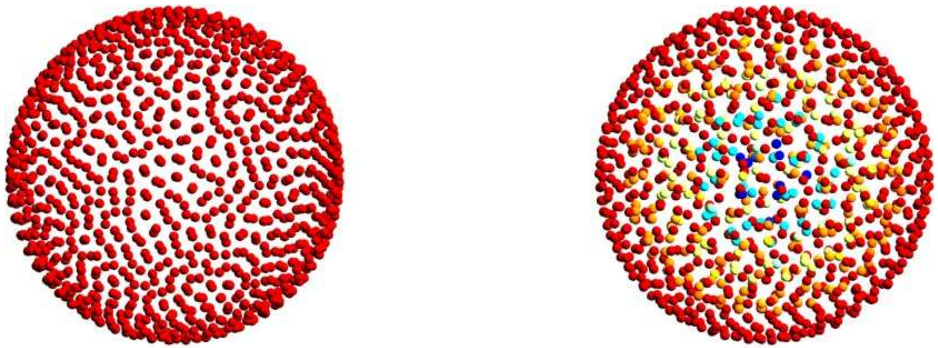
- Apply the **Saalschütz Theorem** to simplify

$$ {}_3F_2\left(\begin{matrix} p+1, l+1, -l \\ p+2, 1 \end{matrix}; 1\right) = \frac{\Gamma(l-p)\Gamma(p+2)}{\Gamma(l+p+2)\Gamma(-p)}.$$

Generalized Lennard-Jones interaction

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

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



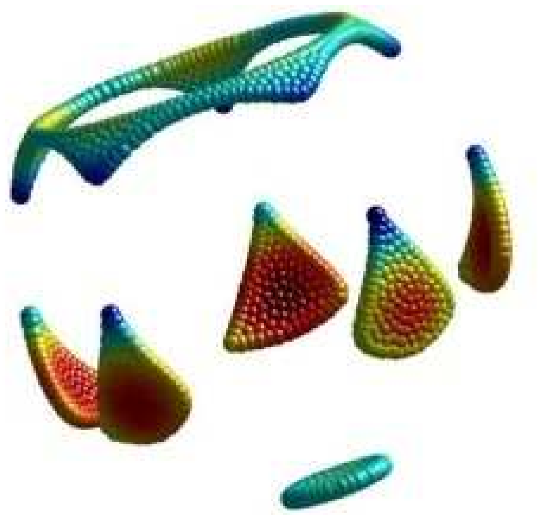
(a) (b)

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.

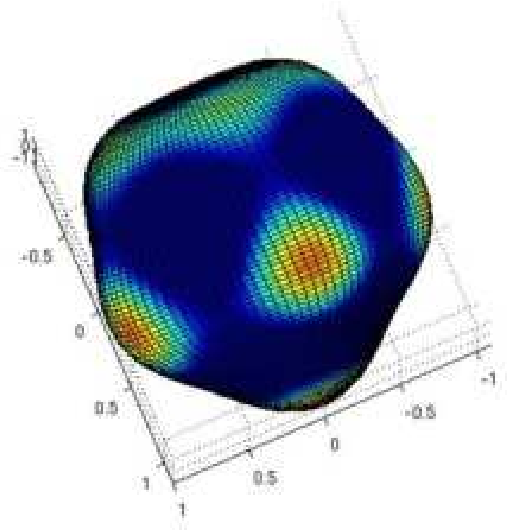
Custom-designed kernels

- 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

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?

Bounded states of constant density

Claim. Suppose that

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

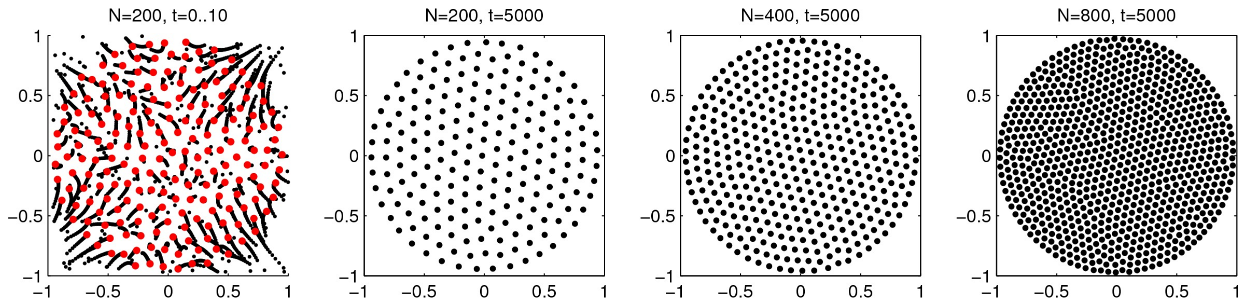
Then the aggregation model

$$\rho_t + \nabla \cdot (\rho v) = 0; \qquad v(x) = \int_{\mathbb{R}^n} F\left(|x-y|\right) \frac{x-y}{|x-y|} \rho(y) dy.$$

