Automated Tile Design for Self-Assembly Conformations

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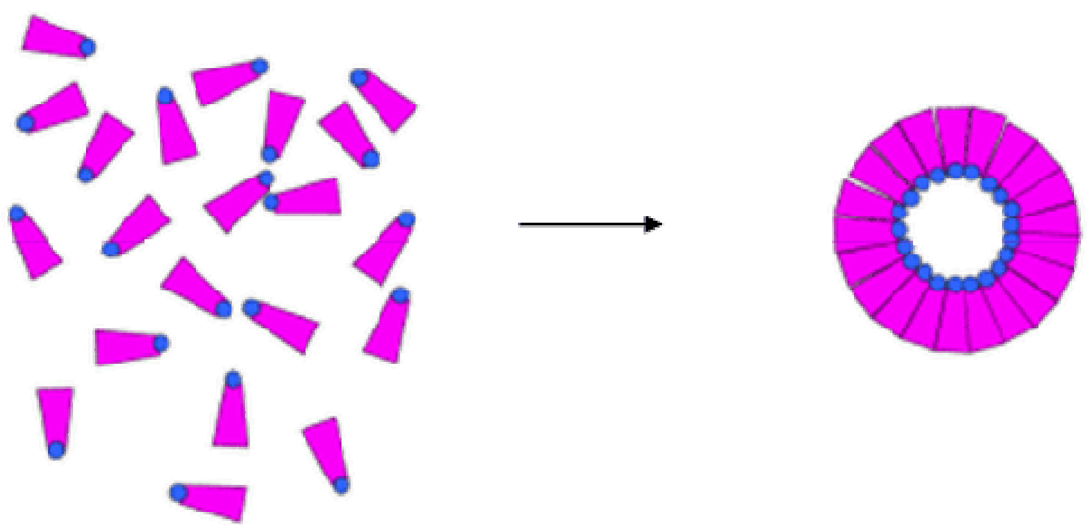
Outline

- Self-assembly
- Wang Tiles model
- Design by evolution
- Experiments & Results
- Self-assembly analysis
- Future work

Self-Assembly

- Distributed asynchronous mechanism
- Hierarchical complex structures are built from bottom-up



Self-Assembly

- Properties
  - Set of autonomous individual components
  - Components interact with each other
  - Desired final structure is "encoded" on the components *interactions*
  - Components are (usually)not pre-programmed but rather the interactions are
  - There is no *centralized* master plan
  - There is no external intervention

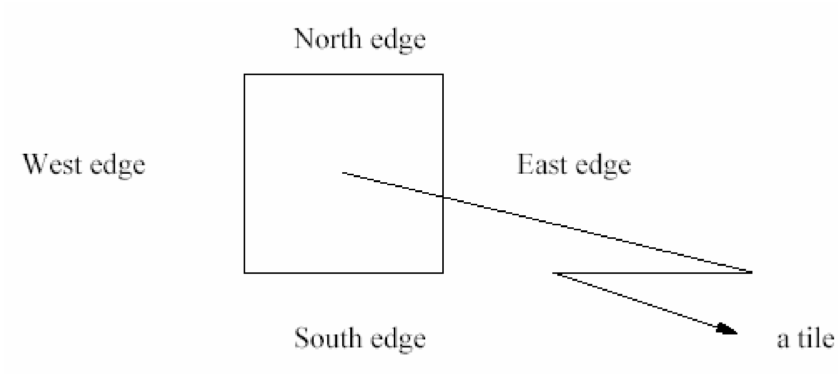
Self-Assembly

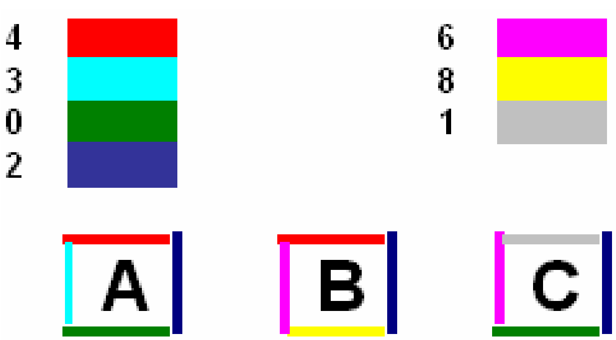
- Ubiquitous in nature at microscopic scale
  - Molecular self-assembly
  - Nanotechnology (nanocrystal assembly, surface patterning, etc.)
  - DNA (strands find the correct match)
  - Protein Folding (aminoacids interaction)

