Crystallographic Defects in Cellular Automata Marcus Pivato Trent University Peterborough, Ontario

http://xaravve.trentu.ca/pivato/Research/#defects

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CA are the 'discrete analog' of partial differential equations. They are *spatially distributed* dynamical systems whose dynamics are driven by *local interactions* governed by *translationally equivariant* rules.

- **Space** is a lattice \mathbb{Z}^D (for $D \ge 1$).
- The **local state** at each point in the lattice is an element of a finite alphabet, e.g. $\mathcal{A} := \{0, 1\}$.
- The **global state** is a \mathbb{Z}^D -indexed configuration $\mathbf{a} : \mathbb{Z}^D \longrightarrow \mathcal{A}$. The space of such configurations is denoted $\mathcal{A}^{\mathbb{Z}^D}$. A generic element of $\mathcal{A}^{\mathbb{Z}^D}$ will be denoted by $\mathbf{a} := \left[a_{\mathbf{z}}|_{\mathbf{z} \in \mathbb{Z}^D}\right]$.
- The evolution is governed by a map $\Phi : \mathcal{A}^{\mathbb{Z}^D} \longrightarrow \mathcal{A}^{\mathbb{Z}^D}$, computed by applying a '**local rule**' ϕ at every point in space.



Example: Elementary Cellular Automaton #62 $\text{Let } D := 1, \ \mathbb{K} := \{-1, 0, 1\}, \ \text{and } \mathcal{A} := \{0, 1\}.$ $\text{Define } \phi_{62} : \{0, 1\}^{\{-1, 0, 1\}} \longrightarrow \{0, 1\} \text{ by:}$ $\phi_{62}(0, 0, 1) = 1; \ \phi_{62}(0, 0, 0) = 0;$ $\phi_{62}(0, 1, 0) = 1; \ \phi_{62}(1, 1, 0) = 0;$ $\phi_{62}(0, 1, 1) = 1; \ \phi_{62}(1, 1, 1) = 0;$ $\phi_{62}(1, 0, 0) = 1;$ $\phi_{62}(1, 0, 1) = 1.$



⁽white=0; black=1)

Such a nearest-neighbour CA on $\{0, 1\}^{\mathbb{Z}}$ is called an **Elementary Cel**lular Automaton. Each ECA is described by an 8-bit binary number (i.e. a number between 0 and 255) as follows:

If $N = n_0 + 2n_1 + 2^2n_2 + 2^3n_3 + 2^4n_4 + 2^5n_5 + 2^6n_6 + 2^7n_7 \in [0...255]$

then $\phi_N(a_0, a_1, a_2) := n_k$, where $k := a_0 + 2a_1 + 4a_2 \in [0...7]$.

For example, the CA here is ECA#62, because $2^1 + 2^2 + 2^3 + 2^4 + 2^5 = 62$.





Emergent Defect Dynamics in ECA#54







Emergent Defect Dynamics in ECA#18

blue

Empirical Work: • P. Grassberger [1983, 1984].

- Steven Wolfram [1983-2005]. (Mainly ECA #110).
- S. Wolfram and Doug Lind [1986]. (Classified defects of ECA #110).
- N. Boccara, J. Naser, M. Rogers [1991]. (ECAs 18, 54, 62, 184).

• James Crutchfield and James Hanson's 'Computational Mechanics' [1992-2001]. (Also Cosma Shalizi, Wim Hordijk, Melanie Mitchell).

• Harold V. McIntosh [1999, 2000].

Theoretical Work: • Doug Lind [1984] conjectured:

(i) Defects in ECA#18 perform random walks.

(ii) Defect density decays to zero through annihilations. Thus, ECA#18 converges 'in measure' to the 'odd' sofic shift $(1 \leftrightarrows (0) \leftrightarrows (0))$.

• Kari Eloranta [1993-1995] proved Lind's conjecture (i); studied quasirandom defect motion in 'partially permutive' CA.

• Petr Kůrka and Alejandro Maass [2000, 2002] studied CA convergence to limit sets through 'defect annihilation'. Kůrka [2003] proved Lind's conjecture (ii).

• S. Wolfram and Matthew Cook [2002, 2004]: ECA #110 is computationally universal (used 'defect physics' to engineer universal computer).

- What is a 'defect'? What is a 'regular background pattern'?
- Is there an 'algebraic structure' governing defect 'chemistry'?
- Why do defects 'persist' over time instead of disappearing? Is this related to aforementioned 'algebraic structure'?
- What is the 'kinematics' by which defects propagate through space?

A subshift is a subset $\mathfrak{A} \subseteq \mathcal{A}^{\mathbb{Z}^D}$ of configurations, defined by stipulating which 'local patterns' may or may not occur around each point in \mathbb{Z}^D .

Topological Markov Shifts: Let D = 1. Let $\mathcal{A} :=$ the vertices of a directed graph. A sequence $\mathbf{a} \in \mathcal{A}^{\mathbb{Z}}$ is admissible iff it describes an infinite directed path through the graph.

 $\mathbf{a} = [\dots,0,1,2,1,2,0,0,0,0,1,2,0,0,1,2,1,2,1,2,0,0,\dots]$

Sofic Shift: Let D = 1. Like a topological Markov shift, but now several vertices might be labelled with the same letter in \mathcal{A} .

A configuration $\mathbf{a} \in \mathcal{A}^{\mathbb{Z}^D}$ is **defective** if there are points in \mathbb{Z}^D where the local pattern in \mathbf{a} is *inadmissible*—i.e. *not* in $\mathfrak{A}_{(r)}$. These points are called **defects**. Let $\mathbb{D}(\mathbf{a}) \subset \mathbb{Z}^D$ be the set of these 'defect points' in \mathbf{a} .

Let $\Phi : \mathcal{A}^{\mathbb{Z}^D} \longrightarrow \mathcal{A}^{\mathbb{Z}^D}$ be a CA. We say \mathfrak{A} is Φ -invariant if $\Phi(\mathfrak{A}) \subseteq \mathfrak{A}$. Empirically, if $\mathbf{a} \in \mathcal{A}^{\mathbb{Z}^D}$ has defects, then so does $\Phi(\mathbf{a})$.

Let $\widetilde{\mathfrak{A}} := \{ \text{configurations with 'finite' defects} \}$. Then $\Phi(\widetilde{\mathfrak{A}}) \subseteq \widetilde{\mathfrak{A}}$.

Wang tilings

Let D = 2. Let $\mathcal{A} :=$ set of square tiles, with notches on their edges which dictate how the tiles can be assembled. These **edge-matching constraints** determine a subshift $\mathfrak{A} \subset \mathcal{A}^{\mathbb{Z}^2}$, called a **Wang tiling**.

A defect corresponds to a 'hole' in the tiling:

Remark: Wang tilings and topological Markov shifts are **subshifts** of finite type (SFTs), meaning they are determined entirely by 'local constraints'. Sofic shifts are a broader class, which may have 'nonlocal' constraints. (Defect theory more complicated, but still possible.)

Generalization to \mathbb{Z}^D : Idea: $\mathcal{A} = \text{set of 'atoms', with certain admissible 'chemical bonds' between them. Thus, an admissible configuration corresponds to a 'crystalline solid'. Defects are 'flaws' in crystal structure.$

- Is there an 'algebraic structure' governing defect 'chemistry'?
- Why do defects 'persist' over time instead of disappearing? Is this related to aforementioned 'algebraic structure'?
- What is the 'kinematics' by which defects propagate through space?

Formalism: Fix $D \in \mathbb{N}$. For any r > 0, let $\mathbb{B}(r) := [-r...r]^D \subset \mathbb{Z}^D$. Fix r > 0. Let $\mathfrak{A}_{(r)} \subset \mathcal{A}^{\mathbb{B}(r)}$ be a set of of **admissible** r-blocks.

The **subshift of finite type (SFT)** determined by $\mathfrak{A}_{(r)}$ is the set

$$\mathfrak{A} := \left\{ \mathbf{a} \in \mathcal{A}^{\mathbb{Z}^D} ; \ \mathbf{a}_{\mathsf{z}+\mathbb{B}(r)} \in \mathfrak{A}_{(r)}, \ \forall \ \mathsf{z} \in \mathbb{Z}^D \right\}$$

For any R > 0, let $\mathfrak{A}_{(R)}$ be the projection of \mathfrak{A} to $\mathcal{A}^{\mathbb{B}(R)}$.

If $\mathbf{a} \in \mathcal{A}^{\mathbb{Z}^D}$ and $\mathbf{z} \in \mathbb{Z}^D$, then \mathbf{a} is **defective** at \mathbf{z} if $\mathbf{a}_{\mathbf{z}+\mathbb{B}(r)} \notin \mathfrak{A}_{(r)}$. The **defect set** of \mathbf{a} is the set $\mathbb{D}(\mathbf{a})$ of all such \mathbf{z} .

Let $\Phi : \mathcal{A}^{\mathbb{Z}^D} \longrightarrow \mathcal{A}^{\mathbb{Z}^D}$ be a CA. We say \mathfrak{A} is Φ -invariant if $\Phi(\mathfrak{A}) \subseteq \mathfrak{A}$. Empirically, if $\mathbf{a} \in \mathcal{A}^{\mathbb{Z}^D}$ has defects, then so does $\Phi(\mathbf{a})$.

We say **a** is **finitely defective** if, $\forall R > 0$, $\exists z \in \mathbb{Z}^D$ with $\mathbf{a}_{\mathbb{B}(z,R)} \in \mathfrak{A}_{(R)}$.

Idea: a may have infinitely large defects, but **a** also has infinitely large 'nondefective' regions. Let $\widetilde{\mathfrak{A}} := \{ \text{finitely defective } \mathbf{a} \in \mathcal{A}^{\mathbb{Z}^D} \}$. $(\mathfrak{A} \subset \widetilde{\mathfrak{A}})$

Lemma: If $\Phi(\mathfrak{A}) \subseteq \mathfrak{A}$, then $\Phi(\widetilde{\mathfrak{A}}) \subseteq \widetilde{\mathfrak{A}}$.

Also, if $\mathbf{a} \in \widetilde{\mathfrak{A}}$ and $\mathbf{a}' = \Phi(\mathbf{a})$, then the any defects in \mathbf{a}' are 'close' to corresponding defects in \mathbf{a} .

The Fine Print: To extend the definition of 'defect' to other subshifts (not of finite type), it is necessary to introduce a 'detection range' R > 0. We must then talk about 'defects of range R'. Let $\mathbb{G}(\mathbf{a}) := \{ \mathbf{z} \in \mathbb{Z}^D ; \mathbf{a} \text{ is not defective at } \mathbf{z} \}$. Let $\mathbb{G}(\mathbf{a}) \subset \mathbb{R}^D$ be the union of all unit cubes whose corner vertices are all in $\mathbb{G}(\mathbf{a})$.

The defect in \mathbf{a} is a **domain boundary**^{*} if $\mathbf{G}(\mathbf{a})$ is disconnected.

Examples: (a) If D = 1, then all defects are domain boundaries.

(b) (*Monochromatic*) Let $\mathcal{A} := \{\blacksquare, \Box\}$. Let $\mathfrak{M}_{\mathfrak{o}} \subset \mathcal{A}^{\mathbb{Z}^2}$ be SFT such that no \blacksquare can be adjacent to a \Box .

The following configuration has a domain boundary defect:

(c) (*Checkerboard*) Let $\mathcal{A} := \{\blacksquare, \square\}$. Let $\mathfrak{Ch} \subset \mathcal{A}^{\mathbb{Z}^2}$ be SFT where no \blacksquare can be adjacent to a \blacksquare , and no \square can be adjacent to a \square .

The following configuration has a domain boundary defect:

(*) If we considering a defect of range R > 0, then technically this is a domain boundary of range

(d) (Square ice) Let
$$\mathcal{I} := \left\{ \overbrace{}^{\wedge}, \overbrace{}^{\wedge}, \overbrace{}^{\vee}, \overbrace{}^{}, \overbrace{}^{\vee}, \overbrace{}^{\backslash}, \overbrace{}^{\backslash}, \overbrace{}^{\vee}, \overbrace{}^{\backslash}, \overbrace{}^{I}, \overbrace{}^{I}, \overbrace{}^{I}, I,$$

Let $\mathfrak{I}_{\mathfrak{ce}} \subset \mathcal{I}^{\mathbb{Z}^2}$ be the SFT defined by obvious edge-matching conditions.

