Ansatz solutions to a problem of mean curvature and Newtonian potential

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Morphogenesis in development.

The Gierer-Meinhardt system with saturation.

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

$$\epsilon^2 \Delta u - u + \frac{u^p}{(1+\kappa u^p)v^q} = 0; \quad d\Delta v - v + \frac{u^r}{v^s} = 0$$

on a domain D with the Neumann boundary condition

$$\frac{\partial u}{\partial \nu}\Big|_{\partial D} = 0; \quad \frac{\partial v}{\partial \nu}\Big|_{\partial D} = 0.$$

$\kappa = 0$: 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.

One interface radial solution of GMS: del Pino (1994), Sakamoto and Suzuki (2004).

Reduction to a nonlocal geometric problem.

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

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 ϵ is small and d is large in the sense $d = \frac{d_0}{\epsilon}$, a subset E of D emerges so that solutions $(u(x), v(x))$ of GMS satisfy

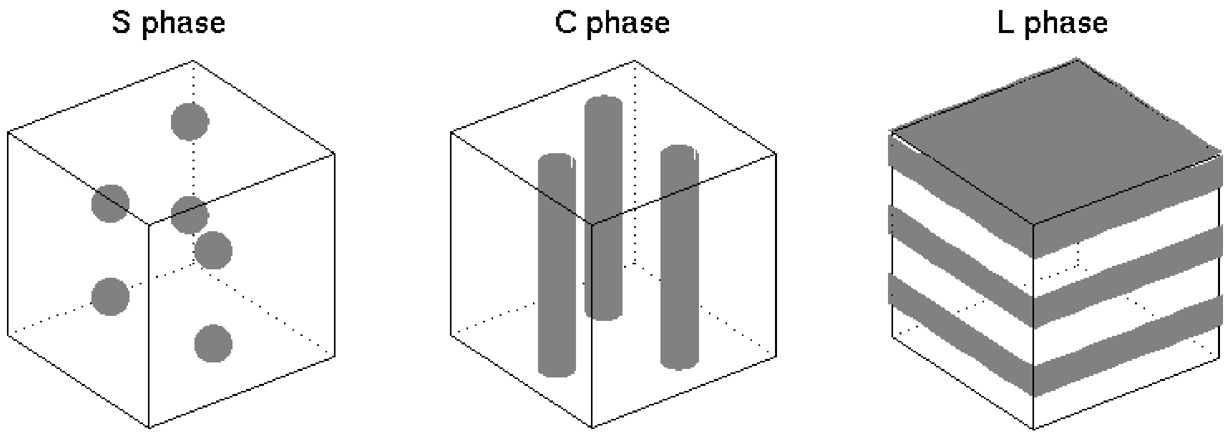
$$(u(x), v(x)) \to (z\chi_E(x), v_0) \text{ as } \epsilon \to 0.$$

On ∂E the equation

$$\mathcal{H}(\partial E) + \gamma(-\Delta)^{-1}(\chi_E - a) = \lambda \tag{2}$$

holds, and $|E| = a|D|$. Here $a \in (0,1)$ and $\gamma > 0$ are derived from the parameters of GMS.

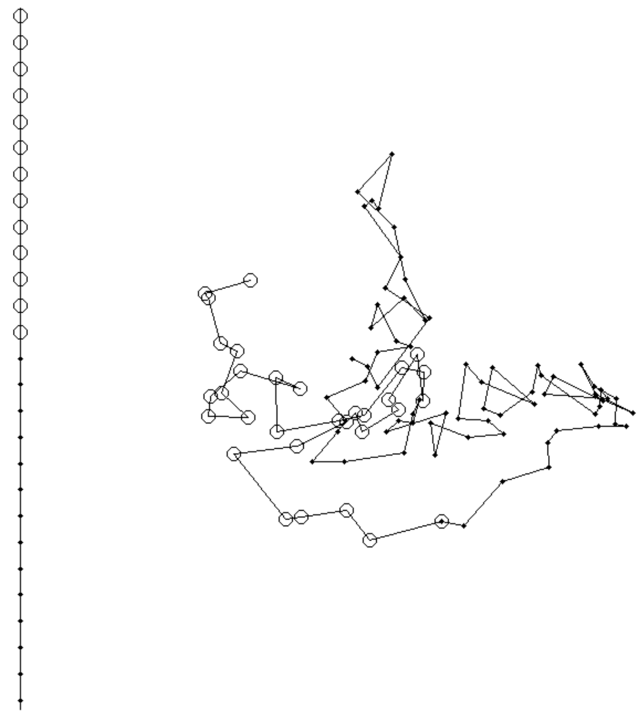
Morphological phases in diblock copolymers.



