Pattern formation in particle systems: from spherical shells to regular simplices

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Slides at 'Talk #' at www.math.toronto.edu/mccann

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Animals forming patterns: flocking, milling, swarming

and schooling

bottom view

Led scientists to make models...

e.g. (very incomplete)
Lennard-Jones (1924) 6-12 potential for molecular interactions
Parr (1927)
Breder (1954) attractive-repulsive power law interaction for fish separation
Keller-Segal (1971) purely attractive, 1st order (2d cell chemotaxis)

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Mogilner and Edelstein-Keshet (1999) 1d attractive-repulsive + diffusion
Levine, Rappel and Cohen (2000) 2nd order, preferred speed
Topaz, Bertozzi and Lewis (2006)
Cucker and Smale (2007) 2nd order, matched speeds

.

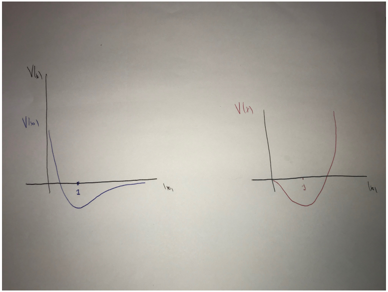
... analyze and simulate
e.g. (just as incomplete) Albi, Balague, Bertozzi, Burchard, Carrillo, Choksi, Craig, Delgadino, Dolbeault, Fetecau, Figalli, Frank, Huang, Hoffman, Kolokolnikov, Laurent, Lieb, Lopes, Pavlovski, Pattachini, Raoul, Shu, Slepcev, Simione, Sun, Topaloglu, Uminsky, von Brecht, Yao ...

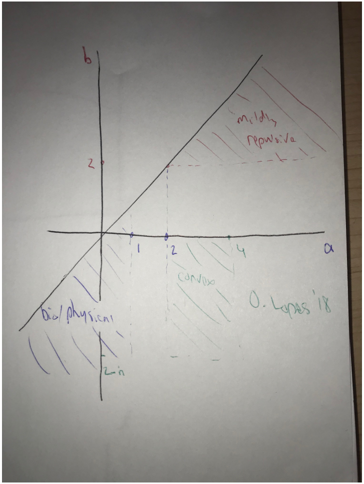
Attractive-repulsive pair potentials on $x \in \mathbf{R}^n$:

$$V_{a,b}(x) := V_a(x) - V_b(x)$$

$$V_a(x) := \frac{1}{a}|x|^a \qquad \text{exponents } a > b$$

- minimized at separation $|x| = 1$





First-order, interacting J particle dynamics

ODE description: $x_k(t) \in \mathbf{R}^n$ for $i \in \{1, \ldots, J\}$:

$$\frac{dx_k}{dt} = \frac{1}{J-1} \sum_{i \neq k} \nabla V_{a,b}(x_i - x_k)$$

PDE description:

the probability measure $\mu(t) := \frac{1}{J} \sum_{i=1}^{J} \delta_{x_i(t)}$ on $\mathbf{R}^n$ satisfies

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which dissipates the quadratic energy

$$E(\mu) = E_{a,b}(\mu) = E_a(\mu) - E_b(\mu) := \int_{\mathbf{R}^n} \int_{\mathbf{R}^n} V_{a,b}(x-y) d\mu(x) d\mu(y)$$

The continuumum $J \to \infty$ limiting dynamics

The aggregation / self-assembly equation

$$\frac{d\mu}{dt} = \nabla \cdot [\mu \nabla (V_{a,b} * \mu)] = \frac{1}{2} \nabla \cdot [\mu \nabla (\frac{\delta E}{\delta \mu})],$$

defines a flow on $\mathcal{P}(\mathbf{R}^n)$, where

$$\mathcal{P}(K) := \{\mu \geq 0 \text{ on } \mathbf{R}^n \mid \mu[K] = 1 = \mu[\mathbf{R}^n]\}$$

denotes the space of Borel probability measures on $K \subset \mathbf{R}^n$ and

$$\mathcal{P}_c^0(K) = \{\mu \in \mathcal{P}(K) \mid \operatorname{spt} \mu \text{ is compact and } 0 = \int_{\mathbf{R}^n} x d\mu(x)\}.$$

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Minimizers of $E_{a,b}(\mu)$ on $\mathcal{P}(\mathbf{R}^n)$ represent attracting fixed points of the flow (as do local minimizers in a suitable topology).

