Traveling Wave of Gray-Scott in Turing Pattern Formation

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Introduction

A. Turing had a seminal idea in 1952:

Complex pattern can be formed in simple reaction-diffusion system by tweaking to change the constant state from stable to unstable.

The chemical basis of morphogenesis. Philos. Trans. Roy. Soc. London Ser. B 237 (1952), no. 641, 37-72.

A lot of theoretical study followed in 1960-80, see

H. Meinhardt, Models of Biological Pattern Formation (Academic, New York, 1982).

Can we realize it in experiment?

Yes, but only 40 years later.

V. Castets, E. Dulos, J. Boissonade, and P. De Kepper,

Experimental evidence of a sustained standing Turing-type nonequilibrium chemical pattern, Phys. Rev. Lett. 64, (1990), 2953-56.

Q Ouyang, HL Swinney,

Transition from a uniform state to hexagonal and striped Turing patterns, Nature, 352, (1991), 610 - 612.

An Outstanding Model

Gray-Scott model (with feeding):

$$(*)\begin{cases} a_t = \Delta a - Eab^2 + F(1-a), \\ b_t = D\Delta b + Eab^2 - kb \end{cases}$$

is one of the two major mathematical models to simulate the experiments, where D, E, F and k are positive parameters.

Observation: **Auto-catalysis is a must for positive feedback.**

An Interesting Phenomenon

J. E. Pearson, **Complex patterns in a simple system,** Science, 261 (1993), 189-192.

W. N. Reynolds, J. E. Pearson, S. Ponce-Dawson, **Dynamics of self-replicating patterns in reaction diffusion systems,** Physical review letters, (1994), 2797-2800,

discovered the following phenomenon:

Traveling Pulse undergoes a self-splitting process

They did it by numerical simulation in spatial dimensions 1 and 2.

Previous Math. Works on Traveling Wave of Gray-Scott

- A. Dolemann et al, 97-03, in
  Phys. D, Nonlinearity,
  SIAM Applied Math.,
  SIAM Appl. Dyn. Sys.
- C. Muratov & V. Osipov, 01-02, in
  Phys. D,
  SIAM Applied Math
- S. Ei et al, 01, in Phys. D.

formal analysis on traveling waves in one dimensional space. But, **no rigorous proof** of any kind!!!

Other Related Works

J. Wei, Nonlinearity 12 (1999), 593-616.

J. K. Hale, L. A. Peletier and W. Troy, SIAM J. Appl. Math. 61 (2000), 102-130.

W. T. Sun, M. J. Ward and R. Russell, SIAM J. Appl. Dyn. Syst. 4 (2005), 904-953.

T. Kolokolnikov and J. Wei, European J. Appl. Math. 16 (2005), 201-237.

T. Kolokolnikov, M. J. Ward and J. Wei, Stud. Appl. Math. 116 (2006), 35-95

Y. C. You, Commun. Pure Appl. Anal. 7 (2008), 947-970.

W. Chen and M. J. Ward, European J. Appl. Math. 20 (2009), 187-214.

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What do we want to do?

We want to

- prove **existence** of traveling wave solutions,
- study **structure** of traveling wave problem, and
- show **stability**

of Gray-Scott and related systems.

Applications

- Chemical Waves and Fluid Mechanics
- Turing Pattern Formations
- Population Dynamics
- Combustion Theory

Case I: Auto-Catalytic System of Order n

$$A + n\ B \to (n+1)B \qquad \text{with rate } ab^n,$$

after simple scaling,

$$(I) \begin{cases} a_t = a_{xx} - ab^n, \\ b_t = Db_{xx} + ab^n, \end{cases}$$

where $D > 0$ and $n \geq 1$ is an integer.

Case II: Gray-Scott without feeding

$$A + n\ B \to (n+1)B \qquad \text{with rate } ab^n,$$

$$B \to C \qquad \text{with rate } kb,$$

after simple scaling,

$$(II) \begin{cases} a_t = a_{xx} - ab^n, \\ b_t = Db_{xx} + ab^n - kb, \end{cases}$$

where $n \geq 1$ is an integer and $k > 0$.
$n = 2$, Gray-Scott model in Pattern Formation.

