Intra-disciplinary bridges for multi-dimensional patterns

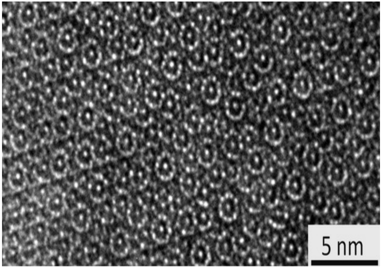
Priya Subramanian

By Frits Ahlefeldt

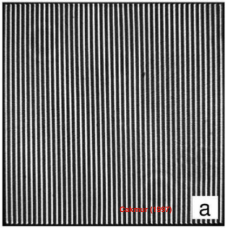
with many collaborators: AMR, AJA, EK, VR, CL, MC, etc.

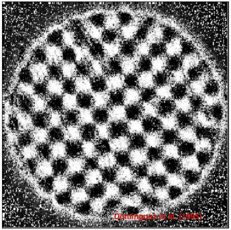
UNIVERSITY OF AUCKLAND
Waipapa Taumata Rau
NEW ZEALAND

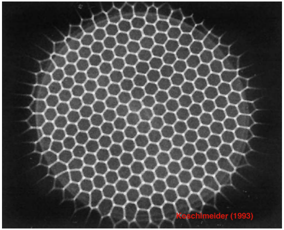
Multidimensional patterns are universal across scales: from kilo- to nano- metres

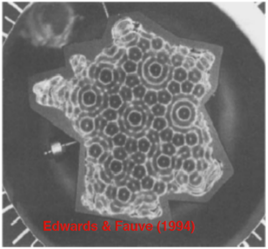


Many nonequilibrium systems in controlled settings also display complicated patterns



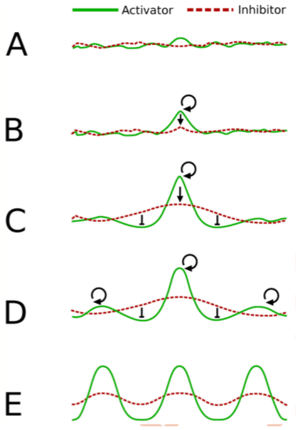






- System can display different patterns at different parameters
- Features: time varying, multiple length scales, localization, symmetries

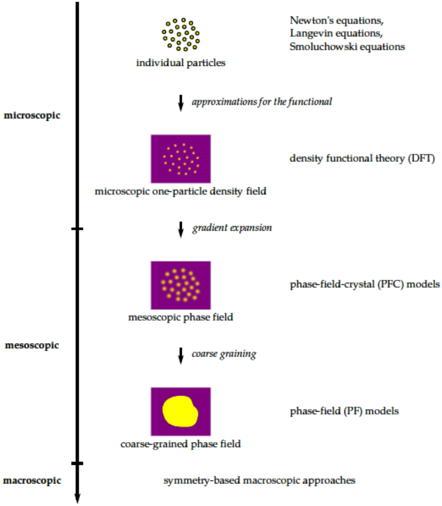
We assume that the underlying mechanism for pattern formation is universal: Turing bifurcation



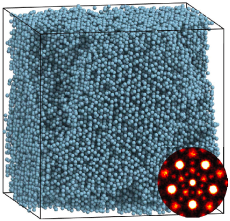
Nogare et. al., PLoS 2017

- A homogeneous state becomes unstable with change in parameter
- Initial perturbations grow and nonlinearities dampen this growth and help form a pattern

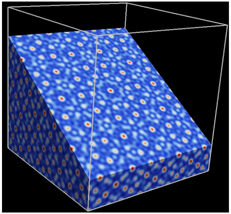
Modelling pattern formation usually involves choosing a level of detail and very often involves arriving at a governing PDE



Emmerich et. al., Adv. in Phys., 2012



Damasceno et. al., JCP 2017



Subramanian et. al., PRL 2016

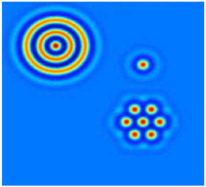
A prototypical PDE for studying pattern formation

Reaction Diffusion equation:

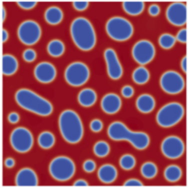
$$\frac{\partial U}{\partial t} = \triangle U + \mathcal{N}[U]\,.$$