S, C, L phases appear as the monomer composition parameter a increases from 0 to 1/2. They repeat as a moves from 1/2 to 1 with the colors reversed.

Diblock copolymers.

Soft materials, fluid-like disorder on the molecular scale, a high degree of order at longer length scales. $a = \frac{N_A}{N_A + N_B}$.



The Ohta-Kawasaki theory (1986).

The free energy of a diblock copolymer melt (formulated by Nishiura and Ohnishi 1995):

$$\mathcal{I}_{D,\epsilon}(u) = \int_D [\frac{\epsilon^2}{2}|\nabla u|^2 + W(u) + \frac{\epsilon\gamma}{2}|(-\Delta)^{-1/2}(u-a)|^2]$$

$$u \in W^{1,2}(D), \quad \overline{u} := \frac{1}{|D|}\int_D u = a$$

u, $1-u$: The relative densities of the A and B monomers.
0 and 1: Two pure monomer states.
W: A balanced double-well function with global minimum value 0 at 0 and 1, e.g. $W(u) = (1/4)u^2(1-u)^2$.
$(-\Delta)^{-1/2}$: $-\Delta$ has the Neumann boundary condition.
ϵ: A small parameter $\sim$ thickness of interfaces.
γ: A parameter $\sim$ the size of the sample.

The Γ-limit.

The Γ-convergence theory (De Giorgi 1975, Modica and Mortola 1977, Modica 1987, and Kohn and Sternberg 1989) is readily applicable. The Γ-limit of $\epsilon^{-1}\mathcal{I}_{D,\epsilon}$ is $\mathcal{J}_D$ given before.

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

$$\chi_E \in BV(D), \ |E| = a|D|$$

Note that u now is replaced by χ_E. $\tau = \int_0^1 \sqrt{2W(s)}\, ds$. In this talk we take $\tau = \frac{1}{n-1}$.

Euler-Lagrange equation:

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

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 λ 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 ∂E meets ∂D, then the two meet orthogonally.

The problem has a variational structure:

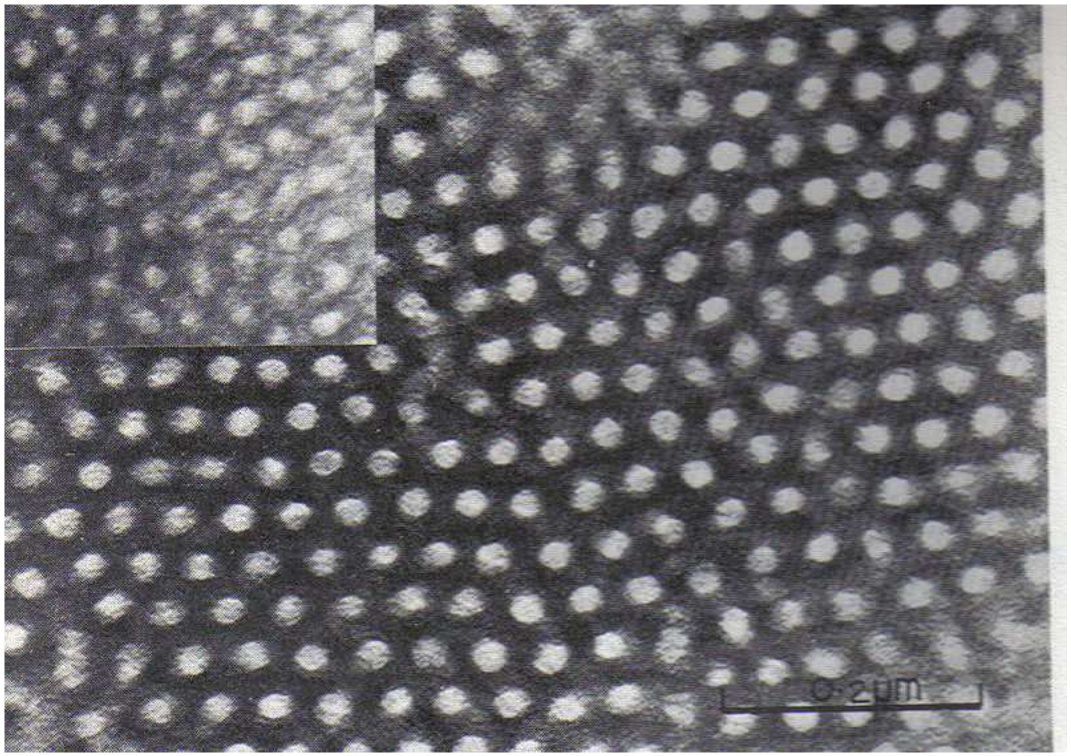
$$\mathcal{J}_D(E) = \frac{1}{n-1}\mathcal{P}_D(E) + \frac{\gamma}{2}\int_D |(-\Delta)^{-1/2}(\chi_E - a)|^2 \, dx$$