Case III: Gray-Scott with feeding

$$A + n\ B \to (n+1)B \qquad \text{with rate } ab^n,$$

$$B \to C \qquad \text{with rate } kb,$$

$$(III) \begin{cases} a_t = a_{xx} - Eab^n + F(1-a), \\ b_t = Db_{xx} + Eab^n - kb, \end{cases}$$

where $n \geq 1$ is an integer and $k > 0$.
$n = 2$, Gray-Scott model in Pattern Formation.

A Traveling Wave Solution of System (I)

$a(x,t) = a(z),\ b(x,t) = b(z)$ with $z = x - vt$ and v a positive constant, satisfying

$$\lim_{z\to-\infty}(a,b) = (0,1), \qquad \lim_{z\to\infty}(a,b) = (1,0), \tag{2.1}$$

$$\begin{cases} a'' + va' - ab^n = 0, & a > 0 \quad \text{in} \quad \mathbb{R}, \\ Db'' + vb' + ab^n = 0, & b > 0 \quad \text{in} \quad \mathbb{R}, \end{cases} \tag{2.2}$$

$D = 1,\ a + b \equiv 1$: Degenerate KPP,

$$b'' + vb' + b^n(1-b) = 0.$$

Earlier Works on System (I)

- Alikakos; Conway & Smoller, Martin & Pierre; Hollis, Martin & Pierre; Masuda, global dynamics in bounded domains (1977-83).
- Bricmont, Kupiainen and J. Xin, global dynamics in R^1 with L^1 initial data (1996).
- Billingham, Merkin and Needham, on Traveling Fronts of quadratic reaction $n = 1$, (1990-1992).
- Focant and Gallay, on Traveling Fronts in quadratic and cubic mixed reactions (1998).

More Related Works

There are a lot of works on KPP ($n = 1$) type or bi-stable type of nonlinearity in the context of

- thermal-diffusive systems
- nano-material processing, and
- population biology

in 2D and 3D in heterogeneous media.
Berestycki, Bourlioux, Constantin, Hamel, Heinze, Khouider, Kiselev, Larrouturou, P. L. Lions, Majda, Oberman, Nolen, Papanicolaou, Ryzhik, Steven, Souganidis, J. Xin, Zlatos, and others.

Most Recent Works

- Shi & Wang, and Zhao et al, on ground states (2006-12)
- Li & Wu, on Traveling Wave Stability when $D \sim 1$ (2013)
- Ai & Huang, on Traveling Fronts of fractional power (2004-06)

Open Question: If $D > 1$, initial values $0 \leq a_0,\ b_0 \in L_\infty$, is (a, b) uniformly bounded for all $0 < t < \infty$?

Old Results on (I)

Theorem (with X. Chen 2007 SIMA)

Suppose $D \geqslant 1$ and $n \geqslant 1$. There exists a positive constant $v_{\min}$ such that (I) admits a travelling wave iff $v \geqslant v_{\min}$. In addition, $v_{\min}$ is bounded by

$$\sqrt{\frac{D}{K(n)}} \leqslant v_{\min} \leqslant \sqrt{\frac{D}{K(n)}}\, \frac{1}{\sqrt{1-(1-\frac{1}{D})\frac{\sqrt{4K(n)+1}-1}{\sqrt{4K(n)+1}+1}}}$$

where $K(n)$ is a positive constant. $K(1) = 1/4$, $K(2) = 2$.

Note:

$$v_{\min} = O(\sqrt{D}) \qquad \text{if } D \gg 1$$

Theorem (with X. Chen 2007)

Suppose $D < 1$ and $n \geq 2$.