Wang Tiles model

- Set of square tiles
- Each tile edge has a colour
- Tiles move randomly
- Tiles self-assemble subject to the stickiness of their edges and the environment’s temperature
- Stickiness is pre-programmed (in a table)

Wang Tiles model





	C_0	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9
C_0	7	2	7	7	3	0	0	1	7	1
C_1	2	7	1	5	7	3	8	2	1	6
C_2	7	1	6	4	8	9	2	2	5	1
C_3	7	5	4	8	5	3	3	7	9	6
C_4	3	7	8	5	8	7	5	0	3	9
C_5	0	3	9	3	7	6	0	3	9	5
C_6	0	8	2	3	5	0	1	8	8	5
C_7	1	2	2	7	0	3	8	3	9	6
C_8	7	1	5	9	3	9	8	9	7	0
C_9	1	6	1	6	9	5	5	6	0	0

Design by Evolution

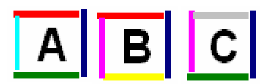
- Given a target shape (e.g. 10x10 tile square)
- Given a Wan Tile "world" model
- Given a GA
- Goal: To evolve sets of tiles that self-assemble in the target shape

Design by Evolution

- Genetic Algorithm
  - Individual = set of tiles randomly created
  - Fitness function = Tile Wan model simulator + shape scanner
  - Crossover = one-point crossover
  - Mutation = mutate tile’s colours
  - Elitist population. Best individual passes to the next population