Swift-Hohenberg equation:

$$\frac{\partial U}{\partial t} = \mu U - (1 + \nabla^2)^2 U + \mathcal{N}[U]\,.$$


Swift-Hohenberg

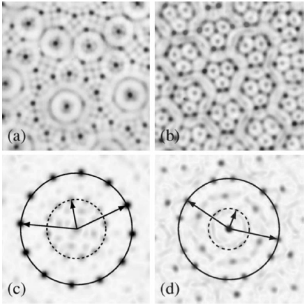

Fitz-Hugh Nagumo


Cahn-Hilliard

- Where $\mathcal{N}$ is a (polynomial) nonlinear function
- The equations are nonlinear and infinite dimensional

Visual PDE

Complicated patterns observed in experiments can be analysed by introducing a second length scale in the problem



Ding & Umbanhowar (2006)

- 12-fold quasipattern and superlattice patterns observed in Faraday wave experiment
- Ratio of two length scales, $0 < q < 1/2$ – superlattice patterns and $0.5 < q < 1$ – quasipatterns

Lifshitz-Petrich model:

$$\frac{\partial U}{\partial t} = \big(r_1 U - c(1+\nabla^2)^2(q^2+\nabla^2)^2 + QU^2 - U^3\big)$$

Extension to model with two independent growth rates:

$$\frac{\partial U}{\partial t} = \mathcal{L}U + QU^2 - U^3$$

Designing a linear operator with two preferred length scales

$\sigma(k)$ associated with $\mathcal{L}$ needs to satisfy the following constraints

- *Reflection and rotation symmetry*
- *Choice of lengthscales*
- *Sharpness of the choice of lengthscales*
- *Large lengthscales are damped*
- *Independent growth rates at two lengthscales*

These conditions amount to:

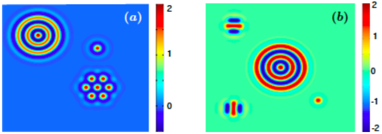
$$\begin{aligned}\sigma(k=1) &= r_1, \quad \sigma(k=q)=r_q, \quad \sigma(k=0)=\sigma_0,\\ \frac{d\sigma}{dk}(k=1) &= 0, \quad \frac{d\sigma}{dk}(k=q)=0, \quad \sigma(k)=\sigma(-k).\end{aligned}$$

The resulting 8^{th} order polynomial in k is

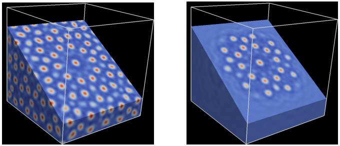
$$\sigma(k)=\frac{k^2(P(k)r_1+R(k)r_q)}{q^4(1-q^2)^3}+\frac{\sigma_0}{q^4}(1-k^2)^2(q^2-k^2)^2$$

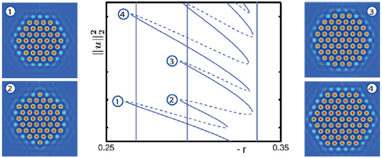
where $P(k)=(k^2(q^2-3)-2q^2+4)(k^2-q^2)^2q^4$ and
$R(k)=(k^2(3q^2-1)+2q^2-4q^4)(k^2-1)^2$.

Observed phenomena in pattern formation that we would like to understand/explain: (i) Spatial localisation

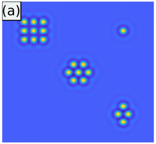


Lloyd et al., 2008

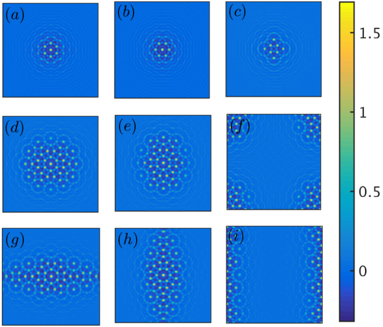




Lloyd et al., 2008

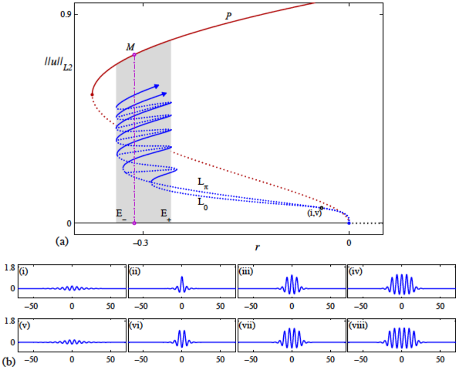


Hill et al., 2022



Subramanian et al., 2018

Spatially localised patterns in 1D occur can be analysed using the approach of spatial dynamics



