Building a Database for the Global Dynamics of Multi-Parameter Systems

Konstantin Mischaikow

Dept. of Mathematics/BioMaPS Institute
Rutgers
mischaik@math.rutgers.edu

Z. Arai, Kyoto
W. Kalies, Florida Atlantic Univ.
H. Kokubu, Kyoto
H. Oka, Ryukoku
P. Pilarczyk

Why do we want Databases of Global Dynamics?

Mathematical Answer: Interesting physical systems often involve many parameters and the dynamics is of fundamental importance. Normal form theory tells us what happens near singularities. Want similar information globally.

Scientific Answer: This is already being done but without the full perspective of dynamical systems.

von Dassow, et. al., Nature 2000, “The segment polarity network is a robust development module”

136 dimensional ode, 50 unknown parameters, phenomonological nonlinearities

240,000 randomly chosen points in parameter space
More than 1,000,000 simulations

The General Framework

$f : X \times \Lambda \to X$ continuous

$$(x, \lambda) \mapsto f(x, \lambda) = f_\lambda(x)$$

X locally compact metric space ($\mathbb{R}^n$)

$\Lambda \subset \mathbb{R}^m$

Goals for a Data-Base

We would like to be able to query to:

- Identify the structure of recurrent dynamics
- Identify gradient-like (non recurrent) dynamics
- Detect and identify bifurcations

Concepts are General

Evolution Equation:

$$u_t = F(u)$$

$$\begin{aligned} \varphi : [0,\infty) \times X &\to X \\ \varphi(0,u) &= u \\ \varphi(t+s,u) &= \varphi(t,\varphi(s,u)) \end{aligned}$$

$$\begin{aligned} f : X &\to X \\ f(u) &= \varphi(\tau,u) \end{aligned}$$

Time Series Data:

$$u_0, u_1, u_2, u_3, \ldots$$

$$x^i = (u_i, u_{i+1}, u_{i+2}) \in \mathbb{R}^3$$

$$\begin{aligned} f : X &\to X \\ x^i &\mapsto x^{i+1} \end{aligned}$$

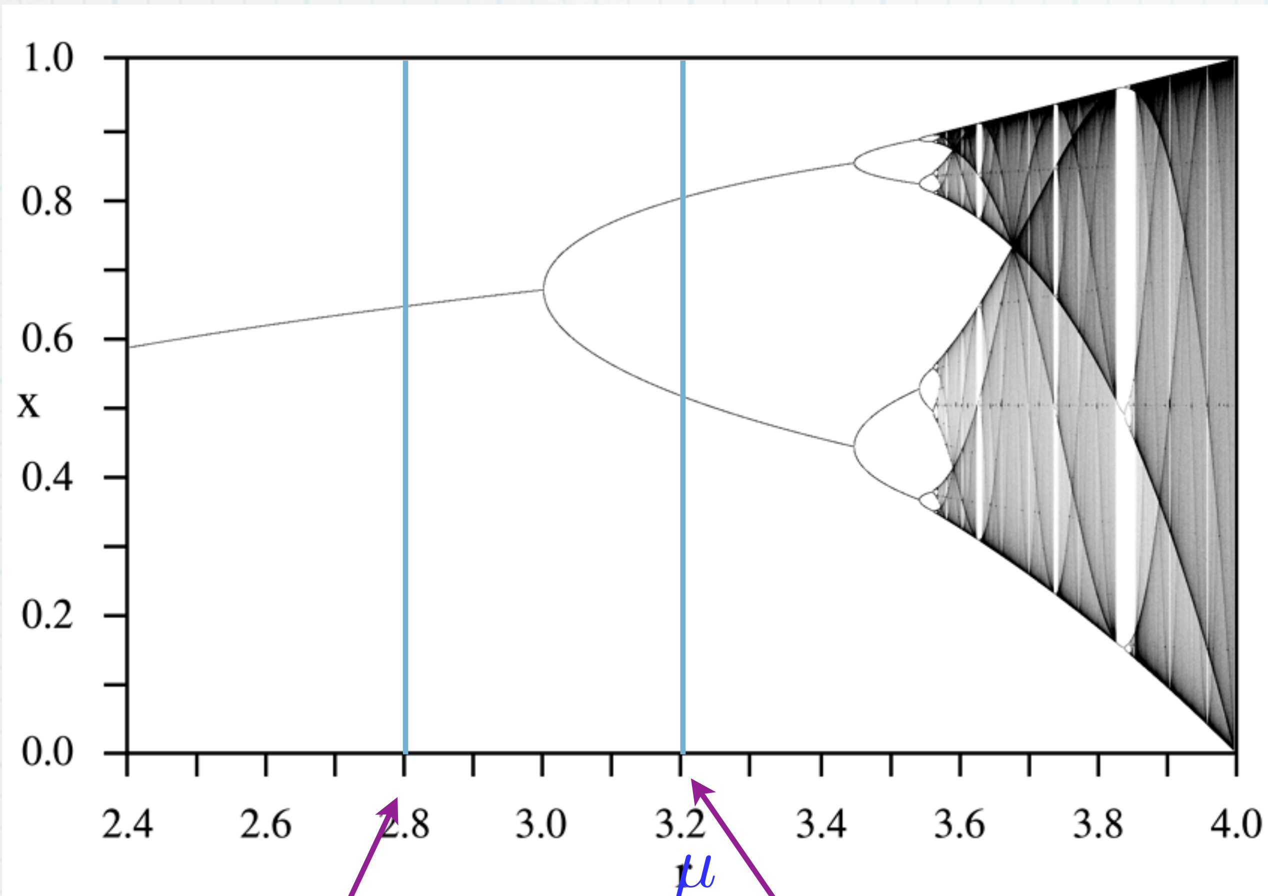
The Basic Problem

- Chaotic dynamics implies sensitivity with respect to initial conditions.
- Solution: Focus on invariant sets. $f_\lambda(S_\lambda) = S_\lambda$
- Bifurcation theory implies structural stability is not generic. Discussed in Stefano's opening lecture in CANDY08 workshop.
- Solution: Focus on isolating neighborhoods and isolated invariant sets.

$$S_\lambda = \mathrm{Inv}(N, f_\lambda) \subset \mathrm{int}(N)$$

Implies moving beyond classical ideas of bifurcations and structural stability.

Form of the Data-Base



Example: The Logistic Map

$$f : \mathbb{R} \times [1,4] \to \mathbb{R}$$

$$f_\mu(x) = f(x,\mu) = \mu \cdot x \cdot (1 - x)$$

stable equilibrium

unstable equilibrium

gradient-like dynamics

stable period 2 orbit

$1 < \mu < 3$

$3 < \mu < 1 + \sqrt{6}$

Data in Data-Base

Directed Graph
(gradient structure)

Algebraic Topology
(recurrent structure)

Some Notation

$f : X \times \Lambda \to X$

Parameterized Dynamical System $F : X \times \Lambda \to X \times \Lambda$

$$F(x, \lambda) = (f_\lambda(x), \lambda) = (f(x, \lambda), \lambda)$$

Given $\Lambda_0 \subset \Lambda$ denote the restriction of F to $X \times \Lambda_0$ by

$$F_{\Lambda_0} : X \times \Lambda_0 \to X \times \Lambda_0$$

Observe: $F = F_\Lambda$

f_λ can be identified with $F_{\{\lambda\}}$.

A Simple Population Model

A density dependent Leslie model:

first year population
second year population

$$\begin{bmatrix} x \\ y \end{bmatrix} \mapsto \begin{bmatrix} (\theta_1 x + \theta_2 y)e^{-c(\theta_1 x + \theta_2 y)} \\ (1-\mu)x \end{bmatrix}$$

Mathematically:

$$f : \mathbb{R}^2 \times \mathbb{R}^4 \to \mathbb{R}^2$$

$$f(x, \theta, \mu, c) = \frac{1}{c} f(cx, \theta, \mu, 1)$$

To communicate the ideas I want to show pictures:

$$\begin{bmatrix} x \\ y \end{bmatrix} \mapsto \begin{bmatrix} (\theta_1 x + \theta_2 y)e^{-0.1(\theta_1 x + \theta_2 y)} \\ 0.7 \cdot x \end{bmatrix}$$

$$f : \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R}^2$$

$$(x, y; \theta_1, \theta_2)$$

$$f : \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R}^2 \qquad \begin{bmatrix} x \\ y \end{bmatrix} \mapsto \begin{bmatrix} (\theta_1 x + \theta_2 y)e^{-0.1(x+y)} \\ 0.7x \end{bmatrix}$$
$$(x, y; \theta_1, \theta_2)$$

Parameterized Dynamical System

$$F : \mathbb{R}^2 \times [10, 50]^2 \to \mathbb{R}^2 \times [10, 50]^2$$

A1: There exists a compact set $R \subset \mathbb{R}^n \times \Lambda$ which is an isolating neighborhood for F.

$$S := \mathrm{Inv}(R, F)$$

Not true for Leslie model, but $f_\theta(R \setminus \{0\}) \subset \mathrm{int}(R \setminus \{0\})$ where

$$R := \{(x_1, x_2, \theta_1, \theta_2) \mid 0 \le x_1 \le \theta_1 + \theta_2,\ 0 \le x_2 \le 0.7(\theta_1 + \theta_2)\}$$

Want to describe: $S_\theta \qquad \theta \in [10, 50]^2$

Reasonable Questions for a Population Model

Global Dynamics:

Are there multiple basins of attraction?

How large are the basins of attraction?

Should we expect extinction?

Local Dynamics:

Are there equilibria and/or periodic orbits?

Is there chaotic dynamics?

Bifurcations:

Are there period doubling bifurcations?

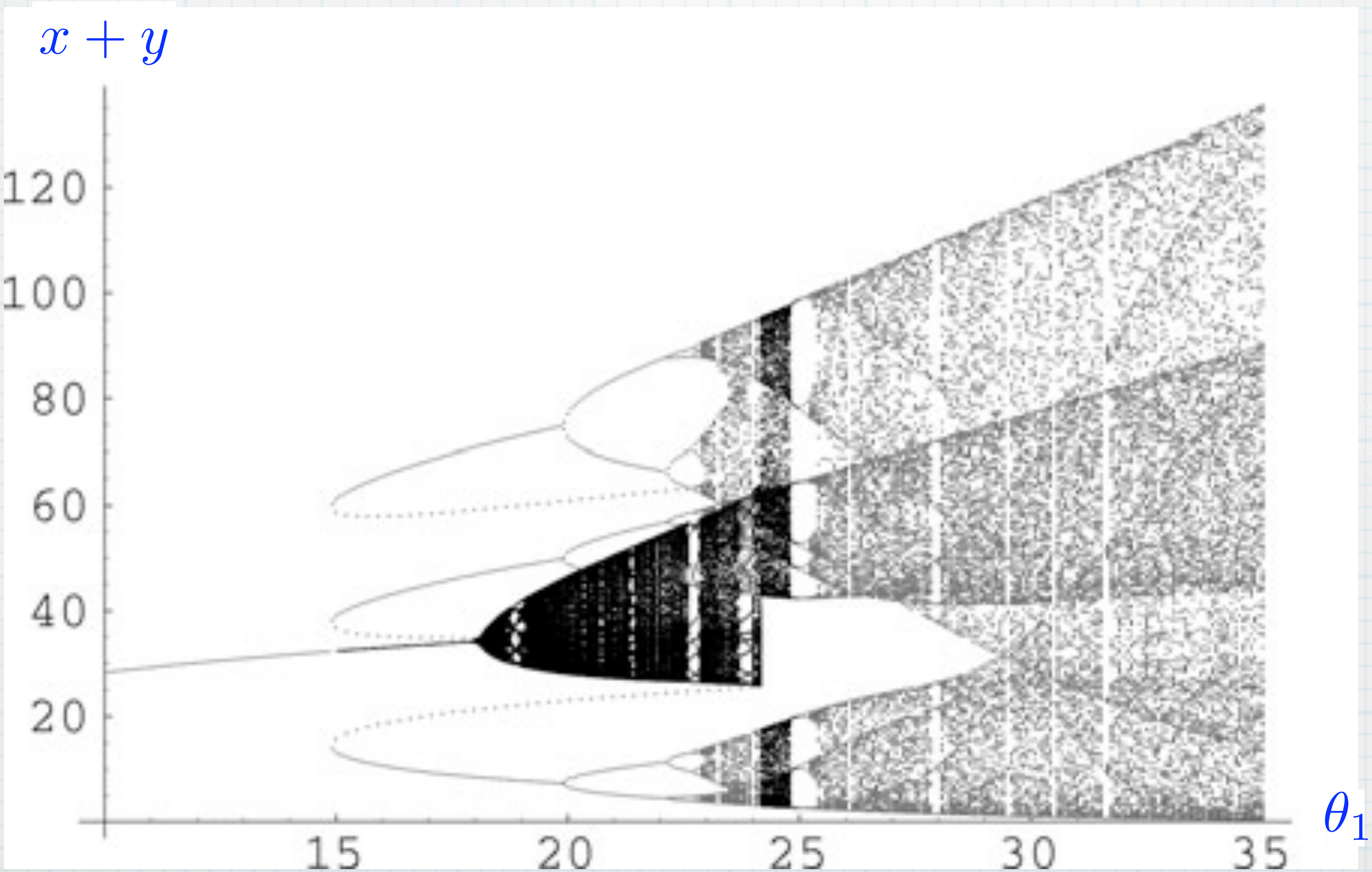
Are there saddle node bifurcations?

