Ansatz solutions to a problem of mean curvature and Newtonian potential

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Morphogenesis in development.
Plecosomus Catfish, Fan Dancer Goby, Vampire Plecosomus.

Abramite Head Standers, Altolamprologus, Cyphotilapia Frontosa.
The Gierer-Meinhardt system with saturation.

This is a reaction diffusion system of the activator-inhibitor type. Its steady states satisfy

\[ \epsilon^2 \Delta u - u + \frac{u^p}{(1 + \kappa u^p)v^q} = 0; \quad d\Delta v - v + \frac{ur}{vs} = 0 \]

on a domain \( D \) with the Neumann boundary condition

\[ \frac{\partial u}{\partial \nu} \bigg|_{\partial D} = 0; \quad \frac{\partial v}{\partial \nu} \bigg|_{\partial D} = 0. \]

\( \kappa = 0 \): non-saturation case. \( \kappa > 0 \): saturation case.

There is a large body of literature on the non-saturation GM system. The saturation case (GMS) is not as well studied.

Reduction to a nonlocal geometric problem. Let

\[ f(u, v) = -u + \frac{u^p}{(1 + \kappa u^p)v^q}. \]  

(1)

As a function of \( u \), \( f(u, v) \) is bistable with three zeros.

\( \exists v_0 \) such that \( f(\cdot, v_0) \) is balanced, i.e. \( \int_0^z f(u, v_0) \, du = 0 \), where \( z \) is the largest zero of \( f(\cdot, v_0) \).

When \( \epsilon \) is small and \( d \) is large in the sense \( d = \frac{d_0}{\epsilon} \), a subset \( E \) of \( D \) emerges so that \( u(x) \) of a solution \( (u, v) \) is close to \( z \) if \( x \in E \) and close to 0 if \( x \in D \setminus E \).

To describe \( u \) near \( \partial E \) let \( Q(\xi, s) \) be the traveling wave solution of

\[ Q_{\xi\xi} + c(s)Q_{\xi} + f(Q, s) = 0, \]  

(2)

\[ \lim_{\xi \to -\infty} Q(\xi, s) = 0, \quad \lim_{\xi \to \infty} Q(\xi, s) = \text{largest zero of } f(\cdot, s). \]

The (unknown) constant \( c(s) \) is the velocity of the traveling wave.
Let $d(x)$ be the signed distance function from a point $x$ to $\partial E$. $d(x)$ is positive if $x$ is in $E$ and negative if $x$ is in $D \setminus E$. We assume that approximately

$$u(x) \approx Q\left(\frac{d(x)}{\epsilon}, s\right)$$

where $s$ is constant, discussed later. Insert this $Q$ into the first equation of the GMS system to find

$$Q_{\xi \xi} |\nabla d|^2 + \epsilon Q_{\xi} \Delta d + f(Q, v) = 0.$$ 

It is known that on $\partial E$, $|\nabla d| = 1$ and $\Delta d(x) = \mathcal{H}(x)$ where $\mathcal{H}(x)$ is the mean curvature of $\partial E$ at $x$, viewed from $E$. Therefore we obtain

$$Q_{\xi \xi} + \epsilon \mathcal{H} Q_{\xi} + f(Q, v) = 0.$$ 

Comparing (4) to (2) we deduce

$$c(s) = \epsilon \mathcal{H}, \quad v = s \text{ on } \partial E.$$
Now consider $c(s)$. Unlike $u(x)$, $v(x)$ changes slowly in $x$ so that $v(x) \approx v_0 + \epsilon w(x)$. On the other hand $c(s) = c(v) \approx c(v_0) + \epsilon c'(v_0)w$. Since $v_0$ is the point where $f(\cdot, v_0)$ is balanced, $c(v_0) = 0$. Hence (5) implies that

$$H = c'(v_0)w. \tag{6}$$

It remains to find an equation for $w$. In the second equation of GMS we deduce

$$\frac{d_0}{\epsilon} \Delta(v_0 + \epsilon w) - (v_0 + \epsilon w) + \frac{u^r}{(v_0 + \epsilon w)^s} = 0.$$