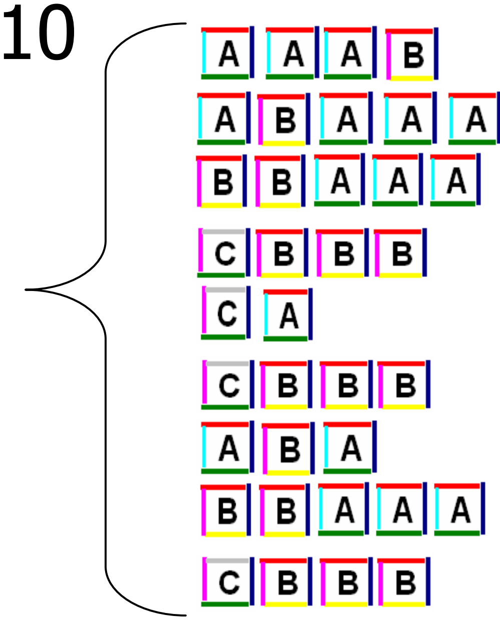
Design by Evolution

- Individual
  - Set of tiles



  - Randomly created
  - Maximum length of 10

- Population:
  - Set of individuals

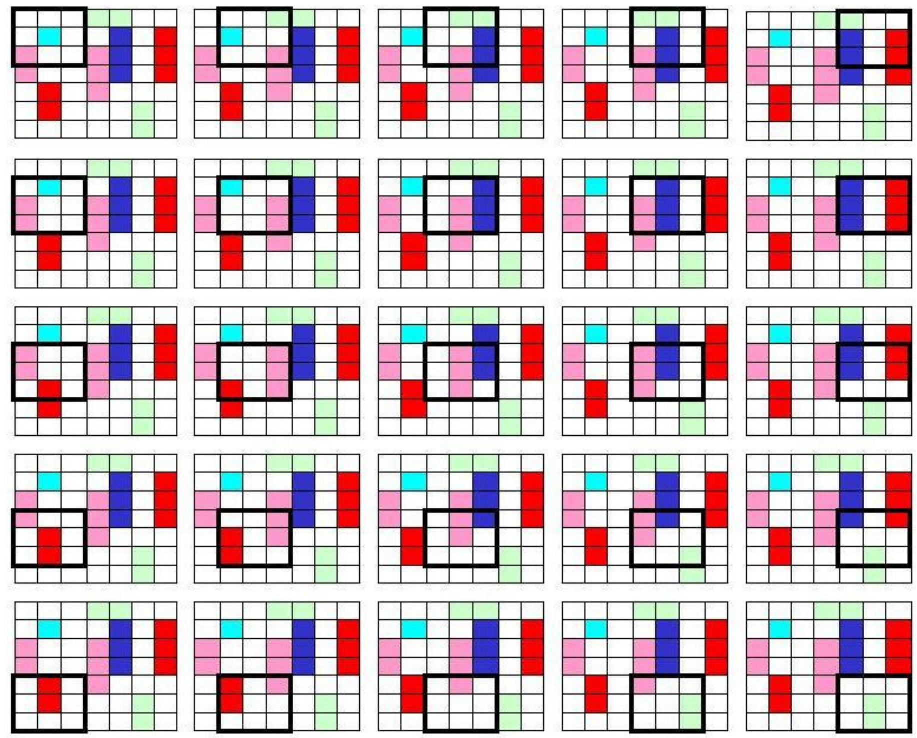


Design by Evolution

- Tile Simulator
  - Receive a set of tiles with lifetime
  - Tiles move randomly across a lattice
  - Tiles attach subject to the stickiness value of their adjacent edges and a temperature