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

References. One dimensional case: R. and Wei 2000; Fife and Hilhorst 2001. Global minimizers in higher dimensions: Alberti, Choksi, and Otto 2009; Muratov; Sternberg and Topaloglu 2011.

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 ρ by $K\pi\rho^2 = a|D|$.

1. For every $\epsilon > 0$ there exists $\delta > 0$, depending on ϵ, 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.

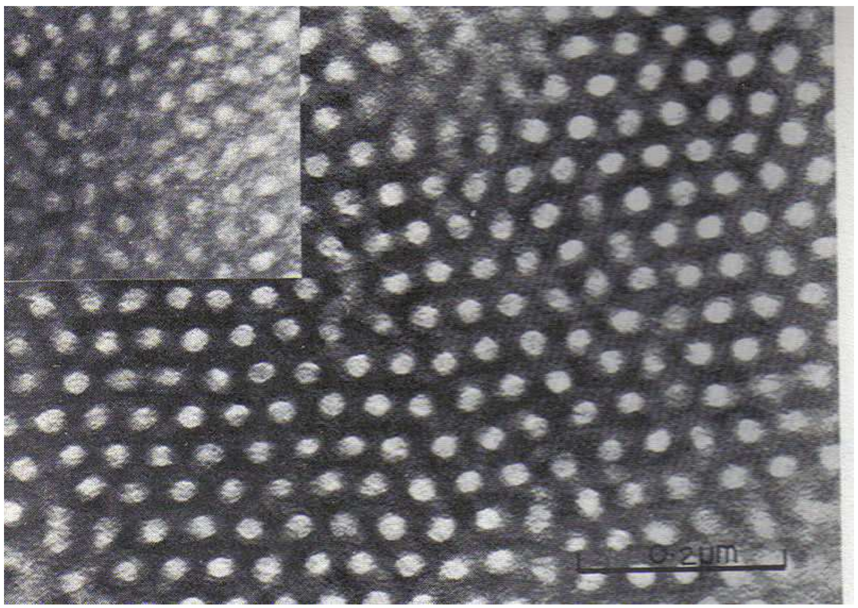
2. Each disc is approximately round with the same radius ρ.