As $\epsilon \to 0$, we find

$$d_0 \Delta w - v_0 + \frac{z^r}{v_0^s} \chi_E = 0 \tag{7}$$

where $\chi_E$ is the characteristic function of $E$. 
The equations (6) and (7) form a system for $\partial E$:

$$H = c'(0)w \text{ on } \partial E, \quad d_0 \Delta w - v_0 + \frac{z^r}{v_0^s} \chi_E = 0 \text{ in } D. \quad (8)$$

The Neumann boundary condition for $v$ implies the same boundary condition for $w$ and hence

$$\int_D (-v_0 + \frac{z^r}{v_0^s} \chi_E) \, dx = 0 \implies |E| = \frac{v_0^{s+1}}{z^r} |D|.$$  

Define

$$a = \frac{v_0^{s+1}}{z^r}, \quad \gamma = -\frac{c'(v_0) z^r}{d_0 v_0^s}, \quad (9)$$

to write (8) as

$$H(\partial E) + \gamma(-\Delta)^{-1}(\chi_E - a) = \lambda \quad (10)$$

which holds on $\partial E$. 
Recapitulation.

A physical/biological system occupies a bounded domain $D$ in $\mathbb{R}^n$. Given two parameters: $a \in (0, 1)$ and $\gamma > 0$, find a subset $E$ of $D$ and a constant $\lambda$ such that $|E| = a|D|$, and on $\partial E \cap D$ the equation

$$\mathcal{H}(\partial E) + \gamma(-\Delta)^{-1}(\chi_E - a) = \lambda$$

holds. If $\partial E$ meets $\partial D$, then the two meet orthogonally.

The problem has a variational structure:

$$\mathcal{J}_D(E) = \frac{1}{n-1} \mathcal{P}_D(E) + \frac{\gamma}{2} \int_D |(-\Delta)^{-1/2}(\chi_E - a)|^2 \, dx$$

where $\mathcal{P}_D(E)$ is the perimeter of $E$ in $D$, i.e. the size of $\partial E \cap D$.

Self-organization.

A cross section of a diblock copolymer in the cylindrical phase (TEM micrograph taken by Lewis).

Is there an $E \subset D \subset \mathbb{R}^2$ which is a union of small discs arranged in a hexagonal pattern and solves $\mathcal{H}(\partial E) + \gamma(-\Delta)^{-1}(\chi_E - a) = \lambda$?
**Theorem** (R. and Wei 2007). Let $D \subset \mathbb{R}^2$. Suppose that $K \geq 2$ is an integer, and define $\rho$ by $K \pi \rho^2 = a|D|$.

1. For every $\epsilon > 0$ there exists $\delta > 0$, depending on $\epsilon$, $K$ and $D$ only, such that if $\rho < \delta$, and $\gamma \in \left(\frac{1+\epsilon}{\rho^3 \log \frac{1}{\rho}}, \frac{12-\epsilon}{\rho^3}\right)$, then there exists a stable solution with $K$ discs.

2. Each each is approximately round with the same radius $\rho$.

3. Let the centers of these discs be $\zeta_1, \zeta_2, \ldots, \zeta_K$. Then $(\zeta_1, \zeta_2, \ldots, \zeta_K)$ is close to a global minimum of a function $F$:

$$F(\xi_1, \xi_2, \ldots, \xi_K) = \sum_{k=1}^{K} R(\xi_k, \xi_k) + \sum_{k=1}^{K} \sum_{l=1 \atop l \neq k}^{K} G(\xi_k, \xi_l)$$

where $G$ is the Green’s function of $-\Delta$ on $D$, and $R$ is the regular part of $G$. 

