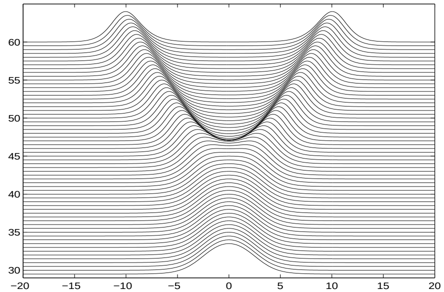
A simple model of self-replication



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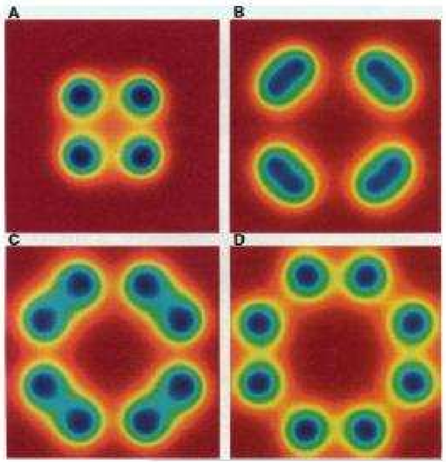
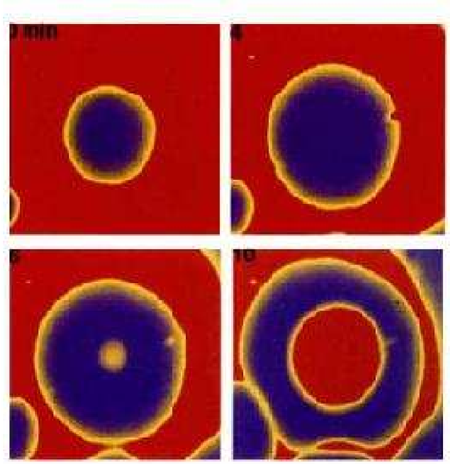
Introduction

- In 1993, Pearson reported self-replicating spots in the Gray-Scott model [J.E. Pearson, Science, 261, 189 (1993)].

- Experiments using Ferrocyanide-iodate-sulphite reaction (which GS models) confirmed numerical observation [Lee et.al, Nature, 1994].



Pearson (1993, numerics)



Lee et.al. (1994, lab)

- Self-replication was found in many other models, including chemial reactions, material science and nonlinear optics.

Autonomous models

- **Simplest model:**
$$u_t = \varepsilon^2 \Delta u - u + u^p \tag{1}$$
  - Admits a steady-state spot-solution with $u \to 0$ as $|x| \to \infty$
  - Spot solution is ***unstable*** in time
  - ***No self-replication*** is possible

- **Shadow system:**
$$u_t = \varepsilon^2 \Delta u - u + \frac{u^p}{\int u^{p+1}} \tag{2}$$
  - Occurs naturally as a limiting case for GS model in the low-feed regime
  - Steady state is the same as for (1)
  - The nonlocal term $\int u^{p+1}$ ***stabilizes*** the ground state
  - ***No self-replication*** is possible

Gray-scott model

- Models a chemical reaction

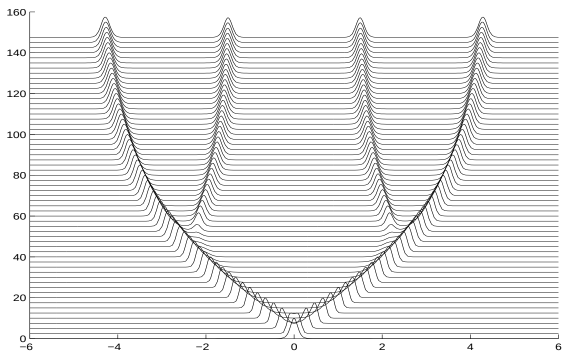
- Consists of a ***system***

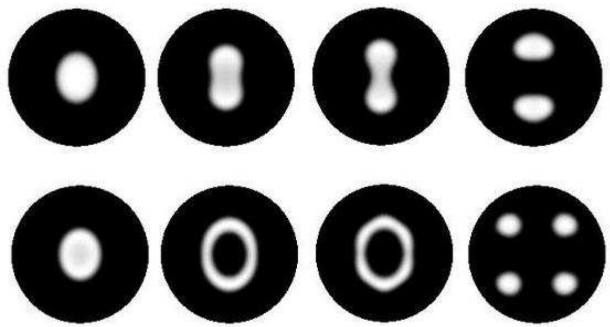
$$\begin{cases} u_t = D_v \Delta u - (F + k)u + vu^2 \\ v_t = D_u \Delta v + F(1 - v) + vu^2 \end{cases}$$