The following configuration has a domain boundary defect:

(e) (Domino Tiling) Let $\mathcal{D} := \left\{ \square, \square, \square, \square \right\}$.

Let $\mathfrak{D}_{\mathfrak{om}} \subset \mathcal{D}^{\mathbb{Z}^2}$ be the SFT defined by obvious edge-matching conditions. The following configurations have domain boundary defects:

Let $\Phi : \mathcal{A}^{\mathbb{Z}^D} \longrightarrow \mathcal{A}^{\mathbb{Z}^D}$ be a CA, with $\Phi(\mathfrak{A}) \subseteq \mathfrak{A}$. Let $\mathbf{a} \in \widetilde{\mathfrak{A}}$. The defect in **a** is Φ -persistent if $\Phi^t(\mathbf{a})$ also has a defect, for all $t \ge 0$.

Question: These defects seem to be persistent. Are they? Why?

Essential Defects _

A defect is **essential** if it can't be removed through a local change. That is, $\forall R > 0$, if $\mathbf{a}' \in \mathcal{A}^{\mathbb{Z}^D}$ is obtained by modifying \mathbf{a} in an R-neighbourhood of defect, then \mathbf{a}' is also defective.

Proposition: If $\Phi : \mathfrak{A} \longrightarrow \mathfrak{A}$ is bijective (e.g. if $\mathfrak{A} \subseteq \mathsf{Fix}[\Phi]$ or $\mathfrak{A} \subseteq \mathsf{Fix}[\Phi^p]$ or $\mathfrak{A} \subseteq \mathsf{Fix}[\Phi^p \circ \sigma^q]$), then any essential defect is Φ -persistent. \Box

Question: These defects to be seem essential. Are they? Why?

Suppose $\mathfrak{A}_{(r)}$ breaks into two (or more) disjoint subsets $\mathfrak{A}_{(r)} = \mathfrak{B}_{(r)} \sqcup \mathfrak{C}_{(r)}$ (called (F, σ) -transitive components), such that, for each $\mathbf{a} \in \mathfrak{A}$,

either **a** is totally covered by $\mathfrak{B}_{(r)}$ -blocks,

- or **a** is totally covered by $\mathfrak{C}_{(r)}$ -blocks,
- but **a** cannot have a mixture of $\mathfrak{B}_{(r)}$ -blocks and $\mathfrak{C}_{(r)}$ -blocks.

An **interface** is a domain boundary between a $\mathfrak{B}_{(r)}$ -covered region and a $\mathfrak{C}_{(r)}$ -covered region. Such a boundary is necessarily an essential defect.

Example: Let \mathfrak{M} be the *monochromatic* shift. Then $\mathfrak{M}_{(1)} := \mathfrak{B}_{(1)} \sqcup \mathfrak{W}_{(1)}$, where $\mathfrak{B}_{(1)} := \left\{ \blacksquare \right\}$ and $\mathfrak{W}_{(1)} := \left\{ \blacksquare \right\}$. The defect at right is an interface.

Example: (ECA #184) Let $\mathcal{A} = \{\Box, \blacksquare\}$. Let $\mathfrak{G}_{(1)} := \mathfrak{B}_{(1)} \sqcup \mathfrak{W}_{(1)} \sqcup \mathfrak{C}_{(1)}$, where $\mathfrak{B}_{(1)} := \{\blacksquare\blacksquare\blacksquare\}$, $\mathfrak{W}_{(1)} := \{\Box\Box\Box\}$, and $\mathfrak{C}_{(1)} := \{\blacksquare\Box\blacksquare, \Box\blacksquare\Box\}$. This yields 6 possible interfaces:

α^- :	$\mathfrak{C}_{(1)}$ \mathfrak{mess}
ω^- :	$\mathfrak{W}_{(1)}$ $\mathfrak{C}_{(1)}$
ϵ :	$\mathfrak{B}_{(1)} \ \overline{\qquad} \mathfrak{D}_{(1)} \ \overline{\qquad} \mathfrak{M}_{(1)} \ \overline{\qquad} \mathfrak{M}_{(1)}$

 $\Phi_{184}(\mathfrak{G}) \subseteq \mathfrak{G}$, and the Φ_{184} -propagation of these interfaces is as follows:

Theorem: If $\Phi : \mathfrak{A} \longrightarrow \mathfrak{A}$ is surjective, then all interfaces are Φ -persistent defects. \Box

 \mathfrak{A} is (Φ, σ) -transitive if $\bigcup_{t \in \mathbb{N}} \bigcup_{\mathbf{z} \in \mathbb{Z}^D} \Phi^{-t} \sigma^{-\mathbf{z}}(\mathfrak{O})$ is dense in \mathfrak{A} , for any

nonempty open $\mathfrak{O} \subset \mathfrak{A}$. (Equivalent: most (Φ, σ) -orbits are dense in \mathfrak{A}).

Suppose \mathfrak{A} is not transitive, but $\mathfrak{A} = \mathfrak{A}_1 \sqcup \cdots \sqcup \mathfrak{A}_K$, where $\mathfrak{A}_1, \ldots, \mathfrak{A}_K$ are clopen (Φ, σ) -transitive components.

 $(\mathfrak{A}_1, \ldots, \mathfrak{A}_K \text{ are clopen}) \Rightarrow (\text{indicator functions are locally determined})$ i.e. $\exists r > 0$, and function $\kappa : \mathfrak{A}_{(r)} \longrightarrow [1...K]$ such that, $\forall \mathbf{a} \in \mathfrak{A}$,

 $(\mathbf{a} \in \mathfrak{A}_k) \quad \Longleftrightarrow \quad \left(\kappa(\mathbf{a}_{\mathbb{B}(r)}) = k\right).$

 $\forall \mathbf{z} \in \mathbb{Z}^D$, let $\kappa_{\mathbf{z}}(\mathbf{a}) := \kappa(\mathbf{a}_{\mathbb{B}(\mathbf{z},r)})$. Then $\kappa_{\mathbf{z}}(\mathbf{a})$ is also well-defined for any $\mathbf{a} \in \widetilde{\mathfrak{A}}$ such that $\mathbf{a}_{\mathbb{B}(\mathbf{z},r)}$ is \mathfrak{A} -admissible.

If $\mathbf{y}, \mathbf{z} \in \mathbb{Z}^D$, then \mathbf{a} has an **interface**[†] between \mathbf{y} and \mathbf{z} if $\kappa_{\mathbf{y}}(\mathbf{a}) \neq \kappa_{\mathbf{z}}(\mathbf{a})$.

Example: $\mathfrak{M}_{\mathfrak{o}}$ has two σ -transitive components: \mathfrak{M}_{0} := all-black, and \mathfrak{M}_{1} := all-white. This defect is an interface.

Nonexample: This is *not* an interface, because \mathfrak{D}_{om} is σ -transitive [Einsiedler, 2001]. Instead this is a 'gap' defect.

Interfaces always form domain boundaries. Let $\mathbb{Y}_1, \ldots, \mathbb{Y}_N$ be the connected components of $\mathbb{G}(\mathbf{a})$. There is a function $\mathcal{K}: [1...N] \longrightarrow [1...K]$ such that for any $n \in [1...N]$ and any $\mathbf{y} \in \mathbb{Y}_n$, $\kappa_{\mathbf{y}}(\mathbf{a}) = \mathcal{K}(n)$.

(†) Technically, this is an interface of range r, and this concept only makes sense for domain boundaries of range $R \ge r$.

A connected component \mathbb{Y}_n of \mathbb{G} is **projective** if, for all R > 0, $\exists \mathbf{y} \in \mathbb{Y}_n$ with $\mathbf{a}_{\mathbb{B}(\mathbf{y},R)} \in \mathfrak{A}_{(R)}$. (i.e. \mathbb{Y}_n contains arbitrarily large \mathfrak{A} -admissible patches.)

Lemma: The interface in **a** is essential if there are two projective components \mathbb{Y}_n and \mathbb{Y}_m with $\mathcal{K}(n) \neq \mathcal{K}(m)$. \Box

Signature of the interface := restriction of \mathcal{K} to projective components.

Example: Let $\mathfrak{A} \subset \mathcal{A}^{\mathbb{Z}}$. Suppose $\mathbf{a} \in \widetilde{\mathfrak{A}}$ has defects $\mathbf{d}_1, \ldots, \mathbf{d}_N$ with $\mathbb{Y}_0, \ldots, \mathbb{Y}_N$ being the \mathfrak{A} -admissible intervals between these defects: $-\mathbb{Y}_0 \longrightarrow \mathbf{d}_1 \longleftarrow \mathbb{Y}_1 \longrightarrow \mathbf{d}_2 \longleftarrow \mathbb{Y}_2 \longrightarrow \cdots \longleftarrow \mathbb{Y}_{N-1} \longrightarrow \mathbf{d}_N \longleftarrow \mathbb{Y}_N - \cdots$

Projective components: $\mathbb{Y}_0 \& \mathbb{Y}_N$. : Interface is essential if $\mathcal{K}(0) \neq \mathcal{K}(N)$.

Theorem: If $\Phi : \mathfrak{A} \longrightarrow \mathfrak{A}$ is surjective, then all essential interfaces are Φ -persistent. If $\mathbf{a} \in \widetilde{\mathfrak{A}}$ has an essential interface, then $\Phi(\mathbf{a})$ also has an essential interface, with the same signature as \mathbf{a} . \Box

Example: (ECA #184) Let $\mathcal{A} = \{\Box, \blacksquare\}$. Let $\mathfrak{G} := \mathfrak{G}_0 \sqcup \mathfrak{G}_1 \sqcup \mathfrak{G}_*$, where $\mathfrak{G}_0 := \{\overline{\blacksquare}\}, \mathfrak{G}_1 := \{\overline{\Box}\}, \text{ and } \mathfrak{G}_* := \{\overline{\blacksquare\Box}, \overline{\Box\blacksquare}\}$. (Here, $\overline{\blacksquare} := [\ldots \blacksquare \blacksquare \blacksquare \blacksquare \ldots]$ and $\overline{\blacksquare\Box} := [\ldots \blacksquare \blacksquare \blacksquare \Box \ldots]$, etc.

Then $\mathfrak{G}_0 \cup \mathfrak{G}_1 \subset \mathsf{Fix} [\Phi_{184}]$, while $\Phi_{184}|_{\mathfrak{G}_*} = \sigma$.

The Φ_{184} -propagation of these defects is as follows:

Dislocations (intuitive version)

Suppose \mathfrak{A} has a *spatiotemporally periodic* structure. In any \mathfrak{A} -admissible configuration, certain patterns must recur periodically in space and time.

A **dislocation** is a domain boundary between two regions which are 'out of phase' with respect to this periodic structure. Such a domain boundary is necessarily an essential defect.

Example: The checkerboard shift \mathfrak{Ch} is both vertically and horizontally 2-periodic in space. The domain boundary at right is a dislocation.

The spatiotemporally periodic structure of \mathfrak{A} is described by a subgroup $\mathbb{K} \subset \mathbb{Z}^{D+1}$. Each dislocation is characterized by a **displacement** $\delta \in \Delta$, where $\Delta := \mathbb{Z}^{D+1}/\mathbb{K}$ is the quotient group.

Example: (ECA#62) Let \mathfrak{D} = orbit of $[\ldots \blacksquare \blacksquare \square \blacksquare \square \blacksquare \square \ldots]$. Then $\Phi_{62|_{\mathfrak{D}}} = \sigma$, so $(\mathfrak{D}, \Phi_{62})$ is 3-periodic in both space and time, and $\Delta \cong \mathbb{Z}_{/3}$.

Here are two dislocations in \mathfrak{D} and their displacements:

Theorem: If $\Phi : \mathfrak{A} \longrightarrow \mathfrak{A}$ is surjective, then any nontrivial dislocation is a Φ -persistent defect. Furthermore the displacement of each dislocation is constant over time.