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Numerical calculations. Let $D$ be a unit disc. Then $G$ and $R$ are known explicitly.

The TEM micrograph by Lewis on the left; a numerical minimization of $F$ with $K = 100$ on the right.

A profile problem is needed to isolate each component (an ansatz) from the pattern. It ignores component to component interaction.
A profile problem of mean curvature and Newtonian potential.

Let $m > 0$ and $\gamma > 0$. Find a set $E$ in $\mathbb{R}^n$ and a number $\lambda$ such that $|E| = m$ and

$$\mathcal{H}(\partial E) + \gamma \mathcal{N}(E) = \lambda$$

holds on $\partial E$. $\mathcal{H}(\partial E)$ is the mean curvature of $\partial E$.

$$\mathcal{N}(E)(x) = \begin{cases} \int_{E} \frac{1}{2\pi} \log \frac{1}{|x-y|} \, dy & \text{if } n = 2 \\ \int_{E} \frac{1}{4\pi|x-y|} \, dy & \text{if } n = 3 \end{cases}$$

is the Newtonian potential of $E$. Variational structure:

$$\mathcal{J}(E) = \frac{1}{n-1} \mathcal{P}(E) + \frac{\gamma}{2} \int_{E} \mathcal{N}(E)(x) \, dx, \quad |E| = m.$$  

$\mathcal{P}(E)$ is the perimeter of $E$, i.e. the size of $\partial E$.

The two parameters $m$ and $\gamma$ can be reduced to one. Take $m = 1$ (or any other convenient number).
**Definition.** An ansatz is a solution of the curvature-potential equation, used as a building block for periodic patterns.

Ansätze in $\mathbb{R}^2$:


Ansätze in $\mathbb{R}^3$:

The disc ansatz.

For any $\gamma > 0$ the disc $\{x \in \mathbb{R}^2 : |x| < 1\}$ is a solution of the curvature-potential equation

$$\mathcal{H}(\partial E) + \gamma \mathcal{N}(E) = \lambda.$$ 

The disc is stable if $\gamma \in (0, 12)$ and unstable if $\gamma > 12$.

**Application.** The disc ansatz is used for the construction of the stable multi-disc solution to

$$\mathcal{H}(\partial E) + \gamma (-\Delta)^{-1} (\chi E - a) = \lambda$$

on a bounded domain $D \subset \mathbb{R}^2$.

1. Make $K$ copies of the ansatz, and scale them down so their radii $\sim \rho$.
2. Add a small perturbation to each small disc.
3. Place the perturbed small discs properly in $D$. 

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Ring droplets.

Ring droplets on freshwater ray; the ring ansatz.

**Theorem** (Kang and R. 2009). There exists $\gamma_0 > 0$ such that if $\gamma > \gamma_0$, the curvature-potential equation $\mathcal{H}(\partial E) + \gamma \mathcal{N}(E) = \lambda$ admits a ring shaped ansatz $E = \{x \in \mathbb{R}^2 : R_1 < |x| < R_2\}$ and $|E| = \pi$. The solution is stable if $\gamma > \gamma_1$ and unstable if $\gamma \in (\gamma_0, \gamma_1)$. 
Ring droplet solutions and mixed droplet solutions.

On a bounded domain the geometric problem has ring droplet solutions and solutions of co-existing rings and discs if $a$ small and $\gamma$ is sufficiently large (Kang and R. 2010).

In the first picture, all the rings have approximately the same size and their locations are determined by a minimum of the same $F$ for the disc droplet solutions. In the second picture, the rings and the discs have approximately the same area.
The ball ansatz.

The story in $\mathbb{R}^3$ is more interesting.

For any $\gamma > 0$, the ball $\{x \in \mathbb{R}^3 : |x| < 1\}$ is a solution of

$$\mathcal{H}(\partial E) + \gamma \mathcal{N}(E) = \lambda.$$ 

The ball is stable if $\gamma < 15$.