- Self-replication reduces to study a fully-coupled 4-th order ODE:

$$\begin{cases} \Delta U - U + U^2 V = 0 \\ \Delta V - U^2 V = 0 \\ V'(0) = 0 = U'(0), \quad V'(\infty) = B \end{cases}$$

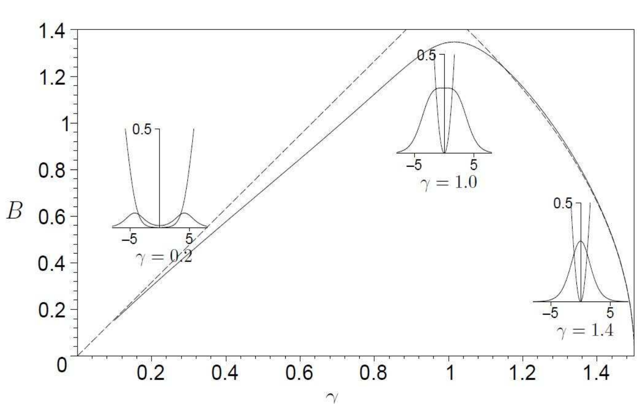
- Replication has been observed in 1D and 2D (two different types):

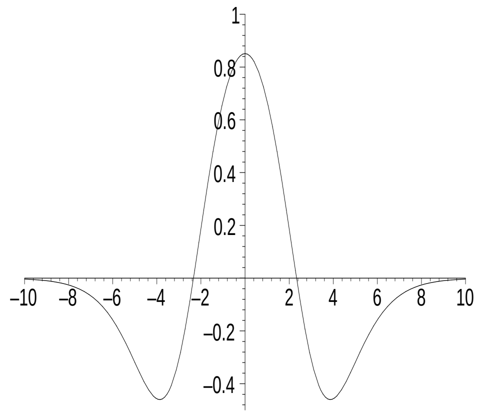




Criteria for self-replication

- Four criteria, proposed by Nishiura and Ueyema (1999):
  1. The disappearance of the ground-state solution due to a fold point.
  2. The existence of a ***dimple eigenfunction*** at the fold point, responsible for the initiation of the self-replication process.
  3. Stability of the steady-state solution on one side of the fold point.
  4. The alignment (or cascade) of the fold points for K spots.
- Verification of these conditions is usually done numerically
- Analytic verificationis an open problem for the GS model; order too high.





Simpler self-replication model in $\mathbb{R}^N$

$$u_t = \Delta u - u + \frac{(1 + a|x|^q)\, u^p}{\int_{\mathbb{R}^N} (1 + a\,|x|^q)\, u^{p+1}}; \quad \nabla u(0,t) = 0 \tag{3}$$

- Reduces to the shadow model for $a = 0$
- Steady state satisfies (after rescaling):

$$0 = u_{rr} + \frac{N-1}{r} u_r - u + (1 + ar^q)\, u^p; \;\; u'(0) = 0, \;\; u > 0 \tag{ss}$$

- Existence of ground state depends on a, q, p
- ***Main result:*** Self-replication occurs if a is gradually increased from 0, provided that

$$p > 1 \text{ and } \; q > \frac{(p-1)N}{2} \text{ if } N = 1 \text{ or } 2$$
$$1 < p < \frac{N+2}{N-2} \text{ and } q > \frac{(p-1)(N-1)}{2} \text{ if } N \geq 3.$$