Let $\mathfrak{G}_* = \text{orbit of } [\ldots \square \square \square \square \ldots]$. Then $\Phi_{184}|_{\mathfrak{G}_*} = \sigma$, so $(\mathfrak{G}_*, \Phi_{184})$ is 2-periodic in both space and time, and $\Delta \cong \mathbb{Z}_{/2}$.

Here are two dislocations, both with displacement $1 \in \mathbb{Z}_{/2}$:

Dislocations in ECA#110

Then $\Phi_{110}|_{\mathfrak{E}} = \sigma_{\mathfrak{Z}}^{\mathfrak{L}}$ so $(\mathfrak{E}, \Phi_{110})$ is spatiotemporally periodic, and $\Delta \cong \mathbb{Z}_{/14}$. Here are seven dislocations in \mathfrak{E} :

Displacement Algebra and Defect Chemistry

When two displacement defects collide, the outcome can be partially predicted by the algebra of the displacement group Δ .

Dislocations (fomal version)

Let $\mathfrak{A} \subset \mathcal{A}^{\mathbb{Z}^D}$ be a Φ -invariant subshift. Let $\boldsymbol{\lambda} := (\lambda_0; \lambda_1, \dots, \lambda_D)$ be a (D+1)-tuple of complex roots of unity. A **rational eigenfunction** of \mathfrak{A} with **eigenvalue** $\boldsymbol{\lambda}$ is a function $F : \mathfrak{A} \longrightarrow \mathbb{C}$ such that:

 $F \circ \Phi = \lambda_0 F$, and $F \circ \sigma^z = \lambda^z F$, $\forall z \in \mathbb{Z}^D$. Here, if $\mathbf{z} = (z_1, \dots, z_D)$, then we define $\lambda^z := \lambda_1^{z_1} \cdots \lambda_D^{z_D}$.

Any rational eigenfunction is **locally determined** i.e. $\exists r > 0$, and function $f : \mathfrak{A}_{(r)} \longrightarrow \mathbb{C}$ such that, $\forall \mathbf{a} \in \mathfrak{A}, F(\mathbf{a}) = f(\mathbf{a}_{\mathbb{B}(r)}).$

 $\forall \mathbf{z} \in \mathbb{Z}^D$, let $f_{\mathbf{z}}(\mathbf{a}) := f(\mathbf{a}_{\mathbb{B}(\mathbf{z},r)})$. Then $f_{\mathbf{z}}(\mathbf{a})$ is also well-defined for any $\mathbf{a} \in \widetilde{\mathfrak{A}}$ such that $\mathbf{a}_{\mathbb{B}(\mathbf{z},r)}$ is \mathfrak{A} -admissible. If $\mathbf{x}, \mathbf{y} \in \mathbb{Z}^D$, then \mathbf{a} has an (\mathfrak{A}, Φ) -dislocation[‡] between \mathbf{x} and \mathbf{y} if $f_{\mathbf{x}}(\mathbf{a})/f_{\mathbf{y}}(\mathbf{a}) \neq \boldsymbol{\lambda}^{\mathbf{x}-\mathbf{y}}$.

Example: Define $F : \mathfrak{C}_{\mathfrak{h}} \longrightarrow \{\pm 1\}$ by local rule $f : \{\blacksquare, \square\} \longrightarrow \{\pm 1\}$ where $f(\blacksquare) = 1$ and $f(\square) = -1$. Then F is σ -eigenfunction with eigenvalue (-1, -1).

Nonexample: This is *not* a dislocation, because $\mathfrak{D}_{\mathfrak{om}}$ is σ -mixing [Einsiedler, 2001], and thus, has no nontrivial eigenfunctions [Keynes & Robertson, 1969].

Instead this is a 'gap' defect.

Dislocations always form domain boundaries. Let $\mathbb{K} := \{ \mathbf{k} \in \mathbb{Z}^D ; \mathbf{\lambda}^{\mathbf{k}} = 1 \}$. For any connected components \mathbb{X}, \mathbb{Y} of $\mathbb{G}(\mathbf{a}), \exists$ unique **displacement** $\boldsymbol{\delta} \in \mathbb{Z}^{D+1}/\mathbb{K}$ such that, for any $\mathbf{x} \in \mathbb{X}$ and $\mathbf{y} \in \mathbb{Y}, \quad \frac{f_{\mathbf{x}}(\mathbf{a})}{\mathbf{\lambda}^{\mathbf{x}-\mathbf{y}} f_{\mathbf{y}}(\mathbf{a})} = \mathbf{\lambda}^{\boldsymbol{\delta}}$.

(‡) Technically, this is a dislocation of range r, and this concept only makes sense for domain boundaries of range $R \ge r$. **Lemma:** The dislocation in **a** is essential if \exists two projective components X and Y with a nontrivial displacement between them. \Box

If **a** has N projective components, then the **displacement matrix** is the antisymmetric $N \times N$ matrix of $(\mathbb{Z}^{D+1}/\mathbb{K})$ -valued displacements between them. Essential dislocations are persistent:

Theorem: If $\Phi : \mathfrak{A} \longrightarrow \mathfrak{A}$ is surjective, then all essential dislocations are Φ -persistent. If $\mathbf{a} \in \widetilde{\mathfrak{A}}$ has essential dislocation, then $\Phi(\mathbf{a})$ also has essential dislocation, with the same displacement matrix as \mathbf{a} . \Box

Example: (ECA#62) Let $\mathcal{A} = \{\blacksquare, \square\}$. Let \mathfrak{D} be the three-periodic σ -orbit of $\blacksquare\blacksquare\square$. Then $\Phi_{62|_{\mathfrak{D}}} = \sigma$.

Let $\lambda := e^{2\pi \mathbf{i}/3}$. Define $F : \mathfrak{D} \longrightarrow \mathbb{C}$ by $F(\overline{\blacksquare\blacksquare}) = \Box$, $F(\overline{\blacksquare\blacksquare}) = \lambda$, and $F(\overline{\blacksquare\blacksquare}) = \lambda^2$. Then $F \circ \sigma = \lambda F = F \circ \Phi_{62}$, so F is eigenfunction with eigenvalue (λ, λ) .

 $\mathbb{K} = \mathbb{Z}(3,0) \oplus \mathbb{Z}(1,2)$, so displacements are elements of $\Delta \cong \mathbb{Z}_{/3}$.

Below are three rational dislocations in \mathfrak{D} and their displacements.

The β and γ defects are essential, hence persistent by the theorem.

The α defect is *not* essential, but is still persistent (not because of the theorem).

Let $\mathfrak{B} := \mathfrak{B}_0 \sqcup \mathfrak{B}_1$, where \mathfrak{B}_0 is the 4-periodic σ -orbit of $\blacksquare \blacksquare \square \blacksquare$ and \mathfrak{B}_1 is the 4-periodic σ -orbit of $\square \square \blacksquare \square$.

Then $F \circ \sigma = \mathbf{i}F = F \circ \Phi_{54}$, so F is eigenfunction with eigenvalue (\mathbf{i}, \mathbf{i}) . $\mathbb{K} := \mathbb{Z}(2, 2) \bigoplus_{\mathbf{i} \in \mathbf{i}} \mathbb{Z}(0, 4)$, so displacements are elements of \mathbb{Z}^2/\mathbb{K} . Here are four equational dislocations in ECA#54 and their displacements:

All four have nontrivial displacement, so they are essential, $\therefore \Phi_{54}$ -persistent.

Persistence of Dislocations in ECA #110 _

Let $\lambda := e^{\pi i/7}$. Let $F : \mathfrak{E} \longrightarrow \{\lambda^k\}_{k=0}^{13}$ be a σ -eigenfunction with $F \circ \sigma = \lambda F$. Then $F \circ \Phi_{110} = \lambda^4 F$, so F is a (Φ_{184}, σ) -eigenfunction with eigenvalue $(\lambda^4; \lambda)$. $\mathbb{K} = \mathbb{Z}(0, [\mathfrak{F}_4] \oplus \mathbb{Z}(1, 10))$, so displacements are elements of $\mathbb{Z}^2/\mathbb{K} \cong \mathbb{Z}_{/14}$. Here are seven rational dislocations in \mathfrak{E} :

All have nontrivial displacement, so they are essential and $\Phi_{110}\text{-}\text{persistent}.$

Persistence of Dislocations in ECA #184 _____ Let $\mathfrak{G}_* = \{\Box \blacksquare, \blacksquare \Box\}$. Then $\Phi_{184}|_{\mathfrak{G}_*} = \sigma$. Define $F : \mathfrak{G}_* \longrightarrow \{\pm 1\}$ by $F(\Box \blacksquare) = 1$ and $F(\blacksquare \Box) = -1$. Then $F \circ \sigma = -F = F \circ \Phi_{184}$, so F is eigenfunction with eigenvalue (-1, -1). $\mathbb{K} = \mathbb{Z}(2, 0) \oplus \mathbb{Z}(1, 1)$, so displacements are elements of $\mathbb{Z}^2/\mathbb{K} \cong \mathbb{Z}_{/2}$. Here are two dislocations and their displacements:

$$\begin{array}{cccc} \gamma^+ & & & & & \\ \gamma^- & & & & \\ \end{array} \end{array} \overbrace{}^{\bullet} & & & \\ \end{array} \overbrace{}^{\bullet} & & & \\ \end{array} \overbrace{}^{\bullet} & & \\ \end{array}$$

Both have nontrivial displacement, so they are essential and Φ_{184} -persistent.

_Displacement Algebra and Defect Chemistry ____

When two displacement defects collide, the outcome can be partially predicted by the algebra of the displacement group $\mathbb{Z}^{D+1}/\mathbb{K}$.

The Fine Print: Our definition of 'displacement' here is somewhat oversimplified. The 'real' definition is that a displacement is a *character* on the spectral group of $(\mathfrak{A}, \Phi, \sigma)$. This is necessary to extend the theory of dislocations to *irrational* eigenvalues (e.g. in Sturmian shifts or multidimensional SFTS) or *discontinuous* eigenfunctions (e.g. on sofic shifts, as in ECA#18).

Let $\mathfrak{A} \subseteq \mathcal{A}^{\mathbb{Z}^D}$ be a subshift. Let (\mathcal{G}, \cdot) be a (discrete) group. A \mathcal{G} -valued **cocycle** is continuous function $C : \mathbb{Z}^D \times \mathfrak{A} \longrightarrow \mathcal{G}$ satisfying **cocycle equation:**

 $C(\mathbf{y} + \mathbf{z}, \mathbf{a}) = C(\mathbf{y}, \sigma^{\mathbf{z}}(\mathbf{a})) \cdot C(\mathbf{z}, \mathbf{a}), \quad \forall \mathbf{a} \in \mathcal{A}^{\mathbb{Z}^{D}} \text{ and } \forall \mathbf{y}, \mathbf{z} \in \mathbb{Z}^{D}.$ **Examples:** (a) Let $\Im_{\mathbf{ce}} \subset \mathcal{I}^{\mathbb{Z}^{2}}$ be square ice. Define $c_{1}, c_{2} : \mathcal{I} \longrightarrow \{\pm 1\}$ by $c_{1}(\{ \mathbf{x}, \mathbf{x} \}) := +1 =: c_{2}(\langle \mathbf{x}, \mathbf{x} \}) \text{ and } c_{1}(\{ \mathbf{x}, \mathbf{x} \}) := -1 =: c_{2}(\langle \mathbf{x}, \mathbf{x} \}) ('*' \text{ means } (\mathbf{x}, \mathbf{x}))$ 'anything'). Define cocycle $C : \mathbb{Z}^{2} \times \Im_{\mathbf{ce}} \longrightarrow \mathbb{Z}$ as follows:

$$\forall \mathbf{i} \in \mathfrak{I}_{\mathfrak{c}}, \ \forall \mathbf{z} = (z_1, z_2) \in \mathbb{Z}^2, \ C(\mathbf{z}, \mathbf{i}) := \sum_{x=0}^{z_1-1} c_1(i_{x,0}) + \sum_{y=0}^{z_2-1} c_2(i_{z_1,y}).$$

This is a **height function** (a Z-valued cocycle). These arise in tilings [e.g. K. Eloranta 1999-2005, H.Cohn & J.Propp] and statistical mechanics [R.Baxter 1989].