$$\begin{bmatrix} x \\ y \end{bmatrix} \mapsto \begin{bmatrix} (\theta_1 x + \theta_2 y)e^{-0.1(x+y)} \\ 0.7x \end{bmatrix}$$

Ugarcovici & Weiss, Nonlinearity '04

$10 \leq \theta_i \leq 50$ $\theta_1 = \theta_2$

Limitations to Presentation:



Single parameter

Only see the attractors

Can't easily probe or extend the results

A Review of Conley Theory

Morse Decompositions

Conley Index

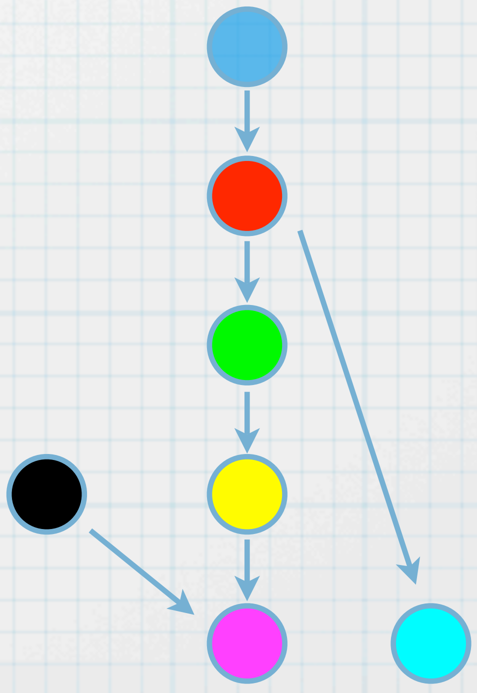
A Morse decomposition of S_{Λ_0} is a finite collection of disjoint isolated invariant subsets of S_{Λ_0}, called Morse sets,

$$\mathbf{M}(S_{\Lambda_0}) := \{M_{\Lambda_0}(p) \subset S_{\Lambda_0} \mid p \in \mathcal{P}_{\Lambda_0}\},$$

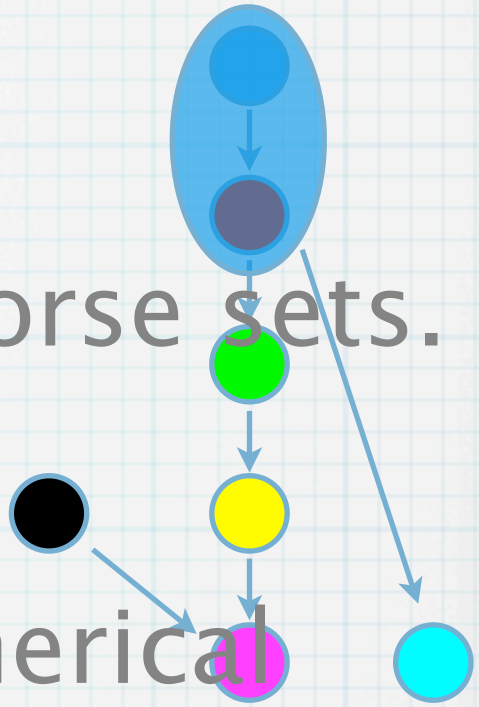
for which there exists a strict partial order $>_{\Lambda_0}$, called an admissible order, on the indexing set $\mathcal{P}_{\Lambda_0}$ such that for every $(x,\lambda) \in S_{\Lambda_0} \setminus \cup_{p\in\mathcal{P}} M_{\Lambda_0}(p)$ and any complete orbit γ of (x,λ) in S_{Λ_0} there exists indices $p >_{\Lambda_0} q$ such that under F_{Λ_0}

$$\omega(\gamma) \subset M_{\Lambda_0}(q) \quad \text{and} \quad \alpha(\gamma) \subset M_{\Lambda_0}(p)$$

Since $\mathcal{P}_{\Lambda_0}$ is a partially ordered set, a Morse decomposition can be represented as an acyclic directed graph $\mathcal{MG}(\Lambda_0)$ called the Morse graph.



Remarks about Morse Decompositions:



- All recurrent dynamics occurs within Morse sets.
- Morse Decompositions are not unique.
- The empty set can be a Morse set (Numerical artifacts).
- Given a Morse decomposition

$$\mathbf{M}(S_{\Lambda_0}) := \{M_{\Lambda_0}(p) \subset S_{\Lambda_0} \mid p \in (\mathcal{P}_{\Lambda_0}, >_{\Lambda_0})\}$$

if $\Lambda_1 \subset \Lambda_0$ then

$$\{M_{\Lambda_1}(p) \subset S_{\Lambda_1} \mid p \in (\mathcal{P}_{\Lambda_0}, >_{\Lambda_0})\}$$

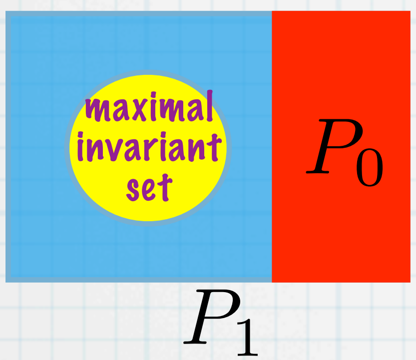
is a Morse decomposition of S_{Λ_1} under F_{Λ_1} where

$$M_{\Lambda_1}(p) := M_{\Lambda_0}(p) \cap (X \times \Lambda_1)$$

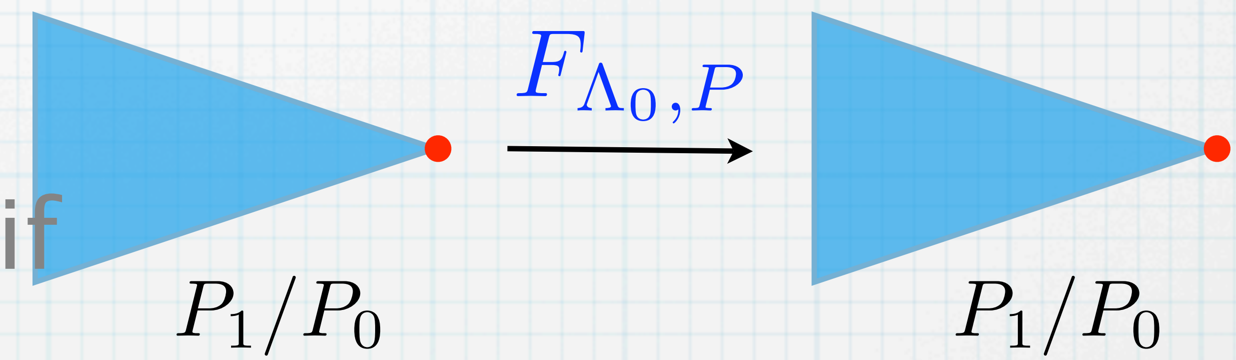
Conley Index

Let $P = (P_1, P_0)$ with $P_0 \subset P_1$ be a pair of compact sets in $X \times \Lambda_0$.

Define $F_{\Lambda_0,P} : P_1/P_0 \to P_1/P_0$ by



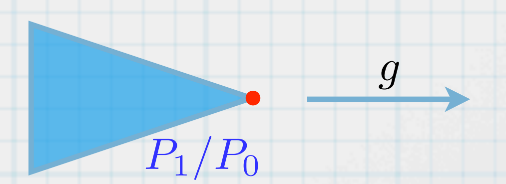
$$F_{\Lambda_0,P}(x) = \begin{cases} F_{\Lambda_0}(x,\lambda) & \text{if } (x,\lambda), F_{\Lambda_0}(x,\lambda) \in P_1 \setminus P_0 \\ [P_0] & \text{otherwise} \end{cases}$$



P is an index pair for $F_{\Lambda_0,P}$ if

- $F_{\Lambda_0,P}$ is continuous.
- $\mathrm{cl}(P_1 \setminus P_0)$ is an isolating neighborhood

Fact: If no iterate of $F_{\Lambda_0,P}$ is homotopic to the trivial map, then $\mathrm{Inv}(\mathrm{cl}(P_1 \setminus P_0), F_{\lambda_0}) \neq \emptyset$



Corollary: If $F_{\Lambda_0,P*} : H_*(P_1/P_0, [P_0]) \to H_*(P_1/P_0, [P_0])$ is not nilpotent, then $\mathrm{Inv}(\mathrm{cl}(P_1 \setminus P_0), F_{\Lambda_0}) \neq \emptyset$.

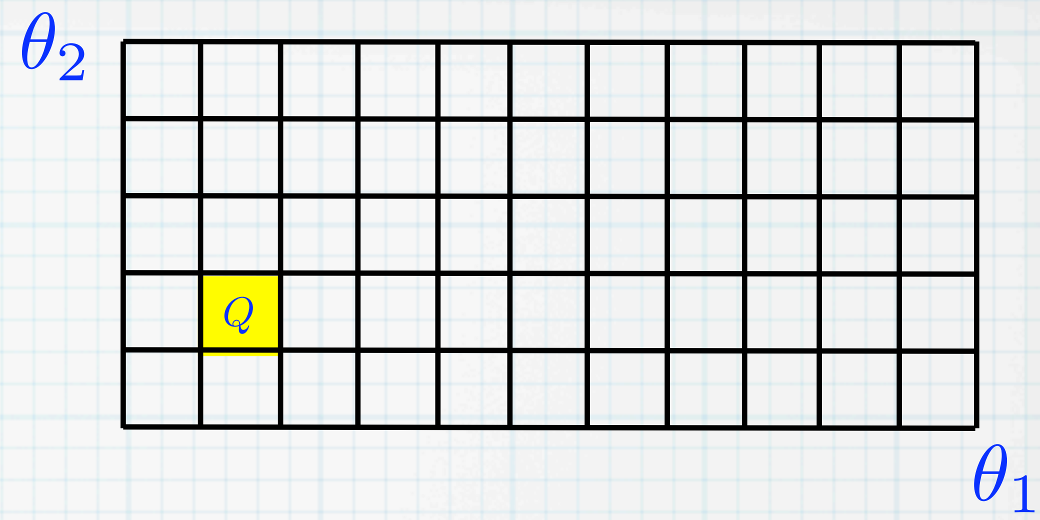
The Conley index is the shift equivalence class of

$$F_{\Lambda_0,P*} : H_*(P_1/P_0, [P_0]) \to H_*(P_1/P_0, [P_0])$$

Theorem: Let $S_{\Lambda_0} := \mathrm{Inv}(\mathrm{cl}(P_1 \setminus P_0), F_{\Lambda_0})$
If Λ_0 is simply connected then the Conley index of S_{Λ_0} and S_λ are equivalent for all $\lambda \in \Lambda_0$.