Piecewise linear force laws

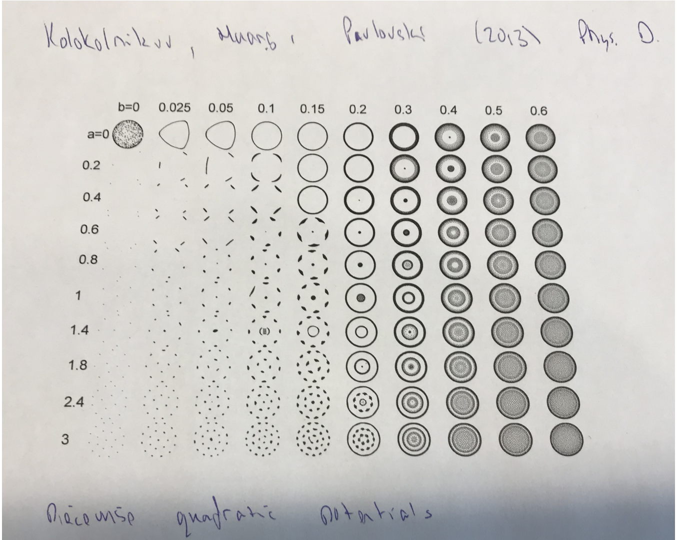
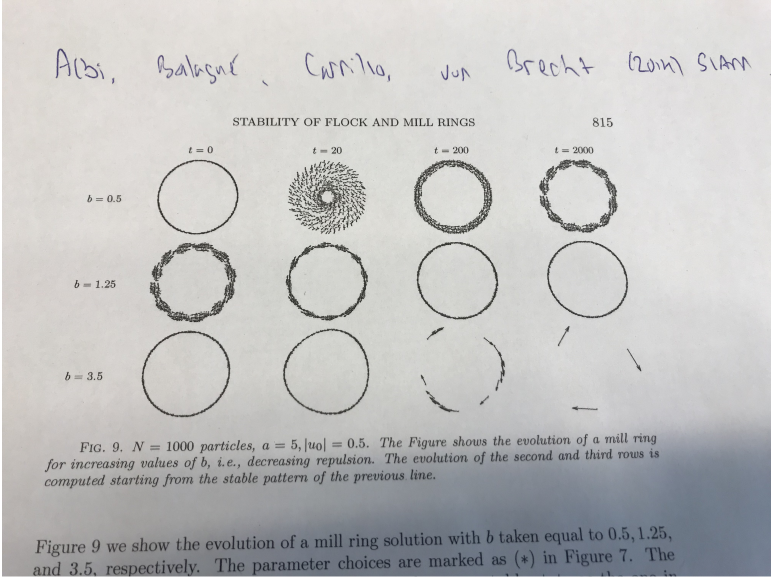


Figure 1: Steady states of (1) with $F(r) = \min(ar + b, 1 - r)$, using $N = 1000$ particles and with a, b as indicated. A snapshot at $t = 10,000$ is shown. Integration was performed using forward Euler method with stepsize 0.5.

Power law potentials



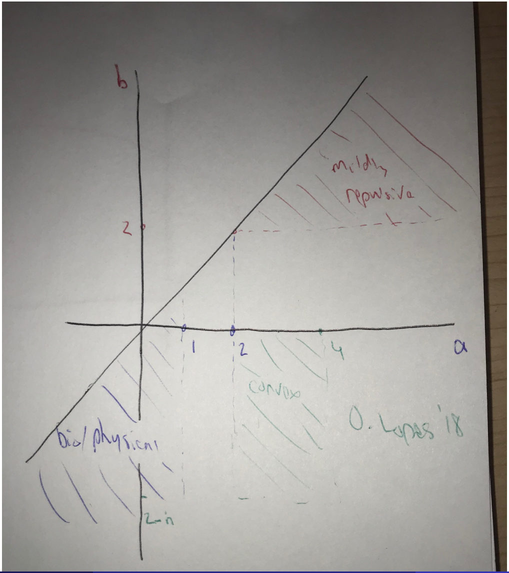
Albi, Balagué, Carrillo, von Brecht (2014) SIAM

STABILITY OF FLOCK AND MILL RINGS 815

Fig. 9. $N = 1000$ *particles,* $a = 5, |u_0| = 0.5$. *The Figure shows the evolution of a mill ring for increasing values of* b, *i.e., decreasing repulsion. The evolution of the second and third rows is computed starting from the stable pattern of the previous line.*

Figure 9 we show the evolution of a mill ring solution with b taken equal to $0.5, 1.25$, and 3.5, respectively. The parameter choices are marked as $(*)$ in Figure 7. The

Parameter space



Some related results

M. '94, '05 introduced d_∞-local minimization to find stable rotating stars

Balague, Carrillo, Laurent, Raoul '13: showed d_∞-local minimimizers μ of $E_{a,b}$ on $\mathcal{P}(\mathbf{R}^n)$ have support with Hausdorff dimension at least $2 - b$.

