Pattern formation

surprising structure in a chaotic world

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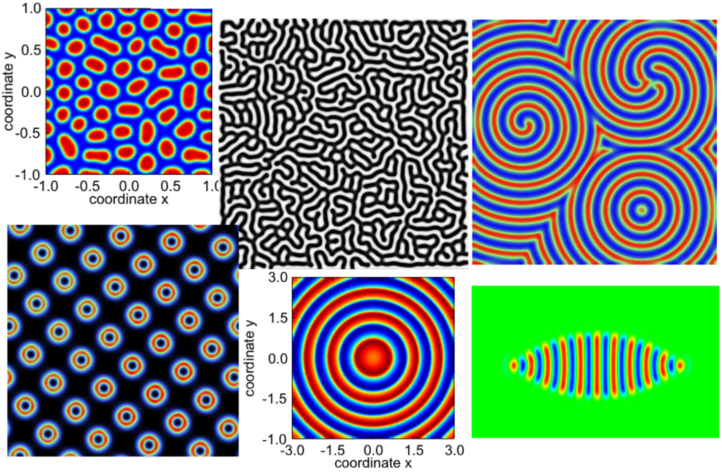
Outline

1. Introduction

Patterns in nature

Patterns in nature

Patterns in mathematical models, e.g. PDEs



Evolution equations

- Abstract setting of most models: *evolution equations*

$$\frac{\partial u}{\partial t} = \mathcal{F}[u], \quad u \in \mathbb{R}^n$$

with

$$u : \Omega \times \mathbb{R}_+ \to \mathbb{R}^n, \quad x \in \Omega \subset \mathbb{R}^m$$

and $\mathcal{F}$ is a set of evolution rules, for example, partial (spatial) derivatives of u:

$$\mathcal{F}[u_x, u_x x, u_y, u^2, uu_x, \text{etc}]$$

(can also contain integrals, delay terms, ...)

- Stationary patterns are *equilibria* of evolution: solution to

$$\mathcal{F}[u] = 0$$

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Stationary patterns

Problem: Generally impossible/difficult to find analytical solution to system of nonlinear PDEs $\mathcal{F}[u] = 0$

Approach: Focus on spatial dimension = 1

$$\Rightarrow x \in \Omega \subset \mathbb{R}, \quad u : \mathbb{R} \times \mathbb{R}_+ \to \mathbb{R}^n$$

- Existence equation $\mathcal{F}[u] = 0$ is now system of ODEs in x
- System of ODEs = dynamical system in independent 'time' variable $x \Rightarrow$ use dynamical system techniques!
- Patterns can often be described effectively as "1-dimensional section $\times$ Euclidean symmetry" (translation, rotation)
- Related to what we define/perceive as "patterns" $=$ spatially regular phenomena

2. Geometric singular perturbation theory

Reaction-diffusion systems

Modelling framework:

$$\begin{cases} \dfrac{\partial U}{\partial t} = \Delta U + F(U,V) \\ \dfrac{\partial V}{\partial t} = \Delta V + G(U,V) \end{cases}$$

Specific choices for reaction terms $F(U,V)$ and $G(U,V)$: models from literature

- Developmental biology: Gierer-Meinhardt (morphogenesis)
- Chemistry: Gray-Scott (autocatalysis)
- Physics: Ginzburg-Landau (phase transitions, superconductivity), nonlinear Schrödinger (optics, wave propagation, Bose-Einstein condensates)
- Ecology: Schnakenberg (desertification, predator-prey)

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Pattern formation research

Goal: Use **analytical techniques** to get insight in behaviour of solutions to these models.

- Beyond model specific model simulations: use results as inspiration/guidance for analysis
- Beyond abstract ’existence & uniqueness’ results: use insights from functional analysis
- In between computational and pure mathematics: study general classes of models, but obtain concrete, specific results

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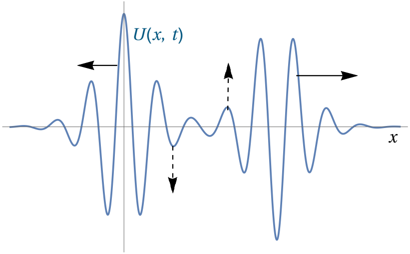
One spatial dimension

$$\begin{cases} \dfrac{\partial U}{\partial t} = \dfrac{\partial^2 U}{\partial x^2} + F(U, V) \\ \dfrac{\partial V}{\partial t} = \dfrac{\partial^2 V}{\partial x^2} + G(U, V) \end{cases}$$



1. What does the pattern look like? (existence/construction)
2. How does the pattern move/behave? (stability/dynamics)
   - Decay, blow-up, colliding peaks, splitting peaks, etc.