Burke & Knobloch 2007

- At a steady solution, the PDE becomes a fourth order spatial ODE
- We can convert in into four first order ODEs for

$$\xi = (U, U_y, U_{yy}, U_{yyy})^T$$

Spatial dynamics system: ill-posed IVP, but we can analyse the bifurcation structure

$$\xi_y = \mathcal{A}\xi + \mathcal{N}[\xi]$$

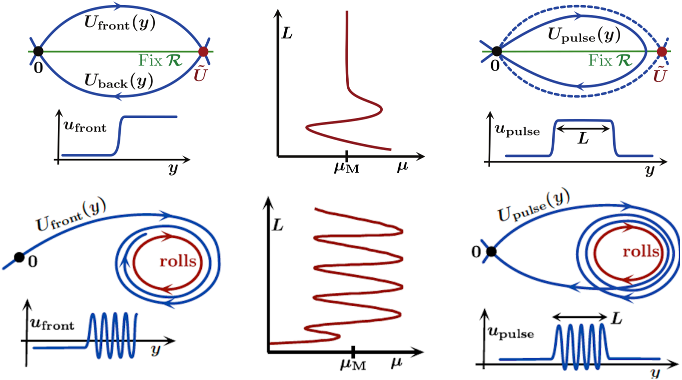
reversible with respect to the reverser

$$\mathcal{R} : (U, U_y, U_{yy}, U_{yyy})^T \to (U, -U_y, U_{yy}, -U_{yyy})^T$$

- The spatial dynamical system is conservative - energy functional values remain constant
- Fronts connecting to the trivial state are only possible when the energy functional corresponding to the patterned state also vanishes: Maxwell point
- Unstable manifold of trivial state intersects the stable manifold of the patterned state transversally within the zero level set of the energy functional
- Homoclinic orbits bifurcating from such a heteroclinic connection will exist over an open parameter interval

Avitabile et al. 2010

Two scenarios that can occur are the non-snaking and snaking scenarios



Avitabile et al. 2010

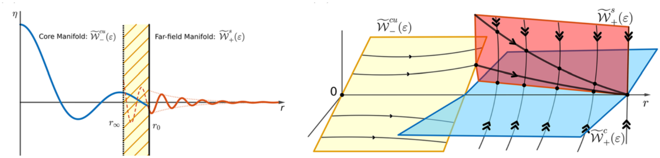
- Heteroclinic cycles between two reversible equilibria lead to branches of symmetric homoclinic orbits with vertical asymptote at Maxwell point
- Heteroclinic cycles between an equilibrium and a reversible periodic orbit lead to two branches of symmetric/asymmetric homoclinic orbits that oscillate between two distinct parameter values

How can we extend a similar method to analyse spatial localisation in 2D/3D? Or to more complicated PDEs?

By Frits Ahlefeldt

Some ideas so far...

- Core-Farfield decomposition for dihedral patterns:



Hill et al. 2021

- Analysis for a truly 2D pattern, even in a prototypical pattern forming PDE requires new methods/bridges
- Long way from analysing snaking observed in fluid flows modelled using Navier Stokes equation

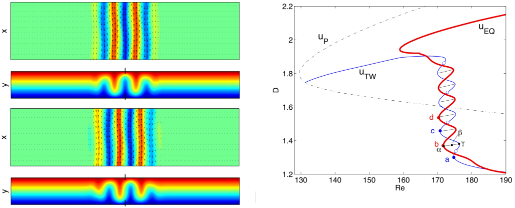
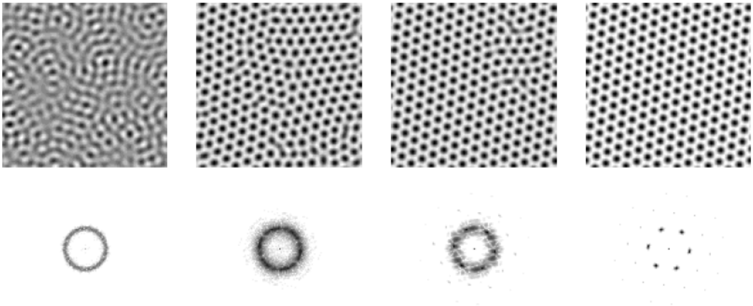