Computing the Dynamics

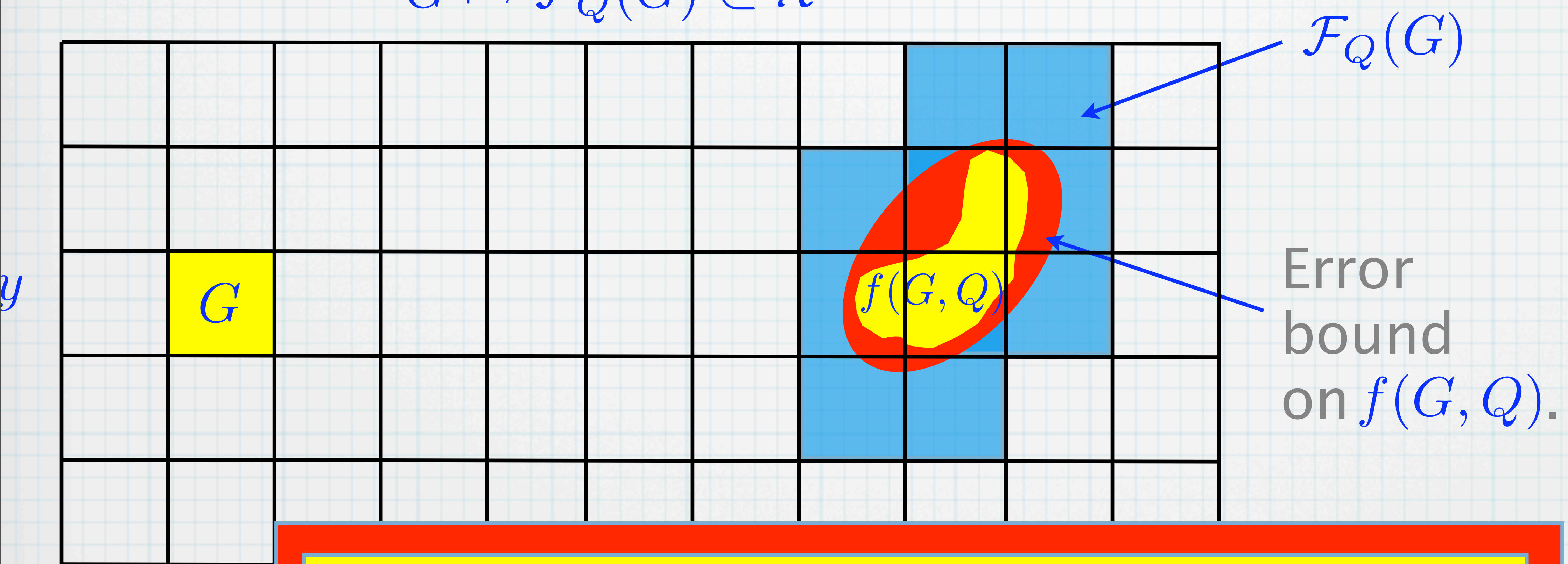
Choose a cubical grid $\mathcal{Q}$ that covers Λ.



Choose a cubical grid $\mathcal{X}$ that covers X.

Construct a combinatorial multivalued map $\mathcal{F}_Q : \mathcal{X} \rightrightarrows \mathcal{X}$.

$$G \mapsto \mathcal{F}_Q(G) \subset \mathcal{X}$$



A multivalued map $\mathcal{F}_Q : \mathcal{X} \rightrightarrows \mathcal{X}$ is an outer approximation of $f : X \times Q \to X$ if

$$f(G,Q) \subset \operatorname{int}\left(|\mathcal{F}_Q(G)|\right) \quad \forall\, G \in \mathcal{X}$$

Let $\mathcal{F} : \mathcal{X} \rightrightarrows \mathcal{X}$ be an outer approximation for $f : X \times Q \to X$

Think of $\mathcal{F}$ as a directed graph: Vertices $G \in \mathcal{X}$

Edges $G \to H$ if $H \in \mathcal{F}(G)$

The recurrent set for $\mathcal{F}$ is

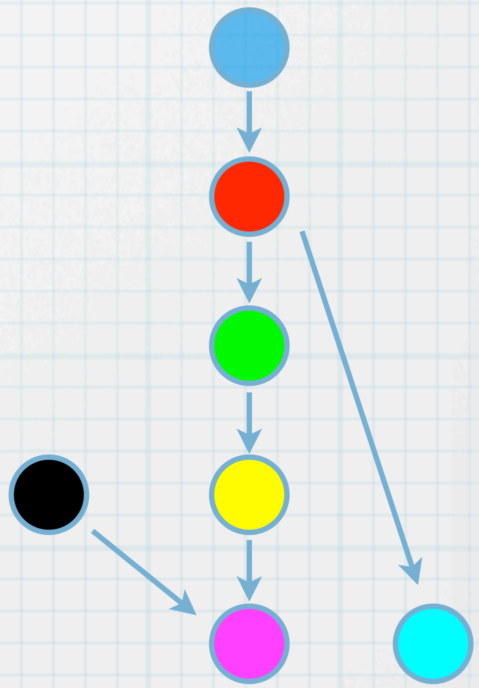
$$\mathcal{R}(\mathcal{F}) := \{G \in \mathcal{X} \mid \exists \text{ nontrivial path from } G \text{ to } G\}$$

A Morse set of $\mathcal{R}(\mathcal{F})$ is an equivalence class:

$G \sim H \quad \Leftrightarrow \quad$ There exists a path from G to H and a path from H to G.

Fact: There exists an algorithm $O(|\mathcal{X}| + |\mathcal{F}|)$ that produces a function $\kappa : \mathcal{X} \to \mathbb{Z}$ such that $\forall H \in \mathcal{F}(G)$

1. $G \sim H \quad \Rightarrow \quad \kappa(G) = \kappa(H)$
2. $G \not\sim H \quad \Rightarrow \quad \kappa(G) > \kappa(H)$

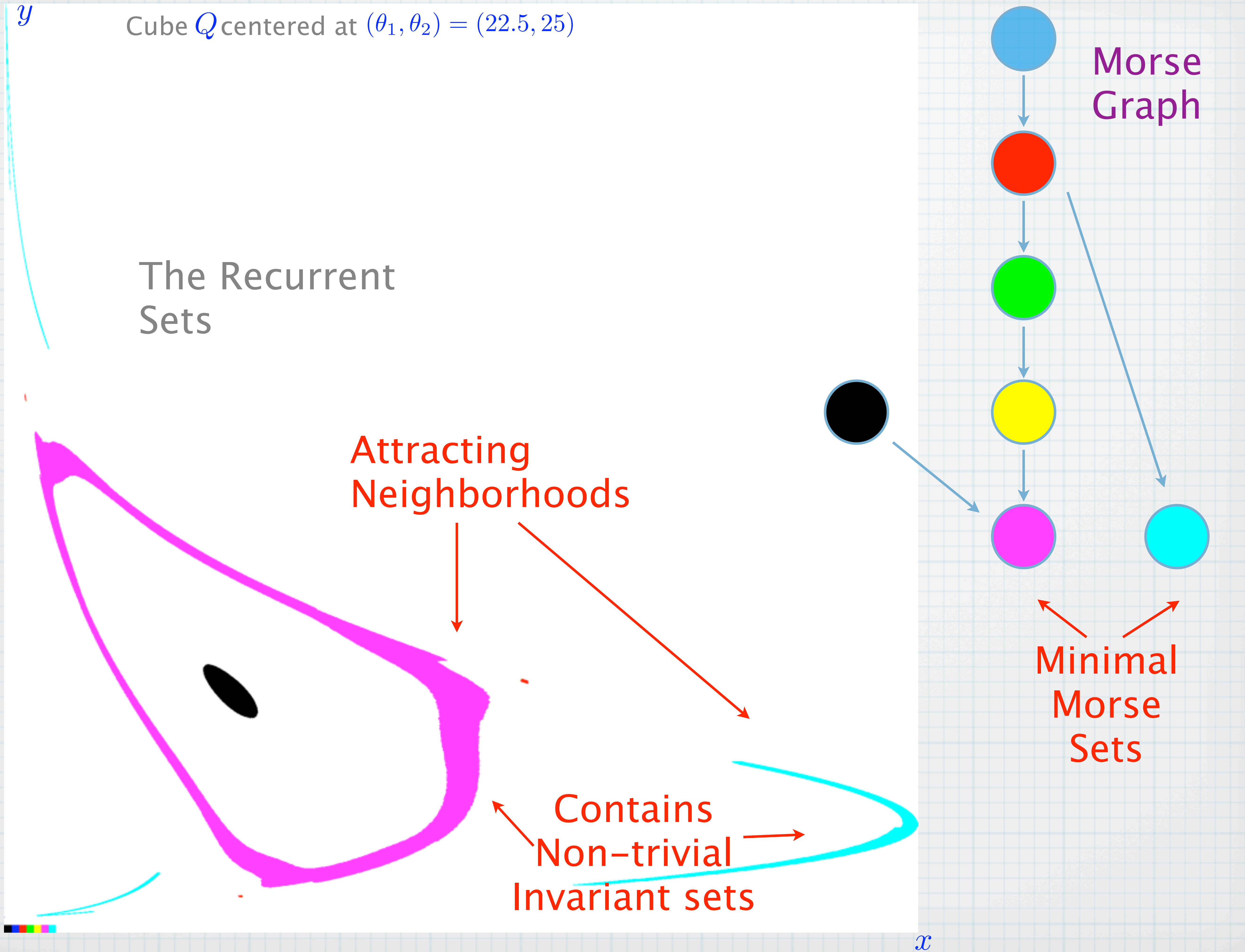


Corollary: There exists a partial ordering (acyclic directed graph) relating the Morse sets of $\mathcal{F}$.

We have a Morse Graph!

Prop: Let $\{\mathcal{M}_Q(p) \mid p \in (\mathcal{P}_Q, >_Q)\}$ be the Morse sets for $\mathcal{F}_Q$. Then $\mathbf{M}(S_Q) := \{M_Q(p) \mid p \in (\mathcal{P}_Q, >_Q)\}$ where $M_Q(p) := \mathrm{Inv}(|\mathcal{M}_Q(p)|, F_Q)$ is a Morse decomposition for S_Q.

The acyclic directed graph that represents the Morse sets for $\mathcal{F}_Q$ define a Morse graph $\mathcal{MG}(\mathcal{F}_Q)$ for a Morse decomposition of S_Q


y
Cube Q centered at $(\theta_1, \theta_2) = (22.5, 25)$
The Recurrent Sets
Attracting Neighborhoods
Contains Non-trivial Invariant sets
x
Morse Graph
Minimal Morse Sets

We have a Conley-Morse Graph!

Prop: $|\mathcal{M}_Q(p)|$ is an isolating block for F_Q.