(c) If $b : \mathfrak{A} \longrightarrow \mathcal{G}$ is continuous, then function $C(\mathbf{z}, \mathbf{a}) := b(\sigma^{\mathbf{z}}(\mathbf{a})) \cdot b(\mathbf{a})^{-1}$ is a cocycle, called a **coboundary**.

(d) Let \mathbf{X} = topological space. Let \mathcal{H} =homeo(\mathbf{X}). Then \mathcal{H} -valued cocycles are the fibre-wise maps of a skew product extension of the σ -action on \mathfrak{A} to a \mathbb{Z}^{D} -action on $\mathfrak{A} \times \mathbf{X}$. [R.Zimmer 1976-80, J.Kammeyer 1990-93]

Two cocycles C and C' are **cohomologous** $(C \approx C')$ if \exists continuous **transfer function** $b : \mathfrak{A} \longrightarrow \mathcal{G}$ such that

$$C'(\mathbf{z}, \mathbf{a}) = b(\sigma^{\mathbf{z}}(\mathbf{a})) \cdot C(\mathbf{z}, \mathbf{a}) \cdot b(\mathbf{a})^{-1}, \quad \forall \mathbf{z} \in \mathbb{Z}^{D}, \text{ and } \mathbf{a} \in \mathfrak{A}.$$

Let \underline{C} := cohomology equivalence class of the cocycle C.

 $\mathcal{Z}^1(\mathfrak{A}, \mathcal{G}) := \{\mathcal{G}\text{-valued cocycles}\}.$

 $\mathcal{H}^1(\mathfrak{A},\mathcal{G}) := \{ \text{cohomology equivalence classes in } \mathcal{Z}^1(\mathfrak{A},\mathcal{G}) \}.$

If (\mathcal{G}, \cdot) is abelian, then $\mathcal{Z}^1(\mathfrak{A}, \mathcal{G})$ is a group (under pointwise multipication), and $\mathcal{H}^1(\mathfrak{A}, \mathcal{G})$ is a quotient group, called the **1st cohomology group** of \mathfrak{A} (with coefficients in \mathcal{G}). [see e.g. K.Schmidt (1995, 1998) for discussion]

_Trails and locally determined cocycles _____

Let
$$\mathbb{E} := \{ \mathbf{z} \in \mathbb{Z}^D ; \mathbf{z} = (0, ..., 0, \pm 1, 0, ..., 0) \}$$
. A **trail** is a sequence
 $\zeta = (\mathbf{z}_0, \mathbf{z}_1, \dots, \mathbf{z}_N) \subset \mathbb{Z}^D$, where, $\forall n \in [1...N], \ \mathbf{z}'_n := (\mathbf{z}_n - \mathbf{z}_{n-1}) \in \mathbb{E}$.
Let $r > 0$. Let $c : \mathbb{E} \times \mathfrak{A}_{(r)} \longrightarrow \mathcal{G}$ be such that, $\forall \mathbf{e}, \mathbf{e}' \in \mathbb{E}, \quad \forall \mathbf{a} \in \mathfrak{A}$,
(a) $c(\mathbf{e}', \mathbf{a}_{\mathbb{B}(\mathbf{e},r)}) \cdot c(\mathbf{e}, \mathbf{a}_{\mathbb{B}(r)}) = c(\mathbf{e}, \mathbf{a}_{\mathbb{B}(\mathbf{e}',r)}) \cdot c(\mathbf{e}', \mathbf{a}_{\mathbb{B}(r)})$. i.e. $c(\uparrow) = c(\downarrow)$
(b) $c(-\mathbf{e}, \mathbf{a}_{\mathbb{B}(\mathbf{e},r)}) = c(\mathbf{e}, \mathbf{a}_{\mathbb{B}(r)})^{-1}$. i.e. $c(\downarrow) = c(\uparrow)^{-1}$

Then $c(\zeta, \mathbf{a}) := \prod_{n=1}^{N} c(\mathbf{z}'_n, \mathbf{a}_{\mathbb{B}(\mathbf{z}_{n-1}, r)})$ depends only on \mathbf{z}_0 and \mathbf{z}_N , not ζ .

Example: If ζ is **closed** (i.e. $\mathbf{z}_N = \mathbf{z}_0$) then $c(\zeta, \mathbf{a}) = e_{\mathcal{G}}$.

Define cocycle $C : \mathbb{Z}^D \times \mathfrak{A} \longrightarrow \mathcal{G}$ as follows: $\forall \mathbf{a} \in \mathfrak{A}, \mathbf{z} \in \mathbb{Z}^D$, $C(\mathbf{z}, \mathbf{a}) := c(\zeta, \mathbf{a})$, (where ζ is any trail from 0 to \mathbf{z}). We say C is **locally determined** with **local rule** c of **radius** r.

If \mathcal{G} is discrete, then \forall continuous \mathcal{G} -valued cocycles are locally determined. For any r > 0, let $\mathcal{Z}_r^1(\mathfrak{A}, \mathcal{G}) :=$ radius-r cocycles on \mathfrak{A} . **Proposition:** Let $\mathfrak{A} \subset \mathcal{A}^{\mathbb{Z}^D}$ be a subshift. Let $\Phi : \mathcal{A}^{\mathbb{Z}^D} \longrightarrow \mathcal{A}^{\mathbb{Z}^D}$ be a cellular automaton with $\Phi(\mathfrak{A}) \subseteq \mathfrak{A}$. Let \mathcal{G} be a group.

- (a) Let $C \in \mathcal{Z}^1(\mathfrak{A}, \mathcal{G})$ be cocycle. Define $\Phi_*C : \mathbb{Z}^D \times \mathfrak{A} \longrightarrow \mathcal{G}$ by $\Phi_*C(\mathsf{z}, \mathbf{a}) = C(\mathsf{z}, \Phi(\mathbf{a}))$. Then Φ_*C is also a cocycle on \mathfrak{A} .
- (b) If Φ has radius R, and C is locally determined with radius r, then Φ_*C is locally determined with radius r + R.
- (c) Let $C, C' \in \mathcal{Z}^1(\mathfrak{A}, \mathcal{G})$. If $C \approx C'$, then $\Phi^*C \approx \Phi^*C'$. Thus, Φ induces a function $\Phi_* : \mathcal{H}^1(\mathfrak{A}, \mathcal{G}) \longrightarrow \mathcal{H}^1(\mathfrak{A}, \mathcal{G})$.
- (d) If (\mathcal{G}, \cdot) is abelian, then Φ_* is a group endomorphism.

We will see that the Φ -persistence of certain kinds of defects depends critically on the surjectivity of the endomorphism Φ_* .

Question: When is Φ_* surjective?

Gap Defects: Definition

Some domain boundaries exhibit divergence in cocycle asymptotics.

Let $C \in \mathcal{Z}_r^1(\mathfrak{A}, \mathbb{Z})$ be a range-r cocycle (i.e. 'height function').

Let $\mathbf{a} \in \widetilde{\mathfrak{A}}$. Let \mathbb{X} be an infinite, simply-connected component of $\mathbb{G}_r(\mathbf{a})$. Fix $\mathbf{x}^* \in \mathbb{X}$. For any $\mathbf{x} \in \mathbb{X}$, we define the **height difference**:

$$\mathbf{C}_{\mathbf{a}}(\mathbf{x}^*, \mathbf{x}) \quad := \quad c(\zeta, \mathbf{a}),$$

where $c: \mathfrak{A}_{(r)} \longrightarrow \mathbb{Z}$ is 'local rule', and ζ is any trail in \mathbb{X} from \mathbf{x}^* to \mathbf{x} .

(Well-defined independent of ζ because X is a simply-connected.) Note:

 $|C_{\mathbf{a}}(\mathbf{x}^*,\mathbf{x})| \quad \leq \quad K \cdot d_{\mathbb{X}}(\mathbf{x}^*,\mathbf{x}),$

where $K := \max_{\mathbf{a} \in \mathfrak{A}_{(r)}} |c(\mathbf{a})|$, and $d_{\mathbb{X}}(\mathbf{x}^*, \mathbf{x}) := \min$ length (X-trail from \mathbf{x}^* to \mathbf{x}).

Let \mathbb{Y} be another infinite connected component of $\mathbb{G}_r(\mathbf{a})$. Fix $\mathbf{y}^* \in \mathbb{Y}$. For any $\mathbf{y} \in \mathbb{Y}$, define $C_{\mathbf{a}}(\mathbf{y}, \mathbf{y}^*)$ in the same way as $C_{\mathbf{a}}(\mathbf{x}^*, \mathbf{x})$ above. We then define

$$\mathbf{C}(\mathbf{y},\mathbf{x}) \quad := \quad C(\mathbf{y},\mathbf{y}^*) + C(\mathbf{x}^*,\mathbf{x}).$$

If X and Y were the same connected component (or if we could remove the defect in **a** so that they were), then we expect

$$C(\mathbf{y}, \mathbf{x}) \leq K \cdot d_{\mathbb{X}}(\mathbf{y}, \mathbf{x}) + \text{const.} \approx K|\mathbf{y} - \mathbf{x}| + \text{const.}$$

We say there is a *C*-gap between X and Y if $\sup_{\mathbf{y}\in\mathbb{Y}, \mathbf{x}\in\mathbb{X}} \frac{|C(\mathbf{y},\mathbf{x})|}{|\mathbf{y}-\mathbf{x}|} = \infty.$

(This suggests that the defect separating X and Y is essential.)

Fine print: If $\mathcal{G} \neq \mathbb{Z}$, we can also define gaps for \mathcal{G} -valued cocycles, by first defining an appropriate *pseudonorm* $\|\bullet\| : \mathcal{G} \longrightarrow \mathbb{R}$ which satisfies the triangle inequality and is invariant under conjugation.

Example: Consider the defective configuration in $\mathfrak{T}_{\mathfrak{ce}}$ shown above, and let $\{\mathbf{x}^*, \mathbf{x}_1, \mathbf{x}_2, \ldots\} \subset \mathbb{X}$ and $\{\mathbf{y}^*, \mathbf{y}_1, \mathbf{y}_2, \ldots\} \subset \mathbb{Y}$ be as shown. Let $C \in \mathcal{Z}^1(\mathfrak{T}_{\mathfrak{ce}}, \mathbb{Z})$ be the cocycle with local rule

Then $C(\mathbf{x}^*, \mathbf{x}_n) = n$ and $C(\mathbf{y}^*, \mathbf{y}_n) = -n$, so $C(\mathbf{x}_n, \mathbf{y}_n) = 2n, \forall n \in \mathbb{N}$.

But $|\mathbf{x}_n - \mathbf{y}_n| = 2$, $\forall n \in \mathbb{N}$, so $\lim_{n \to \infty} \frac{|C(\mathbf{x}_n, \mathbf{y}_n)|}{|\mathbf{x} - \mathbf{y}|} = \lim_{n \to \infty} \frac{2n}{2} = \infty$; hence there is a gap between X and Y.

Let $\mathcal{Z} := \{ \text{cyclic subgroup generated by } vh \} \subset \mathcal{G}.$ Then $(\mathcal{Z}, \cdot) \cong (\mathbb{Z}, +),$ and for all $\mathbf{d} \in \mathfrak{D}_{om}$ and $2\mathbf{z} \in 2\mathbb{Z}^2, \ C(2\mathbf{z}, \mathbf{d}) \in \mathcal{Z}.$

Let $\mathcal{D}_2 \subset \mathcal{D}^{2\times 2}$ be the alphabet of \mathfrak{D}_{om} -admissible 2×2 blocks. Let $\mathfrak{D}_2 \subset \mathcal{D}_2^{\mathbb{Z}^2}$ be 'recoding' of \mathfrak{D}_{om} in this alphabet. Then $2\mathbb{Z}^2$ acts on \mathfrak{D}_2 in the obvious way, and C yields a cocycle $C' : 2\mathbb{Z}^2 \times \mathfrak{D}_2 \longrightarrow \mathcal{Z} \cong \mathbb{Z}$.