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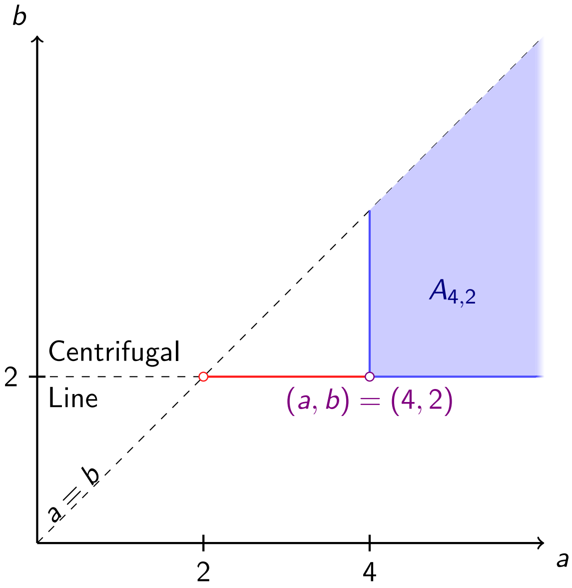
Carrillo, Figalli, Patachini '17: showed if $b > 2$ then d_∞-local minimimizers are supported only at isolated points (and indeed only finitely many such points in the case of global energy minimizers).

Kang, Kim, Lim, Seo '19+: catalog d_∞-local and global minimizers in $n = 1$ dimension

Our results:



Transition from spherical shells to regular simplices

Theorem (Minimizing attraction with mild repulsion for $n \geq 2$)

1. (Spherical shells) If $4 > a > b = 2$ then $E(\mu)$ is uniquely minimized on $\mathcal{P}_c^0(\mathbf{R}^n)$ by uniformly distributing the mass of μ over a sphere

2. (Critical point) If $a/2 = b = 2$, every measure on the sphere of radius $r = \sqrt{\frac{n}{2n+2}}$ with $\frac{r^2}{n} Id$ as its second moment tensor minimizes E on $\mathcal{P}_c^0(\mathbf{R}^n)$

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3. (Regular simplices) There is a continuous strictly decreasing function $a_n : [2, \infty] \longrightarrow [-\infty, 4]$ *such that* $a_n(2) = 4$ *and: if* $a > b \geq 2$ *then* $E(\mu)$ *is minimized on* $\mathcal{P}_c^0(\mathbf{R}^n)$ *by equidistributing the mass of* μ *over the vertices of a regular simplex*

$$\mu = \hat{\mu} = \frac{1}{n+1} \sum_{i=0}^{n} \delta_{x_i} \qquad \text{where } |x_i - x_k| = 1 \text{ for all } 0 \leq i < k \leq n$$

if and only if $a \geq \max\{b, a_n(b)\}$; *the only minimizers are rotations of* μ *if the inequality holds strictly*

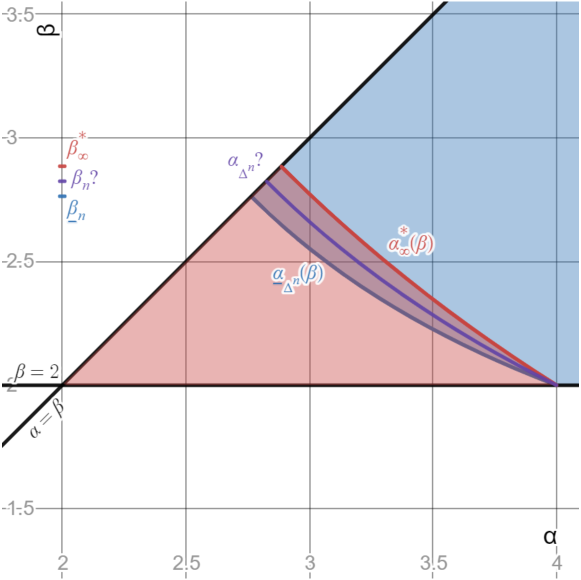
4. (Estimating the transition threshold)
In the region $a > b$ of interest, $a_n(b) \in [\bar{a}_n(b), \bar{a}_\infty(b)]$