Bifurcation structure in 1-D $(p = 2)$

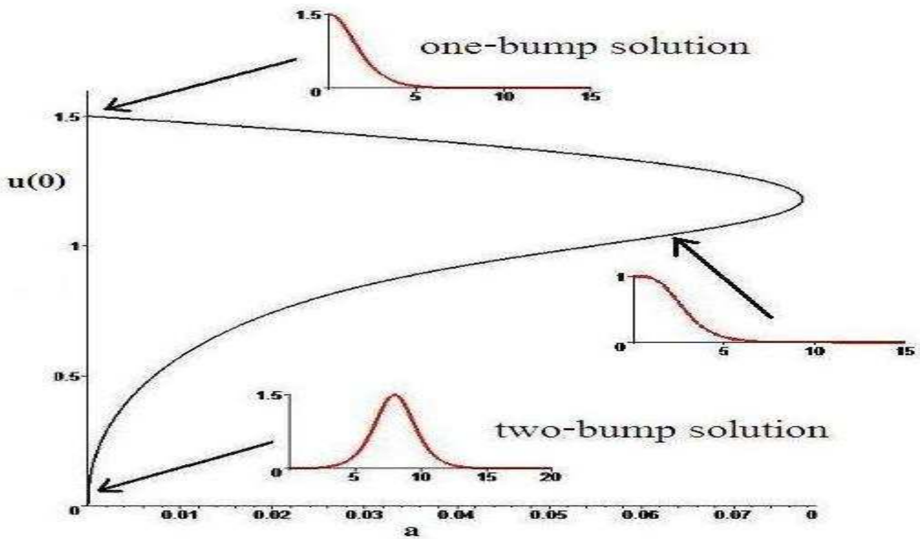
- If $a = 0$ then $u_{rr} - u + u^2 = 0$, there exists a ***unique*** ground-state solution,

$$u(0) = \frac{3}{2}\text{sech}^2\left(\frac{r}{2}\right) \tag{B1}$$

- When $0 < a \ll 1$, there exist ***many*** solutions consisting of 1, 2, 3, ... bumps. A one-bump solution is given by (B1). A ***two-bump*** solution is

$$u(r) \sim \frac{3}{2}\text{sech}^2\left(\frac{r - r_0}{2}\right) \qquad \text{where} \qquad \frac{e^{-2r_0}}{r_0^{q-1}} \sim \frac{aq}{30}.$$

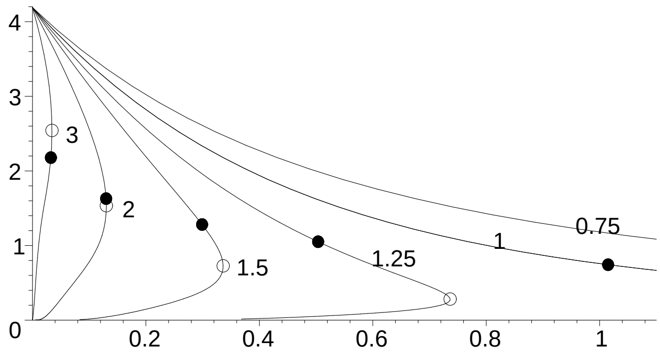
- Two-bump solution connects to one-bump solution in a fold-point bifurcation. This is the ***first condition for self replication.***



Bifurcation structure in $N \geq 3$

Main result:

1. If $q > \frac{(N-1)(p-1)}{2}$, there is a solution with $a \ll 1$, $u(0) \ll 1$ given by
$$u(r) \sim Cw\left(r - r_0\right) \text{ where } r_0 = \left(\frac{1}{a}\right)^{1/q} \left(\frac{(N-1)(p-1)}{2q - (N-1)(p-1)}\right)^{1/q}$$
where $w'' - w + w^p = 0$ is a 1-D ground state, C some constant.
2. If $q < \frac{(N-1)(p-1)}{2}$, there is a solution for $a \gg 1$ (no fold point)
3. If $q = \frac{(N-1)(p-1)}{2}$, there is a solution with $a \gg 1$, $u(0) \ll 1$ given by
$$u(r) \sim Cw\left(r - r_0\right) \text{ where } r_0 = O\left(\ln a\right)$$



$p = 2, \quad q$ as indicated

Main theorem about steady states of

$$u_{rr} + \frac{N-1}{r} u_r - u + (1 + ar^q) u^p, \quad u'(0) = 0, \quad u > 0 \qquad \text{(ss)}$$

(i) There exists a constant C such that $a < C$ provided that

$$q > \begin{cases} \frac{(p-1)(N-1)}{2}, & \text{if } N \geq 3 \\ \frac{(p-1)N}{2}, & \text{if } N = 1, 2 \end{cases} \qquad (4)$$

(ii) If $N \geq 3$ then the solution to (ss) exists for all $a \geq 0$ provided that

$$\left(\frac{N-2}{2}\right)\left(p - \frac{N+2}{N-2}\right) < q < \frac{(p-1)(N-1)}{2} \quad \text{and} \quad q \geq 0 \qquad (5)$$

- (i) shows that there is a fold point when (4) holds
- (ii) is a generalization of [Ding-Ni, 1986] (they show (ii) when $p < \frac{N+2}{N-2}$).
- Note that solution can exist even if $p > \frac{N+2}{N-2}$, e.g. $N = 3, \; p = 6, \; 1/2 < q < 6.$
- ***Open question:*** in 1D, numerics indicate fold point exists for all $q > 0$; but we can prove it only for $q > (p-1)/2.$
- ***Open question:*** in 3D, numerics indicate fold point ***does not*** exist when (ii) holds; but can only prove some special subcases.