FIG. 2: (color online). Snaking of the localized u_{TW}, u_{EQ}

Schneider et. al., 2010

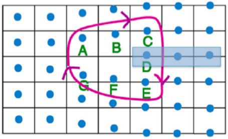
Observed phenomena in pattern formation that we would like to understand/explain: (ii) Pinning of defects



$$u_t = \mu u - (1 + \nabla^2)^2 u + Qu^2 - u^3 \qquad \mu = 0.1 \qquad Q = 0.5$$

- Hexagons are preferred when quadratic nonlinearity is activated.
- In the nonlinear phase, patches of hexagons exhibit penta-hepta defects, which are destroyed until a uniform pattern of hexagons remain.

Defects can be classified into two groups: topological defects and non-topological defects



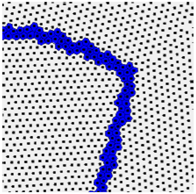
Griffin & Spaldin 2017

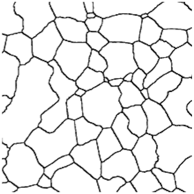
Defects are studied in an amplitude-phase formulation where U is written as

$$U = \epsilon^{1/2} \sum_{j=1}^{3} B_j exp(i(k_j + \triangle k_j)r) + \mathrm{c.c}$$

- Topological defects are associated with zeros of the amplitudes B_j where the phase becomes undefined
- Topological defects need to interact with another defect in order to be eliminated
- Non-topological defects (e.g. Penta-Hepta defects) were thought to 'heal' by themselves - without interactions with another defect

However, defects found at grain boundaries can get pinned to the background





Boissoniére et al. 2021

Subramanian et al. 2021

We look at the Swift-Hohenberg model

Reminding ourselves of the dynamical equation for u

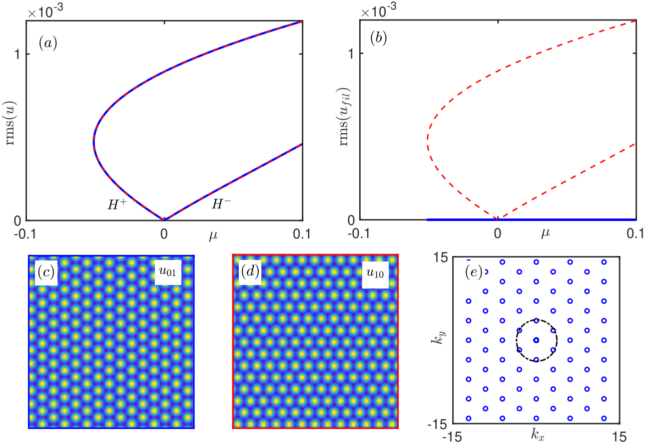
$$\frac{\partial u}{\partial t} = \mu u - (1 + \nabla^2)^2 u + Q u^2 - u^3$$

associated with a free energy,

$$\mathcal{F}[u] = \int \left[-\frac{1}{2}\mu u^2 + \frac{1}{2} u (1 + \nabla^2)^2 u - \frac{1}{3} Q u^3 + \frac{1}{4} u^4 \right] \mathrm{dx}$$

- We consider a periodic domain in 2D of length 30 wavelengths of the characteristic mode ($k = 1$) and consider a system with $Q = 0.75$
- Time evolutions are obtained pseudospectrally using second-order exponential time differencing
- Pseudo-arclength numerical continuation is used to obtain the bifurcation behaviour for varying μ

Choosing one extended state as the reference pattern

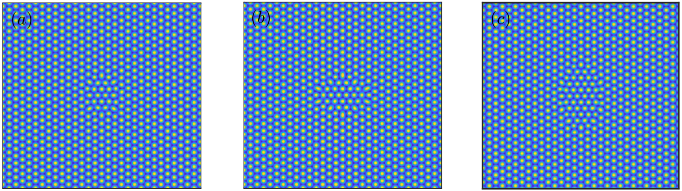


$$\text{Spectral filter: } \mathcal{P} = \begin{cases} 0, & \text{components of } \hat{u} \in RLV(u_{01}) \ , \\ 1, & \text{otherwise} \, . \end{cases}$$