Shape of pattern

Look for stationary (time independent) solutions to reaction-diffusion system: obtain 4-dimensional ODE system

$$\left\{ \begin{array}{rcl} u' & = & p \\ p' & = & -F(u,v) \\ v' & = & q \\ q' & = & -G(u,v) \end{array} \right.$$

Spatial pattern

=

Special solution to dynamical system

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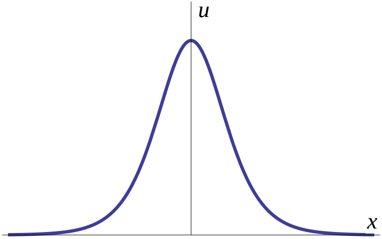
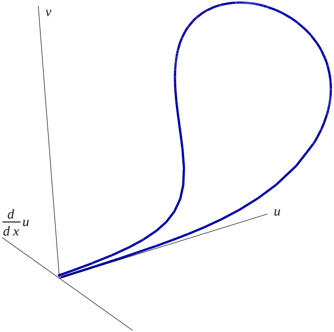
Shape of pattern

Pulse solution in reaction-diffusion system



Homoclinic solution to ODE system

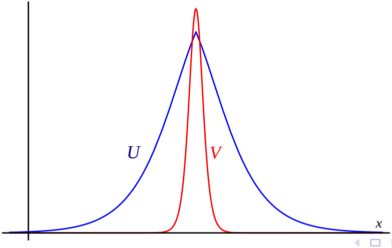


Geometric singular perturbation theory

Small parameter ε in reaction-diffusion system, $0 < \varepsilon \ll 1$:

$$\begin{cases} \frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} + F(U,V) \\ \frac{\partial V}{\partial t} = \varepsilon^2 \frac{\partial^2 V}{\partial x^2} + G(U,V) \end{cases}$$

causes behaviour on different spatial/time scales



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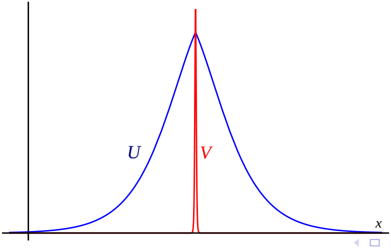
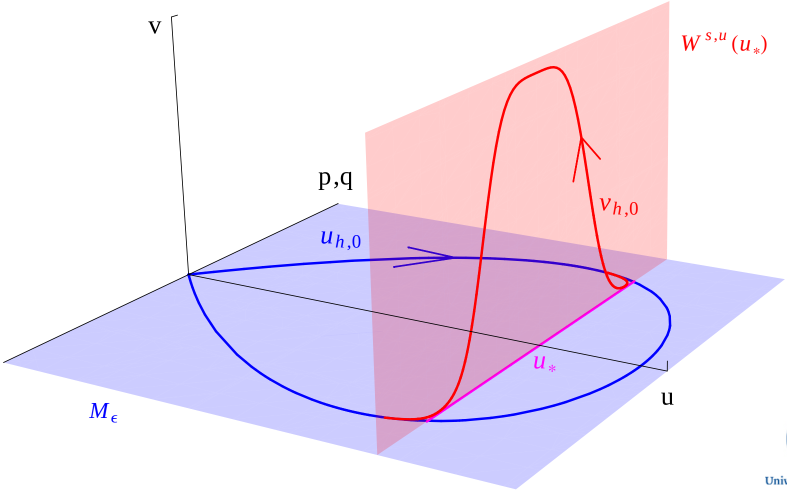


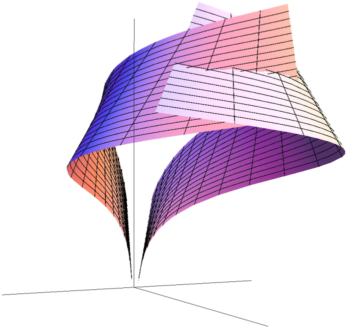
Geometric singular perturbation theory



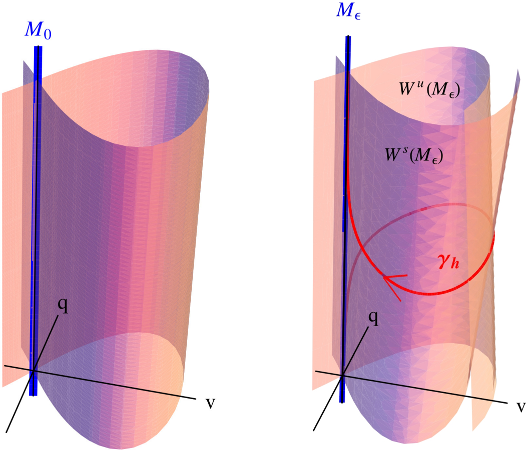
Geometric singular perturbation theory

Define and study geometric objects such as slow/fast stable/unstable manifolds, fibres; when do they intersect?