admits a steady state of the form

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

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:

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

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 $M = \int_{\mathbb{R}^n} \rho(y)dy = MR^2 \implies R = 1$.

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

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

and continuity equations become

$$\begin{aligned} \rho_t + v\rho_x &= -v_x \rho \\ &= (M - 2\rho)\, \rho \end{aligned}$$

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

$$\frac{d}{dt} X(t; x_0) = v; \qquad X(0, x_0) = x_0$$

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

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

Solving we get:

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

Solving for characteristic curves

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:

$$w_t + v w_x = 0$$

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

$$\frac{d}{dt}X = 2w_0 - M(X+1); \quad X(0; x_0) = x_0$$

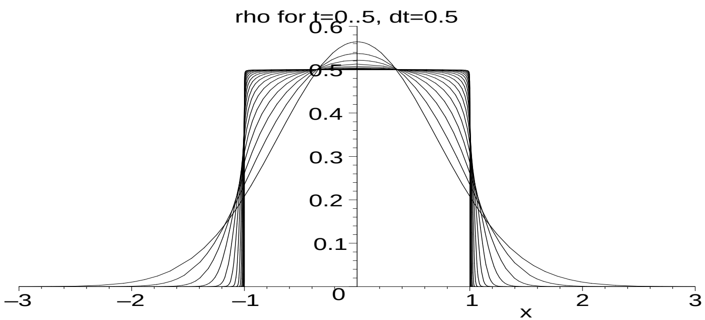
Summary for $F(r) = 1 - r$ in 1D:

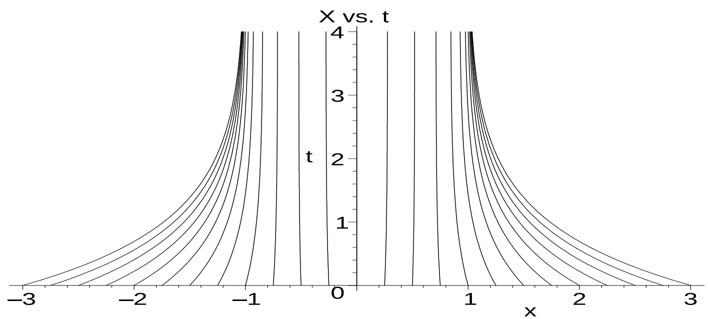
$$X = \frac{2w_0(x_0)}{M} - 1 + e^{-Mt}\left(x_0 + 1 - \frac{2w_0(x_0)}{M}\right)$$

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

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

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





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

$$\rho(x, \infty) = \begin{cases} M/2, & |x| < 1 \\ 0, & |x| > 1 \end{cases} \tag{10}$$

- 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,

$$\nabla \cdot v = 2\pi\rho(x) - 4\pi M;$$

$$\begin{aligned} \rho_t + v \cdot \nabla\rho &= -\rho\nabla \cdot v \\ &= -\rho\,(\rho - 2M)\,2\pi \end{aligned}$$

- Along the characterisitics:

$$\frac{d}{dt}X(t;x_0) = v; \qquad X(0,x_0) = x_0$$

we still get

$$\frac{d}{dt}\rho = 2\pi\rho(2M - \rho);$$

$$\rho(X(t;x_0),t) = \frac{2M}{1 + \left(\frac{2M}{\rho(x_0)} - 1\right)\exp\left(-4\pi Mt\right)} \tag{11}$$

- 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

$$\det \nabla_{x_0} X(t;x_0) = \frac{\rho_0(x_0)}{2M} + \left(1 - \frac{\rho_0(x_0)}{2M}\right) \exp\left(-4\pi M t\right).$$

- If ρ is **radially symmetric**, characteristics are also radially symmetric, i.e.