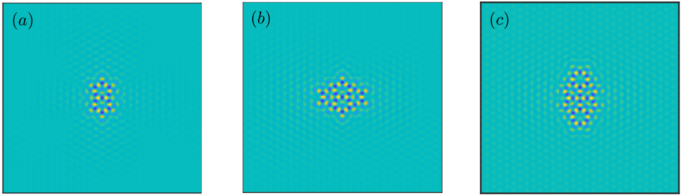
$$\text{Measure: } \quad \text{rms}(u_{fil}) = \sqrt{\frac{1}{A} \int [\text{IFFT}(\mathcal{P}\hat{u})]^2 \, dA}$$

We place a patch of u_{10} with a background of u_{01} as an initial guess for numerical continuation

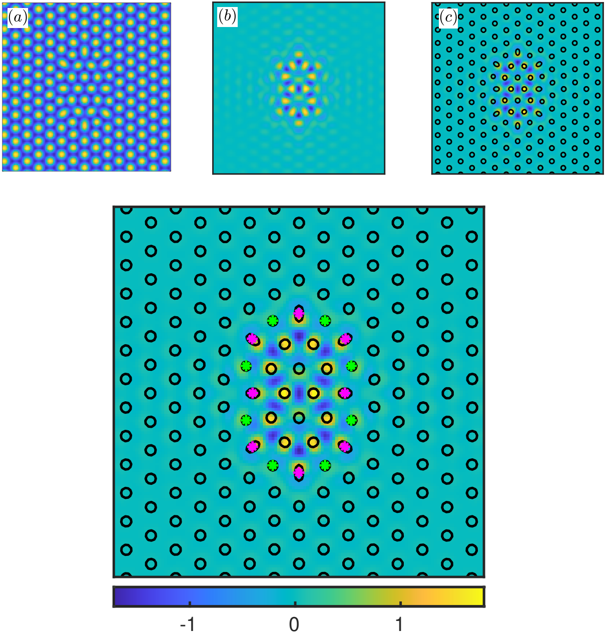
We obtain multiple equilibria at the same parameters that have different size/shape of the patch



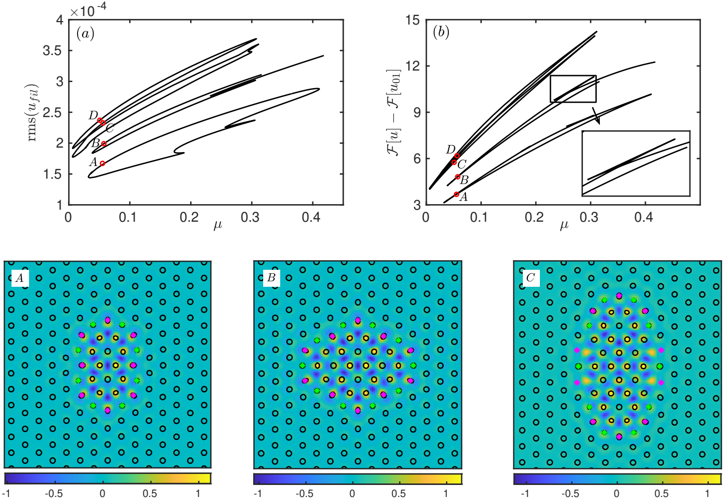
Viewing the u_{fil} field shows the differences more clearly



Where are the penta-hepta defects located?



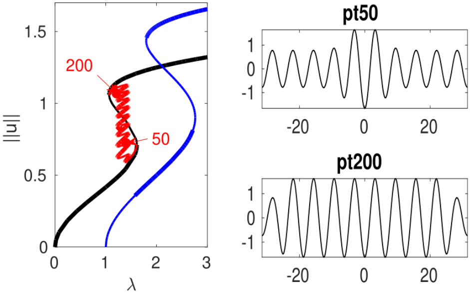
States with defects exist over a wide range of parameters



- How can we explain the snaking of non-topological defects?
- What is the smallest stationary stable defect that can exist?

Pinning of defects in 1D is currently being analysed

- Defects have been obtained between two patterned equilibria numerically



Knobloch et. al., 2019

- Current work (by DJL) is looking to use spatial dynamics to analyse this as a Periodic-to-Periodic homoclinic connection

How can we extend a similar method to analyse pinning of defects in 2D/3D?

