Growth and patterns in nature

Ryan Goh - Boston University November 19th, 2019

Pattern formation in nature

• How does nature form its structures?













Lets focus on one: CDIMA reaction

"Simple set of chemical reactions can create spatial patterns"

 $\begin{array}{rll} {\rm MA} &+ {\rm I}_2 & \longrightarrow {\rm IMA} + {\rm I}^{{\scriptscriptstyle -}} + {\rm H}^{{\scriptscriptstyle +}} \\ {\rm ClO}_2 + {\rm I} & \longrightarrow {\rm ClO}_2^{-} + 0.5 \ {\rm I} \\ {\rm ClO}_2^{-} + 4{\rm I}^{-} + 4{\rm H}^{+} \longrightarrow 2{\rm I}_2 + {\rm Cl}^{-} + 2{\rm H}_2{\rm O} \end{array}$

Well-stirred vat of chemicals feeds into gel suspension, slows down diffusion of chemical species —>

Chemical reaction occurs in a spatially non-constant manner: Striped and spotted states form at *random orientations*.

How does this happen?



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[Epstein '12 et. al]
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Mathematical modeling of patterns

• Alan Turing:

1.5

0.5

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THE CHEMICAL BASIS OF MORPHOGENESIS

By A. M. TURING, F.R.S. University of Manchester

(Received 9 November 1951—Revised 15 March 1952)

Turing's idea: Reaction + Diffusion = spatial patterns





Figure 2. (*a*) The morphogen pattern in a ring of cells as deduced by Turing. The greyscale indicates concentration differences. (*b*) Turing's hand-calculated 'dappled pattern' created by a morphogen scheme in two dimensions [1, fig. 2]. (*c*) The resemblance to animal markings (here a cheetah) was obvious, albeit at this point no more than qualitative.

0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 3. Concentrations of Y in the development of the first specimen (taken from table 1). ---- original homogeneous equilibrium; ///// incipient pattern; —— final equilibrium.

- Mathematics reveals how simple physical mechanisms can combine and lead to complicated spatial behavior
 - Foundational work inspiring whole area(s) of research

Chemical reaction

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Lets start with no spatial variation in the model: (ordinary differential equation)

• In a well-stirred mixture there exists a chemical equilibrium:

$$F(U_*) = 0 \qquad \Longrightarrow \ U_t = 0$$

Dynamics near equilibrium: Taylor expand about $U=U_*$

$$V_t = F(U_* + V) = F(U_*) + DF(U_*)V + O(|V|^2)$$

- 2D-Linear system: $V_t = AV$, $A = DF(U_*) = \begin{pmatrix} \partial_u f & \partial_v f \\ \partial_u g & \partial_v g \end{pmatrix}$
 - Stability: Do solutions V(t) grow or decay in time?

Linear system

$$V_t = AV, \qquad A = DF(U_*) = \begin{pmatrix} \partial_u f & \partial_v f \\ \partial_u g & \partial_v g \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

Study the eigenvalues of $A: \quad \lambda_{\pm} = \frac{\tau \pm \sqrt{\tau^2 - 4\delta}}{2}, \qquad \tau = a_{11} + a_{22}, \quad \delta = a_{11}a_{22} - a_{12}a_{21}$

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Stability condition:



Upshot: If well-stirred, chemical concentrations will approach a stable equilibrium state.

Reaction - Diffusion

Now allow the chemical species to spread or *diffuse* in space (i.e. fed them into a gel):

$$u_{t} = d_{u}u_{xx} + a - bu - \frac{4uv}{1 + u^{2}} - \phi$$
$$v_{t} = d_{v}v_{xx} + \sigma(bu - \frac{uv}{1 + u^{2}} + \phi)$$

What effect does the diffusion have?