In the $\widetilde{\mathfrak{D}_{om}}$ -configuration shown above, $C'(\mathbf{x}^*, \mathbf{x}_n) = (vhvh)^n \cong 2n$, while $C'(\mathbf{y}^*, \mathbf{y}_n) = h^{2n} \cong 0$, so $C'(\mathbf{y}_n, \mathbf{x}_n) = n$, for all $n \in \mathbb{N}$.

But
$$|\mathbf{x}_n - \mathbf{y}_n| = 4$$
, $\forall n \in \mathbb{N}$, so $\lim_{n \to \infty} \frac{|C'(\mathbf{x}_n, \mathbf{y}_n)|}{|\mathbf{x} - \mathbf{y}|} = \lim_{n \to \infty} \frac{n}{4} = \infty$.

In the $\widetilde{\mathfrak{D}_{om}}$ -configuration shown above, $C'(\mathbf{x}^*, \mathbf{x}_n) = (vhvh)^n \cong 2n$, while $C'(\mathbf{y}^*, \mathbf{y}_n) = (hvhv)^n \cong -2n$, so $C'(\mathbf{y}_n, \mathbf{x}_n) = -4n$, $\forall n \in \mathbb{N}$. But $|\mathbf{x}_n - \mathbf{y}_n| = 4$, $\forall n \in \mathbb{N}$, so $\lim \frac{|C'(\mathbf{x}_n, \mathbf{y}_n)|}{|\mathbf{x}_n - \mathbf{y}_n|} = \lim \frac{-4n}{4} = -\infty$.

Theorem: If $\Phi: \mathcal{A}^{\mathbb{Z}^D} \to \mathcal{A}^{\mathbb{Z}^D}$ is a CA, $\Phi(\mathfrak{A}) \subseteq \mathfrak{A}$, and endomorphism $\Phi_*: \mathcal{H}^1(\mathfrak{A}, \mathbb{Z}) \ni C \mapsto C \circ \Phi \in \mathcal{H}^1(\mathfrak{A}, \mathbb{Z})$

is surjective, then any gap is Φ -persistent.

Example: If $\mathcal{I} := \{ \begin{array}{c} & & \\ & & \\ \end{array}, \begin{array}{c} & & \end{array}, \end{array}, \begin{array}{c} & & \\ \end{array}, \begin{array}{c} & & \\ \end{array}, \end{array}, \begin{array}{c} & & \end{array}, \end{array}, \begin{array}{c} & & \\ \end{array}, \end{array}, \begin{array}{c} & & \end{array}, \end{array}, \begin{array}{c} & & \\ \end{array}, \end{array}, \begin{array}{c} & & \end{array}, \end{array}, \begin{array}{c} & & \end{array}, \end{array}, \begin{array}{c} & & \end{array}, \end{array}, \end{array}, \begin{array}{c} & & \\ \end{array}, \end{array}, \end{array}, \end{array}, \begin{array}{c} & & \end{array}, \end{array}, \end{array}, \begin{array}{c} & & \\ \end{array}, \end{array}, \end{array}, \end{array}, \end{array}, \end{array}, \begin{array}{c} & & \\ \end{array}, \end{array}, \end{array}, \end{array}, \end{array}, \end{array},$, \end{array}, \end{array}, \end{array}, \\, \end{array}, \end{array}, \end{array}, \end{array}, , \end{array}, \end{array}, \end{array}, \\, \end{array}, \end{array}, \end{array}, \end{array}, \\, \end{array}, \end{array}, \end{array}, \\, \end{array}, , \end{array}, \end{array}, \\, \end{array}, \end{array}, \end{array}, , \end{array}, \\, \end{array}, , \end{array}, , \end{array}, \\, \end{array}, \\, \end{array}, , \end{array}, , \end{array}, , \end{array}, , \end{array}, , \end{array},

Proof idea: First show that C-gaps depend only on cohomology class of C, i.e.:

Lemma: If $C \approx C'$, then any C-gap is also a C'-gap.

Now suppose **a** has C-gap. Now Φ_* is surjective, so find $C' \in \mathbb{Z}^1$ such that $\Phi_*C' \approx C$. Then **a** also has (Φ_*C') -gap. But this implies that $\Phi(\mathbf{a})$ has C' gap. \Box

_Sharp Gaps are Essential ____

A gap in $\mathbb{G}_r(\mathbf{a})$ is **sharp** if, for all $R \geq r \geq 0$, there exists constant $K = K(R, r) \in \mathbb{N}$ such that, for any $\mathbf{y} \in \mathbb{G}_r(\mathbf{a}), \exists \mathbf{x} \in \mathbb{G}_R(\mathbf{a})$ in same connected component \mathbb{X} of $\mathbb{G}_r(\mathbf{a})$ as \mathbf{y} , with $d_{\mathbb{X}}(\mathbf{x}, \mathbf{y}) \leq K$.

Idea: The gap does not ramify into lots of 'tributaries'.

Example: If \mathfrak{A} is a subshift of finite type, and defect set $\mathbb{D}(\mathbf{a})$ is confined to a thickened hyperplane [as in previous three examples] then the gap is sharp.

Theorem: Sharp gaps are essential defects.

Proof idea: First show:

Thus, we can always move our basepoint x^* and 'gap-detection' sequence $\{x_1, x_2, \ldots\}$ far away from gap. Thus, a gap is 'detectable' from any distance; hence it cannot

 \diamond

A domain boundary is a defect of **codimension 1**.

Fix $r \in \mathbb{N}$. Let $\mathbb{G}_r(\mathbf{a}) := \{ \mathbf{z} \in \mathbb{Z}^D ; \mathbf{a}_{\mathbb{B}(\mathbf{z},r)} \in \mathfrak{A}_{(r)} \}$. (Loosely, this is the complement of a radius-r neighbourhood around the defects in \mathbf{a} .)

Let $\mathbf{G}_{\mathbf{r}}(\mathbf{a}) :=$ union of all unit cubes whose corners are all in $\mathbb{G}_r(\mathbf{a})$.

We say **a** has a (range r) **codimension** (k + 1) defect if the kth homotopy group $\pi_k [\mathbf{G}_r(\mathbf{a})]$ is nontrivial^(*).

Examples of Codimension-Two Defects:

The sequence of inclusions $\mathbb{G}_1(\mathbf{a}) \supseteq \mathbb{G}_2(\mathbf{a}) \supseteq \mathbb{G}_3(\mathbf{a}) \supseteq \cdots$ yields sequence of homomorphisms

$$\pi_k \left[\mathbf{G}_1(\mathbf{a}) \right] \longleftarrow \pi_k \left[\mathbf{G}_2(\mathbf{a}) \right] \longleftarrow \pi_k \left[\mathbf{G}_3(\mathbf{a}) \right] \longleftarrow \cdots$$

Define $\pi_k [\mathbf{G}_{\infty}(\mathbf{a})] :=$ inverse limit of this sequence^(†) (detects 'extremely large scale' homotopy properties).

Say **a** has a **projective** codimension (k+1) defect if $\pi_k [\mathbf{G}_{\infty}(\mathbf{a})] \neq \{0\}$.

- (*) Strictly speaking, we must fix a basepoint and a connected component of \mathbf{G}_r .
- (†) We must fix a proper base ray, and assume \mathbf{G}_r has unique connected component for large r.

Trail Homotopy

Let $\mathbb{Y} \subseteq \mathbb{Z}^D$ and let ζ and ζ' be trails in \mathbb{Y} .

 ζ and ζ' are **homotopic in** \mathbb{Y} (notation: $\zeta \approx \zeta'$) if we can move from ζ to ζ' through a sequence of transformations like:

If **Y** is connected, then every homotopy class of $\pi_1(\mathbf{Y})$ can be represented as a (trail) homotopy class of trails in \mathbb{Y} .

Hence regard $\pi_1(\mathbb{Y}) = \{ \text{group of } \mathbb{Y} \text{-homotopy classes of } \mathbb{Y} \text{-trails} \}.$

Lemma: Let $C \in \mathcal{Z}_r^1(\mathfrak{A}, \mathcal{G})$. Let $\mathbf{a} \in \widetilde{\mathfrak{A}}$. Let ζ be closed trail in $\mathbb{G}_r(\mathbf{a})$.

- (a) If $\zeta \approx \zeta'$ in $\mathbb{G}_r(\mathbf{a})$, then $C(\zeta, \mathbf{a}) = C(\zeta', \mathbf{a})$. (e.g. If ζ is nullhomotopic in $\mathbb{G}_r(\mathbf{a})$, then $C(\zeta, \mathbf{a}) = e_{\mathcal{G}}$.)
- (b) Suppose (\mathcal{G}, \cdot) is abelian. If $C \approx C'$ then $C(\zeta, \mathbf{a}) = C'(\zeta, \mathbf{a})$.

We say that **a** has a *C*-pole if $C(\zeta, \mathbf{a}) \neq e_{\mathcal{G}}$ for some closed trail $\zeta \in \pi_1[\mathbb{G}_r(\mathbf{a})]$.

Proposition: Let $\mathbf{a} \in \widetilde{\mathfrak{A}}$. Let $C \in \mathcal{Z}_r^1(\mathfrak{A}, \mathcal{G})$.

(a) $\operatorname{Res}_{\mathbf{a}} C : \pi_1[\mathbb{G}_r(\mathbf{a})] \ni \underline{\zeta} \mapsto C(\zeta, a) \in \mathcal{G} \text{ is a group homomorphism.}$

(b) If (\mathcal{G}, \cdot) is abelian, and $C \approx C'$ then $\operatorname{Res}_{\mathbf{a}} C = \operatorname{Res}_{\mathbf{a}} C'$. Thus, we get group homomorphism

 $\operatorname{Res}_{\mathbf{a}}: \mathcal{H}_{dy}(\mathfrak{A}, \mathcal{G}) \times \pi_1[\mathbb{G}_{\infty}(\mathbf{a})] \times \ni (\underline{C}, \underline{\zeta}) \mapsto C(\zeta, a) \in \mathcal{G}.$

The configuration \mathbf{a} has a \mathcal{G} -pole if $\operatorname{Res}_{\mathbf{a}}$ is nontrivial homomorphism. The function $\operatorname{Res}_{\mathbf{a}}$ acts as an algebraic 'signature' of the defect in \mathbf{a} .

Theorem: \mathcal{G} -poles are essential defects.

Persistence of Poles

Theorem: If the function $\Phi_* : \mathcal{H}^1(\mathfrak{A}, \mathcal{G}) \ni C \mapsto (C \circ \Phi) \in \mathcal{H}^1(\mathfrak{A}, \mathcal{G})$ is surjective, then all \mathcal{G} -poles are Φ -persistent.

Example: If $\Phi : \mathcal{I}^{\mathbb{Z}^2} \longrightarrow \mathcal{I}^{\mathbb{Z}^2}$ was a CA with $\Phi(\mathfrak{Ice}) \subseteq \Phi(\mathfrak{Ice})$, and Φ_* was surjective, then the ice pole would persist under Φ .

Proof idea: Let $R := \operatorname{radius}(\Phi)$. If $\mathbf{a} \in \widetilde{\mathfrak{A}}$ and $\mathbf{a}' := \Phi(\mathbf{a})$, then $\mathbb{G}_{r+R}(\mathbf{a}) \subseteq \mathbb{G}_r(\mathbf{a}')$.

This yields homomorphisms $\Phi_{\dagger} : \pi_1[\mathbb{G}_{r+R}(\mathbf{a})] \longrightarrow \pi_1[\mathbb{G}_r(\mathbf{b})]$, for all $r \in \mathbb{N}$.

Lemma: For all $\zeta \in \pi_1[\mathbb{G}_{r+R}(\mathbf{a})]$ and $C' \in \mathcal{Z}_r^1(\mathfrak{A}, \mathcal{G})$, if $\zeta' := \Phi_{\dagger}(\zeta)$ and $C \approx \Phi_*(C')$, then $C'(\mathbf{a}', \zeta') = C(\mathbf{a}, \zeta)$.

Now, if **a** has a *C*-pole for some $C \in \mathcal{Z}^1(\mathfrak{A}, \mathcal{G})$, then there exists $\zeta \in \pi_1[\mathbb{G}_{r+R}(\mathbf{a})]$ with $C(\mathbf{a}, \zeta)$ nontrivial.