Sketch of proof

- **Step 1:** To show $u(0)$ is bounded, we study the limiting ODE

$$u_{rr} + \frac{N-1}{r} u_r + r^q u^p = 0 \tag{6}$$

ODE (6) has a scaling symmetry and phase plane analysis can be used.

- **Step 2 [non-existence]:** Taking limit $a \to \infty$ and rescaling, we get

$$u_{rr} + \frac{N-1}{r} u_r - u + r^q u^p = 0 \tag{7}$$

Usual Pohozhaev identity: multiply by $r u_r$ and integrate. Then we get $q < \frac{(p-1)N}{2}$. This is not enough!

New identity (for radial solutions with $N \geq 3$ only): Multipy by u_r and integrate. Then we get $q < \frac{(p-1)(N-1)}{2}$.

- **Step 3:** If no solution when $a = \infty$ then no solution for large a.

- **Step 4 [existence if $q > \frac{(p-1)(N-1)}{2}$]:** Generalization of [Ding-Ni 1986] result using generalized Sobolev exponent.

Corrollary: Nishiura-Ueyema condition 1

- For $N = 1$: multi-bump solutions exist for all $q > 0$; ***there is always a fold point if*** $q > (p-1)/2$;
- For $N \geq 3$: multi-bump solutions exist and ***there is always a fold point if*** $q > \frac{(N-1)(p-1)}{2}$
- Conjecture: fold point exists iff there are multi-bump solutions [this is proved for $N \geq 3$; still open for $N = 1, 2$].

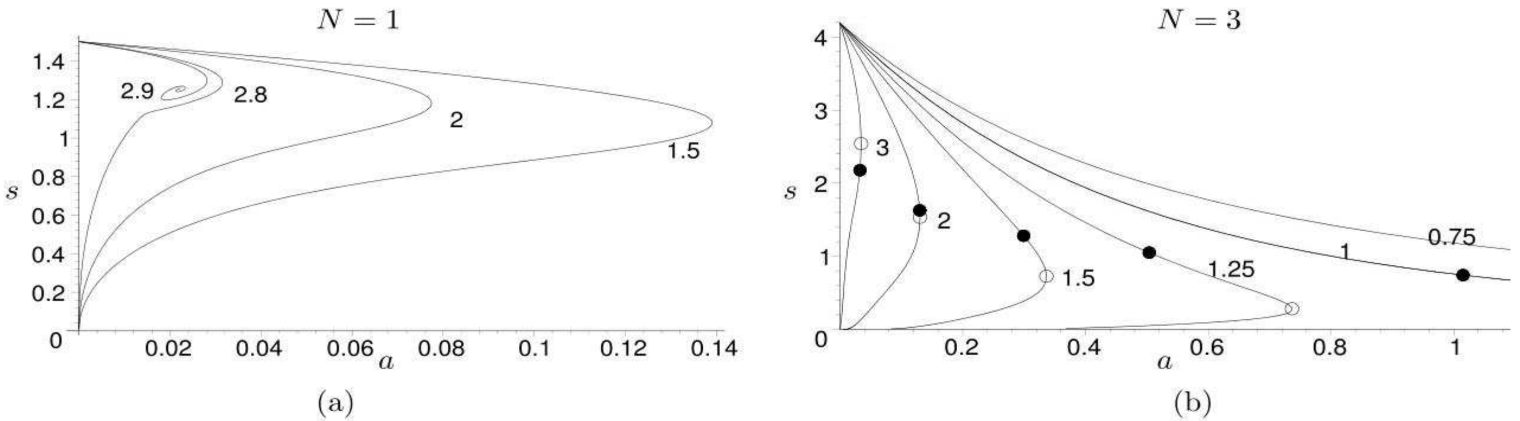


FIGURE 2. Bifurcation diagram for (4) of a vs. $s = u(0)$ with $p = 2$ and for several different values of q as indicated. **(a)** $N = 1$. There is a fold point for all values of q. The bifurcation graph changes its topology at around $q = 2.8$, but is bounded for all q. **(b)** $N = 3$. Fold point is indicated by an empty circle. Nonradial instability threshold is indicated with filled circle. If $q > 2.1$ then fold-point instability dominates. If $q < 2.1$ then non-radial instability dominates. The fold point exists if $q > 1$; the bifurcation graph is unbounded if $q < 1$.