(i) *there exists a unique TW solution to (I) if*

$$v \geq \frac{4D}{\sqrt{1+4D}}$$

(ii) *there does not exist any solution if*

$$v < \sqrt{\frac{D}{K(n)}}\,\frac{1}{\sqrt{1-(1-\frac{1}{D})\frac{\sqrt{4K(n)+1}-1}{\sqrt{4K(n)+1}+1}}}.$$

Note:

$$v_{\min} = O(D) \qquad \text{if } D \ll 1$$

Theorem (with X. Chen 2009 JDE)

Suppose $D < 1$ and $1 < n < 2$.

$$(i)\textit{there exists a unique TW solution to (I) if}$$

$$v \geq \frac{2D}{(-D^2+\nu^2)^{1/2}}$$

$$(ii)\quad \textit{there does not exist any solution if}$$

$$v < \sqrt{\frac{D}{K(n)}}\,\frac{1}{\sqrt{1-(1-\frac{1}{D})\frac{\sqrt{4K(n)+1}-1}{\sqrt{4K(n)+1}+1}}},$$

where

$$\nu = \frac{n-1+\sqrt{(n-1)^2+8(3-n)D+16D^2}}{4}.$$

New Result on (I) -Existence of Minimum Speed

Theorem (with X. Chen & G. Liu, 2017 JDE)

Suppose $D > 0$ and $n > 1$. There exists a $v = v^*(n, D) > 0$ such that there is a TW solution with speed with speed v to (I) iff $v \geq v^*$.

That is, we have exactly the mono-stable case of scalar equation. Result vaild for More general setting with ab^n replaced by $ag(b)$ with $g(b) > 0$ on $(0, 1)$, $g(0) = g'(0) = 0$

Stability

Theorem (with X. Chen 2008 SIAP)

Suppose $n = 1$, $D > 1$ *and* $a(x, 0) \equiv 1$ *and* $b(x, 0) \geq 0$ *continuous and has compact support.*

1. *Let* $m(t) = 2t - 3(\log[3 + t] - \log 3)$*. Then for each* $t > 0$ *and* $x \in [-m(t), m(t)]$, $(a, b) \sim (0, 1)$ *in the following sense*

$$a(x; t) \leq e^{-\mu[m(t)-|x|]}, \quad |1 - b(x, t)| \leq \frac{C}{\sqrt{1 + m(t) - |x|}},$$

with μ *and* C *positive constants.*

2. *On the other-hand, when* $x \in R^1 \setminus [-m(t), m(t)]$, $(a, b) \sim (1; 0)$ *in the sense that*

$$|1 - a(x, t)| + b(x, t) \leq C\,\{1 + |x| - m(t)\}\, e^{m(t)-|x|}.$$

Challenge to Study Stability

- No Maximum Principle,
- No Variational Structure,
- Non-Monotone System.

Key to our analysis:

- Iterative estimates;
- Hard analysis involving heat kernel.

A case of interest-mixed reactions

A mixture of

$$A + n\ B \to (n+1)B, \qquad \text{and} \qquad A + m\ B \to (m+1)B,$$

$$(MN) \begin{cases} a_t = a_{xx} - ab^m - kab^n, \\ b_t = Db_{xx} + ab^m + kab^n, \end{cases}$$

where $n > m \geq 1$ are integers and the constant $k > 0$.

Theorem (with X. Chen JDE 2009)

Suppose $D \geqslant 1$ *and* $n > m \geqslant 1$. $\exists v_{\min}$ *such that (MN) admits a TW iff* $v \geqslant v_{\min}$. *In addition,* $v_{\min}$ *is bounded by*

$$\sqrt{\frac{D}{L(m,n,k)}} \leqslant v_{\min} \leqslant \sqrt{\frac{D}{L(m,n,k)}}\,\frac{1}{\sqrt{1-(1-\frac{1}{D})\frac{\sqrt{\Delta+1}-1}{\sqrt{\Delta+1}+1}}},$$

where $\Delta = 4L(m,n,k)(1+k)$, *with* $L(m,n,k)$ *a positive constant.*

In particular, when $m = 1, n = 2$,

$$2\sqrt{D} \leq v_{\min} \leq \frac{2\sqrt{D}}{\sqrt{1-(1-\frac{1}{D})\frac{\sqrt{2+k}-1}{\sqrt{2+k}+1}}} \qquad \text{if } k \leq 2,$$

$$\sqrt{D}\left(\sqrt{\frac{k}{2}}+\sqrt{\frac{2}{k}}\right) \leq v_{\min} \leq \sqrt{D}\left(\sqrt{\frac{k}{2}}+\sqrt{\frac{2}{k}}\right) \times \frac{1}{\sqrt{1-(1-\frac{1}{D})\frac{k}{2(k+1)}}} \qquad \text{if } k > 2.$$