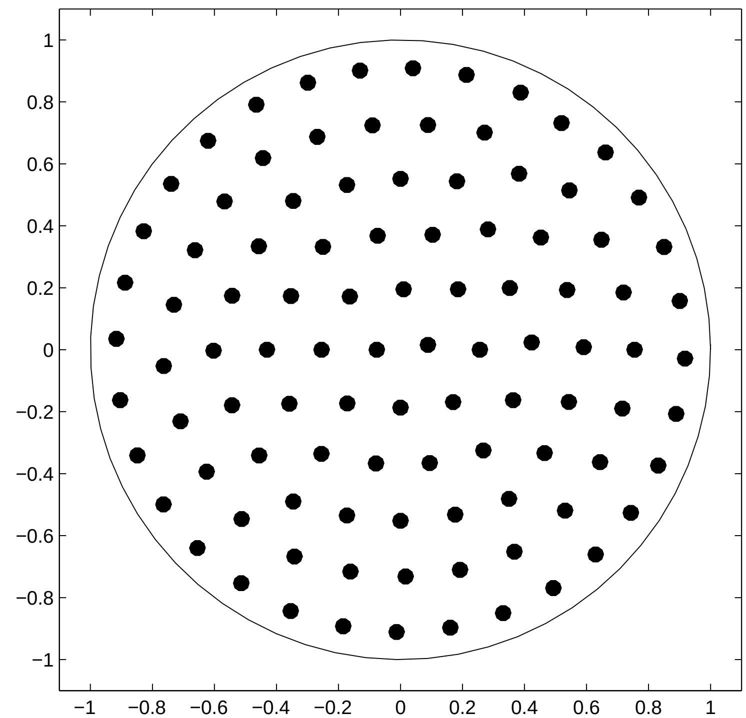
3. Let the centers of these discs be ζ_1, ζ_2, ..., ζ_K. Then $(\zeta_1, \zeta_2, ..., \zeta_K)$ is close to a global minimum of a function F:

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

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

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. Only self-interaction is considered.

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 λ such that $|E| = m$ and

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

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

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

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 ∂E.

The two parameters m and γ 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.

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 $D \subset \mathbb{R}^2$ (R. and Wei 2007).

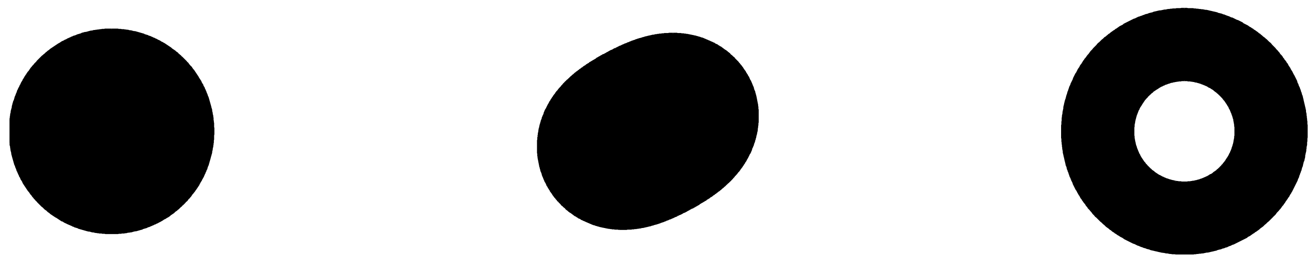
1. Make K copies of the ansatz, and scale them down so their radii $\sim \rho$.

2. Add a small perturbation to each small disc.

3. Place the perturbed small discs properly in D.

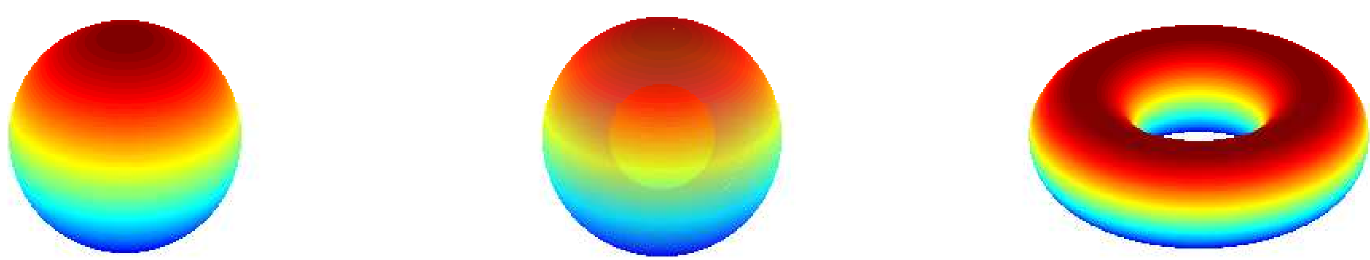
Ansatze in $\mathbb{R}^2$:

1. Disc ansatz, 2. Oval ansatz, 3. Ring ansatz.

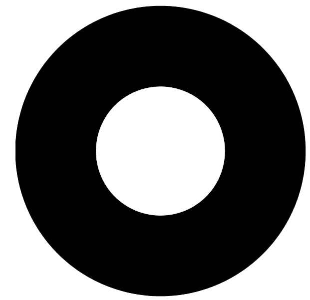


Ansatze in $\mathbb{R}^3$:

1. Ball ansatz, 2. Shell ansatz, 3. Toroidal ansatz.



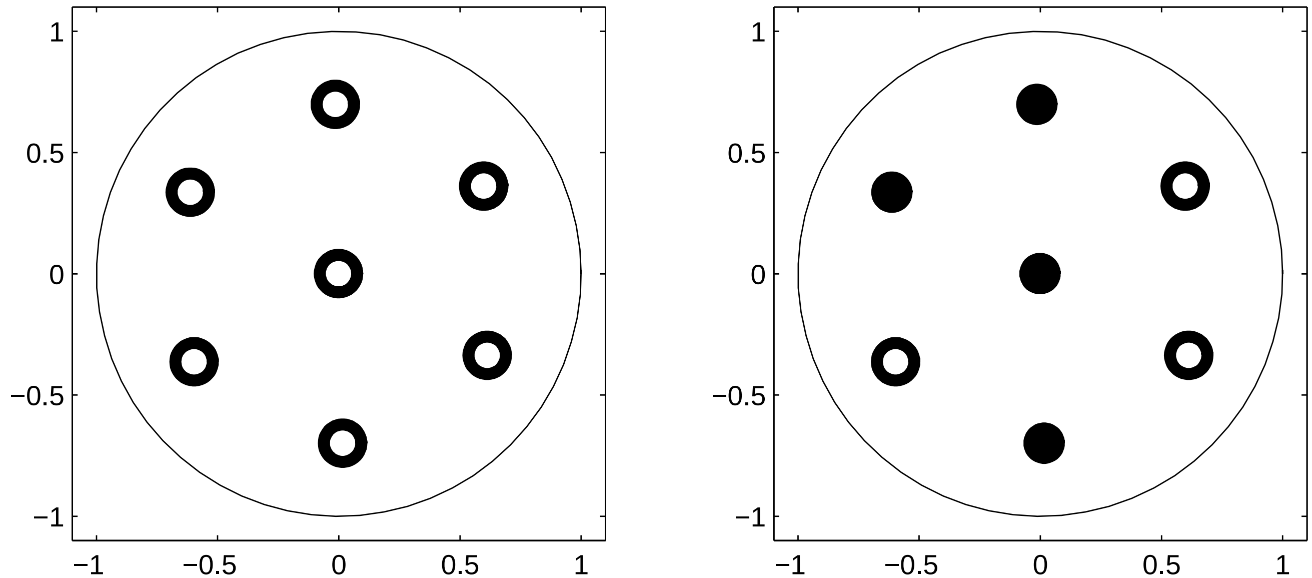
Ring droplets.



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 γ 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.

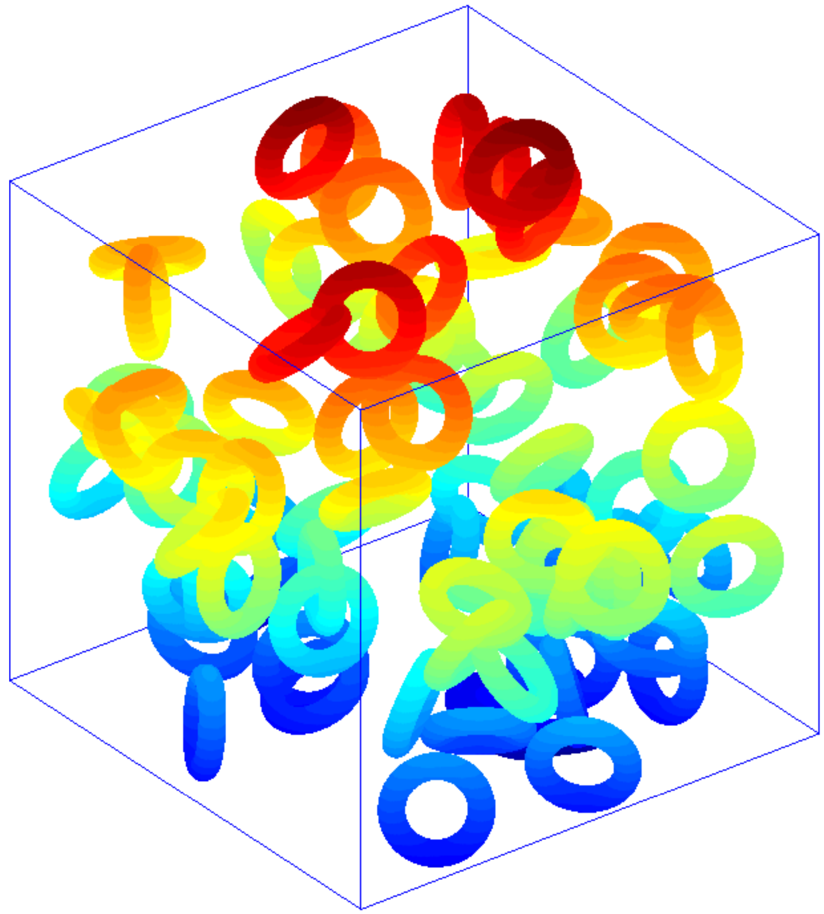
The toroidal tube ansatz.