Radial stability

- Consider a more general model

$$u_t = \Delta u - u + u^p h(x;a) \frac{1}{\int u^{p+1} h(x;a)}$$

(where $h(x;a) = 1 + a\,|x|^q$).

- The stability problem leads to ***Non-local Eigenvalue Problem***:

$$\lambda Z = LZ - u^p h(p+1) \int Z u^p h. \qquad \text{(NLEP)}$$

where $LZ := \Delta Z - Z + u^{p-1} h p Z$.

- The ***local*** problem

$$\lambda Z_0 = LZ \qquad \text{(LEP)}$$

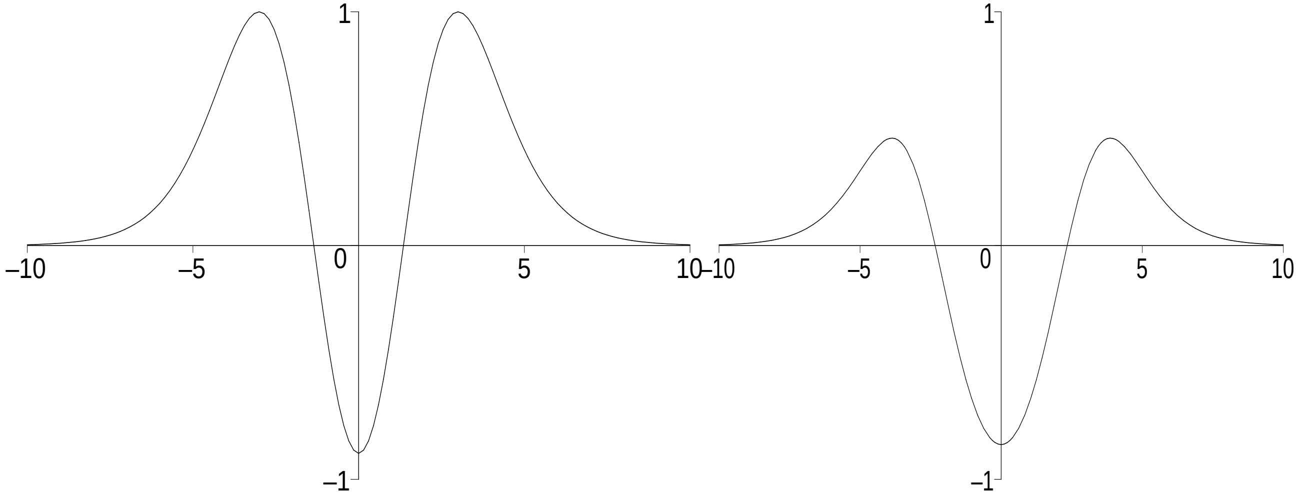
has an unstable eigenvalue $\lambda_0 > 0$.

- The ***nonlocal*** term $\int Z u^p h$ in (NLEP) stabilizes λ_0 [Similar to shadow model].

- Let $s(a) = u(0; a)$, then

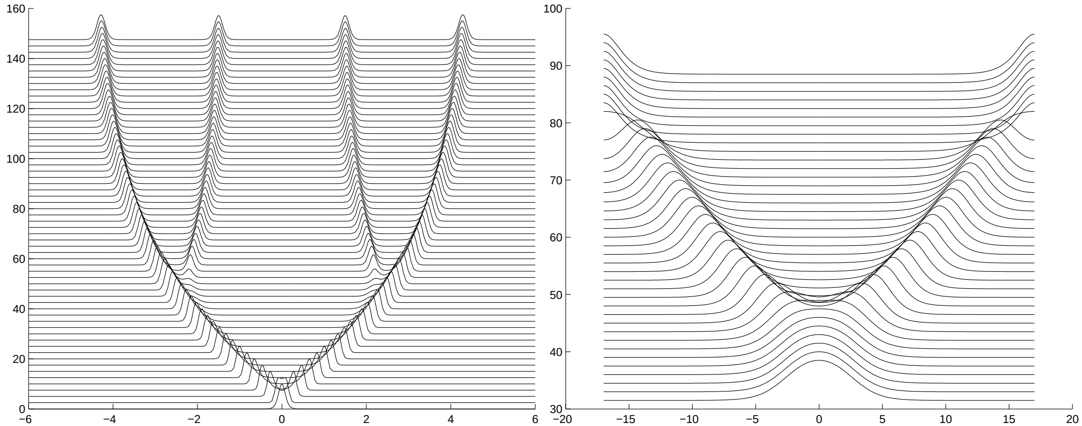
$$L\left(\frac{\partial u}{\partial s}\right) = -u^p h_a \frac{\partial a}{\partial s}. \tag{8}$$