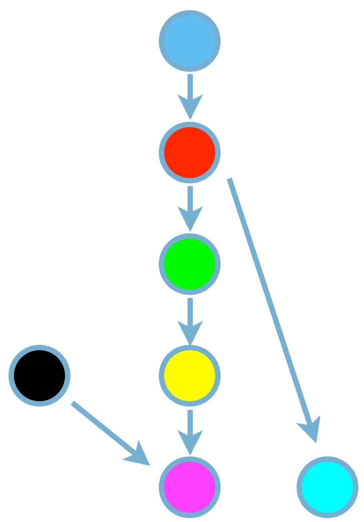
Given an outer approximation $\mathcal{F}_Q$ there exist algorithms for producing index pairs $P = (P_1, P_0)$ and computing

$$F_{\Lambda_0, P*} : H_*(P_1/P_0, [P_0]) \to H_*(P_1/P_0, [P_0])$$

Reference: Computational Homology
T. Kaczynski, K. M., M. Mrozek

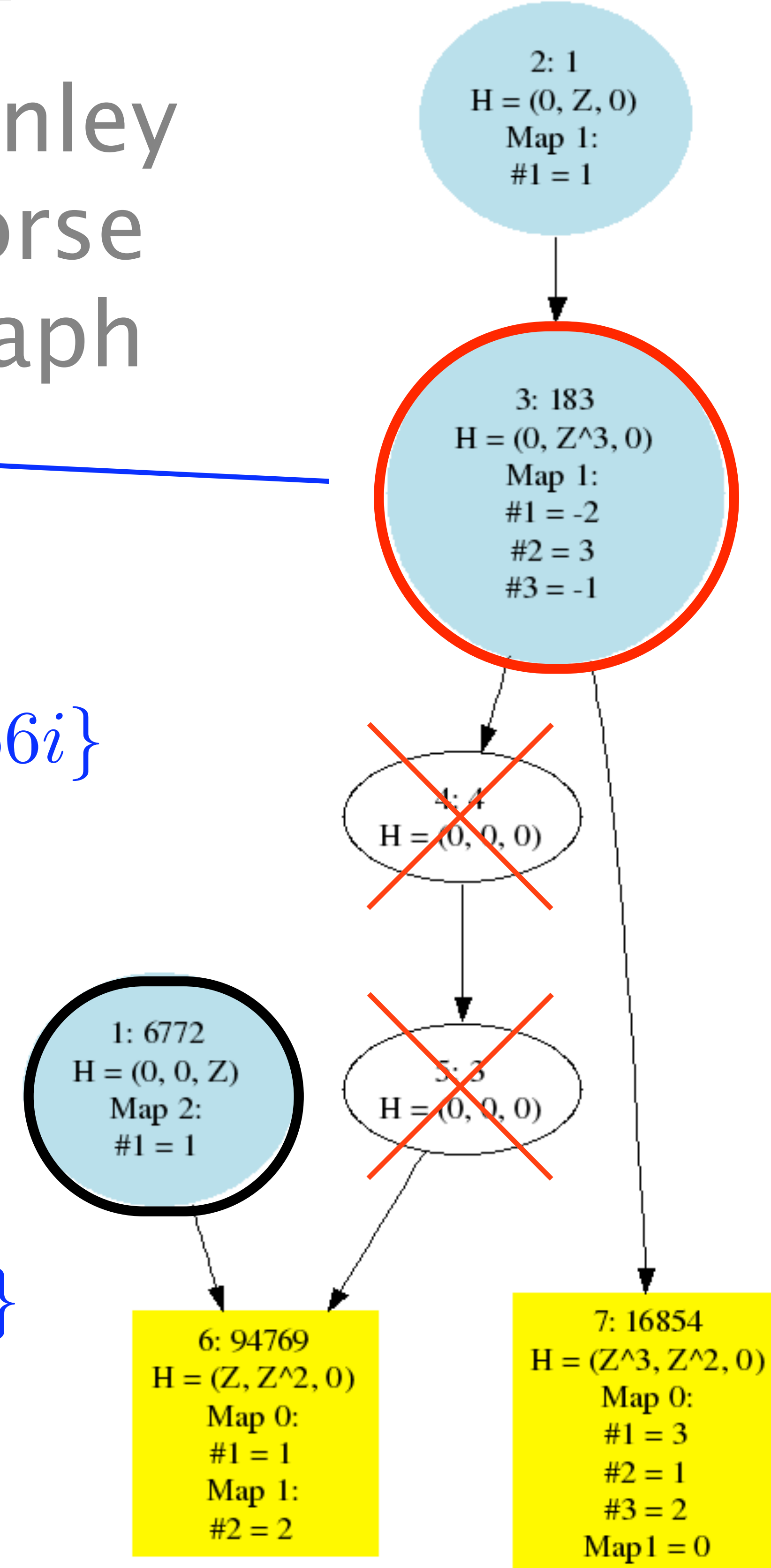
Software: http://chomp.rutgers.edu/

Conley Morse Graph



$$\begin{bmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

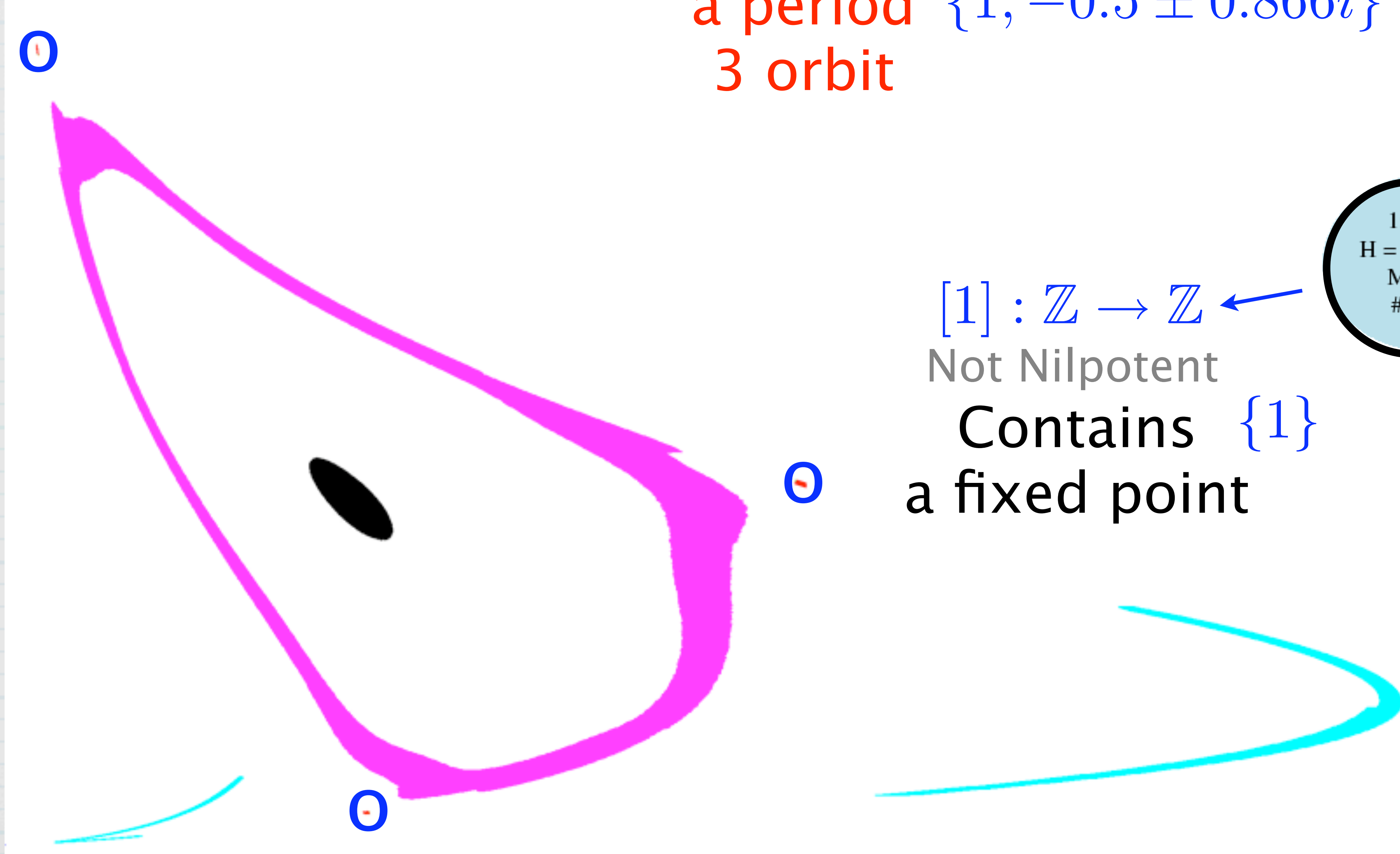
Contains a period 3 orbit $\{1, -0.5 \pm 0.866i\}$



$[1] : \mathbb{Z} \to \mathbb{Z}$

Not Nilpotent

Contains a fixed point $\{1\}$



Relating the Computations

Consider $Q_0, Q_1 \in \mathcal{Q}$ such that $Q_0 \cap Q_1 \neq \emptyset$.

How should we define $\mathcal{CMG}(\mathcal{F}_{Q_0}) \cong \mathcal{CMG}(\mathcal{F}_{Q_1})$?

We have the Morse sets for outer approximations:

$\{\mathcal{M}_{Q_0}(p) \mid p \in (\mathcal{P}_{Q_0}, >_{Q_0})\}$ $\{\mathcal{M}_{Q_1}(q) \mid q \in (\mathcal{P}_{Q_1}, >_{Q_1})\}$

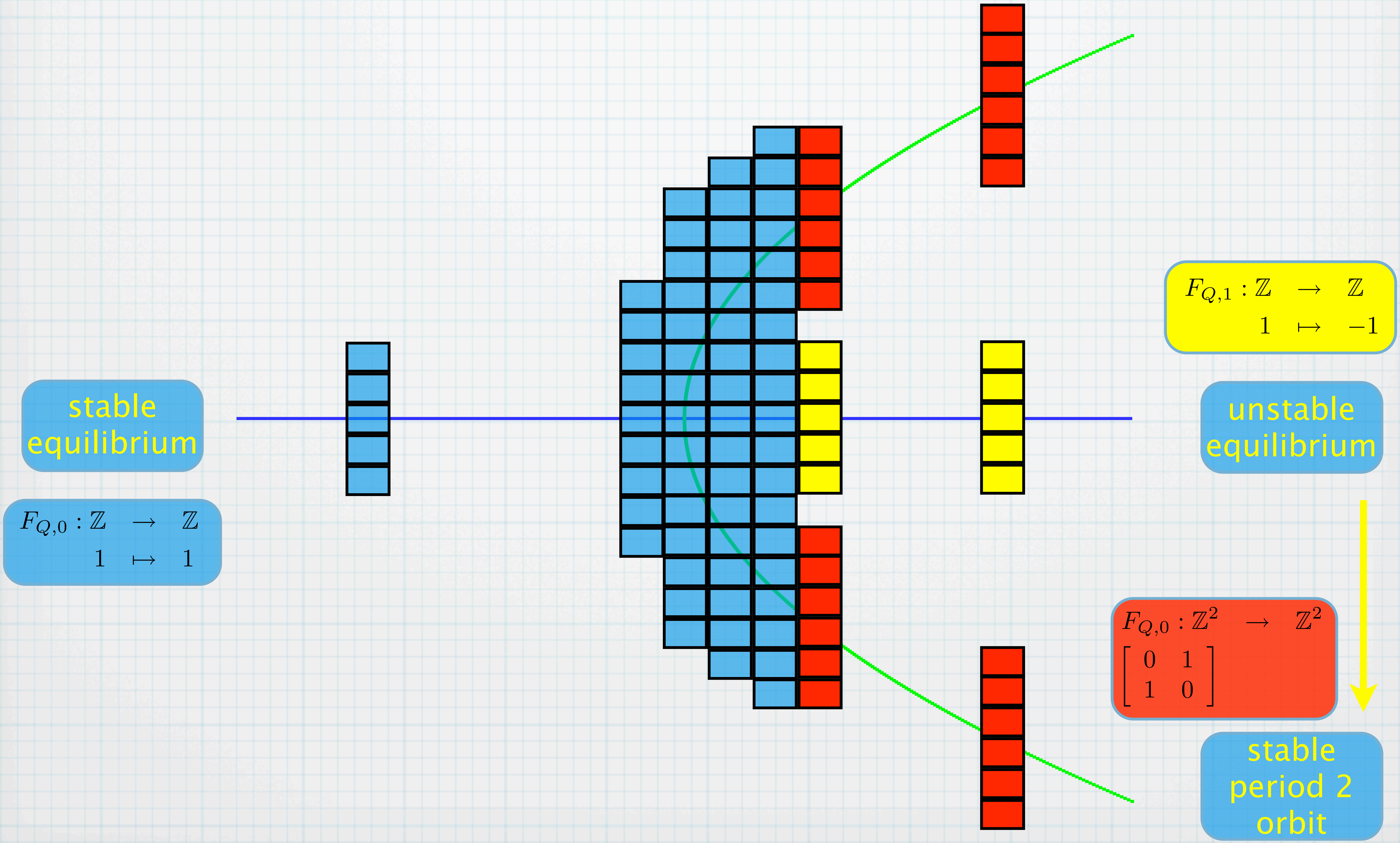
Construct relation ι_{Q_1,Q_0} with relations $p_i \to q_j$ if