- Prove existence of solutions
- Know their shape



Geometric singular perturbation theory



$\varepsilon = 0 \qquad \longrightarrow \qquad \varepsilon > 0$

Stability

How does the pattern move/behave?

- Travelling wave: analysis similar to stationary solution
- Otherwise:
  1. perturb stationary solution $\Phi_0(x)$ with small perturbation $\delta\phi(x,t)$
  2. substitute $\Phi_0(x) + \delta\phi(x,t)$ in reaction-diffusion system
  3. obtain 4-dimensional eigenvalue problem

$$\frac{d\phi}{dx} = (A(x,\varepsilon) - \lambda I)\,\phi$$

$A(x,\varepsilon)$ depends on x: difficult to solve!
Solution: use techniques similar to geometric analysis: *scale separation*

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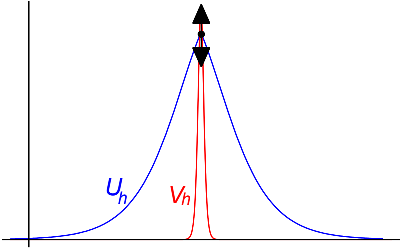
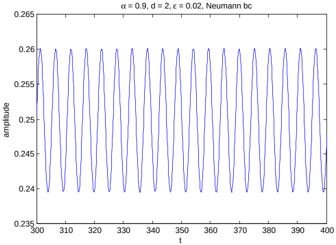
Example: breathing pulses





Using geometric techniques, we can understand and quantify this behaviour in the *general* reaction-diffusion system (for general $F(U, V)$ and $G(U, V)$)!

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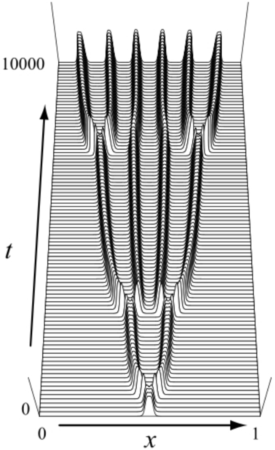
Example: pulse splitting

- When do pulses split?
- Is the splitting symmetrical in space?
- How fast do the pulses move apart?
- Can pulses merge again? (is the splitting symmetrical in time?)
- Is the length of the domain important?

Not yet fully understood!



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Closed orbit, periodic pattern

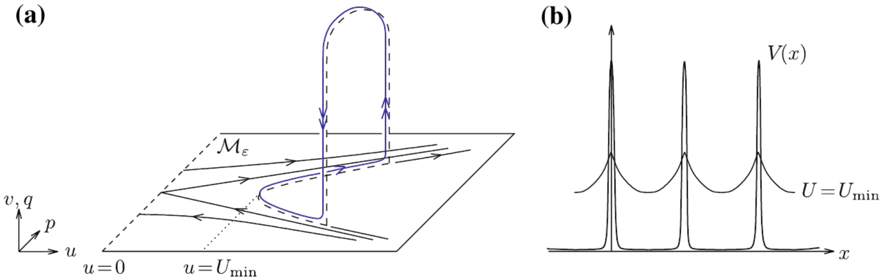

Fig. 2 **a** Schematic illustration of the constructed periodic orbit and the singular skeleton structure on which it is based (*dashed lines*). A *single arrow* means slow flow, a *double arrow* means fast flow. Note that $\mathcal{M}_\varepsilon = \mathcal{M}_0$ can be chosen as large as one wishes, so that it will contain the orbit in $\{v = q = 0\} \supset \mathcal{M}_\varepsilon$ that is part of the singular orbit. **b** Sketch of the corresponding periodic pattern $(U(x), V(x))$

source: G. Hek, JMB 60 (2010)