Linear stability analysis about U_* : insert $U = U_* + V_*$

Taylor expand and truncate at linear order in V:

$$\frac{d}{dt}V_k = A(k)V_k, \qquad A(k) := \begin{pmatrix} -d_u k^2 & 0\\ 0 & -d_v k^2 \end{pmatrix} + DF(U_*)$$
$$DF(U_*) = \begin{pmatrix} \partial_u f & \partial_v f\\ \partial_u g & \partial_v g \end{pmatrix}$$

Eigenvalues: $\lambda_{\pm}(k) = \tau(k) \pm \sqrt{\tau(k)^2 - 4\delta(k)},$

 $\tau(k) = a_{11} + a_{22} - k^2 (d_u + d_v),$ $\delta(k) = (a_{11} - d_1 k^2)(a_{22} - d_2 k^2) - a_{12}a_{21}$

node" \overline{x} | |----d

Re
$$e^{ikx} = \cos(kx)$$
 Spatial "m

$$2\pi/k$$
 = spatial period

(partial differential equation)

"Turing" instability

Choose parameters correctly: typically $d_u \ll 1$ and $d_v \sim 1$ (short range activation, long range inhibition), obtain an unstable eigenvalue $\lambda_+(k)$ with non-zero wavenumber



"Linear growth of spatially non-constant modes"

In two spatial dimensions, this corresponds to an annulus of wavenumbers becoming unstable





If no diffusion, then no spatial patterns!

Light-sensitivity of CDIMA reaction

- Light suppresses spatial patterns
- Traveling mask speed *selects* pattern and *mediates* defects
- Experimental model for a growing organism



FIG. 1. Schematic of the experiment. A moving opaque mask image creates a growing shadow domain where Turing patterns can develop. In the illuminated domain the pattern is suppressed.



Homogeneous medium, [Epstein et. al. '12]



Heterogeneous medium, [Miguez et. al. '06]

Patterns and Growth

How does growth or spatial heterogeneity mediate or select patterns?

- External mechanism travels through system, or system domain grows, mediating pattern formation.
- Aim is to more efficiently and effectively form novel materials at various length-scales, and understand growth processes in nature.



Quenching/solidifcation in Eutectic Lamellar Crystals



Ion bombardment of alloys

Early stage digit-patterning

Chemical precipitation

Nonlinear Dynamics viewpoint

Existence, Stability, Bifurcation, and Dynamics of nonlinear coherent states, which organize behavior

• Simple ODE example: $u_t = \mu u - u^3$ $u \in \mathbb{R}, \mu$ - bifurcation parameter

 $u_* = 0$ equilibrium, changes stability at $\mu = 0$



- Bifurcation indicated by a linear instability of $u_* = 0$, at $\mu = 0$: $v_t = \mu v$
- Dynamics saturated by nonlinearities, non-trivial states u_{\pm} attract nearby trajectories
- What is the "basin of attraction" of each non-trivial state u_{\pm} ?

Dynamics of spatial patterns?

Can we study patterns in a simpler setting compared with coupled system: so a *scalar* equation?

Could introduce (2D) spatial dependence by adding in diffusion:

 $u_t = \Delta u + \mu_0 u - u^3, \qquad \Delta := \partial_x^2 + \partial_y^2$ "Diffusion" "Reaction" <u>Allen-Cahn equation</u>

but patterned solutions are unstable, or not persistent

Turns out... a simple way to get stable patterns, in scalar PDE:

$$u_t = -(1+\Delta)^2 u + \mu_0 u - u^3,$$

Swift-Hohenberg equation

[SH-'77], [Cross, Hohenberg '93]





Pattern forming model: The Swift-Hohenberg equation

$$u_t = -(1+\Delta)^2 u + \mu_0 u - u^3, \quad u : \mathbb{R}^n \to \mathbb{R},$$

- μ_0 -bifurcation/"onset" parameter: $u \equiv 0$ stable/unstable for $\mu_0 \leq 0$
- Originally derived for Rayleigh-Bénard convection —>
- Universal model for many phenomena:
 - In fact Turing was working on a similar equation! [Dawes '15]
 - "Outline of development of the Daisy" [Turing, unfinished draft]
 - Been used as a model for liquid crystals, soft-materials, plant phylotaxis, reaction-diffusion
- Nice starting point because much is rigorously known:

Grain Boundaries

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Hexagons





Zig-Zags



[SH-'77], [Cross, Hohenberg '93]

FIG. 1. Schematic picture of Rayleigh-Bénard convection showing fluid streamlines in an ideal roll state.