- In fact, $\int \frac{\partial u}{\partial s} u^p h = 0$ [follows by integration by parts] so that $\frac{\partial u}{\partial s}$ ***is an eigenfunction of (NLEP) corresponding to zero eigenvalue at the fold point*** when $\frac{\partial a}{\partial s} = 0$.
- ***Main result:*** (NLEP) is stable w.r.t. radial functions iff (LEP) admits exactly one unstable eigenvalue. So the steady state is stable on one side of the fold point, unstable on the other. This verifies Nishiura-Ueyema condition 3
- Since $\int u_s u^p h = 0$ and $u, h > 0$, u_s must have a positive root. Thus ***eigenfunction at the fold point has a dimple shape.*** This verifies Nishiura-Ueyema condition 2



Dimple eigenvalue for simplified model (left) and for GS model (right)

Comparison with GS model



Left: GS model. Right: Simplified model.

- GS model: a cascade of self-replication events, resulting in multiple interior spikes.
- Simplified model: only one self-replication event; the spike moves to and merges with the boundary.
- Initial stages of self-replication mechanism are similar for the two models.

Nonradial stability $(N = 3)$

- Using spherical coordinates we decompose

$$Z(x, y, z) = \Phi(r) Y_l^m(\theta, \phi); \; l = 0, 1, \ldots; \quad m = 0, \pm 1 \ldots \pm l$$

where Y_l^m are the spherical harmonics.

- For $l \geq 2$, The nonlocal term in (NLEP) disappears since $\int hZu^{p-1} = 0, \; l \geq 2$ and we get

$$\lambda_l \Phi = \Phi_{rr} + \frac{2}{r}\Phi_r - \frac{\gamma}{r^2}\Phi - \Phi + phu^{p-1}\Phi; \qquad \gamma = l(l+1), \; l \geq 2. \qquad \text{(NREP)}$$

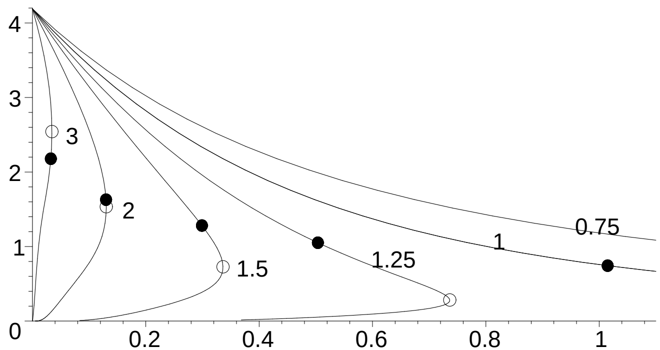
- In the threshold case $q = p - 1$ and $a \gg 1$,

$$u(r) \sim Cw\left(r - r_0\right) \text{ where } r_0 = O\left(\ln a\right)$$

so that (NREP) becomes (LEP):

$$\lambda_l \Phi \sim \Phi_{rr} - \Phi + phu^{p-1}\Phi$$

which is ***unstable!***



Threshold case: $N = 3,\ q = p - 1$

- Nonradial instability exists if $a \gg 1$; need to show the system is radially stable.

- Non-degeneracy: radial instability can only occur at the fold point.

- Uniqueness of steady state $\implies$ no fold point $\implies$ non-radial bifurcation

- For the case $N = 3, p = 2, q = 1$, can use theorem of [Kam-Li, Trans. AMS. 1992]: Solution to $v_{ss} + F(s)v + v^p = 0$ is unique if $F(s)$ is Λ-shaped.

- Can transform (ss) to get

$$F(r) = \left(g'' + \frac{N-1}{r} g' - g\right) g^3 r^{2(N-1)}; \quad g = h^{\frac{1}{-3-p}} r^{\frac{2(N-1)}{-3-p}}.$$

- In case $h = 1 + ar$, $F' = 0 \iff 25r^4a^2 + 50r^3a - \left(75a^2 - 50\right) r^2 - 45ar - 12 = 0.$

- By Descartes rule of signs, there is only one root $\implies$ F is Λ-shaped $\implies$ uniqueness.