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.

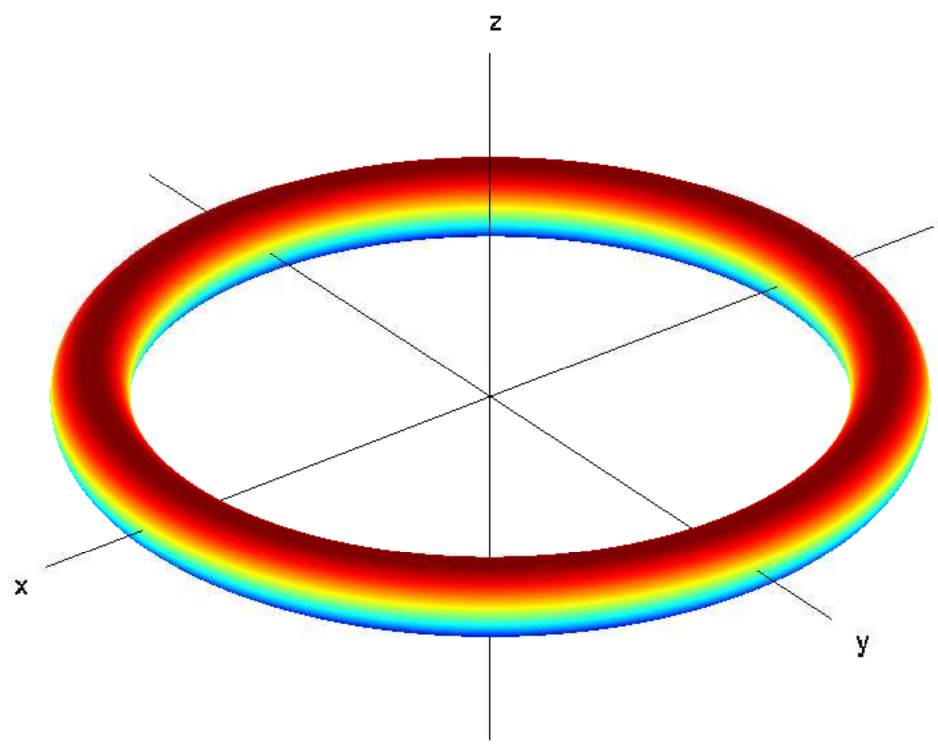
In a quntuam fluid, a vortex ring is formed by a loop of poloidal quantized flow pattern. It was detected in superfluid helium by Rayfield and Reif, and more recently in Bose-Einstein condensates by Anderson, *et al*.