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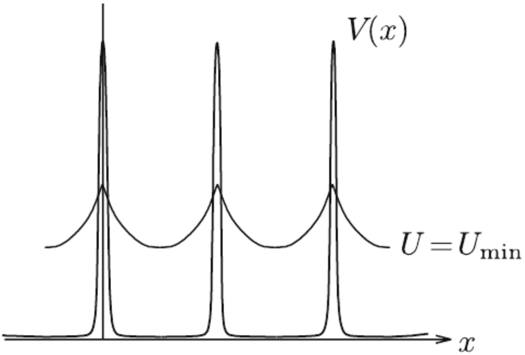
Spatial scale separation

- Note the *spatial scale separation* between the components: U long scale (x), V short scale ($\xi = \frac{x}{\varepsilon}$)



- Observing such a scale separation in a pattern in nature can give guidance to the modelling of the underlying processes

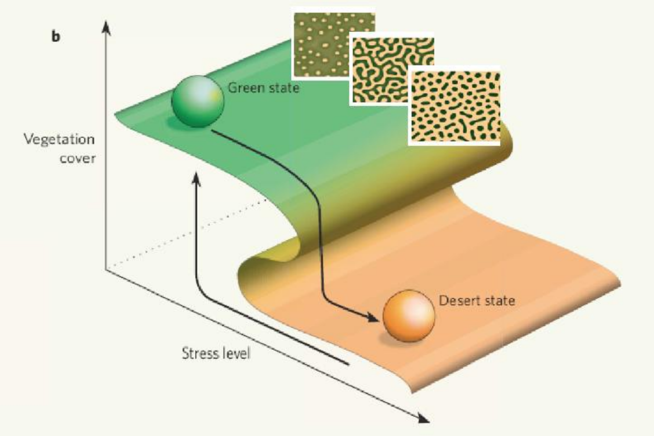
3. Examples and applications

1: Vegetation patterns

Patterns of tiger bushes in arid environment (Negev desert, Israel)

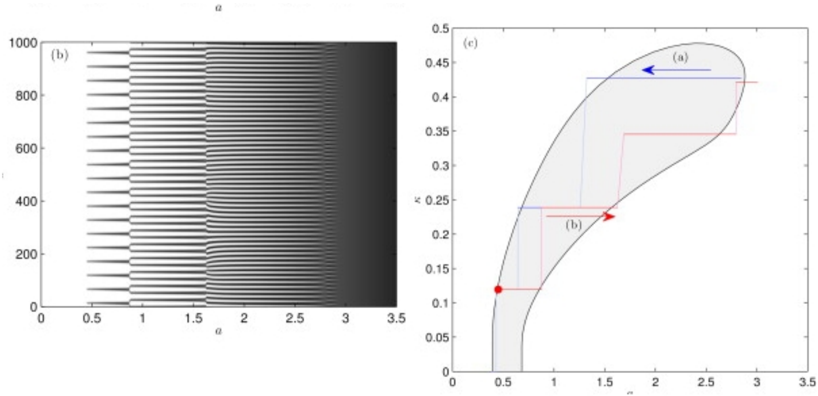
- Underlying vegetation-water mechanics: Klausmeier model, nonlinear reaction-diffusion system
- Study influence of climate change on ecosystem: patterns indicate state of the system

Desertification: sudden collapse of vegetation



Ecological question: Are patterns an *early warning signal*?

Decreasing rainfall: pattern selection



Busse balloon: region in (parameter, wave number)-space where stable patterns exist

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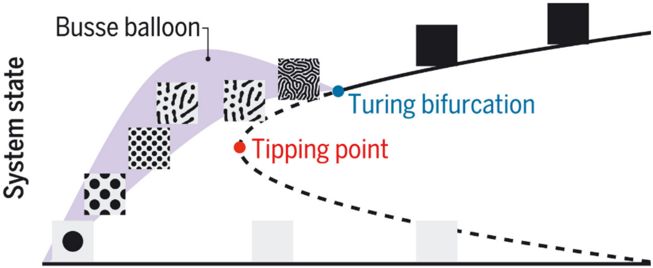
Alternative pathway to desert state



source: Rietkerk et al., Science 374 (2021)

Self-organisation through patterns occurs before tipping point, and patterns persist *beyond* tipping point

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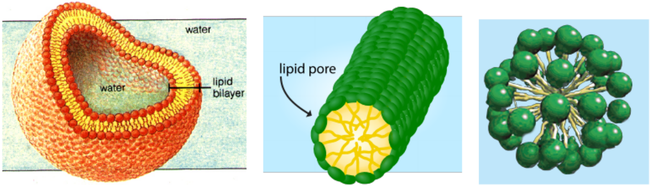
2: Amphiphilic molecules & interfaces