 Φ_* is surjective, so $\exists C' \in \mathcal{Z}^1(\mathfrak{A}, \mathcal{G})$ with $\Phi_*C' \approx C$. Let $\zeta' := \Phi_{\dagger}(\zeta) \in \pi_1[\mathbb{G}_r(\mathbf{a}')]$. Then $C'(\mathbf{a}', \zeta') = C(\mathbf{a}, \zeta)$ is nontrivial. Thus \mathbf{a}' has a C'-pole. \Box

Remark: We can also characterize poles using the *fundamental cocycles* of [K.Schmidt, 1998].

The Conway-Lagarias Tiling Group

Let \mathcal{W} be a (finite) set of notched square prototiles (to tile \mathbb{R}^2). The **tile complex** of \mathcal{W} is a 2-dimensional cell complex **X** defined as follows:

• For each $z \in \mathbb{Z}^D$ and each $w \in \mathcal{W}$, there is a *w*-shaped 2-cell in **X**, positioned in space 'over' z. Each notched edge of w is a 1-cell in **X**.

• If \mathbf{z} and \mathbf{z}' are adjacent in \mathbb{Z}^2 , and tiles w and w' 'match' along the corresponding edge, then glue together tiles (w, \mathbf{z}) and (w', \mathbf{z}') in \mathbf{X} .

Example: (Piece of tile-complex for \mathfrak{Dom}). Each square contains four 2-cells $\{ \square, \square, \square, \square, \square \}$. Between each vertex-pair \exists two edges $\{ |, \rangle \}$.

 $\exists \text{ natural projection } \Pi : \mathbf{X} \longrightarrow \mathbb{R}^2 \text{ (sending the vertices of } \mathbf{X}^0 \text{ into } \mathbb{Z}^2 \text{)}.$ $\left(\text{Admissible } \mathcal{W}\text{-tiling } \mathbf{w} \text{ of } \mathbb{R}^2\right) \cong \left(\text{Continuous } \Pi\text{-section } \varsigma_{\mathbf{w}} : \mathbb{R}^2 \longrightarrow \mathbf{X}\right)$ $\left(\text{'Partial' } \mathcal{W}\text{-tiling } \mathbf{w} \text{ of } \mathbf{U} \subset \mathbb{R}^2\right) \cong \left(\text{'Partial' } \Pi\text{-section } \varsigma_{\mathbf{w}} : \mathbf{U} \longrightarrow \mathbf{X}\right)$ In the second case, $\varsigma_{\mathbf{w}}$ defines homomorphism $\varsigma_{\mathbf{w}}^* : \pi_1(\mathbf{U}) \longrightarrow \pi_1(\mathbf{X})$. Then: $\left(\mathbf{U}^{\complement}\text{-hole in } \mathbf{w} \text{ can be admissibly filled}\right) \implies \left(\varsigma_{\mathbf{w}}^*\text{-image of any loop in } \mathbf{U} \text{ is nullhomotopic}\right) \iff \left(\varsigma_{\mathbf{w}}^* \text{ is trivial}\right).$ $\pi_1(\mathbf{X}) = \text{'tile homotopy group' [J.H.Conway & J.C.Lagarias, 1990; W.Thurston, 1990]}$

_Higher homotopy/homology groups for Wang tiles ____

Let \mathcal{W} be a (finite) set of D-dimensional notched hypercubic Wang tiles (to tile \mathbb{R}^D). Build a D-dimensional cell complex \mathbf{X} analogous to before. Get projection $\Pi : \mathbf{X} \longrightarrow \mathbb{R}^D$ such that $\Pi(\mathbf{X}^0) = \mathbb{Z}^D$.

(Admissible
$$\mathcal{W}$$
-tiling \mathbf{w} of \mathbb{R}^D) \cong (Continuous Π -section $\varsigma_{\mathbf{w}} : \mathbb{R}^D \longrightarrow \mathbf{X}$)
('Partial' \mathcal{W} -tiling \mathbf{w} of $\mathbf{U} \subset \mathbb{R}^D$) \cong ('Partial' Π -section $\varsigma_{\mathbf{w}} : \mathbf{U} \longrightarrow \mathbf{X}$).
In this case, for all $k \in \mathbb{N}$, the section $\varsigma_{\mathbf{w}}$ defines homomorphisms:

$$\begin{aligned} \pi_{\mathbf{k}}\varsigma_{\mathbf{w}} &: \pi_{k}(\mathbf{U}, u) \longrightarrow \pi_{k}(\mathbf{X}, x); & (x, u = \text{suitable basepoints}) \\ \mathcal{H}_{\mathbf{k}}\varsigma_{\mathbf{w}} &: \mathcal{H}_{k}(\mathbf{U}, \mathcal{G}) \longrightarrow \mathcal{H}_{k}(\mathbf{X}, \mathcal{G}); & ((\mathcal{G}, +) = \text{some coefficient group, e.g. } \mathcal{G} = \mathbb{Z}) \\ \mathcal{H}^{\mathbf{k}}\varsigma_{\mathbf{w}} &: \mathcal{H}^{k}(\mathbf{U}, \mathcal{G}) \longrightarrow \mathcal{H}^{k}(\mathbf{X}, \mathcal{G}) \end{aligned}$$

(Hole in **w** is fillable) \Longrightarrow ($\pi_k \varsigma_{\mathbf{w}}$, $\mathcal{H}_k \varsigma_{\mathbf{w}}$ and $\mathcal{H}^k \varsigma_{\mathbf{w}}$ are trivial, $\forall k \in \mathbb{N}$).

$_$ Homotopy/homology groups for subshifts of finite type $_$

Let \mathcal{A} be a finite alphabet. Let $\mathfrak{A} \subset \mathcal{A}^{\mathbb{Z}^D}$ be a subshift of finite type of radius r > 0. Fix $R \ge r$. Treat $\mathcal{W} := \mathfrak{A}_{(R)}$ as Wang tiles with obvious edge-matching conditions. Get tile complex \mathbf{X}_R . Then:

$$(\mathbf{a} \in \mathfrak{A}) \cong (\mathcal{W}$$
-admissible tiling of $\mathbb{R}^D) \cong (\Pi$ -section $\varsigma_{\mathbf{a}} : \mathbb{R}^D \longrightarrow \mathbf{X}_R)$.
Idea: Use homotopy/(co)homology groups of \mathbf{X}_R as invariant for \mathfrak{A} (and get algebraic invariants for codimension- $(k+1)$ defects in $\widetilde{\mathfrak{A}}$).

Problems:

[i] There \exists many different Wang representations for \mathfrak{A} . None is 'canonical'. Different Wang representations may yield non-isomorphic groups.

[ii] Wang representations (and hence, their homotopy/homology groups) do not behave well under subshift homomorphisms (i.e. CA).

Solution: There are natural surjections $\mathbf{X}_r \leftarrow \mathbf{X}_{r+1} \leftarrow \mathbf{X}_{r+2} \leftarrow \cdots$

Get homomorphisms $\pi_k(\mathbf{X}_r, x_r) \leftarrow \pi_k(\mathbf{X}_{r+1}, x_{r+1}) \leftarrow \pi_k(\mathbf{X}_{r+2}, x_{r+2}) \leftarrow \cdots$

(Here, $\{x_k\}$ are basepoints determined by some fixed $\mathbf{a} \in \mathfrak{A}$.)

Define kth **projective homotopy group** $\pi_k(\mathfrak{A}, \mathbf{a})$:= inverse limit of this sequence. (If k = 1 this is the *projective fundamental group* of W.Geller & J.Propp, 1995).

Likewise, we define kth projective (co)homology groups

$$\begin{array}{ll}
\mathcal{H}_{\mathbf{k}}(\mathfrak{A},\mathcal{G}) &:= & \lim_{\longleftarrow} \left(\mathcal{H}_{k}(\mathbf{X}_{r},\mathcal{G}) \leftarrow \mathcal{H}_{k}(\mathbf{X}_{r+1},\mathcal{G}) \leftarrow \mathcal{H}_{k}(\mathbf{X}_{r+2},\mathcal{G}) \leftarrow \cdots \right) \\
\mathcal{H}^{\mathbf{k}}(\mathfrak{A},\mathcal{G}) &:= & \lim_{\longrightarrow} \left(\mathcal{H}^{k}(\mathbf{X}_{r},\mathcal{G}) \rightarrow \mathcal{H}^{k}(\mathbf{X}_{r+1},\mathcal{G}) \rightarrow \mathcal{H}^{k}(\mathbf{X}_{r+2},\mathcal{G}) \rightarrow \cdots \right)
\end{array}$$

• Isomorphism invariants of \mathfrak{A} . • Detects codimension (k+1) defects.

$_Basepoint Freedom _$

The definition of $\pi_k(\mathfrak{A})$ depends upon a chosen 'basepoint' $\mathbf{a} \in \mathfrak{A}$.

We say \mathfrak{A} is **basepoint free** in dimension k if, for any $\mathbf{a}, \mathbf{a}' \in \mathfrak{A}$, there is a canonical isomorphism $\pi_k(\mathfrak{A}, \mathbf{a}) \cong \pi_k(\mathfrak{A}, \mathbf{a}')$.

Proposition:

(a) Suppose $\Pi_r^0 : \mathbf{X}_r^0 \longrightarrow \mathbb{Z}^D$ is injective for all large enough $r \in \mathbb{N}$. Then \mathfrak{A} is basepoint-free in all dimensions.

Suppose (\mathfrak{A}, σ) is topologically weakly mixing [i.e. the Cartesian product $(\mathfrak{A} \times \mathfrak{A}, \sigma \times \sigma)$ is topologically transitive]. Then:

(b) If $\pi_1(\mathfrak{A}, \mathbf{a})$ is abelian, then \mathfrak{A} is basepoint free in dimension 1. (c) If $\pi_1(\mathfrak{A}, \mathbf{a})$ is trivial, then \mathfrak{A} is basepoint free in all dimensions. \Box

Projective Groups and Cellular Automata

Proposition: Let $\Phi: \mathcal{A}^{\mathbb{Z}^D} \longrightarrow \mathcal{A}^{\mathbb{Z}^D}$ be a CA with $\Phi(\mathfrak{A}) \subseteq \mathfrak{A}$. Then Φ induces group endomorphisms:

$$\pi_{\mathbf{d}} \Phi \colon \pi_{d}(\mathfrak{A}, \mathbf{a}) \longrightarrow \pi_{d}(\mathfrak{A}, \mathbf{a}') \quad (\cong \pi_{d}(\mathfrak{A}, \mathbf{a}) \text{ if basepoint free})$$

$$\mathcal{H}_{\mathbf{d}} \Phi \colon \mathcal{H}_{d}(\mathfrak{A}, \mathcal{G}) \longrightarrow \mathcal{H}_{d}(\mathfrak{A}, \mathcal{G})$$

$$\mathcal{H}^{\mathbf{d}} \Phi \colon \mathcal{H}^{d}(\mathfrak{A}, \mathcal{G}) \longrightarrow \mathcal{H}^{d}(\mathfrak{A}, \mathcal{G}).$$

Proof: (Idea) If Φ has radius q, then Φ induces a cellular map $\Phi_* : \mathbf{X}_{R+q} \longrightarrow \mathbf{X}_R$ for all $R \geq r$, which yields corresponding homotopy/(co)homology homomorphisms. The resulting infinite commuting ladder of homomorphisms defines a homomorphism of the inverse/direct limit groups. \Box

Recall that $\pi_{\mathbf{k}}[\mathbb{G}_{\infty}(\mathbf{a})] :=$ inverse limit of $\pi_{k}[\mathbb{G}_{r}(\mathbf{a})]$ as $r \to \infty$.

Likewise define $\mathcal{H}^k[\mathbb{G}_{\infty}(\mathbf{a})]$ (direct limit) and $\mathcal{H}_k[\mathbb{G}_{\infty}(\mathbf{a})]$ (inverse limit), $\forall k \in \mathbb{N}$.