$$X(t;x_0) = \lambda\left(\left|x_0\right|, t\right) x_0$$

then

$$\det \nabla_{x_0} X(t;x_0) = \lambda(t;r)\left(\lambda(t;r) + \lambda_r(t;r) r\right), \quad r = |x_0|$$

so that

$$\lambda^2 + \lambda_r \lambda r = \frac{\rho_0(x_0)}{2M} + \left(1 - \frac{\rho_0(x_0)}{2M}\right) \exp\left(-4\pi M t\right)$$

$$\lambda^2 r^2 = \frac{1}{M}\int_0^r s\rho_0(s) ds + 2\exp\left(-4\pi M t\right)\int_0^r s\left(1 - \frac{\rho\left(s\right)}{2M}\right) ds$$

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
  $$\frac{d\rho_{\max}}{dt} \le (aR^{q-2} - b\rho_{\max})\rho_{\max}$$
  $$\frac{dR}{dt} \le c\sqrt{\rho_{\max}} - dR^{q-1};$$
  where a, b, c, d are some [known] positive constants.

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

- **Theorem:** For $q \ge 2$, 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

$$\rho(x) = \begin{cases} b_0 + b_2 x^2 + b_4 x^4 + \ldots + b_{2n} x^{2n}, & |x| < R \\ 0, \quad |x| \geq R \end{cases} \tag{12}$$

Define the following quantities,

$$m_{2q} := \int_0^R \rho(r) r^{2q} dr. \tag{13}$$

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

$$F(r) = 1 - a_0 r - \frac{a_2}{3} r^3 - \frac{a_4}{5} r^5 - \ldots - \frac{a_{2n}}{2n+1} r^{2n+1} \tag{14}$$

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:

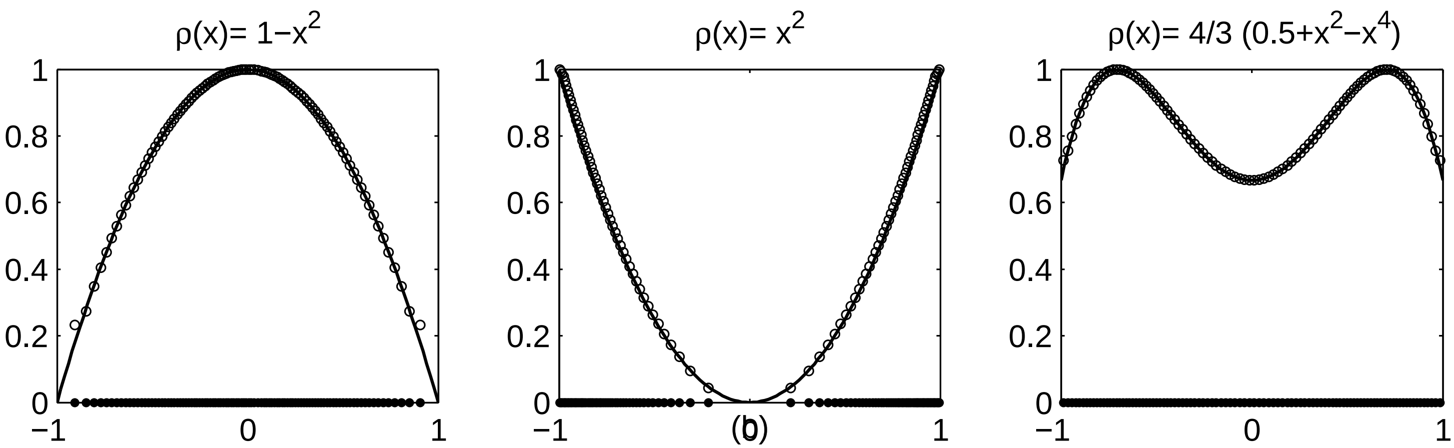
$$b_{2k} = \sum_{j=k}^{n} a_{2j} \begin{pmatrix} 2j \\ 2k \end{pmatrix} m_{2(j-k)}, \qquad k = 0 \ldots n. \tag{15}$$

Example: custom kernels 1D

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

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

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



Ex.1 Ex.2 Ex.3

Inverse problem: Custom-designer kernels: 2D

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

$$\rho(r) = \begin{cases} b_0 + b_2 r^2 + b_4 r^4 + \ldots + b_{2n} r^{2n}, & r < R \\ 0, & r \geq R \end{cases} \tag{16}$$