where $a = \bar{a}_n(b) > b$ uniquely solves $f_n(a) = f_n(b)$ for

$$f_n(a) := \frac{n - (2 - \frac{2}{n+1})^{a/2} - n(1 - \frac{2}{n+1})^{a/2}}{a}$$

and

$$f_\infty(a) := 1 - \frac{2^{a/2}}{a} = \lim_{n\to\infty} f_n(a)$$


3.5
β
3
β^*_∞
β_n?
$\underline{\beta}_n$
α_{Δ^n}?
$\alpha^*_\infty(\beta)$
2.5
$\underline{\alpha}_{\Delta^n}(\beta)$
$\beta = 2$
$\alpha = \beta$
1.5
α
2
2.5
3
3.5
4

$n = 2$

5. (Characterizing the transition)
If $a = a_n(b) > b$ and $\mathcal{P}_{\Delta^n}$ denotes the set of rotations and translations of balanced measure $\hat{\mu}$ on the unit simplex, then at least one of the following two containments is strict:

$$\mathcal{P}_{\Delta^n} \subsetneq \arg\min_{\mathcal{P}(\mathbf{R}^n)} \mathcal{E}_{a,b} \quad \text{or} \quad \operatorname{spt} \hat{\mu} \subsetneq \arg\min_{\mathbf{R}^n} (V_{a,b} * \hat{\mu}).$$

Bifurcation must be discontinuous...

Ideas of proof: 1.

Lopes '18: for $2 < a < 4$ implies strict convexity of $E_a(\mu)$ on $\mathcal{P}_c^0(\mathbf{R}^n)$: for neutral $\rho = \mu_0 - \mu_1$ Fourier transform yields positive-definite

$$\frac{1}{a}\iint |x-y|^a d\rho(x)d\rho(y) = (\rho * V_a, \rho) = C_n(a)\int |k|^{-n-a}|\hat{\rho}(k)|^2 dk;$$

• in this range the minimizer must be unique and spherically symmetric

1. follows from the Euler-Lagrange equation $\mu[\arg\min_{\mathbf{R}^n} \frac{\delta E_{a,b}}{\delta\mu}] = 1$, plus

• the (highly non-trivial) fact that spherical symmetry of $d\mu(x) = d\mu(|x|)$ implies $r \in (0, \infty) \mapsto \frac{\delta E_{a,2}}{\delta \mu}(r) = (V_{a,2} * \mu)(re_1)$ has positive third derivative, hence a unique global minimum $r_* > 0$ in this range.

2. the critical point $a = 4 = 2b$

- $E_2(\mu) = \mathrm{Tr}\, I(\mu)$ is affine (linear) on $\mathcal{P}_c^0(\mathbf{R}^n)$, while

- $t \in [0, 1] \mapsto E_4((1-t)\mu_0 + t\mu_1)$ is strictly convex iff $I(\mu_0) \neq I(\mu_1)$, where

$$I_{ij}(\mu) := \int x_i x_j d\mu(x)$$

is the second moment tensor $I(\mu) = (I_{ij}(\mu))_{i,j=1}^n$

• thus $E_{4,2} = E_4 - E_2$ admits a spherically symmetric minimizer, and all other minimizers share its moment of inertia tensor $I(\mu) = c \cdot Id_n$

• among μ with $I(\mu) = c \cdot Id_n$, Jensen's inequality shows

$$\begin{aligned} 2E_{4,2}(\mu) &= \int |x|^4 d\mu(x) + (\mathrm{Tr}\, I(\mu))^2 + 2\,\mathrm{Tr}(I(\mu)^2) - 2\,\mathrm{Tr}\, I(\mu) \\ &\geq (\int |x|^2 d\mu(x))^2 + (nc)^2 + 2nc^2 - 2nc \\ &= 2nc(nc + c - 1) \end{aligned}$$

with equality forcing $|x|^2 = cn$ to hold μ-a.e. (and $c = \frac{1}{2n+2}$ optimizing)

3. a simple but powerful monotonicity

Theorem (Northeast comparison principle)