[Kraitzman&Promislow, 2014]

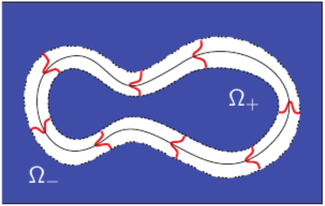
Functionalised Cahn-Hilliard free energy:

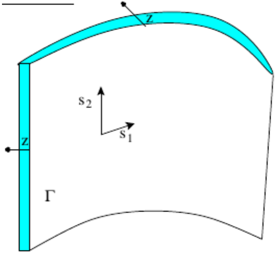
$$\mathcal{F}[u] = \int_\Omega \frac{1}{2}\left|D^2\varepsilon^2\Delta u - F(u)\right|^2 - \varepsilon^p P(u,\nabla u)\,\mathrm{d}x$$

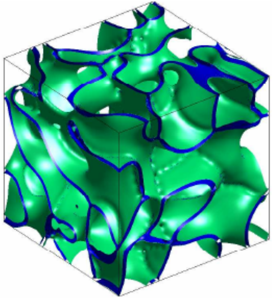
u mixture composition, ε interfacial thickness,
P functionalisation terms

Bilayer interfaces

- A *bilayer interface* is a codim-1 structure with small thickness (of $\mathcal{O}(\varepsilon)$)
- Bilayer structures are formed by 'dressing' codim-1 structures with pulse profiles:

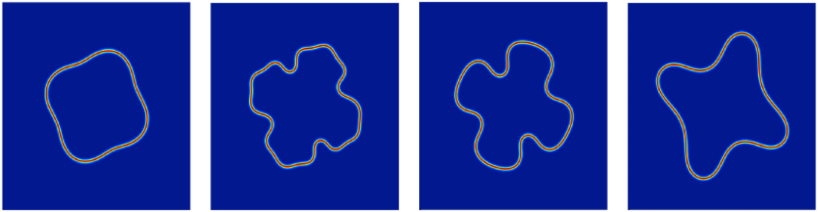






Stability of bilayer interfaces

Spectral analysis yields two major instabilities:
meandering and *pearling*



[Doelman et al., 2014]

Meandering (‘long wavelength’): associated with zero (translational) eigenvalue linear operator

- Meandering instability is *slow* and *benign*

Stability of bilayer interfaces

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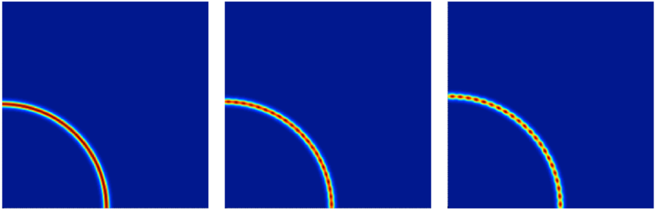
meandering and *pearling*



[Doelman et al., 2014]

Pearling (‘short wavelength’): leads to breakup of bilayer interface

- Pearling instability is *fast* and *destructive*

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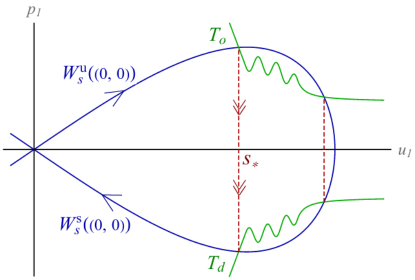
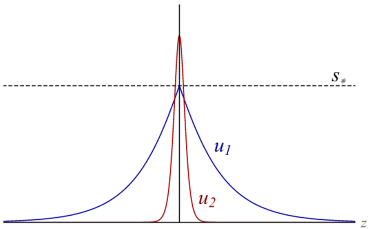
Multicomponent mixtures

Problem: Analysis shows that pearling generically occurs in one-component mixtures $u(x,t) \in \mathbb{R}$

Idea: Introduce multicomponent mixture to try and stabilise the bilayer





Stabilisation through second component

Bilayer stability is determined by spectrum of

$$\left[D\partial_z^2 - \nabla F(u_*)^\dagger\right]\left[D\partial_z^2 - \nabla F(u_*)\right]$$

square of *n*-component, second order differential operator

- Use GSPT & related stability analysis techniques to determine spectrum
- Outcome: a second component can *prevent* pearling / breakup of the bilayer
- **Necessary:** spatial scale separation between components $\Rightarrow$ different length of amphiphilic molecules in mixture
- Biological application: stabilising role of cholesterol on cell membranes