Stripes



Patterns in Swift-Hohenberg equation

 $u_t = -(1+\Delta)^2 u + \mu_0 u - u^3, \quad u : \mathbb{R}^n \to \mathbb{R},$

Turing Patterns: "Pitchfork" bifurcation of a family of spatially periodic equilibria

Turing instability: insert $u = re^{i\mathbf{k}\cdot\mathbf{x}+\lambda t}$ into linear equation yields $\lambda = -(1-k^2)^2 + \mu_0$, $k = |\mathbf{k}|$



Linear instability of base state $u = 0 \implies$



Nonlinear bifurcation of family of stable "roll"/stripe equilibrium states $u_p(x) = \sqrt{4(\mu_0 - \kappa)/3} \cos(kx) + \mathcal{O}(|\mu_0 - \kappa|^{3/2}),$ $\kappa = k^2 - 1, k \sim 1$

Rotational invariance -> all orientations of stripes are solutions

$$u_p(\mathbf{k}\cdot\mathbf{x};k)$$



Swift-Hohenberg equation

$$u_t = -(1+\Delta)^2 u + \mu_0 u - u^3, \quad u : \mathbb{R}^2 \to \mathbb{R},$$



Growth model in Swift-Hohenberg equation

• Spatially progressive bifurcation: jump heterogeneity changes stability of u=0 for $x - ct \ge 0$

$$u_t = -(1+\Delta)^2 u + \mu(x-ct)u - u^3, \quad \mu(\xi) = -\mu_0 \operatorname{sgn}(\xi)$$





• Similar behavior to experimental RD system

Perpendicular stripes t=500, c =0.5 8π 0.8 0.6 0.4 4π 0.2 > 0 0 -0.2 -0.4 4π -0.6 -0.8 8π -100 -50 50 0 х Oblique stripes t=500, c =2 8π 0.8 0.6 0.4 4π 0.2 > 0 0 -0.2 -0.4 4π -0.6 8π -100 -0.8 50 -50 0 х Parallel stripes t=500, c =2.5 8π 0.8 0.6 0.4 4π 0.2 > 00 -0.2 -0.4 4π -0.6 -0.8 8π -100 -50 50 0

х

Swift-Hohenberg

Light Sensing RD system



1-D patterns in Swift-Hohenberg

$$u_t = -(1 + \partial_x^2)^2 u + \mu (x - ct)u - u^3 \qquad \mu(\xi) = \mu_0 \text{sgn}(-\xi)$$

Study existence of pattern-forming fronts, characterize wavenumber dependence on growth speed c



Curves $k_x(c)$ give mechanism and prescription for control of pattern formation process

Fast speeds

$$u_t = -(1 + \partial_x^2)^2 u + \mu (x - ct)u - u^3 \qquad \mu(\xi) = \mu_0 \text{sgn}(-\xi)$$



behind inhomogeneity.

faster than you're letting it

pattern for $c > c_{inv}$

Co-moving frame: $\xi = x - ct$



Fast speeds:



Spatial Dynamics approach

$$\omega u_{\tau} = -(1+\partial_{\xi}^2)^2 u + \mu(\xi)u - u^3 + cu_{\xi} \qquad \xi = x - ct, \tau = \omega t$$

- Look for front solutions as trajectories in a dynamical system with space ξ as evolution variable, in phase space of τ periodic functions,
- non-autonomous in ξ (but *only* piece-wise constant!)

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- Look for front solutions as heteroclinic orbits:
- Intersections of *invariant manifolds* $W^{cu}_{-}(u_p) \cap W^{s}_{+}(0)$ of asymptotic states
 - $W^{s/u}(0) := set of trajectories which converge to state in forwards/backwards evolution$
- Geometry of intersection gives wavenumber predictions!



 $u_{\xi} = v,$

 $v_{\xi} = w,$

periodic orbits



Exploring 2-dimensional patterns

- How to characterize relationship between patterns and growth speed?
- $\bullet \quad {\rm Rigorous \ analysis \ requires \ application/development \ of \ new \ techniques}$
- Explore (k_y, c) parameter space first using direct simulations
- Fix a vertical period k_{y} :

 $\omega u_{\tau} = -(1 + \partial_{\xi}^2 + k_y^2 \partial_y^2)^2 + \mu u - u^3 + c \partial_{\xi} u \qquad y \in [0, 2\pi/k_y)$

- Exponentially growing quenching/growth front $\mu(x-\zeta(t)t), \quad \zeta(t)\sim \mathrm{e}^{\epsilon t}$
- Freeze pattern in the wake (gets rid of possible secondary instabilities)