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 2011). When γ 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

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

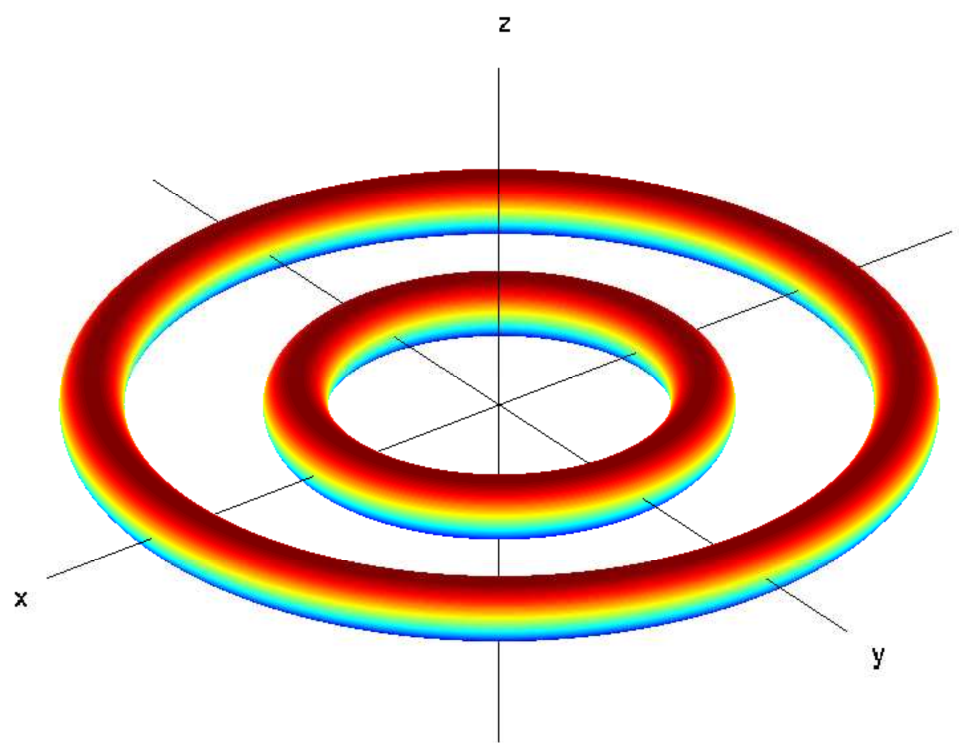
Let p and q be the two radii of the torus ($p > q$). Then $2\pi^2 pq^2 = 1$ and

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

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 γ 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 (Π_1, Π_2) is a minimum of the function

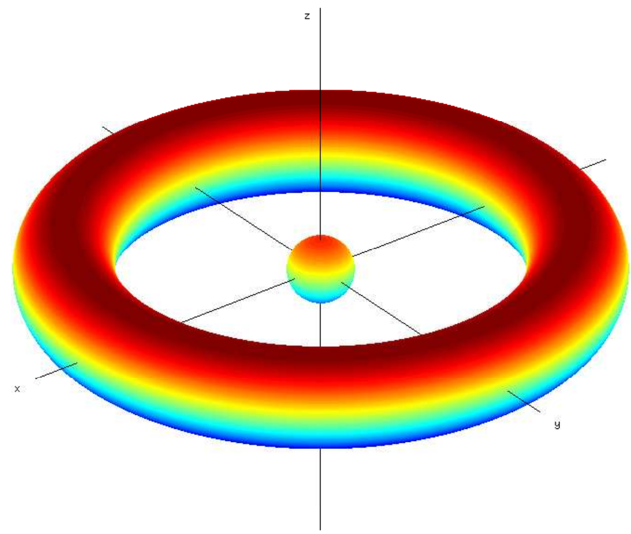
$$(P_1, P_2) \to \sum_{j=1}^{2} \Big(\frac{P_j}{16} + \frac{\pi P_j}{2} G_1(P_j, 0, P_j, 0) \Big) + \pi P_1 G(P_1, 0, P_2, 0).$$

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:

$$\begin{aligned} G(r, z, s, t) &= \frac{s}{4\pi} \int_0^{2\pi} \frac{d\sigma}{\sqrt{r^2 + s^2 - 2rs\cos\sigma + (z-t)^2}} \\ &= \frac{1}{2\pi} \log \frac{1}{|(r, z) - (s, t)|} + G_1(r, z, s, t). \end{aligned}$$

A ball and a torus.

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

Solutions	Stability	A Stability	A+M Stability
Torus	?	Yes	Yes
Double Tori	No	No	Yes
Ball-Torus	No	No	No