**Theorem** (R. and Wei 2008). Let $D \subset \mathbb{R}^3$. Suppose that $K \geq 2$ is an integer, and $\rho = (\frac{3a|D|}{4K\pi})^{1/3}$. For every $\epsilon > 0$ there exists $\delta > 0$, depending on $\epsilon$, $K$ and $D$ only, such that a stable solution of $K$ ball droplets exists if $\rho < \delta$ and $\gamma \in \left(\frac{1.5+\epsilon}{\rho^3}, \frac{15-\epsilon}{\rho^3}\right)$.

Again the balls are located at a minimum of the function

$$F(\xi_1, \xi_2, \ldots, \xi_K) = \sum_{k=1}^{K} R(\xi_k, \xi_k) + \sum_{k=1}^{K} \sum_{l=1, l \neq k}^{K} G(\xi_k, \xi_l).$$
The shell ansatz.

**Theorem** (R. 2009). There exists $\gamma_0 > 0$ such that the curvature-potential equation has a shell ansatz solution of the volume $\frac{4\pi}{3}$ when $\gamma > \gamma_0$.

The shell ansatz is unstable for all $\gamma > \gamma_0$. 
The toroidal tube ansatz.

Toroidal objects are fascinating. Known as the vortex ring in fluid dynamics, it is a region of rotating fluid where the flow pattern takes on a toroidal shape.

In a quantum fluid, a vortex ring is formed by a loop of poloidal quantized flow pattern. It was detected in superfluid helium by Rayfield and Reif, and more recently in Bose-Einstein condensates by Anderson, et al.

In 2004 Pochan, et al, found a toroidal morphological phase in a triblock copolymer.
An illustration of a toroidal supramolecule assembly.
Theorem (R. and Wei). When $\gamma$ is sufficiently large, the curvature-potential equation $\mathcal{H}(\partial E) + \gamma \mathcal{N}(E) = \lambda$ has an approximately torus shaped, tube like solution in $\mathbb{R}^3$ of volume 1.
Define a function $f = f(\gamma)$ via its inverse

$$\gamma = \frac{2}{f^3 \log \frac{1}{2\pi^2 f^3}}, \quad \lim_{\gamma \to \infty} f(\gamma) = 0.$$ 

Let $p$ and $q$ be the two radii of the torus $(p > q)$. Then $2\pi^2 pq^2 = 1$ and

$$\lim_{\gamma \to \infty} \frac{q}{f(\gamma)} = 1 \quad \text{and} \quad \lim_{\gamma \to \infty} 2\pi^2 f^2(\gamma)p = 1$$

A cross section of this ansatz is only approximately a round disc. The ansatz is not a perfect torus.
Double tori.

**Theorem** (R. and Wei). The curvature-potential equation has a disconnected solution of two approximate tori of combined volume 2 in $\mathbb{R}^3$, if $\gamma$ is sufficiently large.
Let $p_1$ and $q_1$ be the larger and the smaller radii of the inner torus and $p_2$ and $q_2$ be the two radii of the outer torus. Then

$$\lim_{\gamma \to \infty} \frac{q_j}{f(\gamma)} = 1 \quad \text{and} \quad \lim_{\gamma \to \infty} 2\pi^2 f^2(\gamma)p_j = \Pi_j, \quad j = 1, 2.$$

Here $(\Pi_1, \Pi_2)$ is a minimum of the function

$$(P_1, P_2) \to \sum_{j=1}^{2} \left( \frac{P_j}{16} + \frac{\pi P_j}{2} G_1(P_j, 0, P_j, 0) \right) + \pi P_1 G(P_1, 0, P_2, 0).$$

In this function $G$ is the kernel of the Newtonian potential operator for axisymmetric sets in the cylindrical coordinates, and $G_1$ is the second term in the expansion about the singularity of $G$:

$$G(r, z, s, t) = \frac{s}{4\pi} \int_0^{2\pi} \frac{d\sigma}{\sqrt{r^2 + s^2 - 2rs \cos \sigma + (z - t)^2}}$$

$$= \frac{1}{2\pi} \log \frac{1}{| (r, z) - (s, t) |} + G_1(r, z, s, t).$$
A ball and a torus.