Define the following quantities,

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

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

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

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:

$$b_{2k} = \sum_{j=k}^{n} a_{2j} \begin{pmatrix} j \\ k \end{pmatrix}^2 m_{2(j-k)+1}; \quad k = 0 \ldots n. \tag{19}$$

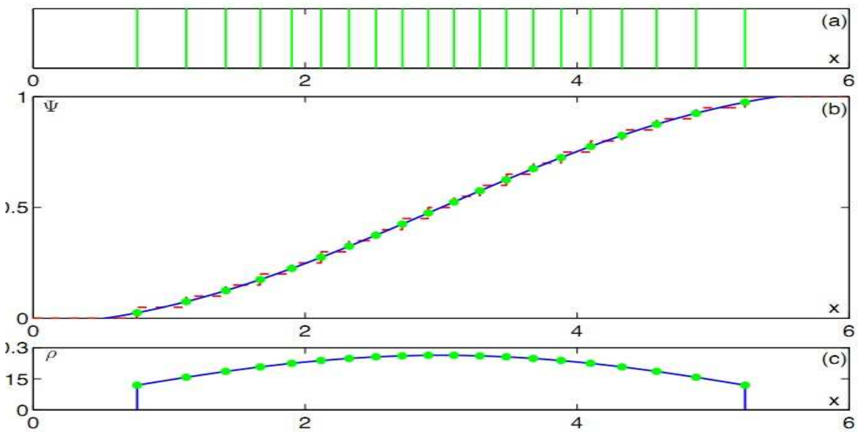
This system always has a unique solution for provided that $m_0 \neq 0$.

Numerical simulations, 1D

- First, use standard ODE solver to integrate the corresponding discrete particle model,

$$\frac{dx_j}{dt} = \frac{1}{N} \sum_{\substack{k=1...N \\ k \neq j}} F\left(|x_j - x_k|\right) \frac{x_j - x_k}{|x_j - x_k|}, \quad j = 1 \ldots N.$$

- How to compute $\rho(x)$ from x_i? [Topaz-Bernoff, 2010]
  - Use x_i to approximate the cumulitive 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

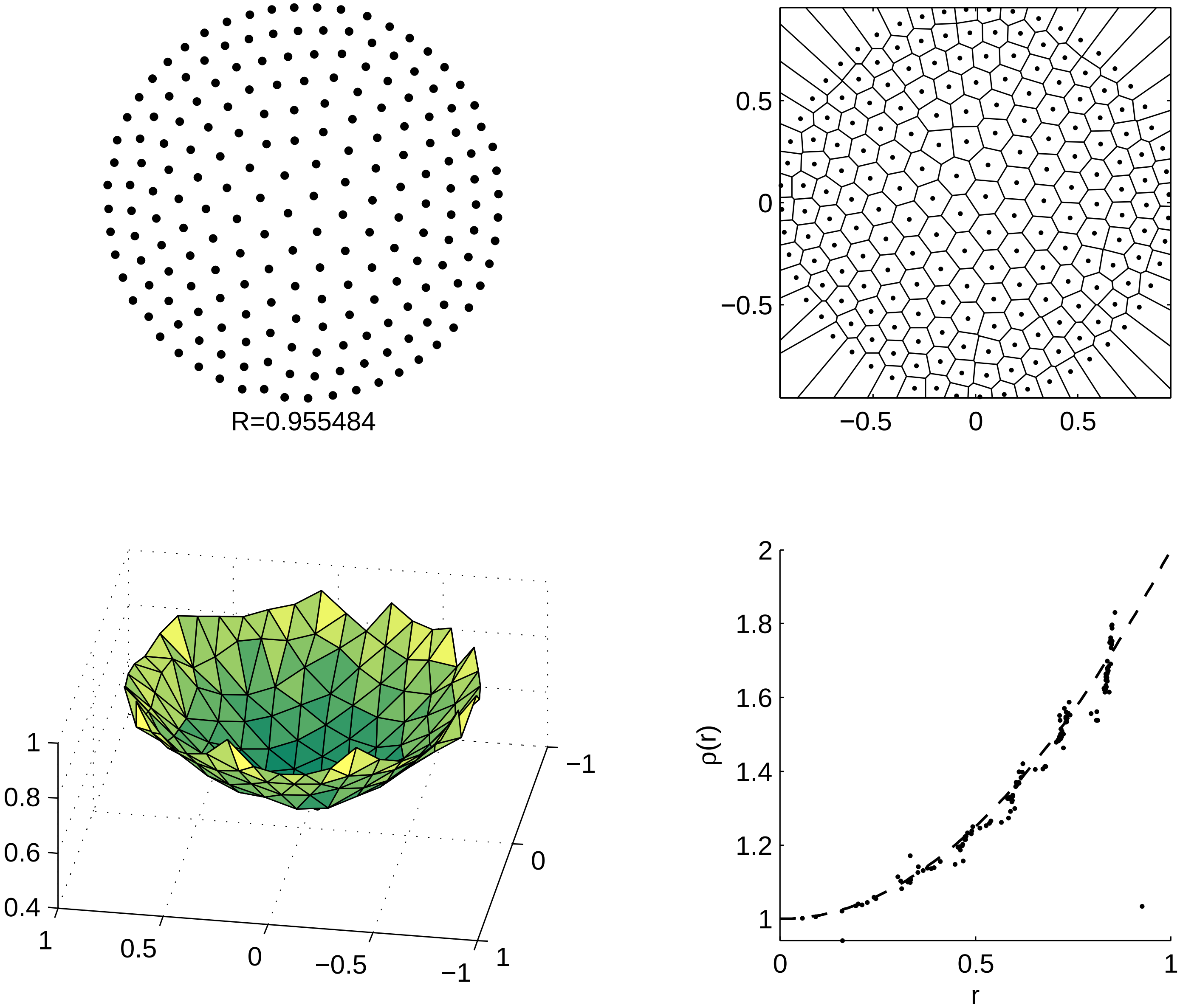
- Solve for x_i using ODE particle model as before [$2N$ variables]
- Use x_i to compute **Voronoi diagram**;
- Estimate $\rho(x_j) = 1/a_j$ where a_j is the area of the voronoi cell around x_j.
- Use **Delanay triangulation** to generate smooth mesh.
- **Example:** Take