  - Simulation ends when all tiles are attached or lifetime expires

Design by Evolution

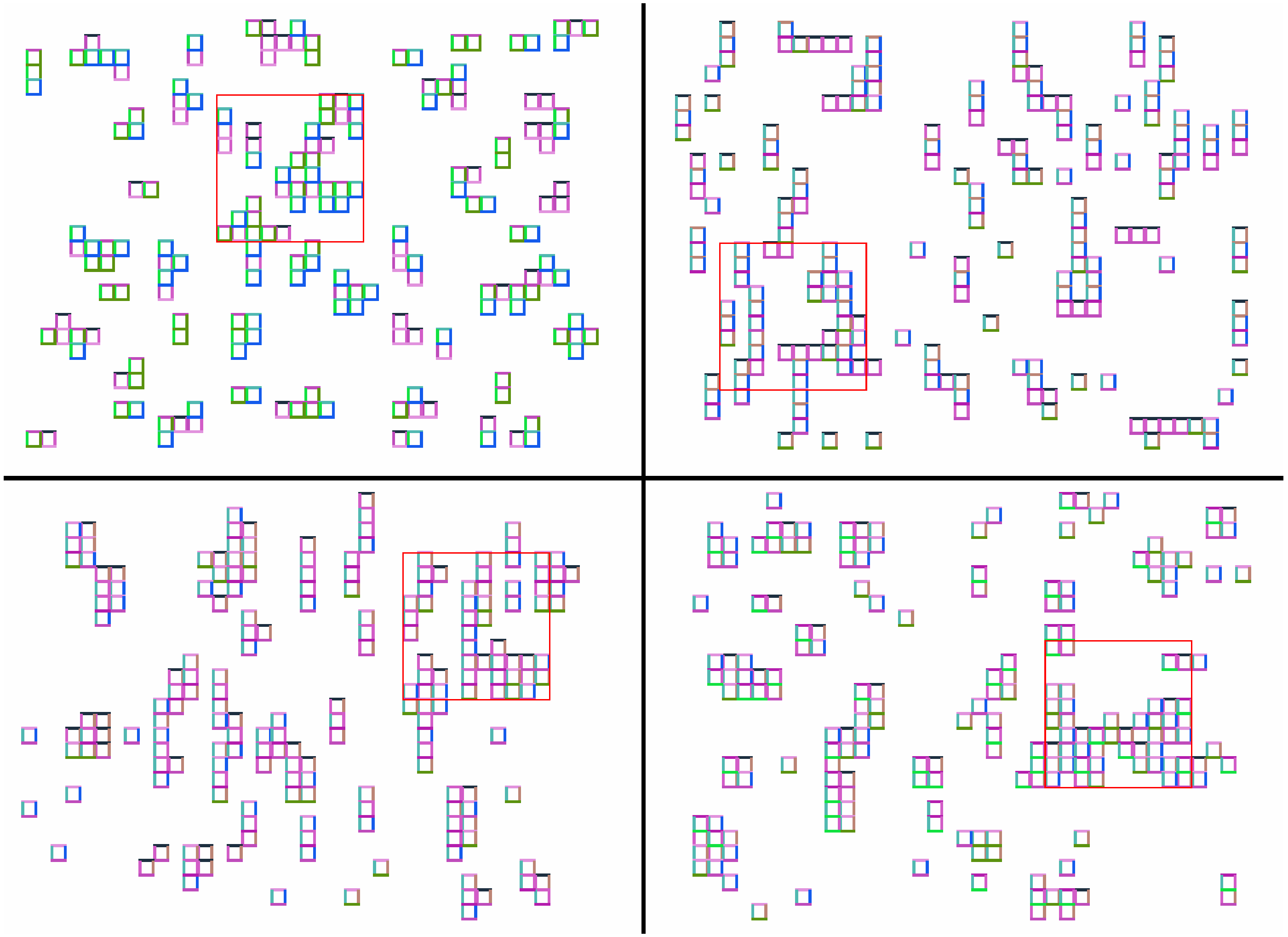
- Shape Scanner
  - Takes a target shape as a parameter
  - Receives the final lattice configuration from the simulator
  - Looks for the lattice region with most semblance to the target shape. Returns its # of matching tiles.