Oscillatory behavior past saddle-nodes

- Take c just above one of the saddle-node values
- Phase sees the "ghost" of the heteroclinic solution of MTW:
- Dynamics similar to saddle-node on a limit cycle:
 - Period of oscillation scaling like $\sim (\delta c)^{-1/2}$











Organize/represent solutions: "Moduli space"

MTW $\begin{cases} \omega \partial_{\tau} u = -(1 + \partial_{\xi}^2 + k_y^2 \partial_{\tau}^2)^2 u + \mu(\xi) u - u^3 + c \partial_{\xi} u, \quad u(\cdot, \tau) = u(\cdot, \tau + 2\pi) \\ \lim_{\xi \to -\infty} u(\xi, \tau) \to u_p(k_x \xi + \tau, k), \quad \lim_{\xi \to \infty} u(\xi, \tau) \to 0, \quad \mathbf{k} = (k_x, k_y), \omega = c k_x \end{cases}$

 $\mathcal{M} := \{(k_y, c, k_x) \in \mathbb{R}^3 : \text{MTW has a solution}\} \longrightarrow \text{Each point on surface represents a striped pattern}$





Boundaries of pattern transitions governed by bifurcation curves

Moduli space \mathcal{M} is the "pattern cookbook": how to create and select a given pattern





Other systems: how do patterns behave?



<u>Reaction-Diffusion systems</u> $u_t = d_u u_{xx} + \mu (x - ct)u - u^3 - v$ $v_t = d_v u_{xx} + u - \gamma v$





Other types of growth

• For example: radial growth front



Patterns in experiment

Precipitation and Vapor deposition

$$a_t = D\Delta a - f(a, b) + h(t, x; c)$$
$$b_t = \Delta b + f(a, b)$$



<u>Gastrulation in embryos</u>

$$A_t = D_A \Delta A + \frac{s_A A^2}{k_I + I} - k_A A$$
$$I_t = D_I \Delta I + s_I A^2 - k_I$$

CDX2/BRA/SOX2





[S. Chhabra, L. Liu, RG, A. Warmflash,'19]

w/ P. Shipman, S. Thompson

Summary

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- Nature is incredibly capable of forming patterns and structure
- Growth is a useful way to mediate pattern formation in natural and experimental settings
- Mathematics can characterize the phenomena:
 - Dynamics and Functional Analysis are powerful viewpoint to illuminate the underlying structure/mechanisms in PDE models
 - 1-D patterns: existence and wavenumber selection for fast and slow growth speeds
 - 2-D patterns: Transitions between different orientations of stripes, many interesting dynamics and phenomena!
 - Use the moduli space representation as a *pattern cookbook*
 - Yields explicit qualitative/quantitative predictions for pattern selection
 - Many of these predictions can be used in other PDE models

- There is much more to be done, using a variety of tools and approaches:
 - Rigorous approaches, formal asymptotics, numerics...

Some good references to get into this area

- "Forging patterns and making waves from biology to geology: a commentary on Turing (1952) 'The chemical basis of morphogenesis', Ball, Phillip, Phil. Trans. R. Soc. B 370: 20140218.
- The Chemical Basis of Morphogenesis A. M. Turing, Phil. Trans. R. Soc. B 237: No. 641. (Aug. 14, 1952), pp. 37-72
- Nature's Patterns: a tapestry in three parts, Phillip Ball
- Pattern Formation: An Introduction to methods, Rebecca Hoyle









Career as an academic mathematician

My path

- Always liked math, was decent at it (mom was a high-school math teacher)
- Started reading non-technical books on math (non-Euclidean geometry, Riemann Hypothesis, Gödel's incompleteness) one stuck out:
 - *Chaos*, by James Gleick
- (2007-2011) Attended Michigan State University: B.S. in math, B.A. in physics
 - Research in dynamics of piecewise-linear maps, and ODE modeling of dyesensitized solar cells
 - Attended an REU at Univ. of Minnesota with Arnd Scheel
- (2011-2016) PhD in Mathematics at University of Minnesota: studied dynamical systems, functional analysis, partial differential equations, with applications to formation of coherent structure in nature
- (2016-2019) Postdoctoral fellowship at Boston University, mentored by Prof. C.
 Eugene Wayne
- (2019-) Tenure-track assistant professor at Boston University



Undergrad studies in math/applied math

Explore!!!