Theorem (with X. Chen 2009)

Suppose $D < 1$. Then, there exists no TW to (MN) if

$$v < \sqrt{\frac{D}{L(m,n,k)}}\,\frac{1}{\sqrt{1-(1-\frac{1}{D})\frac{\sqrt{\Delta+1}-1}{\sqrt{\Delta+1}+1}}}.$$

But, there exists a TW to (III) if

$$v \geq \begin{cases} \frac{4D(1+k)}{\sqrt{1+4D(1+k)^{1/2}}} & \text{if} \quad m \geq 2 \\ \frac{2D}{(-D^2+\nu^2)^{1/2}} & \text{if} \quad 1 < m < 2, \end{cases}$$

where where $\Delta = 4L(m,n,k)(1+k)$,

$$\nu = \begin{cases} \frac{(m-1)(1-D)+\sqrt{(m-1-4D)^2+4(5-m)D(1+k)}}{5-m} & \text{if } n \leq 2m; \\ \frac{m-1+\sqrt{(m-1-4D)^2+16D(1+k)}}{4} & \text{if } n > 2m. \end{cases}$$

Traveling Wave problem of (II)

$$a(x,t) = a(x - Ct), b(x,t) = b(x - Ct),$$

$$\begin{cases} a'' + Ca' = ab^n, & a > 0 & \text{in } \mathbb{R}, \\ Db'' + Cb' = b - ab^n, & b > 0 & \text{in } \mathbb{R}, \\ a(-\infty) = a_0, \quad b(-\infty) = 0, & b(\infty) = 0, & a(\infty) < \infty. \end{cases} \tag{3.1}$$

All equilibrium points are taking the form $(A, 0)$.

Recent Works

- Zhou & Shi and Zhao et al on BVP of steady states,
- Guo & Tsai on TW when $ab^n - kb$ is replaced by $ab^n - kb^n$ with $n > 1$,
- Huang, Ai & Huang on TW when $n = 1$,
- Smith and Zhao on Global Dynamics and TW for a special case, when $n = 1$,

Solution Structure of $n = 1$

- b is **always** bell-shaped;
- It is TW if $b > 0$ in R^1,
- consequently, $b \searrow 0$ exponentially when $x \nearrow \infty$;
- It is TW if $C \geq C^*(a_0, D, k)$.

Preliminary Analysis

- Every equilibrium is of the form $(a_0, 0), \; a_0 \in R^1$.
- It is a saddle point if $a_0 > 0$.
- Non-TW positive solution possible,

$$\lim_{x \to \infty} b(x) x^{1/n} \qquad \text{and} \qquad \lim_{x \to \infty} a(x) x^{(n-1)/n}$$

exist and positive.

New Results

Theorem (Q 2015 JDE)

Suppose $n > 1$ and $k > 0$. There exists TW for all a_0 large if C suitably large, $D > 1$ but close to 1 and

$$(D-1)C^2 = k.$$

Theorem (with Chen & Zhang 2016 JDE)

Suppose $n > 1$, $D > 0$, $k > 0$ and $a_0 > 0$.

- *There exists TW for some $C > 0$.*
- *Moreover, for a_0 fixed, the set of speed of TW must be in a bounded interval.*

Surprising New Results

Let us use h **for** a_0 and consider $h \gg 1$.
Make the change of variables:

$$\varepsilon = h^{-\frac{n}{n-1}}, \quad a = [1 + \varepsilon\alpha]h,$$
$$\beta = h^{-\frac{1}{n-1}} b, \quad C = c\varepsilon,$$

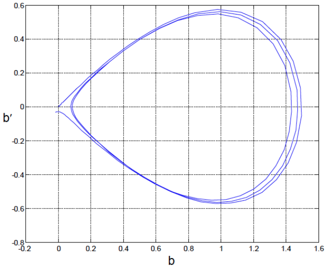
$\exists$ of TW is equivalent to finding (α, β, c) which satisfy