Experiments

- GA parameters
  - Generations = 100
  - Population = 100
  - Ind. length <= 10
  - XProb = 0.3
  - MProb = 0.01
  - Shape 10x10
  - Fitness accuracy = 20
  - 25% of strips (H & V)
- Simulator parameters
  - Lattice 40x30
  - Temperature = 4
  - Colors = [0, 9]
  - Tile lifetime = 300
  - Matrix size = 10x10

Generations 0, 15, 30, 45 ...



Generations … 60, 75, 90, 99

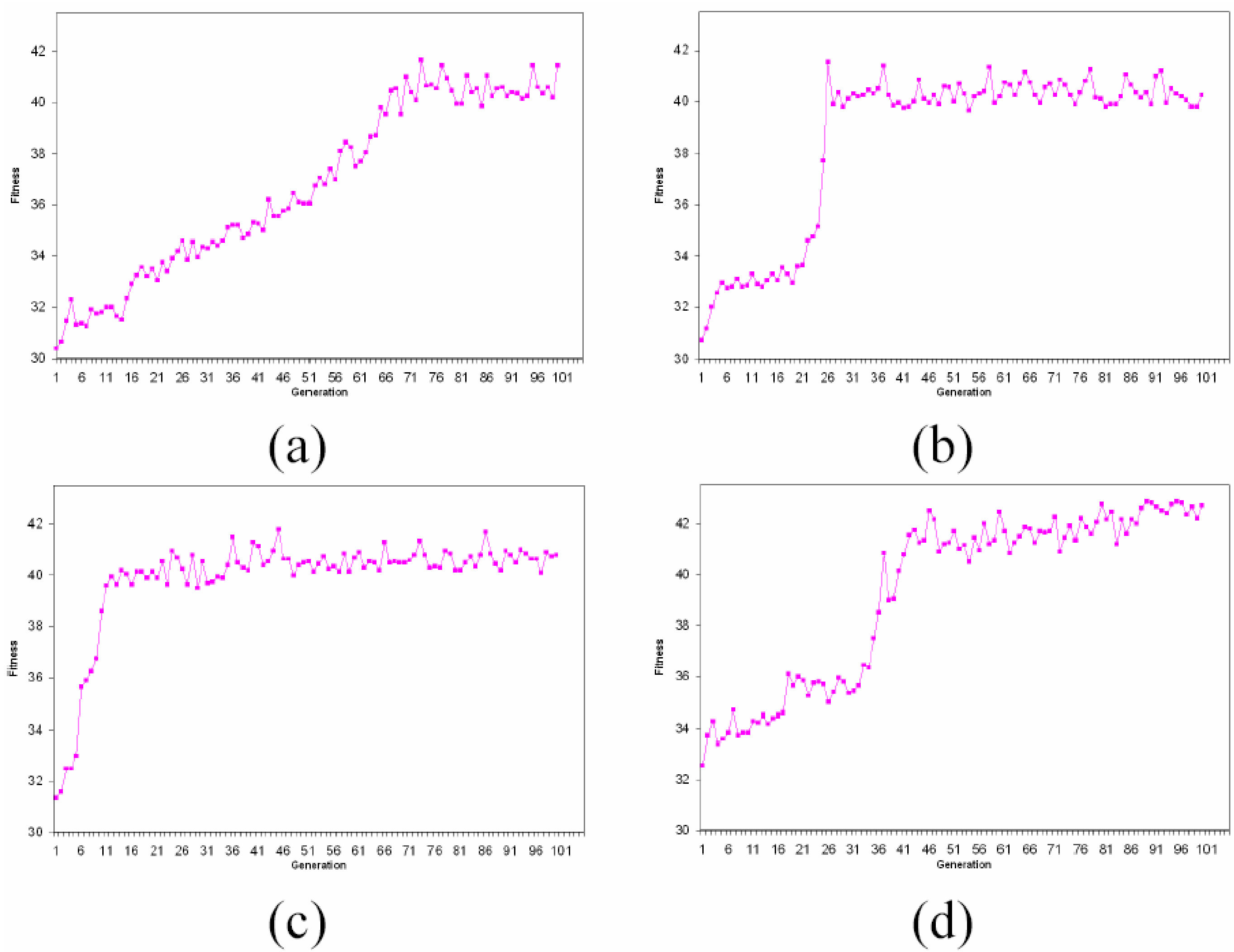
Results

- While the evolution takes place
  - Noise among conformation decreases through generations
  - Small islands of conformations appear approaching the target shape
  - Horizontal and vertical strips guide the GA to get the target shape

Results

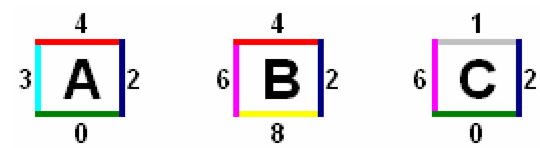
- Learning curve
  - Initial fitness values start from 30 or 33 due to the strips
  - Fitness rise up to 40 or 41
  - Best fitness is reached in early generations
  - Considerable changes in the genome take place at short periods

Results



Self-assembly analysis

- How self-assembly was achieved by a particular individual ?

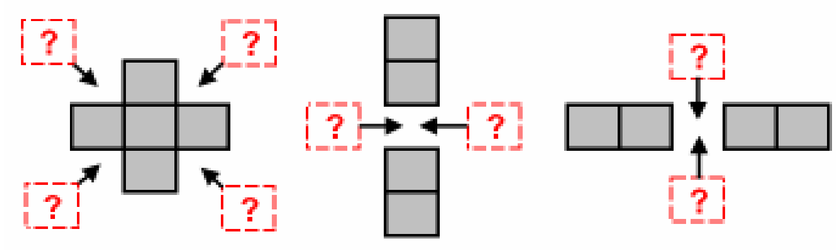


- There are **no two-tile** combinations cooperating
  - No combination of colours greater than temperature
  - Temperature = 4

	C_0	C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9
C_0	7	2	7	7	3	0	0	1	7	1
C_1	2	7	1	5	7	3	8	2	1	6
C_2	7	1	6	4	8	9	2	2	5	1
C_3	7	5	4	8	5	3	3	7	9	6
C_4	3	7	8	5	8	7	5	0	3	9
C_5	0	3	9	3	7	6	0	3	9	5
C_6	0	8	2	3	5	0	1	8	8	5
C_7	1	2	2	7	0	3	8	3	9	6
C_8	7	1	5	9	3	9	8	9	7	0
C_9	1	6	1	6	9	5	5	6	0	0

Self-assembly analysis

- **Three-tile** combination
  - Considering binding sites



  - And considering the Normalized Average Free Energy (NAFE)

$$\frac{\sum_{1}^{|T|}(G(t_i^e,t_?^w)+G(t_j^n,t_?^s))}{|T|}$$
(a)

$$\frac{\sum_{1}^{|T|}(G(t_i^e,t_?^w)+G(t_j^s,t_?^n))}{|T|}$$
(b)

$$\frac{\sum_{1}^{|T|}(G(t_i^w,t_?^e)+G(t_j^n,t_?^s))}{|T|}$$
(c)

$$\frac{\sum_{1}^{|T|}(G(t_i^w,t_?^e)+G(t_j^s,t_?^n))}{|T|}$$
(d)