- Remark: This method does not for general $p > 1, q = p - 1$, though numerics indicate solution is still unique.

Radial vs. nonradial instability, $N = 3$

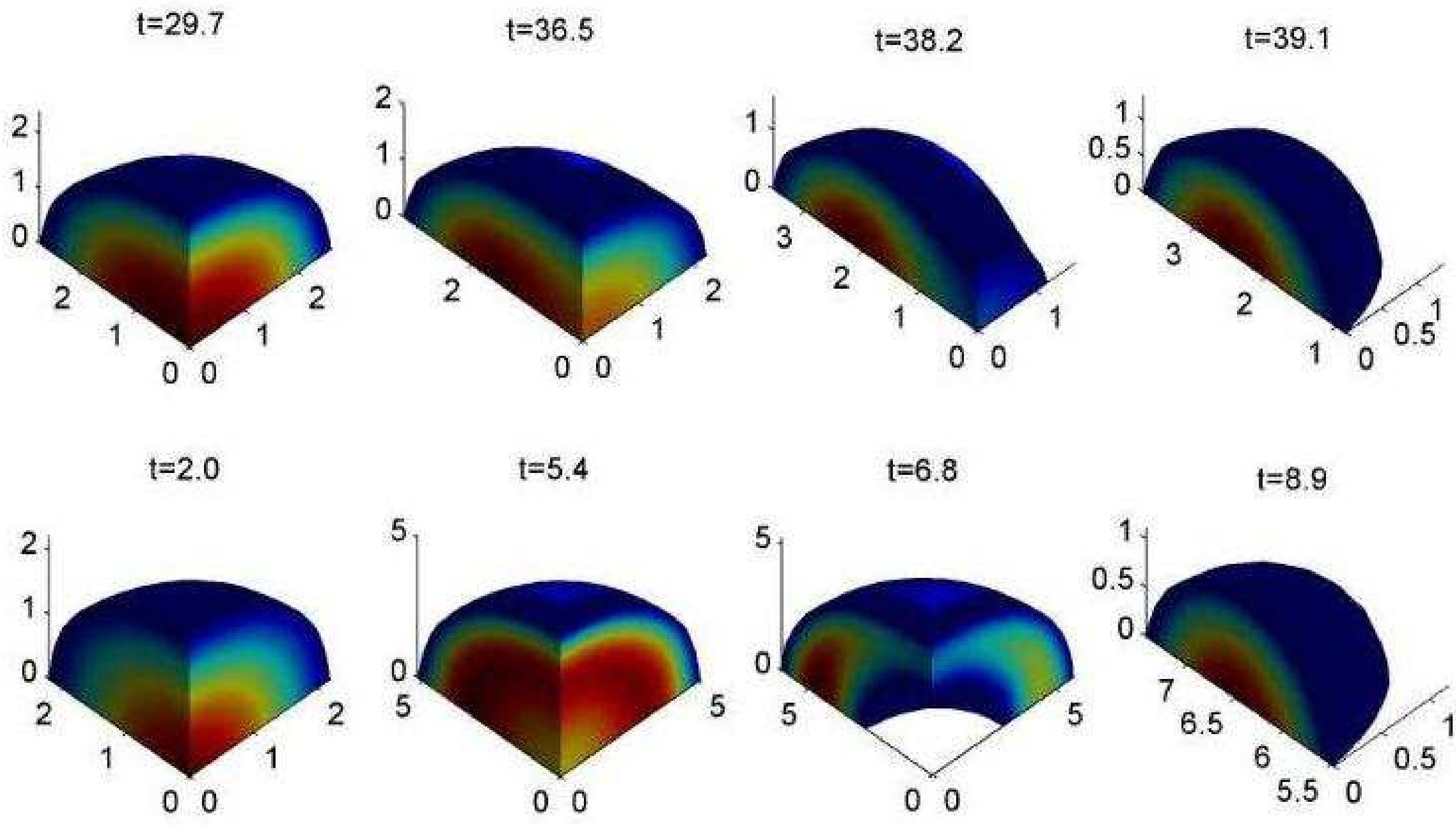
- Take $p = 2$; for a given q, follow the bifurcation curve and solve (NREP) numerically.
- Determine a when fold point occurs and when (NREP) becomes unstable. Whichever comes first determines the instability type.