If the unit simplices $\hat{\mu}$ minimize $E_{a,b}(\mu)$ on $\mathcal{P}_c^0(\mathbf{R}^n)$, then (a) they uniquely minimize $E_{a+\epsilon,b}(\mu)$ and $E_{a,b+\epsilon}(\mu)$ for all $\epsilon > 0$ and (b)

$$\mathrm{spt}\,\hat{\mu} = \arg\min_{\mathbf{R}^n}(\hat{\mu} * V_{a+\epsilon,b}) = \arg\min_{\mathbf{R}^n}(\hat{\mu} * V_{a,b+\epsilon})$$

Proof: If $v_{a,b}(r) := \frac{1}{a}r^a - \frac{1}{b}r^b$ then by the concavity of log

$$\bar{v}_{a,b}(r) := -\frac{v_{a,b}(r)}{v_{a,b}(1)} = \frac{br^a - ar^b}{a-b} = \bar{v}_{b,a}(r)$$

satisfies

$$a\frac{\partial}{\partial b}\bar{v}_{a,b}(r) = \frac{a^2 r^b}{(a-b)^2}(r^{a-b} - 1 - \log r^{a-b}) \geq 0$$

for $r > 0 \neq a \neq b$, with equality only at $r \in \{0, 1\}$. □

Theorem (LM21: Local minima pervade mildly repulsive regime)

If $a > b > 2$ and $0 < m_0 \le \cdots \le m_n$ with $1 = \sum_{i=0}^{n} m_i$ then

$$\mu = \sum_{i=0}^{n} m_i \delta_{x_i} \qquad \text{where } |x_i - x_k| = 1 \text{ as above}$$

is a d_∞-local minimizer of $E(\mu)$ (mininimizing strictly up to rigid motions).

Bifurcation must be discontinuous...

SIMIONE '14: in the plane $n = 2$ these d_∞-local minimizers (and other ring type solutions) enjoy certain nonlinear stability properties;

• the existence of finer ring type solutions approximating the spherical shell implies the latter cannot be attractors (i.e cannot be asymptotically stable); in what sense might they be stable?

Kantorovich-Rubinstein-Wasserstein L^p-transport metric d_p

Given $p > 1$ and $K \subset \mathbf{R}^n$ compact,

$$d_p(\mu, \nu) := \left(\inf_{\gamma \in \Gamma(\mu,\nu)} \int_{\mathbf{R}^n \times \mathbf{R}^n} |x - y|^p d\gamma(x, y) \right)^{1/p}$$

metrizes the weak topology on $\mathcal{P}(K)$, where

$$\Gamma(\mu, \nu) := \left\{ \gamma \in \mathcal{P}(\mathbf{R}^{2n}) \mid \begin{array}{ll} \mu[U] = & \gamma[U \times \mathbf{R}^n], \\ & \gamma[\mathbf{R}^n \times U] \quad = \nu[U] \end{array} \forall U \subset \mathbf{R}^n \right\}$$

denotes the set of joint measures with given marginals.

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denotes the set of joint measures with given marginals.

$$d_\infty(\mu, \nu) := \lim_{p \to \infty} d_p(\mu, \nu)$$

metrizes a much finer topology.

Lemma (Lyapunov)

If $E : X \longrightarrow \mathbf{R}$ *is a coercive function on a metric space* (X, d) *— meaning* $E^{-1}((-\infty, h])$ *is compact for each* $h \in \mathbf{R}$ *— then for each* $\epsilon > 0$ *there exists* $\delta > 0$ *and* $h \in \mathbf{R}$ *such that*

$$(\arg\min_X E)^\delta \subset E^{-1}((-\infty, h)) \subset (\arg\min_X E)^\epsilon,$$

where

$$Y^\epsilon := \{x \in X \mid d(x, Y) := \inf_{y \in Y} d(x, y) < \epsilon\}.$$

Theorem (Lyapunov stability)

6. For $0 < b < a < \infty$ and $a \geq 1$, the hypotheses of the lemma are satisfied by $E = E_{a,b}$ and $(X, d) = (\mathcal{P}_c^0(\mathbf{R}^n), d_a)$. Any energy non-increasing curve $(\mu(t))_{t \geq 0}$ which starts within δ of a minimizer therefore remains within distance ϵ of an energy minimizer, with δ and ϵ from Lyapunov's lemma.

Proof: Two applications of Jensen's inequality, combined with the bounded compactness of $(\mathcal{P}_a^0(\mathbf{R}^n), d_a)$...

Thank you