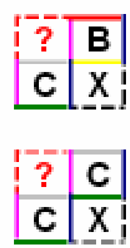
$$\frac{\sum_{1}^{|T|}(G(t_i^s,t_?^n)+G(t_j^n,t_?^s))}{|T|}$$
(e)

$$\frac{\sum_{1}^{|T|}(G(t_i^e,t_?^w)+G(t_j^w,t_?^e))}{|T|}$$
(f)

- We define **EQ classes** among conformations split by its NAFE

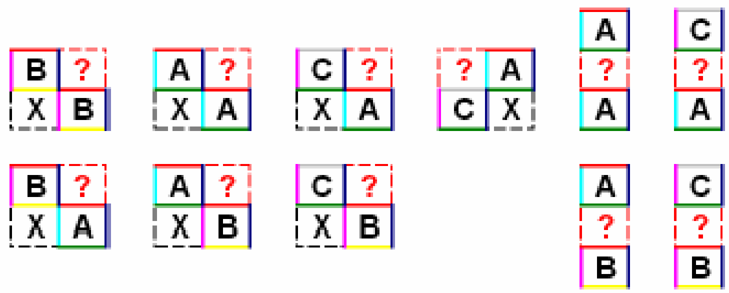
EqC	NAFE	Qty	Het	EqC	NAFE	Qty	Het
i	5.00	7	Y	vi	4.66	10	Y
ii	5.33	8	Y	vii	6.66	5	Y
iii	5.66	11	Y	viii	4.33	8	Y
iv	3.66	2	N	ix	6.33	1	N
v	7.00	2	N				

- Elements of EQ Class IV are **unlikely** to start self-assembly unless another tile locates at the west of "?"

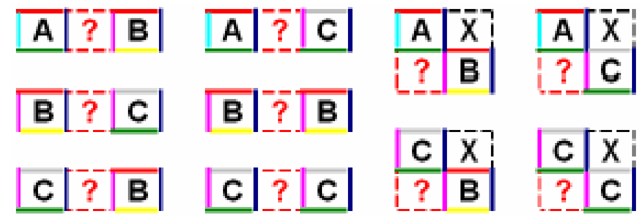


(Eq. Class iv)

- The most populated classes are likely to build conformations

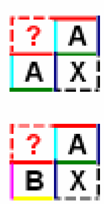


(Eq. Class iii)

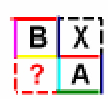


(Eq. Class vi)

- The less populated classes are less populated but have the highest NAFE (except Eq iv)



(Eq. Class v)



(Eq. Class ix)