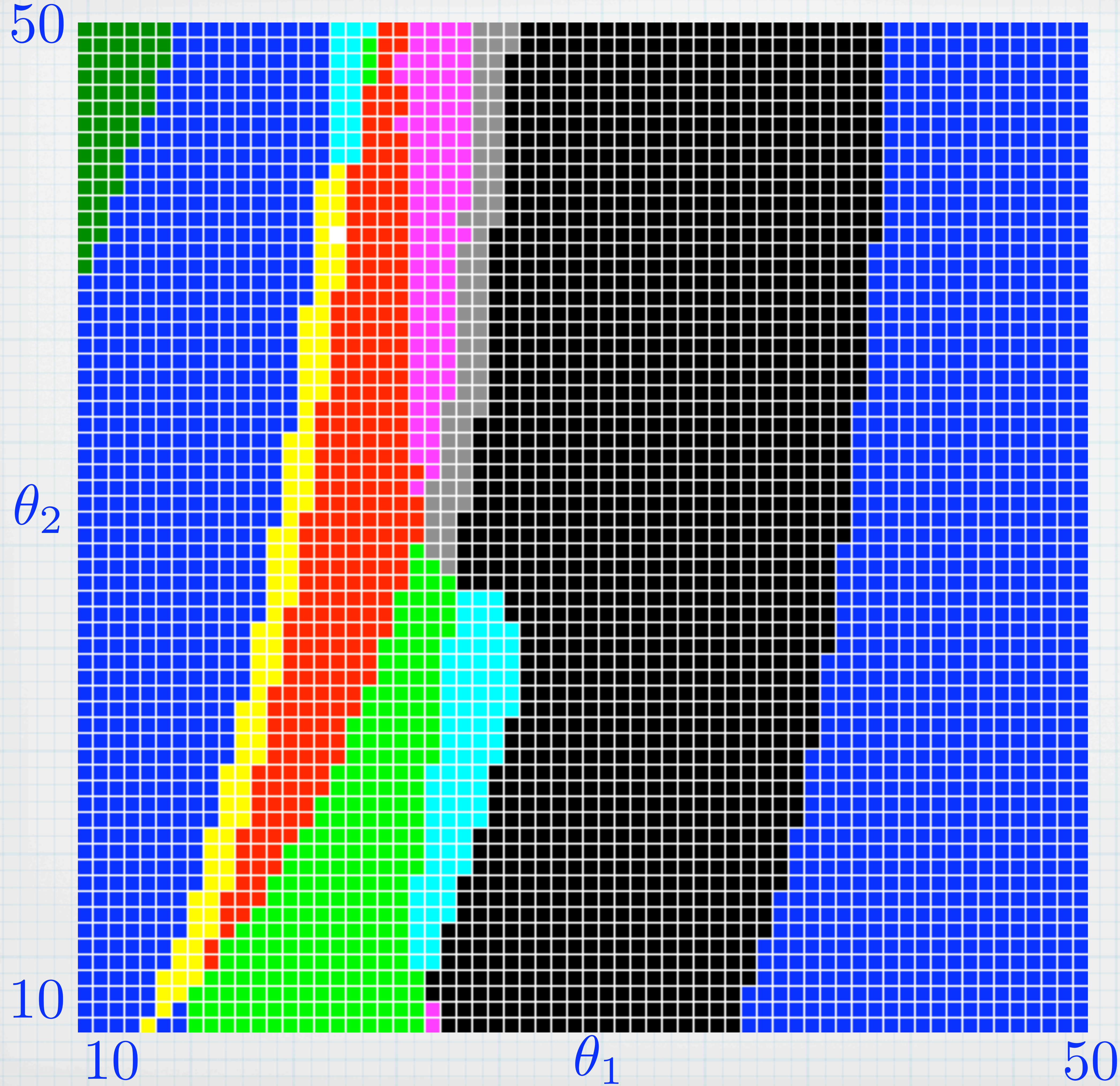
$$\mathcal{M}_{Q_0}(p_i) \cap \mathcal{M}_{Q_1}(q_j) \neq \emptyset$$

Defn: $\mathcal{CMG}(\mathcal{F}_{Q_0})$ and $\mathcal{CMG}(\mathcal{F}_{Q_1})$ are phenotypically equivalent if ι_{Q_1,Q_0} is a directed graph isomorphism.

An Example

Period Doubling Bifurcation $f : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$





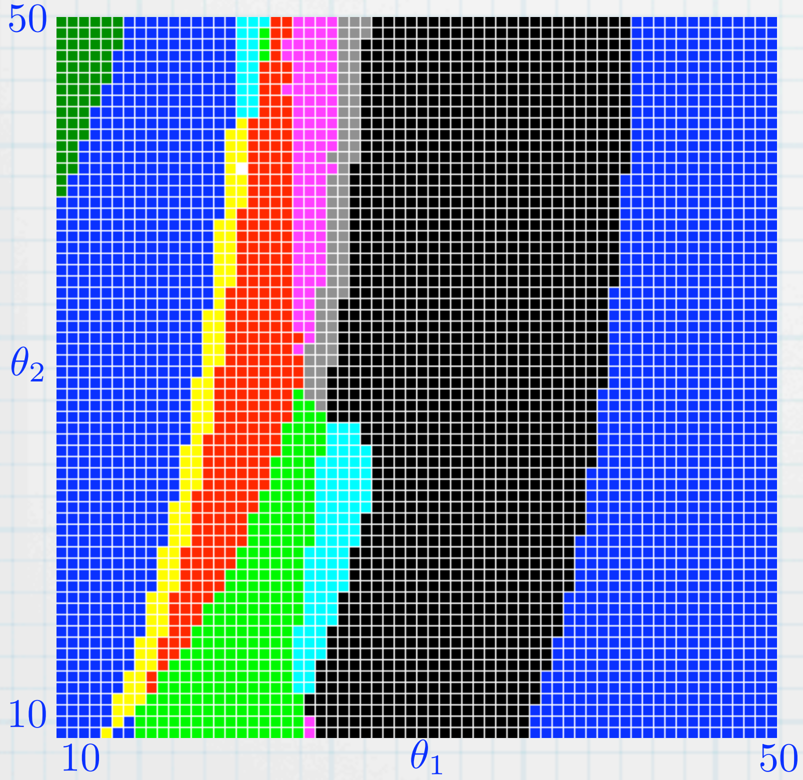
The Data Base!

Different colors represent different phenotypic dynamics

Recall: N is an isolating neighborhood if $\mathrm{Inv}(N, f) \subset \mathrm{int}(N)$

Thus: If N is an isolating neighborhood for f_{λ_0} then N is an isolating neighborhood for f_{λ_1}.

Theorem: (Conley, Montgomery) The space of isolated invariant sets is a sheaf over Λ.



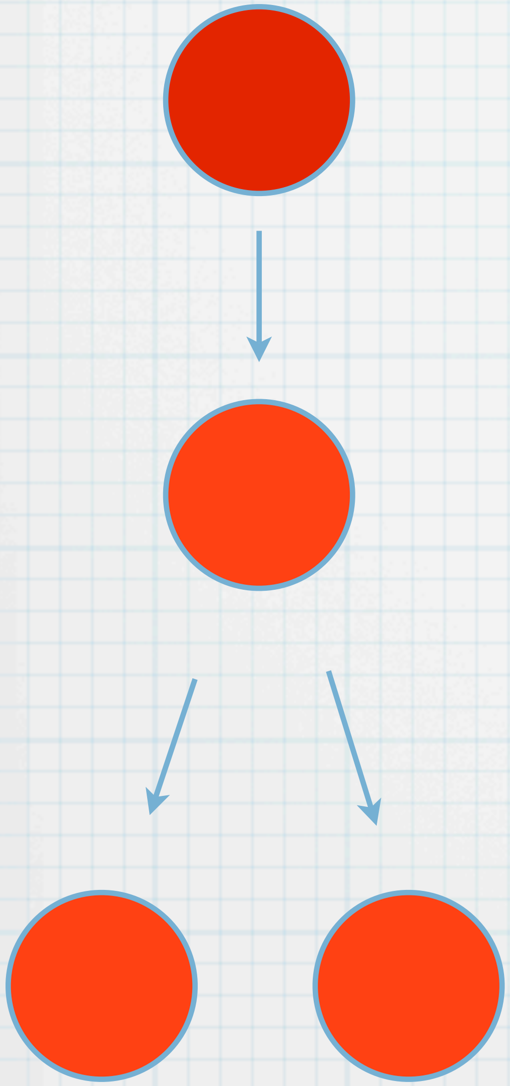
Remark 1: We have built a bundle
fiber = Conley–Morse graph
over each colored region in parameter space.

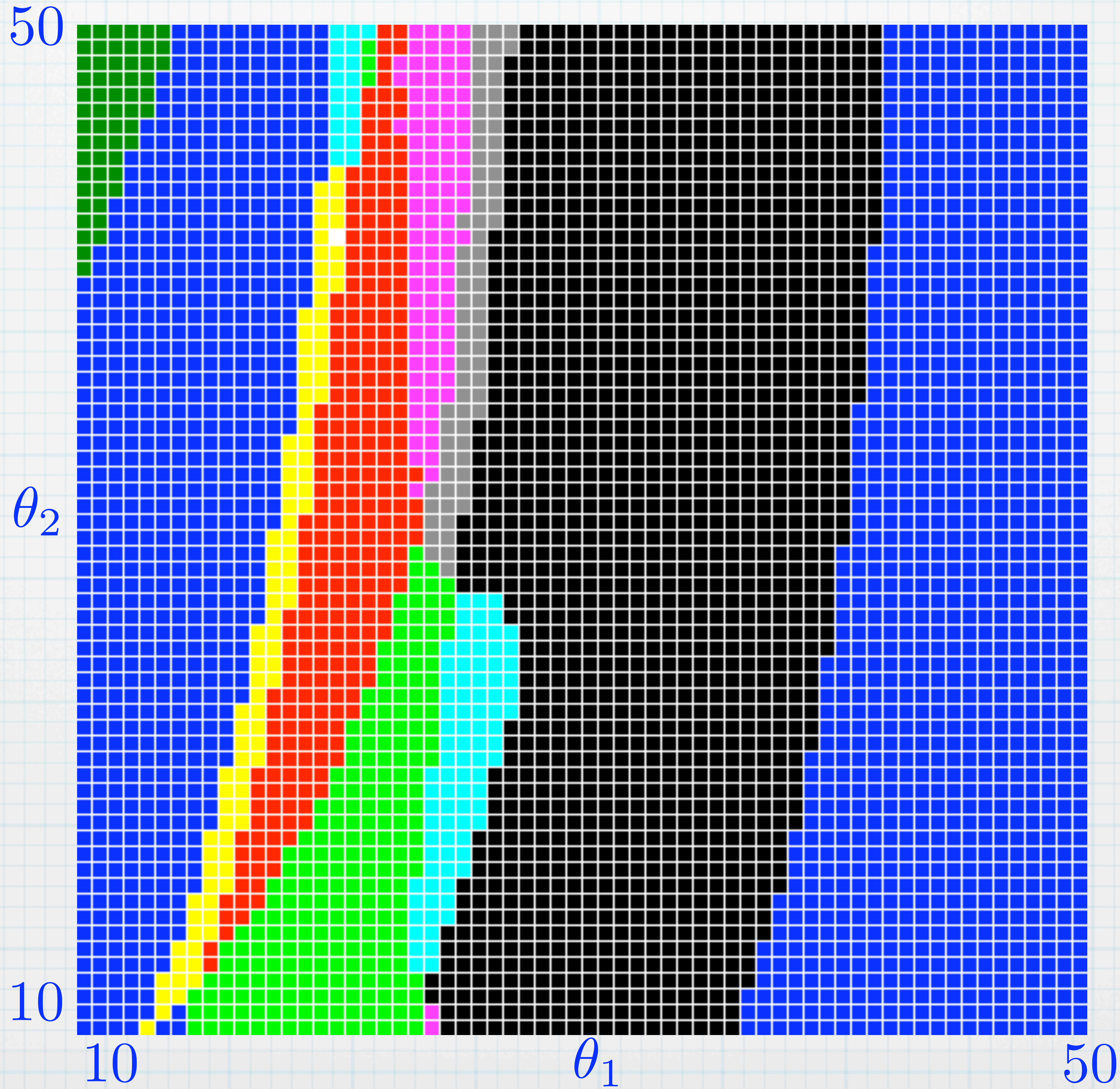
Remark 2: If these bundles are nontrivial, then there must be global bifurcations.