If $\mathbf{a} \in \widetilde{\mathfrak{A}}$, then \mathbf{a} defines 'partial' Π -section $\varsigma_{\mathbf{a}} : \mathbf{G}_R(\mathbf{a}) \longrightarrow \mathbf{X}_R$ for all $R \geq r$. This induces group homomorphisms:

$$\begin{aligned} \mathcal{H}_k \mathbf{a} \colon \mathcal{H}_k [\mathbb{G}_R(\mathbf{a}), \mathcal{G}] &\longrightarrow \mathcal{H}_k(\mathbf{X}_R, \mathcal{G}); \\ \mathcal{H}^k \mathbf{a} \colon \mathcal{H}^k(\mathbf{X}_R, \mathcal{G}) &\longrightarrow \mathcal{H}^k [\mathbb{G}_R(\mathbf{a}), \mathcal{G}]; \\ \pi_k \mathbf{a} \colon \pi_k [\mathbb{G}_R(\mathbf{a})] &\longrightarrow \pi_k(\mathbf{X}_R). \end{aligned}$$

The resulting infinite commuting ladders of homomorphisms define homomorphisms of the inverse/direct limit groups. Thus, we have:

Theorem: (a) Any $\mathbf{a} \in \widetilde{\mathfrak{A}}$ induces group homomorphisms: $\mathcal{H}_{\mathbf{k}}\mathbf{a} \colon \mathcal{H}_{k}[\mathbb{G}_{\infty}(\mathbf{a}), \mathcal{G}] \longrightarrow \mathcal{H}_{k}(\mathfrak{A}, \mathcal{G}) \text{ and } \mathcal{H}^{\mathbf{k}}\mathbf{a} \colon \mathcal{H}^{k}(\mathfrak{A}, \mathcal{G}) \longrightarrow \mathcal{H}^{k}[\mathbb{G}_{\infty}(\mathbf{a}), \mathcal{G}].$ (b) If \mathfrak{A} is basepoint-free in dimension k, then \mathbf{a} also induces a group homomorphism $\pi_{k}\mathbf{a} \colon \pi_{k}[\mathbb{G}_{\infty}(\mathbf{a})] \longrightarrow \pi_{k}(\mathfrak{A}).$

We call $\pi_k \mathbf{a}$ (resp. $\mathcal{H}_k \mathbf{a}$ or $\mathcal{H}^k \mathbf{a}$) the *k*th homotopy (resp. (co)homology) signature of \mathbf{a} ; if it is nontrivial, we say \mathbf{a} has a homotopy (resp. (co)homology) defect of codimension (k + 1). _Persistence of Homotopy/(co)homology Defects _____

Theorem: Let $\mathfrak{A} \subset \mathcal{A}^{\mathbb{Z}^D}$ be SFT. Let $\Phi \colon \mathcal{A}^{\mathbb{Z}^D} \to \mathcal{A}^{\mathbb{Z}^D}$ be CA with $\Phi(\mathfrak{A}) \subseteq \mathfrak{A}$.

- (a) Suppose \mathfrak{A} is basepoint-free in dimension k. If $\pi_k \Phi : \pi_k(\mathfrak{A}) \longrightarrow \pi_k(\mathfrak{A})$ is injective, then every homotopy defect of codimension (k + 1) is Φ -persistent.
- (b) If $\mathcal{H}_k \Phi : \mathcal{H}_k(\mathfrak{A}, \mathcal{G}) \longrightarrow \mathcal{H}_k(\mathfrak{A}, \mathcal{G})$ is injective, then every homology defect of codimension (k+1) is Φ -persistent.
- (c) If $\mathcal{H}^k \Phi : \mathcal{H}^k(\mathfrak{A}, \mathcal{G}) \longrightarrow \mathcal{H}^k(\mathfrak{A}, \mathcal{G})$ is surjective, then every cohomology defect of codimension (k+1) is Φ -persistent. \Box

This follows from:

Theorem: Let $\Phi: \mathcal{A}^{\mathbb{Z}^D} \longrightarrow \mathcal{A}^{\mathbb{Z}^D}$ be a CA with $\Phi(\mathfrak{A}) \subseteq \mathfrak{A}$. Let $\mathbf{a} \in \widetilde{\mathfrak{A}}$ and let $\Phi(\mathbf{a}) = \mathbf{b}$. Then we have commuting diagrams:

If \mathfrak{A} is basepoint-free, we also get a commuting diagram:

$$\begin{array}{cccc} \pi_k[\mathbb{G}_{\infty}(\mathbf{a}),\omega] & \xrightarrow{\pi_k\iota} & \pi_k[\mathbb{G}_{\infty}(\mathbf{b}),\omega] \\ \pi_k\mathbf{a} & & \downarrow \pi_k\mathbf{b} \\ \pi_k(\mathfrak{A}) & \xrightarrow{\pi_k\Phi} & \pi_k(\mathfrak{A}) \end{array}$$

Proof: (Idea) Stick together all the aforementioned infinite commuting ladders to get infinite commuting 'girder', which yields commuting square of inverse limit homomorphisms.

Equivariant (co)Homology

Question: Is there a higher-codimension analog to the codimension-2 'poles' from dynamical cohomology?

Let $k \in \mathbb{N}$. A (cubic) *k*-chain is a formal 'sum' of *k*-dimensional cubes in \mathbb{R}^D with vertices in \mathbb{Z}^D (combinatorial analog of '*k*-dimensional submanifold'). Fix an abelian group $(\mathcal{G}, +)$. Define $\mathcal{C}_{\mathbf{k}} := \{ \text{free abelian group of cubic$ *k* $-chains} \}$. $\mathcal{C}^{\mathbf{k}}(\mathcal{G}) := \{ (\text{cubic}) \ k\text{-cochains} \} = \{ \text{homomorphisms } c : \mathcal{C}_k \longrightarrow \mathcal{G} \}.$

(combinatorial analog of 'k-dimensional differential forms').

 \mathbb{Z}^D acts on \mathbb{R}^D by shifts. This induces \mathbb{Z}^D -action on \mathcal{C}_k , and thus on \mathcal{C}^k .

Let $\mathfrak{A} \subset \mathcal{A}^{\mathbb{Z}^D}$ be subshift. An **equivariant cochain** on \mathfrak{A} is a continuous function $C : \mathfrak{A} \longrightarrow \mathcal{Z}^k(\mathcal{G})$ which commutes with all \mathbb{Z}^D -shifts.

Idea: For any $\mathbf{a} \in \mathfrak{A}$, $C(\mathbf{a})$ is a cochain. If $\zeta \in \mathcal{C}_k$ is any chain, then $C(\sigma^{\mathsf{z}}(\mathbf{a}))[\zeta] = C(\mathbf{a})[\sigma^{\mathsf{z}}(\zeta)].$

Let $\mathcal{C}_{eq}^{\mathbf{k}}(\mathfrak{A}, \mathcal{G}) := \{\text{equivariant } k\text{-chains}\}$. There is a natural **cobound**ary operator $\delta^{\mathbf{k}} : \mathcal{C}_{eq}^{k} \longrightarrow \mathcal{C}_{eq}^{k+1}$. Let $\mathcal{Z}_{eq}^{\mathbf{k}} := \ker(\delta^{k})$ be the group of **equiv**ariant cocycles.

Examples: (a) Recall that a 'dynamical' cocycle is a function c: $\mathbb{Z}^D \times \mathfrak{A} \longrightarrow \mathcal{G}$ such that

$$c(\mathbf{y} + \mathbf{z}, \mathbf{a}) = c[\mathbf{y}, \sigma^{\mathbf{z}}(\mathbf{a})] + c(\mathbf{z}, \mathbf{a}).$$

Any dynamical cocycle defines an equivariant cocycle $C \in \mathbb{Z}_{eq}^1$ as follows: for any chain $\zeta \in \mathcal{C}_k$, treat ζ as a 'trail' and define $C(\zeta, \mathbf{a})$ as before.

(b) (Equivariant cocycle $C \in \mathbb{Z}_{eq}^2$ on 'ice cube' shift) This picture shows how to evaluate C on a single 2-cell (i.e. oriented square). To evaluate C on 2-chain, sum values on all constituent 2-cells.

_Equivariant Cohomology vs. Dynamical Cohomology __ Let $\mathcal{B}_{eq}^{\mathbf{k}} := \operatorname{image}(\delta^{k-1})$ (equivariant coboundaries).

Define equivariant cohomology group $\mathcal{H}^k_{eq}(\mathfrak{A}, \mathcal{G}) := \mathcal{Z}^k_{eq}/\mathcal{B}^k_{eq}$.

 \mathcal{Z}_{eq}^k and \mathcal{B}_{eq}^k are σ -invariant. Thus, σ induces \mathbb{Z}^D -action on \mathcal{H}_{eq}^k . Let

 $\begin{aligned} \mathcal{Z}^{1}_{dy}(\mathfrak{A},\mathcal{G}) &:= \{ \text{dynamical cocycles} \}; \\ \mathcal{H}^{1}_{dy}(\mathfrak{A},\mathcal{G}) &:= \text{'dynamical' cohomology group.} \end{aligned}$

Theorem: Let $(\mathcal{G}, +)$ be abelian. There are canonical isomorphisms:

 $\mathcal{Z}^1_{\text{eq}}(\mathfrak{A},\mathcal{G})\cong\mathcal{Z}^1_{\text{dy}}(\mathfrak{A},\mathcal{G})\quad and\quad \mathcal{H}^1_{\text{eq}}(\mathfrak{A},\mathcal{G})\cong\mathcal{H}^1_{\text{dy}}(\mathfrak{A},\mathcal{G}).$

Proof idea: Given $C \in \mathcal{Z}^1_{dy}$, define $C' \in \mathcal{Z}^1_{eq}$ as follows: for any chain $\zeta \in \mathcal{C}_k$, represent ζ with (sum of) trails ζ' , and then define $C'(\zeta, \mathbf{a}) := C(\zeta', \mathbf{a})$. This sends cocycles to cocycles because $\left(\delta^1 C' \equiv 0\right) \iff \left(C'(\partial_2 \xi, \mathbf{a}) = 0 \text{ for all } \xi \in \mathcal{C}_2\right) \iff \left(C(\zeta', \mathbf{a}) = 0 \text{ for any closed trail } \zeta' \text{ in } \mathbb{Z}^D\right).$

Codimension-k poles _____

Let $\partial_k : \mathcal{C}_k \longrightarrow \mathcal{C}_{k-1}$ be combinatorial 'boundary' operator

Let $\mathcal{Z}_{\mathbf{k}} := \ker(\partial_k) = \{k \text{-dimensional cycles}\}$ ('submanifolds without boundary'). **Example:** $\mathcal{Z}_1 := \{(\text{sums of}) \text{ closed trails}\}.$

If $C \in \mathbb{Z}_{eq}^k(\mathfrak{A}, \mathcal{G})$, and $\mathbf{a} \in \mathfrak{A}$, and $\zeta \in \mathbb{Z}_k$, then $C(\mathbf{a}, \zeta) = 0$.

If \mathcal{G} is discrete, then C is 'locally determined' by rule of radius R > 0.

If $\mathbf{a} \in \widetilde{\mathfrak{A}}$, and ζ stays inside $\mathbb{G}_r(\mathbf{a})$ (for some $r \geq R$), then $C(\mathbf{a}, \zeta)$ is still well-defined.

a has a *C*-pole (of radius *r*) if there is some cycle ζ such that $C(\mathbf{a}, \zeta) \neq 0$. **a** has a **projective** *C*-pole if **a** has a radius-*r* pole for all large $r \in \mathbb{N}$.

Example: Codimension-3 pole in Ice Cube shift

Theorem: Projective poles are essential defects.

Proof idea: Similar to 'dynamical' cohomology proof for codimension-2 poles. \Box

Theorem: Let $\mathfrak{A} \subset \mathcal{A}^{\mathbb{Z}^D}$ be an SFT. Let $\Phi: \mathcal{A}^{\mathbb{Z}^D} \to \mathcal{A}^{\mathbb{Z}^D}$ be a CA with $\Phi(\mathfrak{A}) \subseteq \mathfrak{A}$. Fix $d \in [1...D]$.