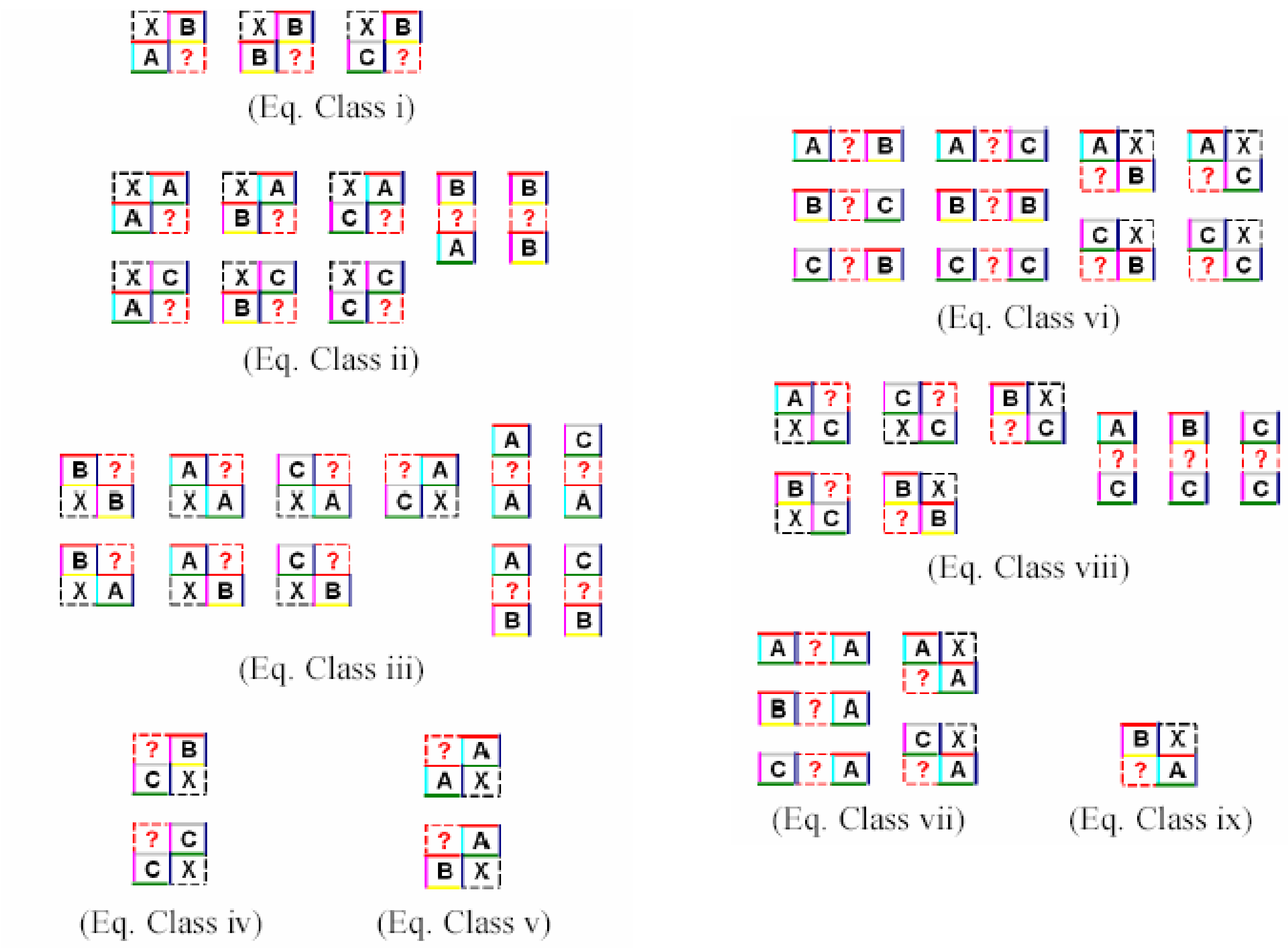
EqC	NAFE	Qty	Het	EqC	NAFE	Qty	Het
i	5.00	7	Y	vi	4.66	10	Y
ii	5.33	8	Y	vii	6.66	5	Y
iii	5.66	11	Y	viii	4.33	8	Y
iv	3.66	2	N	ix	6.33	1	N
v	7.00	2	N				

- Classes could be **heterogeneous** or **homogenous**

EqC	NAFE	Qty	Het	EqC	NAFE	Qty	Het
i	5.00	7	Y	vi	4.66	10	Y
ii	5.33	8	Y	vii	6.66	5	Y
iii	5.66	11	Y	viii	4.33	8	Y
iv	3.66	2	N	ix	6.33	1	N
v	7.00	2	N				

- Heterogeneous classes
  - are more populated
  - NAFE is high in average

- Homogeneous classes
  - are less populated
  - NAFE is low in average.


(Eq. Class i)
(Eq. Class ii)
(Eq. Class iii)
(Eq. Class iv)
(Eq. Class v)
(Eq. Class vi)
(Eq. Class viii)
(Eq. Class vii)
(Eq. Class ix)

Improved Fitness Formulation

- Substantially better results
- Faster!
  - Early generations (bad fitness):
    - Example 1
    - Example 2
    - Example 3
  - Medium generations (reasonable fitness):
    - Example 1
    - Example 2
  - Later generations (good fitness):
    - Example 1
    - Example 2
    - Example 3

But

- More problem specific

Future Work

- Develop a more realistic tile model
  - Rotation
  - Grouping
- Look for the design of more complex shapes using self-assembly

Thank you