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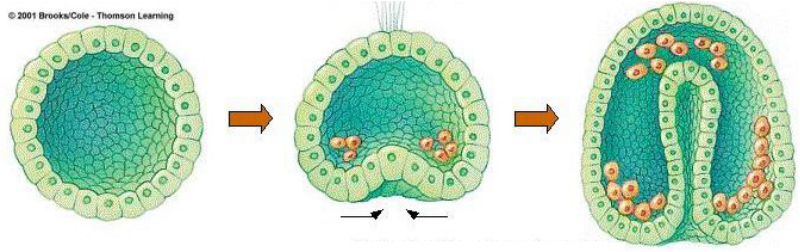
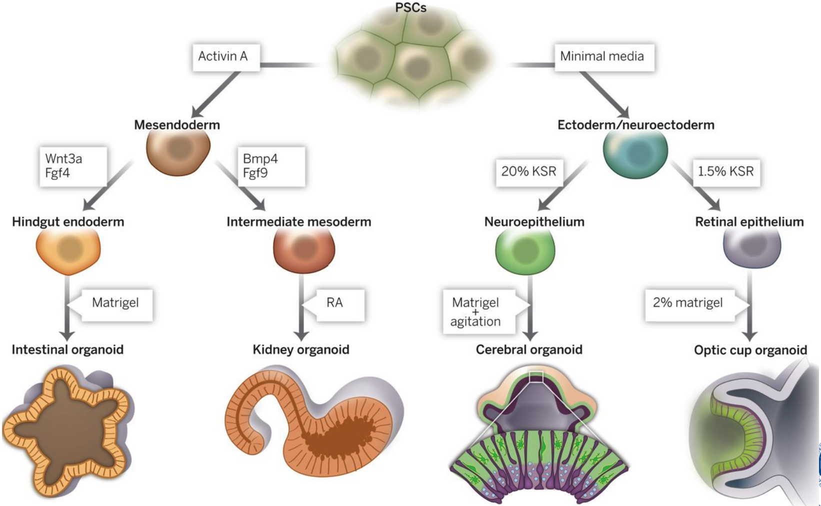
3: Early stages of embryogenesis

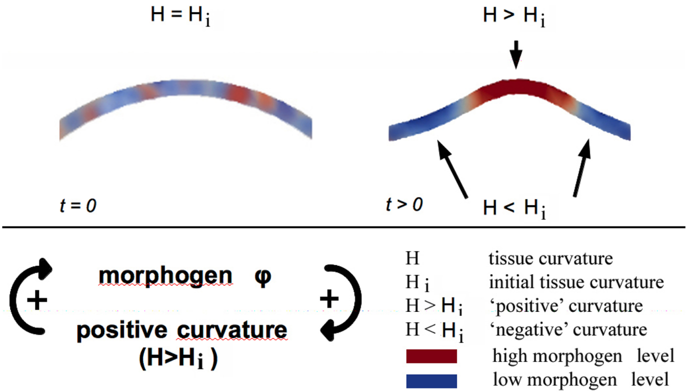


- Symmetry breaking of spherical tissue induces pattern formation
- Pattern formation induces change in shape

Pattern formation process leads to organoids

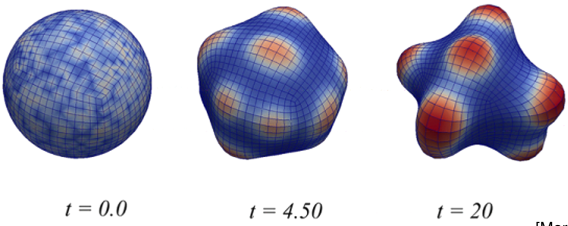


Mechanochemical pattern formation



[Mercker et al., 2013]

Mechanochemical pattern formation



[Mercker et al., 2013]

- Numerical simulations show that mechanochemical model leads to morphogen patterns and surface deformation
- **Question:** Can we investigate these patterns *analytically*? Can we find relations between pattern shapes and model components (e.g. surface stiffness, morphogen reactions)?

Summary

- One-dimensional (reductions of) spatial patterns can be studied using dynamical systems techniques
- In the presence of *spatial scale separation*, we can use **geometric singular perturbation theory** to robustly construct singular orbits $\rightarrow$ scale-separated patterns
- Stability can be determined using same singular perturbation techniques $\rightarrow$ analytical control over pattern stability

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References

Contact: f.w.j.veerman@math.leidenuniv.nl

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