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

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...

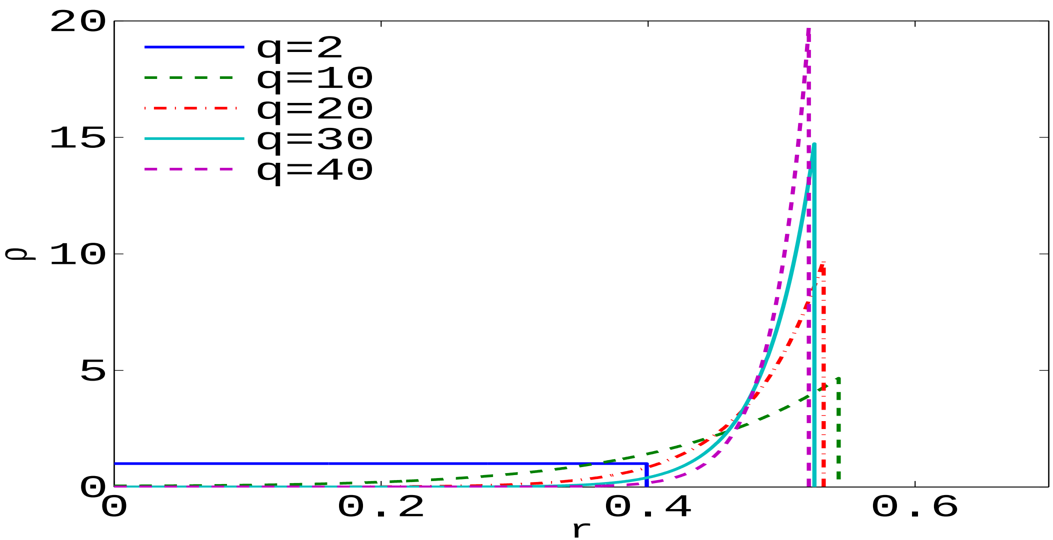

R=0.955484
0.5
0
−0.5
−0.5
0
0.5
1
0.8
0.6
0.4
1
0.5
0
−0.5
−1
−1
0
1
2
1.8
1.6
1.4
1.2
1
ρ(r)
0
0.5
1
r

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 ρ and R, we adjust R until the operator $\rho \to c(q) \int_0^R (r'\rho(r')K(r,r')dr'$ has eigenvalue 1; then ρ 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`

Thank you!