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- Take classes, go to talks, meet with faculty
- Directed/independent study, research project with faculty,
- Summer REU/Interships (academic vrs. industry career paths)
- Maybe teach a little (?), grading, teaching assistant, etc...
- Start thinking about graduate school
 - How to prepare: all the above!, discuss with faculty advisors, start reading and thinking about types of research
 - Choosing one: don't just go on rankings
 - Want a school with at least at least few research areas/faculty that interest you
 - What is the grad student culture/community like?
 - Where do PhD graduates go after?
 - Location and benefits?

Graduate School

- Last place where you just get to learn! (and learn how to learn, establish habits)
- It's hard, but mostly fun! (good to have a support group)
- Learn mathematics more deeply (core subjects algebra, topology, analysis, applied math)
- Learn one or two subjects really, really well
- After introductory course work, start reading papers with faculty, start a small project,
- Typically have to pass written/oral exams
- Stipend support by either Teaching Assistantship, Research support from advisor
- Math is social! (i.e. soft-skills matter too!)
 - Talk with professors (possible collaborations, will need letters)
 - -> Go to workshops/conferences/summer schools, present a poster, give a talk, maybe even collaborate with someone!
 - Organize department events (SIAM, MAA, AMS, AWM student chapters)
- Maybe do internship? (Math PhD's can go into industry!)
- Start thinking about career track: Research University (large/small, public/private), liberal arts 4-year, national lab.

Postdoctoral studies

- Become an independent researcher though typically mentored by a senior faculty
- Move into different research areas
- Gain experience as a lecture/instructor of record (teach various courses, 1 to 2 (maybe 3) a semester)
- Start applying for tenure-track jobs
- Taking on more responsibilities:
 - Mentor undergrad research
 - Organize professional events, referee journal papers
 - Maybe work of multiple projects
 - Help with department functions (write prelims, organize department seminars, ...)

Tenure- Track Assistant Professorship

Research:

- develop and produce high-quality, impactful research (papers, review articles, etc...)
- Maybe recruit a graduate student or two
- Be active in your research community
- Teaching: (one to two courses/a semester, varies depending on institution)
 - high-quality instruction (student evaluations and peer-reviews)
 - Variety of courses (large 100-200 level lectures, 500-advanced undergrad/masters classes, graduate courses)
 - Maybe develop a new course or two?!
- Service:

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- Department: take part in administration and direction of department/school
- University: faculty council, etc...
- Community: academic and public

Academic Career: Pros and Cons

Pros:

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- Get to do math for a living!
- Relatively independent (still have bosses, but less direction than at a company)
 - Academic freedom and tenure
 - No profit incentive (though have to get grants!)
 - Relatively flexible schedule
 - Get to visit a lot of cool places and meet interesting and diverse people
 - Contribute new knowledge to the world
 - Educate/Impact the next generation of mathematicians and scientists
 - Sabbaticals are nice
 - Job security (once you get one...)

Cons:

- Positions are competitive (difficult to get)
- Pay not at the level of industrial job with equivalent experience (though not bad at all!)
- Work/Life balance can be tough (especially during early career)
- Societal/economic trends & broad changes in academia (student debt bubble, etc. . .)
- Need to bring in grant \$\$ for university
- "Publish or perish"

Day in the life (on "teaching day")

- 5:30-6am wake-up, breakfast, get ready, bike in around 7am
- 7:15-7:30am Arrive on campus, respond to emails
- 7:30 9: work on a research problem
- 9-10: teaching prep, review lecture notes, grading, course emails
- 10-11: teach
- 11-12 decompress & send emails (maybe lunch)
- Afternoon (varies):
 - Research collaboration meetings, work on research projects
 - Office hours, student research projects
 - Committee/faculty meetings (undergrad, graduate, etc...)
 - Referee journal articles
 - Other activities for more senior faculty (advising, university committees, editor of academic journals etc...
 - Go to seminar talks
 - 4 6pm: Bike home

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6-8:30pm: Dinner and family time, 8:30-10pm work on a research project, 10-10:30 get ready for bed

Thanks!!

Thanks!

References:

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