By Frits Ahlefeldt

Computer assisted proofs (CAPs) in nonlinear analysis

We want to construct algorithms that provide an approximate solution to a problem together with precise and possibly efficient bounds within which a rigorous exact solution is guaranteed to exist.

This area uses ideas from

- scientific computing
- functional analysis
- approximation theory
- numerical analysis
- topological methods

Consider a general nonlinear problem

$$\mathcal{F}(x) = 0\,.$$

Based on slides from the SIAM Gene Golub Summer School 2025

To solve such a general nonlinear problem in a Banach space X exactly is impossible

The alternative is to find small balls in which it is demonstrated that a unique solution exists

- Let $\bar{x}$ be a numerical approximation to $\mathcal{F}(x) = 0$ using a finite dimensional reduction

To solve such a general nonlinear problem in a Banach space X exactly is impossible

The alternative is to find small balls in which it is demonstrated that a unique solution exists

- Let $\bar{x}$ be a numerical approximation to $\mathcal{F}(x) = 0$ using a finite dimensional reduction
- Construct a linear operator $\mathcal{A}$ that is the approximate inverse of $\mathcal{DF}(x)$

To solve such a general nonlinear problem in a Banach space X exactly is impossible

The alternative is to find small balls in which it is demonstrated that a unique solution exists

- Let $\bar{x}$ be a numerical approximation to $\mathcal{F}(x) = 0$ using a finite dimensional reduction
- Construct a linear operator $\mathcal{A}$ that is the approximate inverse of $\mathcal{D}\mathcal{F}(x)$
- Verify that $\mathcal{A}$ is an injective linear operator

To solve such a general nonlinear problem in a Banach space X exactly is impossible

The alternative is to find small balls in which it is demonstrated that a unique solution exists

- Let $\bar{x}$ be a numerical approximation to $\mathcal{F}(x) = 0$ using a finite dimensional reduction
- Construct a linear operator $\mathcal{A}$ that is the approximate inverse of $\mathcal{DF}(x)$
- Verify that $\mathcal{A}$ is an injective linear operator
- Define a Newton-like operator $T(x) = x - \mathcal{A}\mathcal{F}(x)$ about the numerical approximation $\bar{x}$

To solve such a general nonlinear problem in a Banach space X exactly is impossible

The alternative is to find small balls in which it is demonstrated that a unique solution exists

- Let $\bar{x}$ be a numerical approximation to $\mathcal{F}(x) = 0$ using a finite dimensional reduction
- Construct a linear operator $\mathcal{A}$ that is the approximate inverse of $\mathcal{D}\mathcal{F}(x)$
- Verify that $\mathcal{A}$ is an injective linear operator
- Define a Newton-like operator $T(x) = x - \mathcal{A}\mathcal{F}(x)$ about the numerical approximation $\bar{x}$
- Consider $\mathcal{B}_{\bar{x}}(r) \in X$, the closed ball of radius r centered at $\bar{x}$

To solve such a general nonlinear problem in a Banach space X exactly is impossible

The alternative is to find small balls in which it is demonstrated that a unique solution exists

- Let $\bar{x}$ be a numerical approximation to $\mathcal{F}(x) = 0$ using a finite dimensional reduction
- Construct a linear operator $\mathcal{A}$ that is the approximate inverse of $\mathcal{DF}(x)$
- Verify that $\mathcal{A}$ is an injective linear operator
- Define a Newton-like operator $T(x) = x - \mathcal{AF}(x)$ about the numerical approximation $\bar{x}$
- Consider $\mathcal{B}_{\bar{x}}(r) \in X$, the closed ball of radius r centered at $\bar{x}$
- Find a radius $r > 0$ such that the operator T is a contraction mapping

In summary, we have looked at some current directions in the analysis of multi-dimensional patterns

- Analysis of nonlinear PDEs arising in pattern formation needs expertise in multiple areas of mathematics - need for intradisciplinary bridges
- Observations of spatial localisation and pinning of defects in 2D/3D are very much open problems
- Coming up on Wednesday:
- (i) an outline of CAP for the Swift-Hohenberg equation and
- (ii) a detour to analysing codimension-2 bifurcations using computational algebraic geometry