Let’s Query the DataBase!

Multiple Basins of Attraction

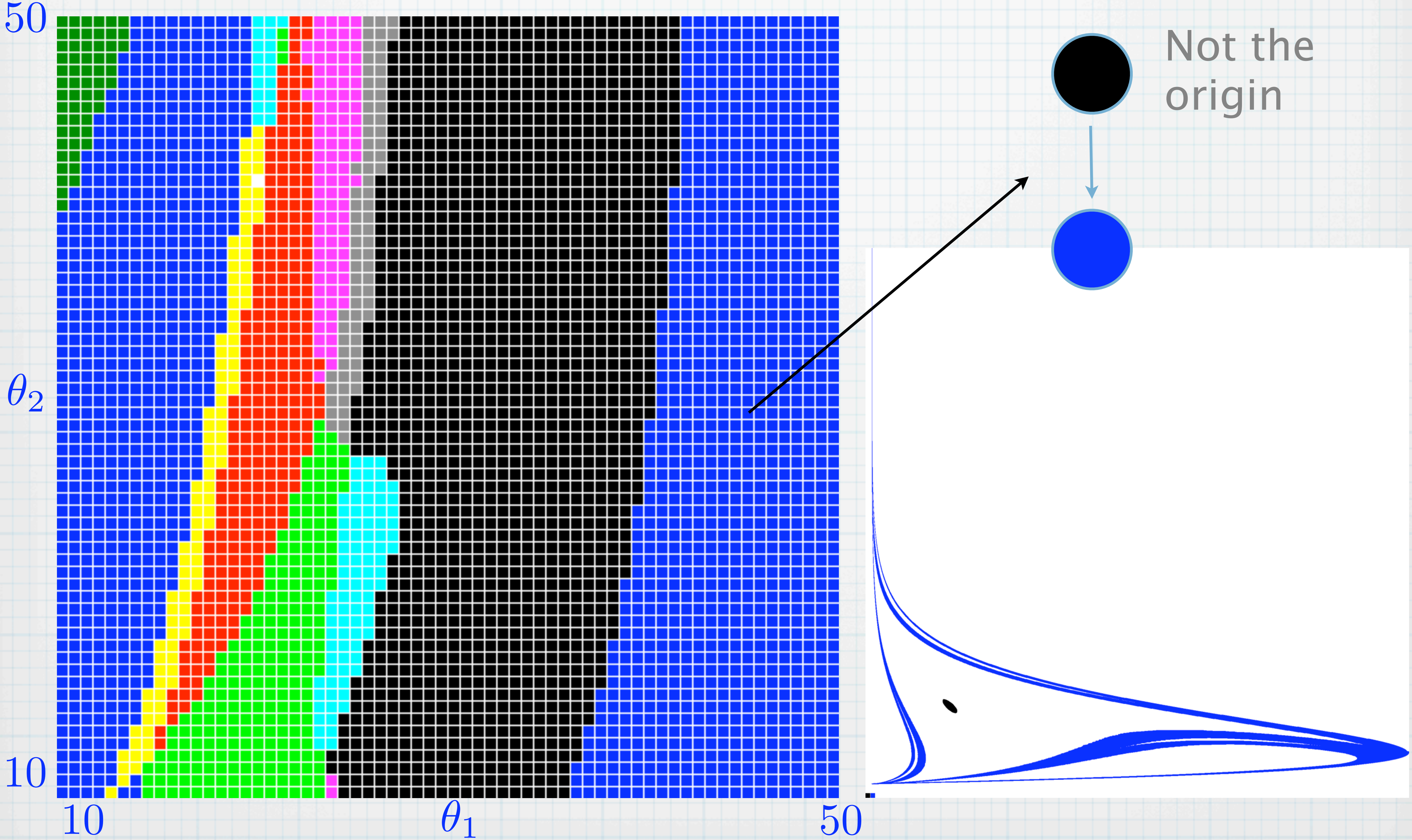
(Multiple minima in directed graph)





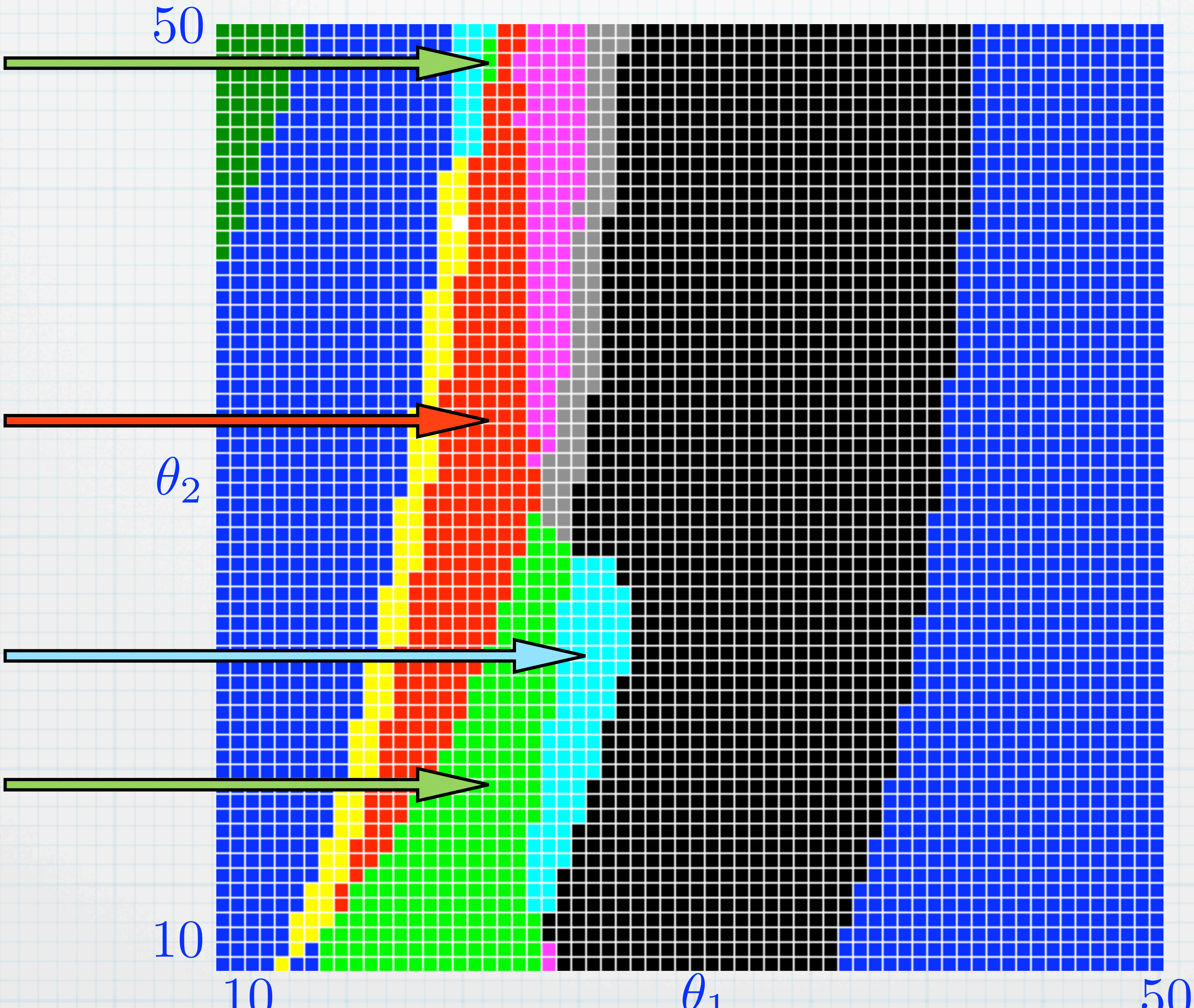
Probable Extinction

(Minimal element of graph contains a cube which intersects origin)



Possible Stable Period 3 Orbit

(Minimal element of graph with index $\left\{1^{1/3}\right\}$)