$p = 2, q = 1.3$			
a	s	λ_r	λ_2
0.0000	4.1895	-0.79	-1.03
0.1104	3.1895	-0.62	-1.02
0.2311	2.2895	-0.44	-0.67
0.4410	1.1395	-0.18	-0.02
0.4523	***1.0895***	-0.17	***0.00***
0.6044	0.3895	-0.005	0.59
0.6046	**0.3395**	**0.005**	0.65
0.5981	0.2895	0.014	0.71
0.4370	0.0895	0.026	0.98
0.1647	0.001	0.0067	1.19

$p = 2, q = 3$			
a	s	λ_r	λ_2
0.0000	4.1895	-0.79	-1.037
0.0183	3.6395	-0.54	-0.99
0.0343	2.5895	-0.024	-0.3
0.0344	**2.5395**	**0.0015**	-0.27
0.0343	2.4895	0.027	-0.23
0.0326	***2.1895***	0.18	***0.00***
0.0314	2.0895	0.23	0.066
0.0229	1.6395	0.42	0.39
0.0128	1.1395	0.46	0.66
0.0003	0.001	0.033	1.19

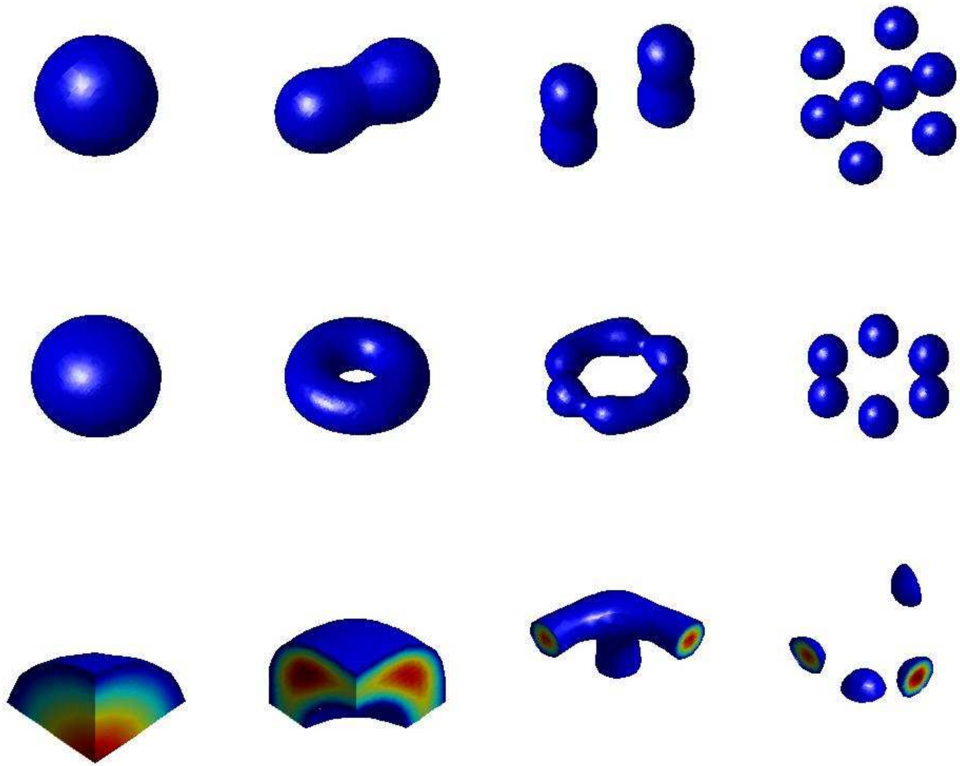
- $q = 1.3 \implies$ nonradial instability as a is increased past 0.4523.
- $q = 3 \implies$ radial instability as a is increased past 0.0344.

Numerical simulations $(N = 3)$



top row: $q = 1.3$. Bottom row: $q = 3$.

Numerical simulations for GM model



Some open questions

- What is relationship between self-replication and multi-bump solutions?
  - In 3D, we proved that self-replication exists whenever multi-bump solutions exist [when $q > (N-1)p/2$]. It appears that for $q < (N-1)p/2$, there is no fold point. Can this be proved?
  - In 1D, multi-bump solutions exist for all $q > 0$ However analytically can only prove self-replication for $q > (p-1)/2$.
- ***Conjecture:*** Show that the problem

$$u_{rr} - u + r^q u^p, \;\; u'(0) = 0, \;\; u > 0$$

  has no solution for all $q > 0$. We are only able to prove it for $q > (p-1)/2$.

- For large q, bifurcation diagram for the problem

$$\Delta u - u + (1 + ar^q)u^p, \;\; u'(0) = 0, \;\; u > 0$$

  has a spiral. Explain.