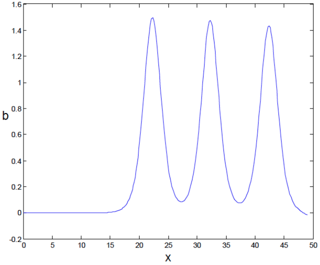
$$\begin{cases} \alpha'' + c\varepsilon\alpha' = [1 + \varepsilon\alpha]\beta^n, & \alpha' > 0 \quad \text{in } \mathbb{R}, \\ D\beta'' + c\varepsilon\beta' = \beta - [1 + \varepsilon\alpha]\beta^n, & \beta > 0 \quad \text{in } \mathbb{R}, \\ \alpha(-\infty) = \beta(-\infty) = 0, & \alpha(\infty) = 0, \quad \beta(\infty) < \infty. \end{cases} \tag{3.2}$$

Theorem (with Chen & Lai & Qin & Zhang 2015)

Suppose $n > 1$.

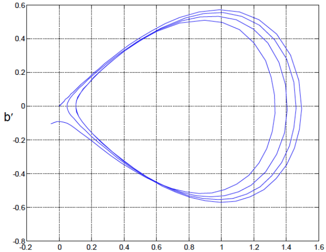
- $\exists$ M_1, M_2, *and* $M_3 > 0$ *depending on* m *and* d *such that* (3.2) *has no solution if* $c \geqslant \max\{\sqrt{M_1/\varepsilon}, M_2\}$ *or if* $c \leqslant \gamma - M_3\varepsilon$.
- $\forall \varepsilon \ll 1$ *and an integer* L *satisfying* $1 \leqslant L \leqslant \varepsilon^{-1/4}$, $\exists$ $c_L = L\gamma[1 + O(\varepsilon + [n-1]^2\varepsilon|\ln\varepsilon|)]$ *s.t. the solution is TW when* $c = c_L$, *It is an* L-**peak solution** *with* $w := [1 + \varepsilon a]^{1/(n-1)} b$ *having exactly* L *local maxima and* $L - 1$ *interior local minima.*

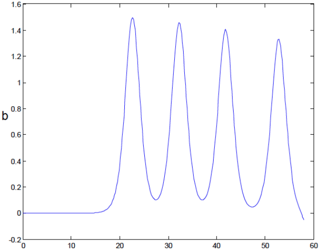




(a) $\varepsilon = 0.00025, \; c = 18$

(b) $\epsilon = 0.00025, \; c = 18$





Solution Structure for $n > 1$

- b can oscillate many times;
- $\exists$ positive solutions which are not TW;
- It is TW only if $b > 0$ in R^1, and $b \searrow 0$ exponentially as $x \nearrow \infty$;
- No *TW* if $C \geq C^*(a_0, D, k, n)$;
- Speed set for TW is not an interval.

Idea of Proof in CQZ

It is a shooting argument in speed C.

$$x_2(C) := \sup\{z \in \mathbb{R} \mid b > 0 \text{ in } (-\infty, z)\}.$$

We denote

$$\begin{aligned}
\mathcal{A} &:= \{C \geqslant 0 \mid x_2(C) < \infty\},\\
\mathcal{B} &:= \{C \geqslant 0 \mid x_2(C) = \infty, \lim_{x\to\infty} u(x,C) = \infty\},\\
\mathcal{C} &:= \{C \geqslant 0 \mid x_2(C) = \infty, \lim_{x\to\infty} u(x,C) < \infty\}.
\end{aligned}$$

- $\mathcal{A}$ is open and $0 \in \mathcal{A}$;
- $\mathcal{B}$ is open and $[M, \infty) \subset \mathcal{B}$. for some $M = M(a_0, k, n) > 0$.

Hence, the existence of TW.

Main Idea of Proof in CLQQZ

Perturbation around a periodic solution of

$$\begin{aligned} W'' &= W - W^n, \\ W(0) &= M, \quad W'(0) = 0, \end{aligned}$$

for $w = [1 + \varepsilon a]^\alpha b$.

Fresh New Result

Theorem (with X. Chen et al)

Suppose $D/k \ll 1$. Then, there exists a traveling wave to $(*)$, the Gray-Scott system with feeding, if

$$\delta \equiv \frac{\sqrt{Dk^3}}{EF^2}$$

is suitably large, in both 1D and 3D.

It is a traveling ring in 3D!!!

Thanks for your attention!!!