Period Doubling Bifurcation

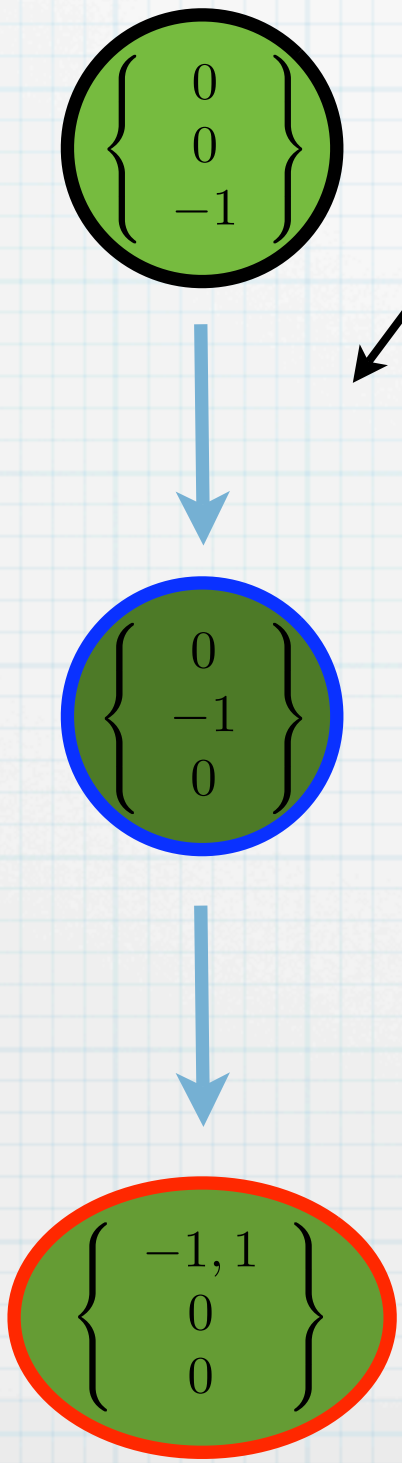
Interpretive *Guide* to Dynamics

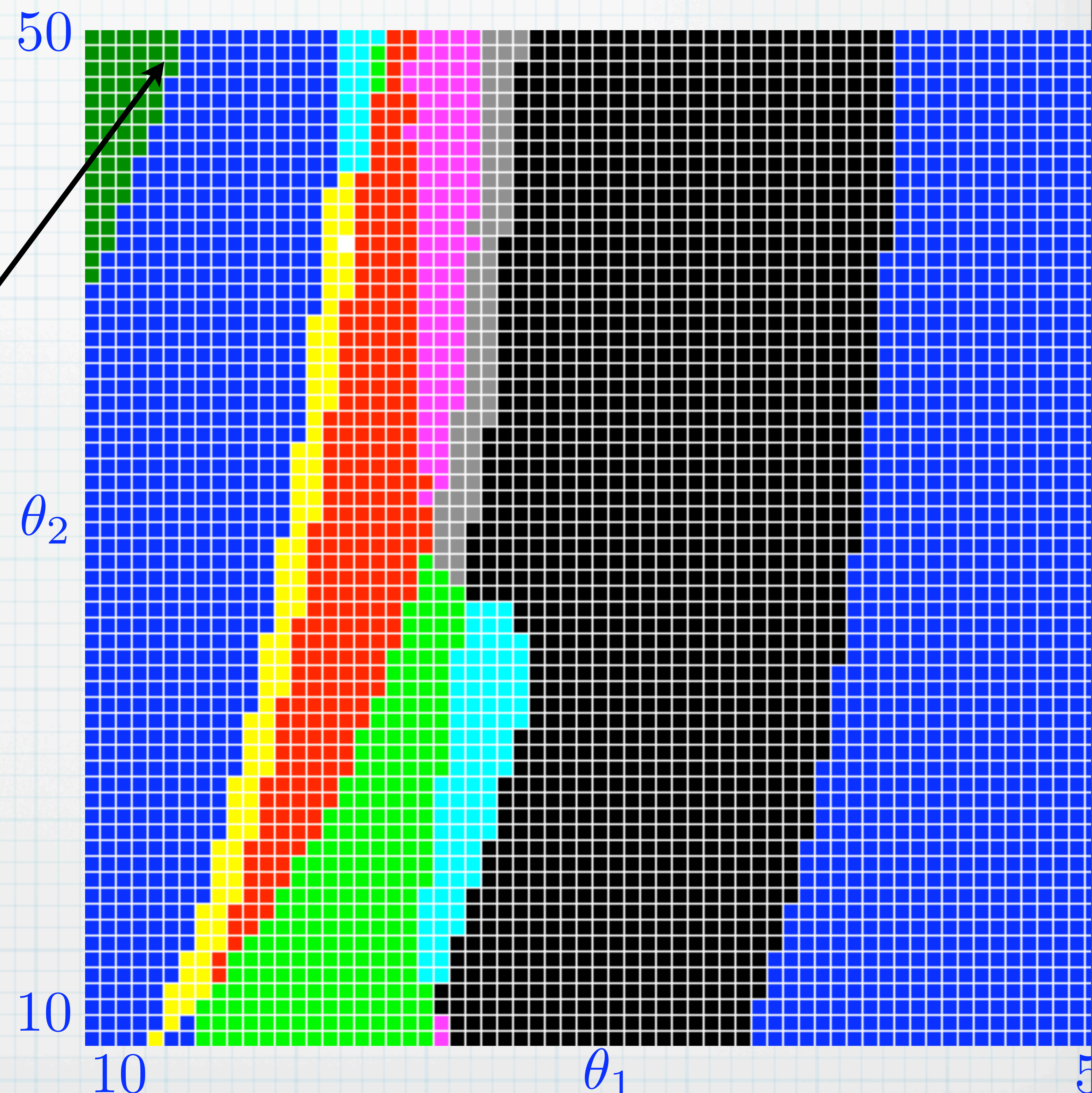
Conley Morse Graph

Equilibrium 2-d unstable manifold with flip

Equilibrium 1-d unstable manifold with flip

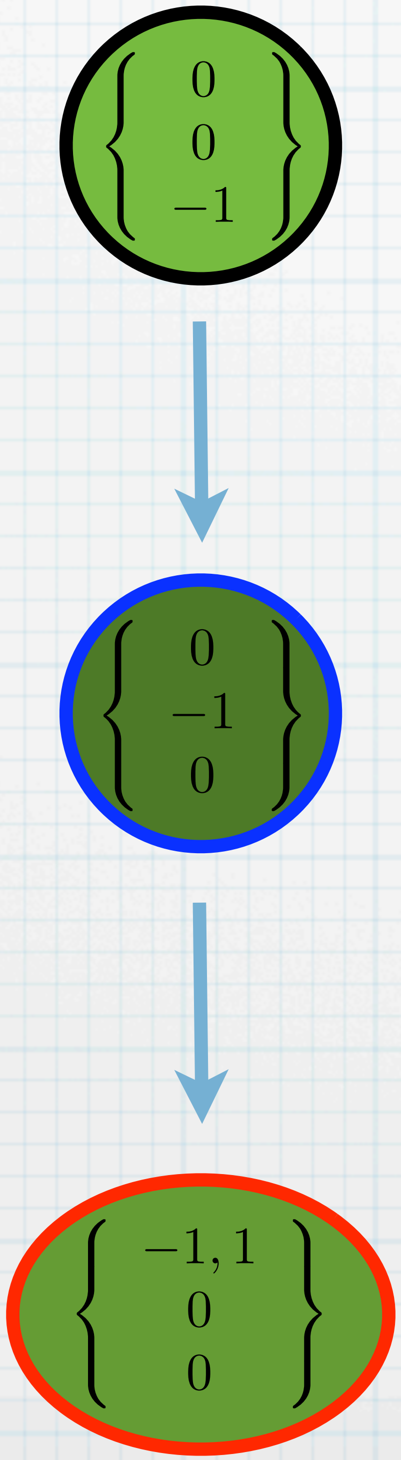
Stable Period 2 orbit





Interpretive *Guide* to Dynamics

Conley Morse Graph



Equilibrium 2-d unstable manifold with flip

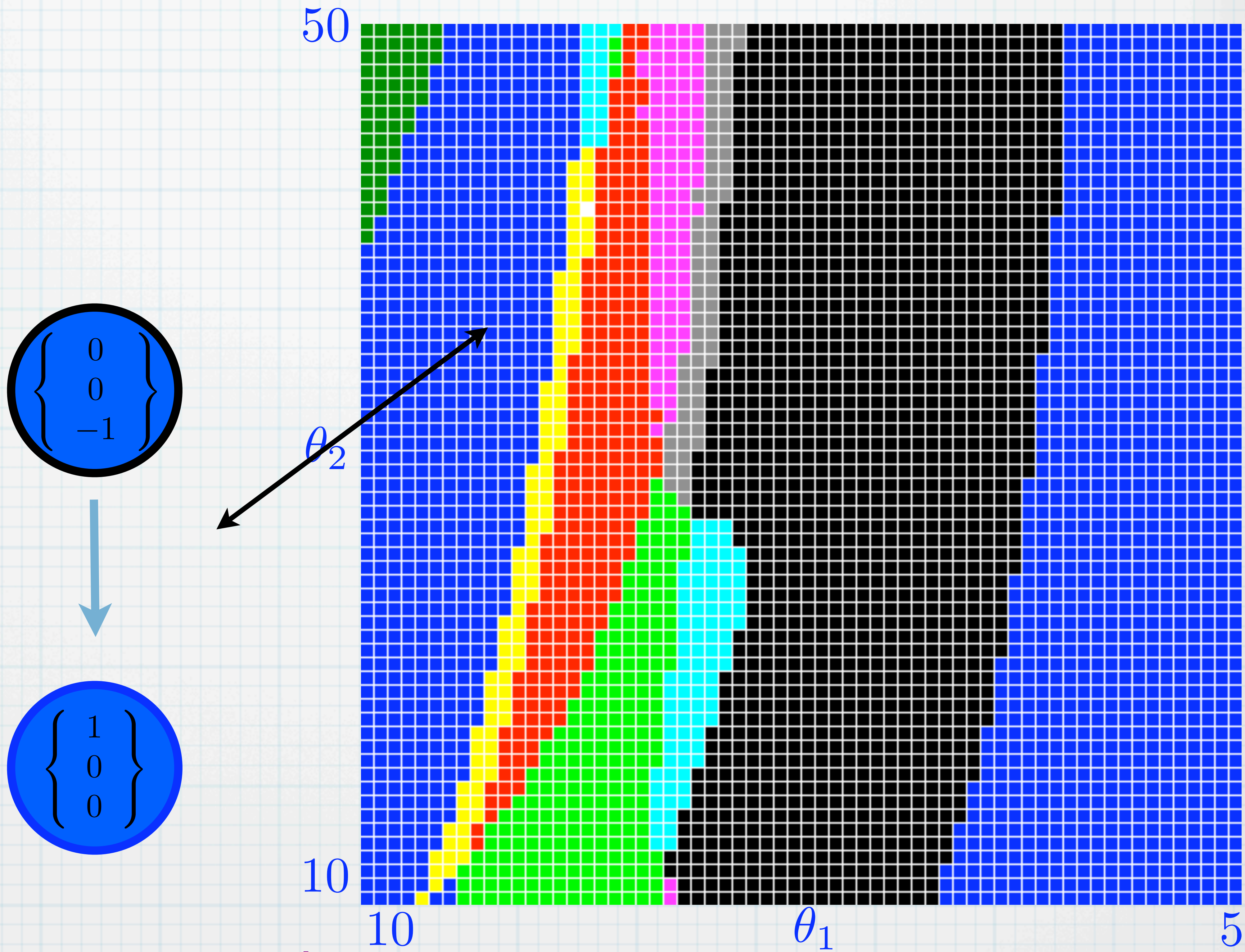
Equilibrium 1-d unstable manifold with flip