Theorem (Pan and R.). The curvature-potential equation in $\mathbb{R}^3$ admits a solution of volume 1, which is the union of an approximate ball and an approximate torus, when $\gamma$ is sufficiently large.

Let $l$ be the radius of the ball, and $p$ and $q$ be the two radii of the torus $(p > q)$. Then $\frac{4\pi l^3}{3} + 2\pi^2 pq^2 = 1$ and

$$\lim_{\gamma \to \infty} \frac{l}{f(\gamma)} = \frac{2}{3}, \quad \lim_{\gamma \to \infty} \frac{q}{f(\gamma)} = 1, \quad \lim_{\gamma \to \infty} 2\pi^2 f^2(\gamma)p = 1.$$
Stability.

A: axi-symmetry about the $z$-axis.

M: mirror-symmetry about the $xy$-plane.

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The non-saturation Gierer-Meinhardt system.

Gierer-Meinhardt system without saturation in $\mathbb{R}^3$:

$$
\epsilon^2 \Delta u - u + \frac{u^p}{v^q} = 0; \quad \Delta v - v + \frac{u^r}{v^s} = 0.
$$

Here $p$, $q$, $r$, and $s$ are positive, and satisfy $0 < \frac{p-1}{q} < \frac{r}{s+1}$.

In one dimension, there are solutions that look like spikes. The activator $u$ concentrates at certain points and is exponentially small away from such points (Wei 1999, Iron, Ward, and Wei 2001).

In two dimensions, spike solutions exist. Their stability and dynamics have been studied (Wei and Winter 1999-2002, Ward, McInerney, Houston, Gavaghan, and Maini 2002).
On the other hand, less is known about the GM model in three or higher dimensions.

For example, the existence of a single spike solution on $\mathbb{R}^3$ is a long-standing open problem.

The only result, before our work, in three dimensions so far is the existence of shell solutions, which are radial solutions that concentrate on two-dimensional spheres (Ni and Wei 2006, Kolokolnikov and Wei 2008).
The smoke-ring.

Before our work solutions found on $\mathbb{R}^3$ were either radially symmetric, or were trivial extensions to $\mathbb{R}^3$ of solutions found on $\mathbb{R}$ and $\mathbb{R}^2$.

We present a non-radial, axisymmetric three dimensional solution: a smoke-ring solution. The activator $u$ concentrates on a circle in $\mathbb{R}^3$. 

![Diagram of a smoke-ring solution in 3D space]
**Theorem** (Kolokolnikov and R.) Consider

\[
e^2 \Delta u - u + \frac{u^2}{v} = 0, \quad \Delta v - v + u^2 = 0, \quad \text{in } \mathbb{R}^3.
\]

If \( \epsilon \) is sufficiently small, the system admits a smoke-ring shaped solution on \( \mathbb{R}^3 \), i.e. a solution whose activator component concentrates on a circle.

The radius \( l \) of the circle is determined from

\[
1 - 2l \int_0^1 \frac{\exp(-2l\tau)}{\sqrt{1 - \tau^2}} d\tau = \frac{\int_0^\infty (\int_0^\rho w^3(t)tdt)w^2(\rho)\rho d\rho}{2\left(\int_0^\infty w^3(\rho)\rho d\rho\right)\left(\int_0^\infty w^2(\rho)\rho d\rho\right)}
\]

where \( w \) is the positive radial solution in \( \mathbb{R}^2 \) of

\[
\Delta w - w + w^2 = 0, \quad \lim_{|x| \to \infty} w(|x|) = 0.
\]