- (a) Define $\Phi_* : \mathcal{C}^d_{eq}(\mathfrak{A}, \mathcal{G}) \longrightarrow \mathcal{C}^d_{eq}(\mathfrak{A}, \mathcal{G}) \ by \ \Phi_*C(\mathbf{a}, \zeta) := C[\Phi(\mathbf{a}), \zeta].$ This induces endomorphism $\mathcal{H}^d_{eq}\Phi : \mathcal{H}^d_{eq}(\mathfrak{A}, \mathcal{G}) \longrightarrow \mathcal{H}^d_{eq}(\mathfrak{A}, \mathcal{G}).$
- (b) Suppose $\mathcal{H}^d_{eq}\Phi$ is an epimorphism.
 - [i] If \mathcal{G} is the additive group of a field (e.g. $\mathcal{G} = \mathbb{Z}_{/p}$ for p prime), then all projective \mathcal{G} -poles are Φ -persistent.
 - [ii] If d = 1 or D, then any projective d-pole is Φ -persistent. \Box

Invariant Cohomology

Questions: (a) What is relationship between the (dynamical) cocycles of \mathfrak{A} and the (co)homology groups of Wang tile cell complex of \mathfrak{A} ?

(b) What is relationship between poles and (co)homology defects?

 $\forall r \geq \mathbf{R} := \operatorname{radius}(\mathfrak{A}), \text{ let } \mathbf{X}_r := \operatorname{radius} r \text{ Wang tile cell complex for } \mathfrak{A}.$

The σ -action on \mathfrak{A} induces natural \mathbb{Z}^D -action on \mathbf{X}_r ; hence on $\mathcal{H}^k(\mathbf{X}_r, \mathcal{G})$.

Let $\mathcal{H}^k_{inv}(\mathbf{X}_r, \mathcal{G})$:= group of \mathbb{Z}^D -fixed elements of $\mathcal{H}^k(\mathbf{X}_r, \mathcal{G})$. We define the *k*th **invariant cohomology group** of \mathfrak{A} :

 $\mathcal{H}^{\mathbf{k}}_{\mathrm{inv}}(\mathfrak{A},\mathcal{G}) := \lim_{\longrightarrow} \left(\mathcal{H}^{k}_{\mathrm{inv}}(\mathbf{X}_{R+1},\mathcal{G}) \to \mathcal{H}^{k}_{\mathrm{inv}}(\mathbf{X}_{R+2},\mathcal{G}) \to \mathcal{H}^{k}_{\mathrm{inv}}(\mathbf{X}_{R+3},\mathcal{G}) \to \cdots \right)$

Theorem: Let $\mathfrak{A} \subset \mathcal{A}^{\mathbb{Z}^D}$ be SFT. Let $(\mathcal{G}, +)$ be discrete abelian group. There is a natural isomorphism $\mathcal{H}^d_{inv}(\mathfrak{A}, \mathcal{G}) \cong \mathcal{H}^d_{eq}(\mathfrak{A}, \mathcal{G})$. In particular, $\mathcal{H}^1_{inv}(\mathfrak{A}, \mathcal{G}) \cong \mathcal{H}^1_{dy}(\mathfrak{A}, \mathcal{G})$.

Thus, poles are $\mathcal{H}^d(\mathfrak{A},\mathcal{G})$ -cohomology defects.

A finite state machine (FSM) has a finite set of internal states S, finite input alphabet \mathcal{I} and output alphabet \mathcal{O} , and update rule

 $\Upsilon: \mathcal{I} \times \mathcal{S} \longrightarrow \mathcal{S} \times \mathcal{O}$

If FSM begins in state s_0 , and receives input stream $i_0, i_1, i_2, \ldots, i_{N-1}$, then it proceeds through states s_1, s_2, \ldots, s_N and produces output o_1, o_1, \ldots, o_N , where, for every $n \in [0...N)$,

$$\Upsilon(\boldsymbol{i_n}, \boldsymbol{s_n}) \quad = \quad (\boldsymbol{s_{n+1}}, \boldsymbol{o_{n+1}})$$

Diagramatically:

$$i_{0} \quad i_{1} \quad i_{2} \quad i_{3} \dots \dots \quad i_{N-1}$$

$$\downarrow \quad \downarrow \quad \downarrow \quad \downarrow \quad \qquad \downarrow$$

$$s_{0} \Longrightarrow s_{1} \Longrightarrow s_{2} \Longrightarrow s_{3} \Longrightarrow \dots \Longrightarrow s_{N-1} \Longrightarrow s_{N}$$

$$\searrow \quad \searrow \quad \searrow \quad \searrow \quad \qquad \searrow$$

$$o_{1} \quad o_{2} \quad o_{3} \quad o_{4} \dots \dots \dots \quad o_{N}$$

A **defect particle** in **a** is a defect which is finite in size and whose size in $\Phi^t(\mathbf{a})$ remains bounded for all t > 0. Defect particles act like FSM:

Internal state = \mathfrak{A} -inadmissible symbol-sequence inside defect.

Input = \mathfrak{A} -admissible symbols on boundary of defect.

Output = Instantaneous verocity.

Example: Defect particles in ECA#54:

Remarks: • The width of inadmissible region fluctuates over time. We define the **width** of the defect to be the maximum width it ever obtains. This defines the effective 'state space' of the FSM representation.

• If \mathfrak{A} is (Φ, σ) -periodic (as in these examples), then the FSM is driven by periodic input, so its long-term behaviour is periodic.

• The defect velocity fluctuates over time, but there is a long-term 'average' velocity obtained by averaging over the period.

A **pushdown automaton** (PDA) is an FSM augmented with 'last in, first out' memory model called a **stack**. The machine can 'push' symbols onto the stack, and later 'pop' them off the stack in reverse order.

A **Turing machine** is an FSM augmented with a biinfinite random access memory model called a 'tape'. The FSM acts has a 'head' which can read/write symbols as it moves along the tape.

One-dimensional CA: Kinematic Regimes _

In one-dimensional CA, the particle kinematics depends upon the kind of subshifts found to the right and left of the particle.

	Defect		Right Side (σ, Φ) -Dynamics				
Kinematic Regimes		σ-dynamics	Zero Entropy, σ -periodic	Right- regular	Nonzero σ-Entropy, Not σ-periodic		
	σ-dynamics	Φ-dynamics	Φ-Periodic or Φ-Fixed	Right- resolving	Φ-Periodic or Φ-Fixed	Anything else	
de (σ,Φ)-Dynamics	Zero Entropy, $\Rightarrow \Phi$ -Periodic σ -periodic or Φ -Fixed		Ballistic	Diffusive	Autonomous PDA	Complicated	
	Left-regular Left-resolving		Diffusive Diffusive		Markov PDA	Complicated	
	Nonzero σ-Entropy,	Φ-Periodic or Φ-Fixed	Autonomous PDA	Markov PDA	Turing Machine	Complicated	
Left Si	Not σ -periodic	Anything else	Complicated		Complicated		

Ballistic: Defect has (Φ, σ) -periodic subshifts on both sides. Acts like FSM driven by periodic input. Moves with constant average velocity through periodic background. **Examples**: ECAs 54, 62, 110, and 184

Diffusive: Regular, Φ-resolving subshifts on one or both sides. Acts like FSM driven by Markov process. Performs generalized random walk. **Example**: ECA #18.

Turing Machine: Defect moves through Φ -fixed, positive σ -entropy background, and modifies background as it goes. Acts like Turing machine: particle is the 'head', and inert background is the 'tape'.

Autonomous Pushdown Automaton: Φ -fixed, positive σ -entropy domain on one side (which acts as a 'stack' memory), and zero-entropy domain on the other side. Acts like a PDA without external input.

Markov PDA: Φ -fixed, positive σ -entropy domain on one side (acts as a 'stack'), and regular Φ -resolving subshift on the other. Acts like a PDA driven by a Markov process.

Regular Markov Subshifts & Resolving CA

 $\forall a \in \mathcal{A}, \text{ let } \mathcal{F}(a) \subseteq \mathcal{A} \text{ be a set of 'admissible followers'. Write } a \rightsquigarrow b$ if $b \in \mathcal{F}(a)$.

The corresponding **Markov subshift** $\mathfrak{A} \subset \mathcal{A}^{\mathbb{Z}}$ is the set of all infinite sequences $[\cdots \rightsquigarrow a \rightsquigarrow b \rightsquigarrow c \rightsquigarrow d \rightsquigarrow \cdots]$ (Every SFT can be recoded thus.)

Let $\mathcal{P}(a) := \{ b \in \mathcal{A} ; b \rightsquigarrow a \}$ be the set of admissible 'predecessors'.

 \mathfrak{A} is **regular** if $\exists F \in \mathbb{N}$ such that $\#[\mathcal{F}(a)] = F$ for all $a \in \mathcal{A}$, and $\exists P \in \mathbb{N}$ such that $\#[\mathcal{P}(a)] = P$ for all $a \in \mathcal{A}$.

frag replacements

Let $\Phi : \mathcal{A}^{\mathbb{Z}} \longrightarrow \mathcal{A}^{\mathbb{Z}}$ be a CA with local rule $\phi : \mathcal{A}^{3} \longrightarrow \mathcal{A}$. Suppose $\Phi(\mathfrak{A}) \subset \mathfrak{A}$. Let $(b \rightsquigarrow c \rightsquigarrow d)$ and let $x := \phi(b, c, d)$.

If $d \rightsquigarrow e$, then $x \rightsquigarrow \phi(c, d, e)$. Thus, we get function $\phi_{c,d} : \mathcal{F}(d) \longrightarrow \mathcal{F}(x)$. We say Φ is **right-resolving** if $\phi_{c,d}$ is bijective for all such (c, d).

If $a \rightsquigarrow b$, then $\phi(a, b, c) \rightsquigarrow x$. Thus, we get function $\phi^{b,c} : \mathcal{P}(b) \longrightarrow \mathcal{P}(x)$. We say Φ is **left-resolving** if $\phi^{b,c}$ is bijective for all such (b, c).

 Φ is **resolving** if it is both left- and right- resolving.

Examples: (a) *Permutative* CA acting on full shift $\mathfrak{A} = \mathcal{A}^{\mathbb{Z}}$.

(b) *Linear* CA acting on Markov subgroup. (Here \mathcal{A} is a group, so $\mathcal{A}^{\mathbb{Z}}$ is a group. $\mathfrak{A} \subset \mathcal{A}^{\mathbb{Z}}$ is a subgroup, and $\Phi : \mathcal{A}^{\mathbb{Z}} \longrightarrow \mathcal{A}^{\mathbb{Z}}$ is endomorphism.)

Diffusive Defect Particle Kinematics

The **Parry measure** μ is the measure of maximal entropy on \mathfrak{A} . It is Markov measure given equal transition probability to all $b \in \mathcal{F}(a)$.

Theorem: Let $\mathfrak{A} \subset \mathcal{A}^{\mathbb{Z}}$ be regular Markov subshift. Let Φ : $\mathcal{A}^{\mathbb{Z}} \longrightarrow \mathcal{A}^{\mathbb{Z}}$ be CA with $\Phi(\mathfrak{A}) \subseteq \mathfrak{A}$ and Φ resolving on \mathfrak{A} . Let $\mu = Parry$ measure on \mathfrak{A} . (Then $\Phi \mu = \mu$.)

Let $\mathbf{l} \in \mathcal{A}^{(-\infty...0)}$ be μ -random, left-infinite \mathfrak{A} -admissible sequence.

Let $\mathbf{r} \in \mathcal{A}^{[W...\infty)}$ be μ -random, right-infinite \mathfrak{A} -admissible sequence.

Let $\mathbf{w} \in \mathcal{A}^{[0...W)}$ be 'defect' word. Set initial condition: $\mathbf{a} := \mathbf{l.w.r}$.

Define $\zeta : \mathbb{N} \longrightarrow \mathbb{Z}$ by $\zeta(t) := position of defect in \Phi^t(\mathbf{a})$. Then ζ is a generalized random walk. [i.e. increments of ζ are a hidden Markov process]. (Generalizes Eloranta [1993-1995]; similar result for 0-width defects in 'partially permutive' CA.)

Proof idea: The defect motion is driven by ' μ -random information' coming in from the left and right, as follows:

Diffusive Defect Particle Kinematics

Scale: 50×50 (space \times time)

Scale: 300×6000 (space × time)