Stable Period 2 orbit

Interpretive *Guide* to Dynamics

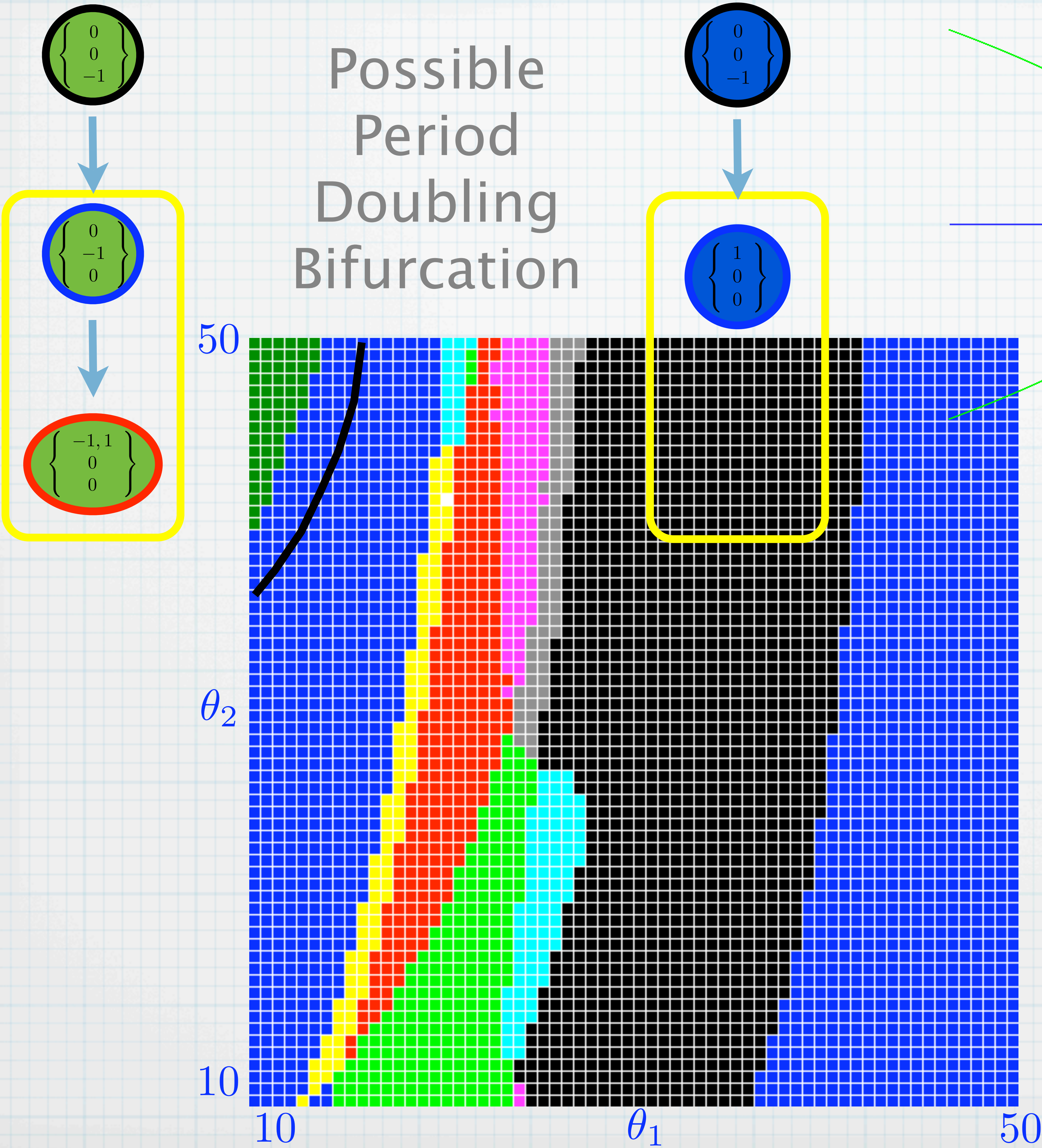
Equilibrium
2-d unstable
manifold

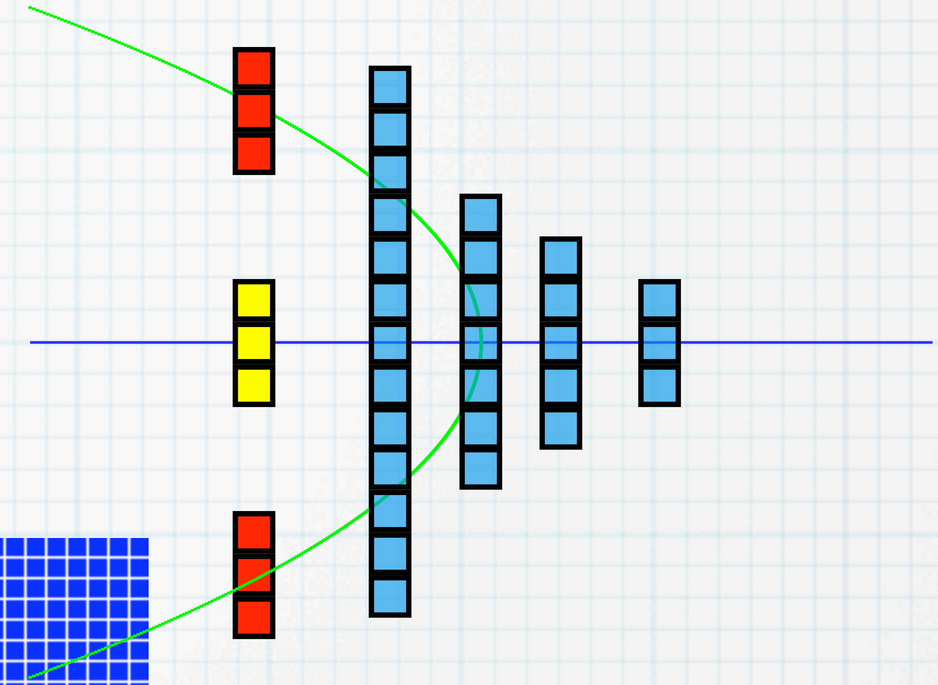
Equilibrium
stable



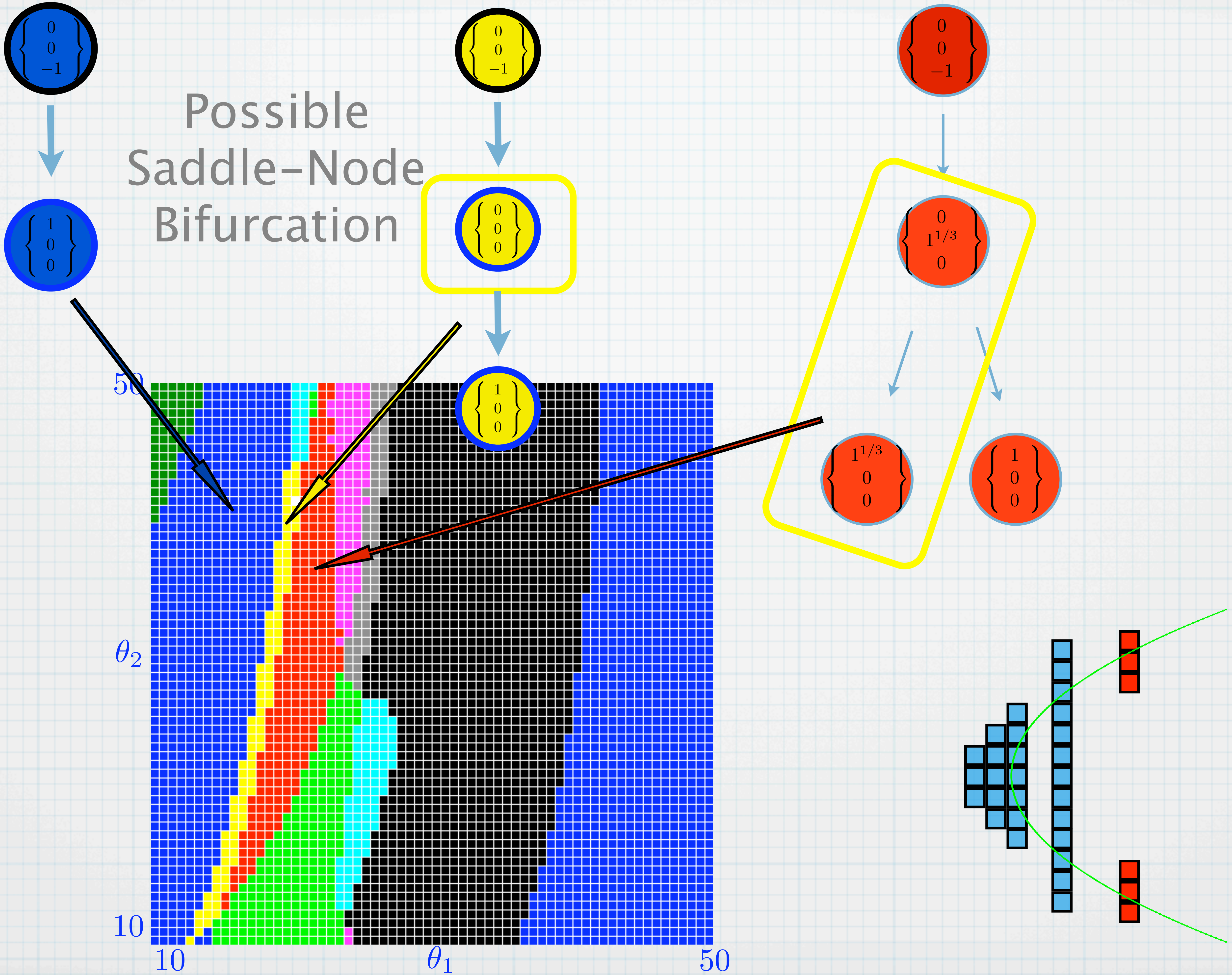
Conley Morse Graph

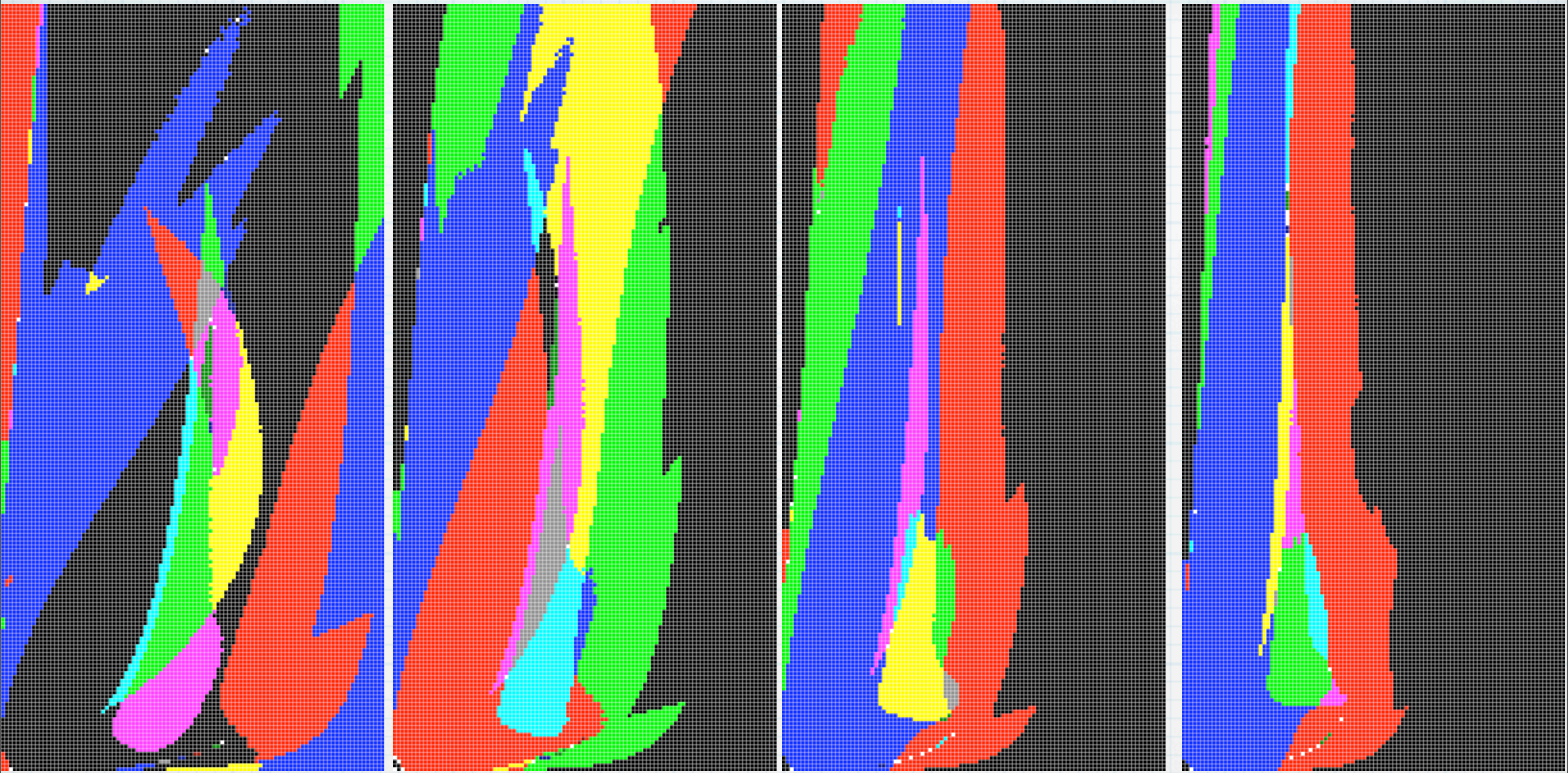
Possible Period Doubling Bifurcation





Possible Saddle-Node Bifurcation





p = 0.6 p = 0.7 p = 0.8 p = 0.9

$$\Lambda = [0, 50] \times [0, 100]$$

Thank-you for your attention

DARPA

National Science Foundation
WHERE DISCOVERIES BEGIN

U.S. DEPARTMENT OF ENERGY